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Fortran 95

Fortran 95

Including Fortran 90, details of High Performance Fortran (HPF), and the Fortran module for variablelength character strings

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First published in 1996 by UCL Press UCL Press Limited University College London Gower Street London WC1E 6BT

> and 1900 Frost Road, Suite 101 Bristol Pennsylvania 19007–1598

This edition published in the Taylor & Francis e-Library, 2005.

"To purchase your own copy of this or any of Taylor & Francis or Routledge's collection of thousands of eBooks please go to www.eBookstore.tandf.co.uk."

The name of University College London (UCL) is a registered trade mark used by UCL Press with the consent of the owner.

British Library Cataloguing in Publication Data A catalogue record for this book is available from the British Library.

Library of Congress Cataloging-in-Publication Data are available

ISBN 0-203-97846-3 Master e-book ISBN

ISBN: 1-85728-367-8 (Print Edition)

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Preface

This is a revised, expanded, and updated version of the original book *Fortran 90* which appeared when Fortran 90 was first launched as an international standard programming language some five years ago. This book conforms to the proposed new Fortran 95 standard, but the new features are clearly marked as such so that the book can be used without difficulty by those who are continuing to use Fortran 90. It is designed to be useful both as a textbook for those new to programming and also as a fully up-to-date reference book for more experienced computer users.

Fortran 95 includes a chapter on High Performance Fortran, the major extension to the language enabling programs to be written to exploit multiple-processor computers to the full. In addition there is an appendix giving details of the module ISO_VARYING_STRINGS, the now-standard extension of the Fortran language to handle variable-length character strings.

As well as dealing with the vocabulary and syntax of Fortran, a number of general programming concepts are explained here. The production of annotated, comprehensible, bug-free, and maintainable code is encouraged. Fortran is a large language and it provides the programmer with plenty of latitude for bad as well as good programming practice, so attention is paid to disciplined methods of programming and to consistent coding conventions. The language has evolved over a long period of time, and it has always been considered important that new versions of Fortran should be backward-compatible with earlier versions so that old programs can continue to be used alongside new. So Fortran 95 contains within it virtually all of Fortran 90, which itself contained all of FORTRAN 77. Just a few features of Fortran 90 have been deleted in Fortran 95: they are listed in the first chapter, and where they arise in the course of the book they are indicated as being non-Fortran-95 features.

As a result of its history Fortran 95 has many redundant features which would nowadays be regarded as obsolete. At the same time there are also elegant modern features, such as derived data structures and modules, which are very powerful and encourage up-to-date programming practice. In the main part of this book we concentrate on the modern core of Fortran 95, but all parts of the language, old and new, are included within this book and are indexed for easy reference.

CHAPTER 1 What is Fortran 95?

This introductory chapter describes the evolution of the Fortran programming language and its new extensions. The nature and structure of a Fortran program, its division into separate program units of different types, the existence of intrinsic procedures, the distinction between declarative and executable statements, and the types of data that can be represented in the language, are introduced. Some comments are made about coding conventions.

1.1

The Fortran language family

Fortran is a world-standard computer programming language approved under the auspices of the International Standards Organization (ISO). It is the leading language for scientific computing and it is an evolving language that has existed for over 40 years in various forms. Fortran 90 replaced FORTRAN 77 a few years ago, and in turn is being replaced now by the latest version, Fortran 95. Fortran's evolution has been the key to its longevity: it has developed in response to progress in computer architecture and to new insights in programming language theory, it has been used for solving an increasingly broad range of problems, and it will certainly continue to develop in the future to enable computer users to take full advantage of innovations to come. Fortran 90 was accepted as an international standard by ISO in 1991 and it was a major expansion of the earlier FORTRAN 77. At the time of writing,

Fortran 95 is expected to gain final ISO approval in mid-1996. Fortran 95 will be a relatively minor revision of Fortran 90 and most programs written in. Fortran 95 will appear very similar to those in Fortran 90. This book can be used equally well for Fortran 90 as for Fortran 95. The next major revision of Fortran, expected to take place very early in the next century, is already being contemplated and is termed "Fortran 2000" or "f2k".

Although Fortran includes an impressive set of mathematical functions, and is the most advanced highlevel programming language for scientific and technical computing, it is not intended only for mathematical work. In fact, Fortran handles text and general datasets with the same flexibility that it handles numbers. So, while containing numerous mathematical examples, this book is intended to be equally valuable to nonmathematicians who will be using Fortran to solve problems of other kinds.

Fortran involves ideas and terminology which have become standard in the world of software engineering, with concepts like "character" and "pointer" and "argument" that are also used in describing other programming languages. These terms have precise technical meanings and are part of the vocabulary that program-writers need to discuss their work. Beginners should try to get used to the terminology even

when it sounds rather pompously long-winded, e.g. "structure constructor", and "relational intrinsic operator". This book deliberately uses accurate technical terms as often as possible, since serious Fortran users will need to become familiar with the terminology as well as learning the keywords and syntax of the language itself.

Uniquely among computer programming languages, the evolution of Fortran is self-consciously progressive and open-ended, and arrangements are in place for the steady development of the language beyond Fortran 95. It is intended that the language should be expanded in a modular fashion, extending but not modifying what is already in existence. A module subprogram, which encapsulates new procedures and derived data types in a self-contained package, is a natural way of implementing such extensions to Fortran. The first such module to gain ISO approval, **ISO_VARYING_STRINGS**, is described in detail in Appendix C.

"High Performance Fortran", or HPF, is a much more elaborate extension to Fortran than **ISO_VARYING_STRINGS**. HPF has arisen because new kinds of computer architecture demand to be exploited as efficiently as possible. HPF is for programmers who need to push against the performance envelope of the most advanced parallel-processing systems that exist today.

1.2 Programs and programming

A computer program is simply a sequence of instructions to be carried out by a computer. A computer is a composite mechanical system that works by the transmission of signals and data between components such as keyboards, optical and magnetic disks, semiconductor chips with micron-scale circuits for storing and processing data, visual display screens and printers. A computer system also includes special programs—system software—whose task is to manage the flow of information around the system itself. "Operating systems" are a species of system software. Some computer systems have sophisticated interfaces with telecommunications systems that connect them with other computers, including the global network of computers known as the Internet, and recent years have seen the evolution of "open systems" in that the boundaries between one computer system and others have become blurred.

But what are computers for? Ultimately, computers exist in order to exercise control over equipment external to the computer, or to make calculations and to solve problems that lie outside computer science. A computer might control a production line, or it might predict the likely result of a presidential election, or the likely course of a tornado. To do such jobs, special-purpose programs must be written. Because a computer is a general-purpose tool, it cannot be expected that a special-purpose program will always be installed on the computer for which it was originally written: it may happen that the program will be used on many different computers, perhaps manufactured by different companies and running under the control of different operating systems. One of the main reasons for having a standardized programming language like Fortran is to ensure that a program will be portable from one computer to another. As long as a computer can understand Fortran, it can run any program written in Fortran. Program portability has always been important, but it is all the more vital now that the Internet makes it possible for a program to be distributed with great ease to large numbers of different computers.

Fortran, then, is a standard programming language to allow general-purpose computers to solve specialized problems. The newcomer to Fortran may be surprised to learn that it is supposed to be an easy language, intended to be used not by experts in computer science but by those whose primary specialism is in some other discipline that might be a branch of engineering, physics, chemistry, mathematics, or the environmental and human sciences. For this reason—as well as for reasons of program portability—Fortran

does not involve the programmer in the "low-level" technical details of exactly how a particular computer system is designed and how it stores and manipulates information internally. This philosophy is an aspect of what is sometimes called "data abstraction"—allowing the programmer to think of data in terms of idealized concepts (such as that of a real number) while not having to think about how that data is represented physically within a particular computer's hardware. If Fortran is not easy to learn, it is because, in response to demand by its users, it has become a sophisticated and powerful modern programming language and is very extensive. However, most programming tasks can be achieved with recourse to only a fraction of Fortran's features, and most program-writers do not attempt to memorize the whole language. The skill lies not in knowing all of Fortran, but in knowing what it can express and being able to refer to what you want when you want it.

A program written in Fortran will be translated (or "compiled", to use the technical term) into the appropriate low-level machine code by the computer system itself. This leaves the programmer free to concentrate on solving the real problem in hand, whether it be in aeronautics, economic forecasting or whatever. Programmers can cultivate their expertise in their specialist subjects and their involvement with computer science need not extend much beyond the strictly defined boundaries of the programming language. The purpose of a programming language, like that of any language, is that the user should not have to cross its boundaries. The compilation of a program from Fortran into machine code is carried out by a part of the system known as a "compiler". A compiler is itself a piece of software, i.e. a computer program, but one that would not normally be written in Fortran. For all its merits, Fortran is not usually the ideal language for writing system software or compilers. Other languages, such as C, come into their own for such purposes. Compiling a program is not the same as running it: compilation puts instructions into a form understandable to the computer, but only when the compiled program is "run" will the instructions be carried out.

Portability between computers has already been mentioned above, but portability in time is just as important as portability in space. There is now an enormous investment in existing programs written by the scientific community in the past using earlier versions of Fortran. To preserve that investment, Fortran 90 was designed for backwards-compatibility with the previous standard version, FORTRAN 77; and apart from the deletion of a few of the obsolete features Fortran 95 is compatible with Fortran 90. Consequently, Fortran 95 includes a number of archaic features that would not have been included in the language if it were being designed from scratch without the burden of history. The archaic features should be avoided by a newcomer; they are no longer functionally necessary, and in this book they are covered only for the sake of completeness.

What we mean by a "program" generally takes the form of a length of text divided into lines. There might be a couple of dozen lines in a very simple program, or a few hundred in a medium-sized one, or many tens of thousands of lines in sophisticated programs written and maintained by teams of programmers.

Any program will have a starting point and an end point, and instructions between the start and the end will be "executed" in turn when the program runs. Many of the instructions will manipulate data in some way—multiplying numbers together, for example, or concatenating strings of text. However, some instructions can permit a program to branch out into alternative paths, and so in practice most programs are not executed in a fixed linear sequence of instructions. There can be branches, loops, conditionally executed blocks of instructions, and other structures, and a program may have several different possible points of termination.

1.3

Program structure

In general a Fortran program consists of a number of separate "program units", namely

- A "main program" When the program as a whole is run, it always starts at the first statement of the main program.
- An arbitrary number of other program units These can be called into play when needed by special statements within the main program or within other program units.

A short program could consist only of a main program, but in practice there are usually several program units. Apart from the main program, the other program units fall into two classes:

- "external subprograms", or "external procedures" (introduced in Chapter 7).
- "modules" (dealt with in Chapter 10) that can, for example, be used to contain data that will be made available to different subprograms.

There is a third class of program unit, now outmoded and unnecessary, known as **BLOCK DATA**. Throughout the chapters of this book, small type like this is used when referring to old Fortran features whose use is no longer recommended.

The difference between a module and an external subprogram is that a module contains information made permanently accessible to the program unit that invokes it: invocation is by a once-and-for-all declaration at the start of that program unit. A subprogram, on the other hand, is invoked dynamically (and perhaps repetitively) by action statements during program execution.

Subprograms can be invoked from the main program or from other subprograms. There is even the possibility of "recursive" subprograms that invoke themselves. Subprograms fall into two classes, namely "subroutines" and "functions", differing according to exactly how they are invoked. Normally subroutines are used to switch the flow of execution of the program, while functions are used for repeated calculations.

It should be noted that the terms "procedure" and "subprogram" are synonyms in the Fortran context. They are used interchangeably in this book.

There is another kind of subprogram not so far mentioned, namely a "module subprogram". A module subprogram is a procedure encapsulated within a module. Module subprograms, like external subprograms, are classified as either subroutines or functions, but putting a group of them together in a module can be a useful way of setting out a group of subprograms that have a special relationship with one another and need access to a shared pool of data. Technically, module subprograms are not classified as program units in their own right: it is the module that contains them that is classed as a "program unit".

1.4

Intrinsic procedures

"Intrinsic procedures" are a kind of toolkit provided for the programmer in Fortran. They are a generalpurpose set of subprograms that can be invoked from any Fortran program. For example, to calculate the square root of a number a program only needs to use the expression **SQRT(...)**, inserting the number in question between the brackets. **SQRT** is a Fortran "keyword" that simply causes the square root to be calculated. Procedures like **SQRT** are just there, waiting in the background in case they are needed. They are an intrinsic part of the Fortran language. There are well over 100 intrinsic procedures in Fortran 95, and almost all of them (including **SQRT**) take the form of a "function", like a mathematical function, and are called "intrinsic functions". A function is a procedure that can be referred to simply by mentioning its name, even in the middle of a complicated expression; for example **SQRT**(**21–SQRT**(**25**)) is an acceptable Fortran expression that calls the **SQRT** function twice and is equal to 4.0.

Fortran's intrinsic procedures include several standard mathematical functions such as the common trigonometrical and hyperbolic functions. They also include some very useful procedures for frequently needed numeric manipulations, such as finding the absolute magnitude of a number or picking out the largest from a given set of numbers. There are other intrinsic procedures that operate not on numbers but on strings of characters. Yet others are useful for checking up on the characteristics of the computer being used: for example the intrinsic inquiry function **PRECISION** will tell your program what is the limit of your computer's decimal precision. Inquiry functions like this would be unnecessary if all computers were identical, but are very valuable for writing programs to be portable between computers with different characteristics.

There are still other intrinsic procedures that are used for handling vectors and matrices, and for manipulating binary "bits", and for tasks such as the generating of random numbers. They are introduced gradually through this book, but are all listed in Appendix F.

1.5

Statements

A Fortran program or subprogram consists of an ordered sequence of "statements", and the statements can carry out different sorts of tasks. Some statements ("assignment" statements) give a value to a variable quantity: for example

n = 256

is an assignment statement that sets a variable called n equal (for the time being!) to 256. Assignment statements always have an = sign in them. Other kinds of statement are indicated by special keywords, for example a statement that writes out data will begin with the keyword **WRITE**. Fortran statement types are listed in Appendix E; it is a long list, and rather bewildering at first sight, but in practice most programs, like most people's conversation, is built up predominantly out of statements of relatively few kinds.

Statements can be divided into two important classes: "declarative" statements and "executable" statements. The declarative statements can be imagined to take effect once and for all when the program is compiled: they establish what kinds of data are to be manipulated by the program (or subprogram), allow memory space to be allotted to data, and may set up certain relationships between items of data.

The executable statements take full effect only when the program is run: they are action statements that cause items of data to be altered or moved in some way, or that make decisions. Executable statements are sometimes called "procedural" statements and, when the program runs, the computer proceeds through them in turn.

Within a program or subprogram, the declarative statements must be grouped together at the beginning and they are followed by the executable statements in sequence. The difference between a declarative statement and an executable statement is quite fundamental. It is a little like the difference between an adjective and a verb in English. Consider the following program:

Cinderella is beautiful Sisters are ugly, and coarse, and there are two of them The Prince is rich Dress Cinderella Nullify the Sisters Take Cinderella to the dance Marry the Prince

The first three of these statements do not actually do anything but they set the scene. They could have been stated in any order. They are declarative. The last four statements are executable, in the sense that changes are made to some of the entities referred to in the first three statements. For the executable statements, the order is important.

All Fortran program units have the same basic structure as the Cinderella example above. However, one should be aware that there are different styles and fashions in programming and some programmers prefer to emphasize declarative aspects of programming while others prefer the procedural approach. Fortran is historically a procedural language and earlier versions of it were much more limited in their repertoire of declarative statements than Fortran 95 is.

There are several kinds of declarative statement in Fortran, but by far the most important is known as the "type declaration statement" or TDS. It is so important that most of Chapter 8 is devoted to describing all its possible variations. The TDS can be regarded as Fortran's archetypal declarative statement, the archetypal executable statements being the assignment statement and the IF statement that enables the flow of program execution to be controlled according to the values that variables are found to have at the time.

1.6 Data

Items of data may be "constants", unchanging throughout the execution of a program, or they may be "variables" able to be changed. Every variable is identified by a "name". In the example of an executable statement given earlier,

n = 256

the letter n is the name of a variable and the number 256 is a constant. In fact, a set of similar data items may be grouped together in an "array" under a common name: this makes it possible to manipulate large sets of data with very simple statements. Mathematically, these sets of data may be sequences of numbers, or vectors, or matrices, or tensors, or whatever you like, and they may be organized in many different dimensions; they can still be named and handled as single entities. "Array" is the general term used for a set of data going under a single name. Fortran works very flexibly with arrays of almost arbitrary size and can be used to exploit vector-processing facilities on computers of advanced architecture. In fact, the statement above could actually cause a large number of data items each to be set equal to 256 if it had been arranged

for the name n to represent an array of numbers. The arrangement would be made by stating n to be an array in a declarative statement (a TDS) at the start of the program. Thus, the meaning and effect of an executable statement may depend profoundly on the attributes that items of data have been declared to have.

Likewise, most of Fortran's intrinsic mathematical functions will work for arrays: an expression like SQRT(x), if x is the name of an array, will calculate the square roots of all the numbers in the array x.

Data items may be of a number of different "types". For example, integer numbers and complex numbers are different types. The word "type" is not used loosely: it is a technical term that refers to the nature, and not the particular value, of a single data item. Most programming languages allow for a few different types of data, but Fortran 90 allows, in principle, for an arbitrary variety of types. This is because of a feature known as "user-defined types" or "derived types", by which the programmer may construct a definition of a fresh type of data relevant to the problem in hand. It is easy to draw examples from advanced mathematics: for example, a programmer interested in four-dimensional geometry could define four-component vectors and 4×4 transformation matrices, and could also define what would be meant by the sums and products of such entities. As a more down-to-earth example, the latitude and longitude of a geographical point together comprise a special sort of data item and could be set up as a user-defined type obeying its own rules according to the programmer's wishes. User-defined types can be more flexible than arrays: an array is a set of items all of which must be of the same type, but a user-defined type can be a complicated structure incorporating data of quite different basic types, e.g. mixing numbers and words. So, a single Fortran "name", like x, could in this way refer to a mixed package of data such as a person's name, address, telephone number and age.

Another interesting feature in Fortran is that of "pointer" data. The concept of a pointer is not easy to appreciate at first, but one way to illustrate the idea is to take the example at the end of the previous paragraph, of a set of data consisting of a person's name, address, telephone number and age. Imagine that we have a large list of information of this sort. Suppose that we want the set of data for each person to include also a cross-reference to the corresponding information for the person's spouse. There are various ways in which this might be achieved. One way might be to give an index number to each person listed, and to include the spouse's index number in the data set for each person who is married. However, the simplest method in Fortran is to include a "pointer" to a spouse's details. The pointer would have the appearance of an additional data item encapsulating all the spouse's personal details; but in reality it would simply "point" to the other area of memory where the spouse's details are already listed in his/her own right. Using pointers, there is no need to take up unnecessary memory space by repeating chunks of data, nor to set up special codes for cross-referencing between data.

Modules are another very valuable feature of Fortran, and were mentioned above in Section 1.3. Like pointers, modules are difficult to appreciate in the abstract. You have to use them, in real programs, to see how effective they can be. Modules are useful in the architecture of large programs or systems of programs, where they can be used to organize plug-in sets of procedures for particular purposes. In smaller programs, modules are most useful for memory access, i.e. for containing data that is to be used by more than one procedure.

1.7 Writing Fortran

In practice, any Fortran program takes the form of text divided into lines. Each line may be up to 132 characters in length. Usually there is one Fortran "statement" per line. Within the line, the statement does not have to start at the first character or end at the end of the line: there may be blank spaces leading or

trailing behind the statement. As a rule, blanks may be used to space out parts of a statement to improve legibility.

If desired, it is possible to have several statements on one line, using the semi-colon as a separator. It is also possible to spread one statement over several lines, using an ampersand (&) to mark the break. Also, it is easy to annotate the program with comments—pieces of text which do not actually form part of the program and will be ignored by the compiler. This way of laying out a program is known as "free source form" to distinguish it from an older "fixed form", the latter being a tightly constrained statement layout which originated historically in the format of the now-long-vanished 80-column punched card.

It is important to understand that Fortran will not, usually, solve a conceptual problem for the programmer. The programmer has to solve it. Fortran itself has no creativity, but simply allows the programmer to express the solution (or "algorithm")in a form that can be read and acted upon by a computer. However, although Fortran will not of itself solve the problem facing the programmer, a methodical approach to writing Fortran can assist by helping the programmer to analyze the problem efficiently and perhaps to reduce it to a number of simpler sub-problems. The pattern of program units in a Fortran program often reflects the logical reduction of the original problem into separate parts. In this sense, Fortran is a powerful thinking tool and it can be claimed that you do not really understand the solution to a problem unless you can express it as a successful Fortran program!

Fortran usually offers the programmer more than one correct way of expressing an algorithm. Choices are therefore involved and can be made on the basis of various considerations such as mathematical elegance, speed of computation, economy of memory, and the transparency of the code to a different human reader. Some of these considerations may be irrelevant: for example, such is the speed of today's computers that, for a particular problem, the computation time may be negligible however the program is written. But the history of computing is a beautiful illustration of how increasingly complex tasks are attempted to match the resources available to carry them out and of how leading-edge science always seems to work at the limits of current technology. So, in spite of the prodigious speed and memory capacity of present-day computers, it is just as important as it ever was to design programs that will execute as speedily as possible and will utilize memory as economically as possible. Many of Fortran's apparently arcane features—such as "allocatable arrays"—exist for this reason.

1.8

Coding conventions and typography

Fortran 95 offers its users a good deal of scope for establishing their own conventions about the superficial aspects of writing a program, such as the use of upper- or lower-case letters, margins and choices between equivalent ways of expressing the same things such as **ELSEWHERE** as opposed to **ELSE WHERE**. The Fortran code in this book embodies, for the most part, a set of coding conventions that are summarized in Chapter 14. Programmers often like to disagree with one another about coding conventions and it is possible for individual creativity to express itself harmlessly in the way that a program is presented to the human reader. It is not the purpose of this book to promote one set of coding conventions over another. However, consistency of presentation is extremely important both for an individual and, obviously, for any group of programmers who will need to be able to read and check one another's work efficiently. Consistency itself is more important than the particular set of conventions chosen. It may be legal to refer to a variable as **x** in one line of code and as **x** in the next, but it would not be wise. Fortran is a permissive language, but liberty implies responsibility!

One of the coding conventions used in this book is to express all Fortran keywords and intrinsic procedure names in upper-case letters, and the names of data objects in lower case. Fortran is additionally set in **Courier** typeface. For example, as it will be expressed in this book, **REAL** is a keyword referring to a special class of Fortran data whereas "real" is an English word that may refer to the mathematical concept of a real number.

Sometimes, in the text, double quotes ("") are used to clarify the meaning if there is any danger of ambiguity between a technical term, or the name of a data object, and the corresponding English word. This should prevent any confusion over words like "automatic" and "name" which have technical as well as English meanings.

Fortran statements and expressions sometimes need to be expressed in generalized forms in a book like this, and then italics are used. For example, the first statement of a program takes the general form

PROGRAM program-name

but it would never look like that in an actual program: *program-name* merely represents whatever the name of the program might be. If the program is to be called **Extrapolate** then the actual statement would be

PROGRAM Extrapolate

Italics will also be used for other generalizations such as when discussing procedures with optional arguments such as **RANDOMSEED** (*SIZE*, *PUT*, *GET*). It could be misleading to print **RANDOMSEED** (SIZE, PUT, GET) because the false impression might be given that it is a valid fragment of Fortran as it stands.

1.9

Fortran 90 features deleted from Fortran 95

Existing users of Fortran 90 should note that Fortran 95 is expected to exclude real **DO**-loop indices, branching to an **END IF** statement from an outer block, the **PAUSE** statement, the **ASSIGN** statement, and "Hollerith" data editing. All the expected differences between Fortran 90 and Fortran 95 are described in context in the appropriate sections of this book. The new features of Fortran 95 that were not present in Fortran 90 are listed in Appendix D.

CHAPTER 2 Getting started

The characters, "lexical tokens" and format used to construct Fortran 95 programs are described, and a simple example program is discussed in detail. The Fortran statements met are the "assignment statement" and the statements **PROGRAM, REAL, READ, WRITE, IF... THEN, ELSE, END IF, and END PROGRAM.** Arithmetic operators and the intrinsic function SQRTare also encountered.

2.1

The character set

Fortran programs are built up out of the limited set of characters listed below:

Letters: ABCDEFGHIJKLMNOPQRSTUVWXYZ

Digits: 0123456789

The underscore: _

Special characters:

- = Equals
- + Plus
- Minus
- * Asterisk
- / Slash
- (Left parenthesis
-) Right parenthesis
- , Comma
- . Decimal point or full stop
- \$ Currency symbol
- Apostrophe (or single quote)

- : Colon
- ! Exclamation
- " Quote (or double quote)
- % Percent
- & Ampersand
- ; Semicolon
- < Less than
- > Greater than
- ? Question mark Blank

Most of these characters have specified uses in Fortran. For example, the letters crop up in statement keywords like WRITE or STOP; the digits and decimal point are used to represent numbers; characters like

+ and – are used in the usual way for mathematical operations; and so on. Virtually all the Fortran standard characters should exist on any keyboard and it should be possible to display them all on any screen or printer.

It should be noted that Fortran only recognizes one kind of apostrophe or single quote ('). Although a processor may distinguish between an opening apostrophe (') and a closing one ('), they are the same to the Fortran language. A similar thing applies to (double) quote marks—or inverted commas—(").

There are just two exceptional special characters, the currency symbol (\$) and the question mark (?), which have no particular roles in standard Fortran itself. However, such characters occur in real life and so they are likely to crop up in programs as elements of character strings, as in the WRITE statement

WRITE (*,*) "What is your name?"

This is an executable statement that, when the program containing it runs, would cause the standard output device—presumably a screen—to display the string of character between the quotation marks, i.e.

What is your name?

The meaning of (*, *) in the **WRITE** statement will be explained in due course.

With Fortran, output devices will display the characters more or less in the forms tabulated above, although the exact font style may vary. The symbol given as a dollar sign (\$) is regarded as a general currency symbol and could appear as £ or whatever according to the country.

The **WRITE** statement above illustrates an important point: in a specified character string (**"What is your name?"**) one may mix lower-case and upper-case letters and the processor may distinguish between them. Almost all modern computer systems do in fact permit the two kinds of letters, but some equipment does not, so Fortran does not insist on the distinction and no such distinction is made in the syntax of the language itself, e.g. in keywords such as **WRITE**. This is why lower-case letters were not listed separately at the beginning of this chapter. As far as the processor is concerned, the statement given above could equally well appear as

Write (*,*) "What is your name?"

and if the processor is incapable of discriminating between lower-case and upper-case letters, the result of executing the statement might be

WHAT IS YOUR NAME?

Throughout the rest of this book it will be assumed that the processor can discriminate between upper-case and lower-case letters. However, the programmer must always realize that there is no such distinction in the syntax of the Fortran language itself ("What is your name?" is the English language, not Fortran!). So

N = 256

is precisely equivalent to the example statement, n=256, encountered in Chapter 1.

It is advantageous for the programmer to develop a style that exploits lower-case and upper-case letters to improve the readability and editability of programs; for example, it is a good idea always to use upper-case letters for statement keywords (like **WRITE**) and for the names of intrinsic functions, and to use lower-case letters for the names of variables, as in something like

 $x = -b + SQRT(b^{**2} - 4^{*a*c})$

Here, **SQRT** is Fortran's built-in square root function, mentioned earlier in Section 1.4. It should be remembered that a programmer will normally be working through the medium of some sort of text editor while writing or updating a program. It makes no practical difference to Fortran whether you refer to the square root function as **SQRT**, Sqrt or sqrt, but it may make a difference to your editor if, for example, a string-search facility is used to find all the usages of that function within a very large program. Consistency is therefore recommended.

Blank spaces are not always relevant to the syntax of Fortran, but they can be used to space things out to improve appearance. The above statement is precisely equivalent to

x=-b+SQRT(b**2-4*a*c)

but the former is a little easier to read and to check. However, blank spaces may not be embedded within keywords or within the names of procedures. The letters of WRITE and SQRT, for example, may not be broken up with blanks. Furthermore, blanks are not ignored when they appear as elements of fixed character strings such as **"What is your name?"**. In program statements, such strings are always distinguished by being enclosed between quotes or apostrophes.

There is one more important point that must be made about characters in Fortran. It is that any character whatsoever that is representable within the processor may occur in "character context", i.e. as an element of a character string such as "What is your name?". The lower-case letters are a special case of this rule, but it applies equally to any other unusual characters that were not listed in the table earlier but may be available on a particular processor and may appear on keyboards and screens. If a processor is capable of representing the letters of the Greek alphabet, or Japanese kanji characters, or whatever, then they may validly appear in a character context within Fortran. The character set shown at the beginning of this section is a minimum set for conformance with the Fortran standard, but a program may display information in other ways depending on the capabilities of the processor.

2.2 A simple program

PROGRAM Triangle

REAL :: a, b, c, s, areasq, area

WHITE (*,*) "This program calculates the area of a triangle."

WRITE (*,*) "Type in the lengths of the three sides:"

READ (*,*) a, b, c

WRITE (*,*) "Check: you have input the following lengths"

WRITE (*,*) a, b, c

s = 0.5 * (a+b+c) ! Semiperimeter

areasq = s*(s-a)*(s-b)*(s-c) ! Square of area

IF (areasq<0.0) THEN

WRITE (*,*) "Error: that is not a real triangle"

ELSE

area=SQRT(areasq)

WRITE (*,*) "The area of the triangle is", area

END IF

END PROGRAM Triangle

Here, the first two statements are the declarative part of the program. The **PROGRAM** statement serves to introduce the program and to give it a name (Triangle). The statement beginning **REAL** serves the purpose of establishing that **a**, **b**, **c**, **s**, **areasq** and **area** are to be the names of variables which are real numbers. We shall see later that this **REAL** statement (a special form of what is generally known as a "type declaration statement" or TDS) is in fact not strictly necessary here.

After the first two lines is a blank line. This does absolutely nothing—it will be ignored by the compiler but is an allowable way of breaking up the program for display purposes.

We now move on to the program's executable statements. The **WRITE** statements are for the output of data. The statement

WRITE (*,*) "Type in the lengths of the three sides:"

is a Fortran abbreviation for

WRITE (UNIT=*, FMT=*) "Type in the lengths of the three &

&sides."

If a statement is uncomfortably long, or is too long to fit onto one line, ampersands (the & character) can be used to divide it between two lines, as here. It does not really matter where the break between lines occurs. The following statements are equivalent:

WRITE (UNIT=*, FMT=*) "Type in values for the lengths &

&of the triangle's three sides"

and

WRITE (UNIT=*, FMT=*) &

"Type in values for the lengths of the triangle's &

&three sides."

It is no mistake that only one & appears between the first two lines here, but two between the second and the third. The exact rules for continuing a statement from one line to the next are summarized in Section 2.6.

In principle, **WRITE** statements may be used to output data onto any of a variety of devices that may be connected to the processor: printers, a screen, magnetic tape units, or whatever. Fortran expects each device to have a number, the "unit number", and the WRITE statement can specify the unit by including in brackets **UNIT=1**, **UNIT=3**, **UNIT=9**, or whatever. However, to simplify matters any processor is required to have a standard output unit that will automatically be used unless another unit is explicitly specified by number. An asterisk is used to refer to the standard output unit, so we have the specification **UNIT=*** in the **WRITE** statement above. In most modern personal computers the standard output device will be a screen, so this **WRITE** statement will cause the string of characters

Type in the lengths of the three sides:

to appear on the screen.

What about **FMT=*?** This is to do with the format in which a piece of data is to be output (or, for input, the expected format in which it is to be read). Just as the **UNIT** keyword gives the programmer access to the range of available input/output devices, so the **FMT** keyword gives freedom to specify precisely in what style the information is to be displayed: for example, with how many places of decimals a number will be shown. By using the asterisk in **FMT=***, we are taking an easy way out called "list-directed formatting", whereby the format follows certain default conventions according to the nature of the data item (or items) listed in the subsequent part of the WRITE or READ statement. For the time being, list-directed formatting will be sufficient for us. Format specification is a large topic but not, for everybody, an important one. It is covered in detail in Appendix A.

So, in the example program above, (*, *) is a valid abbreviation for (UNIT=*, FMT=*) and it means that standard defaults are being used for the i/o devices and for the i/o formats. For most of this book we will imagine that all input is via a keyboard and all output is onto a screen.

The **READ** statement in the example program is

READ (*,*) a, b, c

and it means that numbers represented by a, b and c are to be input from the keyboard. "Real" numbers are expected, i.e. positive or negative numbers that may include decimal fractions, as opposed to integers or complex numbers or people's names or anything more complicated, a, b and c are "variables", i.e. entities whose values are not necessarily known when the program is written but are determined later on as the program runs and may be altered from one value to another in the course of the program. Inputting the numbers with a **READ** statement is one such way of giving values to the variables a, b and c. Selecting the first three letters of the alphabet as the names of these variables is a completely arbitrary choice. We could have used more or less any letters of the alphabet, or indeed sequences of letters. For example, we could have used instead the statement

READ (*,*) side_a, side_b, side_c

in which case the rest of the program would also have to have a, b and c replaced by **side_a**, **side_b** and **side_c**. The detailed rules for the naming of variables are given in the next chapter.

Fortran normally expects a variable to be a real number if its name begins with a letter of the alphabet in the range a–h or o–z. Names beginning with i, j, k, l, m or n are expected to represent integer variables, corresponding to numbers without fractional parts. If a variable is neither a real number nor an integer, for example if it is a complex number, Fortran requires this fact to be declared explicitly in advance by a type declaration statement along the same lines as the **REAL** statement above.

The default (list-directed) format is such that a, b and c in our example can be input from the keyboard in a form such as

3, 4, 5

or

3, 4, 5

or

345

or even with the numbers on separate lines as in

3(return)

4(return)

5(return)

The "delimiter" between the numbers may be a comma, or a blank, or both, or a series of blanks, or it can be the end-of-record code signified by the **return** or **enter** button on most keyboards. Decimal points could be included as in

3.0, 4.0, 5.0

and obviously the decimal point is mandatory if the variables actually have fractional parts, as in

3.5, 4.333, 5.25

However,

3 1/2, 4 3/4, 5 1/4

would be unacceptable because 1/2, 3/4 and 1/4 are not part of the Fortran character set listed at the start of this chapter.

The final number must be followed by a delimiter (e.g. a blank or a return) otherwise the processor does not know you have finished. More detailed information on the format of "list-directed" input is given in Appendix A.

If we continue with the example program, **Triangle**, there are two **WRITE** statements that display the given lengths of the sides of the triangle as a check. Then we have

s = 0.5 * (a+b+c) ! Semiperimeter

This is the first statement of the program that actually does anything mathematical. It is called an "assignment statement" and it sets the real variable s to be equal to half the sum of a, b and c. The asterisk is Fortran's multiplication sign. Assignment statements do not begin with a keyword but are characterized by the = sign. In general, on the right hand side of the = there must be an expression that the processor can calculate. In this example the processor will just have been given numerical values for a, b and c and these will be used to give a numerical value to s when the assignment statement is executed. It would not matter if the variable s already had a value: if it did, then the previous value would be replaced.

This statement also illustrates the use of the exclamation mark to start a comment. The ! and the text that follows it are treated like blanks by the processor. It is the means by which the programmer can annotate the program.

The next statement is:

areasq = s*(s-a)*(s-b)*(s-c)! Square of area

If a, b and c represent the lengths of the sides of a triangle then **areasq** is the square of the triangle's area. The expression on the right-hand side is a geometrical formula, the knowledge that the programmer must bring to this program. To finish calculating the area we just have to take the square root of **areasq**, and this is done by calling the intrinsic function **SQRT** that we have already met.

However, there is a potential problem: if the user of the program put in silly values for a, b and c (e.g. 1, 1 and 99, which cannot correspond to the sides of a real triangle) then the variable **areasq** could come out to have a negative value. Trying to take its square root would then cause the program to fail, since a negative number does not have a real square root. So the program should first check to make sure that **areasq** is not negative. The check is carried out by control statements that direct the course of the program so that different statements will be executed in different circumstances.

The control statements in our example are the IF...THEN, ELSE, and END IF statements. Their meaning should be obvious, but the details are set out in Chapter 6. In the IF...THEN statement, the expression

areas<0.0

is a "logical expression", that is to say an expression that has not a numerical value but a logical value, i.e. is either true or false. If **areasq** is less than zero then this logical expression has the value "true" and control will then pass to the statement following. If **areasq** is not less than zero, then the logical expression has the value "false" and control will pass down to the statement following **ELSE**. The **END IF** statement indicates the end of the blocks of conditional statements.

Whatever the value of **areasq**, control finally passes beyond the **END IF** statement to the **END PROGRAM** statement that brings execution of the program to a halt. Note that the conditional statements following **IF...THEN** and **ELSE** have been indented to the right purely for cosmetic reasons. Leading blank spaces have no significance in Fortran syntax, but by indenting statements in this way we can make a program considerably easier to read and understand.

The above example has been discussed in fine detail. We have encountered the statement types **PROGRAM, REAL, WRITE, READ,** Assignment (=), **IF...THEN, ELSE, END IF and END PROGRAM**. We have discussed numeric variables and the names that can be used to represent them, and used **READ** and **WRITE** statements to input and output values of real variables by list-directed formatting on the standard default i/o devices (keyboard and screen). We have encountered real and logical expressions. The real expressions

0.5 * (a+b+c)

and

s*(s-a)*(s-b)*(s-c)

illustrate the use of the arithmetic operators * (for multiplication), + (for addition), and - (for subtraction) and of brackets to make sure that things are done in the right order (s*s-a*s-b*s-c would be not be same thing at all!). Arithmetic operators in general are described in the next section.

2.3 Arithmetic operators

Fortran's complete list of arithmetic operators is:

**	exponentiation, i.e. raising to a power (e.g. 3**4 is equal to 81)
* and /	multiplication (e.g. 5*6 equals 30) and division
+ and –	addition and subtraction (e.g. 9-27 is equal to -18)

These are "binary operators" in the sense that they go between two numbers and produce a result that depends on the two. (However, the minus sign can also be used as a "unary" operator, applied to just one number, e.g. –b is the negative of b. The plus sign, too, can be a unary operator in the trivial sense that +10 is equal to 10.)

The arithmetic operators above can be combined with variables and constant numbers to form expressions such as $b^{**2}-4^*a^*c$.

The descending order of the operators listed above is their order of precedence, i.e. the order in which they are normally carried out when different kinds occur in the same expression. However, brackets are used to over-ride that order of precedence. In the example just mentioned, b is first of all squared, then 4*a*c is evaluated, then 4*a*c is subtracted from b**2. The result is as if we had instead

(b**2) - (4*a*c)

When there are two or more operators together on the same level of precedence, the expression is evaluated left to right, i.e. 4*a*c is equivalent to (4*a)*c. With a chain of multiplications, of course, the order does not usually make any difference: (4*a)*c is the same as 4*(a*c). But in many cases the order is significant, e.g.

16/8/2 is equivalent to (16/8)/2, equal to 1 16/8*2 is equivalent to (16/8)*2, equal to 4

12-6-3 is equivalent to (12-6)-3, equal to 3

The left-to-right rule applies to all the above examples, but there is an exception in the case of the exponentiation operator. When a number of exponentiations are strung together they are evaluated from right to left: so 2.0**0.5**(-1) is equivalent to 2**(0.5**(-1)), and is equal to 4.0.

Note that $2^{**0.5^{**-1}}$ would not be a permissible expression because the rules of Fortran do not allow two consecutive numeric operators (in this case, $^{**-}$). Another limitation is that the exponentiation operator should not be used to raise a negative real quantity to a real (as opposed to integer) power: so you should not expect (-3.375)**(0.333333) to have the value -1.5. Expressions of this sort should either be avoided or should be handled using complex numbers (Chapter 3).

Here are a few more examples of the rules of operator precedence in Fortran expressions:

```
3*5+7-9 = (((3*5)+7)-9) = 13

21/3*5/7 = (((21/3)*5)/7) = 5

2**2**2**2 = (2**(2**(2**2))) = 65536

4**4/2*2**2 = ((4**4)/2)*(2**2) = 512
```

However, in practice it is wise to sidestep the question of operator predence by the liberal use of brackets when writing Fortran statements.

2.4 Exercises 2.A

2.A Check which of these are in the Fortran character set:

1 **# A \$ @ % [: ; >** 2.A Evaluate the following: 2

(i) 3**2**3	(ii) 4+6/12*2
(iii) 18/4/2** (-1)	(iv) SQRT (4**3**2)
(v) 9/8*7/6*5/4*3/2	(vi) 9*8/7*6/5*4/3*2
(vii) 6–4+1	(viii) 16.0**3.0/2.0
(ix) (-1)** 0.5 **(-1)	(x) 2–1**0.5**(–l)

2.A If a, b, c, d and e are the names of real variables, write Fortran expressions for: 3

- (i) The average of a, b, c, d and e;
- (ii) The root-mean-square of a, b and c;
- (iii) b, expressed as a percentage of the total of a, b, c, d and e;
- (iv) The geometric mean of a and b.
- 2.A Input into a computer the example program (Triangle) given earlier. Run the program and test it with 4 different values for a, b and c. Enhance the program to make it calculate and display not only the area of the triangle but also its perimeter.
- 2.A Write a program to input two numbers and to output the larger of them. The program should 5 communicate clearly with the user, and should use only the elements of Fortran that appear in Triangle.

2.5

Names and other lexical tokens

In the discussion so far we have encountered several of what are called "names" in Fortran terminology. These examples were as follows:

the name of a program: Triangle the names of variables: a, b, c, s, areasq, area, side_a, side_b, side_c an intrinsic function: SQRT

The names of variables are sometimes referred to a "identifiers". Fortran also permits names for subprograms (user-written functions, subroutines and modules), for user-defined data types, and for certain other objects such as "namelist" groups. The general rule is that names must begin with a letter and may consist of up to 31 "alphanumeric" characters. The alphanumeric characters are the letters, the digits and the underscore.

A blank is not regarded as an alphanumeric character, so blanks may not be included in names, and nor may the other special characters listed in Section 2.1.

Names are just one of the six kinds of "lexical tokens" that Fortran syntax is built up out of. The six are:

Names	(see above)
Keywords	e.g. PROGRAM, WRITE, READ, IF, FMT, UNIT
Constants	e.g. numeric constants such as i.0, 365 and -66.896; and character-string constants
	such as "Error: that is not a real triangle" (in quotes or inverted commas)
Operators	e.g. +, -, **, = and >
Delimiters	e.g. ! and brackets (parentheses)
Statement labels	(see Chapter 14)

From Fortran's point of view it is possible for names to be identical to keywords, but this is best avoided as it could obviously lead to confusion in the programmer's mind.

We have been using a particular convention for the capitalization (i.e. upper case or lower case) of letters of the alphabet. This convention is just that —a convention—and is not obligatory within Fortran, but it is extremely important to use some sort of capitalization convention to achieve orderly, consistent and attractive programming, particularly when teams of programmers are working together. There is nothing worse than a lengthy program in which the use of upper and lower case is arbitrary or inconsistent.

Our suggested capitalization convention can be summarized as follows:

Upper-case:

Statement keywords (such **READ**) Names of intrinsic procedures (such as **SQRT**) Keywords for arguments of intrinsic procedures

Lower-case, but with an initial capital letter:

Name of a program or a program unit Keywords for arguments of non-intrinsic procedures Namelist group names

Derived types

Lower-case

Names of variables or of constants

Some of the terms mentioned above may not be meaningful at this stage, but they are listed here for the sake of completeness. You may, of course, choose a different convention from this.

2.6 Fortran source form

The Fortran "source form", i.e. the general format according to which programs should appear, can be of two alternative kinds, namely "free" or "fixed" source form. The latter is now of historical interest only and is summarized further below. Free source form has already been used in the examples of Fortran given so far, and the details are as follows:

- (a) A program is divided into records (i.e. "lines") each up to 132 characters in length. Except as mentioned in (g) below, blank characters have no significance, other than to make the code more readable, and they are ignored by the processor.
- (b) Normally there is one "statement" per line. A statement may start with a keyword (such as PRINT) or it may be an assignment statement (assigning a value to a variable by use of the = sign). A statement may be preceded on the line by blank characters, i.e. it may be indented, and it may be followed by blanks. A statement may also be preceded by an integer number used as a "statement label", a common but generally inelegant feature of Fortran programming discussed in Chapter 14.
- (c) Comments may be inserted after statements to guide readers of the code. A comment must always be separated from the statement by the ! character. The ! terminates the statement as far as the processor is concerned, and everything on that line after the ! is treated as commentary. A line is permitted to contain only a comment, and no statement at all, if it begins with a !. A completely blank line will be ignored. However, it must be remembered that a ! that occurs within character context, i.e. as part of a character string specified between single or double quotes, does not start a comment.
- (d) A statement may be continued from one line to the next. Continuation is indicated by having an ampersand (&) as the last non-blank character in a line, with the effect that the subsequent line is tacked on to whatever immediately preceded the &.

However, a comment cannot be continued in this way: an & occurring within a comment has no special effect. Also, an & occurring in character context will not normally continue the string on the next line, i.e. it will just be taken as part of the character string, in the same way that a ! in character context has no special effect. However, in a case where it is necessary to continue a character string to the next line, the effect can be achieved by using two &s, putting one at the end of the first line and the other at the beginning of the second.

In fact, it is always acceptable to put an ampersand at the beginning of the continuation line as well as at the end of the preceding line, but unless you are in character context the second ampersand is optional rather than compulsory. When an ampersand starts a continuation line it need not be the first character of the line: there may be leading blanks that the compiler will ignore. It was mentioned above that the ampersand should be the last non-blank character on a line that is to be continued: but in fact it may be followed by a ! and a comment except when the continuation is within character context.

- (e) A statement may be continued over many lines. The only limitation is that a statement may not contain more than 2640 characters.
- (f) It is possible to have more than one statement per line. The semi-colon (;) then serves to separate one statement from the next. However, a semicolon in character context does not have this effect.
- (g) Blanks are generally irrelevant to Fortran and they can be used generously to make a program easy to read. However, blanks are significant in one or two respects. They may not be embedded in lexical tokens. A keyword adjacent to a name must be separated from it by a blank. Blanks are not ignored in character context. In most double-keyword combinations a dividing blank is not mandatory but it is good practice to include it.

In a statement like

END PROGRAM Triangle

the blank between END and PROGRAM is not strictly necessary, i.e.

ENDPROGRAM Triangle

would be equally valid. The Fortran keyword-pairs (and in one case, triplet) that are allowed to be run together without a blank space are as **follows: BLOCKDATA, DOUBLEPRECISION, ELSEIF, ELSEWHERE, END-BLOCKDATA, ENDDO, ENDIF, ENDINTERFACE, ENDMODULE, ENDPROGRAM, ENDSELECT, ENDSUBROUTINE, ENDTYPE, ENDWHERE, GOTO, INOUT, and SELECTCASE**. Needless to say, for the sake of clarity, it is recommended that the blanks be inserted.

The following contrived examples, all legal Fortran, may help to make the rules clear:

ENDPROGRAM Triangle

would be equally valid. The Fortran keyword-pairs (and in one case,

PROGRAM Master ! Version 6

READ (*,*)indata

WRITE (*,*) "We're off!"

weightedsumofcubes = a * alpha**3 &

+ b * beta**3 &

+ c * gamma**3

remark = "When a statement is continued from one line &

&to the next, but without breaking a character string &

&like this, it doesn't matter whether or not the &

&continuation line starts with an ampersand or not. &

&The two ampersands are only necessary in a character &

&string."

x=a1; y=a2; z=a3; sum=x+y+z ! 4 statements, 1 line.

this = & ! One statement, two lines

that

! This & does not turn the next line into a comment.

These are:

- a **PROGRAM** statement with lots of blank spaces and a comment at the end;
- **READ** and **WRITE** statements with leading blank space;
- an assignment statement spaced by ampersands over three lines;
- a character-string assignment statement spaced over six lines with pairs of ampersands;
- a set of four assignment statements on one line, followed by a comment;
- an assignment statement split into two lines and with a comment after the first part; and finally
- a statement consisting only of a comment.

Fixed source form

There is an alternative to the source form described above, namely "fixed" source form that was the usual form in earlier versions of Fortran and is therefore retained in Fortran 95 for the sake of backward compatibility. Fixed source form originated when programs were stored on 80-column punched cards, of which the first 72 columns could be used for Fortran. So, in fixed source form each line must contain 72 characters.

The first six character positions in each line are reserved for the following special purposes:

- (i) If the first character is c or *, the whole line is taken as a comment.
- (ii) Characters 1 to 5 may contain an integer statement label (see Chapter 14).
- (iii) The sixth character is normally blank. A continuation line is indicated by having any non-blank character (other than zero) in sixth position.

Fortran keywords, names, etc. would normally follow after the sixth character. Therefore, in fixed source form, each line may only contain 66 characters of actual code.

2.7 Program structure

When a program is to be written, it is important to approach the task by planning what is to be done before actually starting to do it. I did not write this book by starting at the beginning and working through to the end. I started by clarifying the purpose of the book, then I planned the structure it should have so that it would fit together logically with nothing being left out or duplicated. Only then did I actually start to write it. Planning a laboratory experiment is rather similar: the first step, which is often surprisingly difficult, is to establish precisely what the purpose of the experiment is. The second step is to plan what will be the experimental procedure (analogous to drawing up a structure plan for a computer program). Only then should one actually do the experiment.

This is an aspect of what is sometimes called the "top-down" design philosophy. One starts by taking a broad view, defining the purpose of the task and planning the overall structure of the program that is to be written. Often, at this stage it will become clear that it would be advantageous for the program to be broken down into a number of quasi-independent program units. It must always be borne in mind that a program (or program unit) does not only do calculations: it must also communicate with the outside world (or with other program units) so that data can be passed in and out, otherwise there is no point in doing anything. And of course, it is essential to define at the outset what sort of data is being dealt with, e.g. whether we are doing integer or real-number arithmetic.

It can sometimes be helpful to consider a program as having the general form:

PROGRAM statement

Declarative statements (data definition)

Executable statements (data processing):

data input

calculations

data output

END PROGRAM statement

The program Triangle, the example given at the start of Section 2.2, can be written as follows in an annotated form to make that structure clear:

PROGRAM Triangle

! Declarative statements:

REAL :: a, b, c ! The lengths of a triangle's sides

REAL :: s ! The semiperimeter of the triangle

REAL :: areasq ! The square of the triangle's area

REAL :: area ! The area of the triangle

! Data input:

WRITE (*,*) "This program calculates the area of a &

&triangle."

WRITE (*,*) "Type in the lengths of the three sides:"

READ (*,*) a, b, c

WRITE (*,*) "Check: you have input the following lengths"

WRITE (*,*) a, b, c

! Calculations:

s = 0.5 * (a+b+c)

```
areasq = s^{(s-a)*(s-b)*(s-c)}
```

IF (areasq<0.0) THEN

WRITE (*,*) "Error: that is not a real triangle"

ELSE

```
area=SQRT(areasq)
```

! Data output:

WRITE (*,*) "The area of the triangle is", area

END IF

END PROGRAM Triangle

Comparison with Section 2.2 shows that this version has been made rather more understandable by the liberal use of annotations, particularly where the variables are declared, and by the clear separation between the three phases of execution. Another thing, which may help to make the program easier to read, is that the statements whose execution is conditional on the IF and ELSE statements are indented to the right. This is an example of a widely used indentation convention for blocks of code controlled by statements such as IF. The indentation convention is particularly valuable for its visual impact when dealing with lengthy blocks of conditionally executed code, especially when there is a complex structure of "nested" blocks.

2.8 Exercises 2.B

2.B Which of these are valid Fortran names?

1

(i) aramaic	(ii) zhq5	(iii) balance\$
(iv) p998530	(v) 99 in	(vi) top_mark
(vii) bakers dozen	(viii) baker's dozen	

(ix) state _population_estimate_1997

2.B Write a program to read in two numbers and calculate and write the magnitude of their difference as a 2 percentage of their sum.

2.B Write a program called Quad to solve a quadratic equation expected to have real solutions. The 3 coefficients in the equation are to be input and the solutions output.

2.B Write a program (Mean) that will input six numbers, calculate and display their average, and calculate 4 and display their root-mean-square deviation from that average.

2.B Write a program to convert temperatures in either direction between Celsius and Fahrenheit.

5

CHAPTER 3 Types of data

Fortran 95 can deal with data items of many different types: in fact with an indefinite range of data types, since there is a facility for "derived" (or "userdefined")data types constructed by the programmer. Derived data types will be explained in Chapter 12. In this chapter we will cover the "intrinsic" data types INTEGER, REAL, COMPLEX, LOGICAL and CHARACTER. This chapter also deals with the simple but invaluable IF statement, the intrinsic functions ABS, AIMAG, CMPLX, COS, EXP, HUGE, INT, LOG, LOG10, MOD, REAL, SIN, TRIM and LEN, and finally the ASCII character set and the associated functions ACHAR and IACHAR.

3.1

Integers

As their name implies, integers in Fortran are the whole numbers 0, 1, 2, 3, 4,... and including the negatives -1, -2, -3,

Examples of integer constants are

137

+365 (the + sign is unnecessary but may be included)

-9

0

299792458

Constant integers may appear explicitly in programs. Integers may alternatively be represented by names. The usual convention is to represent an integer by a name beginning with a letter in the range i–n. Unless otherwise specified (by a type declaration statement, Section 3.6 and Chapter 8) variables with names like

istructure j57 mlight

nyear izero ides_april

will be therefore be taken by Fortran 95 to be integers.

Arithmetic can be done with integers using the arithmetic operators introduced in Chapter 2. If i2=2 and i3=3,

i2**i3 has the value 8
i2*i3 has the value 6
i2+i3 has the value 5
i2-i3 has the value -1

and more surprisingly

i2/i3 has the value 0

The final example arises because of the way the ratio of two integers is interpreted: the exact ratio is calculated, then the fractional part of it is discarded if an integral result is required. Thus, 365/7 has the value 52. Where negative numbers are concerned, the ratio is cut back towards zero, i.e. -365/7 has the value -52. If we had an assignment statement such as

r = i2/i3

with i2 and i3 as above, and r being a real variable, the result would still be zero, because the expression i2/ i3 is first interpreted as an integer-valued expression; assigning an integer value to a real variable is something made clearer in the next section.

Fortran has an intrinsic function, **MOD**, which can be very useful in integer arithmetic. MOD(J, k) is the value of j modulo k, i.e. the remainder when j is divided by k. To be more precise,

MOD(j, k) is equivalent to j - ((j/k)*)

where j/k is the integer quotient calculated according to the rounding-down rule mentioned above. Thus

MOD(365, 7) has the value 1

MOD(-365, 7) has the value -1

MOD(9, 6) has the value 4

Below is an example of a program using the MOD function.

PROGRAM Miles

! Display Information and input a number

WRITE (*,*) &

"This program converts a large number of inches into &

&miles, yards and inches."

WRITE (*,*) "Type in the distance in inches:"

READ (*,*) inches

! Calculation

inch = MOD(inches, 36)

nyards = inches/36

nyard = MOD(nyards, 1760)

mile = nyards/1760

! Output the results

WRITE (*,*) "The result is:"

IF (mile>1) WRITE (*,*) mile,"miles"

IF (mile==1) WRITE (*,*) mile,"mile"

```
IF (nyard>1) WRITE (*,*) nyard," yards"
```

IF (nyard==1) WRITE (*,*) nyard," yard"

IF (inch>1) WRITE (*,*) inch,"inches"

IF (inch==1) WRITE (*,*) inch,"inch"

END PROGRAM Miles

This program uses statements of the kind introduced in Section 2.2, except for the **IF** statements. An **IF** statement is simply a conditional form of some other single statement: the keyword **IF** is followed by a bracketed logical expression, followed by something else (in the above examples, **WRITE**) that will be executed only if the logical expression is true. Note that an **IF** statement is not quite the same thing as what is called an **IF** "construct". Using **IF** constructs we would have blocks of code like

IF (miles>1) THEN WRITE (*,*) miles," miles" END IF but in a case like this, where only one action is contingent on the IF, it can be put into one **IF** statement as in the program above.

It should be noted that the program Miles, above, has no declaration statements at the beginning to state what are the variables to be used (inches, inch, nyards, nyard, mile) and what types of variable they are (integers). This is because of the capitalization convention by which these variables, having names starting with letters in the alphabetical range i–n, are automatically taken to be variables of integer type, as desired. It would do no harm to add the type declaration statement

INTEGER :: inches, inch, nyards, nyard, mile

immediately after the **PROGRAM** statement, simply to make it beyond doubt, for anyone reading the program, that these variables are integers. In fact, many authorities on Fortran would insist that type declaration statements should always be included for all the variables in a program for the sake of clarity even when one is not strictly necessary.

One may ask how large an integer may be in Fortran. Obviously a finite processor cannot cope with all of the infinite mathematical set of integers. In fact, the maximum-sized integer is not specified by the Fortran 95 standard but will depend on the processor. It may therefore be important within the running of a program to check what the processor's largest permissible integer is. For this purpose there is an intrinsic inquiry function **HUGE**. If i is any variable of type integer, then **HUGE** (i) returns with the largest integer number representable in the processor. (It does not really matter what the value of i is.) For example, the statement

IF (ABS(nyears)>HUGE(1)/100) CALL Error

will transfer control to a subprogram called Error if the variable **nyears** gets within two orders of magnitude of the largest permissible integer. The keyword **CALL** is explained in **Chapter 7**. **ABS** is an intrinsic function that calculates the absolute value of its argument, i.e. a positive number is unchanged but a negative one is changed in sign to become positive.

As well as **HUGE** there is another enquiry function, **RANGE**, which will return the maximum number of digits allowed. In other words, **RANGE** (i) = INT(LOG10(HUGE(i))), LOG 10 being an intrinsic function calculating the logarithm (to base 10) of its argument, and the function INT being as described in the next section.

3.2 Real numbers

"Real" numbers are positive or negative numbers not restricted to integral values, in general having fractional parts. They are sometimes called "floating point" numbers and are usually expressed in decimal notation. Real numbers may appear in programs explicitly (i.e. as "real literal constants") in forms such as:

-78.915443 1877724. +3.000 4.65E-9 -0.3E12 -.1E+6 666E6

where the last four examples introduce the notation of the "exponent letter" **E** followed by a power of ten, positive or negative, which is to multiply the number. The last example is therefore equal to 666 million. The number **4.65E–9** is equal to $4.65 \times 10-9$. Note that a + sign is always optional both with the number itself (the "significand") and with the exponent. A decimal point should always appear somewhere unless there is an exponent letter: otherwise the processor cannot distinguish a real number from an integer.

Real variables should normally be represented by names beginning with a letter in the range **a-h** or **o-z**.

It is easy to convert integers into the corresponding real numbers, and vice versa, bearing in mind that when a real number is converted into an integer the fractional part will be discarded. One method of conversion is just to use an assignment statement such as

r = i

and then if i=1, r will be set equal to 1.0. With

i = r

we would get i=9 if r=9.9. This works because, according to Fortran's rules for assignment statements, type conversion will automatically take place between real and integer numbers if a variable of one type is set equal to an expression of the other type. More elegantly, there is an intrinsic function INT that always replaces a real argument by the corresponding integer: so the above example is shorthand for

i = INT(r)

The function INT may of course be combined into expressions, as in

ksum = INT(radius_1) + INT(radius_2)

and you should perceive that this is not necessarily equal to

ksum = INT(radius_1 + radius_2)

To convert integers into real numbers, Fortran has an intrinsic function **REAL**, and r=i is exactly equivalent to

r = REAL(i)

In practice the function **REAL** is not often needed in Fortran, since implicit type conversion will happen anyway if an integer appears in a context demanding a real number. However, if we pick up an example from Section 3.1, the **REAL** function may be important in a statement such as

r = REAL(12)/REAL(13)

which is not equivalent to r=i2/i3.

It is easy to fall into confusion about how an expression is evaluated if it includes both real and integer numbers. There is a very important rule concerning the effect of a binary arithmetic operator (+, -, *, /, or **) on data of real and/or integer types. Any such operator comes between two "operands", which is why it is called "binary". The rule is that if both operands are integers, the result is an integer, but if one or both of the operands is real then the result is real. So if we have integers **i2=2** and **i3=3** as in our earlier example,

i2**i3

is an integer. Because this rule applies to expressions as well as individual variables,

i2*(i2**i3)

is also an integer. On the other hand,

REAL(i2)/i3

is real, because one of the operands is real, and this would be exactly equivalent to

i2/REAL(i3)

With an expression like

r1/i2/i3

care is needed because the result may depend on the order in which the divisions occur. In fact, because of the left-to-right rule for operators of the same precedence (Section 2.3), this statement is equivalent to

(r1/i2)/i3

The expression in brackets is real (because one of its operands is real) and then the whole expression is real because the first operand of the second division is a real expression. However, if we had

r1/(i2/i3)

then the second division would operate first and would give an integer result because both of its operands are integers. Subsequently the first division, operating between a real variable and an integer expression, would give a real result to the expression as a whole. So, (r1/i2)/i3 and r1/(i2/i3) are both expressions of real type, but of course they have different values.

The lesson to learn from this is that for trouble-free code you should make liberal use of brackets to simplify complicated expressions, and use the **REAL** and **INT** functions explicitly, allowing implicit type conversions to occur only in the simplest cases.

The intrinsic function **HUGE** and **RANGE**, mentioned earlier in connection with integers, can be used with a real argument, in which case the value of **HUGE** is the largest real number representable on the processor and **RANGE** is the number of powers of ten that can be spanned by representable non-zero positive real numbers (normally from 1.0 up to **HUGE**).

IF (condition) conditional-statement

where condition is a relationship that is either true or false, like mile>1. Technically, condition is known as a "logical expression", something explained more fully in Section 3.9 below. The *conditional-statement* can be any kind of executable statement, except another IF statement.

The IF construct has the general form

Name: IF (condition) THEN conditional statements ELSE IF (condition) THEN Name conditional statements Z. ELSE Name conditional statements END IF Name

The construct may, optionally, be given a Name. If so, the same name must appear before a colon at the start of the **IF...THEN** statement that opens the construct, and at the end of the **END IF** statement. The same name may also be inserted, optionally, at the end of an ELSE IF statement or an **ELSE** statement.

After the opening **IF...THEN** statement, there follows a set of one or more statements that are executed if, and only if, the condition in the **IF...THEN** statement is satisfied. If it is not satisfied, the condition in the **ELSE IF** statement is scrutinized and, if satisfied, the set of statements following that are executed. There can be any number (including none) of **ELSE IF** statements and associated sets of conditional statements. If the **IF..THEN** condition is not satisfied, nor any conditions attached to **ELSE IF** statements, then finally statements following an **ELSE** statement will be executed. However, it is not necessary for an **ELSE** statement to be present. So the simplest kind of **IF** construct would consist only of three statements such as

IF (miles>1) THEN

WRITE (*,*) miles," miles"

END IF

having no name, no secondary (ELSE...IF) conditions, no default (ELSE) statements, and only one statement being executed if the IF...THEN condition is satisfied. As we have seen, an IF construct as simple as this could equally well be replaced by a single IF statement.

A slightly more complex IF construct is the following:

Rootover: IF (snakeskin>0.0) THEN

droop = 1.0/SQRT(snakeskin)

ELSE IF (snakeskin==0.0) THEN

droop = 0.0

ELSE

snakeskin = -snakeskin

droop = 1.0/SQRT(snakeskin)

END IF Rootover

Giving the construct a name (Rootover) makes no difference to the execution of the construct, but can help the programmer to keep track of what is going on in code where there may be several IF constructs. It is possible for one IF construct to be nested inside another, as in

```
First: IF (a>b) THEN

a = a/2

Second: IF (a<1.0) THEN

b = b^{**2}

a = a^*b

END IF Second

b = a + b

IF (b>a) b = b - 1.0

END IF First
```

which also includes an IF statement for good measure. This example should make it clear that complex systems of alternative actions can be coded with IF constructs.

3.4

Intrinsic procedures

We have now met a number of Fortran's intrinsic functions: SQRT, MOD, HUGE, ABS, RANGE, EXP, INT, LOG10, and REAL. Others introduced later in this chapter are AIMAG, CMPLX, COS, LOG, SIN, and TRIM.

They are invoked simply by having an expression of the general form

FUNCTION (argument)

where *FUNCTION* is the Fortran name for the intrinsic procedure in question, and *argument* is the variable of which the function is being calculated. In some cases (**HUGE** and **RANGE**) the value of the function does not, oddly enough, depend on the value of the argument, but only on what type of data item it is. In other cases (**MOD** and **CMPLX**) there may have to be two or even more arguments.

Fortran's intrinsic functions carry out different kinds of task and are classified accordingly. Some of the classifications are:

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- "Numeric" functions such as ABS, AIMAG, CMPLX, INT, MOD and REAL. These do not actually calculate anything but manipulate numeric data in various ways. Many of them are to do with the converting of data from one numeric type to another.
- "Mathematical" functions such as COS, EXP, LOG, LOGIC, SIN and SQRT, which calculate standard mathematical functions.
- "Character" functions, operating on textual data. The character function TRIM is explained in Section 3.10 below.
- "Numeric inquiry" functions such as HUGE and RANGE.

All the intrinsic functions are listed in Appendix F and it is worth looking there to see the full variety of classifications and complete descriptions of each procedure.

3.5 Exercises 3.A

3.A What are the values of the following integer expressions, if **n=-8**?

(i) n**2–2	(ii) n/2/2	(iii) MOD(42, n+11)
(iv) MOD(n, -3)	(v) ABS(n**3-n)	(vi) 2**n

3.A Express as ordinary decimal numbers

2	

3

(i) 666E–3	(ii) 0.024E6	(iii) 1E+1
and use the exponent letter	r (E) notation to express the	e following compactly as Fortran real
constants:		
(iv) 2700000000.0	(v) 0.0000101	(vi) 10⁻¹⁶

3.A What are the values of the following real-number expressions, if a=-9.0 and t=l4.8?

(i) s+t/2–1	(ii) s**2t+t	(iii) ABS(s+t)
(iv) MOD (s, t)	(v) MOD(t, s)	(vi) n**2/s, with n=-8
(vii) 2.0**n, with n=-2		

3.A Write a program to convert a sum of British currency expressed in pounds and new pence to the old-4 style pounds, shillings and old pence (a pound contained 20 shillings, each of 12 old pence).

3.A The Bohr radius for a very heavy nucleus is given by the formula

5

$$a_{\infty} = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$$

In these units, write a program to calculate and write out the values of a and r_e . Write a program to read the coordinates of two points in the two-dimensional plane and to calculate and write out the equation of the line joining them.

3.6 The type declaration statement

This section is a preliminary description of a sort of statement that is not dealt with in full detail until Chapter 8.

It has been said that integer numbers are represented by variables whose names start with the letters i, j, k, l, m and n, and real numbers by variables starting with other letters of the alphabet. However, this rule can be overridden by a "type declaration statement" that can take forms like

REAL :: negentropy

REAL :: joules, kelvin_temp, energy

INTEGER :: days, weeks, months

i.e. the keyword **REAL** or **INTEGER**, followed by a double colon, followed by a list of one or more names. The variables named are thereby declared to be of real or integer type whatever their initial letters might be.

The double colon

In type declaration statements we show a double colon between the type keyword and the list of variables. In fact, the double colon is usually optional and can be omitted except in more complicated cases that will be covered in Chapter 8. Nevertheless, it is best to use the double colon as a general rule, because it is never wrong to do so and it is the distinctive signature of the type declaration statement.

These **REAL** and **INTEGER** statements fall into the special class known as "nonexecutable" or "declarative" statements. They are used to define the nature of data objects once and for all when the program is compiled, but do not change anything during execution. Such statements must occur at the very beginning of the program (or subprogram) immediately after the **PROGRAM** statement. Declarative statements may not be mixed up with executable statements.

Other kinds of type declaration statement are the **COMPLEX**, **LOGICAL** and **CHARACTER** statements introduced in the remainder of this chapter.

Although it is not always necessary for variables to be declared in type declaration statements, it is recommended that they should be except in the case of the very simple integer variables known as "loop indices" that have not yet been introduced. If variables are always declared, it does not really matter whether the capitalization convention (i–n for integers, other letters for reals) is used or not; but nevertheless it is recommended that the capitalization convention be adhered to firmly to make it straightforward for readers of a program to distinguish immediately between integers and real numbers. It is not really too hard to think of suitable names starting with appropriate letters!

3.7

Kinds of real numbers

In fact, real numbers in Fortran are a little more complicated than the discussion in Section 3.2 suggests. The language actually allows for at least two different kinds of real numbers, with different degrees of precision. The first, sometimes called "default precision", is the sort of real number we have been using so far: it provides ample precision for most calculations and is provided automatically by the processor if the programmer does not explicitly demand still higher precision. The second kind of real number, providing more accuracy, is sometimes called "double precision" because on many processors it corresponds to doubling the number of bytes used to store a real number (e.g. from four to eight bytes). Double-precision

constants can be set up by using the exponent-letter notation but using a D instead of an E as in the examples

4.65D–9 –0.3D12 –.1D+6 666D6 0.DO

The names of double-precision variables should be declared by means of the **REAL** statement, the keyword being followed by the specification of a parameter called **KIND**. For example, this statement could set up five double-precision numbers:

REAL(KIND=2) :: splithair, x, y, z, difference

It might be possible to use other values of **KIND** for numbers of still greater precision. However, the actual values of **KIND** that might be valid (including **KIND=2**) may vary from one processor to another and, for the sake of program portability, it would be necessary to use special intrinsic inquiry functions (described in Chapter 5) to establish which values of **KIND** are applicable to a particular processor. On a processor representing double precision by **KIND=2**, the above declaration statement would be valid and variables could be assigned by statements such as

splithair = 4.65D-9

There is also another way of writing a real constant, including its KIND parameter, by following the number itself by an underscore followed by the value of the **KIND** parameter. The above statement could therefore be written

splithair = 4.65E-9_2

as long as KIND=2 corresponds to double precision, and the other constants listed above could be written

-0.3E12_2 -100000.0_2 666000.0_2

0.0_2

In fact, in expressions like this the **KIND** parameter may be expressed by a named integer constant as in the example

6666000.0_maxprecision

(See **PARAMETER**, Chapter 8.)

Optionality of the KIND parameter

In type declaration statements such as that given above, **KIND=** may be omitted, i.e. a statement like

REAL(2) :: splithair, x, y, z, difference

would be valid.

Double precision

Instead of a statement such as

REAL(KIND=2) :: splithair, x, y, z, difference

one may write

DOUBLE PRECISION :: splithair, x, y, z, difference

In general, **DOUBLE PRECISION** specifies real numbers having a precision greater than the processor's default real kind. **DOUBLE PRECISION** is equivalent to **REAL** (**KIND=KIND** (**0. DO**)), in terms of the intrinsic **KIND** function explained later!

3.8

Complex numbers

Fortran allows for complex numbers as long as the names of complex variables are declared by statements like

COMPLEX :: z1, z2, z3, z4

COMPLEX :: omega

COMPLEX :: i

Complex constants can be specified by the usual mathematical notation of giving, in brackets, the real part followed by the imaginary part. Examples are

z1=(3.756, 0.051) z2 = z1**2 - (0.0, 1.0) z3 = SQRT(z2) - (0.0, -1.0)

omega = (-1.0, 0.0)**(1.0/3.0)

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i = (0.0, 1.0)

The brackets are needed even in a case like

i = SQRT((-1.0,0.0))

because, here, one pair of brackets is needed to set apart the argument of the SQRT function and another to contain the parts of the complex number.

As the above examples show, complex numbers may be combined in expressions using the usual arithmetic operators. The SQRT function works with a complex argument: if the argument is complex, so is the result. In Fortran, the following intrinsic functions are either real functions of real arguments or complex functions of complex arguments, according to the argument types:

SQRT	Square root
SIN	Sine
COS	Cosine
EXP	Exponential function
LOG	Natural logarithm (i.e. the logarithm to base e)

The trigonometrical functions measure angles in radians. The complex **SQRT** function normally yields the principal value with positive real part, and the complex **LOG** function yields the principal value with imaginary part between $+\pi$ and $-\pi$. There is one intrinsic function that always has to have a complex argument and a complex value:

CONJG Complex conjugate

The following functions may have complex arguments but give real or integer values:

REAL	Real part
INT	Real part, truncated to an integer
AIMAG	Imaginary part
ABS	Absolute value

Note that if z is complex, **INT**(**Z**) is the same as **INT**(**REAL**(**Z**)), and that **AIMAG** ((1.0,2.0)) is equal to 2. 0, not (0.0,2.0). The function **LOG10**, which was mentioned briefly in Section 3.4 and gives a base-10 logarithm, is not permitted to have a complex argument.

Finally there is a function, **CMPLX**, which generally has two real arguments and a complex value. It simply forms a complex number, the real and imaginary parts respectively being given as arguments. **CMPLX** is discussed further in Section 5.3.

It is possible to mix complex, real and integer data in Fortran expressions built up out of the arithmetic operators. When each operator takes effect, if either operand is complex, then the result of that operation is complex. This is just an extension of what happens with real and integer data, where an operation gives a real result if either operand is real.

3.9 Logical data

"Logical" data is a non-numeric data type that we have already encountered indirectly: for example, as the logical expression in brackets within the statement

IF (miles>0) THEN

In general we may have constants, variables and expressions of logical type. They have only two possible values, true and false, and can be thought of as "bits" of information like binary digits. The names of logical variables must be declared initially using the **LOGICAL** type declaration statement, e.g.

LOGICAL :: error_flag

LOGICAL :: checksum, kexists, ifmiles

A statement like

```
ifmiles = miles>0
```

is a valid assignment statement, setting the logical variable ifmiles to be true or false according to whether or not the integer miles is greater than zero. The IF statement given earlier could then take the form

IF (ifmiles) THEN

Logical constants are written as either **.TRUE**, or **.FALSE**., the surrounding dots being an essential part of the syntax. Logical constants could crop up in code like

```
LOGICAL :: condition_1, condition_2
```

INTEGER :: j, k

READ (*,*) j, k

condition_1 = .TRUE. ; condition_2 = .TRUE.

IF (j>k) condition_1=.FALSE.

IF (k>0) condition_2=.FALSE.

```
IF (ABS(j+k)>0) condition_1=condition_2
```

There is a set of special operators available for use on logical variables only, namely:

.NOT. Negation

.AND. And

.OR. Or

.EQV. Logical equivalence

.NEQV. Logical inequivalence

.NOT. is a unary operator that flips the value of whatever logical quantity follows it. Thus, if **checksum** is a logical variable, **.NOT.checksum** has the value **.FALSE.** if **checksum** has the value **.TRUE.** and vice versa. Obviously, **.NOT. .TRUE.** is equal to **.FALSE.** and **.NOT. .FALSE.** is equal to **.TRUE.** The other operators in the list above give results depending on the relationship between two items of logical data. They are binary operators, and stand between the two logical quantities to which they relate. Their meanings are summarized in Table 3.1, with **p** and **q** representing logical variables (or logical constants or expressions). In this table *t* stands for **.TRUE.** and **.FALSE.** by a declaration like

LOGICAL, PARAMETER :: t=.TRUE., f=.FALSE.

which sets up fixed logical constants called t and f instead! (For the details of the attribute **PARAMETER**, see Chapter 8.)

The logical operators discussed above may be combined to form more complicated logical expressions like

q.AND..NOT.p.NEQV.q.OR.r

In evaluating such an expression the operators have an order of precedence. **.NOT.** comes before **.AND.** which comes before **.OR.** which comes before

р	q	p.AND.q	p.OR.q	p.EQV.q	p.NEQV.q	
t	t	t	t	t	f	
t	f	f	t	f	t	
f	t	f	t	f	t	
<u>f</u>	f	f	f	t	f	

Table 3.1 Relationships between logical data.

.EQV. or .NEQV.. That is why they were listed in that order above. So, the above example is equivalent to

(q.AND. (.NOT.p)) .NEQV. (q.OR.r)

Since .EQV. and .NEQV. have the same level of priority, an expression like

q.EQV.p.NEQV.r.EQV.S

could be ambiguous: but then in a case like this Fortran works from left to right, so the expression is equivalent to

((q.EQV.p) .NEQV.r) .EQV.s

Brackets may always be used to over-ride the normal order of precedence, as for the arithmetic operators, and even when brackets are not strictly necessary the programmer should use them to make the meaning of an expression as clear as possible. If brackets are always used, it is unnecessary to memorize the order of precedence!

In addition to the operators discussed above, which operate on logical-type data and produce logical values, there are "relational" operators that act on numerical data (and, in some cases, character strings) to produce logical values. In fact one or two of these have already been met: in Section 2.2 we used the expression **areas<0.0**, and in Section 3.1 we used expressions such as **miles>0**. The full set of relational operators that can be used between numerical data is:

==	Equal
/=	Not equal
<	Less than
<=	Less than or equals
>	Greater than
>=	Greater than or equals

It is important to realize that these operators, although used to form logical expressions, cannot be used between logical data items. If p and q are logical, we must use **p.EQV.q** rather than **p==q**. Also, the double equals sign (==) has a meaning quite different from the single equals sign (=). The = is used in assignment statements and changes the value of whatever is on the left-hand side. The == just compares the existing values of the objects on either side of it and changes neither.

Using both sorts of relational operator we can form quite complicated logical expressions, as in the statement

IF (((j/=k) .AND. (m>k)) .EQV. ((j+m)==k)) THEN

where j, k and m are integers. Because Fortran has a default order of precedence for all operators it is often possible to get away without all the brackets: the relational operators take precedence over the logical operators and arithmetic operators take precedence over both, so the above statement is equivalent to

IF (j/=k.AND.m>k.EQV. j+m==k) THEN

but, as said before, the best practice is always to use brackets freely to make the meaning of the code as clear as possible.

Alternative forms of the relational operators:

The operators ==, /=, <, <=, >, and >= have also the synonymous forms **.EQ.**, **.NE.**, **.LT.**, **.LE.**, **.GT.**, and **.GE.** respectively.

3.10

Characters and strings

So far we have met the numeric data types **INTEGER**, **REAL** and **COMPLEX**, and the non-numeric type **LOGICAL**. The next data type for us to deal with is **CHARACTER** data.

"Character constants" and "character variables" are not quite the same things as "characters". A character is an explicit individual symbol, such as a letter of the alphabet. Characters can be drawn from the list given at the beginning of Chapter 2, i.e. from the letters, the decimal digits, the underscore, and 21 special characters. In addition, characters could in principle include other more exotic symbols: the total number of permissible different characters is processor-dependent. Usually, upper- and lower-case letters are regarded as distinct characters.

A character constant is an explicit "string" of characters. For example, **"aeiou"** is a character constant. In fact we have already met character constants: early in the previous chapter we used **"What is your name?** *, which is a character constant or fixed-value character string. A character string may be only one character in length; in fact it may have zero length, i.e. have no characters in it at all. In Fortran, character constants are given between a pair of double or single quotes, although in this book we will generally stick to double quotes for this purpose.

We can also have character variables, i.e. names that could represent arbitrary characters or strings of characters. We will often use the common term "character string", or just "string", to denote any character variable or character constant.

Here is a simple example of how character strings can be manipulated within a program:

soft = "aei" hard = "ou" vowels = soft//hard WRITE (*,*) vowels

which will yield the output

aeiou

In this example there are three character variables: **soft, hard** and **vowels**. These words are being used as the names of character strings, just as they could have been used as the names of numeric variables. The first two statements set the variables **soft** and **hard** to be equal to the constants "**aei**" and "**ou**". The third statement sets the variable vowels to be the "**concatenation**" of **soft** and **hard**. The double-slash (//) is the concatenation operator, making a single longer string out of the two strings on either side of it. The concatenation operator can be used with character variables or with character constants: thus

vowels="aei"//"ou"

or

vowels = "aei"//hard

vowels = soft//"ou"

would all have exactly the same effect as **vowels = soft//hard** in the above example.

The "length" of a character string is the number of characters in it (including blanks, which are significant in this context). Strings may obviously have various lengths. **soft, hard** and **vowels,** in the above example, have lengths of three, two and five respectively. Before a character variable is used, it must be declared to be of character type: otherwise the name will be assumed to represent a real or integer number. At the same time its length should normally be specified. The example above should therefore be preceded by type declaration statements of the form

CHARACTER(3) :: soft

CHARACTER(2) :: hard

CHARACTER(5) :: vowels

the lengths of the strings being in brackets after the keyword **CHARACTER**. The lengths of character variables are, of course, unrelated to the lengths of their names.

If there is no bracketed number after **CHARACTER**, the string is taken to have length one, i.e. it consists of just a single character:

CHARACTER :: dollarsign, shriekmark, ampersand

sets up three character variables each of which will be just a single character; but this statement is exactly equivalent to

CHARACTER(1) :: dollarsign, shriekmark, ampersand

and many programmers take the view that the length of the character strings should always be declared explicitly even when it is equal to the default value of one.

LEN

In a character type declaration statement, the string length may be preceded by LEN= thus:

CHARACTER(LEN=5) :: vowels

In practice, we may not know in advance the lengths of character variables and the declaration statements will need to allow for the maximum number of significant characters that the variable might contain. For example, consider this:

PROGRAM Nomination

CHARACTER(20) :: forename, surname

CHARACTER(41) :: name CHARACTER(1) :: initial1, initia12 CHARACTERS) :: initials WRITE (*,*) "What is your first name?" READ (*,*) forename WRITE (*,*) "What is your surname?" READ (*,*) surname name = TRIM(forename)//" "//TRIM(surname) WRITE (*,*) "Thank you. You are", TRIM(name) initial1=forename initial2=surname initial2=surname

WRITE (*,*) "Your initials are ", initials

END PROGRAM Nomination

The **READ** statements here will fill the strings **forename** and **surname** with the names that are input, but there will be blank spaces at the ends to make up 20 characters for each. **TRIM** is an intrinsic Fortran function that takes any string and returns it with trailing blanks removed. The variable **name** will contain the person's forename and surname with one blank space between them, and with trailing blanks to make up its full length of 41 characters. The third **WRITE** statement will output **name** without the trailing blanks. The assignment statements involving **initials1** and **initials2** exploit the fact that a truncation will take place if a longer string is assigned as the value of a shorter string.

Besides the function **TRIM**, mentioned above, another important intrinsic function that has a character string as its argument is called **LEN**, and its value is simply the length of (i.e. the number of characters in) the string. For example, the expression **LEN**("Gum") is an integer equal to 3.

3.11 The ASCII character set

The ASCII code is a correspondence between a set of characters and the numbers ranging from 0 to 127 (Table 3.2). Since 127 is 1111111 in binary notation, i.e. 128 is 2⁷, ASCII is a seven-bit code. Because computer systems use eight-bit "bytes", there is a "spare" bit that means that it is possible to have additional characters corresponding to the numbers 128 to 255: but they are not specified by the ASCII standard. Most

of the ASCII "characters" are ordinary printable characters. Those that are not are omitted from Table 3.2, except for some whose usual meaning is indicated in parentheses.

The correspondence between characters and ASCII code numbers would be irrelevant to Fortran if it were not possible to translate the one into the other.

Character	Code	Character	Code	Character	Code
(null)	0	<	60	٨	94
(bell)	7	=	61	_	95
(backspace)	8	>	62	,	96
(return)	13	?	63	а	97
(delete)	16	@	64	b	98
(escape)	27	А	65	с	99
(blank)	32	В	66	d	100
!	33	с	67	e	101
•	34	D	68	f	102
ŧ	35	Е	69	g	103
\$	36	F	70	h	104
%	37	G	71	i	105
&	38	Н	72	i	106
	39	Ι	73	k	107
,	40	J	74	Ι	108
)	41	Κ	75	m	109
*	42	L	76	n	110
+	43	Μ	77	0	111
	44	Ν	78	Р	112
	45	0	79	q	113
	46	Р	80	r	114
1	47	Q	81	S	115
)	48	R	82	t	116
1	49	S	83	u	117
2	50	Т	84	V	118
3	51	U	85	W	119
4	52	V	86	Х	120
5	53	W	87	у	121
6	54	Х	88	Z	122
7	55	Y	89	{	123
3	56	Z	90	Ι	124
9	57	[91	}	125
:	58	Ň	92	~	126
	59	1	93	(delete)	127

Table 3.2 The ASCII character set.

This can be achieved by two intrinsic functions, **ACHAR** and **IACHAR. IACHAR'S** argument is a single character, and its value is the integer corresponding to that character in the ASCII code. **ACHAR** is the inverse function: its argument is an integer and its value is the corresponding character. So **ACHAR (78)** is equal to "N", and **IACHAR ("m")** is equal to 109. If c is the name of a character variable, **ACHAR** (**IACHAR(c)**) is equal to c. An example of the use of the **ACHAR** and **IACHAR** functions is given in Section 7.3.

3.12 Exercises 3.B

3.B Which of these are legal Fortran constants? What are their types?

(i) .	(ii) 3.	(iii) 3.1
(iv) 31	(V) 0.	(vi) +2
(vii) –E18	(viii) "ACHAR(61)"	(ix) 3 500
(x) 4,800,000	(xi) "X or Y"	(xii) "X"//"Y"
(xiii) 4.8E6	(xiv) 5000E-3	(xv) "VAT 69"
(xvi) 6.6_big	(xvii) (1, -1)	(xviii) 007
(xix) 1E	(xx) -630958813365	

3.B Write type declaration statements to declare

2

1

- (i) Three real variables called power1, power2 and creeper;
- (ii) Two integers called kappa and kappa_prime;
- (iii) A **KIND=3** real variable called fine tune;
- (iv) Two strings, each of four characters, called v and w.
- 3.B Using a type declaration statement and three assignment statements, set up complex variables called c1, 3 c2 and c3, and give them the values of the cube roots of -2.
- 3.B Write a program to solve a quadratic equation (with real coefficients) allowing for complex roots.

3. If gum1 and gum2 are logical variables both with the value **.TRUE.**, what are the values of B5

- (i) gum1.NEQV.gum2.EQV. .NOT.gum1;
- (ii) (gum1.NEQV.gum2) .EQV. .NOT.gum1;
- (iii) gum1.OR. .NOT.gum2 .NEQV.gum1.AND.gum2.
- (iv) What is the value of (iii) above if gum1 is .TRUE. and gum2 is .FALSE.?
- 3.B Write a Fortran logical expression depending on five integers n1, n2, m1, m2 and k, which will be true 6 if (and only if) the absolute magnitude of the difference between n1 and n2 exceeds that between m1 and m2 by at least the magnitude of k.
- 3.B Write a program to read in two strings of 12 characters each and to write out the first if the second is 7 "satisfactory". (If it is not, write out a message saying so.)

- 3.B Write a program to read four real numbers, taken to be the lengths of the sides of a trapezium in cyclic 8 order, and calculate and write out the area of the trapezium.
- 3.B With a distance to be travelled being input, produce a table of the journey times for average speeds 9 ranging from 40 to 140kph (in steps of 10kph).
- 3.B Write a program to read in a sequence of three single characters. If they are all hexadecimal digits the
- 10 program is to write out the decimal equivalent of the hexadecimal integer that the characters represent. If one or more of the characters cannot be interpreted as hexadecimal digits, an appropriate error message should be written. (Use only the elements of Fortran, including the IF construct, that have so far been introduced. Other features of the language, to be introduced later on, will shorten the program considerably!)

CHAPTER 4 Introducing arrays

This chapter begins with how array variables are declared and used. Then "array constructors" and "array sections" are explained, followed by information about the notation for specifying character substrings and sections of character arrays. The WHERE statement and the WHERE construct are described. Finally a number of intrinsic functions for arrays are introduced: ALL, ANY, COUNT, MAXVAL, MINVAL, PRODUCT and SUM.

4.1 Declaring arrays

Up to now we have looked at data that may consist of a real or integer number, a complex number or a logical element. We have also looked at items of character data consisting of a string of characters. These have all been "scalar" objects, in the sense that a constant or the name of a variable refers to a single integer, or a single string of characters, and so on. It does not matter that a long string of characters will take up much more memory than a single logical datum: both are regarded as individual scalar data items. An "array", on the other hand, is an ordered set of data items, all of the same type, that can be referred to collectively by a single name. Arrays are an invaluable feature of Fortran and in practice only the very simplest of problems are solved without recourse to them.

A statement like

CHARACTER(30) :: surname

will establish that **surname** is the name of a variable whose form is a string of 30 characters. It is equally simple to set up instead a list of 50 people's surnames, the declaration statement then taking the form

CHARACTER(30) :: surname(50)

On either side is it possible to have a space before opening the brackets, so it would be equally valid to write

CHARACTER (30) :: surname (50)

By following the name (surname) with a positive integer in brackets, it is implied that the variable is a onedimensional array (sometimes called a "vector") with that number of members. There is an equivalent alternative notation, namely

CHARACTER(30), DIMENSION(50) :: surnames

Here the keyword DIMENSION is known as an "attribute specifier", specifying that the variable is an array and indicating how many members it has. This form is convenient if you want to declare several similar arrays: for example

CHARACTER (30), DIMENSION (50) :: surnames, forenames, &

nationalities

sets up three arrays each of 50 character strings, each string being 30 characters long, i.e. 4500 characters in all. Each string is an "element" of a 50-strong array.

Arrays of other types can be declared in similar ways, e.g.

REAL, DIMENSION(100) :: height, weight

INTEGER, DIMENSION(100) :: kage

However, the attribute DIMENSION may always be omitted if the dimensions of the arrays are given in brackets after their names, as in

REAL :: height (100), weight (100) INTEGER :: kage (100) COMPLEX :: roots (25) LOGICAL :: maskmatrix (32,32)

These are all variations of the type declaration statement (Chapter 8). For simplicity it is recommended that the **DIMENSION** attribute be always avoided, and in the rest of this book arrays are indicated simply by specifying their dimensions after the names of the variables as in examples immediately above.

The final example above, the logical array called **maskmatrix**, is an example of a two-dimensional array, specified by having two integers between the brackets following the name. It may be imagined as a matrix with 32 rows and 32 columns, and therefore with 1024 elements in all. An array's number of dimensions is known as its "rank", and may be up to seven, i.e. we could have a seven-dimensional array like

INTEGER :: iternary(3, 3, 3, 3, 3, 3, 3)

this example having 2187 different elements. The total number of elements in an array is called its "size". In general an array may have a different "extent" in each dimension, and the total size is the product of the extents. So,

REAL :: hash (1024, 8, 26, 2)

declares an array of rank 4 and size 425984. This array has an extent of 1024 in its first dimension, 8 in its second, and so on. The set of extents (**1024**, **8**, **26**, **2**) is known as the "shape" of the array.

Incidentally, it is possible for an array to have an extent of only one in one or more of its dimensions. The array

REAL :: oddity (1, 1, 1)

is, technically speaking, a three-dimensional array, in spite of the fact that it has only one element that might just as well have been expressed as a scalar variable. In fact, it is even possible for an array to have a zero extent in one of its dimensions, and therefore to contain no elements at all. The sense of this will become clearer later when array sections and arrays of variable shape are discussed.

4.2

Using arrays

In the declaration statements given as examples in the above section, the array names are followed by bracketed lists of the extents of the arrays in each dimension. In assignment statements, or in expressions, a similar notation is used to specify a particular single element of an array, e.g.

surnames(12) = "Johnson"

assigns a value to the 12th element of **surnames**. It does not mean that **surnames** has rank 12. However, **surnames** must have rank of at least 12 in order for **surnames** (12) to exist. To take an example where an array element is on the right-hand side of an assignment statement,

x = 1.0 - SQRT(hash(98, 1, 14, 2))

takes one element out of the four-dimensional real array hash, and uses it to calculate x.

To refer to all the elements of an array it would be possible to use a construct like a **DO** loop (see Chapter 6), such as

Cuberoots: DO 1=1, 30

croots(i) = REAL(i)**(1.0/3.0)

END DO Cuberoots

and this would set up a table of cube roots. But this sort of construction is generally not necessary: arrays really come into their own in Fortran because a reference to an array name by itself is equivalent to a reference to all the elements individually. For example, if \mathbf{x} and \mathbf{y} are one-dimensional arrays of size 12, then

x = y**2

As a rule, array assignment statements may refer to Fortran's intrinsic functions, as in

x = SQRT(y)

this being equivalent to 12 scalar assignments and involving 12 calls to the function **SQRT**, if **x** and **y** both have size 12. Functions that can be used like this in array assignment statements are called "elemental" functions because they operate on all the elements of the array that is given as their argument. Other valid statements would be, for example,

x = SQRT(x)

and

 $\mathbf{x} = \mathbf{y}/\mathbf{z}$

The variables x, y and z here could be arrays of any shape, but their shapes must be the same. In the latter example, x(1) is set to y(1)/z(1), x(2) to y(2)/z(2), and so on.

An array assignment statement must have an array on the left-hand side with the same shape as the array (or array expression) on the right-hand side, but an exception to this rule is that we may have a scalar on the right-hand side, in which case all elements of the array are set equal to that same value. For example, going back to the first example of this section,

surnames = "Johnson"

would set all elements of the array called **surnames** to the same string **"Johnson"**. To show how an array might be used in a program, here is something equivalent to the program shown in Section 2.2:

PROGRAM Triangle

REAL :: side(3)

WRITE (*,*) "This program calculates the area of a triangle."

WRITE (*,*) "Type in the lengths of the three sides:"

READ (*,*) side

WRITE (*,*) "Check: you have input the following lengths"

WRITE (*,*) side

s = 0.5 * SUM(side) ! Semiperimeter

areasq = s*PRODUCT(s-side) ! Square of the area

IF (areasq<0.0) THEN

WRITE (*,*) "Error: that is not a real triangle"

ELSE

area = SQRT(areasq)

WRITE (*,*) "The area of the triangle is ", area

END IF

END PROGRAM Triangle

This is no shorter than the earlier version of this program and it uses two intrinsic functions (**SUM** and **PRODUCT**) that will be explained at the end of this chapter. However, it illustrates how three variables (originally a, b and c) can be referred to under one name (side) so that the program reflects the mathematical symmetry of the problem. Note that **READ** and **WRITE** statements can be used with arrays, with the same effect as if each element of the array had been listed. So, the statement

WRITE (*,*) side

is equivalent to

```
WRITE (*,*) side(1), side(2), side(3)
```

On the other hand,

WRITE (*,*) sided)

would only write the first element.

4.3

Array constructors

So far, we have looked at how variables are declared to be arrays, and at how arrays can be used in assignment statements and **READ** or **WRITE** statements. But how do we initially set values for the elements of an array? It is possible to set each element individually, as in

REAL :: x(3)

x(1) = 3.76; x(2) = -7.4; x(3) = 5.19

but for rank-1 arrays there is a simpler syntax known as an "array constructor" that looks like

x = (/3.76, -7.4, 5.19/)

The array has its elements specified as a list between a (/ and a /). This notation can be used in an assignment statement, or it can be used when array variables (or named constants) are initially declared, as in

REAL :: x(3) = (/3.76, -7.4, 5.19/)

or

INTEGER, PARAMETER :: months(12) = &

(/31, 28, 31, 30, 31, 30, 31, 31, 30, 31, 30, 31/)

(The **PARAMETER** attribute is explained in Chapter 8.) The list in an array constructor may include items that are themselves arrays, so

INTEGER :: u(3), v(3), w(3), uvw(9) u = (/1, 2, 3/) v = 4 w = (/3,2,1/) uvw = (/u,v,w/)

has the effect of giving uvw the value

(/1,2,3,4,4,4,3,2,1/)

Also, arrays within array constructors may themselves be array constructors, if you see what is meant. For example, uvw above could have been written

uvw = (/(/1,2,3/),v,(/3,2,1/)/)

Furthermore, a form of implied DO can be used in an array constructor. As an example, the table of cube roots given in the previous section is equivalent to

croots = (/ (REAL(i)**(1.0/3.0), i=1,30) /)

The meaning of this notation should be fairly clear even though the syntax is based on the idea of the DO loop described in Chapter 6. Within its own pair of brackets there is a structure comprising an expression, then a comma, then an index ranging between limits separated by another comma. The index name i is arbitrary, and the expression may be a function of the index. This structure creates an array element in the structure constructor for each value of the index over the range specified, i.e. 30 elements in the above case.

Another example is

ten_units = (/ (1.0, i=1,10) /)

which is equivalent to

ten_units = 1.0

as long as ten_units was declared to be a rank-one array of size 10.

One should be aware that an array constructor cannot be used as the parent array in the specification of an array element or array section, i.e. something like

neat = (/1,2,3,4,4,4,5,6,7/)(7)

is an illegal statement and cannot be used to pick out the seventh element of the constructed array. However, if **miasma** is the declared name of a nine-element rank-one integer array, then

miasma = (/1,2,3,4,4,4,5,6,7/)

neat = miasma(7)

does the trick.

.

Since an array constructor is a one-dimensional sequence of values, it can be used to construct only onedimensional (rank-one) arrays. A one-dimensional array can be reshaped into a multidimensional array of the same size, using a special intrinsic function **RESHAPE**, but details of this are deferred until Chapter 9.

4.4

Array sections

We have so far considered arrays whose elements are labelled by integers ("subscripts")ranging from 1 up to the maximum extent in each dimension. However, subscripts may run from starting points other than 1 with a notation where both the lower and upper subscript limits are given, separated by a colon. For example,

REAL :: annual(1900:2025)

declares an array with 126 elements, i.e. **annual(1900)**, **annual(1901)**, **annual(1902)**,..., **annual(2025)**. In a case like this items such as annual (1) simply do not exist. This notation can equally well be used for multidimensional arrays, as in

LOGICAL :: flipper(-10:10,32,0:20)

which is a rank-three array with total size $21 \times 32 \times 21$.

The colon notation is also used to refer to what is called an "array section", which is a subset of a previously declared array. We could have

REAL :: annual(1900:2025), decade(10)

decade = annual(1981:1990)

where, in the assignment statement, **annual (1981:1990)** is an array section, i.e. a particular set of ten elements from the larger array **annual**. The elements of the array **decade** are being set equal to **annual (1981)**, **annual (1982)**,..., **annual (1990)**. In fact, for array sections, the notation can be extended to allow sets of elements that are not sequential in the original array, by specifying a "stride" after a second colon. So,

annual(1904:1996:4)

is an array section consisting of every fourth element starting from **annual(1904)** and going up to **annual** (**1996**). The three bracketed numbers, separated by colons, are a "subscript triplet" and the general rule is that the processor starts from the first and moves on to the second in steps equal to the third. If **leaps** is a rank-one real array of size 24, then

leaps = annual(1904:1996:4)

picks out leap years. The stride may be negative and, if it is equal to -1, the effect is to give an array section with elements in the reverse order from the original array. Note that sections of the same array may occur on both sides of an assignment statement, as in

decade = decade(10:1:-1)

which reverses the order of the elements in decade, or

```
tenfold = tenfold + tenfold(10:1:-1)
```

where tenfold is a rank-one array of size 10. This array assignment statement is a bit like

```
tenfold(1) = tenfold(1) + tenfold(10)
```

```
tenfold(2) = tenfold(2) + tenfold(9)
```

.

```
tenfold(10) = tenfold(10) + tenfold(1)
```

except for the very important difference that when we write it out the long way, with ten scalar assignment statements, the last five statements will have quantities on the right-hand side that were changed by the first five statements. The array assignment statement, on the other hand, always uses the original values of all the

elements on the right-hand side and the result is therefore not dependent on the order in which a processor might evaluate the elements of the array on the left-hand side.

By applying this notation to each dimension in turn we can form sections of multidimensional arrays. With the rank-three array given by

INTEGER :: matrices(4,4,200)

it is possible to have sections such as

```
matrices(1:4, 1:4, 1)
matrices(1:4, 4, 98)
matrices(4:1:-1, 4:1:-1, 1:200)
```

The first of these fixes the third subscript as 1 and so gives a two-dimensional array with 16 elements in total, i.e. a "size" of 16. In the second case both the second and third subscripts are fixed, leaving a one-dimensional array of size four. The final example is like the full array but with the element order reversed along two of the three dimensions.

In an array section, any subscript limit may be omitted, in which case it is taken to be the array's lower bound (before the colon) or upper bound (after the colon). So, with the array **matrices** as above, the examples could be written more compactly:

matrices(:,:,1) matrices(:,4, 98) matrices (4:1:-1, 4:1:-1,:)

There are some subtleties to the syntax associated with array sections. An array section is an array even if it has only one element or even if it has no elements at all. For example,

r(1:0) = 1.0

is valid but does nothing because the array section on the left has no elements. Bear in mind that an assignment statement can have an array on the left and a scalar on the right. But,

r(1:0) = (/1.0/)

is illegal because on the right we have an array of size one (not a scalar!) which is not conformable with the zero-sized array on the left.

In view of the importance of the subscript triplet notation for array sections, it is stated concisely for future reference in Section 4.6 below.

4.5 Exercises 4.A

- 4.A Write statements, which should be as concise as possible, to set up the following one-dimensional 1 arrays:
 - (i) The square roots of the first ten positive integers;
 - (ii) (/-1,-i,... (repeated30times), 1, 1,... (repeated30times)/);
 - (iii) The first ten powers of π .
- 4.A Write declaration statements to set up two-dimensional arrays to contain examination marks (0–100) 2 and corresponding letter grades (A–F) for each of 300 students in each of 12 subjects. Write code to rescale all the marks so that the average mark is 60 per cent in every subject, and then convert the marks into grades in a sensible way.
- 4.A Write code to set up a two-dimensional array of the binomial coefficients, i.e. the numbers of ways in 3 which m objects may be selected from n, n being a positive integer up to 50.
- 4.A A statistical exercise: if x_n (n = 1, ..., N) is a set of N values drawn from a distribution with mean X and 4 variance a, then estimates of X and a are given by

$$X = \Sigma x_n / N$$

$$\sigma^2 = \Sigma (x_n - X)^2 / (N - 1)$$

and the uncertainty in the estimate X is $\sigma/N1^{/2}$.

On this basis, write a program to read in a series of numbers that are assumed to come from a distribution having a particular mean. The program is to calculate and write out an estimate, X, of the mean of the distribution, together with the uncertainty in it.

4.6 Subscript triplets

Before proceeding further, for future reference it will be useful to define in general terms the notation using colons that was described above to specify array sections. A section of an array specified by array-name is defined by

array-name (section-subscript, section-subscript, &

section-subscript, ...)

there being one *section-subscript* for every dimension of the array.

What is a *section-subscript*? A *section-subscript* is either a *subscript-triplet* or a single integer. (A third possibility, a "vector subscript", is introduced in Chapter 9.) If a *section-subscript* is an integer, it could be either a constant or a variable or an integer-valued expression, but it must be a scalar.

However, to form an array section, it would not be permissible for every *section-subscript* to be an integer. If they were all integers, the expression would be a valid one but, instead of representing an array section, it would simply represent a single element of the array and would be a scalar. On the other hand, as long as at least one *section-subscript* is a *subscripttriplet*, then we will be forming an array section and it is

important to realize that an array section is itself a kind of array. The array section has a rank equal to the number of *subscript-triplets* among the *section-subscripts*.

What is a subscript-triplet? It is

subscript1: subscript2: stride

a construction in which only the first colon is compulsory and may not be omitted. The effect of the *subscript-triplet* is to pick out the elements of the array whose indices (in this particular dimension) run from *subscript1* to no more than *subscript2* in increments of *stride*. Note that *subscript1*, *subscripts* and stride must be integers (constants, variables or expressions). If *subscript1* is omitted, the effect is as if it were equal to the index at the lower bound of the array in this dimension. If *subscript2* is omitted, it is as if the upper bound were specified. If *stride* is omitted, it is as if it were equal to 1.

Note that *subscript2* would normally be greater than *subscript1*, but it could be the other way round if *stride* were negative, in which case the selected array elements would be reversed in order from the original array. Note also that an array section will contain no elements (but will still exist!) if there is a *subscript-triplet* that generates no valid index. This would happen, for example, if **stride** were positive but *subscript2* were less than *subscript1*.

If quintessence is a rank-five array,

```
quintessence(:,:,:,:,:)
```

is no different from

quintessence

but

quintessence(:, 1, : ,6, :)

is a rank-three array section and

```
quintessence(1,1, 9, 6,2)
```

is just one element of quintessence, and is a scalar. In

```
quintessence(:,:,:,:,2:1:1)
```

the fifth *subscript-triplet* is **2:1:1**, which generates no indices because you never get to 1 by adding units to 2; so this array section is a rank-five array with no elements at all!

4.7

Character substrings and arrays of character strings

The subscript triplet notation is very similar to a notation that may be used to pick out a part of a character string. If **lines (10)** is an array of ten character strings, what will the processor understand by **lines (1:5)**? The answer is, it means the first five elements of the array lines, in accordance with all that has been said above. On the other hand, **lines (1) (1:5)** would actually represent the first five characters of the first element of the array!

The situation is that if *character-name* represents any scalar character-string, then

character-name (position1 : position?)

represents the character string formed by taking the sequence of characters within *character-name* starting from position *position1* and going forward to *position2*. It is a "substring" of *character-name*. If *position1* is omitted, it is taken to be 1, and if positions is not given, it is taken to have its maximum value, i.e. the length of the string *character-name*. If L is the length of character-name, we must have

1 position1 position2 L

unless

position1 > position2

in which case the substring exists but contains no characters, i.e. it has zero length. The pair

position1 : position2

is known as a "substring range". So, the substring c (i : j) would be equal to

C(i) //c(i+1) //c(i+2)//...//c(j-1)//c(j)

if j is sufficiently greater than i.

Now, if we pick up the example given at the start of this section,

lines(1:4) (1:5)

is an array section consisting of four substrings, i.e. the first five characters from each of the first four elements of the array lines. On the other hand,

lines (1:5) (1:4)

is an array section consisting of five substrings each of four characters. Symbolically, the notation for a subobject of a rank-one character array is

character-array-name (section-subscript) (substring-range)

and if the rank is greater than one there must be that number of *section-subscripts*. If *substring-range* is omitted then we simply have a section of the array as defined in Section 4.6. The *section- subscripts* may not be omitted, i.e.

character-array-name (substring-range)

is not legal, but the desired effect may be got by writing

```
character-array-name (:,:,:,...,:) (substring-range)
```

where the number of colons is the rank of *character-array-name*. The following example may make the notation clear:

```
CHARACTER (30) :: words (2000), test (25)
```

```
CHARACTER(10) :: shorter (2000) , check
```

. test = words(176:200) shorter = words(1:2000)(1:10) check = words(99)(1:10)

The first two of these assignment statements give values to arrays. The third gives a value to the scalar character string check. The last two statements could equally well be written

```
shorter = words(:)(:10)
check = words(99)(:10)
```

since an omitted index is taken to have the lowest or highest value possible, according to whether it is before or after the colon. Similar rules apply to multidimensional arrays, as in

CHARACTER(30) :: words (30, 60,200), halfpage (30, 30)

. .

CHARACTER :: capitals(30,60,200)

halfpage = words(:,:30,57)

capitals = words(:,:,:)(:1)

Array sections and substrings can also be used in array constructors, as in

CHARACTER, PARAMETER :: digits(0:9) = (/ ("01235456789"&

(k:k), k=1,10) /)

CHARACTER, PARAMETER :: octals(0:7) = digits(:7)

This syntax is made clearer in Chapter 8. As a final example, if we have

CHARACTERS) :: concept(3) = (/&

"origin","cattle","potato"/)

then concept(2:)(4:5) is equal to (/"t1", "at"/). Incidentally, an array constructor is taken to have the same type as the first element in it, and a character-type array constructor consists of strings whose lengths are all the same as those of the first element. So, the character constant

(/"or", "cattle", "potato"/)

is exactly equivalent to (/"or", "ca", "po"/), because the longer elements will be truncated just as they would be if they were given as values to length-two strings by assignment statements.

Remember that the substring notation may not be applied to an expression other than a constant or a variable. So,

a//b(i:j)

concatenates a string with a substring; it does not take a substring of the concatenation of two strings. And it is not permissible to specify a substring of a substring directly as in

p = q(1:m)(n:)

which could actually mean something quite different, as we will see in the next chapter when arrays are explained in more detail.

4.8 Masks

The concept of a "mask" arises in the WHERE statement, to be explained below, and in several of the intrinsic functions commonly used with arrays.

A mask is a logical array, i.e. an array whose elements are data items of LOGICAL type. The word "mask" is appropriate because arrays of this type are most often used to mask arrays of other types, i.e. to identify a subset of their elements on which some other operation is to be carried out.

Suppose, for example, that a and b are REAL arrays of the same shape. Then a>b is a logical expression, whose value is .TRUE, whenever a>b, and it is itself an array of the same shape as a and b. It is a logical array, i.e. a mask.

Logical arrays can be manipulated by assignment statements like any other type of array, e.g.

pickneg = a<0.0

evens = (/.FALSE.,.TRUE.,.FALSE.,.TRUE.,.FALSE.,.TRUE./)

4.9 WHERE

Normally, an array assignment statement a=b will set each element of a equal to the corresponding element of b. However, the assignment may be made conditional with a statement such as

WHERE (b>a) a = b

or

WHERE (a<0.0) a=0.0; a=SQRT(a)

The expression **b**>**a** is a mask of the same shape as the arrays **a** and **b**, and **a**<**0**. 0 has the same shape as **a**. The logical array **b**>**a** could be expressed in array constructor notation as

(/ b(1)>a(1), b(2>a(2), b(3)>a(3), /)

The general syntax of the WHERE statement is

WHERE (m) a = b

Here, m must be of logical type: it could be a variable, or a constant, or an expression. It is necessary for a to be an array (otherwise, we could have had IF instead of **WHERE**). If m, a and b are all arrays, they must have the same shapes. The assignment a=b then takes place conditionally, element by element, according to whether the corresponding element of m is true or false. The logical object m could be a scalar, in which case the statement is equivalent to

IF (m) a = b

If b is a scalar and m and a are arrays, then the value of b is given to all the elements of a that correspond to true elements of m.

Here is another simple example:

REAL :: angles(500)

WHERE (angles>360.0) angles = MOD(angles, 360.0)

Going beyond the simple **WHERE** statement, there is a **WHERE** construct by which a number of conditional array assignment statements may be tied together. If x, x1 and xr are real arrays of the same shape, we could have:

WHERE (x>0.0) x1 = LOG(x) xr = SQRT(x) ELSEWHERE x1 = -99.0 xr = 0.0 END WHERE

This **WHERE** construct consists of an opening statement with the keyword **WHERE** followed just by a bracketed logical array; then there is a sequence of array assignment statements; then there can be an **ELSEWHERE** followed by assignment statements conditional on the inverse of the original logical array. Finally, the construct is terminated by an **END WHERE** statement. The **WHERE** construct forms a unit and must not be interspersed with other types of statement. The **WHERE** construct may only contain assignment statements and not (for example) **WRITE** statements.

The **WHERE** statement, and assignment statements within a **WHERE** construct, are often called "masked" array assignments.

Fortran 95 feature not in Fortran 90

WHERE constructs may be nested, and may be named, in the same way as IF constructs. An example is

```
Outer: WHERE (out)

a = b

c = d

Inner: WHERE (narrow)

e = f

Innermost: WHERE (inside)

x = y
```

END WHERE Innermost

g = h

END WHERE Inner

i = j

WHERE (outlook) k = 1

END WHERE Outer

This consists of three **WHERE** constructs nested inside one another, and a **WHERE** statement that is within the outer **WHERE** construct. For simplicity no ELSEWHERE statements are included in this example, but in principle they could also occur.

In Fortran 95, a WHERE construct may contain a series of masked ELSE WHERE statements, like ELSE IF statements in the IF construct, as well as a non-masked ELSEWHERE that is analogous to ELSE. (Notice that, although Fortran does not distinguish between ELSE WHERE and ELSEWHERE, it is as well to follow the English language and use ELSE WHERE when another mask follows it, but ELSEWHERE for an unmasked catch-all final part of the construct).

In a Fortran 95 **WHERE** statement or **WHERE** construct, if the data is of a userdefined derived type, then the assignment must be an "elemental" assignment defined by an elemental subroutine (Section 11.3).

4.10

Arrays and intrinsic functions

Arrays can make use of many of Fortran's intrinsic functions, and in this chapter we have already encountered the SQRT and LOG functions being applied to arrays. Functions that can be applied to arrays are known as "elemental" functions. Fortran's numeric, mathematical and character functions are all elemental, and so are the bit manipulation functions (Appendix B). However, inquiry functions and so-called "transformational" functions that operate on whole arrays are not elemental. Examples of transformational functions are

ALL(masA) ANY(mask) COUNT(mask) MAXVAL(array) MINVAL(array) PRODUCT(array)

SUM (array)

where the arguments are one-dimensional arrays but the results returned are scalars. The use of multidimensional arrays with these functions is slightly more complicated and additional arguments may be applicable.

The names of these functions make it easy to remember what they do. The argument of ALL must be a logical array, and the result is a scalar of logical type and is true if and only if all elements of the argument are true. The function **ANY** likewise returns a true result if any of its elements is true. The function **COUNT** has an integer value equal to the number of true elements in its argument. MAXVAL and MINVAL operate on arrays that may be of real or integer type, and the results are the highest (MAXVAL) or lowest (MINVAL) values to be found among the elements. So,

MINVAL ((/5, 99,0,-5, 1/))

is equal to -5. The functions PRODUCT and SUM operate on arrays that may be real, integer or complex and the result is the product of all the elements or the sum of them. Thus,

PRODUCT((/(0.0,1.0),(0.0,1.0)/))

is equal to (-1.0,0.0).

Note that MAXVAL, MINVAL, PRODUCT and SUM have values that are of the same data type as their arguments. For example,

SUM((/1,-1,1,-1/))

is equal to the integer 0 because the argument is an integer array. Because these functions are not specific to a single data type they are called "generic" functions.

4.11 **Exercises 4.B**

4.B What are the substrings

(i) "mulligatawny" (7:8)

(iii) "mulligatawny" (6:6)

4.B Write type declaration statements to declare

2

1

(i) A zero-length string called null;

(ii) Three strings, each of length 24, called s1, s2 and s3;

(iii) A character-string constant named me whose value is your surname;

(iv) A named character constant of length 1 called bs whose value is the backslash character (\).

4.B Write statements, which should be as concise as possible, to set up the following one-dimensional 3 arrays:

- (ii) "mulligatawny" (1:4) (iv) "mulligatawny" (10:8)

(i) (/.TRUE., .FALSE., .TRUE., .FALSE., ..., (repeated for 50 pairs) /);

(ii) (/"a","ab","abr","abra", ..., "abracadabra"/);

- (iii) The array razamatazz but with its elements in reverse order and omitting every third element, where razamatazz is the name of a size-30 vector.
- 4.B Write a program to read a list of ten real numbers (real parts) and then another list of the same length 4 (imaginary parts) and then to form the array of complex numbers comprised by the corresponding real and imaginary parts. Then calculate which of the complex numbers has the greatest magnitude, and write it. (Note that CMPLX and ABS are elemental functions.)
- 4.B If the array s is given by
 - 5

CHARACTER (5) : : S (6)

s = (/"light","trick","witch","hazel","beach","shore"/)

use structure constructors to write down the values of

(i) s(1:2)	(ii) s(5:)	(iii) s(4:3 :-1)
(iv) s(1:2) (3:4)	(v) s(1) (5:5)	(vi) s(5:1:-1)(5:)

For example, the answer to (vi) is (/"ch", "e1", "ch", "ck", "ht"/).

- 4.B Write a program to input a string of up to 80 characters that will be interpreted as a line of text. Obtain 6 the words from this string (a "word" being any sequence of letters with non-letter characters at both ends of the sequence) and search the words for palindromes. A palindrome is a word that reads the same in both directions, like "deed". The program should write out any palindromes that it finds.
- 4B. Write code to convert a sequence of *x*, *y*, *z* coordinate triplets into the corresponding sequence of radial 7 coordinates (r, θ , ϕ), and then write out the radial coordinates of the point nearest to the origin. (Hint: look up **MAXLOC** in Appendix F.)
- 4.B Use a WHERE statement to halve all the elements of an integer array that are even numbers. 8
- 4.B Write a program to input a string of up to 20 characters and replace any blank in the string (but not 9 trailing blanks) by an asterisk. Then write out the string, excluding trailing blanks.
- 4.B Write code to take a string that is a series of words (separated by blanks) and reduce it to a string made 10 of their capital letters (e.g. "**North Dakota**" being reduced to "ND").

4.B Use a WHERE construct to manipulate three two-dimensional square arrays (i.e. matrices) of real type

- 11 called a, b and c. The object is to double the values of the elements of a that correspond in position to negative elements of b, unless the corresponding element of c is also negative, in which case it is the element of b that is doubled in value; and subsequently it is necessary to replace each element of b by the greater of the corresponding elements then to be found in a and c.
- 4.B Use a WHERE construct to look at an integer-valued array called nibble and form a real-valued array
- 12 called **chew**. The elements of **chew** are to be the square roots of the elements of **nibble** where the latter are positive and odd, but the cube roots in all other cases.
- 4.B Given an array of 100 real numbers, called data, write a WHERE construct to halve each element of
- 13 **data** that exceeds the average value of all of the elements initially in **data**, and to double those which are less than the average.

- 4.B Write another WHERE construct, again looking at the array data as in the previous example, but
- 14 halving each element that is closer in value to the largest than to the smallest, and doubling those closer in value to the smallest.
- 4.B Again looking at the array data of the previous two examples, write a statement which, if any element
- 15 of **data** is negative, will add to each element a number (the same for each element) sufficient to bring the value of the lowest element up to zero.

CHAPTER 5 Intrinsic procedures

Intrinsic procedures are facilities provided as a ready-coded adjunct to Fortran and they can be used to carry out a number of commonly-needed tasks and calculations. Here we discuss the procedure DATE_AND_TIME as an example of an intrinsic subroutine, introduce the CALL statement, and then turn to the mathematical intrinsic functions SQRT, SIN, COS, EXP, LOG, LOG10, TAN, SINH, COSH, TANH, ASIN, ACOS, ATAN, and ATAN2.

The numeric functions ABS, AIMAG, CMPLX, INT, MOD, REAL, AINT, ANINT, CEILING, CONJG, DIM, FLOOR, MAX, MIN, MODULO, NINT, and SIGN are explained, and then the numeric enquiry functions HUGE, PRECISION, TINY, RANGE, and EPSILON, leading to a more detailed discussion of the KIND parameter for data types. Then after covering the intrinsic subroutines SYSTEM_CLOCK, CPU_TIME, RANDOM and RANDOMSEED, the final part of this chapter is devoted to the array-related functions MAXLOC, MINLOC, ALL, ANY, COUNT, MAXVAL, MINVAL, PRODUCT, SUM, SIZE, CSHIFT, EOSHIFT, TRANSPOSE, MERGE, PACK, UNPACK, SPREAD, DOTPRODUCT and MATMUL and to the floating-point manipulation functions RADIX, DIGITS, MAXEXPONENT, MINEXPONENT, TINY, EXPONENT, FRACTION, NEAREST, SPACING, RRSPACING, SCALE and SETEXPONENT.

5.1

An intrinsic subroutine: DATE_AND_TIME

One of Fortran's intrinsic subroutines is entitled **DATE_AND_TIME** and can be invoked by a statement of the form

CALL DATE_AND_TIME &

(ALL=list, COUNT=nticks, MSECOND=millisecs, &

SECOND=nsecs, MINUTE=nmins, HOUR=nhours, DAY=nday, &

MONTH=nmonth, YEAR=nyear, ZONE=minaadvance)

This subroutine is taken as an example to explain a number of points about intrinsic procedures in general.

Some intrinsic procedures are functions, but some are subroutines, and those in the latter category can only be invoked by a CALL statement, an executable statement which has the general form

CALL subroutine-name (arguments)

although the call may be the "action" part of an IF statement such as

IF (time==.TRUE.) CALL DATE_AND_TIME (MSECOND=ms)

Unlike a function, a subroutine does not have a "value". Information may be passed to and/or from a subroutine through the values of its arguments.

DATE_AND_TIME has ten arguments, indicated by the keywords ALL, **COUNT**, **MSECOND**, and so on. These keywords are part of the language and are fixed (except, of course, that it would not matter if lower-case letters were used for them).

The effect of the call is to set the variables represented above by *list, nticks, millisecs*, etc. to values that will tell the program what the time and date are at the moment the statement is executed. Note that the names *nticks, millisecs, nsecs*, etc. are arbitrary, and any names for integer variables could be inserted in their place.

The statement

CALL DATE_AND_TIME &

(ALL=list, COUNT=nticks, MSECOND=millisecs, &

SECOND=nsecs, MINUTE=nmins, &

HOUR=nhours, DAY=nday, MONTH=nmonth, &

YEAR=nyear, ZONE=minadvance)

would have exactly the same effect as

CALL DATE_AND_TIME &

(list, nticks, millisecs, nsecs, nmins, nhours, &

nday, nmonth, nyear, minadvance)

i.e. it is optional to include the attributions of the variables to the keywords. However, it is generally advisable to use the keywords and it is very useful to do so when (as is usually the case with the **DATE_AND_TIME** subroutine) not all the information contained in all the ten arguments is required. If the keywords are not used, then all the arguments must be included, in the correct order, at least as far as the last of them that is needed. So, if the value of the argument **minadvance** is needed, and if keywords are not being used, then all the preceding nine arguments must be included in the argument list before **minadvance**. On the other hand, if only **list** is required, the statement

CALL DATE_AND_TIME (list)

would be sufficient. The advantage of the argument keywords is that they can appear in any order and they need not all be present. For example, the statement

CALL DATE_AND_TIME (MONTH=k1, DAY=k2)

could be used if it were only necessary to find the values of the seventh and eighth arguments.

As the keywords suggest, the **DATE_AND_TIME** subroutine yields the local time and date in milliseconds, seconds, minutes, hours, days in the month, months in the year, and years according to the Gregorian calendar. ZONE gives the number of minutes that local time is in advance of Coordinated Universal Time. **COUNT** provides a processor-dependent "stopwatch". All the arguments of **DATE_AND_TIME** are integers. The keyword **ALL** can provide a neat way of getting all the information of the other keywords: the corresponding argument, called list above, must be an array with nine elements and would be filled with the values **COUNT**, **MSECOND**, etc. in that order. This is our first example of an array being an argument of a subroutine.

Incidentally, a piece of code like

CALL DATE_AND_TIME (ZONE=minutes); longitude=minutes/4

could give a very rough indication of where the processor is!

There are keywords that may be used with all the arguments of all Fortran's intrinsic procedures, functions as well as subroutines, although it is common to omit the keywords in the cases where there are only one or two arguments anyway and so there is little danger of confusion between them. For example, the intrinsic function **SQRT** could be invoked by an expression such as **SQRT** (x=3 6.0) using the keyword x, but there is no advantage over omitting the keyword and writing **SQRT** (36.0).

It is possible to omit the keywords for some arguments but not for others, as long as those for which they are omitted (and which are therefore distinguished from one another by their positions in the list) all precede the arguments for which the keyword is included. For example,

CALL DATE_AND_TIME (listarray, nods, YEAR=j, DAY=k)

would be a valid statement.

DATE_AND_TIME is unusual because of the large number of its arguments and because all of them are optional. Most intrinsic procedures have at least one argument which must always be present. Since **DATE_AND_TIME** has no obligatory argument, the statement

CALL DATE_AND_TIME ()

could in theory be written although it would be useless. A subroutine with no arguments does not even need the pair of brackets, i.e. we could just have

CALL DATE_AND_TIME

These remarks are not pointless because it will be seen later that there can be "external" (user-written) subroutines that have no arguments but nevertheless carry out useful tasks.

The situation is slightly different with intrinsic (and external) functions. In the few cases where it makes sense to refer to a function without giving it an argument, the brackets cannot be omitted. For example, **NULL** () is permissible but not simply **NULL**. The reason is that, without the brackets that follow it, a function name would be indistinguishable from the name of an ordinary variable. A subroutine, however, is always distinguished by following the keyword **CALL** and so the brackets may be omitted without ambiguity.

5.2 Mathematical functions

The intrinsic procedures can be divided into several categories, one being the mathematical functions. A complete list of these follows, and more detailed specifications are given in Appendix F. The letter x is used to represent the argument, and may be used optionally as an argument keyword, although we will not use a keyword when the function has only one argument.

The following may have either a real or a complex argument and a result of the same type:

SQRT(x) square root

SIN(X) sine

cos(x) cosine

EXP (X) exponential (power of e)

LOG (x) natural logarithm

So, **SQRT**((-1.0, 0.0)) is equal to (0.0, 1.0). The functions **SQRT** and **LOG** are not allowed to have a negative real argument, and the argument of **LOG** may never be zero. The following functions must have a real argument, and yield a real result:

LOG10(X) logarithm to base 10

TAN(X) tangent

SINK(X) hyperbolic sine

COSH(X) hyperbolic cosine

TANH(X) hyperbolic tangent

ASIN(X) inverse sine (between $\pm \pi/2$)

ACOS(X) inverse cosine (from 0 to π)

ATAN(X) inverse tangent (between $\pm \pi/2$)

ATAN2(Y,X) inverse tangent (in range $\pm \pi$)

In spite of the requirement of non-integer arguments, it is in fact possible to insert integers as arguments of any of these functions, just as an integer may appear on the right-hand side of an assignment statement giving a value to a real or complex variable named on the left. What happens is that implicit type conversion takes place, the effect being as if the function **REAL** had been used for explicit type conversion. For example, the evaluation of **EXP(5)** is equivalent to **EXP(REAL (5))** and is the same as **EXP(5.0)**.

In all the functions above, angles are always taken to be in radians, not degrees.

The last function, **ATAN2**, is unusual in having two arguments. In effect it is very similar to **ATAN**, but its two arguments can be regarded as the coordinates of a point of which **ATAN2** is the bearing and that can lie in the full angular range between $\pm \pi$. Another way of saying this is that **ATAN2** (y, x) is the "argument", in the mathematical sense, of the complex number (x, y). In a statement like

bearing = halfpi + ATAN2 (to_north, to_east)

the arguments of ATAN2 must be in the correct order to avoid ambiguity and they are then called "positional" arguments. Alternatively, using the argument keywords x and Y,

bearing = halfpi + ATAN2(Y=to_north, X=to_east)

and

bearing = halfpi + ATAN2(X=to_east, Y=to_north)

are equivalent to one another and to the previous example.

5.3 Numeric functions

The "numeric" functions are a group that carry out simple manipulations of numbers. They include the following, introduced in the previous chapter:

ABS(A)	Absolute value of A (argument of any numeric type)	
AIMAG(Z)	Imaginary part of Z (complex argument)	
CMPLX (X,Y,KIND)	Forms a complex number (real or integer X and Y)	
INT (A, KIND)	The fractional part of A is removed, giving the integer nearest to A whose magnitude does not exceed the magnitude of A (argument of any numeric	
	type, but INT(A) = INT (REAL (A)) if A is integer or complex.)	
MOD(A,P)	Remainder if p is repeatedly subtracted from A (real or integer arguments A and P).	
REAL (A, KIND)	Converts A to real type (argument of any numeric type)	

Most of these will require no further explanation. The function **MOD** may have either real or integer arguments and the result is of the same type as the argument **A**. The function **REAL** can be used to extract the real part of a complex number, or to convert an integer into real type. It is important to realize that this is

a different usage of the word **REAL** from that in a type declaration statement: arguably it is a defect of Fortran that **REAL** could represent either a data type, or this function, and for that matter could also be used as the name of a variable. However, the pathological statement

REAL :: real = REAL (0)

is illegal because a name (of a variable, constant, construct, procedure, derived type or namelist group) may not be used in the same subprogram (technically, within the same "scoping unit") to identify two things. The above statement is illegal because real and the second REAL are both names, indistinguishable to Fortran, but the former refers to a variable and the latter to an intrinsic procedure. The first REAL is not a name at all, but a statement keyword, and so

REAL :: real

involves no clash of names and would be a legal statement (albeit an unwise one because it would preclude any reference to the REAL function elsewhere in the same subprogram).

The **KIND** argument is always optional where it is mentioned in the list above, and if present it can specify a non-default KIND parameter for the result's type (see Section 3.7 for non-default real numbers). For example we could have

x = REAL (A=nunber, KIND=k)

and in this example number is an integer variable being converted to a real number (x) with a **KIND** parameter given by the variable **k**. The **REAL** function could be used to convert between real types, as in

xhigh = REAL(A=xlow, KIND=2)

Similarly, CMPLX can be used to form a complex number as in

z = CMPLX(X=horiz, Y=vert)

or to convert a complex number from one KIND to another as in

zhigh = CMPLX(X=zlow, KIND=2)

So, for **CMPLX**, **X** and **Y** may be integer or real, and **X** may be complex if **Y** is absent. The other numeric intrinsic functions are:

AINT(A, KIND)	Truncation of A to a whole number (similar to INT , but with real A and a real result)
ANINT(A, KIND)	Nearest whole number to A (real A and a real result)
CEILING (A)	Nearest integer not less than A (real A but an integer result)
CONJG(X)	Complex conjugate of X (complex argument and result).
DIM(X, Y)	Difference (unsigned) between X and Y (X , Y and the result must all be real or all
	integer).

FLOOR (A)	Nearest integer not greater than A (real A but integer result).
MAX(A1,A2,A3)	Highest number (indefinite number of arguments).
MIN(A1,A2,A3)	Lowest number (indefinite number of arguments).
MODULO (A, P)	A modulo P.
MINT (A, KIND)	Nearest integer to A (real A but an integer result).
SIGN(A,B)	Gives the first argument the sign of the second.

AINT simply removes the fractional part of a real number, and **ANINT** does a very similar job but goes to the nearest whole real number; so AINT(-1.7) = -1.0, AINT(-0.7) = 0.0, and AINT(1.7) = 1.0, but ANINT(1.7) = 2.0.

The **CEILING** function is very similar, but its result is of integer type: **CEILING** (A) gives the integer immediately above A in value, i.e. **CEILING** (1.3) = 2 and **CEILING** (-5.8) = -5. The function **CONJG** must have a complex argument and its result is the complex conjugate of it. The **DIM** function must have two arguments and they can be either both real or both integer. **FLOOR** is another function along the lines of **CEILING**. The argument of **FLOOR** must be real and its result is the integer immediately below. Consequently, if **X** is any number with a fractional part, **FLOOR**(**X**) is equal to **CEILING**(**X**) are both equal to **INT**(**X**).

MAX and **MIN** are very useful functions which may have any number of arguments; the arguments may be real or integer, but not a mixture of the two types. The result is simply the largest (**MAX**) or smallest (**MIN**) of the arguments, i.e. **MIN**(-9, -5, 0, 2) is -9.

MODULO is subtly different from **MOD**, the distinction being relevant if either argument is negative. To be precise,

MODULO(A,P) = A-P*FLOOR(REAL(A)/REAL(P))

whereas

MOD(A,P) = A-P*INT((A/P)

The final two functions listed above, **NINT** and **SIGN**, have real or integer arguments and the result is of the same type as the arguments.

DBLE and **DPROD**

There are two intrinsic functions to do with "double precision" real data. **DBLE(A)** is like **REAL** (A) but the result is of double precision type. **DPROD(X, Y)** calculates the double-precision-real product of the default-real arguments X

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The **CEILING** and **FLOOR** functions may also have a **KIND** argument (as **INT** and **NINT** may) to give a result of the specified **KIND** of integer.

The **SIGN** function may be used for a special purpose if the processor is configured (as some are) to offer a distinction between real variables of positive and negative zero values.

If the second argument of **SIGN** is a variable or expression of zero value, the value of **SIGN** may be positive or negative. This facility is provided in Fortran 95 because some processors, following an IEEE standard, have one bit pattern for positive zero and another for negative zero.

5.4 Numeric inquiry functions

The precision of real number arithmetic, and the maximum and minimum sizes of real numbers, depend on the processor. To monitor and manage precision Fortran provides a number of utility functions. The functions available include:

HUGE(X)	The largest representable number
PRECISION (X)	An integer equal to the maximum decimal precision, i.e. the maximum number of
	significant figures
TINY(X)	The smallest representable non-zero positive number
RANGE (X)	An integer equal to the order of magnitude of the largest representable number or, if
	greater, of the inverse of the smallest. So, RANGE (X) is equal to the greater of INT
	(LOG10 (HUGE(X)) and INT(-LOG10 (TINY(X)))
EPSILON(X)	A positive real number almost negligible in comparison with unity, convenient when
	you simply want to use as small a number as the processor will support (e.g. for
	numerical differentiation).

Different kinds of real number are distinguished by the **KIND** parameter, which was introduced in Chapter 3. It is a parameter that may be specified in a type declaration statement and it must have a non-negative integer value. When a real constant appears, the **KIND** parameter may follow the value after an underscore, as in

-78.915443_normal

1877724. _quad

4.65E-9_hiprec

where normal, quad and hiprec are named constants given previously in type declaration statements (with the **PARAMETER** attribute, Chapter 8) and having values corresponding to **KIND** parameters valid for this processor.

The KIND parameter could alternatively be given explicitly, as in

-78.915443_2

but this sort of code is unsafe as it may not be portable between processors: the actual values of the **KIND** parameters (2 in this instance) are not laid down in Fortran. The best thing to do is to use a special intrinsic function, **KIND**(x), which returns the value of the **KIND** parameter for the number **X**. The default **KIND** parameter is given by, say, **KIND**(0.0). Real numbers of higher precision can always be specified by a **KIND** parameter as defined by, say,

INTEGER, PARAMETER :: hiprec = KIND(0.0D0)

where 0.0D0 is a "double precision" number, as mentioned in Section 3.7. Notice that the word **KIND** can be used in three different ways: as a parameter when real data is declared, as an argument keyword in several intrinsic functions, and as the name of a particular intrinsic function. Examples of the three sorts of use are the statements

REAL (KIND=hiprec) :: sensitivity

q = REAL(A=k, KIND=2) - AINT(A=1.0, KIND=2)

IF (KIND(r).NE.2) THEN

Another example will be given at the end of this section. In addition to **KIND**, there is another intrinsic function provided to help control the use of real numbers of different kinds. It is the function **SELECTED_REAL_KIND(P, R)**, which returns an integer equal to the minimum **KIND** value used by the processor for real numbers of a given precision and range. The argument P is the required decimal precision and R is the required exponent range, and it is not necessary for both arguments to be present. **SELECTED_REAL_KIND** could be used in a type declaration statement (see Chapter 8) such as

INTEGER, PARAMETER :: nreal = SELECTED_REAL_KIND(P=15)

which sets nreal to be a named integer constant equal to the **KIND** parameter necessary for 15-figure decimal precision. Variables requiring this precision can subsequently be declared by statements like

REAL (KIND=nreal) :: x, y, z

However, one should first check that **nreal** is positive, because the **SELECTED_REAL_KIND** function will return a negative value if the processor cannot attain the required precision or range. In any program doing serious number crunching it is advisable for the programmer to decide in advance what precision and range are going to be needed. You could have a statement such as

IF (SELECTED_REAL_KIND(P=15, R=80) &

/= SELECTED_REAL_KIND(0.0)) STOP

to check that non-default kinds are not needed, or

IF (SELECTED_REAL_KIND(P=20, R=100)<0) STOP

to check that kinds of real numbers are available that will be capable of achieving the needed precision and range. (The **STOP** statement is mentioned in Section 6.7.)

Normally the default precision will be amply good enough for most calculations. Arguably, a program is badly designed if it relies on exceptionally high decimal precision. In the remainder of this book, little more will be said about non-default kinds of data.

Among the intrinsic functions discussed so far there have been the functions **REAL** and **KIND**. It is worth emphasizing yet again that these functions should not be confused with the keywords or parameters **REAL** and **KIND** that can occur in type declaration statements. The statement

REAL(KIND=KIND(0.0D0)) :: giga=REAL(2**30)

is really quite tricky because it uses the keyword REAL, meaning that the data object **giga** is to be of real type, and also the function **REAL**, which converts the integer **2**30** into a real number; and also there is the **KIND** function, which yields the parameter needed by this processor to specify a double-precision number such as **0.0D0**, and the **KIND** keyword that applies that parameter to **giga**!

5.5

Exercises 5.A

5.A Write programs to read a number from the keyboard and calculate and display the value(s) of its 1

- (i) secant
- (ii) inverse hyperbolic sine (arcsinh)
- (iii) logarithm to the base 16
- 5.A Write a program to input a sum of money, an interest rate and a time in years, and to calculate what the 2 sum has grown to after that time if the interest is compounded monthly.
- 5.A A straight line (chord) divides a circle into two unequal parts. Write a program to calculate the area of 3 the smaller part, given the circle's radius and the length of the chord.
- 5.A Write code to find the number of the current month of the year (using **DATE_AND_TIME**) and output 4 its name.
- 5.A If x is a real variable, write a line of code to calculate the natural logarithm of the complex number 5 whose real and imaginary parts are cosh(x) and sinh(x).
- 5.A Write a program which will simulate the tossing of a coin (writing out **head** or **tail**) using the 6 millisecond counter of **DATE_AND_TIME** to give an integer of practically random parity.
- 5.A Write a program which will input a sequence of ten integers and calculate their average when the largest 7 one and the smallest one are disregarded.
- 5.A Write a program to find and write the order of magnitude of the number given by **EPSILON** on your 8 processor. Also, find out if the square of this number is representable as distinct from zero.
- 5.A The intrinsic function SIGN(A, B) gives the first argument the sign of the second. Write code to do the 9 same job without using this function.

5.6

More intrinsic subroutines: SYSTEM_CLOCK, CPU_TIME, RANDOM and RANDOMSEED

Besides **DATE_AND_TIME**, described at the start of this chapter, there are two other intrinsic subroutines used for timekeeping, namely **SYSTEM_CLOCK** and (in Fortran 95) **CPU_TIME**.

SYSTEM_CLOCK has up to three arguments and is called by a statement of the form

CALL SYSTEM_CLOCK (COUNT=i, COUNT_RATE=j, COUNT_MAX=k)

The arguments are scalar integers with the keywords **COUNT**, etc. as shown. The **COUNT** argument measures time in the processor's own basic units or "clock counts". It is the same as the **COUNT** argument in the **DATE_AND_TIME** subroutine. **COUNT_RATE** allows the programmer to connect values of **COUNT** with real elapsed time, **COUNT_RATE** being the number of counts per second. **COUNT_MAX** gives the maximum count after which the clock is reset to zero. If the processor does not possess a clock then **COUNT_RATE** and **COUNT_MAX** are returned as zero. **SYSTEM_CLOCK** could be used by statements like

CALL SYSTEM_CLOCK(COUNT_RATE=nsec)

IF (nsec>0) THEN

CALL SYSTEM_CLOCK(COUNT=n)

milliseconds = 1000*n/nsec

END IF

Note that all three arguments of **SYSTEM_CLOCK** are optional, although obviously there is no point in calling it if none are present.

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CPU_TIME is an intrinsic subroutine that has one argument, of real type, measuring the "processor time" in seconds. The precise definition of processor time will in general be dependent on the processor. **TIME** is a scalar in standard Fortran 95, but a parallel processor could provide an enhanced version of **CPU_TIME** returning an array of processor times.

There is a very useful pair of intrinsic subroutines used for generating random numbers, **RANDOM** and **RANDOMSEED. RANDOM** has a single argument, of real type, which is returned to the program with a random value in the range between 0 and 1. It does not matter what value (if any) the argument had before

RANDOM is called. If it is an array variable, then an array of different random numbers will be returned. So, if x is a real scalar variable,

CALL RANDOM(x)

gives x a random value between 0. 0 and 1. 0 (to be precise, $0.0 \le x < 1.0$). A more complex usage is the following:

REAL :: radvec(3) = 99.0

DO WHILE (SUM(radvec**2)>1.0)

CALL RANDOM(radvec)

END DO

The **DO WHILE** syntax is explained in the next chapter. This code finds a random point within the threedimensional unit sphere. It does so by picking a point within a cubic volume and checking to see if it is also within the enclosed sphere. The coordinates are preset to a large value merely to satisfy the WHILE condition when the DO loop is first entered: subsequently the loop is repeated until a point within the sphere is found.

The subroutine **RANDOMSEED** is to do with the initializing of the random number generator that **RANDOM** will invoke. **RANDOMSEED** has three optional arguments, but no more than one may be present in a particular call, so we could have any of the following

CALL RANDOMSEED

CALL RANDOMSEED(SIZE=nintS)

CALL RANDOMSEED(PUT=intseedin)

CALL RANDOMSEED(GET=intseedout)

Now, **RANDOM** generates random numbers (or, more technically, "pseudorandom" numbers) using internally a set of integers known as the "seed" that changes from one call to the next. The seed determines the subsequent sequence of random numbers. A call to **RANDOMSEED** with no argument will simply reset the seed, and might be used at the beginning of a program to make sure that different runs of the same program would give different sequences of random numbers. A call with the argument keyword **GET** is used to obtain from the processor the current value of the seed. The **PUT** keyword lets the program specify the seed value. Calls with **GET** and **PUT** could be used to record the value of the seed at the start of a

simulation, say, and to repeat the run later with the same sequence of random numbers. A complication is that the seed might not be a single integer but a set of integers in a rank-one array. The size of that array (i.e. the number of integers in the seed) is processor-dependent but can be found in a program by calling **RANDOMSEED** with the **SIZE** keyword. Obviously the variables used to hold the seed must be arrays of sufficient size, i.e. in the above example, intseedin and intseedout must be of size equal to or greater than nints.

Although **RANDOM** generates real numbers between 0 and 1, it is a simple matter to scale the results to simulate, say, the throw of a set of seven dice:

REAL :: x(7) INTEGER :: n(7), ntotal CALL RANDOM(X) n = 1 + INT(6.0*x)

ntotal = SUM(n)

5.7 Functions for arrays

The intrinsic functions described in this section are

MAXLOC	Location of an array's largest element
MINLOC	Location of the lowest element
ALL	True if all an array's elements are true
ANY	True if any element is true
COUNT	The number of true elements
MAXVAL	Value of the largest element
MINVAL	Value of the lowest element
PRODUCT	Product of all the elements
SUM	Sum of all the elements
CSHIFT	Shift the elements cyclically
EOSHIFT	Shift the elements "end-off"
TRANSPOSE	The transpose of a matrix
MERGE	Merge two arrays selectively
PACK	Pack an array into a rank-one array

Each of these will be discussed briefly below, with indications of the argument keywords and their meanings. In many cases it is obvious what the keywords mean, e.g. **ARRAY** always refers to an array argument. At first reading, the descriptions below will inevitably seem very complex and you may wonder what on earth these functions are really needed for. In fact, they are very useful for testing, manipulating and reordering the elements of arrays, and doing so with great flexibility and conciseness. They are powerful tools for the programmer who needs to work with arrays of data.

MAXLOC (**ARRAY**, **MASK**) looks into an array of real or integer numbers and returns the set of subscripts giving the location of the largest element. The value of **MAXLOC** will be a rank-one array containing the subscripts, so the size of **MAXLOC** is equal to the rank of **ARRAY.MASK** is an optional second argument: if present it must be a logical array (or expression) with the same shape as **ARRAY**, and elements of **ARRAY** are disregarded if the corresponding elements of **MASK** are false. For example, if y is the array (71946,1932,1945,1949, 1936/) then

MAXLOC(ARRAY=y, MASK=y<1946)

is equal to the array (/3/). **MINLOC(ARRAY, MASK)** is exactly like **MAXLOC** except that it indicates the minimum-valued array element.

ALL (MASK, DIM), and others following it in the list above, were introduced in a simple form in Chapter 4. Its first argument is a logical array, MASK. In the simple case, where the optional argument DIM is absent, ALL is a logical function true if all the elements of MASK are true. If DIM is present, DIM (short for "dimension")must be a scalar integer no greater than the rank of MASK, and the function then sees if all the values of MASK are true along the DIMth dimension: the result is then an array of rank one less than that of MASK. In other words, ALL suppresses the DIMth dimension of MASK to a value that is true only if all MASK'S elements along that dimension are true. For example, if q is a six-dimensional logical array and

f = ALL(MASK=q, DIM=4)

then f is a five-dimensional array such that f (i, j, k, m, n) is equal to

ALL(MASK=q(i, j, k, : , m, n))

ANY (MASK, DIM) is like **ALL** except that the result (or an element of the result) is true if any of **MASK'S** elements (or its elements along a particular dimension) is true.

COUNT (MASK, DIM) also operates on logical arrays. In the simple case when the optional argument DIM is absent, the function has an integer (not logical) value equal to the number of MASK'S true elements. If **DIM** is present, then (as for ALL and ANY) the result **COUNT** is an array whose shape is reduced from that of MASK by the elimination of the DIMth dimension. Continuing the previous example,

ntrue = COUNT(MASK=q, DIM=4)

gives an array such that ntrue(i, j, k, m, n) is equal to

COUNT(MASK=q(i,j,k,:,m,n))

MAXVAL (ARRAY, DIM, MASK) operates on an array of type integer or real and looks for maximum element values. MASK is an optional logical array that, if present, must be of the same shape as ARRAY; it causes the function to ignore elements of ARRAY corresponding to false elements of MASK. If DIM is present, it has an effect similar to that for the functions ALL, ANY and COUNT, and the result is an array. MINVAL(ARRAY, DIM, MASK) is similar to MAXVAL but finds the minimum-valued element, or elements, of ARRAY. PRODUCT (ARRAY, DIM, MASK), just like MAXVAL, has optional arguments DIM and MASK that make it possible to do more complicated things than were mentioned when we introduced this function in Chapter 4. For example, if

kit = (/1,0,6,-5,3,0,0,-2,10/)

then

PRODUCT(ARRAY=kit,MASK=kit/=0)

is equal to 1800.

SUM(**ARRAY**, **DIM**, **MASK**) is just like **PRODUCT** except that it adds rather than multiplies. The function **SIZE** (**ARRAY**), as its name implies, yields the size (i.e. total number of elements) of the array; it may also be used with an optional argument **DIM**, and **SIZE**(**ARRAY**, **DIM**) is the extent of the array along its **DIMth** dimension. A simple example of the use of **SIZE** and **SUM** is the calculation of the root mean square (rms) of the elements of an array x, by the statement

nms = SQRT(SUM(x**2)/SIZE(x))

If we wanted the rms value only of alternate members of the array x, that could be achieved by

rms_odd = SQRT(SUM(x(1::2)**2)/SIZE(x(1::2)))

or

rms_even = SQRT(SUM(x(2::2)**2)/SIZE(x(2::2)))

and if we wanted these two things to be paired as a size-two array, we could have

rms_alternates = (/ (SQRT(SUM(x(i: :2) **2)/&

SIZE(x(i::2))), i=1,2) /)

CSHIFT (**ARRAY**, **DIM**, **SHIFT**) is a function we have not encountered before. It operates on an array of any type. The result **CSHIFT** is also an array and it is of the same type and shape as **ARRAY**. In the simplest case, where **ARRAY** is one-dimensional, DIM must be equal to 1 and the effect of the function is to perform a circular shift of the elements of ARRAY. The shift is through SHIFT places, SHIFT being a scalar integer. So,

y = (/"a","b","c","d", "e","f"/)

```
z = CSHIFT (ARRAY=y,DIM=1,SHIFT=-2) &
```

```
//CSHIFT (ARRAY=y, DIM=1, SHIFT=1)
```

gives

(/"eb","fc","ad","be","cf","da"/)

If ARRAY has more than one dimension, then shifting will take place along the dimension specified by DIM. DIM must be a scalar integer lying in the range from 1 up to the rank of ARRAY. In this case, SHIFT may be a scalar integer and all elements of ARRAY will be shifted by SHIFT places around the DIMth dimension; but alternatively the different sections

ARRAY(i,j,k...,:,...)

(where a colon appears in the DIMth position) may be shifted DIM-wise by different numbers of places, SHIFT then being an array whose shape is reduced from that of ARRAY by the suppression of the DIMth dimension (cf. ALL, ANY etc. above).

EOSHIFT (ARRAY, DIM, SHIFT, BOUNDARY) is just like CSHIFT except that the shifting of elements is not circular, i.e. elements disappear when they fall off one end of a dimension and are not transferred to the other end. EOSHIFT is an acronym for "end-off shift". With an array y defined as previously,

EOSHIFT (ARRAY=y, DIM=1, SHIFT=2)

is equal to

(/" ", " ", "a", "b", "c", "d"/)

i.e. as we move the array to the right, vacancies are created on the left and these are filled with blank strings of the appropriate length. In the case of numeric or logical data, zero or **.FALSE.** is inserted. If different infill values are required, they can be specified through the optional argument **BOUNDARY**, which like **SHIFT** may be a scalar or an array. For example, if

n = (/ (k, k=1,10) /)

then

EOSHIFT (ARRAY=EOSHIFT (ARRAY-n, DIM=1, SHIFT=4, &

BOUNDARY= 0), DIM= 1, SHIFT= -2, BOUNDARY= 10)

is equal to (/0,0,1,2,3,4,5,6,10,10/).

TRANSPOSE (MATRIX), by contrast with the above functions, is extremely simple. It obtains the transpose of a matrix, in the mathematical sense. MATRIX, the only argument, must be a rank-two array and may be of any type. If MATRIX is an array m with shape (n1,n2) and elements m(i, j), and **t=TRANSPOSE(m)**, then t has shape (n2,n1) and elements t(i,j) = m(j,i).

MERGE(TSOURCE, FSOURCE, MASK) is an elemental function returning either TSOURCE or FSOURCE according to whether MASK is true or false. MASK must be of logical type; TSOURCE and FSOURCE may be of any type, but the same, and if they are arrays they must have the same shape. If MASK is an array it must have the same shape as TSOURCE and FSOURCE. If TSOURCE and FSOURCE are logical, then MERGE is equivalent to

(TSOURCE.AND.MASK) .OR. (FSOURCE.AND. .NOT.MASK)

The MERGE function acts as a sort of switch, as in the expression

MERGE(TSOURCE=1, FSOURCE=0, MASK=veracity)

which could be used to convert a logical variable (veracity)into integer type.

PACK (ARRAY, MASK, VECTOR) can transform an array whose rank is two or more (**ARRAY**) into a rank-one array. This can be done selectively, keeping only those elements corresponding to **MASK** being true. In other words, **PACK** is constructed by forming the elements of **ARRAY** into a one-dimensional list. The order is determined by running through the subscript values of **ARRAY** from the left as in:

ARRAY(1,1,1,...),

ARRAY(2,1,1,...),

ARRAY(3,1,1,...,,

ARRAY(1,2,1,...),

ARRAY(2,2,1,...) ...

This is called "array element order". Another example should make the principle clear: if the array s is declared by

REAL :: S(2,3)

then PACK(S) is the one-dimensional array

(/ s(1,1), s(2,1), s(1,2), s(2,2), s(1,3), s(2,3) /)

It is permissible for **ARRAY** to have rank one, in which case PACK will be very similar to **ARRAY** but excluding elements for which MASK is false. Thus, the expression

PACK(ARRAY=characters, MASK=(characters/=""))

eliminates all the blanks from an array of single characters.

The size of **PACK** will be the number of elements in **ARRAY** for which **MASK** is true, but to get a result of predetermined size the optional argument **VECTOR** can be used: it must be a rank-one array whose size will be the size of PACK and whose latter elements provide values to pad out **PACK** in default of sufficient **MASK=.TRUE.** elements from **ARRAY.** For example,

PACK(ARRAY=(/5,4/3,2,1/),MASK=.TRUE.,VECTOR=(/k,k=1,10/

has the value

(/5, 4, 3, 2, 1,6, 7, 8, 9, 10/)

UNPACK (**VECTOR, MASK, FIELD**) can be regarded as the inverse of PACK. If VECTOR is a rankone array of any type, its elements will be distributed into the array FIELD to form the result **UNPACK**. FIELD may have any shape, but its type must be the same as **VECTOR'S**. The unpacking of VECTOR into FIELD is done under the control of MASK. Running through the elements of FIELD in the usual array element order (see **PACK**), elements from **VECTOR** are inserted sequentially to replace those elements of **FIELD** for which **MASK** is true. Where **MASK** is false, or where the elements of **VECTOR** have already been used up, **FIELD** is unchanged. To take a simple example, if there is such a thing,

UNPACK (VECTOR= (/ 1 , 2 /) , &

MASK=(/.TRUE., .FALSE., .FALSE., .TRUE./),&

FIELD=(/9,8,7,6/))

is (/1,8,7,2/).

SPREAD (SOURCE, DIM, NCOPIES) will replicate the array SOURCE by adding an extra dimension of extent NCOPIES; each element of SOURCE is repeated NCOPIES times along the new dimension. The argument DIM indicates in which position the new dimension is to be inserted in the list of extents defining the shape of SOURCE. So, if the shape of g is (4,4,200),

SPREAD (SOURCE=g, DIM=3, NCOPIES=10)

has the shape (4,4,10,200). Amore complicated example : the code

v1 = .FALSE.

```
v2 = EOSHIFT(ARRAY=v1,DIM=1,SHIFT=1,BOUNDARY=.TRUE.)
```

m1 = SPREAD (SOURCE=v2, DIM=2, NCOPIES=d)

m2 = CSHIFT(ARRAY=m1, DIM=2, SHIFT=(/ (i-1,i=1,d) /))

m3 = 0.0

diagonal_matrix = UNPACK (VECTOR=vector, MASK=m2, FIELD=m3)

where the vs are size-d vectors and the ms are d X d square matrices, is a way of forming a diagonal matrix from the elements of vector.

DOTPRODUCT(VECTOR_A,VECTOR_B) forms the dot product (or "scalar product") of the two vectors that are its arguments. If the vectors are integer or real numbers, the dot product is the sum of the products of corresponding pairs of elements. If they are complex (to be more precise, if VECTOR_A is complex) then the complex conjugates of the elements of VECTOR_A are multiplied with the elements of VECTOR_B. If the vectors u and v are of logical type, then DOTPRODUCT(u,v) is equivalent to ANY (u. AND. v).

MATMUL(MATRIX_A,MATRIX_B) forms the matrix product of two numeric matrices. The shapes of the two arguments must fit together, i.e. if MATRIX_A has shape (i, j) and MATRIX_B has shape (j,k) then MATMUL has shape (i, k). Alternatively, one of the two arguments may be a vector, in which case MATMUL takes the product between the vector and the matrix in the conventional way. MATMUL may be used with logical instead of numeric data: if u and v are logical matrices and w=MATMUL(u,v), then w(i,j) is ANY(u(i,:) .AND.v(:,J)).

5.8

Floating-point manipulation functions

The next set of intrinsic functions to be looked at is to do with the way in which numbers are represented internally within the computer. Although we almost always work with numbers displayed in decimal form, the computer itself may use a base other than ten. There is an intrinsic inquiry function RADIX (X) that returns an integer equal to the internal number base being used for real numbers (if x is real) or for integers (if x is an integer). In fact, most computers use the binary (base two) system. Below, it is assumed that RADIX is equal to 2.

The processor represents a real number x in a form that may be modelled as

x = ±1 * 2**e * 0.1...

where the exponent e is a positive or negative integer and 0.1... is any binary fraction in the range 0.1000... to 0.1111... (i.e 0.5 to almost 1.0 in decimal). The integer e might typically be formed from eight bits and could then range from -126 to +127. (To represent the case of x=0, e and all the digits in the binary fraction are set to zero.) The binary fraction might run to, say, 24 places, and since the first place is always 1 this corresponds to 23 bits of information. With the sign bit and the eight bits forming e, we therefore have 32 bits representing a real number. This is a common system for representing default-real data in processors with 32-bit "words", but real data of higher-precision KIND may use, say, 64 bits and have a higher exponent range and more significant figures. To find out the situation on a particular processor, for numeric data of particular type and kind, there are intrinsic inquiry functions DIGITS(X), MAXEXPONENT(X) and MINEXPONENT(x), as well as the function RADIX(X) already mentioned. The argument just specifies the type and kind of data (e.g. DIGITS (0.0) specifies default real data). DIGITS returns the number of

significant binary digits, while MAXEXPONENT and MINEXPONENT return the maximum and minimum values of the exponent e. The function TINY(X) returns the value of the smallest positive number that can be represented on the processor.

Other functions give details of the representation of particular numbers. EXPONENT (X), for real x of a specific value, gives the (integer) value of the exponent e as defined above. FRACTION(X) gives the value of the binary fraction 0.1... defined above, but expressed as a real decimal fraction. NEAREST (x, s) returns the real number that the processor will allow nearest to (but not equal to) X; the real argument s is a flag to indicate whether NEAREST is to be above x or below it, according to whether s is positive or negative. SPACING(X) returns the minimum spacing between two real numbers in the neighbourhood of x. (If SPACING is itself too small to be represented, TINY(X) is returned instead.) Another function, RRSPACING(X), returns the very large number that is the reciprocal of the relative minimum spacing between two real numbers near x. The definitions are such that

RRSPACING(X) * SPACING(X) = ABS(x)

for any value of x. There is a function SCALE (x,I) that scales up a real number x by the Ith power of the processor's internal base, i.e. usually by 2**I. Finally, there is SETEXPONENT (x, I), a function that changes the exponent part of X to the power I; in other words, e is replaced by I in the expression for X given near the start of this section.

Specific names of intrinsic functions

Fortran's intrinsic functions have been introduced under names that are "generic". This usually means that the function can accept arguments of more than one type and that the function result has the same type as the argument. For example, SIN(X) is real if x is real, complex if X is complex, and has "double precision" if x has double precision. SIN is therefore said to be a "generic" function name. Likewise, HUGE is "generic" because HUGE(X) is a large integer if x is an integer and a large real number if x is real. However, Fortran also allows for a number of "specific" names, i.e. names under which functions may be referenced when the argument is restricted to being of a specific type. In the case of the SIN function, there are specific names CSIN and DSIN that can be used if the argument and result are to be restricted to complex or double-precision-real types respectively.

In Appendix F there is a complete list of specific names for generic Fortran functions. As a rule there is no point in using specific names and they are a hangover from earlier versions of Fortran in which different function names had to be used for arguments of different types.

What we mean by "specific" and "generic" names can cause confusion. The situation is that all intrinsic functions have a generic name. In many cases (especially the non-mathematical functions like HUGE and ACHAR) there is only the generic name. Furthermore, the fact that the name is "generic" does not necessarily mean that arguments or results of more than one type are possible: for example ACHAR by its nature can only be a character function of an integer variable, but this is still regarded as a "generic" function name. At the same time, some generic names can also be used as specific names when the context demands it: SIN is an example.

These complications are best avoided by using only the generic procedure names that we have been using so far and that are listed in Appendix F.1. The "specific" names in Appendix F.2 can be avoided altogether, except in connection with the use of procedure names as the arguments of other procedures, a usage that crops up only very rarely and discussion of which is deferred to Chapter 14.

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- 5.B Under the MERGE function, a way was pointed out for converting an item of data from logical to 1 integer type. Write an expression to do the converse, i.e. to convert a binary digit into logical type.
- 5.B Being consistent with the account of MATMUL given above, express as clearly as you can in words 2 what MATMUL (x, y) would mean if x were a logical vector and y a logical matrix.

CHAPTER 6 Execution control

Within any program unit, statements are normally executed in the sequence in which they appear, but often it is necessary for program execution to branch along different paths or to loop repeatedly through the same set of statements. Branching and looping may depend on conditions (such as values of data to be read in) that are not known before the program starts to run. Fortran has five "constructs" for controlling the flow of execution through different blocks of executable statements: **CASE, IF, DO, WHERE** and **FORALL**.

Besides covering all the details of CASE, DO and FORALL, this chapter includes reviews of the IF and WHERE constructs and describes the STOP statement.

6.1

CASE

Different blocks of code may be selected for execution according to different possible values of an expression (the "case expression")which may be of integer, logical or character type. The construct begins with a SELECT CASE statement, then there are one or more blocks each starting with a CASE statement, and finally an END SELECT statement. This very simple example makes a selection according to the value of a logical expression:

Switch: SELECT CASE (input(1:1)=="Y")

CASE (.TRUE.)

. (case block)

END SELECT Switch

The case expression is specified in brackets at the end of the SELECT CASE statement. A CASE construct may be given a name, here Switch, and if so the name precedes the keywords SELECT CASE and is followed by a colon. Here the case expression is the logical expression

input (1:1) =="Y"

In this example there is only one case block, following the statement

CASE (.TRUE.)

and it would be a section of code to be executed if and only if the first letter of the character string input is a Y. The END SELECT statement closes the case construct, and unconditional execution of the program continues. Since the construct has a name, its name must be specified at the end after the keywords **END SELECT**.

Here is a more complicated example, with a selection being made according to the value of an integer nyears:

```
Wars: SELECT CASE (nyears)
CASE (1853:1856)
war = "Crimean War"
CASE (1899:1902)
war = "Boer War"
CASE (1914:1918)
war = "WW1"
CASE (1939:1945)
war = "WW2"
CASE DEFAULT
war = "Peace"
END SELECT Wars
```

A character variable (war) is being given different values according to whether the case expression (nyears) lies in certain ranges. The colon notation is used to specify lower and upper (inclusive) limits for the values of the case expression. Both limits need not be present, i.e. CASE (1914:) would be satisfied by any value greater than 1913, and CASE (: 1914) would be satisfied by any value below 1915, while CASE (1914) would be satisfied only by the value 1914. In any CASE construct, the ranges satisfied by the different

blocks may not overlap, so that whatever the value of the case expression there can be no more than one block selected. A CASE DEFAULT statement may be used to define a default block that will be selected if the case expression matches none of the other blocks. Obviously there can be no more than one default block.

The next example is a section of code with two CASE constructs. The first selects according to the value of an element of a character string and the second according to the value of an integer. The DO construct will be explained in proper detail shortly, but here it means that everything between the DO and END DO statements will be executed repeatedly with the integer i taking the values from 1 up to the length of a character string called text.

! Interpret input text as a number

! Initialization

string = " "; npoints = 0

Rune: DO i = 1, LEN(text)

Digit: SELECT CASE (text(i:i))

CASE ("0":"9")

string=string//text(i:i)

CASE (",")

WRITE (*,*) &

"NB Commas are disregarded"

CASE (".")

npoints=npoints+1

string=string//"."

CASE ("O")

WRITE (*,*) &

"An O has been interpreted as a zero"

string=string//"0"

CASE ("I")

WRITE (*, *) &

"An I has been interpreted as a 1"

string=string//"1"

CASE (" ")

WRITE (*,*) &

"A blank has been disregarded"

CASE DEFAULT

WRITE (*,*) &

"There is a fatal error"

STOP

END SELECT Digit

END DO Rune

Points: SELECT CASE (npoints)

CASE (0)

WRITE (*,*) &

"Check: There was no decimal point"

CASE (2:)

WRITE (*,*) &

"There was more than one decimal point"

STOP

CASE DEFAULT

WRITE (*,*) &

"Your number was "//string

END SELECT Points

text = string

The first SELECT CASE statement specifies that the ith character of the string text is the case expression. In the seven blocks following, different actions are taken if this character is a numerical digit, a comma, a decimal point, a letter o or I, or a blank, or something else. When the construct has been executed the required number of times, i.e. after the END DO statement, the character variable string will contain a modified version of the original text. There is then a second CASE construct looking at the number of decimal points that were encountered. The STOP statement is explained in Section 8.4.

To summarize: in general the case construct takes the form

construct-name: SELECT CASE (case-expression)

CASE (case-value-range-list)

CASE ...

CASE DEFAULT

.

.

END SELECT construct-name

where construct-name is an optional name, *case-expression is* an expression and *case-value-range-list* is a value, a range of values around a colon, or a set of such values and/or ranges separated by commas. Each value may simply be a constant or it may be an expression of some sort (technically, an "initialization expression"). Valid CASE statements are

CASE (p.NEQV.q) CASE ("A","E","I","O","U") CASE (SIZE(array)) CASE (1914:1918,1939:1945) CASE (10**5+1:10**6) CASE ("A":"Z","a":"z")

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The last example illustrates a possible difficulty when the case expression is of character type and a CASE statement specifies a range of values. The problem is that the range is interpreted according to the processor's own character collation sequence, not necessarily the ASCII sequence, and this may differ from one processor to another. For fully portable code, it would be safer to have something like

SELECT CASE (IACHAR(Char))

. . CASE (65:90,97:122)

to select characters which are letters of the alphabet.

6.2 IF: review

The IF statement and the IF construct, described in Section 3.3, are briefly reviewed here. The IF statement is, of course, a single statement of the general form

IF (condition) conditional-statement

where conditional-statement can be any executable "action" statement except a further IF statement or an END PROGRAM or END SUBROUTINE statement (Chapter 7).

Technically, a statement such as

IF (convergence==TRUE.) END FUNCTION Iterate

could be permitted in Fortran, but this is something of an anomaly and the usage is not recommended.

By the definition of an action statement, the conditional-statement is also forbidden to be the start or end of a CASE, DO, or WHERE construct, or a CASE, ELSE, ELSE IF, or ELSEWHERE statement, but it may be a CYCLE or EXIT statement (Section 6.4) or a single WHERE statement.

Examples are

IF (r>0.0 .AND. s>0.0) qfunc = SQRT(LOG(r)*LOG(s))

IF (SIZE(a)==SIZE(b)) WHERE (b==0.0) b=a

The IF construct, whose general form is given in Section 3.3, consists of a series of blocks of code separated by IF...THEN, ELSE IF, ELSE and END IF statements:

```
IF ... THEN

.

ELSE IF ... THEN

.

ELSE IF ... THEN

.

.

ELSE

END IF
```

where each block contains executable statements. They are not restricted only to the "action" statements that may be used in a single IF statement (see above), but may also include further IF statements and additional CASE, IF, DO and WHERE constructs. However, when these constructs are nested inside one another, the integrity of each construct must be respected, i.e. if one construct contains another then it must contain all of it. One construct may not overlap another. For this reason

```
Allowance: IF (allow.EQV..TRUE.) THEN
```

Permission: IF (chance.EQV..FALSE.) THEN

 $q = r^{*}(f+p/2.0)$

END IF Allowance

r = 0.0

END IF Permission

is forbidden even if it were not muddle-headed. The desired effect in this instance, if it is the desired effect, could be achieved with a properly nested pair of IF constructs:

Permission: IF (chance.EQV..FALSE.) THEN

Allowance: IF (allow.EQV..TRUE.) THEN

 $q = r^{*}(f+p/2.0)$

END IF Allowance

r=0.0

END IF Permission

Of the series of blocks of code within a particular IF construct, divided by the ELSE IF and ELSE statements, at most one block will be executed each time the construct is executed. What happens is that the logical conditions associated with the IF and ELSE IF statements are evaluated in sequence and, as soon as a true condition is found, the associated block is executed. Subsequent ELSE IF are ignored. The ELSE block is executed only if all the conditions attached to the preceding IF and ELSE IF statements are found to be false. When there is an ELSE statement, then exactly one block of code within the construct will be executed. Without an ELSE, it is possible that no blocks will be executed.

More examples of IF constructs are:

IF (initialized) THEN; i=0; j=0; k=0; END IF

Clear: IF (x<1.0) THEN

Sign: IF (x<0.0) THEN

 $\mathbf{x} = -\mathbf{x}$

ind = .TRUE.

END IF Sign

x = x + 1.0

ELSE Clear

x = x - 1.0

END IF Clear

6.3 Exercises 6.A

- 6.A Write a program, using a CASE construct for execution control, to solve a quadratic equation whose 1 coefficients are real but that may have complex roots.
- 6.A Use a CASE construct to look at the initial letter of a character string. If it is a lower-case letter, 2 convert it to upper case. If the string starts with a non-letter character, replace it with an x, but if it

starts with a blank just remove it.

6.A Repeat Exercise 6.A2 but using an IF construct instead of CASE.

3

6.A Given an integer, write a program that will check if it is the square or the cube (but not both) of a 4 smaller integer and, if so, write a message saying so.

6.4 DO

The CASE and IF constructs allow a program to execute one block of statements selected from a set of alternative blocks. The DO construct (or "DO loop") allows a program to execute a single block of statements repeatedly. The block must be enclosed between DO and END DO statements. In its simplest form, the construct is

DO

. (block)

END DO

and this causes execution to loop through the block an indefinite number of times. The following example calculates the value of the number e by summing an infinite series:

e=1.0; k=1; j=1 DO

```
e=e+1.0/REAL(j); k=k+1; j=j*k
```

END DO

The problem here is that the program will apparently never stop unless there is some way of escaping from the DO loop. In practice, it will keep looping until an error condition arises when j exceeds the processor's range of integers. So how do we get out of a DO loop? There is a special statement, EXIT, which does this and passes control to whatever statement follows the END DO, as in

```
INTEGER :: ifib(100), i
ifib(1)=1; ifib(2)=1; i=3
DO
ifib(i) = ifib(i-1) + ifib(i-2)
i=i+1
```

IF (i>100) EXIT

END DO

You can also escape from a DO loop by a STOP (see Section 6.7) or, in a subprogram, by a RETURN statement. Another construction is

DO WHILE (logical expression)

END DO

.

Here, each time the program is at the top of the loop, the value of the bracketed logical expression is checked, and, if it is not true, then the loop will not be executed and control passes to the statement after END DO. The DO WHILE construct is exactly equivalent to

DO

IF (.NOT. (logical expression)) EXIT

· · · END DO

Since the DO...WHILE syntax does not enable Fortran to do anything it could not otherwise do, some authorities disapprove of its use.

Note that DO loops, like IF and CASE constructs, may be named. Loop names are not functionally necessary, but it is a good idea to use them as a form of program annotation and self-checking especially when there are nested loops. A loop name, if used, must be given before a colon at the start of the DO statement, and must also appear at the end of the END DO statement. Here is an example of a named DO loop:

x = 1.0; y = 1.0; z = 1.0; ncount=0

Lorenz: DO WHILE ((x**2 + y**2 + z**2)<100000.0)

xplus = $10.0^{*}(y-x)$

yplus = $x^{*}z + 28.0^{*}x - y$

 $zplus = x^{*}y - 8.0^{*}z/3.0$

test = ABS(xplus) + ABS(yplus) + ABS(zplus)

IF (test <= 0.000001) EXIT

ncount = ncount + 1

IF (MOD(ncount, 20) == 0) WRITE (*,*) ncount, &

"iterations"

x = x + xplus

y = y + yplus

z = z + zplus

WRITE (*,*) x, y

END DO Lorenz

Another type of statement that is used for DO loop control is CYCLE. The CYCLE statement is a way of jumping to the bottom of the block and thence back to the top again, but unlike EXIT it does not jump right out of the loop:

DO

```
WRITE (*,*) "Type the password"
READ (*,*) inword
IF (inword/=password) CYCLE
WRITE (*,*) "That's right. Now type a new password"
READ (*,*) password
WRITE (*,*) "The new password is ",password
EXIT
```

The user never gets out of this loop unless the correct password is typed in.

Another way of controlling a DO loop is with a variable known as a loop index. Historically, this was the usual way of constructing DO loops in earlier versions of Fortran. The syntax is

DO i = i1, i2, i3 . . . END DO

where the loop-control quantities *i*, *i1*, *i2* and *i3* are of scalar integer type. A loop name, of course, may also be included as in the earlier example.

The first loop-control quantity, here called *i*, is the "loop index" and it is a local variable whose name is arbitrary. The integers i1,i2 and i3 may be variables, constants or expressions, but they must have definite values at the start of the loop. The loop is executed for values of i starting with i1 and going up to *i*2 in steps ("strides") equal to *i*3. The stride *i*3 may be omitted from the DO statement, in which case its default value is 1.

Here are two simple examples with constant loop parameters:

```
WRITE (*,*) "Table of cubes:"
```

DO k = 0, 20 WRITE (*,*) k, k**3 END DO WRITE (*,*) "Table of cubes:" DO k = 0, 1000, 5 r = REAL(k)/1000.0 WRITE (*,*) r, r**3 END DO

The first of these tabulates the cubes of the integers from 0 to 20, and the second tabulates the cubes of numbers from 0 to 1 in steps of 0.005.

A loop index may have negative stride (i3) if its starting point (i1) is greater than its end point (i2) as in

WRITE (*,*) "Table of cubes:"

DO i = 20, 0, -1

WRITE (*,*) i, i**3

END DO

which does the same thing as an earlier example but in the reverse order. Loop control parameters may also be more complicated expressions, as in

DO icount = MIN(intalpha, intbeta, intgamma), &

MAX(intalpha, intbeta, intgamma), jumper+1

The loop control parameters are set up when the DO statement is first encountered, before looping actually starts, and they cannot be altered by statements within the block. The loop index (i.e. the variable called i or k or icount in the above examples) increases by the "stride" each time the loop repeats, but it should not be altered by statements within the block.

The nesting of loops is a very useful feature of the language, as in

Decades: DO nyear = 1910, 2000, 10 prod=0.0; res=0.0 Ten: DO n = nyear-9, nyear prod = prod + oil(nyear) res = res + found(nyear) END DO Ten WRITE (*,*) nyear, prod, res

END DO Decades

It is important not to mix up your loop indices and not to have overlapping loops. It is always a good precaution to name the loops, as in the scheme

Outer: DO

Middle: DO

- .
- .
- .

Inner: DO

- .
- .
- .

END DO Inner

- .
- .

END DO Middle

- .
- .

.

.

END DO Outer

The EXIT and CYCLE statements usually have effect with respect to the deepest loop level where they appear, but they can refer to any level if names are appended. If you EXIT or CYCLE from an inner loop to an outer one, the inner loop will be finished and cannot be re-entered without re-initializing the inner loop index. The following is a fairly complex structure:

Outer: DO

. .

.

CYCLE Outer

Middle: DO

•

.

-

- .
- .
- .

EXIT Middle

- .
- .

Inner: DO

- . .
- .

EXIT Outer

- .
- .

CYCLE Middle

- .
- .

END DO Inner

•

. . END DO Middle . .

END DO Outer

In this example, CYCLE Outer has the effect of transferring control down to the END DO Outer statement, but it does not actually terminate looping at this level. EXIT Middle does stop looping at the middle level because it transfers control to whatever statement follows after END DO Middle (not to END DO Middle itself) and so it leaves only the outer loop operative. EXIT outer transfers control to the statement after END DO Outer, so no loops remain active. CYCLE Middle transfers control to END DO Middle, terminating the inner loop but leaving the other loops still active.

A complicated example like this is bound to seem confusing at first, but in practice nested loops are extremely useful and the EXIT and CYCLE statements are soon mastered.

DO loops with statement labels:

There is a form of the DO loop that uses a statement label (see Chapter 14) to indicate the bottom of the loop. In this type of DO statement, a numerical "statement label" follows the keyword DO, and the END DO statement must start with the same label. (Alternatively, the labelled END DO statement may be replaced by a labelled CONTINUE statement.) An example is

sumsq = 0.0; DO 6 k=1, kmax

sumsq = sumsq + datum(k)**2; 6 CONTINUE

which is equivalent to

sumsq = 0.0; DO k=1, kmax

```
sumsq = sumsq + datum(k)**2; END DO
```

and of course, most simply, to

sumsq = SUM(ARRAY=datum(1:kmax)**2)

6.5 FORALL (Fortran 95 feature not in Fortran 90)

The FORALL statement provides a way of controlling the execution of assignment statements involving sets of "subobjects", i.e. array sections and character substrings, of which the elements are identified by indices. FORALL is a bit like a cross between IF and WHERE. Like IF and WHERE, FORALL may be used either in the form of a single statement or in the form of a construct containing a block of code.

FORALL is primarily intended to allow for the possibility of the parallel processing of assignment statements. The assignments could be applied in parallel for all the elements of specified data objects. An example will help to make the idea clear:

FORALL (i=1:n, j=1:n, upside(i,j)/=0.0) &

down(i,j) = 1.0/upside(i,j)

which takes the inverses of all the non-zero elements of upside. This is much the same as

WHERE (upside/=0.0) down = 1.0/upside

but the advantage of a FORALL statement is that the logical condition may involve the values of the indices of the elements within upside as in

FORALL (i=1:n, j=1:n, upside(i,j)/=0.0.AND.i.NE.j) &

down(i,j) = 1.0/upside(i,j)

that inverts only the non-diagonal non-zero members of upside.

The general form of the FORALL statement is

FORALL (triplet-spec, triplet-spec, ..., triplet-spec, &

mask) assignment-statement

There must be at least one triplet-spec, and a triplet-spec refers to an index of a data object and takes the general form

index-name = subscript1: subscript2: stride

the index-name being the name of a scalar variable. This follows a very similar syntax to an array section, i.e. it picks out values of index-name going from *subscript1* to *subscript2* in leaps of stride. The stride is taken to be 1 if the second colon and *stride* are omitted in the statement, but neither *subscript* can be omitted. Note that a *subscript* or a stride is not allowed to refer to an index-name from the same list of *triplet-specs, i.e.*

FORALL (i=1:n, j=1:i, upside(i, j) / = 0.0) &

down(i,j) = 1.0/upside(i,j)

is not permissible. Incidentally, an index-name only has meaning within the scope of the FORALL statement (or construct, below) and does not interfere with any variable of the same name outside it.

The assignment-statement must have, on the left of the = sign, a variable that is a subobject identified by the set of index-names. If it is an element of a rank-n array, there will be *n triplet-specs* and therefore *n* indexnames. The assignment statement is executed for the elements picked out by the *triplet-specs*, which may be subject also to the truth of a condition *mask*.

The optional condition *mask*, if present, is a scalar logical expression that may involve the index-name variables as well as other variables. If *mask* involves the invocation of procedures, they must be PURE procedures (see Section 11.2) such as Fortran's intrinsic functions.

The *assignment-statement* must be an assignment statement (or a pointer assignment statement, see Chapter 13) giving a value to a subobject. The subobject must involve all the *index-names* as indices. No *index-name* may be redefined by the statement. The expression on the right of the assignment statement, like a *mask*, must not involve procedures that are not **PURE**.

The general form of the FORALL construct is

Name: FORALL (triplet-spec, triplet-spec, ..., &

triplet-spec, mask)

. . . statements .

END FORALL Name

And this follows much the same rules as a single FORALL statement. The statements may be assignment statements, following the same rules as mentioned above. Additionally, the statements block may include other FORALL statements, WHERE statements, and nested FORALL and WHERE constructs. Here is an example of a WHERE statement within a FORALL construct:

REAL :: x(10,30), y(10,30), z(10)

FORALL (1=2:10:2, z(i)>0.0) WHERE (x(i, :)==0.0) x(i,:) = REAL(i) y(i,:) = REAL(i)/x(i,:)

END FORALL

.

In the following example, the notionally parallel nature of FORALL execution is important:

REAL :: a(10, 300)

FORALL (m = 1:10) WHERE ((m /= 1) AND (m /= 10)) a(m, :) = a(m-1, :) + a(m+1, :) ELSE WHERE (m == 1) a(m, :) = a(10, :) + a(2, :) ELSEWHERE a(m, :) = a(9, :) + a(1, :) END WHERE END FORALL

Here, the right-hand sides of some assignments involve elements of a that are changed by being on the lefthand sides of other assignments. But what is intended, and what will happen, is that the right-hand sides should all refer to the elements of a as they were before the FORALL was entered. What will happen is that all the mask expressions are first calculated, then all the right-hand expressions are calculated where (and only where) the mask is true, and only then will the left-hand variables (the elements of a in this case) have their values changed.

It should be remembered that the keyword FORALL may not be split into FOR ALL.

6.6 WHERE: review

The WHERE statement and WHERE construct, described in detail in Section 4.9, are to carry out masked array assignments. Broadly speaking, IF is more appropriate for scalar assignment statements and FORALL for assigning values to array elements or array sections dependent on the values of indices.

In the example above,

WHERE (x(i,:)==0.0) x(i,:) = REAL(i)

is a valid WHERE statement. Whenever it is executed, the integer i will have a particular value, so that the array section x(i,:) will be a one-dimensional array with thirty elements, and REAL (i) is a scalar.

- In Fortran 90, WHERE constructs may only contain array assignment statements.
- In Fortran 95, a WHERE construct may also contain further WHERE statements and nested WHERE constructs. Although a WHERE construct may be nested in a FORALL, the reverse is not true.
- In Fortran 95, an assignment may be an elemental (Section 11.3) defined assignment.

Ideally, WHERE statements and constructs should allow a parallel-processing system to carry out array assignments on all elements of the array independently, i.e. "elementally". The benefit may be lost if the calculations for the different elements are interdependent or if non-elemental functions are involved. For example,

WHERE (x>0.0) y = LOG(x)

works elementally and (if the processor permits) in parallel, and the LOG function is only called for the elements of x that have positive values; but

WHERE (x>0.0) y = LOG(x)/SUM(LOG(x))

involves a non-elemental function (SUM) of the logarithms of all the elements of x, not just the individual elements selected by the mask x>0.0. Apart from being unsafe code (because it could fail by trying to calculate the logarithm of a non-positive number) this statement is wasteful because calls to LOG will be duplicated.

IF (time>overrun) STOP

The STOP statement may, optionally, be followed by a "stop code" or "access code" consisting of either a character constant or a string of up to five digits. The idea is that the stop code should be accessible to the user after the program has stopped and can be used to indicate exactly where it stopped. This is important for debugging lengthy programs that may have numerous STOP statements dotted about them. So, we can have statements like

CASE 109

IF (time>overrun) STOP "Too Late"

or

CASE (1999); STOP 1999

Exactly how the stop code is output is a matter for the processor's operating system, not for Fortran, since by definition it happens when the Fortran program is no longer running.

PAUSE

The statement PAUSE can be used to halt execution of the program temporarily, with the possibility of resumption under the user's control. PAUSE can be followed, like STOP, by a stop code.

6.8 Exercises 6.B

6.B Use a DO loop to calculate the factorial of an integer.

1

- 6.B Given a character string which consists of letters of the alphabet, write code to put the letters into 2 alphabetical order and produce a new string consisting of the reordered letters.
- 6.B Write a program that will calculate an integer value from a character-string sequence of digits, i.e. to 3 calculate the value 10 from the string "10".
- 6.B Write a program that will find the largest prime factor of an integer.
- 6.B Write a program to test whether a character string would be valid as the name of a Fortran variable. 5
- 6.B Write a program to input a word and write out its vowels.
 - 6

4

- 6.B Write a program that repeatedly reads words typed in until a predetermined password is encountered. 7
- 6.B Picking up the example at the end of Section 6.6, given a rank-one array x of 100 real numbers, write 8 code to produce an array that contains the logarithms of the positive-valued elements of x, but normalized (i.e. scaled) by the average of the logarithms so that the average value of the array produced is 1. Note that the size of the array produced will depend on the number of positive elements of x, and therefore it cannot be declared at the outset. Since allocatable arrays etc. (Chapter 12) have not yet been introduced, the array produced will have to take the form of an expression or an array section, not a whole named array.

6.B Calculate and display the average of an arbitrary number of input numbers.

9

CHAPTER 7 Introducing external procedures

We have already come across several of Fortran's intrinsic procedures, both functions and subroutines. This chapter explains how the programmer can write and use additional "external" functions and subroutines. External procedures are not only useful for carrying out calculations not covered by the intrinsic procedures; they are necessary also for the clear organization and subdivision of any large Fortran program.

The statements covered here are **FUNCTION**, **SUBROUTINE**, **END FUNCTION**, **END SUBROUTINE**, and **CALL**. The important keyword **INTENT** is also introduced. This chapter includes extended sets of exercises.

7.1

Functions

A function is used to calculate a result whose value will generally depend on the values of "arguments" given each time that the function is invoked. A function is like a mini-program and has an overall structure deliberately similar to a main program: it starts with a title statement, followed by non-executable declaration statements, and then the series of executable statements finishing finally with a version of the END statement. An example is

FUNCTION Cot(x)

REAL :: Cot

REAL, INTENT(IN) :: x

REAL :: s, c

IF (x==0.0) THEN

WRITE (*,*) "Error: cotangent function called with &

&zero argument"

Cot = HUGE(x)

ELSE

s = SIN(x); c = COS(x); Cot = c/s

END IF

END FUNCTION Cot

This piece of code would be provided alongside a main program. Whenever there is any reference to Cot in the main program (or for that matter anywhere else in the program as a whole, including other functions) this function will be entered and the cotangent will be calculated. When the END FUNCTION statement is reached, control returns back to wherever the reference to Cot was made.

With the function Cot defined as above, references to cot must have one argument, and the argument must have a real value. This argument is called *x* within the function, but elsewhere a reference to cot can have as its argument the name of any variable, or a constant, or an expression. The name x as it appears above is an arbitrary choice, and x is called a "dummy" argument, because it stands in for whatever "actual" argument will be supplied when the function is invoked. Valid invocations of Cot (occurring in the main program, for example) are the expressions

Cot(y)

Cot(0.1)

Cot(pi - SQRT(q**2 + p**2))

or even

Cot(alpha + ATAN((Cot(beta)+Cot(gamma)))

the Cot function being called three times by the last example.

It is fundamental to understand clearly the distinction between "dummy" arguments and "actual" arguments. A dummy argument is a variable with a name local to the function itself, and should be declared at the start of the function along with other variables used in the calculation of the function's value. An "actual" argument is supplied at execution time when the function is referred to elsewhere in the program, and the actual argument need not be the name of a variable. The actual arguments in the above examples are

у

0.1

 $pi - SQRT(q^{**}2 + p^{**}2)$

alpha + ATAN((Cot(beta)+Cot(gamma))

beta

gamma.

Leaving aside techniques involving modules (Chapter 10), it should be considered that a function's arguments are the only way in which data can enter it. Except as arguments, a function does not have access to data items used elsewhere in the program. Conversely, data items used within a function (except the arguments) are internal to the function and are unknown to the rest of the program, even if the names of variables in the function and variables elsewhere have similar names. Variables internal to the function statements within it.

In the example of the Cot function above, the first statement

FUNCTION Cot(x)

declares that this is the start of a subprogram that is an external function and it gives it the name Cot. (The use of an initial capital is a suggested convention, not a necessity. COT or cot would have the same effect.) After the name, (x) means that the function has a single argument that is being given the local ("dummy") name x.

After the FUNCTION statement is a set of declarative statements that set up the necessary variables. First we have

REAL :: Cot

and this is needed because a function (unlike a subroutine) has a value in its own right, and Cot is intended to have a value of REAL type.

As a matter of fact, there is another way of specifying that the function Cot has a real value: the FUNCTION statement itself may be prefixed by the keyword REAL as in

REAL FUNCTION Cot (x)

The function name does not then need to appear in a type declaration statement. Corresponding prefixes can be used also for function values of other types, e.g.

INTEGER FUNCTION Nfactorial(n)

COMPLEX FUNCTION Gamma(z)

CHARACTER(20) FUNCTION All_Upper_Case(string)

LOGICAL FUNCTION Cone(z)

DOUBLE PRECISION FUNCTION Finetune(p, q)

The function type is never mentioned, however, in END FUNCTION statements.

Since it is not necessary to use type-prefixed FUNCTION statements, and sometimes it can be cumbersome to do so (in Chapter 11 we shall meet other prefixes!), the practice is not recommended.

The next statement in cot,

REAL, INTENT(IN) :: x

declares that the variable x, which is the argument of the function, is of real type. It also specifies what is known as an INTENT attribute for x. The INTENT of an argument is whether it represents information flowing into the procedure or out of it. In this example, it is obvious that the former is intended, i.e. the function receives the value of x when the function is invoked. Later, however, we shall come across cases of external procedures that use arguments as a way of passing information out. The IN above means that information goes in, and if it were going out we would have INTENT (our). It is also possible to have INTENT (IN our) for an argument that can be used to pass information either way.

At this stage it will seem rather pointless to declare the INTENT of any argument, because any argument can be used to pass data either in or out, or both, if the INTENT attribute is omitted entirely. Instead of the above statement we could have simply

REAL :: x

The specification of the INTENT attribute is optional in almost all cases. It is for the sake of more advanced applications, when the INTENT specification can be useful to the compiler, and for the sake of program clarity, that it is recommended that all procedure arguments should have specified INTENT.

The remainder of the function Cot is straightforward to understand. The final declarative statement,

REAL :: s, c

affirms that s and c are variables of REAL type. The executable statements

IF (x==0.0) THEN WRITE (*,*) "Error: cotangent function called with & &zero argument" Cot = HUGE(x) ELSE s = SIN(x); c = cos(x); cot = c/s

END IF

calculate the required cotangent, and assign a value to Cot accordingly. It is obligatory that a value be given to Cot. Finally we have

END FUNCTION Cot

which ends the subprogram and, on execution, returns control to the point in the main program or elsewhere from which cot was invoked.

Instead of

END FUNCTION Cot

the statement can have the abbreviated form END FUNCTION or even just END.

It has to be understood that the data type of a function's name is the type of its value, and this is not necessarily the same type as its argument or arguments. For example, a logical function cone could have a complex argument, the function value being true or false according to whether the complex argument z has a real part of greater or lesser magnitude than its imaginary part:

FUNCTION Cone(z)

LOGICAL :: Cone

COMPLEX, INTENT(IN) :: z

Cone = .FALSE.

IF (ABS(REAL)z))>ABS(AIMAG(z))) Cone = .TRUE.

END FUNCTION Cone

Functions may have more than one argument, as in

FUNCTION Average (r1, r2, r3, r4) REAL :: Average REAL, INTENT(IN) :: r1, r2, r3, r4 Average = 0.25 * (r1 + r2 + r3 + r4)

END FUNCTION Average

In this example the four arguments are all of the same type, and their order is immaterial, but in general it has to be ensured that the proper order of the dummy arguments is adhered to whenever the function is called. This is obvious from the cases of some of the intrinsic functions already met: for example CMPLX(a,b) is not the same as CMPLX(b,a).

It is usually best for a function to receive information through its argument and return information through its value, i.e. to have arguments of INTENT (IN) only. But, if argument values are changed within a function, then the new values will be passed back to the program unit from which the function was called. When arguments are to be changed, it is often more appropriate to use not a function, but the other type of procedure, namely a subroutine.

Statement functions

Within a program unit it is possible to have a sort of simplified one-line function that can be used only within that program unit. It is specified by a non-executable statement that might typically look like this:

$Fun_name(x, y, z) = x/y + y/z + z/x$

i.e. an arbitrary function-name, followed by a bracketed list of arguments, followed after an = by an expression giving the value of the function in terms of the arguments. All arguments and other quantities must be scalars or single elements of arrays. Here is another example:

Croot (a) = a**(1.0/3.0) ! Cube Root Function

Such a statement is known as a "statement function" and must appear before any of the executable statements. Its use is not recommended.

There is one final point that needs to be made about functions. A function may involve ancillary variables (such as s and c in Cot above) that are not arguments. If the function is called repeatedly as the program executes, such variables are not "remembered" from one call to the next. Until we meet the attribute SAVE in Chapter 11, and ways of "pooling" data in modules (Chapter 10), all local variables within functions (and also within subroutines) must be regarded as strictly temporary. Anything that a function calculates must be recalculated afresh each time the function is called.

7.2 Exercises 7.A

7.A Write a function to calculate the volume of a sphere given its radius.

1

7.A Write a complex function to calculate the inverse sine of its (complex) argument.

- 2
- 7.A Write as simple a function as you can to calculate the sine of an angle by adding up the terms of the 3 series

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \dots$$

until additional terms do not seem to make much difference. Do not use any Fortran intrinsic functions, and do not use the power operator (**).

- 7.A The escape velocity from a star or planet is $(2GM)^{1/2}/R$ where G is equal to $6.673 \times 10^{-11} Nm^{-2} kg^{-2}$.
 - 4 Write a function that calculates the escape velocity as a fraction of the velocity of light c = 299792 kms⁻¹. The function must include a logical argument of INTENT (our) which is returned false if the object is
 - a Black Hole.
- 7.A Write a function called **Ind_int_arcsin** to calculate the indefinite integral of the inverse sine function 5 using the equation

$$\int \arcsin(x) \, \mathrm{d}x = x \arcsin(x) + (1 - x^2)^{1/2}$$

7.A The "radiation length" L_R for a material of atomic weight A and atomic number Z is given by 6

$$L_R = Z^2 B / (716.4A)$$

where $B = \ln(184.15/Z^{1/3}) + Z^{-1} \ln(1194/Z^{2/3}) - 1.202.(\alpha)^2 .Z^2 + 1.0369(\alpha)^4 .Z^4 - 1.008(\alpha)^6 .Z^6 / (1 + (\alpha)^2 .Z^2)$

 $\log_{10} x = a_1 t + a_3 t^3$

and the value of a is 1/137.036. Express the radiation length as a Fortran function.

7.A A logarithm to base 10 can be computed approximately by the formula

7

where t = (x-1)/(x+1), and $a_1 = 0.86304$, $a_3 = 0.36415$, as long as x is within the range $(10)^{-1/2} = x$ (10)^{1/2}.

Use this to calculate the logarithm to base 10 of any positive number. The square root of 10 is 3. 162277660 and its inverse, of course, is 0.3162277660. Your function should be as fast as possible and should not defeat the object of the exercise by calling any of the Fortran intrinsic functions or using the power operator (**).

- 7.A Try to write an integer square root function, i.e. calculating the square root of an argument that can be 8 assumed to be a perfect square. It should not rely on real-number arithmetic and should be faster (and more reliable) than using **INT(SQRT(I))!**
- 7. Write a function to calculate the natural logarithm of any positive real number. Use the approximation A9 $\ln(1 + x) = a_1 x + a_2 x^2 + \ldots + a_8 x^8$

where the "a"s are as follows:

$a_1 = 0.99999 64239$	$a_5 = 0.16765 \ 40711$
$a_2 = -0.49987 41238$	$a_6 = -0.09532\ 93897$
$a_3 = 0.33179\ 90258$	$a_7 = 0.03608\ 84937$
$a_4 = -0.24073\ 38084$	$a_8 = -0.00645 \ 35442$

This approximation is valid in the range 0 x 1 so it can be used to get the logarithm of a number between 1 and 2. To calculate the logarithm of a number below 1, use $\ln(y) = -\ln(1/y)$. To calculate the logarithm of a number greater than 2, use the relation $\ln(y) = \ln(2) + \ln(y/2)$, dividing the number by 2 repeatedly until we have a number in the right range for the series approximation above and using $\ln(2) = 0.693147180559945$.

7.A Using RANDOM, write an integer function that will simulate the throw of two dice, adding their 10 results. If a double is thrown, an extra throw is allowed in addition.

7.3

Subroutines

Subroutines are simpler than functions. While a function has a value, and is called by any mention of its name, a subroutine is called only by a special kind of statement, the CALL statement, as in the main program

PROGRAM Process

CALL Read_Data

CALL Analyze

CALL Display_Results

END PROGRAM Process

Read_Data, Analyze, and Display_Results are the names of subroutines to which execution is directed in turn by the CALL statements. They do not themselves have values and, in this example, they do not have arguments either. A subroutine can be more or less any block of code, not necessarily calculating anything in particular. At the end of it, control returns back to the calling program at the point immediately following the CALL statement. In the above example three subroutines are called from the main program, but in general any subroutine may be called from anywhere in the program as a whole, including functions and other subroutines.

Information may be passed into and/or out of a subroutine through arguments, as in:

PROGRAM Process

REAL :: x(100), y(100), xprime(100), yprime(100)

LOGICAL :: readcheck

CALL Read_Data(x, y, readcheck)

IF (readcheck) CALL Analyze (x, y, xprime, yprime)

CALL Display_Results (xprime, yprime, readcheck)

END PROGRAM Process

This illustrates, incidentally, that procedure arguments may be arrays. A subroutine is written very much like a main program except that it usually has arguments after its name and it begins with a SUBROUTINE statement. The above program could call the subroutine

SUBROUTINE Display_Results (a, b, go)

REAL, INTENT(IN) :: a(100), b(100)

LOGICAL, INTENT(IN) :: go

IF (.NOT.go) THEN

WRITE (*,*) "The data was not input correctly"

ELSE

(Display a scatter diagram of a against b)

.

END IF

END SUBROUTINE Display_Results

Here, as in a function, we have dummy arguments (a, b and go) whose names are local to the subroutine and need not be the same as the names of the actual arguments in the calling program. The dummy arguments here are associated with the actual arguments xprime, yprime, and readcheck by their corresponding positions in the argument lists in the CALL and SUBROUTINE statements. The arrays xprime and yprime have the same shapes as the dummy arguments a and b, i.e. they are rank-one arrays of 100 elements. Although other possibilities exist, and these will be explained in Chapter 11, for the time being it can be taken that actual arguments and dummy arguments, when they are arrays, must be declared to have matching shapes. It is also possible for procedures to have arguments that are character strings, in which case the actual and dummy argument strings need not be of exactly the same lengths, but the actual argument may not be shorter than the dummy argument.

SUBROUTINE Compare_Strings_20 (string1, string2, equivalent)

CHARACTER (20), INTENT (IN) :: string1, string2

LOGICAL, INTENT (OUT) :: equivalent

CHARACTER (20) :: s1, s2

equivalent = .FALSE.! Initialization

! Sees if two character strings are equivalent to one

! another, disregarding the distinction between upper-case

land lower-case letters.

! Work on s1 and s2, leaving string1 and string2 unchanged,

s1 = string1; s2 = string2

! The matter is immediately settled if there are different

Inumbers of trailing banks.

IF (LEN(TRIM(s1)) /= LEN(TRIM(s2))) RETURN

! Replace all upper-case letter case by the corresponding

```
lower-case ones
```

DO n = 1, 20

```
j1 = IACHAR(s1(n:n)); j2 = IACHAR(s2(n:n))
```

IF (j1>64.AND.j1<91) THEN

j1 = j1 + 32

s1(n:n) = ACHAR(j1)

END IF

IF (j2>64.AND.j2<91) THEN

j2 = j2 + 32

s2(n:n) = ACHAR(j2)

END IF

END DO

```
IF (s1==s2) equivalent = .TRUE.
```

END SUBROUTINE Compare_Strings_20

In this example, two of the arguments are 20-character strings. When the subroutine is called, the corresponding arguments must also be character strings each containing at least 20 characters, and their leftmost 20 characters are transmitted to the subroutine as the values of string1 and string2. The subroutine would be called by a statement such as

CALL Compare_Strings_20(teststring,&

"North Dakota ", check)

as long as teststring is the name of a sufficiently long character string and is defined when the call is made, the second argument has enough trailing blanks to make at least 20 characters, and check is the name of a logical variable.

The above subroutine includes a new type of statement, RETURN. The RETURN statement, which may occur in any subroutine or function, has the same effect as jumping down to the END FUNCTION or

END SUBROUTINE statement and returning immediately to where the procedure was called from in the calling program. In the case of a function, though, it has to be remembered that the function must have been given a value before you return from it.

Although the use of a RETURN statement can sometimes be handy, it is never necessary, as execution control constructs can be used so that the actual return always takes place at the END FUNCTION or END SUBROUTINE statement that finishes the procedure. It is therefore suggested that the RETURN statement be avoided.

There are a number of commonsense restrictions on the way that actual arguments may be associated with dummy arguments in subroutines and in functions. A variable that is an actual argument may be accessible within the subroutine, not only via the corresponding dummy argument, but also in some other way: this could happen through host or use association in relation to modules (Chapter 10) or simply via an additional argument. In such circumstances, the value of the variable may only be altered within the procedure via the dummy argument.

If there is any overlap among the actual arguments given to a procedure, then the overlapping bits may not be defined or redefined within the procedure. An example is a subroutine with two arguments, both of which are tenelement arrays, called by the statement

CALL MIX (x(1:10), x(6:15))

Because the arguments overlap with the elements x (6:10), these particular elements may not be redefined within MIX. Similar comments would also apply if we were talking about overlapping substrings of characters. As another example of the same sort of thing, consider

SUBROUTINE Product (a, b, ab)

REAL :: a, b, ab

ab = a * b

END SUBROUTINE Product

This is all very well, but

CALL Product (alpha, beta, alpha)

is illegal because the dummy arguments a and ab are here being made to overlap (in alpha) and so it is illegal for the subroutine to redefine either of them (specifically, ab). However,

CALL Product (alpha, alpha, beta)

is legal because, although the first two arguments are being made to overlap, the subroutine does not attempt to redefine either a or b. Declarations of INTENT help to make things clearer:

SUBROUTINE Product (a, b, ab)

REAL, INTENT (IN) :: a, b

REAL, INTENT (OUT) :: ab

ab = a * b

END SUBROUTINE Product

and the illegality of

CALL Product (alpha, beta, alpha)

can then be interpreted in terms of the rule that an INTENT (IN) argument must remain unchanged by the procedure.

ENTRY

Usually a procedure is invoked by the name supplied in its first statement, the FUNCTION or SUBROUTINE statement, and it starts executing from that statement; but it is possible to allow a procedure to be entered at different points under different names and with different arguments. This is done by inserting an ENTRY statement at each alternative entry point. A silly example is:

SUBROUTINE Powers(x) REAL:: x ; STOP ENTRY Fifth (x) ; x=x**5 ; RETURN ENTRY Fourth (x) ; x=x**4 ; RETURN ENTRY Cube (x) ; x=x**3 ; RETURN ENTRY Square (x) ; x=x**2 ; RETURN END SUBROUTINE Powers

This is not intended to be called at all under the name Powers, but by statements like CALL Fifth(y) or CALL Fourth(z) that will return with y or z raised to the power 5 or 4. In general an ENTRY statement consists simply of the keyword ENTRY followed by the name by which it will be called, followed by a bracketed list of arguments. Multiple ENTRY statements may also be used in a function subprogram, in which case the appropriate entry names (rather than the overall function name) must be given a value.

Internal procedures

Functions and subroutines are normally either "intrinsic" or "external" or are "module procedures" (Chapter 10). A fourth possibility is that of "internal procedures". An internal procedure looks very much like an external procedure, but is placed inside another "host" program or subprogram. It must be inserted towards the end of its host, immediately before the host's END statement and following a special separator

statement, CONTAINS. An internal procedure may only be accessed from its host, not from other parts of the program. Unlike an external procedure, an internal procedure has automatic access to all the variables defined in its host program as well as the data transmitted as its arguments.

7.4

Exercises 7.B

7.B Write a subroutine to arrange three numbers in increasing order of magnitude.

1

7.B There is a simple way of finding the day of the week for any date in the twentieth century. You take the 2 two-digit year number (i.e. without the "19"), add to it what you get when you divide it by 4 (rounding down to a whole number), add on to that the number of the day within the month, and then add on a "month code" equal to:

0 for January	1 for May	5 for September
3 for February	4 for June	0 for October
3 for March	6 for July	3 for November
6 for April	2 for August	5 for December

Finally, take the result of this modulo 7 (i.e. take the remainder when you divide by 7) and the number you are left with points to the day of the week, i.e. 1 for Monday, 2 for Tuesday, and so on. Write a subroutine to do this. Three arguments should be the integers forming the date (input to the subroutine) and a fourth argument (output) should be the character-string name of the day.

7.B Write a subroutine to return the probability value for a non-negative integer n from the Poisson 3 distribution of mean A. The probability value is

$A^n . \exp(-A)/n!$

where n! is the factorial function of n. Having done that, extend the function so that it will give an appropriately interpolated result if it is called with a (positive) non-integer value for n.

7.B Write a subroutine to solve a quadratic equation

4

$$ax^2 + bx + c = 0$$

where the coefficients a, b and c may be complex numbers and the solutions of the equation may be complex values of x.

7.B The "error function" that is defined mathematically by

5

$$\operatorname{erf}(x) = 2\pi^{-1/2} \int_{0}^{x} \exp(-t^{2}) dt$$

can be well approximated for non-negative values of x by

$$erf(x) = 1 - exp(-x^2) \cdot (a_1 t + a_2 t^2 + a_3 t^3)$$

where $t=(1 + px)^{-1}$; p=0.47047; and the *as* are: $a_1 = 0.3480242$, $a_2 = -0.0958798$, $a_3=1-a_1-a_2$

Using the fact that erf(-x) = -erf(x), write a Fortran function to yield erf(x) for anyreal x.

7.B Write a subroutine to solve the general cubic equation, allowing for complex coefficients and complex 6 solutions. A cubic equation may be written in the standard form

$$x^3 + a_2 x^2 + a_1 x + a_0 = 0$$

Notice that if we started with an equation in which x^3 had a different coefficient, i.e.

$$a_3x^3 + a_2x^2 + a_1x + a_0 = 0$$

then we could get to the standard form by dividing through by a_3 . To solve the cubic equation in the standard form, two auxiliary quantities must first be computed:

$$q = a_1/3 - a_2^2/9$$

$$r = (a_1 a_2 - 3a_0)/6 - a_2^3/27$$

Then, let $T = q^3 + r^2$ and $t = T^{1/2}$.

If T>0, the equation has one real solution and a conjugate pair of complex solutions. If T<0, all the solutions are real. If T=0, all the solutions are real but at least two are equal to one another. To calculate the solutions, more auxiliary quantities must be computed:

$$s_1 = (r+t)^{1/3}$$
 $s_2 = (r-t)^{1/3}$

and then the solutions are

$$x_1 = (s_1 + s_2) - a_2/3$$

$$x_2 = -(s_1 + s_2)/2 - a_2/3 + i\sqrt{3}(s_1 - s_2)/2$$

$$x_2 = -(s_1 + s_2)/2 - a_2/3 - i\sqrt{3}(s_1 - s_2)/2$$

where *i* is the imaginary unit. Incidentally, the solutions satisfy the symmetry relations

$$x_{1} + x_{2} + x_{3} = -a_{2}$$
$$x_{1}x_{2} + x_{2}x_{3} + x_{3}x_{1} = a_{1}$$
$$x_{1}x_{2}x_{3} = -a_{0}$$

When the calculations are made, t may be imaginary and s_1 and s_2 may be complex. In taking the cube roots to get s_1 and s_2 when they are complex, it may be necessary to know that the Fortran operation

y ** z

computes the "principal value" of EXP (z * LOG(y)). The LOG function may not have zero argument, and if it has a complex argument then the LOG is taken to have an imaginary part between $\pm \pi$. If s_1 and s_2 are complex, they should be complex conjugates.

7.B When a particle moves with velocity β through a medium of refractive index *n*, the "Cerenkov angle" 7 θ_c is given by

 $\theta_c = \arccos(1/\beta n)$

The velocity β must be high enough for βn to exceed 1. The particle will emit Cerenkov light, the number of visible-spectrum photons per metre of pathlength being approximately

$$N_{\rm y} = 50000 \sin^2(\theta_c)$$

z3 = 0.5*(z1 + z2) + c*(z1 - z2)

Write a subroutine yielding θ_c and $N\gamma$ when β and *n* are given.

7.B From two successive complex numbers z1 and z2, a third is generated by taking

8

where c is an imaginary constant. Hence, an indefinite sequence of complex numbers can be generated, given two to start things off. Write a program to model what is going on and investigate the convergence of the sequence for different values of c.

CHAPTER 8 More about data; the type declaration statement

This chapter begins with a closer look at characters, including the definition of character constants and the operators used with character data. The intrinsic functions LEN, LEN_TRIM, TRIM, IACHAR, ICHAR, ACHAR, CHAR, LGE, LGT, LLE, LLT, ADJUSTL, ADJUSTR, INDEX, SCAN, VERIFY, and REPEAT are explained.

Then the type declaration statement is described in detail: all the possible type specifications, attribute specifications, and ways of declaring character-string lengths and array shapes. Finally, defined operators are covered and there is an introduction to procedure interfaces.

8.1

More about characters

Fortran's handling of character data has already been introduced in preceding chapters. Unlike other data types, character data involves the complication that a single item may be a string consisting of an arbitrary number of individual characters. Character constants are specified simply by putting them between quotation marks or apostrophes. So 9 is an integer, 9.0 is real, "9" is a character, and "Nine" is a character string. A string may be of any length, including zero or one, so a single character is just a special case of a character string. As in the cases of numeric and logical data, names are used to represent variable character data. Names may also be used as a convenience to stand in place of character constants. Apart from cases where an IMPLICIT statement has been used (see end of Section 8.4) the names of character strings must always be declared, using a CHARACTER type declaration statement, at the start of the program or subprogram. Normally the lengths of the strings must also be specified at that time.

The character constants mentioned above, "9" and "Nine", were specified as usual between double quotes. But what happens if quote marks are going to crop up in the character string itself? The assignment statement

remark = "Use "==" instead of ".EQ.", please."

does not make a string containing

Use "==" instead of "EQ", please.

To get over this problem, there are two additional rules.

First, a character constant may be enclosed in single quotes (apostrophes) rather than in double quotes, in which case double quotes may occur freely between the single quotes. (Conversely, single quotes may occur freely in a string delimited by double quotes.) So, we could have statements like

remark = 'Use "==" instead of ".EQ.", please.' class = 'CONFIDENTIAL' quote = ''' apostrophe = "''' destination = "It's a cul-de-sac"

Second, if the delimiting character itself is to occur within the string, this can be achieved by showing it twice successively. So,

remark = "Use ""=="" instead of "".EQ."", please." quote = """" apostrophe = "" destination = 'It' 's a cul-de-sac'

are equivalent to the corresponding statements above. More complicated examples can be contrived, like the character constant

'Distinguish "it' 's" from "its' ' " '

which actually looks like

Distinguish "it's" from "its"

and

"Between quotes, """" means """

which looks like

Between quotes, "" means "

In practice the choice of two kinds of delimiter, and the doubling convention if a delimiter is to appear in the string, together give the programmer plenty of flexibility. In fact, it is possible to stick always to one sort of delimiter for all character constants, using the doubling convention when necessary. In this book, double quotes (") will be used as the delimiter.

It should be remembered that the Fortran character set does not distinguish between opening and closing double quote marks ("and"), nor between opening and closing single quote marks ('and'). In the ASCII character set these characters are ACHAR(147), ACHAR(148), ACHAR(145) and ACHAR(146) respectively, but do not appear on a standard keyboard. The keyboard has an angled single quote ACHAR (96), as well as a straight single quote, ACHAR(39) (often used as an apostrophe) but there is only one kind of double quote mark ("), ACHAR(34). If single quotes (apostrophes) are used to delimit a character string constant, they must be the straight quote from the keyboard as in 'James', not 'James' (or 'James').

Non-default character types

Just as a processor may support more than one kind of integer, and more than two kinds of real number, it may also support character data of more than one kind. For example, if a processor uses KIND=2 to specify a set of two-byte characters, then we might have for example **CHARACTER** (KIND=2) :: runder = 2_"r"

(The KIND parameter in a character constant must come in front, the reverse of the case with real numbers!)

8.2

Operators and intrinsic functions for character data

There are a number of operators and intrinsic functions that may be applied to character data. We have already encountered the concatenation operator, //. Other operators that can be used are the relational operators ==, /=, >, >=, <, and <=, giving logical results. For example,

(string1=="Sir").AND.(string2>string3)

is a logical expression with the value .TRUE, if string1 is "Sir" and if also string2 is "greater than" strings. When strings are compared in this way, if their lengths are different, then the shorter of the two is first padded out to the right with blanks. Then, strings are compared one character at a time, working from the left, until differing characters are encountered. The "greater" is then defined by the character which occurs later in the processor's character collating sequence (see the functions CHAR and ICHAR below).

Rather than use >, >=, <, and <= to compare character strings, it is usually better to use the special character functions LGT, LGE, LLT and LLE, explained below, which give an ordering according to the ASCII sequence and are therefore processor-independent.

The intrinsic functions for characters or character strings are listed in Table 8.1, showing the keywords that may be used with the arguments and with an indication of the types of the arguments and results (c=character, I=integer, L=logical).

The first of these, LEN, simply returns the length of the character string given as the argument. So, LEN ("New Zealand") is an integer with value 11. A line of code that calculates the number of times a given character (char)

Name	Argument type	Result type
LEN(STRING)	С	I
LEN_TRIM (STRING)	С	Ι
TRIM (STRING)	С	С
IACHAR(C)	С	Ι
ICHAR(C)	С	Ι
ACHAR (I)	I	С
CHAR(I)	I	С
LGE (STRING_A, STRING_B)	CS	L
LGT (STRING_A, STRING_B)	CS	L
LLE (STRING_A, STRING_B)	CS	L
LLT (STRING_A, STRING_B)	CS	L
ADJUSTL (STRING)	С	С
ADJUSTR (STRING)	С	С
INDEX (STRING, SUBSTRING, BACK)	CS (BACK=L)	Ι
SCAN (STRING, SET, BACK)	CS (BACK=L)	Ι
VERIFY (STRING, SET, BACK)	CS (BACK=L)	Ι
REPEAT (STRING, NCOPIES)	STRING=C, NCOPIES=I	С

Table 8.1 Intrinsic functions for character or character strings.

appears in a given string (string), using LEN and the logical array function COUNT, is

COUNT((/ (char==string(i,i), i=1, LEN(string)) /))

LEN_TRIM is similar but does not count trailing blanks, i.e. LEN_TRIM ("Four") is 4. The function TRIM returns a character string with the trailing blanks removed. Obviously, LEN(TRIM(c)) is equal to LEN_TRIM(c) for any character string c. TRIM could be used in a statement such as

WRITE(*,*) TRIM(output)," is the answer."

to display some text without having to worry about the number of significant characters in it.

The functions IACHAR and ICHAR convert a character into an integer code, and their arguments must therefore be individual characters, i.e. strings of length one. In the case of IACHAR the resulting integer is the standard ASCII seven-bit code (0–127) corresponding to the character: thus, IACHAR("0") has value 48. The ASCII codes are given in Table 3.1. For a character outside the ASCII set the result may be processor-dependent. With the function ICHAR the code may be a different non-ASCII one, according to the particular processor. Note that the character set could in principle be much larger than the ASCII set; IACHAR and ICHAR could yield values above 127, and even above 255 if the processor allowed characters to be defined by more than one byte.

ACHAR and CHAR are the inverse functions to IACHAR and ICHAR: they yield a character corresponding to the integer code given as the argument. With ACHAR, the codes are the ASCII codes in the range 0–127, and for larger arguments the result will be processor-dependent. For example, ACHAR (97) is "a", ACHAR (36) is the currency symbol, and ACHAR(13) is a carriage return. With CHAR, the codes may depend on the processor in a sequence consistent with the ICHAR function. For most purposes the IACHAR and ACHAR functions should be sufficient, and ICHAR and CHAR can be avoided.

To illustrate the use of IACHAR and ACHAR, a lower-case letter can be converted to upper case by:

n=IACHAR(letter)

IF (n>=97.AND.n<=122) letter=ACHAR(n-32)

Note that ACHAR can be used to specify characters beyond the Fortran standard character set and perhaps not appearing on your keyboard:

CHARACTER, PARAMETER :: bell=ACHAR(7), cent=ACHAR(91)

The functions LGE, LGT, LLE and LLT are for comparing character strings according to the ASCII codes of the individual characters taken left-to-right. Since the alphabet is a subset of the ASCII set, these functions may be used to test the alphabetical ordering of strings, but it must be borne in mind that uppercase and lower-case letters have different ASCII codes. LGE means "lexically greater than or equal to", LGT is "lexically greater than", and so on. For example, LGE (STRING_A= "A", STRING_B= "z") is . FALSE . because STRING_A does not follow STRING_B in the ASCII collating sequence, because A does not follow Z in the alphabet. However, lower-case letters follow upper-case ones, SO LGE (STRING A="a", STRING B="Z") is .TRUE..

Also, LGE(STRING_A="Six",STRING_B="Sixty") is .FALSE., because, in comparing strings of different lengths, the shorter string is extended with blanks to the right to match the length of the longer string, and the blank character (ASCII code 32) comes before any of the alphabet.

ADJUSTL and **ADJUSTR** are string-to-string functions that replace leading blanks by trailing blanks (**ADJUSTL**) or trailing blanks by leading blanks (**ADJUSTR**). Thus the value of **ADJUSTL** ("**Preface**") is "**Preface**", but on the other hand **ADJUSTR**("**Chapter One**") is "**Chapter One**". It is useful that the function-of-a-function **TRIM**(**ADJUSTL** (...)) will remove both leading and trailing blanks from a string.

INDEX is a function that carries out the useful job of looking for substrings within strings. If c2 is a substring of c1, then **INDEX(STRING=C1, SUBSTRING=c2)** yields the first starting point (counting characters from the left) of an occurrence of c2 within c1. So the expression

INDEX(STRING="Birmingham", SUBSTRING="ming")

is equal to 4, and

INDEX(STRING="Birmingham", SUBSTRING="i")

is equal to 2. INDEX is zero if SUBSTRING is not a substring of STRING. If SUBSTRING has zero length, INDEX is normally returned with the value 1. The optional argument BACK is a logical variable taken to be . FALSE . if it is not otherwise specified, but if BACK=.TRUE., the function looks for the last (instead of first) occurrence of SUBSTRING within STRING; in other words

INDEX(STRING="Birmingham", SUBSTRING="i", BACK=.TRUE.)

is equal to 5. If BACK=.TRUE. and SUBSTRING has zero length, INDEX is given a value of one more than the length of STRING.

SCAN (STRING, SET, BACK) does a job similar to INDEX, but it looks for any of a number of individual characters within STRING. The argument SET is a string defining a set of individual characters, and INDEX points to the first occurrence of any one of them within STRING. For example,

SCAN(STRING="Strength", SET="aeiou")

has the value 4. As in the case of the INDEX function, the optional BACK argument will make SCAN look for the position of the last occurrence, i.e. SCAN(STRING="Counihan", SET="aeiou", BACK=.TRUE.) has the value?

VERIFY (STRING, SET, BACK) is, in a sense, the opposite of SCAN. It checks to see if all the characters in STRING occur within SET, and if not it yields the position (within STRING) of the first character not found in SET. If BACK is present with value .TRUE., VERIFY gives the position of the last character in STRING that is not in SET. If every character in STRING occurs in SET, VERIFY has the value zero whether BACK is .TRUE. or .FALSE. For example, the logical expression

VERIFY(STRING=intprint, SET="0123456789")==0

has the value .TRUE. if intprint is the name of a string containing only decimal digits.

Finally, REPEAT is a function that concatenates a number of copies of the same string, i.e. REPEAT (STRING=" ",NCOPIES=80) is a character string consisting of 80 blanks.

8.3 Exercises 8.A

8.A What are the values of:

1

(i) LEN("Test_string")	(ii) TRIM('' '')
(iii) ACHAR(111)	(iv) CHAR (" ")
(v) LGE(''Q'', ''S'')	(vi) LLE (" T ", "α")
(vii) LLE("6","1")	(viii) LLE("5","e")

- 8.A Write code to remove the first character of a string called x if (and only if) that character is a numeric 2 digit.
- 8.A Write code to trim off all leading blanks of a string called x, replace them by trailing blanks and write 3 the result.

8.4 The general form of the type declaration statement

A simple form of the type declaration statement (TDS) was introduced as early as Section 2.2, and since then several elaborations of it have been mentioned when necessary. At this point it is appropriate to give complete details of the syntax of the TDS, although there are still one or two features that will not be fully explained until later chapters. In its various forms the TDS is probably the second most common statement type in Fortran (after the assignment statement) and it is essential to understand it well.

The purpose of a TDS is to declare the characteristics of named data items. The statement may at the same time serve the additional purpose of giving initial values to them.

In general a TDS consists of three parts in this order: first a single "type specification", second an optional list of "attribute specifications", and third an "entity declaration list". The type specification and the attribute specifications which may follow it are separated by commas. The attribute specifications are separated by a double colon from the entity declaration list.

Omitting the colon in a TDS

In the simplest cases where there are no attribute specifications and initial values are not given to any data, it is permissible for the entity declaration list to follow the type specification without the intervening double colon. However, it is recommended that the double colon should always be used.

A simple example of a TDS is

LOGICAL, SAVE :: a, cq, cr

where LOGICAL is the type specification, SAVE is an attribute specification, and the entity declaration list contains the three names a, cq, cr. A more complicated example is

CHARACTERS), PARAMETER :: unit(3) = (/"mm", "cm", "dm"/)

and here the type specification is CHARACTER (2), there is one attribute specification, PARAMETER, and the entity being declared is the array called unit (3). Initial values are being given to the elements of unit (3).

The primary purpose of a TDS is to declare the existence of data objects of a certain type. A single TDS must refer to a single type. The type is given by the type specification and it must be one of the following:

INTEGER (*KIND*=...) REAL (*KIND*=...) COMPLEX (*KIND*=...) LOGICAL (*KIND*=...) TYPE (type-name) CHARACTER (*length-selector, KIND*=...)

DOUBLE PRECISION

The bracketed KIND parameters that may occur here are optional and can usually be forgotten about. After the type specification there can be the following range of possible attribute specifications, which will be discussed in turn further below.

PARAMETER SAVE PUBLIC PRIVATE EXTERNAL INTRINSIC OPTIONAL INTENT (*specification*) POINTER TARGET ALLOCATABLE

DIMENSION (specification)

Finally, there are the entities actually being declared. The entity declaration list at its simplest is a series of the names of entities that are of the type given in the type specification and which have special qualities indicated by the attribute specifications. These entities are usually variables, but could be named constants or even the names of functions. Their names must follow the usual Fortran naming rules. A name in the

entity declaration list of a TDS may have additional information appended to it if it is an array or if it is of character type, and it may be given an initial value.

The possible type specifications are explained in more detail below.

INTEGER (KIND=...)

This indicates that the data declared here is of integer type. There may be a KIND parameter if the processor may support integers of unusual precision, but Fortran does not require this to be possible, so this specification will almost always consist simply of the keyword INTEGER. An example is:

INTEGER :: i, j, k, input_unit, gamma

It is recommended that the names of integer data should have initial letters in the range i-n.

Although it is usually recommended that every variable should be declared in a type declaration statement, exceptions can be made for the trivial integers used as indices in DO loops or in the "implied DO" syntax of (say) an array constructor.

REAL (KIND=...)

This indicates data of real type. The bracketed KIND parameter will rarely be needed, but it allows for real numbers of unusual precision. Examples:

REAL :: estimate_1, estimate_2, result, error

REAL (KIND=KIND(0.0D0)) :: hairsbreadth_x, hairsbreadth_y

It is recommended that the names of real data should start with letters outside the range i-n.

For simple scalar data objects of real and integer type, whose names fit the initial-letter convention and which have no special attributes, there is no need to use a TDS at all although it is recommended that one does so.

COMPLEX (KIND=...)

The data following this would be complex numbers. The KIND parameter, if present, means that each complex number is equivalent to a pair of real numbers of the specified kind of precision. Example:

COMPLEX :: omega1, omega2, z

COMPLEX, PARAMETER :: i = (0.0, 1.0)

LOGICAL (KIND=...)

This specification indicates data of logical type. The KIND parameter, as in the case of integers, allows for processors to have more than one way of representing such data, but this would be meaningless on most processors and we can disregard it. Example:

LOGICAL :: decision

TYPE (type-name)

This type specification makes it possible to declare data objects of special userdefined types, or "derived" types. Derived types are described in Chapter 14.

CHARACTER (length-selector, KIND=...)

This indicates data of character type. Whenever character data is declared, the length of each item must be indicated and this can be done by means of a length selector following the keyword CHARACTER. The selector specifies a length that will apply to all the items listed later in the statement.

The length-selector here is not mandatory, because the same job can be done by means of a selector appended to each item's name in the entity declaration list. There is a superficial advantage in specifying character string lengths in the entity declaration list, because then strings of different lengths may be declared in the one statement. However, on balance, it is recommended that the lengths should be specified after CHARACTER even if this demands more statements, since the syntax can otherwise become more confusing.

A KIND parameter may be specified with the CHARACTER keyword if the processor supports non-default character sets.

As a result of Fortran's history, the CHARACTER keyword, with the length selector following it, may take any one of the forms below:

CHARACTER CHARACTER (*expression*) CHARACTER (LEN=*expression*) CHARACTER *(*expression*) CHARACTER *c*onstant* CHARACTER (*) CHARACTER (LEN=*) CHARACTER *(*)

The first of these, with no length selector, could be used to declare character strings of length one, i.e. individual characters, and is therefore equivalent to **CHARACTER(1)**.

The three forms in the following group are equivalent and one may as well stick to the first form, i.e.

CHARACTER (expression)

Here, *expression*, the length of the character string, must be an expression of non-negative scalar integer type. It may simply be a constant, or a constant expression, or it may be a more complicated expression involving variables. However, if it involves variables then they must be accessible and have values when this TDS appears. Accessibility could be through a data module, or (within a procedure) through a dummy argument, or by reference to an intrinsic function. We could have, for example,

CHARACTER (128)

```
CHARACTER (64*128)
```

CHARACTER (n)

CHARACTER (1 + LEN(TRIM(z)))

as long as the integer n, and the character string z, have been previously made accessible. In this way, lengths of strings can be set dynamically rather than fixed when the program is compiled. When a non-constant expression is used to declare the length of a string that is not a dummy argument, the string is known as an "automatic" data object.

Another form listed above was

CHARACTER * constant

and here *constant* would simply be a non-negative integer value. In other words, lengths can be specified by things like

CHARACTER *128

but this notation offers no advantage over

CHARACTER (128)

and is best avoided. The list of forms given above ended with three more which are equivalent to one another, i.e.

CHARACTER (*)

CHARACTER (LEN=*)

CHARACTER *(*)

all of which use an asterisk to mean that the length of the character string is to be assumed from elsewhere. Sticking to the first and simplest of these forms,

CHARACTER (*)

should be used:

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- (a) when the length can be taken from an explicit initial value given to the string later in the statement;
- (b) in a procedure, to declare a dummy character-string argument whose length will be taken from the program unit where the call is made; or
- (c) in a function whose value is a character string, when declaring the name of the function; the asterisk can be used if its length is to be assumed from a declaration made in the program unit from which the function is called.

In cases (b) and (c), the length will therefore be determined, not on compilation, but on execution and could be different each time the procedure is actually called.

Here are a few more examples of character TDSs:

CHARACTER(1) :: initial1, initial2, initial3

CHARACTER(20) :: name_of_state, name_of_city

CHARACTER(12*nwords + 24) :: page

CHARACTERS) :: input_data

CHARACTER(1) :: letter

CHARACTER(20) :: forename, midname, surname

CHARACTER(12) :: q = "CONFIDENTIAL"

CHARACTER, PARAMETER :: Star = "*"

CHARACTER(*), PARAMETER :: origin = "Made in Thailand"

CHARACTER(nchars+6) :: line1, line2, line3, line4

CHARACTERS) :: surname = "Spock"

CHARACTERS) :: title = "Mr. "//surname

CHARACTER(1) :: bell = ACHAR(7)

In summary: the CHARACTER TDS should begin with

CHARACTER(*expression*)

where the expression is equal to the lengths of the strings declared in the statement. If the expression is not merely a constant but is a "specification expression" evaluated at execution, we have an "automatic" length. Alternatively, the statement may begin with

CHARACTER(*)

when the length is going to be ascertained from an explicit initial value given later in the statement, or by argument-passing (or function-name-passing) to a procedure. To minimize the likelihood of confusion, it is recommended that other forms of syntax be avoided.

IMPLICIT

Unless declared by a TDS to be of a different type, variables are assumed to be of integer type if their names begin with letters of the alphabet in the range i–n. Otherwise, they are assumed to be real. This initial-letter convention may be changed within a program unit by a special non-executable statement, IMPLICIT. Some examples will make its use clear:

IMPLICIT REAL (a-z)

means that all variables are interpreted by default as real numbers.

IMPLICIT INTEGER (a, e, i, o, u), REAL (b-d, f-h, j-n, p-t, v-z)

means that names starting with a vowel are to be taken as integers, and others as real numbers.

IMPLICIT CHARACTER (a-z)

means that all names (unless individually specified otherwise) are taken to be the names of character strings.

IMPLICIT TYPE(Encrypt) (a-z)

means that all names will refer by default to the data type Encrypt. Since Encrypt is not an intrinsic type this must be a derived type (see Chapter 12). Finally,

IMPLICIT NONE

means that there is no initial-letter data type convention imposed in this part of the program, and therefore that the programmer will specify explicitly the types of all variables.

The usage of the IMPLICIT statement is controversial among Fortran programmers. The view taken in this book is that (i) it is helpful to adhere to the standard initial-letter convention to distinguish between real and integer data, but at the same time (ii) it is recommended that the types of all variables should be declared explicitly anyway, except for integer DO loop indices, and (iii) the IMPLICIT statement, being unnecessary, should not be used.

8.5 Attributes

The set of possible attribute specifications in a TDS was listed in the previous section. Each attribute may be specified no more than once in one TDS. Many of the attributes are mutually exclusive and many can apply only to certain sorts of data (e.g. to procedure arguments), so in practice it is unusual for a TDS to

include more than one or two attribute specifications. When there is more than one attribute specification, they may be given in any order. The meaning of each attribute is explained below.

PARAMETER

A data object with the PARAMETER attribute has a fixed value, i.e. it is a "named constant" that will not be changed during the running of the program. The value must be appended to the name in the statement's entity declaration list (see Section 8.7). Examples:

REAL(KIND=2), PARAMETER :: e = 2.718281828459045235

CHARACTER(*), PARAMETER :: country = "Lithuania"

SAVE

This is an attribute that may apply to data items (other than arguments) occurring in subprograms. It means that the items will retain their values after the subprogram has executed. In other words, SAVE is a way of retaining the value of data between subsequent calls to a function or subroutine. The SAVE attribute has no effect if it is specified in a main program. Example:

INTEGER, SAVE :: number_of_times_called

PUBLIC and PRIVATE

These two "accessibility attributes" are only applicable to data items declared in a module (Chapter 10). PRIVATE means that the items are not accessible (via a USE statement) to any other program unit outside the module. It could be advisable for data to be declared PRIVATE if it is used only within module procedures and if there could be an unintended clash of names with other data in program units using the module. PUBLIC means the opposite, i.e. that the data is accessible by another program unit using the module. Example:

REAL, PRIVATE :: input_buffer(1025)

EXTERNAL This is applicable not to ordinary data items but only to the names of functions. It indicates an external function. It is important to declare the EXTERNAL attribute with a function name if that name is to be passed as an argument to another procedure (Chapter 14). Within such a procedure, EXTERNAL can indicate the dummy argument that corresponds to that function name.

INTRINSIC

The INTRINSIC attribute means that a function name is that of a Fortran intrinsic function. This attribute needs to be specified only in rather unusual circumstances.

OPTIONAL

This attribute can be used when the dummy arguments of procedures are declared. It indicates arguments that need not necessarily be included in the actual argument list when the procedure is called. A procedure with optional arguments must have an interface (see Section 8.9). Examples:

COMPLEX, OPTIONAL :: croot1, croot2

REAL, OPTIONAL, EXTERNAL :: Smoothing_function

INTENT (specification)

Like OPTIONAL, this is an attribute that may apply to procedures' dummy arguments. INTENT permits the programmer to ensure that an argument is used

- (a) only for data coming in to the procedure;
- (b) only for data going out; or
- (c) for data flowing both ways.

This is done by a specification, in brackets, which may be IN, our or IN our respectively. An argument with INTENT (IN) cannot be changed by the procedure, and one with INTENT (OUT) is initially undefined and must be defined by the procedure. The attribute INTENT(IN OUT) embraces both possibilities and need not be used except as a form of program annotation. Example:

REAL, INTENT(IN) :: vector(3), rotation_matrix(3,3)

REAL, INTENT(OUT) :: new_vector(3)

It is not normally necessary to specify an argument's INTENT at all. However, INTENT (IN OUT) is not always equivalent to not specifying INTENT. If an actual argument is going to be a constant, then it can only have INTENT (IN) and INTENT (IN OUT) will not do. INTENT (IN OUT) means that it must be possible for information to pass in or out of the procedure through the argument in question.

Fortran 95 feature not present in Fortran 90

The INTENT specification is mandatory for the arguments of PURE and ELEMENTAL procedures (see Chapter 11).

POINTER and TARGET

These two attributes can apply when pointers are being used; they will be discussed in Chapter 13. If a procedure argument has either of these attributes, or if a function's value has the POINTER attribute, the procedure must have an interface (see Section 8.9).

ALLOCATABLE

The ALLOCATABLE attribute is applicable only to arrays. It will be dealt with in Chapter 12.

DIMENSION (specification)

The DIMENSION attribute is used only with arrays. DIMENSION indicates that array variables are being declared and it is followed by a bracketed specification of the shape of the arrays.

Alternatively, shapes may be given for individual arrays as part of the entity declaration list, in which case they override a shape specified with DIMENSION. The situation is rather like that for character strings,

where string lengths may be given globally, for the whole set of entities declared in a statement, or individually.

Because arrays may be declared simply by specifying a shape for each array in the entity declaration list, the DIMENSION attribute is not actually necessary at all. So, the TDS

COMPLEX, DIMENSION (4,4) :: gamma1, gamma2, gamma3, &

gamma4, gamma5

is equivalent to

COMPLEX :: gamma1 (4, 4), gamma2 (4, 4), gamma 3 (4,4), &

gamma4 (4,4), gamma5 (4, 4)

Array specifications following DIMENSION, and array specifications following an item in the list, can be constructed in exactly the same ways. These ways are covered in more detail in the next section.

Statements equivalent to data attribute specifications

All the data attributes (PARAMETER, SAVE, etc.) that may occur in a TDS may, equivalently, be given by separate statements, "attribute specification statements" (ASSs). An ASS does not specify the data objects' types, which must still be given in a TDS or assumed from the initial letter of the names. An ASS may not duplicate or contradict an attribute already given in a TDS. Some examples of ASSs are:

SUBROUTINE Integrate (Rfunction, g, h, i, j, name)

REAL :: Rfunction

EXTERNAL Rfunction !Double colon forbidden!

INTEGER :: g, h

INTENT (IN) :: g, h, i, j !Double colon optional!

CHARACTER (*) :: name

OPTIONAL :: name !Double colon optional!

SAVE :: ncalls !Double colon optional!

DIMENSION iflags(6) !Double colon forbidden!

PARAMETER (del=0.0002) !Double colon forbidden!

In addition, in a module (Chapter 10) there may be a PRIVATE statement such as

PRIVATE :: workspace !Double colon optional!

This may happen without any list of variables, i.e. we can have just the PRIVATE keyword by itself:

PRIVATE

which means that all data declared in the module are PRIVATE. Subsequent to this, a PUBLIC statement

PUBLIC :: x, y, z !Double colon optional!

will make the named objects accessible outside the module again.

ASSs had their origin at a time when many programmers avoided TDSs and relied on the initialletter convention alone to specify real and integer data. However, it is now recommended that TDSs should be written for virtually all data objects, and all data attributes should be specified in a TDS, avoiding the need for ASSs.

8.6 Array specifications

The simplest kind of array specification is the sort shown in the above example, where the shape of the array is given by a list of its extents in each dimension. A shape (4, 4) means that there are two dimensions, i.e. a rank of two, and a total of 16 elements making up the whole array. This is a simple example of an "explicit shape" specification list. In fact, Fortran distinguishes between four different sorts of array specification, namely "explicit shape", "assumed shape", "deferred shape" and "assumed size" arrays.

Explicit shape

Explicit shape specification lists such as (4, 4) or (3, 3, 3) or (100) or (4, 20, 2) declare arrays whose elements would be referenced by indices running from 1 to 4 (twice), 1 to 3 (three times), 1 to 100, and in the final case 1 to 4, 1 to 20, and 1 to 2. Alternatively, starting points different from 1 can be set using the colon notation, the shape (4, 4) being equivalent to (1:4, 1:4). If we have

REAL :: alpha(-3:3,0:9)

then the array's rank is two and there are 70 elements, and individual elements can be referenced by expressions such as array (n, m) with n taking any integer value from -3 to 3 and m from 0 to 9 inclusive. It is possible to have mixed declarations in that some, but not all, dimensions are given with the colon notation:

REAL :: alpha(-3:3,0:9), beta(20,0:1), gamma(20,20)

Moreover, the bounds need not be given as specific integers. A declaration like

REAL :: xyz(3, npoints), r(npoints, npoints), checksum(0:k)

is possible if npoints and k are the names of integer constants. In fact, when the declaration is made in a procedure and the object is not a dummy argument, the bounds need not even be constants: they can be integer variables or expressions as long as they will have ascertainable values when the TDS is encountered. The array is then known as an "automatic array", since its shape is not fixed until the procedure is called (and may differ from one call to another). Here is an example:

```
SUBROUTINE Falsetto (n, w)
USE Printer_data
INTEGER, INTENT(IN) :: n
CHARACTER(*), INTENT(IN):: w
REAL :: r(0:n-1,0:n-1)
CHARACTER(1) :: ch(2*LEN(w))
CHARACTER(1) :: page(linelength, pagelength)
.
```

This subroutine uses the argument n to fix the bounds of both dimensions of a rank-two array r, and it uses the length of the character string argument win order to determine the size of an array ch containing single characters. The dimensions linelength and pagelength are presumably specified within the module Printer_data.

The bounds of explicit-shape arrays may be given by fairly complicated "specification expressions", but there are certain restrictions. In particular, a specification expression may not normally involve a reference to any non-intrinsic function. In the example above, LEN is of course an intrinsic Fortran function. Obviously, in order to have a definite value a specification expression must include only variables that are accessible as dummy arguments or (using modules, Chapter 10) as module data or by host association. The situation is the same as for the specification expressions that can be used to set the lengths of automatic character strings (see Section 8.4, under CHARACTER).

Fortran 95 feature not in Fortran 90

Specification expressions may involve PURE external procedures.

Assumed shape

A dummy argument in a procedure may have an assumed shape, which means that its rank is known but its shape is taken from that of the corresponding actual argument whenever the procedure is called. An assumed shape is specified by giving a series of colons, one colon for each dimension. In the following example there are two dimensions, i.e. the array being declared has rank two, but the extents in each dimension will be determined only as and when the function is called. The extents need not be the same, i.e. this need not be a square matrix:

FUNCTION N_positive_elements (matrix)

INTEGER :: N positive elements

```
REAL, INTENT(IN) :: matrix(:,:)
```

- •
- .

With an assumed-shape array it is possible to specify that a lower bound other than 1 will be used in the procedure, by giving the lower bound before the colon. So,

REAL :: matrix(0:,0:)

means that the lower bounds are both 0, but this does not affect the total numbers of elements.

An assumed-shape array can only be a dummy argument within a procedure. Also, it can only be used if the procedure has an INTERFACE in the program unit from which it is called: the meaning of this will become clear in Section 8.9.

Deferred shape

The third kind of array specification is a "deferred shape" specification, but this involves allocatable arrays or array pointers (Chapters 12 and 13) and it would be premature to give details here. Deferred-shape arrays are specified with the same colon notation as assumed-shape arrays, but without the possibility of specifying lower index bounds.

Assumed size

The fourth and final class of array specification is the "assumed size" specification. Like an assumed shape, an assumed size is a possible feature of a dummyargument array in a procedure. Assumed-size arrays are usually regarded as an over-complex and unnecessary feature of Fortran and their use is not recommended. The notation for declaring an assumed size includes an asterisk. To take the simplest example,

REAL FUNCTION Chi (a, b, z)

REAL :: a, b, z(*) . .

means that the arguments a and b are scalars but z is an array. Within the function, z has rank one, but the corresponding actual argument could be an array of any rank. The rank of the actual argument is not passed on and does not become the rank of the dummy argument z. The array z always has rank one. However, z is given the same total number of elements as the actual argument had, i.e. z assumes the size of the actual argument.

In the above example the lower bound of z's dimension would be 1, but as we have previously seen it is possible to give a different lower bound before a colon: with

REAL :: a, b, z(1025:*)

the array z has elements z(1025), z(1026), z(1027), and so on up to an index which will exceed by 1025 the size of the actual argument corresponding to z.

There are one or two further possibilities with assumed-size arrays. For one thing, the actual argument need not be the name of an array, but could just be an array element, in which case what is passed is the series of elements starting at the one given and going on to the end of the array (in normal array element order, see Chapter 15). In other words, with

```
klap = (/2, 5, 7, 1, 1, 0, 7, 9, 5, 4, 0, 0/)
n = 6
CALL Turn (klap(n))
SUROUTINE Turn (k)
INTEGER : : k ( *)
.
```

.

the dummy argument array k in the subroutine will have size seven and the value (/0, 7, 9, 5, 4, 0, 0/).

Things can get a little more complicated with assumed-size character arrays, since the elements of the actual and dummy arguments may be character strings of different lengths! Then, the size assumed for the dummy argument will be whatever is needed to accommodate all the characters in the actual argument array. Suppose we have the following code:

```
toffee = (/"and", "pat", "cob", "try", "owl"/)
```

```
CALL Twist (toffee)
```

•

SUBROUTINE Twist (tripe)

CHARACTER (5) :: tripe(*)

then tripe will be (/"andpa", "tcobt", "ryowl"/), i.e. with size three. As with non-character data, the first part of an array can be left out by giving, as actual argument, one element (or a substring of an element) to be taken as the starting point of what is passed to the procedure:

```
toffee = (/"and", "pat", "cob", "try", "owl"/)
CALL Twist (toffee(3)(2:3))
.
.
.
SUBROUTINE Twist (tripe)
CHARACTER (2):: tripe(*)
```

Here, the actual argument is a substring ("ob") consisting of the second and third characters from the third element of toffee. The subroutine will receive the contents of toffee starting from that substring, giving tripe the value

```
(/"ob", "tr", "yo, "wl"/). The call
```

CALL Twist (toffee(3)(2:2))

would have had exactly the same effect.

So far, in our examples of assumed-size specifications, we have had dummy argument arrays of rank one. Arrays of greater rank are possible, but then all dimensions except the last must be specified as in an explicit shape specification. Only the last dimension is left indeterminate with an asterisk. In the example immediately above, if we had

```
CHARACTER (2) :: tripe(2,*)
```

then tripe would have been a rank-two array taking the shape (2, 2).

8.7 The entity declaration list

Having dealt with type specifications and attribute specifications, it only remains to describe the entity declaration list that comes at the end of a TDS. The task is made easy because the most complicated aspects of entity declaration are those to do with character string lengths and array shapes and these have already been covered exhaustively above.

For scalar data of non-character type, the entity declaration list will simply consist of a series of names separated by commas, each possibly being given an initial value by an "initialization expression" following an = after the name. The following are examples of valid lists:

```
a, b, c, d=0.0, e=5.5, f
```

karavan = 4520988765, k2 = 2**64, kstore1, kstore2, &

kstore3

check1=.TRUE., check2=.TRUE., checks=.TRUE., checksum

q = (0.39967, -1.03847)

There are a number of restrictions on the use of an initialization expression in a TDS. Initialization expressions are compulsory whenever the PARAMETER attribute is present. An initialization expression is forbidden when declaring a dummy argument, function result or automatic object, and it is also incompatible with the ALLOCATABLE and POINTER attributes. Any data object that is declared with an initialization expression will be saved, in the sense that it is given the SAVE attribute even if SAVE was not explicitly included in the attribute list. Note that data initialization takes place once and for all before program execution: data in a procedure may be initialized but are not re-initialized each time the procedure is called.

Initialization expressions are subject to a number of technical restrictions. They may not involve variables and the only functions allowed are intrinsic integer or character functions, inquiry functions (except ALLOCATED), and the transformational functions REPEAT, TRIM, TRANSFER, and RESHAPE. Defined operators (Section 8.9) are not allowed and the exponentiation operator (**) is only allowed with an integer power.

When declaring arrays, array constructors may be used as initialization expressions (if necessary with implied-DO variables) as in

kpow(32) = (/ (2**m, m=1, 32) /)

When declaring character data, initialization expressions may involve substrings and character functions, e.g.

alphabet= (/ ("abcdefghijklmnopqrstuvwxyz" (j:j), j=1, 26) /)

blank_page = REPEAT(" ", 1750)

It has already been mentioned that the length of character data may be specified alongside the name in the entity declaration list. The notation is similar to that which can be used to do the same job after the CHARACTER keyword but is a little more limited. The permissible forms are

charname* (expression)

charname*constant

charname*(*)

where *charname* is the object's name, *expression* is an integer expression as in Section 11.9, *constant* is a specific integer, and the * (*) notation is similar in effect to *CHARACTER*(*). With any of these forms, an array specification could also be inserted between *charname* and the character length specification. In an extreme case, we could therefore have a specification such as

CHARACTER :: chimera(*)*(*)

which is an assumed-size assumed-length character array equivalent to

CHARACTER, DIMENSIONS) :: chimera* (*)

but the simplest notation is of course

CHARACTERS) :: chimera(*)

This variety of different notations arises from the history of Fortran and is not an attractive feature of the language. To keep things simple and clear, it is strongly recommended that you always give character length specifications with the CHARACTER keyword and always give array shapes with the arrays' names, avoiding the use of the DIMENSION keyword. In other words, specify string lengths always on the left of the double colon and array sizes always on the right. So,

CHARACTER(20) :: chimera(30)

is an array of 30 strings each of 20 characters.

Fortran 95 features not in Fortran 90

Pointers (Chapter 13) may be initially disassociated by pointer assignment to NULL (). Initialization of derived-type data is allowed, as in

TYPE (Link), PARAMETER :: empty = Node(0, NULL())

This example involves a derived type (Chapter 12) with a pointer component (Chapter 13).

The DATA statement

As an alternative to initializing data in a TDS, or in an initial assignment statement, there is a special statement type, DATA, which exists in order to give initial values to variables. It works only for ordinary variables, i.e. not for dummy arguments, automatic objects, and the like. As an example, to illustrate the details of the syntax, suppose that variables have been declared by the TDS

INTEGER :: i1, i2, kappa(4), mult(20), ncells(-10; 10, -10:10)

Then initial values could be declared by

DATA 11, 12, 13 /0, 0, 20/, kappa /14, 71, 0, 33/, &

mult /20*1/, ((ncells(, j), i=-10:10), j=-10,10) /441*0/

which is hardly less complicated than it looks. The DATA statement consists of a list of sets, the sets in the above example being

Each set consists of a list of names followed by a list (between slashes) of initial values. The first set puts 11, 12 and 13 equal to 0, 0 and 20 respectively. The second set gives values to the four elements of the array kappa. The third set illustrates a "repeat" notation in the list of values, where an integer before an asterisk is equivalent to that number of occurrences of the value; the 20 elements of the array mult are all set to 1. The final set in our example shows how an implied DO notation can be used to run through elements of an array.

The DATA statement does almost nothing that cannot be done in other ways (especially with array constructors) and it should be avoided. The only thing that a DATA statement can do that is not otherwise possible in Fortran is to allow integer variables to be assigned the values of integer constants specified in binary, octal or hexadecimal form. Such integers are written with their digits within a pair of quotes, and preceded by the letter B, 0 or z (for binary, octal or hexadecimal). Thus, B"10001" and O"21" and z"11" could represent the decimal number 17 in DATA statements.

8.8 Summary

Leaving aside some relatively unimportant options, the type declaration statement should begin with one of

INTEGER REAL or REAL (KIND=KIND (0 . 0D0) COMPLEX or COMPLEX(KIND=KIND(0.0D0) LOGICAL CHARACTER(...) TYPE(...) In the case of CHARACTER, the brackets contain the length of the strings, determined either by a constant or by a non-constant expression ("automatic" data) or by an asterisk ("assumed length"). TYPE is dealt with in Chapter 12. The type specification may be followed by optional attribute specifications:

PARAMETER or SAVE for ordinary variables

EXTERNAL or INTRINSIC for function names

INTENT and/or **OPTIONAL** for dummy arguments

ALLOCATABLE, POINTER, and TARGET: see Chapters 12 and 13

Then there is an entity declaration list consisting of variables' names separated by commas. There may be an array specification after each name. An array specification should be of one of these kinds:

- explicit shape (including "automatic" arrays)
- assumed shape (for dummy arguments, using colons)
- deferred shape (see Chapters 12 and 13)

Finally, the name of a variable may be followed by an = sign and an initialization expression, giving a starting value to the object named. If the PARAMETER attribute is specified, an initialization expression is compulsory and the object is technically a "named constant" rather than a variable.

8.9

Defined operators; introducing interfaces

Just as external functions can be written as a supplement to Fortran's own set of intrinsic functions, likewise it is possible to have user-defined operators to supplement the intrinsic operators (+, -, *, **, //, >, etc.). This section explains how new operators can be created.

Most of Fortran's intrinsic operators are "binary" operators, i.e. they operate between two quantities to produce one result. Sometimes the operation is symmetrical, as for multiplication (*) or addition (+), and sometimes it is not, e.g $p^{**}q$ is not the same as $q^{**}p$. There are two or three "unary" intrinsic operators, operating on a single quantity (+ and – may be used as unary operators, and the logical operator .NOT. is always unary).

A new "defined" operator is linked to an external function of one or two arguments, so that any reference to the operator is a reference to the function. This is achieved with the help of an "interface block".

For present purposes, an interface block is a block of declarative statements that refer to an external procedure and that must be inserted in a subprogram if the procedure in question is to be called from that subprogram. The purpose of an interface block is to tell the calling subprogram something about the called procedure. An interface block contains, within it, the declarative statements that also appear within the external procedure itself. For a defined operator associated with an external function, the interface block has the form

INTERFACE OPERATOR (.op.)

FUNCTION Name (argument1, argument2)

declaration-statements

END FUNCTION Name

END INTERFACE

Here, *op* is the operator being defined, and it must consist of a series of up to 31 letters, surrounded by a pair of dots. The function details must correspond to an external function, and a reference to the operator in an expression of the form

argument1.op.argument2 obtains the value of Name(argument1, argument2).

If the operator is to be unary, only one argument would be specified in the function and the reference would take the form

.op.argument

An example is the interface block

INTERFACE OPERATOR (.Inv.)

FUNCTION Inverse_Vector (v)

REAL :: Inverse_Vector(3)

REAL, INTENT(IN) :: v(3)

END FUNCTION Inverse_Vector

END INTERFACE

which defines . Inv. as a unary operator that can be applied to any real array of rank one and size three. Note that this is a unary operator, with one argument, although the argument happens to be an array with more than one element.

With one argument there may be little to choose between a function-name reference and a definedoperator reference, but with two arguments the usefulness of a defined operator is more apparent. Consider this example:

FUNCTION Vector_Multiplication (v1, v2)

REAL :: Vector_Multiplication

REAL, INTENT (IN) :: v1(*), v2(*)

Vector_Multiplication = DOTPRODUCT(v1, v2)

END FUNCTION Vector_Multiplication

with interface

INTERFACE OPERATOR (.X.)

FUNCTION Vector_Multiplication (v1, v2)

REAL :: Vector_Multiplication

REAL, INTENT (IN) :: v1(*), v2(*)

END FUNCTION Vector_Multiplication

END INTERFACE

This means that expressions like r.x.t or x.X. (/1.89, -5.71, 20.04/) can be used freely to calculate the dot product of any pair of real vectors.

Besides defining operators of a new form (.Inv. and .x. in the examples above) it is possible to redefine Fortran's existing intrinsic operators. If in the example immediately above we had the INTERFACE statement

INTERFACE OPERATOR (*)

this would have the effect of turning the ordinary multiplication operator into a dot product operator in the case of real vectors. This technique is known as "overloading".

It must be emphasized that defined operators arise as a feature not of the procedure itself but of the interface. Since different program units may in principle have different interfaces to the same procedure, different operators could be used for the same task in different parts of a program, or conversely we could have the same operator being used for different tasks. And, with overloading, it is possible to completely confuse Fortran's intrinsic operators: for example the functions of * and / could be interchanged! Unless it is your objective to produce cryptic code, it is best to avoid overloading intrinsic operators and to put all the interfaces to defined operators into one module (Chapter 10) accessed by the whole of your program!

In the evaluation of Fortran expressions, defined unary operators take higher precedence than any other operators, just as if they were single-argument function-name references. By contrast, defined binary operators have a lower precedence than other operators. Naturally, parentheses can and should be used to avoid any ambiguity in the order of evaluation.

As a final example, the following procedure and interface make it possible to concatenate strings using a plus sign (+) as an alternative to the usual / / operator:

FUNCTION Concat (c1, c2)

CHARACTER (*), INTENT(IN) :: c1

CHARACTER (*), INTENT(IN) :: c2

CHARACTER (LEN(c1) + LEN(c2)) :: Concat

Concat = c1//c2

END FUNCTION Concat

INTERFACE OPERATOR (+)

FUNCTION Concat (c1, c2)

CHARACTER (*), INTENT(IN):: c1

CHARACTER (*), INTENT(IN):: c2

CHARACTER (LEN(c1) + LEN(c2)):: Concat

END FUNCTION Concat

END INTERFACE

but notice that this will not work with arrays of character strings.

Procedure interfaces are often required for purposes other than the defining of a new operator. An interface is always required if, as in the above example, we have a character function whose result is not of constant length and cannot be assumed from the program unit that calls the procedure. Although the lengths of the arguments c1 and c2 are assumed from the call, the length of Cone at itself is got from the specification expression LEN(c1)+LEN(c2) and this fact can only be revealed to the calling program by means of an interface. Such an interface starts with the simple interface statement

INTERFACE

if no operator is being defined.

Another circumstance that requires a procedure to have an interface in the calling subprogram is when the procedure has optional arguments.

8.10 Exercises 8.B

8.B

1

- (i) Write a TDS to declare an array (called zbanks) of 30 complex numbers,
- (ii) Write a TDS to declare three optional logical dummy arguments,
- (iii) Write a TDS, intended for use in a procedure, for a 20×20 matrix of real numbers and also a vector of 45 real numbers. All are to have their values saved between calls to the procedure,
- (iv) Write a TDS for an array of 100 named integer constants, called **squares**, with the index running from 0 to 99, fixing their values to be equal to the squares of the integers from 0 to 99.

- (v) Write a TDS for a dummy argument which is of length-12 character type. Its name is to be Julius and it is an assumed-shape array of rank two.
- (vi) Write a TDS for an array of 100 real variables called **inverse_squares.** They are to be given the initial values of the inverse squares of the integers ranging from 1 to 100.
- (vii Write a TDS for a scalar character constant whose value is your name. Call it moniker.

- 8.B Set up a defined binary operator // to concatenate two integers, e.g. to make 1995 out of 19 and 95, the 2 result being an integer.
- 8.B Set up defined binary operators analogous to <, == and > that will operate between character strings to
 - 3 compare the strings according to alphabetical order, ignoring the difference between upper- and lowercase letters and ignoring all non-alphabetic characters.

⁾

CHAPTER 9 Arrays and data manipulation

This short chapter deals with a number of topics to do with the manipulation of data. Some aspects of arrays are covered: array element order, the RESHAPE function, and vector subscripts. "Bits" are introduced. Finally, internal files and the TRANSFER function are explained.

9.1 Array element order; array constructors revisited; RESHAPE

A Fortran array is a set of scalar elements ordered in up to seven dimensions, forming what can be visualized as a hyper-rectangular array. Nevertheless, in a sense any array may be regarded as a continuous linear sequence of elements. Within the processor's memory, an array of any rank will usually be stored in an uninterrupted sequence of memory locations. Moreover, a statement such as

WRITE (*,*) table

where table is an array of any shape, will output a series of values depending on the size, but not the detailed shape, of the array table. In Fortran, all the elements of an array form a sequence in what is known as "array element order", which was mentioned briefly when the PACK function was discussed in Section 5.7. In the trivial case of a rank-one array, this is simply the order of increasing subscript, i.e. the array q(-3:3) gives the sequence

q(-3), q(-2), q(-1), q(0), q(1), q(2), q(3)

For a rank-two array, the array element order is given by letting the first subscript run repeatedly, i.e. the array q(2, 3) gives the sequence

q(1, 1), q(2, 1), q(1, 2), q(2, 2), q(1, 3), q(2, 3)

In general, whatever the rank, "array element order" is given by letting earlier subscripts vary more often than later ones.

Array element order is relevant not only to READ and WRITE statements but also to assumed-size arrays whereby a procedure's argument is passed as a sequence of elements rather than as an array of determinate shape.

It is sometimes convenient to rearrange the elements of an array into another array of different shape. This can be done by assignment statements, looping through all the elements, as in

DO j = 1, 32 DO i = 1, 32 v(32*(j-1)+i) = w(i, j) END DO END DO

which forms a rank-one array from the elements of a rank-two array. Another example is

DO k = 0, 1023 i = 1 + MOD(k, 32) j = 1 + k/32 END DO

which does the opposite. Another way of re-ordering the elements of an array would be to WRITE and READ "internal files", and this will be explained further below. Yet another approach would be to use array constructors with "implied DO" loops, as in

v = (/ ((w(i, j), i= 1, 32), j= 1, 32) /)

or a mixture of techniques:

DO j = 1, 32

w(1:32, j) = (/ v (32*j-31:32*j) /)

END DO

These last two examples do the same jobs as the earlier two above. Array constructors with implied-DO loops can be extremely powerful, although an array constructor can only be used to define a rank-one array. An example of an array constructor with nested implied-DO loops is

```
harlequin = (/ ( (casque(j, 17-i) .OR. (i==j ) , i= 1, 16), &
```

j= 1, 16) /)

which is a rank-one logical array of size 256, whose elements depend on a rank-two logical array called casque.

Any array may be empty, i.e. may have no elements. This is not the same as having elements that are zero-valued (if of numeric type) or blank (if of character type). However, the array constructor

(//)

should not be used to represent an empty rank-one array, because an array constructor must represent not only the elements of the array but their types, and the type is taken as that of the first element in an array constructor. An empty array of, say, REAL type could be written as

(/(0.0, i=1, 0)/)

which has no elements because 0 is below 1, but it is nevertheless real because 0.0 is a real constant. On the other hand,

(/(0.0, 1=1, 1)/)

which is just the same as

(/0.0/)

is a size-one array whose element happens to have the value zero. Bear in mind that a size-one array is not the same as a scalar. Moreover, an empty array or a size-one array could have any shape—it does not have to have rank one, although array constructors can only be written for rank-one arrays.

This discussion began with a consideration of how the elements of an array can be used to form another array of different shape. In fact, the most straight-forward method in Fortran is to use RESHAPE, an array-valued intrinsic function provided specifically for reshaping arrays. RESHAPE can be referenced with the argument keywords

RESHAPE (SOURCE, SHAPE, PAD, ORDER)

and the last two arguments, PAD and *ORDER*, are optional. Let us suppose firstly that *PAD* and *ORDER* are absent. The argument SOURCE can be an array of any sort, and its elements are rearranged to form the result RESHAPE. The elements of RESHAPE are therefore of the same type as those of SOURCE. However, the shape of RESHAPE is given by the argument SHAPE, which is a rank-one integer array specifying, as one would expect, the desired extents of the dimensions of RESHAPE. The rank of RESHAPE is therefore equal to the size of SHAPE, which must be positive and no greater than seven. The effect of the function is to take the elements of SOURCE and place them into RESHAPE in normal array element order, RESHAPE having the shape specified by SHAPE. Using again our earlier examples,

V = RESHAPE (SOURCE=w, SHAPE= (/1024/))

and

w = RESHAPE (SOURCE=v, SHAPE= (/32, 32 /))

If SOURCE has more elements than RESHAPE, the unwanted elements will not be used. If RESHAPE has more elements than SOURCE, then the argument *PAD* must be present, and it must be an array of the same type as SOURCE. The elements of *PAD* are used, in array element order, to fill the remainder of RESULT, if necessary running through PAD more than once. So,

xout = RESHAPE(SOURCE=xin, SHAPE=(/100/), PAD=(/0.0/))

forms the rank-one real array xout using the elements of xin, padding xout with zeros if xin has fewer than 100 elements.

Arrays can of course, have zero size. The SPREAD function allows us to construct zero-size arrays of high rank: starting from the rank-one empty real array

then

empty_2 = SPREAD (empty_1, DIM=1, NCOPIES=0)

is a rank-two zero-sized array, and

empty_3 = SPREAD (empty_2, DIM=1, NCOPIES=0)

is a rank-three zero-sized array, etc., etc.

In RESHAPE, the optional argument ORDER provides an opportunity of placing the elements of the array yielded by RESHAPE not in normal array element order, but as if some of its dimensions were switched around. ORDER must be an integer array of the same size and rank (one) as SHAPE, but containing the integers 1, 2, 3,... in a permuted order. The array ORDER then tells the processor in what order it should run through the dimensions of RESHAPE when fixing its elements. If ORDER is omitted, it is like having ORDER= (/1, 2, 3,.../) and so on up to the rank of RESHAPE. This means that if twist and metric are 4×4 arrays, and

twist = RESHAPE(SOURCE=metric, SHAPE=(/4, 4/), &

ORDER=(/2, 1/))

then twist (i, j) =metric (j, i). In this example, RESHAPE is being used to do what the TRANSPOSE function does.

Using the array transformation functions and array constructors, it is often possible to specify a complex multidimensional array in one statement, as in

iternary = RESHAPE(SOURCE = (/(i, 1=0, 2186)/), &

SHAPE = (/3, 3, 3, 3, 3, 3, 3/), &

ORDER = (/7, 6, 5, 4, 3, 2, 1/))

9.2

Vector subscripts

Section 4.4 dealt with "array sections", i.e. the notation for picking out a subset of the elements of an array. This was done with a colon notation, as in the simple rank-one example

decade(10:1:-1)

The three integers, separated by colons, form what is known as a "subscript triplet", specifying a starting index, a final index, and a "stride" (Section 4.6). "Vector subscripts" are a further tool for forming array sections, permitting a set of indices to be specified in any order. The idea is that, instead of a subscript triplet, a rank-one integer array is given that contains the desired indices in the desired order. Thus, if we have an array

npick = (/10, 9, 8, 7, 6, 5, 4, 3, 2, 1/)

then the array section mentioned above could be specified equally well by

decade(npick)

In other words, an array may have an index that is itself a rank-one array. In **decade (npick)**, **if npick w**ere a scalar integer then we would just have a single element of the array; but because **npick** is an array so is **decade (npick)**. Another example: with the vector subscript

u = (/4, 9, 1, 6/)

the array section x (u) consists of the elements x(4), x(9), x(1) and x(6) in that order.

A vector subscript may be any integer expression of rank one, as long as its elements are within the bounds of the array of which it is a subscript. With the arrays

INTEGER :: matrices(4, 4, 200), triad(3), mum(3, 3)

and if, say,

triad = (/196, 2, 34/)

then

mum = matrices(3:1:-1, 2, triad)

is the rank-two array with elements

mum(1, 1) = matrices(3, 2, 196)

mum(2, 1) = matrices(2, 2, 196) mum(3, 1) = matrices(1, 2, 196) mum(1, 2) = matrices(3, 2, 2) mum(2, 2) = matrices(2, 2, 2) mum(3, 2) = matrices(1, 2, 2) mum(1, 3) = matrices(3, 2, 34) mum(2, 3) = matrices(2, 2, 34)mum(3, 3) = matrices(1, 2, 34)

As this example illustrates, it is possible to have an array section in which different dimensions have different forms of subscript, i.e. we can have a mixture of single subscripts, subscript triplets, and vector subscripts.

A multidimensional array may have more than one vector subscript. For example, if

isquare = RESHAPE(SOURCE=(/ (k**2, k=1, 64) /), &

SHAPE=(/8, 8/))

and we have the vector subscript k3 = (/1, 2, 3/), then

knine = RESHAPE(SOURCE=isquare(k3, k3), SHAPE=(/9/))

is the rank-one array (/1, 4, 9, 81, 100, 121, 289, 324, 361/). Here, isquare is an 8×8 array of integers, and isquare(k3, k3) is an array section with two vector subscripts that happen to be equal. A vector subscript may have more than one element of the same value, in which case it forms what is called a "many-one" array section. For example, given the array of single characters

chars = (/("abcdefghijklmnopqrstuvwxyz_"(i:i), 1=1, 27)/)

and the vector subscript given by

name = (/13, 1, 18, 20, 9, 14, 27, 10, 1, 13, 5, 19, 27, 3, 15, &

21, 14, 9, 8, 1, 14/)

then chars (name) is a many-one array section consisting of 21 single-character elements such that

WRITE (*,*) chars(name)

spells out

martin_james_counihan

If a vector subscript has many repeated elements, the resulting array section could be much greater in size than the array of which it is a section.

There are just a few restrictions on the use of vector subscripts: in particular, a many-one array section may not appear as the variable on the left side of an assignment statement and an array with a vector subscript may not be used as the argument of a procedure that will redefine it (INTENT(IN) should be used). Also, a pointer assignment statement (explained later in this book) may not have as its target an array section with a vector subscript.

There are other games we can play. An array may have itself as a vector subscript, so if, say,

z = (/1, 3, 4, 2/)

then z(z) is (/1, 4, 2, 3/) and z(z(z)) is (/1, 2, 3, 4/).

Also, a vector subscript does not have to take the form of an array constructor: it could be a named array variable or even a rank-one array-valued function result as in the expressions

r(locations_of_cells)

r(Indices_of_Positive_Values(r))

9.3

Bits

The Fortran language allows for a number of different data types, described in Section 8.4, including derived data types constructed out of the basic types real, integer, character, etc.

In addition, it is possible to manipulate data in the form of sequences of binary bits, each bit having the value 0 or 1. In a way, LOGICAL data is binary and a logical array is rather like a sequence of bits, but in fact a data element declared LOGICAL is not normally stored in a single memory bit. So, "bits" in Fortran have nothing directly to do with LOGICAL data. Instead, an item of data declared as INTEGER may be interpreted as a sequence of binary bits. One integer will contain a large number of bits: commonly 32 or 64. The exact number for a particular processor can be ascertained by calling the intrinsic inquiry function BIT_SIZE.

When an integer is being regarded as a sequence of bits, ordinary integer arithmetic will generally be irrelevant. The integer's value when it is taken as an ordinary integer will, in general, differ from its value when the bits are interpreted as a binary number. A Fortran INTEGER, of course, may be negative, but a sequence of binary digits can only be positive. So, instead of the operations of ordinary integer arithmetic, a special set of intrinsic procedures exists so that bits (sometimes called "bitstream" data) can be manipulated. The details are set out in Appendix B.

9.4 Exercises 9.A

9.A Given that r is an array declared by the TDS

1

REAL :: r(4)

(i) r(1:4:1)	(ii) r(1:4)	(iii) r(1:)
(iv) r(1)	(v) r(:4)	(vi) r(:4:1)
(vii) r(4:1)	(viii) r(1::1)	(ix) r(::1)
(x) r(:)	(xi) r(4)	(xii) (/ r(1), r(2), r(3), r(4) /)
(xiii) (/ (r(i), i=1, 4) /)		(xiv) r((/1, 2, 3, 4/))
(xv) r((/ (i, i=1, 4) /))		

which of the following expressions are arrays equal to r?

Using the information in Appendix B, write a function that will convert a length-32 logical array into the corresponding stream of 32 bits, assuming that **BIT_SIZE(1)=32**. Write a function to convert a string of 32 bits (represented as an integer variable, and assuming BIT_SIZE(1)=32) into a positive hexadecimal number (in the form of a length-eight character string representing eight hexadecimal digits). Use RESHAPE in an assignment statement setting the first 48 elements of an 8×8 matrix, in normal array element order, equal to the elements of a size-48 vector. The matrix is called chessboard and the vector is called six_rows. They are to be of logical type. The 16 elements of chessboard which are not filled by six_rows are to be filled with alternating . TRUE . and . FALSE . values. If **vowels = (/"all, "e", "in, "o", "u"/), khard = (/1, 4, 5/)** and **ksoft = (/2, 3 /)** what are the values of

(i) vowels(khard)	(ii) vowels(ksoft)	(iii) khard(ksoft)
(iv) vowels((/4,2/))	(v) vowels(khard)//vowels(2)	

9.5 Internal files; TRANSFER

Some parts of this section will not be completely understandable without reference to Appendix A, which deals with the input and output of data, and in particular to format specifiers (see Appendix A.2).

However, "internal" files are not really files at all: they are simply areas of the processor's memory being treated as if they were sequential-access formatted files. Data can be written to or read from internal files using WRITE and READ statements, but there is no transfer of information outside the processor. Internal files can be very useful for changing the type interpretation of data: you can write to an internal file in one format, then read from it in another format.

Internal files can only be used with the READ and WRITE statements. All the other i/o statements are inapplicable to them, and "non-advancing" i/o is not possible (see Appendix A). An internal file is not only internal to the processor; it is internal to the program and cannot be used to transfer information between different programs or to save data from one program run to another. In fact, an internal file is a local entity that cannot even be used to transfer data between program units except by the usual methods of data association.

An internal file is no more than a character variable. To read or write an internal file, the unit number is replaced by the name of the character variable. An example should make the principle clear:

WRITE (UNIT=digit_string, FMT="(I6)") nref

This statement requires digit_string to have been previously declared in the usual way as a character variable of length six or more. The integer nref, assuming it has a defined value, is written into the string digit_string, taking up six character positions. If the length of digit_string is greater than six, it will be padded out with trailing blanks. The precise meaning of FMT="(I6)" is explained in Appendix A. Subsequently,

READ (digit_string, "(5X, I1)") junits

will yield the last digit of the number. The statement

READ (digit_string, "(F6.0)") ref

will yield the original number but now as a variable of real type. If the integer nref had been, say, 524288, then digit_string would be given the value "524288", junits would be the integer 8, and ref would be the real number 524288.0. Within the processor's memory, the internal representations of nref, digit_string and ref would be quite different, since they are variables of different types.

The next example shows how an internal file WRITE statement can be used for concatenation:

CHARACTER(10) :: title

CHARACTER(30) :: forename, midname, surname

CHARACTER(100) :: name

WRITE (name, "(A, 1X, A, 1X, A, 1X, A)") title, forename, &

midname, surname

This is equivalent to

.

name = title//" "//forename//" "//midname//" "//surname

In the above examples, the internal files called digit_string and name were scalar variables regarded as having one record. If the internal file is an array, then each element of the array is regarded as a "record" of

the internal file, taken in normal array element order. An internal file may be an array section, but not with a vector subscript.

If names is a character array, the statement

READ (names(1:2), "(A12)") forename, surname

reads a file of two records, each being a length-12 string. This statement involves "format reversion" and is equivalent to

forename = names(1); surname = names(2)

except that the READ statement, unlike the assignment statements, will ignore leading blanks in the elements of names. Moreover,

WRITE (names(1:2), "(2A12)") forename, surname

is equivalent to

names(1:2) = (/forename, surname/)

but the WRITE statement will give an error if the elements of names have lengths less than 12. Notice that, in our previous examples, it would be possible for digit_string, nref, junits, ref, title, forename etc. to be arrays as long as they are declared as such and as long as the internal files conform in shape with the data.

When data is input to a Fortran program (say, by reading a magnetic tape) it cannot normally be interpreted properly unless each data item is of a type known within the program. The data types that are read must correspond to the variables named in the input list. This can lead to difficulties when, as sometimes happens, the contents of a file are not known in advance. Suppose intin is a size-100 integer array and we have

READ(UNIT=7, FMT="(100I10)") intin

then what happens if in fact the file contains 100 real numbers? Or an unpredictable mixture of integer and real numbers? Fortunately Fortran provides an intrinsic function, TRANSFER (SOURCE, MOLD, *SIZE*), which can be used to change the type interpretation of a piece of data within the processor, i.e. when it has already been read in. For example, the above statement could be followed by

realin = TRANSFER(SOURCE = intin, MOLD = 0.0, SIZE = 100)

and this would put values into the real-valued array realin by reinterpreting the source data. It is very important to understand that TRANSFER does not convert data between types: the functions REAL, INTEGER, etc. do that. TRANSFER leaves unchanged the bit-patterns within the processor's memory, but simply interprets them in a different way.

TRANSFER (SOURCE, MOLD, *SIZE*) gives a result whose internal representation is exactly the same as SOURCE, but whose type is that of MOLD. SOURCE may be an array. *SIZE* is an optional argument discussed below. TRANSFER works for any data type, including a derived type.

Normally if MOLD is scalar the result is a scalar, whereas if MOLD is an array the result will be a rankone array of sufficient size to hold the contents of SOURCE. The result of TRANSFER is never an array of rank greater than one. For example,

TRANSFER(SOURCE=(1.0, 2.0), MOLD=(/0.0/))

produces a size-two, rank-one real array whose elements are the real and imaginary parts of the complex number (1.0,2.0).

The *SIZE* argument, if it is present, must be a scalar integer. Its effect is to ensure that the result is an array and to fix its size. If *SIZE is* specified and does not match the size of SOURCE, then in forming the function result it is possible that the trailing part of SOURCE may be lost or that the trailing part of the result may be left undefined. So,

TRANSFER(SOURCE=(/1.0, 2.0, 3.0, 4.0/), MOLD=(0.0, 0.0), &

SIZE=2)

produces a size-two complex array whose members are (1.0, 2.0) and (3.0, 4.0). The expression

TRANSFER((/-7.0, 5.1, 6.4/), (0.0, 0.0),1)

has the value (/(-7.0, 5.1)/), while

TRANSFER((/-7.0, 5.1, 6.4/), (0.0, 0.0))

is a scalar with the value (-7.0, 5.1).

If the argument ch is of character type, TRANSFER(SOURCE=ch, MOLD=1) will give an integer-type result of processor-dependent value preserving the bit-pattern of ch; this could be used in conjunction with bit manipulation functions.

Incidentally, TRANSFER (SOURCE=array, MOLD=array) provides a neat way of replacing an array of any shape by the corresponding rank-one array containing the same elements. This could otherwise be done using the RESHAPE function.

The TRANSFER function means that a formatted READ statement can be made very flexible and the data unravelled later, e.g.

READ (UNIT=in, FMT="(A)") chararray

header = TRANSFER(SOURCE=chararray(1:5), MOLD="",&

SIZE=5)

.

length = TRANSFER(SOURCE=chararray(6:10), MOLD=1)

```
IF (length>0.AND.length<(recmax-7)) THEN
```

rdata = TRANSFER(SOURCE=chararray(11:), &

```
MOLD=(/0.0/), SIZE=length)
```

where header, length and rdata are of character, integer and real types respectively. A long program that reads records of different sorts from different devices could in this way use a single generalized READ statement.

Notice that

.

.

.

.

```
REAL :: h (1000)
```

```
INTEGER :: i (1000)
```

```
(read r from an external device)
```

```
.
.
```

i = TRANSFER(SOURCE=h, MOLD=1, SIZE=1000)

allows elements of the data read as real numbers into r to be interpreted instead as integers by referring to i instead of r. This code does a similar job to that sometimes done with the now obsolete EQUIVALENCE statement.

Initialization expressions may make reference to the TRANSFER function, so a declaration of the sort

INTEGER :: i = TRANSFER("counihan", 1)

is possible.

Finally, the point must be clearly understood that TRANSFER is not an alternative to the writing and reading of an internal file. TRANSFER works at a lower level and the effect of TRANSFERring an integer into a real number (say) is not easily predictable and will in general depend on the particular processor's methods of representing integer and real data as sequences of bits. Manipulating internal files, on the other hand, will always translate an integer like 64 into the real number 64.0 because internal files are based on characters, not on bits. The result of TRANSFER will be processor-independent only when the type transfer is between real and complex types, since a complex number is defined in Fortran as an ordered pair of real numbers.

9.6 Exercises 9.B

9.A Write a function that reverses the digits of an integer.

1

9.A Write a function that uses an internal file to convert between a character string and a real number, it 2 being assumed that the string contains digits etc. representing a real number.

CHAPTER 10 Modules

Modules can be of great importance in organizing the structure of any large Fortran program. They enable data to be communicated between subprograms, they are useful for encapsulating sets of related subprograms, and they have a role in the writing of "generic" procedures, which can operate on arguments of different types. This chapter explains the use of modules for sharing data and for containing procedures. There is a discussion of the different forms of data association (argument, host, and USE), a detailed description of the USE statement, and finally an account of how modules can be used in relation to procedure interfaces.

10.1

Data modules

So far we have considered only three different kinds of program units, namely the main program, subroutines, and functions. Program execution always starts with a main program, from which subroutines and functions (collectively called "procedures") may be called. Procedures may call on other procedures in turn. Whenever a procedure is called, a list of arguments is used to pass data in either direction between the two program units, the calling and the called. In the case of functions, of course, the function name itself transfers data back from the function. If a procedure is written to carry out a simple self-contained operation, like calculating a simple mathematical function, then data transmission by argument passing may be good enough, but in general it can be very useful, if not essential, to have a way in which program units can share larger sets of data in a more flexible and open way. Modules provide a method of doing this.

Normally a name given to a variable (or to a named constant) is meaningful only within a particular program unit. A declaration like

CHARACTER(80) :: line(60)

is only known to the main program or procedure in which it appears. If this statement were to be repeated in different program units, the processor would assume that it referred to different things, and distinct areas of memory would be allocated. In other words, the names of variables in Fortran are usually "local" entities. Using modules, however, it becomes possible for the same sets of data to be accessible to a number of different program units.

Suppose, as an example, that a program needs to use an array of character strings representing a page of text together with some integer and logical data items related to it. The form of the data might be specified by the declaration statements

CHARACTER(80) :: line(60)

INTEGER :: linelength, linesperpage, numpage

LOGICAL :: checkin, checkspell, checkout

To have access to this data in different procedures, these declaration statements could be encapsulated in another kind of program unit called a "module", consisting simply of the statements above topped and tailed by MODULE and END MODULE statements:

MODULE Textpage

CHARACTER(80) :: line(60)

INTEGER :: linelength, linesperpage, numpage

LOGICAL :: checkin, checkascii, checkspell, checkout

END MODULE Textpage

The module can then be invoked in any other program unit simply by supplying the statement

USE Textpage

The name Textpage is of course arbitrary. The general form of the MODULE statement is simply the keyword MODULE followed by a name that may be chosen according to the usual Fortran rules, like the name of a variable or a procedure. The END MODULE statement is similar, just like an END FUNCTION or END SUBROUTINE statement, and it is not compulsory to repeat the module's name; in fact END by itself would suffice. As will be seen later, the USE statement can be a little more complicated than is indicated here, but basically it consists of the keyword USE followed by the name of a module.

A program may include many different modules as long as they have different names. A particular program unit may invoke a number of modules by having a series of USE statements. USE statements are non-executable and they must appear at the very beginning of a program unit immediately following the PROGRAM (or SUBROUTINE, etc.) statement and before any other non-executable statements. A module may itself invoke a further module, e.g. we could have

MODULE Textpage

USE Language

CHARACTER(SO) :: line(60)

INTEGER :: linelength, linesperpage, numpage

LOGICAL :: checkin, checkascii, checkspell, checkout

END MODULE Textpage

but it is not permissible for a module to invoke itself, directly or indirectly. So, the module Language may not have a USE Textpage statement, or a circularity would be created.

The next example is a data module containing information about metals, and it shows that a module can be used to hold a database of fairly complex design. It must be stressed that this module does not actually "do" anything. It has no executable statements. Its purpose is to declare the structure of a set of data that can subsequently be utilized in other program units.

MODULE Metals

INTEGER :: number_of_metals, namelengths(100)

CHARACTER(20) :: metal_name(100)

REAL :: weight(100), density_0(100), density_100(100), &

tempmelt(100), conductivity_0(100), &

conductivity_100(100), pricerange(2, 100)

LOGICAL :: data_has_been_read_in

END MODULE Metals

This could be invoked (by the statement USE Metals)in different subroutines to carry out tasks like reading the data from a disk file, modifying the data, rewriting the disk file, and making calculations that need access to this dataset. For example, to estimate the conductivity of a particular metal at a particular temperature we could write a function such as

FUNCTION Conductivity (metal, temperature)

USE Metals

REAL :: Conductivity

REAL, INTENT(IN) :: temperature

REAL :: c0, c100

CHARACTER(20), INTENT(IN) :: metal

Conductivity = -99.0! default function value for an

!unrecognized metal

DO i = 1, number_of_metals IF (metal/=metal_name(i)) CYCLE c0 = conductivity_(i) c100 = conductivity_100(i) Conductivity = c0 + temperature*(c100-c0)/100.0 EXIT END DO

END FUNCTION Conductivity

This is obviously much simpler than transmitting all the data through a long list of arguments.

With a module, a large or complex set of data need only be designed and declared once. This saves memory, keeps programs shorter, avoids error, and avoids passing clumsy long lists of arguments to procedures. In fact subroutines need have no arguments at all. A main program could simply look like

PROGRAM Economic_Prediction

CALL Startup

CALL Calculate

CALL Display

END PROGRAM Economic_Prediction

with the associated subprograms being, say,

SUBROUTINE Startup

USE Basedata

USE Workspace...

SUBROUTINE Calculate

USE Workspace

USE Results...

SUBROUTINE Display

USE Results

USE Output_Formats...

MODULE Basedata...

MODULE Workspace...

MODULE Results...

MODULE Output_Formats...

In this example the four modules could contain all the data declarations and the subroutines could contain only executable statements after the USE statements. The program as a whole consists of eight program units. This sort of design can give the programmer great flexibility: for example, the module called output_Formats could be written in two or three completely different versions to interface with different display devices that could be connected to the processor.

In a module, variables should be declared with the SAVE attribute if their values are intended to be preserved between calls to program units that USE the module (and if the module is not perpetually in USE through the main program). If a module is not perpetually in USE from somewhere or other, unsAVEd variables could become undefined.

Modules encourage a systematic approach to the design, management, and use of a program or system of programs. When important data is kept in modules, the programmer's work can become focused more on the careful design of the data structures rather than on procedures. Modules take on a life of their own, central to how we perceive the program, while procedures can be regarded as mere ancillaries that carry out operations on the data modules. In many application areas that depend on large data sets, this sort of programming style ("declarative" or "data-oriented" programming) is far more appropriate than the "stream-of-consciousness" style that concentrates on the flow of control between subroutines and functions.

This section was headed *Data modules* and we have seen that a module may contain a number of data declarations. The declarations may be type declaration statements of any kind. We shall see later that modules may also contain declarations of derived types (Chapter 12), procedure interfaces (Chapter 11) and namelist groups (Appendix A). They may also include procedures, as explained in the next section.

COMMON

There is an alternative to using a data module for "sharing" data between different program units. The alternative, an old construction that goes back to Fortran's early days, is the "COMMON block". An example of the syntax is

COMMON /Pool/ rnums(10), arr(3, 3, 3), intflag

Between slashes, Pool is the (arbitrary) name of the common block and can be used in different program units to refer to a single shared area of memory. Data are to be found there according to the ordered list of names and array shapes that follows: in this example, some arrays of real numbers and

integers with the local names rnums, arr and intflag. The data does not also need to appear in type declaration statements unless further attributes have to be specified. The data in a common block can have different local names in different program units, i.e. the names and array shapes that follow the slashes can vary, but they will everywhere refer to the same items of data.

The name of the common block can be omitted, in which case the statement refers to a special area of memory known as "blank common". The syntax is like this:

COMMON // rnums(10), arr(3,3,3), intflag

10.2

Exercises 10.A

10. Write a data module to contain in a convenient form the names of the days of the week, the names of A1 the months, and the usual numbers of days in the months.

10. Write a data module to contain the mathematical constants π and e and the first 20 powers of 2. A2

10. Write a data module containing a two-dimensional "spreadsheet" of 30 rows and 10 columns, each cell

A3 containing data in the form of a string of 12 characters. An ancillary array is to contain single-character indicators to say which cells contain values and whether the values are to be interpreted simply as words or as integers or real numbers.

10.3

Module procedures

The procedures we have so far met have been "external" procedures, i.e. subroutines and functions that are external to the main program. External procedures are extremely useful and in practice they form the bulk of almost all large Fortran programs. They have the incidental advantage that they need not necessarily be supplied in the Fortran language: in principle it is possible for a Fortran program to call external procedures that are in another language or in precompiled machine code. Almost everything that can be achieved with Fortran can be done using a set of external procedures, a main program, and data modules.

Nevertheless, Fortran allows for another kind of procedure, "module procedures", which are specified within modules. Like external procedures, module procedures are either of the "subroutine" or the "function" variety; they look very similar to external procedures and are invoked in exactly the same way by CALL statements or function references. However, a module procedure may only be invoked from parts of the program to which the module is plugged in by USE statements (or from another module procedure in the same module). Module procedures must always be supplied in Fortran.

There are a number of reasons why module procedures can be useful. If a module defines the structure of a special set of data, and if there are also some specialized procedures needed for operating on that data, then it can be appropriate to include the procedures as well as the data in the one module. Even if no special data set is involved, it can be handy to use a module to hold a "library" of related procedures. A programmer may create a set of procedures with a frequently encountered problem in mind, e.g. reading disk files in various formats, and putting them into a module that could be copied and used in a number of different programs. Another point is that procedures with the same name can sit in different modules, and then the programmer can switch between different versions of the same procedure just by changing a USE statement.

A special statement, CONTAINS, is required when a module contains module procedures. The general form of a module is

MODULE Name

USE statements

declarative statements

CONTAINS

module procedures

END MODULE Name

When this module is invoked by a USE statement in any other subprogram, that subprogram has access to the data sets declared in the module and may call any of the procedures that follow the CONTAINS statement. It also has access to the additional modules, if any, identified by USE statements at the beginning of this module. The declarative statements may be a mixture of type declaration statements and the other kinds of declaration mentioned at the end of the last section, but may not include executable statements.

After CONTAINS, there is a set of one or more module procedures. Module procedures are exactly the same in form as external subroutines or functions, each starting with a SUBROUTINE (or FUNCTION) statement and finishing with a suitable END statement. All the sorts of subroutines and functions explained in Chapters 7 and 11 may occur as module procedures rather than as external procedures.

There is one very important difference between module procedures and external procedures, namely that a module procedure has direct access to the data declared in the module before the CONTAINS statement. This is called the "host association" of data, and the module is said to be the "host" of its module procedures. Entities declared before the CONTAINS statement are shared by host association among all the module procedures following.

Here is an example of a module with data and procedures:

MODULE Polynomial

REAL :: c(0:3)

CONTAINS

SUBROUTINE Show_Coefficients

WRITE (*,*) C

END SUBROUTINE Show_Coefficients

FUNCTION Poly(x)

REAL :: Poly

REAL, INTENT(IN) :: x $Poly = c(0) + x^*(c(1) + x^*(c(2) + x^*c(3)))$ **END FUNCTION Poly** FUNCTION Inverse_Poly(y) **REAL :: Inverse_Poly** REAL, INTENT(IN) :: y REAL :: scratchpad(4) . (finds an approximate real solution to the cubic equation y=poly(x), . . . with Poly as defined as above) Inverse Poly =... END FUNCTION Inverse_Poly SUBROUTINE Switchback c(0:3) = c(3:0:-1)

END SUBROUTINE Switchback

END MODULE Polynomial

The subroutines Show_Coef f icients and Switchback, and the functions Poly and inverse_Poly, can be accessed by any other program unit that has the statement

USE Polynomial

These module procedures may also access one another: for example the function inverse_poly will include calls to Poly. Moreover, the data declared at the beginning of the module above (the array c) is also directly accessible to all the module procedures and to other parts of the program using the module. To avoid a clash of names, however, the programmer should obviously avoid the use of the name c for any other, different, piece of data in any module procedure.

At the same time, a module procedure may have data items internal to itself and not accessible outside it. This is the situation if a module procedure has some type declaration statements of its own: the items declared will be "local" variables and will not be accessible by host association outside the module procedure. For example, the function inverse_Poly above includes a data array called scratchpad, and this is a local variable not accessible anywhere else. The argument y in inverse_Poly, and also the argument x in Poly, are names local to those procedures and not accessible to the rest of the module, but they are also dummy arguments and are therefore accessible (by "argument association", not "host association"!) from wherever the functions are called.

Note that if one of a module's own data declarations is repeated within a module procedure, the effect is to set up a separate local variable and therefore to prevent the module procedure from accessing the module's data. Consequently,

MODULE Pointless

REAL :: x

CONTAINS

SUBROUTINE Double

REAL :: x

x = 2.0 * x

END SUBROUTINE Double

END MODULE Pointless

will achieve nothing because, within the subroutine, x is a local variable and is not the same piece of data as the x declared before the CONTAINS statement! But, if the subroutine's REAL statement were removed, then its x would be host-associated to the original x, and a statement CALL Double would double the value of x.

10.4 Data association by argument, host and USE

"Local" variables have no significance whatsoever outside the program unit in which they are declared: they have the "scope" of a single program unit. However, data may be shared between program units by "association". There are three distinct forms of association:

- Arguments of procedures allow data to be passed between program units as the program is executing. Just as a door has two sides, an argument exists both as a "dummy" argument in the procedure itself and as an "actual" argument in a calling program. When a procedure is invoked, there is "argument association" between the actual arguments and the dummy arguments. In the case of a function, a similar thing happens with its value. Although "argument association" passes a value between one program unit and another, the names of arguments should be declared separately in the two program units.
- When variables are declared at the beginning of a module that also contains module procedures, then the variables are also accessible within the module procedures by "host association".
- When a USE statement connects a module to a subprogram, the variables declared at the start of the module (i.e. before any CONTAINS statement) are said to be "USE associated" to the subprogram.

The three kinds of association (argument, host and USE association) should be kept quite distinct from one another. A crucial point is that argument association happens dynamically as the program executes, with values being passed from one memory location to another. By contrast, host association and use association are static relationships that are established once and for all when the program is compiled. Host association and use association do not involve any copying or duplication of data: they are merely forms of shared access to particular memory locations.

USE association normally means that all the variables declared in a module (except those local to module subprograms) are accessible within any subprogram which USES the module. However, it can sometimes be helpful to limit this association to a subset of the module's variables. This can be achieved with the help of two attributes that can be applied to type declaration statements in a module, namely PRIVATE and PUBLIC. Data having the PRIVATE attribute cannot be USE-associated, while data having the PUBLIC attribute can. The default situation is PUBLIC, but this can be reversed with the single statement

PRIVATE

which, occurring at the beginning of a module, will make all the data non-USE-accessible unless it is countermanded by specifying PUBLIC in the TDS referring to a particular piece of data. It is also possible to have PRIVATE and PUBLIC statements listing data items that have already been declared in TDSS.

The PUBLIC and PRIVATE attributes can be applied not only to variables but also to other objects such as named constants and the names of module procedures. For example, suppose we have a complicated module called Charsets that, among many other things, defines an operator called . intersect, that identifies the characters that are common to two character strings, i.e.

string1.intersect.string2

is a string consisting of the characters that are to be found both in string1 and in string2. The module Char set must contain a function linked to the .intersect. operator. However, if Charset starts with

MODULE Charset

PRIVATE

PUBLIC :: OPERATOR (.intersect.)

then it makes the operator usable in any program unit that USES Charset, while keeping hidden all the other entities in Charset. This will be made a little clearer by Section 10.6. More generally, to have

MODULE Name

PRIVATE

•

•

.

.

PUBLIC :: list of entities to be accessible from outside

is a more positive and safer way of allowing USE association than doing it the other way around with

MODULE Name

PRIVATE :: list of entities not to be accessible from &

outside

.

.

10.5 USE in detail

USE statements are non-executable statements that must be positioned before anything else after a PROGRAM, SUBROUTINE, FUNCTION or MODULE statement. Each USE statement points to a module and gives the subprogram access to a set of data and/or module procedures. This could, potentially, give rise to problems if the same names have been used to represent different variables in different parts of the program. If there is a data module such as

MODULE Coordinates

REAL :: x(60), y(60), z(60), units

REAL :: xlimits(2), ylimits(2), zlimits(2)

REAL :: scalex, scaley, scalez

INTEGER :: npoints

LOGICAL :: provisional(60)

END MODULE Coordinates

then there would be a conflict if it were used by another subprogram which already had other variables called (say) x and y. To avoid this sort of problem, the USE statement may specify a different local name for data within a module. There is also a form of the USE statement that limits access to a chosen subset of the things in the module. The following examples show the syntax:

USE Coordinates, nplaces => npoints USE Coordinates, xhere => x, yhere => y, zhere => z USE Coordinates, x => y, y => x USE Coordinates, ONLY: xlimits, ylimits, zlimits USE Coordinates, ONLY: z USE Coordinates, ONLY: zhere => z

The first of these gives full access to the module coordinates, but a different local name (nplaces) is to be used here in place of the module's name (npoints) for that particular data item. After this USE statement, the name npoints would not refer to the data in the module at all and could be used for something completely different. The combination => is used to link the new local name with the module name. This is similar to the notation we will come across later for pointer assignment (Chapter 13). In the second example above, the local names xhere, yhere and zhere are linked to the data objects known in the module as x, y and z. Incidentally, when a local name is set up in this way, there is no need to mention it in a TDS in the same subprogram: it is assumed to have the same properties as were declared in the module. So, xhere, yhere and zhere are 60-element arrays.

It is permissible for a program unit to have more than one USE statement referring to the same module and it is possible for one data object to have more than one local name. If the first three statements above were put together at the top of the same subprogram, the effect would be to give access to all the module's data items but with npoints having the local name nplaces, x having the local names xhere and y, y having the local names yhere and x, and z having the local name zhere. All the other data items in the module would keep their original names.

The fourth, fifth and sixth examples above show how the keyword ONLY is used to give partial access to a module. The fourth would be used in a subprogram where access is wanted only to the variables xlimits, y limits and zlimits. The fifth gives access only to z. The sixth also gives access only to z, but imposes the local name zhere. A USE statement with ONLY does not cancel out another less restrictive USE statement;

if a program unit has a USE statement without the ONLY qualifier for a particular module, then all parts of the module are accessible even if the same module is also invoked by a USE ... ONLY statement. A set of USE...ONLY statements gives access to all the items named. If the three final examples above occurred together, the combined effect would be to give access to xlimits, ylimits, zlimits, and z, the last having the local name zhere as well as the name z.

All that has been said above about local names and partial access to modules applies not only to data, but also to module procedures (and other entities, such as interface blocks, that will be met in later chapters). This means that the statement

USE Polynomial, Tell => Show_Coefficients

(referring to the example in Section 10.3) gives full access to the module Polynomial but the subroutine show_coefficients is to be referred to locally as Tell. The statement

USE Polynomial, ONLY: Tell => Show_Coefficients

means that no other parts of the module, apart from this subroutine, are accessible here.

As a rule it is a good idea to avoid renaming data and other entities in USE statements. When the same item is referred to by different names it generally leads to confusion rather than clarity. On the other hand, USE statements with the ONLY keyword are a useful form of "positive vetting", to ensure that data sets in different parts of the program are not inadvertently confused, and they make it easier for the programmer to remember exactly what is to be accessed in each module. For example,

USE locontrol, ONLY: Printer => P6, &

printer_output_format => printer_output_format_6

could be used to select a particular printing function (P6) and associated format data (printer_output_data_6) from a library (Iocontrol) of module procedures and data for input and output.

10.6 Modules and interfaces

Procedure interfaces were introduced in Section 8.9, and will be returned to in Section 11.1. A procedure is given an "explicit" interface in another subprogram by supplying an interface block among the declarative statements at the start of that subprogram. The interface block must contain copies of declarative statements for the procedure in question, declaring the characteristics of the dummy arguments and, where applicable, the function's result. There are many circumstances in which procedures need to be given explicit interfaces and it is potentially a tedious chore to write all the necessary interfaces in many subprograms in a large program involving several different procedures. The chore is simplified considerably, however, by the use of modules to contain interface blocks. For example, if we pick up an example from Chapter 8, the module

MODULE Vector_X

INTERFACE OPERATOR (.X.)

FUNCTION Vector_Multiplication (v1, v2)

REAL :: Vector_Multiplication

REAL, INTENT (IN) :: v1(*), v2(*)

END FUNCTION Vector_Multiplication

END INTERFACE

END MODULE Vector_X

provides an explicit interface to the procedure Vector_Multiplication. Once this module has been set up, it is only necessary to include the statement

USE Vector_X

in any subprogram that is going to make use of the operator .x.. It is envisaged here that Vector_Multiplication is supplied as an external function; but in fact it could equally well be supplied as a module procedure within vector_x, in which case the full interface block is unnecessary because the information required is already available in the module; in other words

MODULE Vector_X

INTERFACE OPERATOR (.X.)

MODULE PROCEDURE Vector_Multiplication

END INTERFACE

CONTAINS

FUNCTION Vector_Multiplication (v1, v2)

REAL :: Vector_Multiplication

REAL, INTENT (IN) :: v1(*), v2(*)

Vector_Multiplication = DOTPRODUCT(v1, v2)

END FUNCTION Vector_Multiplication

END INTERFACE

END MODULE Vector_X

could be used. The meaning of this will be made a little clearer in the next chapter. For present purposes it is sufficient to notice that the module contains the function Vector_Multiplication as a module procedure, and the linkage to the .x. operator is achieved by means of an abbreviated interface block. The USE of this module allows any other subprogram to have access to the operator .x. and to the procedure Vector_Multiplication. If it is desired that the latter should be referenced only indirectly through .x., and never explicitly, then a statement

PRIVATE :: Vector_Multiplication

could be inserted at the start of the module.

10.7 Exercises 10.B

- 10. A database is to consist of a set of up to 3000 names, postal addresses, and telephone numbers, in
- B1 addition to each of which there is a 12-character code for administrative purposes. Design a data module to contain this information in a suitable form. Then, write specifications (in English, not Fortran!) for a number of module procedures that could operate on the database to carry out as many useful tasks as you can think of in ten minutes.
- 10. The inverse hyperbolic functions can be expressed as

B2

$\operatorname{arcsinh}(x) = \ln(x + (x^2 + 1)^{1/2})$	
$\operatorname{arccosh}(x) = \ln(x + (x^2 - 1)^{1/2})$	$(x \ge 1)$
$\operatorname{arctanh}(x) = \frac{1}{2}\ln((1 + x)/(1 - x))$	$(0 \le x^2 < 1)$
$\operatorname{arccosech}(x) = \operatorname{arcsinh}(1/x)$	
$\operatorname{arcsech}(x) = \operatorname{arccosh}(1/x)$	
$\operatorname{arccoth}(x) = \operatorname{arctanh}(1/x)$	

Write these functions as a set of module procedures.

CHAPTER 1 1 More about procedures

Pure, elemental and recursive procedures are explained here, as are procedure interfaces and most of the advanced features that require procedures to have explicit interfaces. The final section deals with the ways in which arrays and character strings can be used as the arguments of procedures or as the values of functions. This chapter includes numerous exercises, some of which could easily form the basis of extended projects.

11.1 Interfaces and procedures

The concept of a procedure interface has been introduced gradually in this book. Section 8.9 explained that a special kind of "interface block" headed by a statement of the form

INTERFACE OPERATOR (.op.)

is needed at the start of a subprogram so that a certain external function will be invoked whenever the defined operator *.op.* is used in that subprogram. It was also mentioned that other kinds of interface blocks are required for certain other purposes. In Section 10.6 it was pointed out that interface blocks to procedures can be placed within modules for convenience, so that only a USE statement needs to appear in the subprograms that call the procedures in question. However, if the procedure is not external but is a module procedure, then what may be needed (in addition to a USE statement for the module procedure itself) is a simplified version of an interface block in which the procedure's name is mentioned in a MODULE PROCEDURE statement.

The concept of a procedure interface is a subtle and important one. Technically, every procedure has an "interface". Its interface is the information that specifies exactly how the procedure can be invoked. The information consists of the procedure's name, the characteristics and attributes of its arguments, the characteristics of its value (in the case of a function) and so on. This information must somehow be available within any subprogram that invokes the procedure, the reason being that a Fortran program will normally be compiled subprogram by subprogram and it cannot be assumed that while the processor is compiling one subprogram it will be able to scrutinize others to get the interface information needed to make sense of a procedure reference.

An important distinction has to be made between an "implicit" interface and an "explicit" interface. An external procedure, when used in the most straightforward way (as in Chapter 7), is said to have an

"implicit" interface because all the information that is needed to invoke the procedure is implicit in how the procedure is referred to. For example, if a subprogram contains the statements

CALL Countout (gong, x, y)

n = Lonsdale (eubank)

then the types and other characteristics of the arguments gong, x, y, and eubank should be known within the subprogram, probably by having been declared in TDSs at the start of it, and no more information need be supplied about the interfaces of countout and Lonsdale to this subprogram.

An intrinsic procedure, on the other hand, is said to have an "explicit" interface, because the form of reference to an intrinsic procedure is explicitly defined as part of the Fortran language, and does not have to be deduced from the context of a particular invocation. A module procedure, likewise, always has an explicit interface because the USE statement that gives access to the module will at the same time give direct access to the declarative statements within the module procedure that define the characteristics and attributes of the arguments.

An interface block starts with an INTERFACE statement. Interface blocks are required (a) if an external procedure's interface needs to be made explicit, or (b) if a module procedure's interface—which is explicit anyway—needs to be enhanced. An interface block is always inserted near the start of the subprogram that is to invoke the procedure in question. In case (a), the "interface block" contains a set of declarative statements, i.e. copies of the FUNCTION or SUBROUTINE statement, the TDSs declaring the dummy arguments and (if applicable) the function result variable, and finally the END FUNCTION or END SUBROUTINE statement. In case (b), the interface block will need a slightly more complex form of the INTERFACE statement, and the module procedure's name is specified with a MODULE PROCEDURE statement. A very simple interface block for an external procedure is:

INTERFACE

FUNCTION Triangle_Area (x1, x2, x3, y1, y2, y3)

REAL :: Triangle_Area

REAL, INTENT(IN) :: x1, x2, x3, y1, y2, y3

END FUNCTION Triangle_Area

END INTERFACE

i.e. it starts with the statement INTERFACE, finishes with the statement END INTERFACE, and between them there is a repetition of the FUNCTION (or SUBROUTINE) statement, argument type declaration statements, and END FUNCTION (or END SUBROUTINE) statements that would also be given in the procedure definition itself. An interface block may contain interfaces to more than one procedure, as in

INTERFACE

FUNCTION Triangle_Area (x1, x2, x3, y1, y2, y3)

REAL :: Triangle_area

REAL, INTENT(IN) :: x1, x2, x3, y1, y2, y3

END FUNCTION Triangle_Area

FUNCTION Quad_Area (x1, x2, x3, x4, y1, y2, y3, y4)

REAL :: Quad_Area

REAL, INTENT(IN) :: x1, x2, x3, x4, y1, y2, y3, y4

END FUNCTION Quad_Area

END INTERFACE

The general form of an interface block is either

INTERFACE

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•

.

interface body to external procedure

interface body to external procedure

interface body to external procedure

.

•

•

END INTERFACE

or alternatively

.

INTERFACE generic-specification

interface body to external procedure

interface body to external procedure

MODULE PROCEDURE proc, proc, ...

MODULE PROCEDURE proc, proc, ...

END INTERFACE

In the former case, the interface simply contains "interface bodies" for an arbitrary number of external procedures that are supplied in any order. Each interface body is a set of declarative statements associated with a particular function or subroutine:

FUNCTION/SUBROUTINE statement

USE statements, if relevant to characteristics of

arguments (and function result)

Type Declaration Statements for arguments (and function

result)

END FUNCTION/SUBROUTINE statement

In the second form of interface block, a *generic-specification* follows the keyword INTERFACE. The *generic-specification* may refer to the definition of an operator (Section 8.9) or to the setting-up of a generic name for several related procedures (Section 11.8) or to a defined assignment (Section 12.10). When there is a *generic-specification*, the external procedures represented by the interface bodies and the module procedures listed in the MODULE PROCEDURE statements must all be connected in that they will be different "specific" procedures corresponding to one "generic" form of invocation.

An external procedure always needs an explicit interface within any subprogram that calls it if any of the following is true:

- 1. the procedure is ELEMENTAL (Section 11.3);
- 2. there are OPTIONAL dummy arguments (Section 11.7);
- 3. a dummy argument is an assumed-shape array (Section 8.6), a pointer or a target (Chapter 13);

- 4. the procedure is a function with an array or pointer as its result;
- 5. the procedure is a function whose value is a character string of "automatic" length, i.e. a non-constant (and non-assumed) length given by a specification expression (Section 11.9).

Even if Conditions 1–5 do not apply, an external procedure needs an explicit interface to a particular subprogram if it is called from that subprogram under any of the following circumstances:

- 1. when it is called with an argument keyword (Section 11.6);
- 2. when it is a subroutine invoked through a defined assignment (Section 12.10);
- 3. when it is a function invoked through a defined operator (Section 8.9).
- 4. when it is invoked by a generic name rather than specific one (Section 11.8); or
- 5. when it is a PURE procedure (Section 11.2), and it is being called in circumstances that require it to be PURE (for example, if it is being called *from* another PURE procedure).

Even if it is not strictly necessary to provide an interface to a procedure, it is not an error to do so and it is wise to provide interfaces liberally rather than depend on remembering the rules listed above. Some authorities on Fortran believe that explicit interfaces should always be provided to all procedures to improve program reliability, since a high proportion of programming errors arise from incorrect data association when procedures are called.

11.2 PURE procedures (Fortran 95 feature not in Fortran 90)

A "pure" procedure is one that has no side-effects.

A pure function calculates and returns its value, but its argument or arguments must have INTENT (IN) and may not be changed within the function. A pure subroutine, however, may have arguments of INTENT (OUT) or (IN OUT), as well as INTENT (IN). In both pure functions and pure subroutines, local variables —those whose scope is limited to the procedure itself—may be manipulated, but not variables of wider scope linked with the procedure by the USE association of a module or by host association.

A pure procedure may not read or write external files or carry out other i/o operations. Internal files may be written or read, but any that are written must have names local to the procedure so that no information may leak out. If a pure procedure makes reference to another procedure, that also must be pure. Otherwise, we could have an illogical situation where the procedure referred to could generate side-effects on the "pure" procedure's behalf.

Intrinsic functions are always pure, and can therefore be referred to from within any other pure procedure. Intrinsic subroutines are pure if they are elemental (e.g. MVBITS) but not otherwise.

A pure procedure is declared as such in its header statement by prefixing the keyword FUNCTION or SUBROUTINE with PURE, e.g.

PURE FUNCTION Quintessence (x)

REAL :: Quintessence

REAL, INTENT(IN) :: x

END FUNCTION Quintessence

The INTENT specification is compulsory: all the arguments of a pure procedure must have declared INTENT, except in the unusual cases of arguments that are dummy procedures (Chapter 14) or pointers (Chapter 13). For the first line, the syntax

REAL PURE FUNCTION Quintessence (x)

or

PURE REAL FUNCTION Quintessence (x)

would also be allowed but neither is recommended. Finally, the END FUNCTION statement does not include the word PURE but the word FUNCTION is not optional and must be there.

If a pure procedure has a dummy procedure name as an argument (Chapter 14), the corresponding actual argument must be pure and it must either be an intrinsic procedure or it must have an explicit interface in the pure procedure where (through its dummy name) it is being referenced.

Pure procedures may not be recursive (Section 11.4 below). Moreover, local variables within a pure procedure may not be saved from one call to the next, so the SAVE attribute is not allowed, and neither may their values be initialized. Also, pure procedures may not STOP!

A pure procedure requires an explicit interface if a reference to it appears in a context that requires the procedure to be pure. An example would be if the procedure is called from within another pure procedure.

It would be fair to ask why the programmer should declare any procedure to be PURE, since to do so involves a number of restrictions and appears to give no additional functionality. Any program with pure procedures would, apparently, be unaffected if the keyword PURE were deleted wherever it occurs. So why bother?

Actually, there are two contexts in which procedures have to be pure, namely in Fortran 95 specification expressions (Section 11.9) and in the FORALL construct (Section 6.5). Specification expressions are a minor issue and, by themselves, would not justify the introduction of the PURE keyword and the rules associated with it. The real reason for specifying PURE procedures is shown by FORALL and is to do with the spread of parallel-processing systems that can take advantage of the fact that multiple calls to pure procedures may be made in any order or simultaneously. Purity, therefore, may not make the programmer's job easier, but in principle it can facilitate greater program efficiency and speed of execution, particularly when the program is to be run on an advanced parallel-processing system.

11.3

ELEMENTAL procedures (Fortran 95 feature not in Fortran 90)

Many of Fortran's intrinsic procedures, both in Fortran 95 and in Fortran 90, are "elemental". In Fortran 95 it is also possible for users to write elemental procedures of their own. An elemental procedure is specified as such by having the keyword ELEMENTAL in place of PURE, e.g.

ELEMENTAL FUNCTION Quintessence (x)

It is never necessary to specify a procedure to be both ELEMENTAL and PURE because all elemental procedures are also pure. In fact, of the prefixes ELEMENTAL, PURE, and RECURSIVE, no more than one can ever be used at once. All the constraints on pure procedures, mentioned in the previous section, apply also to elemental procedures. However, to be elemental involves additional restrictions.

Speaking loosely, the point of an elemental procedure is that it is defined in terms of scalar dummy arguments but can be referenced either with a scalar or with an array as the actual argument; if with an array, the effect is as if the procedure were called repeatedly for each element of the array. This allows whole-array operations to be written compactly and it can simplify the implementation of parallel processing on machines capable of it.

Within an elemental procedure, all the dummy arguments must be scalars and may not be pointers or procedure names. If we have an elemental function, its result must be treated as a scalar within the function. However an elemental function's actual argument, by which it is called from elsewhere, may be an array, in which case the result is also an array of the same shape.

An elemental procedure may be a subroutine rather than a function. When an elemental subroutine is called, either

- 1. all the actual arguments must be scalars, or
- 2. all the actual arguments whose INTENT is OUT or IN OUT may be arrays, but they must have the same shape; and those whose INTENT is IN must either have the same shape again or must be scalars.

An example may help to clarify this:

ELEMENTAL SUBROUTINE Matrix_Diff_Square (a, b, q, z)

REAL, INTENT (IN) :: a, b, q

REAL, INTENT (OUT) :: z

! Each element of z is to be set equal to the square

! of the difference between the corresponding elements

! of a and b, divided by q.

z = ((a–b)**2)/q

END SUBROUTINE Matrix_Diff_Square

This could be invoked elsewhere by code such as:

REAL :: d(10, 10), e(10, 10), f(10, 10), g = 10000.0

CALL Matrix_Diff_Square (d, e, g, f)

In this example, three actual arguments are arrays and, following the rules, they have the same shape. One actual argument (g) is a scalar but in theory it could equally well have been an array as long as its shape was the same (10, 10) as the other arguments. There is just one circumstance - when a dummy argument is used in a specification expression (Section 11.9) - in which the actual argument is restricted to being a scalar.

When one is working with user-defined derived data types (Chapter 12), defined assignments may be elemental. In fact, if the defined assignment is to be used in a WHERE construct, it must be elemental.

Every elemental procedure requires an explicit interface in a program unit that invokes it.

11.4 RECURSIVE procedures

Normally a procedure may not invoke itself, either directly or indirectly. In some circumstances, though, it can be convenient to let this happen, and it is made possible by putting the keyword RECURSIVE before the procedure's name in the first line of the procedure. This can be applied both to functions and to subroutines, but in the case of a function an extension has to be made to the syntax of the FUNCTION statement: if, for example, a function called Iris is to be made recursive, its first line could be

RECURSIVE FUNCTION Iris (juniper) RESULT (berry)

The meaning of RESULT (berry) is explained below. Subroutines are simpler, just requiring the keyword RECURSIVE as in

RECURSIVE SUBROUTINE Metamorphosis (jekyll, hyde)

How can recursive procedures be used? An example is this subroutine to put a sequence of characters into alphabetical order:

RECURSIVE SUBROUTINE Order (caps)

CHARACTER(1):: caps(:), store

LOGICAL :: disorder

disorder = .FALSE.

DO kount = 1, SIZE(caps)-1 IF (LGT(caps(kount), caps(kount+1))) THEN store = caps(kount) caps(kount) = caps(kount+1) caps(kount+1) = store disorder = .TRUE. END IF END DO IF (disorder) CALL Order (caps) END SUBROUTINE Order

This works by putting a disordered sequence into something closer to alphabetical order and then calling itself again. (The colon notation caps (:) is explained in Section 11.9, and SIZE in Section 12.2.) The next example is a recursive subroutine that will show the running total of an indefinite series of input numbers:

RECURSIVE SUBROUTINE Add_In (k) INTEGER :: k, knew, number READ (*, *) number IF (number/=0) THEN ! A zero terminates knew = k + number WRITE (*,*) knew CALL Add_In (knew) END IF END SUBROUTINE Add_In

This is started by CALL Add_in (0), and finished when a zero is input.

In the case of a recursive function, to avoid a possible ambiguity, the function's result value must be given a name different from that of the function itself. The result name that will be used within the function must therefore be specified in brackets after the keyword RESULT at the end of the function statement.

Then, within the function, any reference to the actual function name will be taken as a recursive call to the function.

A popular textbook example of a recursive function is the factorial, which can be written:

RECURSIVE FUNCTION Factorial (n) RESULT (nfac)

INTEGER :: nfac, n SELECT CASE (n) CASE (1) nfac = 1 CASE DEFAULT nfac = n * Factorial (n–1) END SELECT

END FUNCTION Factorial

Here the result is called nfac, a local variable declared in the first line. The result variable nfac and the function value Factorial must necessarily be identical in type, so there is no need to declare both. If their type is not specified by a prefix to the function statement itself, it must be specified by a type declaration statement referring to the result variable. In the above example, the presence of RESULT (nfac) means that the second line may not be

INTEGER :: Factorial, n

Within this recursive function, the name Factorial can only occur as a call to the function and is not used to assign a value to the function.

Recursive procedures can sometimes make life simpler for the program-mer, but they can lead to inefficient code and it is usually possible to carry out the task in another way. The factorial function above can be calculated much more simply by the one-liner

nfac = PRODUCT ((/ (i, 1=1, n) /)) !n!

11.5 Exercises 11.A

11. Write a pure function to convert radians to degrees.

A1

11. Write an elemental function to calculate n!, the factorial of its argument.

A2

11. Write a fast elemental subroutine to calculate the square, cube, fourth and fifth roots of one of its A3 arguments. *Hint:* only call log(x) once.

11. Write a recursive function to calculate a definite integral of the function $\sin^{n}(x)$, the arguments being A4 the power *n* and the limits of integration.

11. Write a recursive subroutine that will find a solution of the equation

A5

It should work by starting from a rough estimate of the solution, finding a better estimate, and then calling itself again, until the estimate is very close to the exact solution. The subroutine's arguments should be the number c and the current estimate of the solution of the equation.

11. The Ackerman function, ACK(m, n) is a function of two non-negative integers. It is defined by: A6

ACK(0, n) = n + 1

ACK(m, 0) = ACK(m - 1, 1)

$$ACK(m, n) = ACK(m - 1, ACK(m, n - 1))$$
 if neither m nor n is zero

 $x - 3\cos(x) = c$.

Write a recursive function to give ACK(m,n), and use it to investigate the function's properties. 11. Write a recursive function to calculate Fibonacci numbers Fib(i), where i is a positive integer, based on

A7 Fib(n) = Fib(n-1) + Fib(n-2)

starting from Fib(1) = Fib(2) = 1. What can you do to make the function work as fast as possible? 11. A program makes frequent use of the functions

A8

$$t_{mn}(\theta) = \sin^m(\theta) . \cos^n(\theta)$$

and of the indefinite integrals

$$T_{m,n}(\theta) = \int t_{m,n}(\theta) \,\mathrm{d}\theta$$

where m and n are positive integers. As long as m + n is not zero, the integrals can be reduced using the formulae

$$T_{m,n}(\theta) = (m+n)^{-1} \cdot t_{m+1,n-1}(\theta) + (n-1)/(m+n) \cdot T_{m,n-2}(\theta)$$
$$= -(m+n)^{-1} \cdot t_{m-1,n+1}(\theta) + (m-1)/(m+n) \cdot T_{m-2,n}(\theta)$$

Write a function procedure for $t_{m,n}(\theta)$ and another for $T_{m,n}(\theta)$, the latter using the reduction formulae above and referring to the former. The functions are to work for any non-negative values of m and n. The procedure for $T_{m,n}(\theta)$ should be written as a recursive function.

Use your procedures to tabulate values of $T_{2k,2k}(2\pi)$ for values of k ranging from 0 to 20.

11. An interesting function of a positive integer (investigated by Dijkstra) is defined by

A9

$$FUSC(1) = 1$$

FUSC(2*n) = FUSC(n)
FUSC(2*n + 1) = FUSC(n) + FUSC(n+1)

Write a recursive function to yield FUSC(n) and use it to look into the function's properties. What is its average value for the values of n lying between 9900 and 10100?

11.6 **Argument keywords**

The idea of argument keywords has already been explained in the context of intrinsic procedures. When a procedure has several arguments, keywords are a foolproof way of avoiding confusion between them, instead of relying simply on the order in which they are specified. With user-written procedures, keywords are not set up in the procedure definition itself, but are set up in an interface block, by listing the desired keyword names in the order of the arguments in the FUNCTION or SUBROUTINE statement. So, with a function like

FUNCTION Distance (x1, x2, y1, y2)

REAL :: Distance

REAL, **INTENT(IN)** :: x1, x2, y1, y2

Distance = SQRT($(x1-x2)^{**2} + (y1-y2)^{**2}$)

END FUNCTION Distance

we could use an interface such as

INTERFACE

FUNCTION Distance (Xa, Xb, Ya, Yb)

REAL :: Distance

REAL, INTENT(IN) :: Xa, Xb, Ya, Yb

END FUNCTION Distance

END INTERFACE

and, in any program unit containing that interface, the function could be called by a statement such as

s = Distance (Xa=1.576, Ya=34.88, Xb=pt3x, Yb=pt3y)

As this example shows, the arguments need not have the same names in the interface block as in the procedure itself (they are all "dummy" arguments), although they must correspond in order. The argument names used in the interface block become the keywords. Where the function is actually called using the keywords, the arguments can be in any order.

Note that a procedure may be given two (or more) different interface blocks in different parts of a program; this means that different keywords may be used in different places for the same procedure! This sort of confusion should, of course, be avoided.

Where an interface block makes it possible for argument keywords to be used, they may nevertheless be omitted, but not beyond a point in the argument list where the order of the arguments differs from that specified in the procedure itself. Thus, the statement above is equivalent to

s = Distance (1.576, Ya=34.88, Xb=pt3x, Yb=pt3y)

and to

s = Distance (1.576, pt3x, Yb=pt3y, Ya=34.88)

Notice that it is only by the occurrence of an = sign that the processor knows that a keyword is being used and it is only through the interface that the name of the keyword is specified.

Whenever one is writing and using external procedures that have multiple arguments, it is good practice to supply interfaces with argument keywords. In fact, one interface block could be put together containing interfaces for all the program's external procedures. This block could be put into a module, and accessed by a USE statement at the start of every program unit.

11.7

Optional arguments

One use of argument keywords is to control a situation where not all of the procedure's arguments need necessarily be present each time it is invoked. (A good intrinsic example of this is the subroutine DATE_AND_TIME, described in Chapter 5.) An argument that need not be given is known as an "optional" argument, and in an external procedure it would be declared by having a special attribute, OPTIONAL, in the TDS. We could have a function starting with

FUNCTION Addemup (s1, s2, s3, s4, s5, s6)

REAL :: Addemup

REAL, INTENT(IN) :: s1, s2

REAL, OPTIONAL, INTENT(IN) :: s3, s4, s5, s6

•

which means that the arguments s3, s4, s5, and s6 need not actually be present. In other words, Addemup may be called with any number from two to six arguments. Within such a function it is usually necessary to have some way of knowing whether or not an optional argument has actually been specified, and this is done with an intrinsic inquiry function, PRESENT, which may be called from within the procedure. If A is the name of an argument, PRESENT (A) is a logical function that is true if and only if A has been specified in this particular call to the procedure. The above function could therefore be completed with the statements

Addemup = s1 + s2

IF (PRESENT(s3)) Addemup = Addemup + s3

IF (PRESENT(s4)) Addemup = Addemup + s4

IF (PRESENT(s5)) Addemup = Addemup + s5

IF (PRESENT(s6)) Addemup = Addemup + s6

END FUNCTION Addemup

If a procedure has any optional arguments, an interface must be supplied. An interface block for the above function could be

INTERFACE FUNCTION Addemup (S1, S2, S3, S4, S5) REAL :: Addemup REAL, INTENT(IN) :: S1, S2 REAL, OPTIONAL, INTENT(IN) :: S3, 84, S5 END FUNCTION Addemup END INTERFACE

and valid forms of reference to the function would be, for example, the statements

a = Addemup(10. 8, 22.1)

b = Addemup(1.0, 2.3, 3.6)

c = Addemup(S1=0.0342, S2=0.0788, S5=0.0066)

d = Addemup(S3=heathrow, S2=gatwick, S1=stansted)

Note that keywords do not necessarily have to be used when there are optional arguments; but without keywords it would only be possible to omit a series of arguments from the back end of the procedure's argument list.

As an example of the use of optional arguments and keywords, suppose that a function, to be called convert_Angle, is to have two arguments, namely an angle in degrees and an angle in radians. Whenever the function is used only one argument must be present and the angle is to be converted from degrees to radians, or from radians to degrees, either way according to which argument is present. The converted value is to be returned as the function's value. The function is to write an error message if neither or both are

present. Whenever the function is used, a keyword must be used to indicate whether the argument is in radians or in degrees. The function could be as follows:

FUNCTION Convert_Angle (radians, degrees)

REAL :: Convert_Angle

REAL, OPTIONAL, INTENT(IN):: radians, degrees

CHARACTER(*), PARAMETER :: err=&

"Convert_Angle should be called with exactly one&

& argument"

LOGICAL :: r, a

r=PRESENT(radians)

d=PRESENT(degrees)

IF (r.EQV.d) THEN

WRITE (*,*) err

Convert_Angle = 0.0

ELSE

IF (r) Convert_Angle=radians*57.2958

IF (d) Convert_Angle=degrees/57.2958

END IF

END FUNCTION Convert_Angle

and a suitable interface would be

INTERFACE

FUNCTION Convert_Angle (Radians, Degrees)

REAL :: Convert_Angle

REAL, OPTIONAL, INTENT(IN) :: radians, degrees

END FUNCTION Convert_Angle

END INTERFACE

11.8 Generic procedures

Procedure interfaces can be extremely useful if we want to use a single name (or a single operator) to invoke any of several different procedures, the choice depending on the nature of the arguments. This is what happens with intrinsic functions when a "generic" name is used and when the result's type depends on the argument's type. To take a very simple example, suppose we want a procedure to "multiply" a character by an integer, and to work whichever way round the arguments are given. This would require two functions such as

FUNCTION Multcn(c, n)

CHARACTER(1), INTENT(IN) :: c

INTEGER, INTENT(IN) :: n

CHARACTER(n):: Multcn

Multcn = REPEAT(c, n)

END FUNCTION Multcn

FUNCTION Multnc(n, c)

CHARACTER(1), INTENT(IN) :: c

INTEGER, INTENT(IN) :: n

CHARACTER(n) :: Multnc

Multnc = REPEAT(c, n)

END FUNCTION Multnc

and either could be invoked through the name Mult as long as there is the generic interface:

INTERFACE Mult

FUNCTION Multcn(c, n)

CHARACTER(1), INTENT(IN) :: c

INTEGER, INTENT(IN) :: n

CHARACTER(n) :: Multcn END FUNCTION Multcn FUNCTION Multnc(n, c) CHARACTER(1), INTENT(IN) :: c INTEGER, INTENT(IN) :: n CHARACTER(n) :: Multnc END FUNCTION Multnc

END INTERFACE

(In this example, Multcn and Multnc are "automatic-length" strings as described in Section 11.9.) Whenever the generic function name Mult is referred to, control will pass either to Multcn or to Multnc according to the order of the arguments. In general, any set of procedures may be referenced by one generic name as long as (a) they are all functions or all subroutines, and (b) the characteristics of the arguments will narrow the choice down to one specific procedure from among the set, so that there is ultimately no ambiguity. The "characteristics" of the arguments means their types, keywords, shapes (if arrays) and whether they are present or not!

Not only can a set of procedures be referenced by a single generic name, but alternatively they may (if functions) be referenced by a single generic operator. The following enables "multiplication" to be defined between integer and logical variables:

FUNCTION Pnm (n, m) INTEGER :: Pnm INTEGER, INTENT(IN) :: n, m Pnm = n*m END FUNCTION Pnm FUNCTION Pnq (n, q) INTEGER :: Pnq INTEGER, INTENT(IN) :: n LOGICAL, INTENT(IN) :: q

END FUNCTION Pnq

FUNCTION Pqn (q, n)

INTEGER :: Pqn

INTEGER, INTENT(IN) :: n

LOGICAL, INTENT(IN) :: q

Pqn = n; IF (.NOT.q) Pnq = -n

END FUNCTION Pqn

FUNCTION Pqr (q, r)

LOGICAL :: Pqr

LOGICAL, INTENT(IN) :: q, r

Pqr = q.AND.r

END FUNCTION Pqr

The interface will be headed by

INTERFACE OPERATOR (*)

and contain all the declarative parts of the external function definitions above. This would permit the asterisk to be used freely between integer and logical data, either way round, with the meaning as defined.

To summarize: the INTERFACE statement may simply take the form

INTERFACE

in which case the interface may be specifying the names of external procedures, the types and shapes of function results, and the types, shapes, keywords and optionalities of the arguments. The number of procedures specified is arbitrary and there need be no connection between them. Alternatively, the statement may take the form

INTERFACE Name

where Name is a "generic name" for a set of two or more related procedures specified in the block. The third possibility is

INTERFACE OPERATOR (.op.)

where *.op.* is the name of an operator, either of the form .XYZ.... or of the same form as an intrinsic operator being "overloaded". The interface block must then contain one or more functions (and no subroutines) and the functions must have either one or two arguments (unary or binary operator). If there is more than one function, the operator is a "generic" one.

A further kind of INTERFACE statement is described in Section 12.10.

In the above examples, the sets of functions being given generic names were external functions. The same sort of thing holds good also for external subroutines. However, things can be done differently in the case of module procedures, because it is not necessary to have explicit interfaces for module procedures within the same module. Instead, an interface block which provides a generic name or operator for a set of module procedures may be of the form:

INTERFACE...

MODULE PROCEDURE list

END INTERFACE

where *list* is just a list of the names of the module procedures being bundled together. Going back to the earlier example, if the functions Pnm, Pnq etc. had been module procedures in the same module, the interface to define the operator could have been simply

INTERFACE OPERATOR (*)

MODULE PROCEDURE Pnm, Pnq, Pqn, Pqr

END INTERFACE

The MODULE PROCEDURE statement can also be used in the context of defined assignment (see Section 12.10).

11.9 Arrays and strings in procedures

It has already been indicated frequently that arrays and character strings may be used in procedures just as they can in a Fortran main program. The purpose of this section is to summarize the rules governing the use of arrays and strings as variables in procedures, especially when the variable is an argument of the procedure or, in the case of a function, is the function's value. Some of what follows has already been mentioned in Section 8.6. Moreover, there remain some usages of arrays that can be important with reference to procedures but still remain to be fully explained in Chapter 12 ("allocatable" arrays) and in Chapter 13 ("array pointers") and that will therefore be referred to only very briefly in this section.

All the techniques described in this section are different ways of making procedures more flexible by allowing them to use arrays (or strings) under circumstances where it would be unduly restrictive to specify their shapes and sizes once and for all when the program is written. In other words, they are ways of permitting procedures to work with variable-shape arrays and variable-length strings.

In a slightly different sense, we have already dealt with a powerful method of invoking procedures with array arguments of arbitrary shape through "array assignment" and WHERE (Sections 4.9 and 6.6), using

elemental procedures (Section 11.3). However, although elemental procedures may be called with arrayvalued actual arguments, they always have scalar dummy arguments, i.e. an elemental procedure has the internal appearance of a procedure whose arguments are all scalars. This section is concerned with nonelemental procedures.

Character strings

A character string must always be declared in a type declaration statement (TDS - Section 8.4) with a length that is specified in some way. In the simplest cases, the length is specified by a scalar integer constant as in

CHARACTER (120) :: line_of_text

When a character string is a dummy argument of a procedure its length may be specified explicitly, as in the above example, as long as the length matches that of whatever the actual argument is when the procedure is invoked.

Alternatively, a dummy argument of character type may have its length specified not by an integer constant but by a scalar integer "specification expression". The concept of a specification expression is an important one since it arises in connection not only with character strings but also with "automatic" arrays.

Specification expressions

A specification expression is a restricted kind of expression that may depend only on:

- 1. variables whose values are known within the procedure by USE association or (for a module procedure) by host association;
- 2. variables that are other dummy arguments of the same procedure;
- 3. references to a number of intrinsic functions, i.e.
 - (a) elemental functions of integer or character type, having integer or character arguments;
 - (b) **SELECTED_INT_KIND, SELECTED_REAL_KIND, TRIM, REPEAT and** TRANSFER, with integer or character arguments;
 - (c) Array enquiry functions (except ALLOCATED), numeric enquiry functions, BIT_SIZE, KIND, LEN and NULL;

except that, when an inquiry function is applied to another dummy argument, the characteristics of that dummy argument should have been specified before this specification expression is encountered. In other words, TDSs (and different entities within them) should appear in the correct order if the specification expression for one dummy argument depends on another;

Fortran 95 feature not in Fortran 90: specification expressions, besides intrinsic functions, may involve nonintrinsic PURE functions (Section 11.2).

The following is a very simple example of how a specification expression may be used to specify the length of a character-type dummy argument:

SUBROUTINE Infiltrate (string, nchars)

.

.

INTEGER, **INTENT**(**IN**) :: nchars

CHARACTER(nchars), INTENT(IN OUT) :: string

The specification expression here is simply the variable nchars. More complicated specification expressions appear in

```
SUBROUTINE Analyze (z, zm, m, a)
USE Database
REAL, INTENT(IN) :: a(:,:)
INTEGER, INTENT(IN) :: m
CHARACTER (SIZE(a) + 1), INTENT(OUT) :: z
CHARACTER (m*SIZE(z) + 1), INTENT(OUT) :: zm
.
```

where the array \mathbf{a} is an assumed-shape array (see Section 8.6, and further below in this section; SIZE is discussed in Section 12.2).

Incidentally, a character string variable does not have to be a dummy argument in a procedure for its length to be given by a specification expression rather than a constant. A character string that is an ordinary local variable may also have its length specified in that way, as long as the specification expression obeys the rules listed above. Such a variable is sometimes called an "automatic" data object. For example, in

SUBROUTINE Double (word, length)

INTEGER, INTENT(IN) :: length

CHARACTER (length), INTENT(IN) :: word

CHARACTER (2*length) :: word2

.

the variable word2 is an automatic object whose length is given by the specification expression 2*length, although word2 is not a dummy argument of the procedure.

Assumed-length strings

Besides using a specification expression, there is another way of allowing a character string which is a dummy argument to have non-fixed length. It is to have an "assumed-length" string, declared using an asterisk as described in Section 8.4. For example,

SUBROUTINE Infiltrate (string)

CHARACTER(*), INTENT(IN OUT) :: string

INTEGER :: nchars

```
nchars = LEN(string)
```

is an alternative method to that given in the similar example above. Another example is

SUBROUTINE Compare (name1, name2, result)

CHARACTERS), INTENT (IN) :: name1, name2

LOGICAL, INTENT(OUT) :: result

.

and of course the strings name1 and name2 must correspond to actual arguments, whose lengths were defined in the calling program. The asterisk in the CHARACTER statement means that the lengths of the dummy arguments name1 and name2 will be determined when the subroutine is called.

Assumed-length character strings may be used a little more widely than just as dummy arguments: they may be used for other character variables or parameters, whose lengths are assumed from initialization expressions (Section 8.7), or for character-valued functions (see below).

Generally speaking, it is preferable for non-fixed-length character-type dummy arguments to be of assumed length, i.e. using the asterisk notation, rather than being declared with specification expressions. In fact, there is a case for avoiding specification expressions altogether for dummy arguments since they tend to make the language over-complex without any great benefit.

Below is an example of a subroutine, Eicheck, with a character string argument of assumed length. Within the subroutine, the length of the argument can be found simply by using the intrinsic LEN function. The subroutine looks into the string for occurrences of the diphthong ei, and changes them to ie except after c:

SUBROUTINE Eicheck(string)

CHARACTER(*) :: string

CHARACTER(*), PARAMETER :: ei="ei", ie="ie", c="c"

INTEGER :: length

length = LEN(string)

IF (length<3) RETURN

DO ipoint=2, length-1

IF (string(ipoint:ipoint+1) /= ei) CYCLE

IF (string(ipoint-1:ipoint-1) == c) CYCLE

string (ipoint:ipoint+1) = ie

END DO

END SUBROUTINE Eicheck

The first CHARACTER statement here declares the dummy argument string to be of assumed length, its length being assumed from the actual argument wherever the subroutine is called. The second CHARACTER statement declares three local character strings also to be of assumed length, except that their lengths (two, two and one) are assumed from the initialization expressions that follow in the same statement.

Character-valued functions

Function values, like arguments, may be character strings of non-fixed length. Again, there are two ways of allocating these. The function's length may be "automatic", given by a specification expression, or it may be indicated by an asterisk and assumed. If it is automatic, the procedure must have an explicit interface.

If the length is assumed (a practice officially declared to be obsolescent in Fortran 95!), it must be assumed from a length specified in the program unit that invokes the function. Thus

FUNCTION All_Upper_Case(string)

CHARACTERS) :: All_Upper_Case

has a value whose length is assumed from wherever it is called from, where it could be specified by a declaration statement such as

CHARACTER(10), EXTERNAL :: All_Upper_Case

As another example, the procedure

SUBROUTINE Caller (n1, n2, n3)

USE Database

.

INTEGER, INTENT(IN) :: n1, n2, n3

CHARACTER(n1+n2+n3), EXTERNAL :: Called

could include a function reference such as

WRITE (*,*) Called (flag)

With the function Called beginning

FUNCTION Called (flag)

USE Database

CHARACTER(*) :: Called

LOGICAL, INTENT(IN) :: flag

Notice that the subroutine caller declares called to be an external function of character type, its length being given by a specification expression. This is then assumed as the length of the function's value within called.

Arrays as arguments

If a procedure has a dummy argument that is an array, there are four different possibilities for how the array's shape might be determined:

- 1. It may have a fixed shape, declared explicitly with bounds that are constants. This shape must correspond exactly to the shape of the actual argument.
- 2. It may have "assumed shape", declared using a colon for each dimension. The shape is assumed from that of the actual argument. Note that an assumed-shape array cannot be anything other than a dummy argument of a procedure. Other arrays cannot have assumed shape.

3. It may have "assumed size" (Section 8.6).

4. It may be an "array pointer", a kind of deferred-shape array described in Section 13.5.

Of these four possibilities, 3 is strongly discouraged, 4 is an advanced feature of Fortran that is not commonly needed, but 2 is recommended for general use whenever a dummy argument is an array. Fixed-shape arrays (1) may be simplest, but they are somewhat restrictive and there is a case for saying that a programmer should always use the "assumed-shape" method when it is necessary for a dummy argument to be an array. As a simple example of an assumed-shape array, if a program unit with an array variable declared by

REAL : : x(0:9)

calls a function called Fun with x as its real argument, and if the function starts with

FUNCTION Fun(z)

.

REAL, INTENT(IN) :: z(:)

then z takes on a size of 10, and its indices range from 1 to 10 (not 0 to 91). If we wanted the indices of z to run up from 0, the final statement could be

REAL, INTENT(IN) :: z(0:)

.

which is still an assumed-shape declaration since the upper bound will assume whatever value is necessary to fit in all the elements that the actual argument might have. It is only the extents of the actual argument in each dimension, not the pairs of index bounds, that are transmitted from the actual to the dummy argument. However, it is only the lower index bound, not the upper, that may be stated in an assumed-shape array declaration. A statement such as

REAL, INTENT(IN) :: x(:99) !illegal!

would be illegal. However, the lower bound is not limited to being a constant integer: it can be determined by any valid specification expression. So, for example, we could have

FUNCTION Fun(z, minimum_index)

INTEGER, INTENT(IN) :: minimum_index

REAL :: z(minimum_index:)

.

.

although it is hard to imagine how this sort of programming would be useful!

A nice example (which was the subject of a discussion initiated by David Serafini on the comp-fortran-90 mailbase discussion list in 1994) is the following:

SUBROUTINE Foo(arg)

INTEGER, INTENT(OUT) :: arg (:,:)

INTEGER :: local (SIZE(arg, 1), SIZE(arg, 2))

The point of this is that the dummy argument arg must have determined characteristics, including a shape, assumed from the actual argument whether the INTENT is IN, OUT, or IN OUT. Specifying INTENT (OUT) just means that the argument's value goes out, it does not mean that its characteristics as a data object do not come into Foo. When Foo is called, there will have to be a defined actual argument that will determine the shape of the variable local. Note that local is an automatic array whose shape is given here by specification expressions using the SIZE function (Section 12.2).

When a dummy argument is an array of non-fixed shape, e.g. when it has assumed shape, the procedure must have an explicit interface.

Finally, it must be emphasized that an elemental procedure (with scalar dummy arguments) is always preferable to a non-elemental procedure (with array dummy arguments) when there is a straight choice between the two.

Arrays as values

A function may have an array as its value, in which case its shape may either be fixed or it may be an "automatic" array with its shape given by a specification expression. The rules governing specification expressions were listed earlier in this section. An array-valued function must have an explicit interface.

This function has an array as its argument and as its value:

FUNCTION Inverse_Vector (v)

REAL :: Inverse_Vector(3)

REAL, INTENT(IN) :: v(3)

Inverse_Vector = v/DOTPRODUCT(v,v)

END FUNCTION Inverse_Vector

and a suitable interface would be

INTERFACE

FUNCTION Inverse_Vector (v)

REAL :: Inverse_Vector(3)

REAL, INTENT(IN) :: v(3)

END FUNCTION Inverse_Vector

END INTERFACE

Inverse_Vector(((1.0, 0.0, 3.0)) is equal to ((0.1, 0.0, 0.3)). Another example is the procedure starting with

FUNCTION Function_title (argument)

REAL :: Function_title (8)

.

.

.

.

whose value is a rank-one array with eight elements. More generally, Function_title could be an automatic array. If the argument were also an array, and if the function's value were to have the same number of elements as the argument, we could have

FUNCTION Function_title (argument)

REAL :: argument (:)

REAL :: Function_title (SIZE(argument))

Here, the value of Function_title is an automatic array but the argument is an assumed-shape array.

Longer examples

A fuller example of a procedure based on an assumed-size array is the following, which fills an array with prime numbers:

SUBROUTINE Primes (p)

INTEGER, INTENT(OUT) :: p(:)

! The subroutine must be called with p having at least

! 3 elements.

LOGICAL :: prime

INTEGER :: n, index

n = SIZE(p) ! We're looking for the first n primes

- P(1) = 2P(2) = 3index = 3 i=3 Odd_Integers: DO i=i+2 ! =5, 7, 9,... prime = .TRUE. Factors: DO j = 3, NINT(SQRT(REAL(i))), 2 IF (MOD (i, j) == 0) THEN prime = .FALSE. **EXIT Factors** END IF **END DO Factors** IF (prime) THEN ! We've found a prime p(index) = iindex = index + 1IF (index>n) EXIT Odd_Integers END IF END DO Odd_Integers
- **END Subroutine Primes**

The next example features fixed-shape function values, an assumed-shape dummy argument, and various automatic arrays:

FUNCTION Polycentroid (vertices)

!

! To calculate the coordinates of the centroid of a convex

! polygon from the coordinates of its vertices.

!

! The argument contains the coordinates of the vertices in

! cyclic order.

!

! This algorithm is valid only for a convex polygon.

INTERFACE

FUNCTION Triarea (t)

REAL :: Triarea

REAL :: t (3,2)

END FUNCTION Triarea

FUNCTION Tricentre (t)

REAL :: Tricentre (2)

REAL :: t (3, 2)

END FUNCTION Tricentre

END INTERFACE

REAL :: Polycentroid (2)

REAL :: vertices (:,:)

```
INTEGER :: nvertices
```

REAL :: triangles (SIZE (vertices, 1)–2, 3, 2)

REAL :: triareas (SIZE (vertices, 1)–2), tricentres(SIZE

(vertices, 1)-2)-2, 2)

REAL :: area, areabycentroid(2)

nvertices = SIZE (vertices, 1)

! initialize summations

area = 0.0

areabycentroid = 0.0

! Set up array of triangles' corners' vertices.

! The i'th triangle's corners are the first, (i+1)'th and

! (i+2)'th vertices of the polygon.

Triangle: DO i = 1, nvertices–2

Corner: DO icorner = 1, 3

IF (icorner==1) ivert = 1

IF (icorner>1) ivert = i + icorner

```
triangles(i, icorner,:) = vertices(i,:)
```

END DO Corner

! Now obtain the area and centroid of each triangle

! and add up their areas

! and make a weighted sum of their centroids.

triareas (i) = Triarea (triangles(i, :, :))

tricentres(i, :) = Tricentre (triangles(i, :, :))

area = area + triareas(i)

areabycentroid = areabycentroid + &

```
tricentres(i, :)*triareas(i)
```

END DO Triangle

! Now calculate the overall centroid

Polycentroid = areabycentroid/area

```
END FUNCTION Polycentroid
```

```
FUNCTION Triarea (t)
```

REAL :: Triarea

```
REAL :: t (3,2)
```

```
!
```

! This function is to return the area of the triangle of

! which the coordinates of the corners (a 3×2 array)

! are supplied as the argument t.

```
!
```

END FUNCTION Triarea

FUNCTION Tricentre (t)

REAL :: Tricentre (2)

```
REAL :: t (3,2)
```

!

! This function is to return the coordinates of the

! centroid of a triangle. The coordinates of the triangle's

! corners (a 3×2 array) are supplied as the argument t.

!

END FUNCTION Tricentre

As a final example, consider a function that calculates the "harmonic mean" *H* of a set of n numbers $a_{1,...,}a_n$. The harmonic mean of a set of numbers is defined by

 $H^{-1} = (a_{11} + a_{2.1} + a_{3.1} + \dots + a_{n.1})/n$

and the function below uses an assumed-shape array as its argument:

FUNCTION Harmonica (array)

! Declarative statements

REAL :: Harmonica

REAL :: array(:), sum

INTEGER :: number

LOGICAL :: nil

! Initialization

Harmonica = 0.0

sum = 0.0

number = SIZE(array)

nil = .FALSE.

! Calculation

```
DO index = 1, number
```

```
nil = (array(index)==0. 0)
```

IF (nil) EXIT

sum = sum + 1.0/array(index)

END DO

! Termination

```
IF (.NOT.nil) Harmonica = number/sum
```

END FUNCTION Harmonica

It is worth noticing that data initialization has not been carried out here in the type declaration statements, i.e. we have not used code like

REAL :: Harmonica =0.0 ! illegal! REAL :: array(:), sum = 0.0 INTEGER :: number = SIZE(array) ! illegal! LOGICAL :: nil = .FALSE. mainly because this kind of initialization only takes place the first time that the function is called. On any subsequent calls the variables will start with the values left behind from the previous call (as if the SAVE parameter had been used). Initialization within a TDS in a procedure means initialization once only and therefore will not have the desired effect in this function. Moreover, the first and third statements above are illegal anyway, because initialization in a TDS is not permitted for a function result (Harmonica) and because an "initialization expression" may not involve the bounds of an array whose shape is assumed.

Although data initialization within a type declaration statement is not appropriate in this example, it may be appropriate for a variable such as a counter that is to keep a running total of how often a function is called throughout the running of the program as a whole; and it is necessary for a fixed-value "named constant" declared with the PARAMETER attribute.

11.10

Exercises 11.B

11. Write a unary operator yielding a randomly-chosen logical value.

B1

11. Write a function which can be called with up to a dozen integer arguments. Its value is to be the integer B2 closest to their average.

- 11. Write a real array-valued function, called Cross, with two arguments both of which are also real arrays.
- B3 The arrays are of rank one and size three, representing three-dimensional vectors, and the result is to be the vector product ("cross product") of the two arguments.
- 11. Write a function called Hebrew, whose argument and value are both character strings of (different)
- B4 variable lengths. The argument is to be any word, and the result is to be the same word but with the vowels removed.
- 11. An operator is needed which, acting between two real numbers, gives their geometric mean. Write a
- B5 function and interface to do the job. What can you do about the case where the two numbers are of opposite signs?
- 11. Write a function and interface with a defined operator so that any real number (including a negative
- B6 one) can be raised to an arbitrary real power. If the result is mathematically a complex number, the function's value is to be equal to its real part. Use the symbol ** as the defined operator, overloading the intrinsic exponentiation operator.
- 11. Look again at the subroutine Eicheck in Section 11.9. Will it always work as intended? What will it do
- B7 to "Pompeii"? "Correct" it!
- 11. Write a subroutine with two arguments: first, an arbitrary-length array of real numbers and, second, a
- B8 single real number. The subroutine is to rescale the elements of the array so that their average becomes equal to the second argument (or, if the second argument is not present, to unity).
- 11. Write a function whose argument is a string of any length, returning a randomly-chosen single B9 character from that string (use the RANDOM function).
- 11. Write a function to say whether or not a number is in the Fibonacci sequence
- B1 1, 1, 2, 3, 5, 8,....
- 0 and another to see if it is in the meta-Fibonacci sequence:

1, 3, 4, 7, 11, 18, 29,....

Then, write a function to say if a number is a super-Fibonacci number, i.e. if it occurs in both the Fibonacci and meta-Fibonacci sequences. These functions should be written for time-efficient multiple

reference, by setting up tables of the different sorts of numbers, not by doing all the calculations from scratch every time.

- 11. Write an operator .s. that will concatenate two strings putting one blank space between them. In other
- B1 words, "Mel".S. "Gibson" is to be equal to "Mel Gibson".
- 11. A set of data consists of n pairs of coordinates x and y, and it is presumed that the data can be fitted to a B1 linear relationship

$$y(x) = a + bx$$

Estimates of *a* and *b* are given by the formulae

$$a = (S_y \cdot S_{xx} - S_x \cdot S_{xy})/D$$

$$b = (S_1 \cdot S_{xy} - S_x \cdot S_y)/D$$

where S_1 is equal to *n* and S_x , S_y , S_{xx} , and S_{xy} are respectively the sums over the *n* coordinate pairs of the quantities *x*, *y*, x^2 , and *xy*. The quantity *D* is given by

$$D = S_1 \cdot S_{xx} - S_x^2$$

This formula assumes equal uncertainties on all the measurements, i.e. gives equal weight in the sums to all the n points. Write a subroutine that will calculate the estimates of a and b given, as input, arrays of values of z and y.

11. Write functions to convert each way between (a) an array of logical data, and (b) an integer which, if B1 expressed in binary form, would represent the logical data as a sequence of is (true) and 0s (false).

3

2

11. Write a recursive function that, by repeated concatenations, converts an array of single characters into a B1 scalar character string.

4

- 11. Write an elemental function Len(integer), i.e. something like the intrinsic character string function LEN
- B1 function but with an integer as argument. It is to give the number of decimal digits in the integer 5 supplied as the argument.
- 11. Write the functions Triarea and Tricentre called by the function Polycentroid in the example in
- B1 Section 11.9.
- 6
- 11. An elemental function is needed for the purpose of calculating square roots as quickly as possible but
- B1 not with high precision. The intrinsic function SQRT would be too slow and unnecessarily accurate. It
- 7 is sufficient to calculate square roots to within one per cent of the precise values. Speed is allimportant, but it does not matter how much memory space is taken up.
- 11. Set up a subroutine Fast_trig to take any angle in radians and return the sine, cosine, and tangent each B1 to within one per cent as quickly as possible.
- B1 to within one per cent as quickly as possible.
- 11. Look at the function PARITY in Section 15.3. Write a version of it that will work for a rank-one
- B1 arbitrary-size array. (The dim argument will not be necessary.)

9

- 11. Look at the POPCNT function in Section 15.3, and refer to Appendix B for information about "bits". Write B2 POPCNT as an elemental external function.
- 0

11. The Mandelbrot set is based on the transformation of a complex number that is obtained by squaring it B2 and adding to it another (constant) complex number c:

1 $z \rightarrow z^2 + c$ Write a complex-valued elemental function Mandelbrot (z,c, iterations) whose value will be the result of carrying out the above transformation a number of times given by the integer argument iterations.

CHAPTER 12 Advanced array features and derived types

This chapter begins with a description of allocatable arrays, involving the statements ALLOCATE and DEALLOCATE and the function ALLOCATED. Then a few further intrinsic functions (LBOUND, UBOUND, SHAPE and SIZE) are dealt with, and details of the different classes of arrays are tabulated. The latter part of the chapter is devoted to derived types ("structures") and to defined assignment.

12.1 Allocatable arrays

"Allocatable arrays" are Fortran's most direct tool for dynamic memory management, in other words for letting arrays have variable bounds. Already, in connection with procedures, we have come across other forms of arrays with non-constant shape (Section 11.9), namely automatic arrays, assumed-shape arrays and assumed-size arrays; but these all involve fixing an array's shape when a procedure is entered. Allocatable arrays have nothing directly to do with procedures.

An allocatable array is a variety of "deferred-shape" array. (There is another variety, the "array pointer", dealt with in Section 13.5.) An allocatable array is initially declared with a certain rank, i.e. a certain number of dimensions, but the extent of each dimension (the "bounds") can be set and may be changed during the running of the program. This can be very valuable when a processor is limited in memory and it means that a program may expand and contract its memory requirements during running to minimize the demands made on the processor. For example, a program may need a large amount of memory to read a database, but may then carry out an analysis using just a small fraction of the input information: using allocatable arrays, most of the memory needed at input could be released by the program when it proceeds to the analysis stage.

An allocatable array is declared in a type declaration statement (TDS) by specifying the attribute ALLOCATABLE, and at that point its rank is specified by giving an array specifier with a series of colons, one colon for each dimension. This is a "deferred-shape" specification. The following are examples of the declarations of allocatable arrays of ranks one, two, three and four:

INTEGER, ALLOCATABLE, SAVE :: bitstream(:)

REAL, ALLOCATABLE :: matrix1(:, :), matrix2(:, :)

CHARACTER(1), ALLOCATABLE :: pages(:, :, :)

LOGICAL, ALLOCATABLE :: truthtable(:, :, :, :)

An allocatable array may not be a function value or a procedure's dummy argument. So, although an allocatable array is declared using the same colon notation as an assumed-shape array, there should never be any confusion between the two: dummy arguments may have assumed shape and other variables may be allocatable, but not the other way round.

The bounds of allocatable arrays are set by a special executable statement, ALLOCATE, that simply lists the names and shapes of the arrays. The ALLOCATE statement causes the required amount of memory space to be allocated to the arrays named. Examples are

ALLOCATE (bitstream(4097))

ALLOCATE (matrix1(45,90), matrix2(45,180), &

pages(65, 30, 1))

Following the usual notation for array shapes, lower and upper bounds may be specified:

ALLOCATE (truthtable(0:1, 0:1, 0:7, 14))

In an ALLOCATE statement the bounds may be expressions. Moreover, they are not restricted to the "specification expressions" allowed for automatic arrays (Section 11.9), but may be scalar integer expressions of more or less any kind, as long as they have definite values when the ALLOCATE statement is executed. So, we could have an arrangement such as

REAL, ALLOCATABLE :: rmem(:)

```
.
.
READ (*,*) n
ALLOCATE (rmem(2 *n))
.
.
```

Statements such as the following would also be possible:

ALLOCATE (workspace(120*nrecords, 15))

ALLOCATE (bytes(npersons, LEN(names))

ALLOCATE (scratchpads(dataset(1:1), 3, SIZE(dataset)))

but not

ALLOCATE (results(npoints), display(SIZE(results)))

because a bound of one array may not depend on an array inquiry function whose argument is another array that is being allocated within the same ALLOCATE statement. (For the meaning of SIZE, see Section 12.2.) However, it would be quite possible to have the sequence of two statements:

ALLOCATE (results(npoints))

ALLOCATE (display(SIZE(results)))

The ALLOCATE statement may have, after the list of arrays, a status variable for the purposes of errorchecking. It is given with the keyword STAT as in

ALLOCATE (display(SIZE(results)), STAT=k)

or

ALLOCATE (a(2), b(3), c(55, 4), STAT=icheck)

The name after STAT= is arbitrary, but it must be a scalar integer variable. After execution of the ALLOCATE statement, the status variable (in this instance, icheck) will be zero if the allocation was successful, but will be positive if there was an error. If STAT= ... is not included, then an error in executing the statement will cause the program to terminate.

The ALLOCATE statement gives space to an array, but the space can be later released with a DEALLOCATE statement. The syntax is just like that for ALLOCATE except that the names of the arrays are not followed by their shapes:

DEALLOCATE (bitstream, matrix1, matrix2, pages, &

STAT=iflag)

DEALLOCATE (truthtable, workspace, bytes)

DEALLOCATE may only be used on allocatable arrays that have actually been allocated, and ALLOCATE may only be used on a previously allocated array if it is deallocated first.

It can be useful to have a way of checking, during program execution, whether or not space has been allocated to an array. To do this there is an intrinsic function ALLOCATED. The ALLOCATED function

has one argument, which must be the name of an allocatable array, and it has the logical value .TRUE. or .F ALSE. according to whether the array is currently allocated. So, it is possible to have statements like

IF (ALLOCATED(scratchpads)) DEALLOCATE(scratchpads)

and

IF (.NOT.ALLOCATED(results)) ALLOCATE(results(4,100))

When allocatable arrays are used, a problem may arise if an array is allocated within a procedure and then the program returns back to the program unit that invoked the procedure. Under these circumstances the array will in effect be lost, even if the procedure is entered again later. In fact, it will not even be possible to deallocate the array later because its allocation status will have become undefined. There are two ways around this problem: one is to give allocatable arrays the SAVE attribute, in which case they are not lost on returning from the procedure, and the other way is to put allocatable arrays into modules. With modules, the arrays are preserved as long as the modules are being used by whatever program units are executing.

Fortran 95 feature not in Fortran 90

Contrary to what is said in the previous paragraph, in Fortran 95 local allocatable arrays that would otherwise get "lost" are automatically deallocated (i.e. without the need for a DEALLOCATE statement) on return from any procedure.

12.2

Intrinsic procedures for arrays

There are intrinsic functions LBOUND and UBOUND that yield the lower and upper bounds on the subscripts of whatever array is given as the argument. If arrays were declared by

REAL :: a(21:30), b(10)

then LBOUND(a) is 21, UBOUND (a) is 30, LBOUND(b) is 1, and UBOUND(b) is 10. The values of LBOUND and UBOUND are, obviously, integers, whatever the types of the arguments. With multidimensional arrays, LBOUND and UBOUND are rank-one integer arrays containing the sets of lower and upper bounds. So with

LOGICAL :: c(0:2, 0:2, 0:2, 0:3)

LBOUND(c) is equal to (/0, 0, 0, 0/) and UBOUND(c) is (/2, 2, 2, 3/).

In fact LBOUND and UBOUND may have an optional second argument, the keywords being LBOUND (ARRAY, DIM) and UBOUND(ARRAY, DIM). If DIM is present it must be a scalar integer no greater than the rank of the argument ARRAY, and then the function yields the subscript bound relevant to the dimension indicated by DIM. Using the previous example, UBOUND (ARRAYS c, DIM=4) is equal to 3. If the argument ARRAY is an array expression or section, rather than just the name of an array variable, then LBOUND will be given equal to 1 and UBOUND will be the extent of the appropriate dimension.

SHAPE is a very straightforward intrinsic function, having a single argument which may be any array. Its value is a rank-one integer array specifying the argument's shape, i.e. with the series of dimensional extents. So, the expression

SHAPE(RESHAPE(SHAPE=a, SOURCE=b))

is just the array a.

The intrinsic function SIZE, which has already cropped up in various examples in the course of this book, is very simple. With a single argument, which must be an array, SIZE is the total number of elements in it. There is an optional second argument, the keywords being SIZE (ARRAY, DIM), in which case SIZE is the extent of ARRAY along the dimension labelled by the integer DIM. So, if SHAPE (a) is (/4,5,100/), then SIZE (a) is equal to 2000 and SIZE(ARRAY=a, DIM=2) is 5.

12.3

Summary: classes of arrays

Fortran's different types of array were mentioned in Section 8.6, when the type declaration statement was being described, and again in Section 11.9 in connection with procedure reference. However, it is such an important topic that it is worth summarizing the situation in Table 12.1.

Constant-shape arrays and automatic arrays are both forms of "explicit-shape" array. Allocatable arrays and array pointers are forms of "deferred-shape" array.

Array type	Context	Comments
Constant shape	Permissible for any purpose	The simplest form of array, but the shape must be fixed when the program is written
Automatic	Not usable for a dummy argument	Declared with a "specification expression"; cannot have SAVE; may be a function value
Assumed shape	Only used for dummy arguments	Declared with colons (and possibly a lower bound)
Allocatable	Not usable as a dummy argument, function value or structure component	Declared with colons alone; permits flexible memory management as the ALLOCATE statement is executable, not declarative
Array pointer	May be used when an allocatable array may not	Declared with colons alone; may use ALLOCATE like an allocatable array; requires pointer syntax
Assumed size	Only dummy arguments	Declared with an asterisk; usage not recommended

Table 12.1 Classes of arrays.

12.4 Exercises 12.A

12.

A1

- (i) Write type declaration statements for an allocatable rank-two array of complex numbers, to be called cmatrix, and an allocatable rank-one array of length-12 character strings, to be called rivernames.
- (ii) Write statements to allocate the shape (4, 4) to cmatrix and allocate 200 elements to rivernames.
- (iii) Write code that will deallocate rivernames if it has already been allocated, and will then allocate 150 elements to it.

12. Write code that will take a character string, of whatever length, and produce a vector of that size A2 containing the individual characters that formed the string.

12. With the array declared by

A3

INTEGER:: spreadsheets (1:12, 1901:2050, 1:20, 0:199)

what are the values of

(i) LBOUND (spreadsheets)

- (ii) SHAPE (spreadsheets)
- (iii) SHAPE (spreadsheets(1:1, :, :, :))
- (iv) **UBOUND** (spreadsheets (1:1, :, :, :))
- (v) SHAPE (spreadsheets (1, :, :, :))
- (vi) **UBOUND** (spreadsheets(1, :, :, :))
- (vii LBOUND (ARRAY=spreadsheets(:, 1967, :, :), DIM=2)

)

(vii SIZE (spreadsheets(1:10, 1967, :, :))

i)

- (ix) UBOUND(LBOUND(spreadsheets(1:10, 1967, :, :))
- (x) **SIZE(SHAPE(spreadsheets(2, :, 1967,:)))**

12.5

Derived types

"Derived types" are special non-standard types of data that may be set up by the Fortran programmer. A derived type is defined in a block headed by a TYPE statement and subsequently data of that type can be declared by a variant of the TDS. Functions and operators, and the meaning of assignment (=), may be defined for use with a derived type.

A derived type (often called a "structure") is built up ultimately from components of intrinsic types. A "derived type constructor", analogous to an array constructor, is used to specify the values of all the components making up a particular structure. To extract an individual component from a structure, there is a special notation involving the % character.

There are two main ways in which derived types are useful. One is to let the programmer use unusual mathematical structures, e.g. geometrical figures, arcane algebras, quaternions, sets, and groups. The other is to set up a short-hand to work with large or complex data sets, whether it be entries in a bibliography, pages of text, printer drivers, or radionuclide decay data.

A block of non-executable code, headed by a derived-type definition statement, must be provided among the declaration statements at the start of any program unit where the new type is to be used. This block of code must declare the name of the type and specify how an item of this type is built up from items of intrinsic type. For example, if complex numbers were not already an intrinsic type in Fortran, they could be derived with the definition block

TYPE Complex

REAL :: x, y

END TYPE Complex

which simply declares that a new data type, Complex, is to consist of a pair of real numbers. The details of complex arithmetic would be a matter for function definitions and operator definitions subsequently.

Usually, the derived-type definition statement simply consists of the keyword TYPE followed by a name. This statement is followed by one or more statements declaring, in order, the components of the structure. These component declarations are very similar in syntax to ordinary type declaration statements, except that:

- 1. the only attribute specifiers available are DIMENSION and POINTER;
- 2. character lengths must be constants;
- 3. array bounds must be constants, except only that a pointer component may be an array pointer (Section 13.5); and
- 4. initial values of components cannot be specified in the derived-type definition.

Finally, the block is finished with an END TYPE statement optionally suffixed by the type-name.

It should be noticed that allocatable arrays are not allowed to be structure components. This is the basic reason why the VARYING_STRING data type (Appendix C) has been implemented in terms of a structure containing an array pointer.

Fortran 95 feature not in Fortran 90

Contrary to (4) above, Fortran 95 allows for the default initialization of derived type objects, as in the type definition

TYPE Coord3

REAL :: x(3) = (/0.0, 0.0, 0.0/)

END TYPE Coord3

A more complex example of a derived type definition is:

TYPE Mail

CHARACTER(10) :: title

CHARACTER :: initials (3)

CHARACTER(30) :: surname

CHARACTER(30) :: address (5)

CHARACTER(10) :: postcode

INTEGER :: telephone

LOGICAL :: gender

INTEGER :: refnumber, spouseref, entrydate

END TYPE Mail

This sets up a data structure that could form the basis of a mailing list. Note that components of different intrinsic types may be included among the components of a structure, and so may arrays.

Once a structure has been defined, variables of that type can be declared by type declaration statements of the form

TYPE (Quaternion) :: rho, sigma, phi

TYPE (Mail) :: newentry, spouse

TYPE (Currency_rates) :: yesterday, today, forward1, &

forward2

It is essential to understand the distinction between a statement like

TYPE Mail

which introduces the definition block for the type itself, and

TYPE (Mail) :: dud

which declares that a particular variable will be of that type. Although both start with the keyword TYPE, these two statements do quite different jobs. The type definition block must come first and could be provided most conveniently by being written once and for all in a module accessible to the whole program. The TDS is really just like any of the TDSs described in Chapter 8; it may have all the possible attribute specifications, just like an intrinsic TDS, and it may declare arrays. For example,

TYPE (Mail) :: retirees (5000)

declares an array with 5000 elements, each being a structure of the type called Mail. If Mail is defined as above, then retirees will actually contain a total of 55000 character strings, 20000 integers, and 5000 logical data items! If a set of coordinates in three-dimensional space is represented by

TYPE Coord3

REAL :: x(3)

END TYPE Coord3

then TDSs using that definition are

TYPE (Coord3) :: neworigin

TYPE (Coord3) :: redgiants(50)

Although Coord3 comprises an array, x(3), it is important to understand that the type Coord3 is not of itself an array or a scalar, any more than the type REAL is of itself either an array or a scalar. The variable neworigin is of type Coord3, but is a scalar, even though the array x subsists in it. The variable redgiants is also of type Coord3, but is an array of size 50.

It will be seen below that a variable of a derived type may be initialized when it is declared by a TDS. Such initialization overrides a Fortran 95 default initialization in the type definition itself.

SEQUENCE

A derived-type definition block may include the single-word statement SEQUENCE after the initial TYPE statement but before the statements defining the components. The effect is to make the derived type a "sequenced" structure, which means that any object of this type will be ultimately resolved into individual numbers or characters in the same way wherever the object is declared. This is necessary if such an object is to appear in a COMMON or EQUIVALENCE statement.

12.6

Structure constructors

It has been explained above how a derived type is defined and how a variable of that type would be declared. But how are actual values given to the components of a derived-type structure? It can be done with a "structure constructor" which takes the general form

Typename (component1, component2, component3,....)

i.e. the values of the components are simply listed in brackets after a reference to the type name. So, using some of the examples from the previous section, we could have assignment statements such as

retirees(1) = Mail ("Prof.", (/"H", "J", ""/), "Wallace", &

(/("", i=1, 5)/), 0, .TRUE., 386740, 386741, 211090)

locus = Coord3 ((/56.923, 20.768, 91.004/))

We can have more complicated expressions such as

locus = Coord3 ((/r*COS(theta)*COS(phi), &

```
r*SIN(theta)*COS(phi), r*SIN(phi)/))
```

Note that array constructors are used when the structure components are arrays. If a structure component were an array of rank greater than one, then the structure constructor could contain a reference to the RESHAPE function, within which the elements could be represented in the form of a rank-one array constructor.

The ordinary rules of assignment apply if there is any difference of detail between the list in the structure constructor and the list that originally defined the structure. So, for example,

```
locus = Coord3 (1)
```

would set all the elements of the array a (3), within locus, equal to 1.0.

Another example (which could define, for example, a plane in three-dimensional space) is the type

TYPE Vtriplet

REAL :: v1(3), v2(3), v3(3)

END TYPE Vtriplet

with variables defined by, say,

TYPE (Vtriplet) :: pa, pb, floor

and with actual values being set by assignment statements such as

pa = Vtriplet (0.0, 0.0, 0.0)

pb = Vtriplet ((/0 .34, 0.81, 0.08/), (/0.88, 0.00, 0.55/), &

(/0.60, 0.28, 0.31/))

floor = Vtriplet (a, b, (/c, d, e/))

where the variables a and b are 3-vectors and c, d and e are scalars.

A structure may be given an initial value, or it may be a named constant, e.g.

TYPE (Vtriplet), PARAMETER :: &

pb = Vtriplet ((/0.34, 0.81, 0.08/), (/0.88, 0.00, 0.55/), &

(/0.60,0.28,0.31/))

12.7

Structure components

Given a variable that is a structure, whose components have defined values, how can the values of those components be obtained? This is the inverse of the task performed by a structure constructor. It is done by giving the component name after the variable's name, separated by the % symbol. With the structure

TYPE Date

INTEGER :: day, month, year

CHARACTER(10) :: dayname

LOGICAL :: holiday, public_holiday

END TYPE Date

and data

TYPE (Date) :: q = Date (25, 5, 1992, "Monday", &

.FALSE., .TRUE.)

then q%day is the integer 25, q%holiday is the logical item .FALSE., and so on. This also holds equally good for variable names, e.g. with

q = Date (n1, n2, n3, daystring, flaga, flagb)

then the expression

q%dayname

is equivalent to the name daystring. This kind of thing can be applied to arrays, e.g. going back to the earlier examples

retirees%telephone

is an array of 5000 integers, consisting of the component telephone from each of the 5000 structures in the array retirees. A similar thing can be done if the component itself is the array, e.g. neworigin%x is simply the array x which is within the structure neworigin of type Coord3. And, with the type vtriplet above, pb% v2 is the array (/0.88,0.00,0.55/). However, this notation is forbidden when the structure itself and the component are both arrays, because an ambiguity would arise: it would not be clear what sort of array

retirees%initials

is supposed to be, since there are three elements of initials in each of 5000 elements of retirees. So, in general,

a%b

means the component called b within the derived-type variable called a, and it is an array if either a or b (but not both!) is an array. Notice that a may be an array element, so we could have

redgiants (1)%x

which would be the 3-vector of the coordinates of the first red giant. However, in a%b it is not permissible for b to be an array element, it must simply be the bare component-name from the structure definition block. This means that the expression

a%b(i)

is the ith element of a%b. It does not necessarily refer to the ith element of b. In fact a%b (i) refers to the ith element of b only if the structure a is scalar and the component b is an array.

12.8

Structures of structures

If derived-type structures were composed only of data items of intrinsic types, life would be interesting but not fascinating. In fact, components of a structure may themselves be derived-type structures. This example sets up a special type, Coord, to represent coordinate pairs in two-dimensional space; and then a further type, circle, is set up to represent circles; but the definition of Circle involves a data item of type Coord:

TYPE Coord

REAL::x,y

END TYPE Coord

TYPE Circle

TYPE (Coord) : : centre

REAL : : radius

END TYPE Circle

This means that structure constructors may be nested, e.g.

ring = Circle (Coord(.0, -1.0), SQRT(2))

and that we can have components of components:

ring%centre%y

would be equal to -1.0. This can be extended over several levels, e.g. the type

TYPE Sixcircles

TYPE (Circle) :: round(6)

END TYPE Sixcircles

which consists of a set of six circles, each based on a coordinate pair and a radius. Then, if hex is a scalar of type Sixcircles, there can be components

hex%round (5) hex%round hex%round (1:3) hex%round%radius hex%round%centre (1)

hex%round%centre%y

These expressions represent respectively the fifth circle in hex, an array (of type circle) of all six circles, an array formed with the first three circles, a real array of the circles' radii, the centre (type Coord) of the first circle, the x component of the centre of the second circle, and an array of the y components of the centres of the six circles!

It is important to remember that a type definition may include other derived-type structures only if the latter have previously been defined. However, a structure may have a component that is of the same type as itself if that component has the POINTER attribute (Section 13.2).

12.9

Procedures and operators with derived types

Like those of intrinsic type, data items of derived type may be used as the arguments of procedures. Functions of derived-type data may be used to define special operators. The following example shows data items representing points and circles in two dimensions, together with a function that will calculate the area of overlap between two circles:

MODULE Ringtypes

TYPE Coord

REAL :: x, y

END TYPE Coord

TYPE Circle

TYPE (Coord) :: centre

REAL :: radius

END TYPE Circle

END MODULE Ringtypes

MODULE Ringover

INTERFACE OPERATOR (.over.)

FUNCTION Overlap(c1, c2)

USE Ringtypes

REAL :: Overlap

TYPE (Circle), INTENT(IN) :: c1, c2

END FUNCTION Overlap

END INTERFACE

END MODULE Ringover

FUNCTION Overlap(c1, c2)

USE Ringtypes

REAL :: Overlap

TYPE (Circle), INTENT(IN) :: c1, c2

REAL :: x1, x2, y1, y2, d, r1, r2, ca1, ca2, s, a1, &

a2, trisq

x1 = c1%centre%x; x2 = c2%centre%x

y1 = c1%centre%y; y2 = c2%centre%y

 $d = SQRT((x1 - x2)^{**}2 + (y1 - y2)^{**}2)$

r1 = c1%radius; r2 = c2%radius

IF (d>(r1+r2)) THEN

Overlap = 0.0; RETURN

ELSE IF (D<ABS(r1-r2)) THEN

Overlap = MAX(r1, r2)**2*3.14159; RETURN

ELSE

 $ca1 = (r1^{**}2 + d^{**}2 - r2^{**}2)/(2.0^{*}r1^{*}d)$

 $ca2 = (r2^{**}2 + d^{**}2 - r1^{**}2)/(2.0^{*}r2^{*}d)$

s = (r1+r2+d)/2

a1 = ACOS(ca1); a2 = ACOS(ca2)

 $trisq = s^{*}(s-r1)^{*}(s-r2)^{*}(s-d)$

Overlap = (a1*r1 + a2*r2 - SQRT(trisq))*2.0

END IF

END FUNCTION Overlap

MODULE Rings

USE Ringtypes ; USE Ringover

END MODULE Rings

Here, the type definition blocks have been put into *a*. module called Ringtypes. The function itself, overlap, is an external function and is not therefore in any module. It is necessary to provide an interface for the function Overlap, because an operator is being defined, and this interface is put into a module called Ringover. The function itself, overlap, uses the derived types and therefore includes a USE Ringtypes statement. Finally, a combination module, Rings, brings together Ringtypes and Ringover so that any program unit using these need contain only the statement

USE Rings

Here is another example where a new type, Location, is defined and may be operated on with a function Distance:

MODULE Locdef

TYPE Location

REAL :: dlatitude, dlongitude

END TYPE Location

END MODULE Locdef

MODULE Interdistance

INTERFACE OPERATOR (.to.)

FUNCTION Distance (a, b)

USE Locdef

REAL :: Distance

TYPE (Location), INTENT(IN) :: a, b

END FUNCTION Distance

END INTERFACE

END MODULE Interdistance

FUNCTION Distance(a, b)

USE Locdef

REAL :: Distance

TYPE (Location), INTENT(IN) :: a, b

REAL, PARAMETER :: rdn = 57.296, rds = 6330000.0

REAL:: ta, tb, pa, pb, ra, rb, direct, aa(3), bb(3), &

absq(3)

ta = a%dlongitude/rdn ; tb = b%dlongitude/rdn

pa = a%dlatitude/rdn ; pb = b%dlatitude/rdn

aa(1) = sin(ta); bb(1) = sin(tb)

ra = cos(ta); rb = cos(tb)

aa(2) = ra*sin(pa) ; bb(2) = rb*sin(pb)

aa(3) = ra*cos(pa) ; bb(3) = rb*cos(pb)

 $absq = (aa - bb)^{**2}$

direct = sqrt(sum(absq))

```
Distance = 2.0*rds*asin(direct/2)
```

END FUNCTION Distance

This function would be invoked by any expression of the form

paris.to.moscow

from any program unit with access to the appropriate modules, if paris and moscow are defined data items of type Location.

In the above examples, derived type data occurs as arguments but the function values themselves are of an intrinsic (real) type. But in general a function result itself may be of derived type, as in

FUNCTION Loop (C)

USE Ringtypes

TYPE (Circle) :: Loop

TYPE (Coord), INTENT(IN) :: c(3)

REAL :: csq1, csq2, csq3, top, bot, xcent, ycent, &

radsq, rad

 $csq1 = c(1)\%x^{**}2 + c(1)\%y^{**}2$

 $csq2 = c(2)\%x^{**}2 + c(2)\%y^{**}2$

csq3 = c(3)%x**2 + c(3)%y**2

 $top = (c(2)\%y - c(3)\%y)^*(csq1 - csq2) - (c(1)\%y - \&$

c(2)%y)*(csq2 - csq3)

bot = $(c(1)\%x-c(2)\%x)^*(c(2)\%y-c(3)\%y) - (c(2)\%x- \&$

 $c(3)\%x)^*(c(1)\%y-c(2)\%y)$ xcent = 0.5 * top / bot ycent = 0.5 * (csq1 - csq2 - 2.0 * xcent * (c(1)%x - & c(2)96x)) / (c(1)%y - c(2)%y) $radsq = (xcent - c(1)\%x)^{**2} + (ycent - c(1)\%y)^{**2}$ rad = SQRT(radsq)Loop = Circle (Coord (xcent, ycent), rad)

END FUNCTION Loop

This function uses the types coord and circle that we met in previous examples, and forms the circle that passes through a set of three points c. It is not mandatory to have an interface for the function Loop because no operator is being defined.

12.10 Defined assignment

Defined operators were covered in Section 8.9, and in some ways it would have been logical to deal with "defined assignments" at the same time. Both are special types of procedure interface; a defined operator permits a function reference to be made through an operator and a defined assignment permits a subroutine to be called through a form of assignment statement (=). However, defined assignment is especially useful in the context of derived types and so has been deferred until this chapter.

First of all, recall that the general form of the assignment statement is

variable = expression

and this simply gives the variable on the left the value of the expression on the right, as long as they are of the same types and have conformable shapes. This applies also to objects of the same derived type: the components of the variable are set equal to the corresponding components of the expression. But we do not always have to have the same types and shapes on each side of an assignment statement. It is permissible for the expression to be a scalar and the variable an array, in which case all the array's elements will be set to the value of the expression. If the variable and the expression are of different numeric types, then the expression will be converted to the variable's type as if by the intrinsic function INT, REAL or CMPLX. If the variable and the expression are character strings of different lengths, the expression will be either truncated or padded to conform to the length of the variable. Those are the rules of "intrinsic" assignment.

"Defined assignment" permits the assignment statement to be given a meaning when it would normally be undefined, i.e. in cases where the variable and the expression are of different types that would normally be incompatible. It also permits the rules of intrinsic assignment to be redefined, or "overloaded", with something different from usual. Defined assignment is specified with a subroutine having exactly two dummy arguments and having an interface of the form

INTERFACE ASSIGNMENT(=)

SUBROUTINE ...

END SUBROUTINE...

END INTERFACE

the first line meaning that the subroutine can be invoked by using the = sign in an assignment statement. When this happens, the variable on the left-hand side will be the first argument of the subroutine and the expression on the right will be the second.

As an example, suppose we want to define the assignment a=b when a is a real scalar variable and b is of the type Circle used in previous examples above. In this case, suppose we want the number a to be set equal to the area of the circle b. This could be achieved with

SUBROUTINE Discus (a, b) USE Ringtypes REAL, INTENT (OUT) :: a TYPE (Circle), INTENT (IN) :: b REAL, PARAMETER :: pi=3.14159265 a = pi * b%radius**2

END SUBROUTINE Discus

where, to define the type Circle, the module Ringtypes has been included. It is necessary to have an interface whenever a subroutine is to be used to define assignment, and in this case there would be

INTERFACE ASSIGNMENT (=)

SUBROUTINE Discus (a, b)

USE Ringtypes

REAL, INTENT (OUT) :: a

TYPE (Circle), INTENT (IN) :: b

END SUBROUTINE Discus

END INTERFACE

There are a few things to notice about this example. The dummy arguments a and b are arbitrarily named and need not even be the same between the subroutine and the interface. The first argument has INTENT (OUT) and the second has INTENT (IN), since the purpose of the subroutine is to give a value to the former based on the latter. In fact, Fortran will assume INTENT (OUT) and INTENT (IN) in these circumstances, so it is not actually necessary to give the INTENT attributes at all in this example. However, it is conceivable that the value of the variable a might depend not only on the expression b but also on the initial value of a; so INTENT (INOUT) is possible for the first argument of a defined assignment.

A defined assignment will be invoked whenever the objects on either side of the = match the combination of types and/or shapes given for the arguments in the interface block. The interface block could contain interfaces to different subroutines, corresponding to different type/shape combinations of the arguments, and it would then be a "generic" interface. Suppose that we wished to define assignments in either direction between integers and single characters: a suitable generic interface would be

INTERFACE ASSIGNMENT (=)

SUBROUTINE C_to_I (i, char)

INTEGER :: i

CHARACTER(1) :: char

END SUBROUTINE C_to_I

SUBROUTINE I_to_C (char, i)

CHARACTER(1) :: char

INTEGER :: i

END SUBROUTINE I_to_C

END INTERFACE

and the corresponding subroutines could be similar but including the executable statements

i = IACHAR(char) - 48

and

char = ACHAR(i + 48)

respectively.

Defined assignments can be great fun, and one more example will not go amiss:

MODULE Gettype

TYPE Grab

CHARACTER(1) :: c

END TYPE Grab

END MODULE Gettype

MODULE Getint

INTERFACE ASSIGNMENT (=)

SUBROUTINE Smash (c, g)

USE Gettype

CHARACTER(1), INTENT(OUT) :: c

TYPE (Grab), INTENT(IN) :: g

END SUBROUTINE Smash

END INTERFACE

END MODULE Getint

MODULE Getget

USE Gettype

USE Getint

TYPE (Grab) :: get

END MODULE Getget

SUBROUTINE Smash (c, g)

USE Gettype

CHARACTER(1), INTENT(OUT) :: c

TYPE (Grab), INTENT(IN) :: g

READ (*,*) C

END SUBROUTINE Smash

With this, in any program unit headed by

USE Getget

a statement such as

qwerty = get

will lead to the character variable on the left (whatever its name) being evaluated by reading in one character from the keyboard.

12.11 Exercises 12.B

12.

B1

- (i) Write a derived-type definition block for a data type to be called Species, which is to describe a species of animal. The type is to be composed of a name (a 12-character string), the average weight, length and height of the animal (three real numbers), how many legs it has (an integer), and whether or not it can swim (logical). Choose sensible names for the components.
- (ii) Write a type declaration statement for four scalar objects of type Species, calling them panda, shark, whale and butterfly.
- (iii) Write a type declaration statement for a rank-one array of objects of type Species, having 15 elements and being named big_cats.
- (iv) Write an assignment statement using a structure constructor to say that the whale, as in (ii) above, is called cetus_____, on average has a weight of 4578.0 kg, a height of 2.86 m and a length of 12.71 m, has no legs, and can swim.
- (v) Write an assignment statement using a structure constructor to say that the fifth element of the big_cats array, as in (iii) above, has the name snow_leopard, average weight 46 kg, height 0.69 m and length 1.35 m, and has four legs, and can swim.
- (vi) Write an assignment statement using a structure component to change the average weight of the whale, first set in (iv) above, to 4287 kg.
- (vii Write an assignment statement using a structure component to say that the snow_leopard, in (v)) above, cannot swim.
- 12. Write derived-type definition blocks for

B2

- (i) a person, the components being a 40-character name and a three-integer date of birth;
- (ii) a married couple, the components being two persons (husband and wife) and a date of marriage; and

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- (iii) a family, the components being a married couple and an array with up to eight children,
- (iv) If robinson is the name of a variable of the family type, as in (iii) above, write expressions for the year of marriage of the couple who head this family, and for the value of the wife's name.

12. B3

- (i) Write a function to calculate the two points of intersection of two circles, following the example in Section 12.8.
- (ii) Write code to allow the + operator to be used between two circles, defining the sum of two circles in a sensible way so that it will be possible also to define the difference between two circles in a consistent way.

12. Write code to set up a special type (Fuzzy) composed of two real numbers to represent an estimate of B4 the value of something together with the statistical error on that estimate. Write functions with defined operators to add, subtract, multiply and divide fuzzys together, combining the errors according to the correct statistical procedure for uncorrelated errors. Using generic interfaces, include other functions so that the proper results are given also when fuzzys are combined with ordinary real numbers. Write a square root function for a fuzzy argument.

12. B5

- (i) Devise a derived type to represent efficiently sparse vectors, i.e. large rank-one arrays of real numbers, almost all of which are zero, only a few being non-zero. Write functions to carry out basic arithmetic operations between sparse vectors.
- (ii) Devise a derived type to represent sparse square matrices, i.e. data equivalent to a real rank-two square array with extents that may be very large but with only a few elements having non-zero values. Allow for a dimensionality up to 1024 X 1024, but with no more than 512 non-zero elements. The idea is to avoid storing all the zeros and thereby save space. Write a function to form the product of two sparse matrices.

12. Write a subroutine and an interface block defining assignment when a variable of integer type is set B6 equal to one of length-one character type. The integer is to be set equal to the ASCII code of the character or to zero for an unrecognizable character.

- 12. The game of "Life" is based on a large two-dimensional rectangular array of cells, each of which is
- B7 either "alive" or "dead". Each cell has eight nearest neighbours, i.e. the cells immediately above, below, to either side, and in the four diagonal directions from it. The state of the array changes generation by generation, with cells dying or being born. Each time, the fate of each cell depends on the number of live neighbours it had in the passing generation. A live cell will die if it had fewer than two or more than four live neighbours and will survive otherwise. A previously dead cell will come to life if it had two or three live neighbours. As parts of a program to model the game of life, devise a derived data type to represent the array of cells and write a subroutine that takes the array from one generation to the next.

There is an alternative set of rules for "Life", i.e. a cell with three live neighbours will become (or remain) alive, a cell with two live neighbours remains however it was, and all other cells become (or remain) dead. Investigate the game and compare the two sets of rules.

- 12. Write a function subprogram that will take (as argument) a rank-one arbitrary-size array of real
- B8 numbers and will return (as the function's value) the geometric mean of the array's elements. Design the subprogram so that it can deal efficiently with very large arrays containing large numbers, taking precautions against overflow and taking appropriate action if there is a zero element. The geometric mean of a set of n numbers is defined as the nth root of their product, i.e. the logarithm of their geometric mean is the mean of their logarithms.
- 12. Set up a user-defined type that is a physically dimensioned real variable, i.e. a real number associated with
- B9 powers of the fundamental MKSA dimensions, mass, length and time; ignore electric current in ampères (A). Write appropriate ancillary procedures, including a special output subroutine to write out a value in an appropriate format.

12. Construct data types to represent lines and planes in three-dimensional space, with a function to B1 calculate the line of intersection of two planes.

0

12. Set up a new derived data type, a "rational" number, being the ratio of two integers not sharing a common B1 factor.

1 This will involve a procedure to reduce two integers by dividing both by their highest common factor. This could use Euclid's algorithm working from the fact that the highest common factor of a and b is the highest common factor of b and c, where c is the remainder left when a is divided by b.

Write functions to carry out all the normal arithmetical operations on rational numbers.

- 12. Design derived data types and operators to manipulate gravitating point masses in three-dimensional
- B1 space. The basic data type should be a point associated with a mass. There should be an "addition"
- 2 (centroid) operator, a totalized gravitational potential function, etc. This could be developed into a system for computing the path of a light test particle through a set of heavy point masses that could have time-varying positions.
- 12. Look at the function COPY_SCATTER in Section 15.3. Write a version of it to be used when all the
- B1 arguments have rank two.
 - 3

CHAPTER 13 Pointers

"Pointers" are a powerful and elegant feature of Fortran, but unfortunately they are notoriously difficult to understand when you first meet them, mainly because it is not immediately clear what sort of problem they are there to solve. This chapter first explains the use of pointers in the simplest of circumstances, in relation to ordinary scalar data of intrinsic type. This is straightforward but will not seem terribly useful. Later sections will extend the idea to derived-type structures (Section 13.2), function results and dummy arguments (Section 13.3), and arrays (Section 13.5), and it is in these contexts that most powerful practical applications of pointers arise.

13.1

Simple pointers

Normally, there are two aspects to any data object in Fortran. First, there are the various attributes that describe what sort of object it is: its type, its name, its shape if it is an array, its length if it is a character string, and the other attributes that can be set by a type declaration statement (TDS). This set of details is sometimes known as the "descriptor" of the data. Second, there is the actual value of the object. When a data object is first declared, the data descriptor is fixed and memory space is set aside to hold the value of the data. If the TDS includes data initialization, that memory space will be filled with the initial data values immediately.

It is very important to distinguish clearly between the data descriptor, which is unaffected by the value of the data, and the value itself. The value may occupy a large amount of memory, especially if the object is a long character string, an array, or a derived-type structure. The descriptor will occupy relatively little space, but is essential for making sense of the data's value, because the content of an area of memory is meaningless unless the processor knows whether it is to be interpreted as a real number, a character, or whatever.

A TDS, then, normally sets up a data descriptor (name, type, etc.) and reserves memory to hold its value, and it may fill that memory with an initial value. A "pointer", however, is a data object that does not have its own reserved area of memory. In other words, a pointer is a data descriptor without its own space for a value. A pointer, as its name suggests, "points" to memory space occupied by the value of some other variable, the "target". At its simplest, a pointer can be regarded as a name that can be associated and disassociated dynamically with memory space occupied by other data. A pointer-name can therefore be used as an "alias".

A particular pointer can only point to data of a particular type. A pointer must be declared with a TDS giving its name, type, etc., and the attribute specification list must include the keyword POINTER. The effect is to establish a data descriptor, including the pointer's name, but without memory of its own to hold a value. It follows that there can be no initial value given when a pointer is declared (except with the NULL function described later below). When the program is executing, the pointer may be associated with a variable of the appropriate type by means of a special statement, a "pointer assignment" statement. Variables to which a pointer may be associated need to be declared initially with a special attribute, TARGET. The TDSs

REAL, TARGET :: a, b, c, d, e, f

REAL, POINTER :: p

set up the pointer p and the six real variables a,..., f which can be targeted. A pointer assignment statement has a form such as

p => a

which would mean that the name p will henceforth refer to the memory space occupied by the value of the target variable a. After such a statement, p could be used as an alternative name for a, either in statements like

$b = p^{**}2/2.0$

WRITE (*,*) p, b

or in

p = c + SQRT(d)

which, since p "points" to a, actually changes the value of a. The pointer assignment statement (=>) by itself does not change the value of anything: it simply connects the named pointer to the named target. The general syntax of the pointer assignment statement is

pname => tname

where *pname* is the name of a pointer (i.e. a variable previously declared with the **POINTER** attribute) and *tname* is the name of a target. As far as we are concerned for the time being, *tname* must be the name of a variable previously declared with the TARGET attribute, but some exceptions to this will be mentioned later. The pointer and the target must be of the same type. Once a pointer assignment statement has been executed, the pointer is said to be "associated" with the target, but if the same pointer subsequently appears on the left side of another pointer assignment statement, the first association is broken and the second takes effect.

There is an intrinsic inquiry function, ASSOCIATED, which can be used to determine whether or not a pointer is associated with a target. ASSOCIATED (pname) is logical and has the value . TRUE . if pname

points to any target and .FALSE. if it does not. This function has an optional second argument which may specify a particular target: the argument keywords are POINTER and TARGET, and the logical expression

ASSOCIATED(POINTER=pname, TARGET= tname)

is true if and only if pname is associated with tname.

As a simple example, this code fragment finds the value of the largest of six numbers:

```
REAL, TARGET :: a, b, c, d, e, f
```

```
REAL, POINTER :: p
```

```
.

p => a

IF (b>p) p => b

IF (>p) p => c

IF (d>p) p => d

IF (e>p) p => e

IF (f>p) p => f

WRITE (*,*) p
```

This is a rather artificial example, since it does no more than

WRITE (*,*) MAX(a, b, c, d, e, f)

but the principle should be clear. The name p is being used to point to one of the six numbers a,..., f. The value of p does not, itself, occupy any additional memory space, because p does not have a "value" in its own right. The above code could be written with p being an ordinary non-pointer variable, and with ordinary assignments (=) instead of the pointer assignment statements, but a little more memory would be

taken up. In the above example, using a pointer has saved a trivial amount of memory space, but later we will come across array pointers that can in principle save a good deal of memory.

Any variable with the POINTER attribute may also be used as a target, and it is not necessary to declare the TARGET attribute as well as POINTER. If we have

```
REAL, POINTER :: p, q, r
```

```
REAL, TARGET :: a, b, c
```

then the statements

r => b p => r

associate r with b and then p with r. Because r is a pointer, the effect of the second statement is actually to associate p with the target currently pointed to by r, i.e. to b. In other words, targeting is "transitive". The statements

r => a q => r p => q

associate p directly with the value of a, and the processor does not "remember" that this happened via q and r. If q or r is subsequently disassociated from a, p still points to a. Note that a target may be pointed to by more than one pointer: the code above leaves the target a pointed to by the three pointers p, q and r.

If r is a pointer and if a statement like

p => r

is executed at a time when r is not associated with a target, the effect is not to link p and r in any way but to leave p "hanging", and if p was previously associated with something else it will become disassociated.

There is a special statement, NULLIFY, which can be used to disassociate a pointer. The keyword NULLIFY is followed by a bracketed list of pointer names. Examples are

NULLIFY (p)

NULLIFY (q, r)

IF (ASSOCIATED(POINTER=p, TARGET=r)) NULLIFY (p)

A pointer declared within a procedure could be left with undefined status on return from that procedure to another program unit, so it is usually wise to declare pointers with the SAVE attribute.

Pointers can be of character type and may point either to a complete character string or to a substring, as long as the pointer was declared with a length matching that of the target. If the target is a substring, it must be part of a string declared with the TARGET attribute. The following code indicates how pointers could be used to work on a long character string while keeping memory utilization to a minimum.

```
! Wipe out the start of chapter 5
CHARACTER(*), TARGET :: document
CHARACTER(9), POINTER :: phrase
CHARACTER(2000), POINTER :: startchapter
CHARACTER(9), PARAMETER :: heading = "Chapter 5"
CHARACTER(1), PARAMETER :: blank = " "
.
.
.
Erase: DO icatch = 1, LEN(document)-1999
phrase => document(icatch:icatch+9)
IF (phrase/=heading) CYCLE
startchapter => document(icatch:icatch+1999)
startchapter = REPEAT(blank, 2000); EXIT
```

END DO Erase

It was explained earlier that a pointer has a name and specifies the attributes of a particular type of data, but does not have its own memory space to hold a value. The pointer assignment statement, however, associates a pointer with memory space containing the value of an ordinary data object, the "target", and the pointer name can then be used as an alias for that target. Besides that, there is another way of associating a pointer with memory space without using a pointer assignment statement. It can be done by using the ALLOCATE statement, which we met in Chapter 12 in connection with allocatable arrays. The ALLOCATE statement can be used with the names of pointers, in which case the effect is simply to associate the pointer with an area of memory for data storage. So, if we have the statements

REAL, POINTER :: x

ALLOCATE (x)

the first establishes x as the name of a real scalar data object and the second allocates space to hold the value of x. Unlike the situation when a pointer is associated with an object previously declared as a target, there is no other name for the piece of data. In fact, the above two statements have much the same effect as

REAL :: x

.

.

ALLOCATE is an executable statement and it allocates memory space during the running of the program. Moreover, memory so allocated may be deallocated by the DEALLOCATE statement, just as for arrays (Section 12.1). This might seem rather pointless in the case of a single real variable, but it could be useful for efficient memory management if, say, a long character string were involved. For example,

CHARACTER (2**20), POINTER :: megabyte

ALLOCATE (megabyte)

DEALLOCATE (megabyte)

sets up a one-megabyte character string and later allocates and deallocates the memory space dynamically. (Note, however, that the inquiry function ALLOCATED must have an allocatable array as its argument and cannot be used to check the allocation status of a pointer.)

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There exists an intrinsic function NULL of pointer type. The "value" of NULL () is a disassociated pointer. It can be used in a type declaration statement to initialize a pointer to have disassociated status, as in

REAL, POINTER :: x => NULL()

For more details, see Appendix F.

POINTER and TARGET

As an alternative to including POINTER or TARGET as an attribute in TDSs, it is possible to use separate "attribute specification statements" such as

TARGET :: x, y, z(12, 12), jswitch

POINTER :: sheet(:, :)

These are declarative statements and must appear near the beginning of a program unit following the type declaration statements.

13.2 Pointers and derived types

Pointers are not restricted to being of intrinsic data types such as REAL or CHARACTER. A pointer may also be of derived type, as in

TYPE (Partnumbers), POINTER :: assembly1, assembly2

and this could point to any variable of that type as long as it has the TARGET attribute, such as those declared by

TYPE (Partnumbers), TARGET :: UKspec, USAspec, Pilotspec

The type Partnumbers could have been defined by the block

TYPE Partnumbers

CHARACTER(24) :: shortname

INTEGER :: nbits, idbit(30), nbit(30)

LOGICAL :: stockflags(30)

END TYPE Partnumbers

and there is no need for POINTER or TARGET specifications to be included within the type definition block. Just as for intrinsic-type data, derived types may be used in pointer assignment statements and as arguments of the functions ASSOCIATED and NULLIFY:

NULLIFY(assembly2)

IF (ASSOCIATED(assembly1)) assembly2 => USAspec

The name of an associated pointer may be used in structure components, e.g.

assembly1 => Pilotspec

item = assembly1%shortname

assembly1%stockf lags = stockstatus

The third of these statements is an array assignment statement, because the component stockf lags is an array, although the complete objects declared to be of type Partnumbers are scalars. The idea that a pointer may itself be an array will be discussed in Section 13.5.

A derived-type pointer, like one of intrinsic type, can have memory space allocated to it dynamically by ALLOCATE and DEALLOCATE statements, as in the scheme

TYPE (Errormatrix), POINTER :: pmeasured, temp, pfitted

ALLOCATE (pmeasured) ! Space for data input

. (read in data "pmeasured")

.

.

.

.

.

ALLOCATE (temp, pfitted) ! Space for calculation

. (using "temp" for temporary workspace,

. calculate "pfitted" from "pmeasured")

DEALLOCATE (pmeasured, temp) ! Space no longer needed

. (write out result "pfitted")

DEALLOCATE (pfitted) ! Space no longer needed

•

Here, the objects called pmeasured, temp and pfitted are derived-type structures and they could occupy a great deal of memory space; their components could include large arrays. The ALLOCATE and DEALLOCATE statements are being used to keep the program's memory requirements to a minimum during program execution.

So far in this section we have been considering pointers to structures of derived type. In addition, it is possible for a structure to have a component that is a pointer. For example,

TYPE Employee

CHARACTER(30) :: name, jobtitle

CHARACTER(10) :: idcode

INTEGER :: ntelephone, idepartment, igrade

CHARACTER(50), POINTER :: salarydatum

END TYPE Employee

The pointer **salarydatum** could be associated with data stored separately, e.g. in the array **salaries** as below:

TYPE (Employee) :: staff(3500)

CHARACTER(50), TARGET :: salaries(3500)

CHARACTER(10) :: code

INTEGER :: iselect

code = staff(iselect)%idcode

DO i = 1, 3500

IF (code==salaries(i)(1:10)) THEN

staff(iselect)%salarydatum => salaries(i)

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EXIT END IF END DO

This selects the identity code (idcode) of a particular employee from the array staff, then runs through the array salaries until an element of salaries is found whose first ten characters correspond to that code. Then the salarydatum pointer for that particular staff member is associated with that element of salaries.

If pointers are used like this, cross-references can be created between different arrays of data. As another example, we could have a bibliography with data objects of the structure given by

TYPE Book

CHARACTER(50) :: title, author, publisher

INTEGER :: iyear, isbn1, isbn2

LOGICAL :: statusflags(6)

CHARACTER(200) :: notes

END TYPE Book

and a title index with elements of the type

TYPE Booktitle

CHARACTER(50) :: title

TYPE (Book), POINTER :: ref

END TYPE Booktitle

and an author index with elements

TYPE Bookauthor

CHARACTER(50) :: author

TYPE (Book), POINTER :: ref

END TYPE Bookauthor

The necessary TDSs might be

TYPE (Book), TARGET :: bibliography(400)

TYPE (Bookauthor) :: authorindex(400)

TYPE (Booktitle) :: titleindex(400)

and there could be procedures to read the bibliography from a disk file, create author and title indices, use the indices to interrogate the bibliography, make changes to the bibliography, and write the modified bibliography back onto disk. The important thing is that the bulk of the information is actually kept in a single array, "bibliography", while the author index and title index are relatively short and can be scanned through relatively quickly. A similar job could be done without pointers, using a system of reference numbers, but the system would then be more complex, probably less memory-efficient, and possibly more errorprone.

It is possible for a structure to have, as a component, a pointer to a data object of the same type as the structure itself. The best-known example of this sort of thing is a "linked list", i.e. a set of data items each of which "points" to another member of the set, thereby linking them all together into an ordered sequence. Consider first the type

TYPE Link

REAL :: x

TYPE (Link), POINTER :: nextlink

END TYPE Link

and suppose that there are several objects of this type:

TYPE (Link), TARGET :: alpha, beta1, beta2, beta3, &

gamma,

then we could have a situation where, say,

alpha%x = 0.34

alpha%nextlink => beta2

beta2%x = 0.79

beta2%nextlink => gamma

gamma%x = 0.04

gamma%nextlink => beta1

and so on. Each Link in the chain contains a real number and a pointer to the next link. We have created a sort of pseudoarray, i.e. a set of data items ordered into a particular sequence. In that example, each link in the chain had its own name (alpha, beta2, etc.). By using ALLOCATE statements, however, it is possible to be much more clever and to create a chain of arbitrary length while giving a name only to the first item. Using the same type Link as above, we could have

TYPE (Link), TARGET :: alpha TYPE (Link), POINTER :: beta, gamma READ (*, *) alpha%x beta => alpha DO i = 1,100 ALLOCATE (gamma) beta%nextlink => gamma gamma%x = SQRT(ABS(1.0 - beta%x**2)) NULLIFY (gamma%nextlink) beta => gamma

END DO

It is worth working through the meaning of this in some detail. First, there is a statement declaring alpha to be a targettable object of type Link. We will see shortly why it is given the TARGET attribute. The second TDS sets up names (beta and gamma) for two pointers of type Link. Being pointers, they have no memory space associated with them at this stage and both of them are going to be used dynamically to represent different data objects at different times as the program runs.

We then start the executable part with the READ statement, which simply allows a value to be given to the first component of alpha.

The DO loop is going to create a linked list of data items of the type Link, starting from alpha, and on each occasion the name beta will be used for the previously created member of the list and gamma will be used for a newly created member. So, before entering the DO loop, we have to start things off by pointing beta to the initial item, alpha. (That is why alpha was given the TARGET attribute.)

The first statement within the DO loop is ALLOCATE (gamma). This has the effect of allocating memory space to hold data under the name of the pointer gamma. This is, as declared earlier, of the type Link.

Next is a pointer assignment statement, and this points the second component of beta to the newly allocated memory space of the object gamma. In other words, the previous member of the list points to the new one that is being created.

Next, a value is given to gamma%x, the first component of gamma: in this example, it is a simple algebraic function of the preceding value beta%x.

The next statement, the NULLIFY statement, defines the association status of the second component of gamma, i.e. the pointer gamma%nextlink. When the statement ALLOCATE (gamma) was executed earlier, the pointer gamma%-nextlink was created but its association status was undefined. In fact, the association status of any pointer is initially undefined. The NULLIFY statement ensures that gamma%nextlink is, for the time being, disassociated, in the sense that it would be given the result. FALSE . by the intrinsic function ASSOCIATED. (A reference ASSOCIATED(gamma%-nextlink) would give an error without the NULLIFY statement.) To summarize: at this point in the DO loop, memory space has been allocated for a new object called gamma, the second component of the previous object (beta) points to gamma, the first component of gamma has been given a value, and the second component of gamma has "disassociated" status.

The final statement within the loop points beta to gamma; this means that beta no longer represents the previous object in the chain, but now represents the new object that has just been set up. The first time we go through the loop, this statement switches beta from pointing to the first object in the chain, alpha, and points it instead to the second object. The second time we go through the loop, this statement stops beta from pointing to the second link and points it to the third: this is interesting because the second link is then left with no name at all, although it consists of actual data occupying actual memory space. Subsequently, it will be possible to get access to this data only through the pointer alpha%nextlink.

When the program goes through the DO loop on the second and subsequent times, the statement ALLOCATE (gamma) causes additional new memory space to be associated with the pointer gamma, and the previous association of gamma is broken off. Incidentally, this situation is different from the case with allocatable arrays: to ALLOCATE a currently allocated array is an error, but to ALLOCATE a currently-allocated pointer is not.

In our example, when the DO loop has been executed 100 times there will be 101 objects in memory, each containing a real value and a pointer to the next one. The first in the chain has the name alpha, and the last is still pointed to by beta and gamma, but the other 99 are not directly accessible. To look through the chain of data we would need code such as

beta => alpha

DO

WRITE (*,*) beta%x

IF (.NOT.ASSOCIATED(beta%nextlink)) EXIT

beta => beta%nextlink

END DO

which uses the pointer beta to run from one link to the next. You know you are at the end of the list when a link is reached whose forward pointer has "disassociated" status.

This example has been explained in detail because it teaches some very important facts about the effect of the ALLOCATE and NULLIFY statements on pointers, because of the interesting concept of nameless data and because it shows how pointers within derived types could be used to invent pseudoarrays if ordinary arrays did not already exist in Fortran!

The type called Link, above, included a pointer component so that one object could point to another. However, if a type were constructed with two pointer components, then each object could point to two others. For example, a family tree could in principle be constructed on the basis of the type:

TYPE Person

CHARACTER(30) :: name

INTEGER :: nyearofbirth

TYPE (Person), POINTER :: mother, father

END TYPE Person

While on the subject of derived-type structures, there is a question that arises about the meaning of assignment statements between structures that have pointer components. Taking the example of the type Person immediately above, and having

TYPE (Person) :: candidate, brother

. . . candidate = brother

the assignment statement is equivalent to

candidate%name = brother%name

candidate%nyearofbirth = brother%nyearofbirth

candidate%father => brother%father

candidate%mother => brother%mother

the last two being pointer assignments and not ordinary assignments. In other words, an ordinary assignment statement between structures is equivalent to ordinary assignments between their non-pointer components and to pointer assignments between their pointer components. Of course, the programmer is at liberty to change this by providing a defined-assignment subroutine as in Section 12.10.

13.3 Pointers and procedures

When a procedure has an argument that is normally an ordinary variable or expression, the actual argument may be a pointer as long as it has a definite target at the time. This is true of intrinsic procedures as well as external procedures or module procedures. Using a pointer in this context is just like using it on the righthand side of an ordinary assignment statement, and the pointer is no more than an alias for its target.

A slightly more complicated situation arises if a dummy argument is declared with the POINTER attribute within a procedure. In that case, the corresponding actual argument must also be a pointer, and an explicit interface to the procedure must be provided so that the processor always "knows" that a pointer argument is expected. When the procedure is referenced, what happens is that the dummy argument pointer is associated with the target of the actual argument. On return from the procedure, the actual argument is associated with the target of the dummy argument, but if the latter target is local to the procedure and is not saved (with the SAVE keyword) then the actual argument will be left with undefined association status. Incidentally, a dummy argument that is a pointer is not allowed to be declared with the INTENT attribute. Here is an example of a procedure with pointer dummy arguments:

SUBROUTINE Switchpoint (a, b) CHARACTER(*), POINTER :: a CHARACTER(*), POINTER :: b CHARACTER(LEN(a)), POINTER, SAVE :: c IF (LEN(a)/=LEN(b)) THEN NULLIFY (a, b) ELSE c => a ! Point c to the target of a a => b ! Point a to the target of b b => c ! Point b to the target of c NULLIFY (c) END IF

END SUBROUTINE Switchpoint

It is also possible for a dummy argument to have the TARGET attribute, but here again it is necessary to provide an explicit interface to the procedure. The following procedure has both TARGET and POINTER arguments:

SUBROUTINE Randomfork (from, toleft, toright)

USE Typedefs

TYPE (Structure), POINTER :: from

TYPE (Structure), TARGET :: toleft, toright

REAL :: x

CALL RANDOM (x)

IF (x>0.5) THEN

from => toleft

ELSE

from => toright

END IF

END SUBROUTINE Randomfork

To round off this section, it remains to consider the case where a function result is a pointer. This is allowed in Fortran, but (as for pointer and target arguments) an explicit interface is then needed. The next example has as its argument a character string object that itself is a pointer, and the function result is a pointer to one individual character within that string:

FUNCTION Pickstar (string) RESULT (star) CHARACTER(1), POINTER :: star CHARACTER(*), POINTER :: String IF (ASSOCIATED(string)) THEN k = SCAN (string,"*") IF (k==0) THEN NULLIFY (star) ELSE star => string(k:k) **END IF**

ELSE

NULLIFY (Star)

END FUNCTION Pickstar

When a function's value is a pointer, the RESULT notation must be used as in a recursive function.

13.4 Exercises 13.A

13. Based on the type Link in Section 13.2, write a program that will read in and store indefinitely long

A1 sequence of integers from the keyboard. The input of the number 99999999 is to be used to indicate that the sequence has ended. After that, the program should calculate and write the average of the numbers.

13. Write a function whose argument is a rank-one assumed-shape real array and that converts the array

A2 into a linked list of the type Link in Section 13.2. The function's result is therefore to be a scalar pointer of derived type.

13. The derived type

A3

TYPE Character_Chain

CHARACTER(1) :: q

TYPE (Character_Chain), POINTER :: qnext

END TYPE Character Chain

could perhaps be used for variable-length chains of characters. This could offer some advantage over ordinary character strings because the latter cannot vary in length during program execution. Try to write a subroutine and interface to define the concatenation operator (//)for these character chains (but not for arrays of them!), a function like the intrinsic LEN function, and a subroutine that will write out a Character_Chain. This project could be developed much further, e.g. with functions to convert data between Character_Chain and ordinary character string types.

13.5

Array pointers

Towards the end of Section 13.1 it was shown that pointers can be used to economize on memory space if they are associated with long character strings. Likewise, pointers can be associated with derived-type structures (Section 13.2). In both these cases the pointers themselves were scalar, although pointing to large or complex structures. But pointers do not necessarily have to be scalar: Fortran allows for pointers to be

arrays, in which case they have properties similar in many respects to the "allocatable arrays" described in Section 12.1.

Array pointers are declared with the POINTER attribute and with an array specification using the same colon notation as an allocatable array, as in the TDSs

COMPLEX, POINTER, DIMENSION(:) :: coefficients, roots

REAL, POINTER :: rates(:,:)

CHARACTER(2048), POINTER :: k2(:)

CHARACTER, POINTER :: tiestring(:, :, :)

TYPE (Person), POINTER :: family(:)

These statements fix the ranks of the arrays by the numbers of colons after each name, but the shapes are not fully determined at this stage.

Array pointers may point to array targets, or to sections of them, which would therefore need to be declared with the TARGET attribute as in

INTEGER, TARGET :: jobcodes(180)

Array pointers cannot be given the ALLOCATABLE attribute, because in a sense they are allocatable anyway. However, array targets may be allocatable arrays:

INTEGER, TARGET, ALLOCATABLE :: jobcodes(:)

Array pointers, like scalar pointers, may be used in pointer assignment statements. The targets need not be whole arrays: array sections are allowed, but not with vector subscripts. If the target is an allocatable array, it needs to have been allocated before the pointer assignment statement is executed.

One effect of an array pointer assignment statement is to determine the shape of the pointer: the pointer's extent in each dimension, and the bounds of its subscripts, are taken from the target array. Once an array pointer is associated with a target, it may be used in an ordinary assignment statement, representing its target's value. The inquiry function ASSOCIATED may be used with an array pointer just as with a scalar pointer.

It is possible to make use of array pointers without having named targets at all, with the statements ALLOCATE, NULLIFY and DEALLOCATE. Although these statements have been met previously in this chapter, it is worth reviewing here what they will do with array pointers as arguments.

ALLOCATE can be used to fix the shape of an array pointer and at the same time to create memory space to which it will point. The syntax is just like that for allocatable arrays and in fact the same statement could allocate a mixture of pointers and allocatable arrays, e.g.

ALLOCATE (rates(0:3, 0:3), family(nlinked), &

jobcodes(143), STAT=mtest)

.

.

.

.

.

.

NULLIFY disassociates target space previously associated with its arguments, but does not deallocate it, i.e. the memory space still exists and may hold data, but is no longer pointed to by this pointer. It is important to remember that the ALLOCATE statement, with a pointer argument, allocates new space but like NULLIFY does not deallocate the old space. ALLOCATE can therefore be used repeatedly with the same pointer argument to create an unlimited amount of "hidden" memory.

The following example illustrates the use of an array pointer, the ALLOCATE statement, and an assumed-shape array:

REAL, POINTER :: x(:, :)

ALLOCATE (x(1000, 1000))

.

.

CALL Analysis(x)

SUBROUTINE Analysis(z)

REAL, INTENT(IN) :: z(:, :)

.

.

When Analysis is called, z takes its shape from x's allocation. Because Analysis has an assumed-shape dummy argument, it needs an explicit interface.

To disassociate a pointer and also to deallocate the memory space it is necessary to use the DEALLOCATE statement, but this is only applicable if the pointer was originally allocated by an ALLOCATE statement: if the pointer was associated with a named target by means of a pointer assignment statement, DEALLOCATE cannot be used. Also, if an array pointer is associated with an allocatable array, then the allocatable array cannot be deallocated through the pointer: in fact, it is not permitted to DEALLOCATE an array pointer that is currently associated with an allocatable array.

To avoid confusion, it is best to distinguish sharply between two styles of array pointer usage:

- not using data with the TARGET attribute, and without using pointer assignment statements, but using ALLOCATE and DEALLOCATE statements, and possibly associating the array pointers to assumedshape dummy argument arrays by procedure reference;
- using named TARGET data (which could be allocatable arrays), associated with the array pointers by use of pointer assignment statements.

Case 1 is very similar to the straightforward use of allocatable arrays described in Section 12.1, but with the crucial difference that an array pointer may be used in circumstances where an allocatable array may not, i.e. as a dummy argument, a function value, or a derived-type structure component. So we have array pointers being used *in place of* allocatable (or other kinds of) arrays.

Case 2 above is more likely to arise if the data is primarily stored in large allocatable arrays and the array pointers are used to latch onto parts of that data, i.e. with array pointers being used as ancillaries *alongside* target arrays of other sorts.

In practice, array pointers tend to be used most effectively in applications of type 1 above, to overcome the limitations of allocatable arrays. In particular, if a derived type is to contain a variable-sized array then it can only be done by using an array pointer. This is the basis of the implementation of the VARYING_STRING data type described in Appendix C.

13.6

Exercises 13.B

13. Set up a system for dealing with a derived data type that is to represent sets of intervals on the real line.

B1 In other words, each object of this type may represent any number of non-overlapping intervals, each interval being defined by two real numbers (x_1, x_2) , where $x_1 < x_2$. (Single-point "intervals" with $x_1 = x_2$ can be excluded for simplicity, i.e. we are dealing with mathematically "open" sets.) Defined operators should be designed to calculate the sum (union) and product (intersection) of interval sets. There can be a function measuring the total extent of an interval set. Generalized forms of elementary mathematical functions (such as the cube root) can be written which map one interval set onto another.

13. Following on from Exercise 12.B5, set up a derived type to handle sparse matrices using array pointers B2 to achieve maximum flexibility in minimum memory.

CHAPTER 14 Overview

A few remaining features of the Fortran 95 language are described in the early part of this chapter. In particular we explain the use of procedure names as procedure arguments, which is important; and the GO TO statement, which is a powerful statement but generally deprecated. This leads to a consideration of coding conventions and the movement towards defining a "core" Fortran 95 language.

The later part of the chapter is devoted to a broader discussion of the programming process including the use of structure plans, the general layout of statements within a program unit, and the design of a program as a set of program units of different kinds.

14.1

Procedure names as procedure arguments

So far we have discussed procedures whose dummy arguments are data objects of various kinds. However, it is also possible for a procedure to have, as an actual argument, the name of yet another procedure. This could be useful if, for example, a procedure is to be written to calculate the integral of an arbitrary function. We could have a subroutine with the structure

SUBROUTINE Integrate (Func, alimit, blimit, result)

REAL, EXTERNAL :: Func

REAL, INTENT (IN) :: alimit, blimit

REAL, INTENT (OUT) :: result

REAL :: x! local variable

- . By references to Func(x), calculate an
- . approximation to the integral of that function
- . between x=alimit and x=blimit.

END SUBROUTINE Integrate

The attribute EXTERNAL in the first REAL statement tells the subroutine that Func is the name of a realvalued function. Note that a dummy argument that is a procedure name may not be given an INTENT attribute. In fact it is always the case that the procedure-name information is conveyed in, not out.

The above subroutine could be called with any actual function name as the first argument, as long as that function is also declared EXTERNAL in the calling program unit and actually exists as an external or module function. Naturally, the actual argument associated with Func must have the same characteristics as Func, e.g. in this example it must be a scalar real-valued function with one real scalar argument. A procedure with a procedure-name argument does not necessarily need to be given an explicit interface in the program unit that calls it.

An actual argument could alternatively be the specific name of an intrinsic function, in which case it should be declared with the INTRINSIC attribute in the calling program unit: but there are awkward restrictions on the names of the intrinsic functions that may be used in this way, so this is best avoided. In most realistic applications a dummy procedure will correspond to an external or module procedure. Even if actual arguments are intrinsic functions, the corresponding dummy arguments should still be declared as EXTERNAL in the procedure itself, because the EXTERNAL designation is used there simply to show that a dummy argument is the name of a procedure (be it external, module or intrinsic) rather than a data object.

The next example is inspired by a feature of the functional programming language Miranda:

FUNCTION Map (Func, array)

REAL, EXTERNAL :: Func

REAL, INTENT (IN) :: array(:)

REAL :: Map(SIZE(array))

INTEGER :: k

k = SIZE(array)

FORALL (i = 1:k) Map(i) = Func(array(i))

END FUNCTION Map

This is a function whose first argument is a function (of a scalar argument) and whose second argument is a rank-one assumed-shape array to all of whose members that function is to be applied. The result is an array of the same length as its second argument. Note that the function Map needs an explicit interface, both because it has an assumed-shape argument and also because it has an array-valued result. However, Map is not particularly useful in Fortran: although it would allow an array expression such as

Map (Cuberoot, dataset)

to be used, a better approach to the problem would be to ensure that functions like Cuberoot are written as elemental (Section 11.3) so that the expression

Cuberoot (dataset)

would do the trick by itself. There are other examples of amusing but not-very-useful procedures with dummy-procedure arrays, such as

FUNCTION Twice (F, x)

REAL, EXTERNAL :: F

REAL :: Twice

REAL, INTENT (IN) :: x

Twice = F(F(x))

END FUNCTION Twice

and

FUNCTION Compose (x. A, B, C, D, E, F, G)

REAL :: Compose

REAL, EXTERNAL, OPTIONAL :: A, B, C, D, E, F, G

REAL, INTENT(IN) :: x

REAL :: store

store = x

IF (PRESENT(A)) store = A(store)

```
IF (PRESENT(B)) store = B(store)
```

IF (PRESENT(C)) store = C(store)

IF (PRESENT(D)) store = D(store)

IF (PRESENT(E)) store = E(store)

IF (PRESENT(F)) store = F(store)

IF (PRESENT(G)) store = G(store)

Compose = store

END FUNCTION Compose

Compose (x) just returns the value of x. Compose (x, EXP) is equivalent to EXP(X). compose (x, EXP, SIN) is equivalent to SIN(EXP(x)), and so on.

In any procedure that calls this function, there must be an explicit interface to Compose because there are optional arguments. Each actual argument corresponding to one of the dummy arguments A–G must be the name of an external or intrinsic function, or it may be the name of an associated module procedure, or it may even be a dummy procedure name within the context of the calling procedure itself (with an EXTERNAL declaration) corresponding in turn to an actual argument in yet another procedure. This rather artificial example illustrates the point:

FUNCTION Arbitrary (aleph) REAL :: Arbitrary, aleph REAL, INTRINSIC : : EXP . . . CALL Caller (EXP) . . . SUBROUTINE Caller (Z) **REAL, INTRINSIC :: SIN**

REAL, EXTERNAL :: Gamma

REAL, EXTERNAL :: Z

INTERFACE

FUNCTION Compose (x, A, B, C, D, E, F, G)

REAL :: Compose

REAL, EXTERNAL, OPTIONAL :: A, B, C, D, E, F, G

REAL, INTENT(IN) :: x

END FUNCTION Compose

END INTERFACE

.

Y = Compose (0.4, SIN, Gamma, Z)

The effect is to calculate EXP (Gamma (SIN(0.4))), whatever the external function Gamma may be. Incidentally, although a self-reference such as

Compose (x, EXP, Compose)

may have a clear mathematical meaning (this would be equal to EXP(X)), it would not be permissible as a Fortran expression because (a) a Fortran procedure is not allowed to refer to itself, directly or indirectly, unless it is defined with the RECURSIVE keyword, and, more to the point, because (b) the characteristics of the real argument Compose and those of the dummy argument B are different and do not match.

In Fortran, the use of procedure names as the arguments of procedures is in fact a rather awkward and inadequate approach to the larger question of allowing variables to represent procedures. For example, it might be nice to have the possibility of code such as

IF (x > 0.0) Trig = SIN IF (x < 0.0) Trig = TAN y = Trig (x)

but this is not permissible in Fortran. No procedure-name may appear on the right of an assignment statement (like SIN and TAN above) without arguments that give it a particular value. It is only as a procedure's dummy argument that a variable may "stand in" for the name of a function, and then only to transmit the name into the procedure, not out of it. The code

CALL Getfunction(Func)

x = Func(y)

to obtain the identity of Func from the subroutine and then apply it to y, could not arise in Fortran because the subroutine Get function could not be written: one might start with

SUBROUTINE Getfunction (Dummyfunc)

EXTERNAL :: Dummyfunc

but then there is no way, in legal Fortran syntax, of associating Dummyfunc and thereby Func with some actual function. There exist "functional" programming languages that allow function names to be manipulated almost as flexibly as data objects, but Fortran is not one of them, although some proposals for a future version of Fortran (Fortran 2000?) have included "procedure variables".

Nevertheless, in practice the range of real-life problems that Fortran can solve seems undiminished by the fact that it is not a "functional" language in the full sense; and Fortran's existing syntax for procedure-name arguments allows adequately for code to calculate such things as integrals, zero-points, and the maxima and minima of arbitrary functions.

14.2

Varying-length character strings

Fortran allows for just five intrinsic types of data: REAL, INTEGER, COMPLEX, LOGICAL and CHARACTER, plus the obsolete type DOUBLE PRECISION. When data of CHARACTER type are declared, the lengths of the character strings must be specified once and for all. For many purposes this is an irksome restriction and it would be more convenient if the programmer could forget about the lengths of strings and leave it to the computer to allocate whatever memory is needed, which could vary during the execution of the program. In fact, Fortran's derived-type facility makes it possible for varying-length strings

to be defined and used. Because of the usefulness of varying-length strings, they have been adopted as an auxiliary to the standard Fortran language. Full details are given in Appendix C.

14.3 INCLUDE

An unusual but potentially useful Fortran feature is the "INCLUDE line", whose general form is

INCLUDE character-string

where *character-string* is a character constant (not just the name of a character constant) that is the name of a file containing Fortran source code. The INCLUDE line is not, technically, a Fortran statement itself: but before compilation it causes one or more statements to be read from the named file and inserted at the position of the INCLUDE line. INCLUDE lines may be nested, i.e. the file referred to may itself contain INCLUDE lines. INCLUDE lines a form of data input, as in

PROGRAM Demonstrate

```
real :: datastream(100) = (/(0.0, i=1,100)/)
```

```
INCLUDE "C:\f95\scratchdata"
```

where the file called "C:\f95\scratchdata" might contain Fortran code such as

datastream = (/2.4, 3.1, 6.0,/)

allowing up to 100 real numbers to be input. For general purposes, a utility subroutine could be written like this:

SUBROUTINE Fortran95_Data (data)

REAL :: data(:)

INCLUDE " /home / counihan/ f 9 5_input_data "

END SUBROUTINE Fortran90_Data

while a file is arranged containing

data = (/...../)

The size of data would have to be declared in the program unit that calls the subroutine Fortran95_Data.

Because INCLUDE works at compilation time, the file to which it refers cannot be written by the program itself while executing. However, if the program runs repeatedly, there is no reason why it should not write a file during one run that will be read via an INCLUDE line and form part of the program for the next run.

14.4 GO TO: the pariah of Fortran

All the Fortran statements that we have met so far must start with a letter of the alphabet. However, before that it is possible to have a sequence of digits serving to label the statement, as in the examples

1 n=1+INT(x) 341 CALL RANDOM(x) 90 nh6 = Firstroot(g1, g2, g3, g4, g5, g6)

8 1=0; 9 j=0; 10 k=0

A label must have at least one non-zero character, it must be separated by at least one blank from the start of the statement itself, it must be unique within its program unit, it may not consist of more than five digits, and it may not have blanks embedded in it. Labels need not be in numerical sequence, although in the examples below they are ordered in the natural way. Labels can be used in Fortran in a number of minor ways that add nothing to the functionality of the language, but they have one important use: to redirect the flow of execution through a *GO TO* statement, which has the simple form

GO TO 341

or whatever might be the number labelling the statement you want to go to at that point. The keyword GO TO must be followed by an actual label, not by an expression or variable name. The GO TO statement may be contingent on an IF, as in

26 IF (x<0.0) GO TO 27

y = SQRT(x)

It can sometimes be handy to have a "do-nothing" statement to hang a label onto; a special statement, CONTINUE, exists for this purpose, so for example

27 CONTINUE

could complete the previous example.

GO TO statements can be used to write extremely opaque code very concisely, as in

READ (*,*) j

j = MAX(1,ABS(j)); k=0 1 If(MOD(j, 2) .EQ.1) GO TO 2 j=j/2; k=k+1; GO TO 1 2 j=j+k; IF(MOD(j, 3) .EQ.1) GO TO 3 GO TO 1 3 j=(j-1)/3 WRITE (*,*) j

Note that there is scarcely any point in ever labelling non-executable statements such as TDSs. It would be an error to GO TO a non-executable statement.

It is arguable that the GO TO statement does nothing that cannot be done with more clarity in Fortran in other ways (e.g. by calling a subroutine). However, GO TO is seductively simple to use and really comes into its own when you want to stitch a modification into a previously existing program. For example,

GO TO 999

```
.
.
```

```
999 CONTINUE
```

will simply bypass all the code between those two statements and could be a useful trick when debugging a program. However,

Bypass: IF (.FALSE.) THEN

END IF Bypass

.

does much the same thing. Because of the potential for its misuse, the once-ubiquitous GO TO statement is deplored by most teachers of Fortran and has become thoroughly disreputable, although it will always occupy a proud place in the history of computing. Nevertheless, GO TO (combined with the IF statement) can be used to simulate all of Fortran's control structures, the array system, and the procedure call system. In fact, a programming language with full mathematical functionality can be made up from little more that IF, GO TO, and the simple assignment statement.

Assigned GO TO

A special statement, ASSIGN, can be used to associate a particular statement label with an integer variable, as in

ASSIGN 10 TO ipoint

The integer variable could subsequently be used instead of a statement label in a GO TO statement, or instead of a format statement label in an i/o statement.

Computed GO TO

GO TO may be followed by a bracketed list of statement labels, and then by an integer expression, as in

GO TO (100, 31, 41, 51) kchoice

and the effect is that control passes to the first, second, third, etc. statement in the list according to whether the integer expression (kchoice in that example) has value 1, 2, 3, etc. If the integer is larger than the number of labels listed, or is less than 1, nothing happens.

Arithmetic IF

A statement such as

IF (handle) 20, 30, 40

transfers control to the statement labelled 20, 30 or 40 according to whether handle is negative, zero or positive. The labels 20, 30 and 40 in this example are arbitrary, but there must be a list of three (not necessarily distinct) labels. The name handle is also an arbitrary example: any real or integer expression may appear between the brackets.

14.5

Coding conventions and "Core" Fortran 95

Because of the language's history, Fortran contains a number of obsolescent or unessential features that a new programmer would be well advised to avoid. These are features which are not functionally necessary, i.e. there's nothing you can do with them that you cannot do without them. Many of them, mentioned only for the sake of completeness, are relegated to small type in this book.

It is strongly recommended that the obsolescent features of Fortran be avoided. Additionally, there are many features whose usage is a matter of taste and personal opinion. At the same time as avoiding obsolescent language features, it is a good idea also to adhere to voluntary conventions that will make your code easier and more pleasant to read, and therefore easier for somebody else to read and understand.

Some recommended coding conventions are, like the avoidance of obsolescent features, implicit in the examples given throughout this book (for example, the avoidance of the DIMENSION attribute). Some worth highlighting are

- 1. Stick to the convention described in Section 2.5 and followed in this book for the use of lower-case and upper-case letters—or, alternatively, use a different convention. But do not mix upper case and lower case indiscriminately!
- 2. Avoid IMPLICIT and stick to the default initial-letter convention for naming real and integer variables. (But beware—many Fortran experts disagree strongly with this!) Ideally all variables should be specified in type declaration statements except for the integers that are used as loop indices *within* statements, e.g. within array constructors.
- 3. If a word already has a meaning in Fortran, e.g. as a keyword in an intrinsic procedure, do not use it as a name for something else.
- 4. Use only double quotes, not single quotes (apostrophes), to delimit character strings.
- 5. In expressions and assignment statements with mixed data types, type conversions should be explicit except in the most trivial of cases (e.g. avoid expressions like x + (1/2) and x == 0 if x is real).
- 6. Use parentheses freely rather than depending on the rules for the order of operations (e.g. do not use expressions such as $x/2^{**}y/2$).
- 7. Always label IF constructs, DO constructs, etc.

This list could be extended considerably. In fact, in many research centres and laboratories where Fortran is used extensively, there are coding conventions that enforce a "house style" of Fortran.

If we go further down this road, it is possible to identify a recommended subset of Fortran 95—"Core Fortran", if you like—which retains all the elegance and power of the language while rejecting large parts of it that are unessential. "Core Fortran" proposals typically involve rather Draconian restrictions such as:

- 1. eliminating GO TO and statement labels entirely;
- 2. drastically pruning the i/o facilities;
- 3. always using generic rather than specific names for intrinsic procedures;
- 4. making all array dummy arguments of assumed shape, and all character dummy arguments of assumed length;
- 5. eliminating non-pure functions;

and, again, the list could be continued. No standard "Core Fortran 95" has been agreed by the programming community, but there is a widely-felt need to create a new, compact language out of the best features that Fortran offers.

14.6

Structure plans; a case study in program design

Of necessity, the bulk of this book has been about the syntax of Fortran and the rules the govern how programs *may* be constructed. Little has been said about how they *should* be constructed, or about how to systematically set about finding the Fortran solution to a complex problem. But, very often, the hardest part of a programmer's task is not the actual coding but the process that must precede the coding—finding out how in principle the problem can be solved, or finding the best solution if there is more than one, or perhaps,

in some cases, establishing that the problem has no solution. And then, if the program is likely to be a large one, there is the skill of designing it as a set of program units. A simple program might be written straightforwardly as a single program unit, and for a slightly more complex problem a few external procedures might be tacked on to the main program unit when the need for them appears; but a much more systematic design process is needed for largescale real-life programming.

This section and the next are an attempt to redress this imbalance by drawing attention to some of the skills involved in program design. In this section, we look at the problem-solving process behind the writing of a single-unit program to carry out a certain mathematical task. In particular, we focus on the concept of a "structure plan". In Section 14.7 we will review the structures of the different kinds of program units that might fit together as parts of a large Fortran program.

The problem we consider in this section is the "zero-point" problem. It is sometimes necessary to be able to find the zero-points of functions: in other words, for a given real function y(x), to find where its curve crosses the x axis. Can we write a Fortran procedure to do this? We will analyze this problem in some detail to see how to proceed in defining a problem, deciding on a mathematical method of solving it, setting out a structure plan for a Fortran program, and finally writing the program itself. However, it is important to understand that there is no unique solution to this problem. No two programmers, no matter how experienced, would approach it in exactly the same way or arrive at exactly the same solution. Indeed, there does not even exist an optimal solution to the problem as posed. Before trying to optimize the solution, further questions would first have to be asked - is it important that the procedure should work quickly? Is memory space at a premium? With what precision is the zero-point to be found? How should the procedure respond to "pathological" functions, such as those having infinite numbers of zeros? Can the procedure assume that y (x) is continuous? Or that it is differentiable? Questions like this are non-nit-picking: they are the important first step towards solving the problem and writing the program. When the answers to such questions are made explicit, they comprise a detailed "specification" of the procedure or program, i.e. a statement of how the procedure is required to perform under any circumstances. The programmer often discovers surprisingly late that the program specification is ambiguous or neglects certain possibilities, or that the problem itself is badly posed. It is no good asking for a programme to calculate the square root of a number without specifying what you will want if the number is negative—a trivial example, but it is mirrored in far-fromobvious ways in the posing of more complex problems.

But let us proceed. Let us write an external function called zeropoint.

What will be the arguments of zeropoint? One argument springs to mind, namely the function y(x) whose zeros are to be found. So, we must write a "function of a function", with the function y being represented by a dummy procedure name. In Fortran, let us use Y as the dummy procedure name. So, we will have a function whose first line might be

FUNCTION Zeropoint (Y)

Then, the first declarative statements must specify the characteristics of Zeropoint and of Y. Zeropoint will be of type REAL, since we are dealing mathematically with real variables. Should zeropoint be a scalar or an array? If the function has more than one zero-point, and we want to find them all, then perhaps zeropoint should be an array. For the time being, let us take it that the task is to find just one zero-point. But this question must be borne in mind and perhaps reconsidered at a later stage.

The function Y, similarly, is of REAL type. Since Y is a function it must be declared here as EXTERNAL: this is just so that the compiler will know that Y is a function rather than an ordinary variable. So we have, so far,

FUNCTION Zeropoint (Y)

REAL :: Zeropoint

REAL, EXTERNAL :: Y

At this stage it is wise to think a little about how this function will be called from elsewhere. Must there be an explicit interface? What are the constraints on the actual argument corresponding to Y?

In fact, as Zeropoint stands, the rules of Fortran do not require it to have an explicit interface, although it would need one if Zeropoint were an array. When Zeropoint is referenced, the actual argument corresponding to Y must be the name of a Fortran function. It may not be a real number or a real constant. To ensure this, the actual argument must, in the calling program, be declared as EXTERNAL or INTRINSIC, or it must be a module procedure accessed by a USE statement or by host association in the calling program. Whichever option is taken, it does not affect the EXTERNAL statement in Zeropoint itself. In the context of the function itself, EXTERNAL is used to indicate the functional character of Y even if the corresponding actual argument will be an intrinsic function. In fact, the simplest way to work will be for the functions whose zeros are to be found to be supplied as external functions in Fortran. To avoid any error or inconsistency, they should have the same characteristics as Y, i.e. they should be scalar-valued real functions of a single real variable.

The mathematical problem

Well, we have started to write the program, but how are we going to solve the problem? For this, some mathematical knowledge and a little imagination are required. Patience may also be needed: few people would be able to think of a good solution without reflecting on the problem for some time.

One possible way forward is for Zeropoint to choose random values of a variable x in the hope of finding by chance a value of Y(x) which is close to zero. This idea immediately raises a number of questions. Can we search the whole range of x, from - to + ? If there is a zero, can we be certain of finding it? With real numbers, the chance of finding an exactly zero value of Y is in most cases infinitesimal, so what do we mean by "close to zero"?

In fact, whatever algorithm might be used, a little thought shows that Zeropoint cannot expect to find a zero-point exactly, but must use some sort of iterative process to approach it. The value of Zeropoint will therefore be an approximation, albeit a good approximation.

Moreover, without checking the value of Y(x) for every possible value of x —an impossibility since x is a real number—we cannot be absolutely certain of finding a zero of Y even if several zeros exist. It is therefore possible that no value can be assigned to zeropoint. And if no zero exists, then of course no value will be found no matter how good the program.

The problems of searching over an infinite range of x are intractable, mathematically and computationally, and should be avoided. In any case, this problem is avoidable. For example, the zeros of the function y(x) over the whole infinite x range are the zeros of the function $y(\tan(\theta))$ over the finite range $(-1/2\pi, +1/2\pi)$ in θ . By changing variables, an infinite range can be converted to a finite one. It is therefore reasonable to modify the specification of zeropoint, and to ask that it looks for a zero-point only within a certain range. Specifying the range with additional arguments, we could have

FUNCTION Zeropoint (Y, xmin, xmax)

REAL :: Zeropoint, xmin, xmax

REAL, EXTERNAL :: Y

There is an additional advantage in doing this. The function Y(x) may not be defined for all values of x, and there may be values for which it is infinite. To avoid errors arising from calls to Y in such circumstances, the call to zeropoint can limit attention to a range in which Y is known to be defined and finite.

Also, in view of the discussion above, zeropoint should allow for the possibility that no zero-point value is found. One way of doing this is by introducing a fourth argument:

FUNCTION Zeropoint (Y, xmin, xmax, f)

REAL :: Zeropoint, xmin, xmax

REAL, EXTERNAL :: Y

LOGICAL :: f

and the logical argument f will be returned with a true value if and only if a zero-point is found. If it is not, f will be false and an arbitrary value (say, zero) will be assigned to Zeropoint itself.

This gives us a possible way of dealing with the problem of multiple zeros. If the Zeropoint function finds a zero of Y(x) at x-xzero, then Zeropoint could be called again with the interval (xmin, xmax) replaced by (xmin, xzero). As long as the specified ranges are interpreted as excluding their boundary points, the latter call will not give a result repeating xzero but will return a second zero-point, if there is one, below xzero. If there is no such point, then we will know because f will be returned false. Having found (or not found) a second zero to the left of xzero, we can then turn our attention to the right of it by looking in the interval (xzero, xmax).

It therefore makes sense to confine the specification of zeropoint to the finding of a single zero-point of the function Y (x). Apart from the fact that we could never be certain of finding all the zeros anyway, a program utilizing the Zeropoint function could easily look for additional zeros, if the programmer wished, by invoking Zeropoint again for the intervals on either side of the first zero to be found. This vindicates the decision above to make Zeropoint a scalar-valued, not array-valued, function.

A structure plan

But how are we to set about actually finding a zero point? The considerations above are important, but we still have not solved the heart of the problem. There are many different ways in which one might proceed, but one way is first to notice that if Y (xmin) and Y (xmax) are different in sign, then Y must pass through a zero value somewhere in the interval. If the chicken gets to the other side, it must cross the road. Unless Y is undefined or has infinite values in the interval, then if Y changes sign between two end points it has a zero between them.

This suggests the following program structure for Zeropoint:

- Step 1. Evaluate Y(xmin) and Y (xmax). For the time being, suppose that their signs are opposite so that...
- Step 2. Y has a zero between xmin and xmax.

- Step 3. Letxmiddle = (xmax-xmin)/2, and evaluate Y(xmiddle).
- Step 4(a) If Y(xmiddle) has the opposite sign to Y(xmin): Y has a zero between xmin and xmiddle. *Replace* xmax by xmiddle. Alternatively,
- Step 4(b) if Y (middle) has the opposite sign to Y(xmax): Y has a zero between xmiddle and xmax. *Replace* xmin by xmiddle.
- Step 5. Since Y(xmin) and Y(xmax) have opposite signs, either 4(a) or 4(b) above must be true. Having replaced either xmin or xmax by xmiddle, we still have an interval within which we know there is a zero of Y; but the width of the interval is half what it was at step 2. Now, go back to step 2 (with the halved interval) and repeat steps 2–5 again and again, halving the interval each time, until the width of the interval is so small that, for all practical purposes, the zero-point has been reached.

This is a "structure plan". It is not Fortran, but it is a way of representing the layout of what might evolve into a Fortran procedure. All programmers use structure plans to some extent, often informally, according to their personal notation, without ever having been taught to do so. A structure plan is not a distraction from the business of writing the Fortran or a sign of intellectual weakness, like counting on your fingers: it is usually the quickest way to arrive at a sound program.

The plan above seems to be an acceptable algorithm for finding the value of Zeropoint: it is an iterative process which is guaranteed to converge on a suitable point. Since the width of the interval is halved at each iteration, an initial interval given by (say) xmin=0 and xmax=1 would give a value of Zeropoint precise to within one part in a million after 20 iterations.

The only remaining problem arises at step 1. What if Y (xmin) and Y (xmax) do not have different signs? If Y (xmax) has the same sign as Y (xmin), then a possible course of action would be to search for a value of x, between xmin and xmax, for which Y (x) has the opposite sign to Y (xmin) and Y (xmax). If such a value of x is found (say, xopp), then a zero-point exists both in the interval (xmin, xopp) and in (xopp, xmax). The algorithm of steps 2-5 above could then be applied to either of those two intervals.

So we need a way of searching the x interval (xmin, xmax) for a value of Y(X) of a certain sign. A suitable method would be simply to pick points at random until a value of Y is obtained having the desired sign. If, after a certain number of tries, no such point is found, then it can be taken that Y(X) possesses no zero in the specified interval and the program must return from Zeropoint with the logical "flag" f set false. How many tries should there be? Mathematically speaking, one can never be absolutely sure that Y does not change sign in the specified interval, as discussed above, but it would be reasonable to give up the search after, say, 10000 tries.

To implement this procedure, step 1 above could be broken down into the following substeps:

- Step 1(a) Evaluate Y(xmin) and Y (xmax). If their signs are opposite move directly to step 2.
- Step 1 (b) Choose a random number (xopp) between xmin and xmax. Evaluate Y(xopp).
- Step 1(c) If Y(xopp) has the same sign as Y (xmin), go back and repeat step 1(b). Do this up to 10000 times, after which go to step 6. If Y(xopp) has the opposite sign to Y(min), then...
- Step 1 (d) Give either xmin or xmax the value of xopp, and pass on to step 2.

Step 6. No zero-point can be found. Set f to be false, give Zeropoint the value 0.0, and return.

Note that, in step 1(d), it does not really matter whether xmin or xmax is replaced by xopp, but it would be more efficient to choose so that the resulting interval is smaller. Having arrived at a suitable structure plan, the function as a whole can be constructed as follows:

FUNCTION Zeropoint (Y, xmin, xmax, f)

REAL :: Zeropoint, x, x1, x2, xmiddle, gap

REAL, INTENT(IN) :: xmin, xmax

REAL, EXTERNAL :: Y

LOGICAL, INTENT (OUT) :: f

! 'epsilon' is used to exclude the ends of the interval

(xmin, xmax):

REAL, PARAMETER :: epsilon = 0.00000000001

! 'fraction' determines how precise Zeropoint is to be:

REAL, PARAMETER :: fraction = 0.000001

! number of times we look for Y to have a different sign:

INTEGER, PARAMETER :: number_of_tries = 10000

! logical variables, true if Y is positive:

LOGICAL :: ipos, ipos1, ipos2

! preset f to be true:

f = .TRUE.

! other auxiliary variables:

gap = fraction*(xmax-xmin)

x1 = xmin + epsilon

x2 = xmax – epsilon

x = 0.0

ipos1 = Y(x1) > 0.0

ipos2 = Y(x2) > 0.0

! Does Y(xmin) have the same sign as Y(xmax)?

Signs: IF (ipos1.EQV.ipos2) THEN

f = .FALSE.

! Look for a Y-value of the opposite sign

Search: DO itry = 1, number_of_tries

CALL RANDOM(x)

x = x1 + x * (x2 - x1)

ipos = Y(x)>0

IF (ipos.NEQV.ipos1) THEN

! We've found one

f = .TRUE.

! Select a new interval

Select: IF ((x - x1)>(x2 - x)) THEN

x1 = x

ELSE Select

x2 = x

END IF Select

EXIT Search

END IF

END DO Search

END IF Signs

! Carry on if a zero-point can be found

Found: IF (f) THEN

! Cut the interval in half

Slice: DO

xmiddle = x1 + (x2-x1)/2

ipos = (Y(xmiddle)>0.0)

! Redefine the interval

IF (ipos.EQV.(Y(x1)>0.0)) THEN

x1 = xmiddle

ELSE

x2 = xmiddle

END IF

! Jump out if we've gone far enough

IF ((x2–x1)<gap) EXIT

END DO Slice

Zeropoint = (x2-x1)/2

ELSE Found

Zeropoint = 0.0

END IF Found

END FUNCTION Zeropoint

This can be regarded as a good first stab at what is required. But this procedure is still very far from perfect. What would be the result of **Zeropoint(TAN, 1.0, 2.0, f)**?

14.7 Program architecture

What about the overall form that a large program unit, or a program consisting of a large set of program units, should have? Unfortunately, in a book of this length it is impossible to give examples of the lengthy programs—running to tens of thousands of statements and more—that have been written to solve real-life problems and that are much closer to the real spirit of Fortran than the very short procedures and code fragments used to illustrate particular points in a textbook such as this.

This section, therefore, gives some indications as to how a large Fortran programme would in practice be designed. We will review the structure that any program unit must have, and particularly the ordering of declarative statements.

A "program unit" may be either a main program, an external subprogram, or a module.

BLOCK DATA

There is another sort of program unit that may occur in Fortran, known as BLOCK DATA, intended merely to preset the values of data items. The syntax is

BLOCK DATA

END BLOCK DATA

where the keyword DATA may optionally be followed by a name. The final statement may be abbreviated to END. Between the two statements shown, one or more COMMON blocks may appear and data items from them may be specified by type declaration statements and/or by DATA statements.

A "subprogram" is either a function or a subroutine. Besides external subprograms, it is possible to have "module subprograms" contained within modules.

Statement functions and internal procedures

There also exist statement functions (Section 7.1) and internal procedures (section 7.3).

The general structure of a program unit may be represented by Table 14.1. Within this and the following tables, the number of the table giving the structure of the entity mentioned is included. For example, Table 14.1 includes reference to interface blocks and derived type definitions, whose detailed structures are given in Tables 14.2 and 14.4 respectively. Table 14.1 also includes reference to module subprograms, which are program units whose structures are themselves of the type given in Table 14.1 itself; this is a case where one program unit may contain another program unit.

An IMPLICIT NONE statement must appear before any other IMPLICIT statement. Apart from IMPLICIT statements, Table 14.1 excludes statements whose usage is not recommended. BLOCK DATA statements are on the same footing as PROGRAM statements. FORMAT and ENTRY statements may appear anywhere between the USE statements and the CONTAINS statement. PARAMETER statements may appear among IMPLICIT statements (but not before an IMPLICIT NONE) or among type declaration statements, interface blocks and derived type definition blocks. DATA statements are on the same footing as type declaration statements, but may also appear among the executable statements. Internal subprograms are on the same footing as module subprograms.

Within Table 14.1, a module subprogram has the same general structure as an external procedure. An interface block has the general structure shown in Table 14.2, within which an interface body has the general structure shown in Table 14.3 Although it is conceivable that an interface block might contain an interface body needing to contain another interface block (e,g. if a procedure

Table 14.1 The general structure of a program unit.

PROGRAM, SUBROUTINE, FUNCTION Of MODULE Statement

USE statements IMPLICIT statements (Section 8.4) Interface blocks (Table 14.2), derived type definition blocks (Table 14.4), and type declaration statements (TDSs) Executable statements CONTAINS statement Module subprograms (Table 14.1) END statement

 Table 14.2 The general structure of a interface block.

INTERFACE statement Interface bodies (Table 14.3) MODULE PROCEDURE statements END INTERFACE

Table 14.3 The general structure of a interface body

FUNCTION or SUBROUTINE statement USE statements IMPLICIT statements Interface blocks (Table 14.2), derived type definition blocks (Table 14.4), and type declaration statements (TDSs) END statement

has a dummy procedure-name argument that is used as an actual procedure-name argument to another procedure) it is rather unusual.

Derived type definition blocks are of the form given in Table 14.4. Here, a PRIVATE statement is allowed only if the block is contained within the declarative part of a module (see cross-reference to Table 14.4in Table 14.1). Also, the type declaration statements (TDSs) here are restricted in form compared with those of program units.

USE statements, type definition blocks, interface blocks and TDSs are all declarative in character and it is often said that they may appear in any order. However, one may depend on another and therefore they should appear in a logical order. For example, the declaration of a variable of derived type should not precede the definition of that type, and an automatic array should not be declared before other objects on whose properties it depends. The presence of

Table 14.4 The form of derived-type defination blocks.

TYPE statement PRIVATE statement Type declaration statements (TDSs) END TYPE statement

Table 14.5 Simplified (non-module) program unit.

PROGRAM, SUBROUTINE, or FUNCTION statement

USE statements **IMPLICIT** statements Type declaration statements (TDSs) Executable statements **END** statement

Table 14.6 Derived-type or interface block module.

MODULE statement USE statements Derived type definition block (Table 14.4) or interface block (Table 14.2) END MODULE statement

specification expressions (Section 11.9), evaluated at execution time, blurs the ideal distinction between declarative (compilation-time) and executable (execution-time) statements.

The scheme can be simplified considerably if the programmer chooses that derived type definitions and interface blocks are *always* to be encapsulated in modules, a convention that will also avoid a good deal of unnecessary repetition in a large program, and also that module subprograms are always to be in modules by themselves. Then the general structure of a program unit reduces to that shown in Table 14.5.

It is a good idea to distinguish sharply between the following different types of module:

Table 14.7 Data module. MODULE statement USE statements IMPLICIT statements PRIVATE or PUBLIC statements Type declaration statements (TDSs) END MODULE statement Table 14.8 Subprogram module. MODULE statement USE statements IMPLICIT statements PUBLIC or PRIVATE statements Type declaration statements (TDSs) for variables to be host-associated among the subprograms following CONTAINS statement Module subprograms (Table 14.5) END MODULE statement

 Table 14.9 Generic external procedure.

MODULE statement USE statements Generic INTERFACE statement Interface bodies to external procedures (Table 14.3) END INTERFACE END MODULE

MODULE Stack

INTEGER, PARAMETER, PRIVATE :: n = 10000

REAL :: array (n)

END MODULE Stack

Table 14.10 Generic module procedure. MODULE statement USE statements referring to subprogram modules (Table 14.8) PRIVATE or PUBLIC statements Generic INTERFACE statement MODULE PROCEDURE statements END INTERFACE END MODULE

- 1. Modules which each contain either an interface block or a derived type definition, as in Table 14.6.
- 2. Modules containing only data, i.e. TDSs, as in Table 14.7. However, it would be unusual to have PRIVATE or PUBLIC statements (or the equivalent accessibility attributes in the type declaration statements) in a module of this sort. If would only arise in a case like

where the programmer wants to declare a large array, and perhaps change its size easily at a later stage, without compromising the use of the name n in any other program unit.

3. Modules containing module subprograms, i.e. with the structure shown in Table 14.8.

- 4. Modules each containing a generic interface to one or more external procedures (Table 14.9); and finally
- 5. Modules each containing a generic interface to one or more module procedures (Table 14.10). The PRIVATE and/or PUBLIC statements here might be to hide the names of the module procedures themselves, making them accessible only through a defined operator or defined assignment.

It is helpful to use USE statements liberally, encapsulating all procedure interfaces and derived types in modules, and it is better to use data modules than to have procedures with confusingly long lists of arguments.

Also, it is wiser to use data modules than to rely on host association. However, there is a danger. The undisciplined use of modules leads to a form of "chinese box" programming that can be opaque and

difficult for anybody else to understand—a modern counterpart of the vice of "spaghetti programming" that arose from over-use of the GO TO statement mentioned in Section 14.5.

The concept of a "scoping unit" may help to clarify the remarks above. A scoping unit can be thought of as a section of a Fortran program within which the variables can have arbitrary names and are not accessible outside the scoping unit. If variables in two different scoping units have the same name, it does not matter and they do not interfere with one another.

A scoping unit is any program unit, but excluding any derived type definition blocks, interface bodies, or (if the program unit is a module) module procedures contained within it. The latter are separate scoping units on their own account.

So, the general program unit in Table 14.1 is a scoping unit, which may contain three sets of other scoping units within it (the module subprograms, the derived type definition blocks, and the bodies in the interface blocks). Consequently, variables that crop up *within* a derived type definition, or that are used *within* an interface block, or which are local variables *within* a module subprogram, are not accessible to (and do not interfere with) the outer program unit in that they are embedded. Of course, the program unit can make use of a derived type—that is why the definition block is there—but it cannot interfere with the variables used to define its internal structure. Nor can the program unit interfere with the variables in an interface block, although of course it can use the keywords that might be defined in such a block.

The simplified program unit in Table 14.5 is a single scoping unit, and the program units in Tables 14.6, 14.7 and 14.9 also each contain essentially a single scoping unit each.

Table 14.8 shows the structure of a module containing subprograms: here, each subprogram is its own scoping unit with its own local variables. As the table indicates, there may be TDSs before the CONTAINS statement, and the variables so declared will be available by host association to all the subprograms that follow. It would probably be better programming practice not to have such data and instead to set up a special data module accessible by a USE statement in each of the subprograms. In other words, it is recommended that host association be avoided: to associate data from one scoping unit with another, USE association and argument association are the simplest and safest methods.

So, it is recommended that in a large program

- Program units should be organized so that, within reason, each program unit is a single scoping unit. Interface blocks, derived type definitions, and module procedures should be individually modularized. Host association should be avoided.
- 2. PRIVATE and PUBLIC statements, and/or the ONLY keyword in USE statements, should be used to avoid the inadvertent association of data between scoping units.
- 3. Data modules should be used freely to avoid lengthy or complicated lists of procedure arguments. For example, all the complications associated with optional arguments can be avoided (except when the

arguments are procedure names!) by putting the data into a module common to the calling and the called procedures.

4. Keep the main program fairly short, with a simple structure that makes the overall working of the program as clear as possible. Do not try to calculate anything in the main program—just use it as a switchyard for controlling the overall flow of the program. The following style has a lot to commend it:

PROGRAM Model USE Data CALL Stage1 CALL Stage2

CALL Stage3

END Program Model

- 5. Use functions to carry out self-contained tasks that depend on limited sets of arguments. A valuable rule (but perhaps an unrealistically harsh discipline!) is that *all* functions should be pure if they are not recursive.
- 6. Use different subprograms to do different sorts of job. For example, try to do all i/o in dedicated subroutines. Also, any processor-dependent code (e.g. something depending on an extended character set) should also be segregated.
- 7. Module procedures are really valuable only when there is a large group of related procedures (for example, to define and manipulate a derived data type) which can be regarded as general-purpose utilities. Such a module can be developed and maintained as an entity in its own right, and easily plugged into any program. The procedures described in Appendix C are an excellent example of this.
- 8. When designing a large program it is helpful to take an "object-oriented" approach and to concentrate initially on the data objects that are being dealt with. Derived-type data structures and arrays can be defined and put into modules as the first step. Functions and subroutines can then be written to carry out standard tasks with that data, e.g. reading it or displaying it. The job of programming is then primarily one of data structure design. With the right data structures in place, the actual flow of program execution will then appear much easier to arrange.

14.8 Exercises 14.A

14. The following are variants of the same basic problem: A1

- (i) Write a function Fix (Proc), where Proc is an external function name, to find a "fixed point" of a complex function of a complex variable. A "fixed point" of a function f(x) is defined as a value of x such that f(x) = x.
- (ii) Write a function Crossover (F, G) to find the value of x for which F(x) = G(x), F and G being real-valued external functions.

(iii) Write a general function-inverter Inverse (F, a) to return the value of x for which a specified function has a specified value. In other words, solve F(x) = a.

14. Write a function Infinite_Range_Integral(F) to calculate the integral of a specified external function

- A2 between plus and minus infinity. *Hint:* a useful mathematical trick might be to make the range of integration finite by a change of variable. For example, taking the inverse tangent of the variable will reduce the range to $(-\pi/2, +\pi/2)$.
- 14. Write a real function Interpol (Intfunc, x) where Intfunc is an integer function of an integer variable and
- A3 x is a real variable. Interpol is to generate a value for Intfunc (x), so to speak, by an appropriate interpolation between the values that Intfunc has for integers on either side of x.
- 14. The module ISO_VARYING_STRINGS is to be implemented in Fortran. You are asked to advise on
- A4 whether the module should be based on representing a variable-length string by an array pointer or by a linked list of characters. Investigate the question and write a brief report making an appropriate recommendation. See also Exercise 13.A3.
- 14. Write a program to try to find an even integer that can be decomposed as the sum of two odd primes in
- A5 only one way, that way being as the sum of two *equal* primes. For example, 6=3+3, but this example does not count because we can also have 6=5+1.

14. The Gamma function $\Gamma(x)$ is similar to the factorial function x! but can have any real argument. It A6 satisfies the recurrence relation

$$\Gamma(x+1)=x.\Gamma(x)$$

which implies

$$\Gamma(1-x) = -x.\Gamma(-x)$$

and these recurrence relations mean that the computation of the Gamma function for any real argument can be reduced to that of computing $\Gamma(x+1)$ for $0 \le 1$. When x *is* in that range, a fairly good approximation is provided by the power series

$$\Gamma(x+1) = 1 + a_1 x + a_2 x^2 + \dots + a_5 x^5$$

with

$a_1 = -0.5748646$
$a_2 = 0.9512363$
$a_3 = -0.6998588$
$a_4 = 0.4245549$
$a_5 = -0.1010678$

Write a Fortran function for $\Gamma(x)$, taking into account that the function is infinite when *x* is zero or is a negative integer. Use your function to find the location of the minimum of $\Gamma(x)$ where *x*>0.

14. Stirling's approximation to the Gamma function is

$$\Gamma(x) = e^{-x} x^{x-(1/2)} (2\pi)^{1/2} S(x)$$

where S(x) is the series

$$S(x) = 1 + \frac{1}{(12x)} + \frac{1}{(288x^2)} - \frac{139}{(51840x^3 - 571)(2488320x^4)} + \dots$$

higher-order terms being generally negligible. It is valid for large positive values of x. Write it as a Fortran function called Stirling (x) and investigate the extent to which it differs from the function written in Exercise

14. when x is less than large. Modify Stirling (x) so that it will write an error message and return a zero A6 value if x is not large enough for the approximation to be good.

- 14. Be a real programmer: do the sieve of Eratosthenes as a one-liner! A program to find prime numbers is
- A8 a common textbook programming exercise, but a more challenging task is to write a single statement that will write out all the prime numbers not exceeding, say, 100.

14. Write a module containing a derived-type definition and miscellaneous procedures for handing data in A9 the form of quaternions.

- 14. A project on derived types and program design:
- A1 A polyhedron can be defined as the set of finite plane surfaces that are its faces. Simplify this 0 representation by breaking down any faces that are quadrilaterals (or polygons with more sides) into triangles. A polyhedron is therefore defined by a set of triangles in 3-space. Each triangle is defined by its vertices. To avoid duplicating the coordinates of the vertices, define the polyhedron as (i) the set of points which are its vertices, and (ii) the triangles which are its faces, defined as ordered triplets of (i). Each of the triangles is to have an inside-or-outside orientation defined by the cyclic order of its three vertices. A method must be found to determine this orientation.

We want to have a logical-valued function Convex (Polyhedron), to determine whether or not a polyhedron is convex, and other procedures to calculate things like the volume and surface area of a polyhedron.

CHAPTER 15 High Performance Fortran

Some basic ideas about parallel-processor computing, and the motivation for High Performance Fortran (HPF), are outlined. The HPF extensions to Fortran's syntax, and its additional array-handing procedures, are listed and explained. Then we come to the heart of the chapter, dealing with the HPF directives and related procedures for aligning and distributing arrays of data among processors. We end with an account of "extrinsic" and "local" procedures, including the HPF Local Library.

High Performance Fortran, usually abbreviated to HPF, is a set of extensions to the Fortran language. HPF has been developed—and is still in a state of development—so that programs can be written in such a way that they will run as efficiently as possible on advanced parallelprocessing computer systems. HPF is a de facto standard in industry and academia (and what follows is based on version 1.1) but it is not an international ISO standard and the implementation of HPF on particular machines is a matter of gradual development. This chapter is written for those who want to gain an insight into the future of Fortran, and of advanced scientific computing, and for those whose research will require them to write programs for parallel-processing computer systems.

We cannot attempt to describe here all aspects of HPF as comprehensively as Fortran 95 has been described in the rest of this book, but all the procedures and directives associated with HPF are mentioned.

15.1 Parallel processing

High Performance Fortran (HPF) is an emerging standard for the programming of advanced computers capable of carrying out data-parallel computation. "Data-parallel" means that similar instructions are being carried out simultaneously, by parallel processors, on several different sets of data.

Although today's conventional single-processor computers (such as the PC) are very much faster than their predecessors, and they continue to grow faster year by year, speed is still the limiting factor that prevents computers from solving certain problems. Because of the way in which science progresses, the solution to one problem always seems to pose new and more difficult problems demanding still more computing power.

One way to speed up a computation is to divide the task into a number of sub-tasks which can be carried out simultaneously and to build a computer with several processing units instead of just one. If the different processors can be efficiently orchestrated and synchronized, then in principle the speed of a computer system can be increased simply by adding extra processors. As long as hardware is relatively cheap, a system could contain hundreds or thousands of separate processors working in parallel, with a combined computation rate far higher than could be achieved by a single processor in the foreseeable future.

It also happens to be the case that large arrays of parallel processors are especially suited to solving some of the most interesting *kinds* of scientific problems that are of current interest. These are problems involving large arrays of data: examples are the lattices used for calculations in quantum chromodynamics in particle physics, simulations of the global climate system, numerical solutions of Einstein's equations in cosmology, simulations of astrophysical events such as supernova explosions, image processing, and the evolution of diverse ecologies of interacting organisms.

The new technology of parallel computation involves both hardware and software. The software problem is that of efficiently controlling a large number of simultaneous threads of calculation, and doing so through a general-purpose programming system based on a standard language. HPF is part of the attack on that problem.

The style of parallel computing reflected in HPF, and suggested by the types of scientific problem mentioned above, is often referred to as "data-parallel" computing. The idea is that identical or very similar instructions will be executed in parallel on all the elements of a large array of data, as opposed to applying an array of different operations to the same item of data. In the latter case, different processors would be supplied with different sequences of instructions, i.e. with different programs, but in data-parallel computing the processors all execute essentially the same instructions but are supplied with different streams of data.

To carry out data-parallel computing as efficiently as possible, the structure of the arrays of data, which is imposed externally by the nature of the problem, needs to be brought into a correspondence with the physical layout of the array of processors. The former needs somehow to be mapped onto the latter through the software that is the bridge between the abstract problem and the hardware that is being used to solve it. The task of mapping the first set of arrays onto the second—the mathematical onto the physical—is undertaken in HPF with compiler "directives", explained in Section 15.4.

15.2

Pure procedures, FORALL and INDEPENDENT

Having been developed before Fortran 95 was defined, HPF is an extension of Fortran 90, not of Fortran 95. However, some of HPF's innovations were also incorporated in the extension of Fortran 90 to Fortran 95 and therefore have already been dealt with elsewhere in this book. In particular, these are "pure" procedures (Section 11.2) and the FORALL statement and FORALL construct (Section 6.5).

Pure procedures, which are constrained to affect only local data, are intended to facilitate parallel computing. If a pure procedure is to be applied to an array of data, then it may be executed simultaneously on separate elements on parallel processors. Elemental procedures, being a sub-category of pure procedures, can also be executed on parallel processors. The keywords PURE and ELEMENTAL can be regarded as advice to the compiler provided so that the system will "know" that parallel execution can be exploited if the hardware supports it.

The FORALL statement and construct are also defined in such a way as to facilitate parallel processing. In a statement such as

FORALL (i=1:n) result(i) = Algorithm(data(i))

the procedure Algorithm must be pure and it must be possible for the assignments to be carried out in any order, or simultaneously, without the result being altered. However, consider a FORALL construct such as

FORALL (i=1:n) data2(i) = Algorithm1(data1(i)) data3(i) = Algorithm2(data2(i)) data4(i) = Algorithm3(data3(i))

END FORALL

Although this could be executed in parallel for each of the n elements of the data arrays, the construct as it stands might still not be optimized for the fastest possible parallel processing. To see why, it must be understood that the code will be executed by:

- 1. calculating Algorithm1(data1(i)) for every value of i, and then
- 2. setting every element of data2 to the corresponding value of Algorithm1, and then
- 3. calculating Algorithm2 (data2 (i)) for every value of i, and then ...

and so on. This may involve parallelism *within* steps 1, 2, 3 etc., but the calculations and assignments are still sequential from one statement to the next. This is lockstep parallelism, with a synchronization across the processors after each step of the calculation. So, the time taken for the *parallel* calculation of the set Algorithm1(data1(i)) will be the longest of the times for the individual values of i. This is like an army marching at the speed of the slowest.

Synchronization may in some cases be a virtue. With code like

```
FORALL (i=1:n)
data2(i) = Algorithm1(data1(i), data1(n–i+1))
data3(i) = Algorithm2(data2(i), data2(n–i+1))
data4(i) = Algorithm3(data3(i), data3(n–i+1))
```

END FORALL

confusion could result if each statement were not fully executed for all values of the index i before proceeding to the next statement. Often, however, it will be possible to relax the synchronization. To achieve this, FORALL can be supplemented in HPF with a "directive" taking the form of the line

!HPF\$ INDEPENDENT

and if this is inserted immediately before the FORALL, then the compiler is advised that the parallel strands of computation are completely independent of one another, and therefore that strong synchronization is not

necessary. If the compiler is capable of making best use of this advice, a considerable saving in execution time may be made.

The line above is not a Fortran statement: it is known as a "directive". Several other HPF directives will be met below in Section 15.4. All HPF directives start with the characters !HPF\$ and it should be noticed that the initial ! means that the whole line will be ignored, as if it were a mere program annotation, by a normal Fortran compiler. So, the presence of HPF directives will not prevent a program from conforming to the Fortran standard, but an HPF compiler will detect the ! HPF\$ string and will interpret the remainder of the line as a directive. A directive is not classed as a statement, and should make no difference whatsoever to what is calculated: it is simply advice to the compiler that should lead to an increase in the speed of the calculation. The directive INDEPENDENT, before a FORALL, does not of itself make the strands of calculation independent of one another: it merely asserts that is the case. If it were not the case (as in the last example above) then INDEPENDENT should not be used.

The INDEPENDENT directive can also be used with the DO construct (Section 6.4). In this context it is even more useful than with FORALL, because a DO loop normally involves no parallelism at all. But if we have

!HPF\$ INDEPENDENT

DO kipper = 1, 1024

mackerel(kipper) = lemon + kipper**2

END DO

then the compiler is informed that the cycles of the loop could, equivalently, be executed in any order or simultaneously. In this rather trivial example, it could be said that the programmer should have used a FORALL instead of a DO anyway, or that a good compiler should detect the independence without having to be told: but in more complex instances it can be far from obvious whether or not a DO loop can be parallelized.

For a DO loop, the INDEPENDENT directive means that no iteration can directly or indirectly affect the result of any other iteration.

With DO loops (but not with FORALL) the INDEPENDENT directive has an extended form including what is known as a "NEW clause". The syntax for this is

!HPF\$ INDEPENDENT, NEW (list-of-names)

where *list-of-names* is a list of one or more variables occurring in the loop. The NEW clause means that the iterations are INDEPENDENT if the named variables are recreated afresh at each iteration through the loop. This amounts to saying that the named variables are local to the loop and need not be "saved" from one iteration to the next. An example is in the pair of nested DOS

!HPF\$ INDEPENDENT, NEW (i)

DO kipper = 1, 1024

mackerel(kipper) = lemon + kipper**2

!HPF\$ INDEPENDENT

DO i = 1, 1024

mullet(i, kipper) = mullet(i, kipper) +&

mackerel(kipper)

END DO

END DO

where the first directive points out that the variable i does not need to be retained from one cycle to the next of the *outer* loop. That is in fact the case, and the outer loop could therefore be parallelized. This example also illustrates that INDEPENDENT directives may be nested with the DO (or FORALL) blocks that they refer to. The second INDEPENDENT means that the iterations of the inner DO loop above could be executed in any order.

15.3 HPF procedures

The Fortran 95 enhancements of the intrinsic functions MINLOC and MAXLOC, which have already been mentioned in this book, are part of the HPF specification. HPF also specifies a new intrinsic function, iLEN (i), useful for some bit-handing problems:

• ILEN (i) returns an integer equal to one less than the number of bits needed to represent i in "two's complement" notation.

More important are two new intrinsic functions that will tell the program about the arrangement of the individual processors comprising a parallel system:

- NUMBER_OF_PROCESSORS (), with no argument, gives the basic information of how many processors there are. On a conventional PC the result is 1. Note that the value of NUMBER_OF_PROCESSORS is not the total physical number of "chips" in the whole computer system: it is, in effect, the number of parallel processing channels.
- PROCESSORS_SHAPE () never has an argument. Its value is an integer rank-one array specifying the notional geometry of the array of processors, analogous to the "shape" of a data array. If there are 64 processors arranged in the form of a two-dimensional square lattice, then PROCESSORS_SHAPE has the value (/ 8, 8 /). The value of PROCESSORS_ SHAPE corresponds to the logical connectedness among the processors and not necessarily to the geometry of their physical positions. It is quite possible, and for some purposes useful, for the processors to form a multidimensional hypercube even though embedded in three-dimensional space!

NUMBER_OF_PROCESSORS has an optional argument, dim, which if specified points to the dimth dimension of the processor array, and the function result is the number of processors along that dimension. In the example just mentioned, NUMBER_OF_PROCESSORS (1) and NUMBER_OF_PROCESSORS (2) are both equal to 8 and no other argument would be meaningful. The

NUMBER_OF_PROCESSORS function will not convey any information that is not already implied in the value of the array **PROCESSORS_SHAPE.**

HPF introduces numerous new functions in a library entitled HPF_LIBRARY. A number of these are to do with how the data is distributed among the processors (see Section 15.5). Other procedures are simply numerical, and would be relevant on any kind of computer, parallel-processing or not:

- LEADZ (i) is an elemental function returning the number of leading zero bits in the representation of the integer i.
- **IALL** (array, *dim, mask*) is a function of an integer array, and carries out a bit-by-bit AND combination of the elements along a particular dimension. It therefore has a concertina effect, the result having a rank of one less than that of array. The optional argument dim indicates along which dimension the elements are to be combined, but if array has rank one then dim may be absent and IALL will reduce the array to a scalar. The logical argument *mask*, if present, means that the AND combination is carried out only among those elements of the array corresponding to true values of *mask*; if *mask* is not a scalar, it must have the same shape as the array.

As an example: if array = (/5, 6, 7/), then in binary it is (/101, 110, 111/) and the IALL function will produce the number represented in binary by 100, i.e. the value 4.

IALL is rather similar to the bit function IAND (Appendix B.2), except that IAND combines its two arguments whereas IALL combines elements from one (array) argument.

- IANY (array, dim, *mask*) does a similar job to IALL, reducing a dimension of array by carrying out a bitwise combination of its elements; but IANY carries out a logical inclusive OR combination rather than IALL'S AND. IANY is therefore analogous to IOR. IANY ((/5, 6, 7/)) produces the binary bit sequence 111, i.e. its value is 7.
- IPARITY (array, dim, *mask*) has a similar syntax to IALL and IANY, but yields the parity of each set of bits. IPARITY ((/i, j /)) is equivalent to iEOR(i, j).IPARITY ((/5, 6, 7/)) is equal to 4.
- PARITY (mask, dim) works not on bits within an integer but on a logical-type array (mask), and its value is a logical scalar or array. If present, dim performs the same role as in the functions above, indicating which dimension of mask is to be collapsed. The basic operation is the exclusive OR combination (i.e. like the NEQV operator) across the appropriate elements of mask.
- POPCNT (i) is an elemental integer function that looks at the sequence of bits within the integer i and returns the number of bits that are equal to 1.
- POPPAR (i) is like POPCNT but yields the parity of the bit sequence within i, i.e. POPPAR is equal to 0 for an even number of 1 bits, and to 1 for an odd number.

We now move on to a series of HPF functions that transform or reconstitute arrays of data. These functions are not simple, but they are much less complicated than they will appear at first sight. We will deal with them in three groups, the first being the following:

ALL_SCATTER (mask, base, indx1, indx2,..., indxn)

ANY_SCATTER (mask, base, indx1, indx2,..., indxn)

COPY_SCATTER (array, base, indx1, *indx2,...,* indxn, mask)

COUNT_SCATTER (mask, base, indx1, *indx2,...*, indxn) IALL_SCATTER (array, base, indx1, *indx2,...*, indxn, mask) IANY_8CATTER (array, base, indx1, *indx2,...*, indxn, mask) IPARITY_SCATTER (array, base, indx1, *indx2,...*, indxn, mask) MAXVAL_SCATTER (array, base, indx1, *indx2,...*, indxn, mask) MINVAL_SCATTER (array, base, indx1, *indx2,...*, indxn, mask) PARITY_SCATTER (mask, base, indx1, *indx2,...*, indxn, mask) PARITY_SCATTER (array, base, indx1, *indx2,...*, indxn, mask) SUM_SCATTER (array, base, indx1, *indx2,...*, indxn, mask)

These all have names of the form XXX_SCATTER, where *xxx* refers in each case to a basic operation similar to one of those carried out by a simpler function that we have already met. For example, ALL_SCATTER can be understood as an extension of the Fortran 95 ALL function. The SCATTER part of the name refers to a process that can be regarded as a generalization of the use of vector subscripts (Section 9.2).

A vector subscript is a way of picking out elements from a rank-one array and arranging them to construct a new array, also of rank one. The vector subscript is itself a rank-one array containing the indices that pick out the desired elements. If

kudos = (/91, 92, 93, 94, 95, 96, 97, 98, 99/)

and if

ipick = (/2, 4, 6, 8, 1/)

then, using ipick as a vector subscript, kudos (ipick) is an array expression equal to

(/92, 94, 96, 98, 91/)

The xxx_SCATTER functions extend the idea of vector subscripts to higher-rank arrays. Where there is an array argument, it contains the fundamental data on which the operation is being carried out. The value of xxx_SCATTER (array,...) will be an array whose shape will in general be different from that of array, being the same as that of the array argument base. The elements of base can be regarded as default values for the elements of the function's result.

Each argument indx1, *indx2*, *indx3*,... is itself an integer array conformable with array. So, each element of array corresponds to a series of elements of indx1, *ind3x2*, *indx3*,.... However, the number of indx integers for each element of array must be equal to the rank of base and therefore to the rank of the function's result. Thus if array has rank two, each element

array (m, n)

will be associated with the element of base:

base (indx1(m, n), *indx2(m, n)*, *indx3(m, n)*,...)

Leaving aside the argument *mask*, each of the functions xxx_SCATTER (array,...) above carries out this association for every element of array, i.e. for every value of m and n spanning the full shape of array. In other words, the elements of array will be "scattered" into a new array having the shape of base. If the optional *mask* argument is present, it must be a logical array conformable to array, and only when the corresponding element *of mask is* true will that element of array be used.

Notice that the indx arrays are generalized vector subscripts, but defined in such as way as to be conformable with the original array rather than with the result—this is opposite to the situation with vector subscripts.

We can now turn to some of the individual functions listed above.

COPY_SCATTER is particularly simple, since it merely copies elements from array into the result without carrying out any mathematical or numerical operation. In other words, the association mentioned above is an equality: if **array** has rank two and if

result = COPY_SCATTER (array, base, indx1, indx2,..., &

indxn, mask)

then its element

result (indx1(m,n), indx2(m,n), indx3(m,n),...)

is in general set equal to the element

array(m, n)

However, if the elements of the indx arrays are such that no element of array is mapped into a particular element of the result, or if mask prevents it, then that element of result will be taken instead from base. On the other hand, if the elements of the indx arrays are such that several elements of array are mapped into the same element of the result, then one of them will be chosen by the processor in an arbitrary way to produce the result of COPY_SCATTER.

Now it starts to get easy! The SCATTER functions with prefixes IALL, IANY, IPARITY, MAXVAL, MINVAL, PARITY, PRODUCT, and SUM have results in which each element is obtained by applying the appropriate numerical operation to the element or elements from array that are scattered there, together with the corresponding element of base. Because IALL_SCATTER, IANY_SCATTER and IPARITY_SCATTER carry out bit-by-bit operations on integers, their arguments must be integers; MAXVAL_SCATTER and MINVAL_SCATTER may have either real or integer arguments.

Note that the base argument in each case serves the purpose not only of determining the shape of the function's result; it also provides default data to ensure that no element of the result will ever be left undefined.

For the special case of a rank-two array and a rank-three base, the effect of, say, SUM_SCATTER could be achieved with the Fortran 95 code

result = 0 !array initialization check = .FALSE. !array initialization DO i=1, SIZE(array, DIM=1) DO j=1, SIZE(array, DIM=2) IF (.NOT.mask(i, j)) CYCLE 1=indx1(i, j) m=indx2(i, j) n=indx3(i, j) result(1, m, n) = result(1, m, n) + array(i,j) check(1, m, n) = .TRUE. END DO END DO

WHERE (.NOT.check) result = base

The xxx_SCATTER functions with the prefixes ALL, ANY and COUNT do not have an argument called array but the logical argument called mask argument takes its place. ALL and ANY have logical-valued results, carrying out the obvious operations on scattered elements of mask with base, base being logical. For COUNT_SCATTER, base is an integer and the function adds the element of base to the number of true elements of mask that are scattered to it.

The next group of HPF functions that we must consider are:

ALL_PREFIX (mask, dim, *segment, exclusive*) ANY_PREFIX (mask, dim, *segment, exclusive*) COPY_PREFIX (array, dim, *segment*) COUNT_PREFIX (mask, dim, *segment, exclusive*) IALL_PREFIX (array, dim, *mask, segment, exclusive*) IANY_PREFIX (array, dim, *mask, segment, exclusive*) IPARITY_PREFIX (array, dim, *mask, segment, exclusive*) MAXVAL_PREFIX (array, dim, *mask, segment, exclusive*) MINVAL_PREFIX (array, dim, *mask, segment, exclusive*) PARITY_PREFIX (mask, dim, *segment, exclusive*) PRODUCT_PREFIX (array, dim, *mask, segment, exclusive*) SUM PREFIX (array, dim, *mask, segment, exclusive*)

These functions carry out operations on the data in their first argument in ways very similar to the xxx_SCATTER functions described above. One difference is that PREFIX functions combine the elements along an indicated dimension (dim) rather than taking elements selected by a generalized vector subscript. The other difference is that the prefix functions do not simply combine all the elements of the array along that dimension (which would give a result whose rank would be one less than that of the first argument). Instead, "running totals", so to speak, are kept as the processor works through the elements. The "running total" at each element forms the corresponding element of the result, and the result has the same shape as the original data. As examples, it will be sufficient for us to look at cases where the first argument is a rank-one array and dim can therefore be omitted. Disregarding for the moment the later optional arguments,

SUM_PREFIX (/6, 3, 0, 8, 8, 6, 9, 1/)

is equal to the array

(/6, 9, 9, 17, 25, 34, 357)

and the phrase "running total" has its literal meaning. PRODUCT_PREFIX, applied to the same array, would give

(/6, 18, 0, 0, 0, 0, 0, 0/)

These are called "prefix" functions because the results involve the elements of the initial data up to and including that corresponding to the particular element of the result.

An optional mask argument allows some of the initial data to be ignored: for example, with

k1 = (/6, 3, 0, 8, 8, 6, 9, 1/)

k2 = PRODUCT_PREFIX(array=k1, mask=(k1/=0))

k2 would have the value

(/6, 18, 18, 144, 1152, 6912, 62208, 62208/)

The argument *segment*, if present, allows the prefix calculation to be made separately for different sections of the data. It is of logical type and of the same shape as the data. As we move from one element to the next, the process is restarted (just as at the first element) if and when there is a flip in the value of the corresponding element of *segment*. So, a new segment within the data is started whenever *segment* switches from false to true or *vice versa*. Following the example above,

t=.TRUE.

```
f=.FALSE.
```

```
k2 = PRODUCT_PREFIX(array=k1, &
```

```
segment=(/t, t, t, f, f, f, t, t/), exclusive=f)
```

yields

(/6, 18, 0, 8, 64, 384, 9, 1/)

The argument *exclusive* is a logical scalar that says whether or not the elements at the boundaries are excluded (in effect, masked out) or included in the computations.

Prefix functions having been understood, there is no need to say much here about the "suffix" functions that form the third group:

ALL_ SUFFIX (mask, *dim, segment, exclusive*)
ANY_ SUFFIX (mask, *dim, segment, exclusive*)
COPY_SUFFIX (array, *dim, segment*)
COUNT_SUFFIX (mask, dim, *segment, exclusive*)
IALL_SUFFIX (array, *dim, mask, segment, exclusive*)
IANY_SUFFIX (array, dim, *mask, segment, exclusive*)
IPARITY_SUFFIX (array, dim, mask, *segment, exclusive*)
MAXVAL_SUFFIX (array, dim, *mask, segment, exclusive*)
MINVAL_SUFFIX (array, dim, *mask, segment, exclusive*)
PARITY_SUFFIX (array, dim, *mask, segment, exclusive*)
PARITY_SUFFIX (array, dim, *mask, segment, exclusive*)
SUFFIX (array, dim, *mask, segment, exclusive*)
SUM_SUFFIX (array, dim, *mask, segment, exclusive*)

These perform in exactly the same way as the prefix functions, but the arrays are scanned the other way around. An element of the result depends on the following, not preceding, elements of the initial data.

The bewildered reader may understand what all these functions do, but may wonder who on earth would want to use them and what problems they might solve. Unlike the frequently-encountered mathematical functions of Fortran 95, such as the trigonometrical functions or those for multiplying vectors and matrices, the HPF functions do not seem to correspond to familiar textbook problems. They are, nevertheless, powerful and useful tools for the construction of fast parallel algorithms.

15.4 Data distribution in parallel-processor systems

All the aspects of HPF mentioned so far have been enhancements to Fortran that could lead to valuable increases in program execution speed on a parallel computer system if the compiler is sufficiently sophisticated to take full advantage of them. However, it was assumed that the compiler itself—not the programmer—is aware of the number and configuration of parallel processors and can choose a good way of distributing the computing among the processors. In practice, however, if the optimum computing performance is to be achieved then the programmer must be aware of the configuration of the hardware and will need to give instructions to the compiler so that the arrays of data can be most efficiently "mapped" onto the array of actual processors.

These instructions are given with the help of a set of HPF directives. Apart from INDEPENDENT (Section 15.2) the possible directives have the keywords

PROCESSORS

DISTRIBUTE and REDISTRIBUTE

ALIGN and REALIGN

TEMPLATE

DYNAMIC

INHERIT

SEQUENCE

Like INDEPENDENT, any of these would actually appear on a line starting with the string !HPF\$. With the exceptions of REDISTRIBUTE, REALIGN and INDEPENDENT, these are classified as "specification directives" and would appear among the declarative statements at the start of a program unit. The other three are "executable directives" and may appear only among executable statements.

The SEQUENCE directive is mainly to handle the disposition of data in Fortran- 77-style COMMON blocks and could be useful if old code is to be converted to run on new parallel computers, but it will not be discussed further here.

Before discussing the above directives in detail, it is necessary to introduce the concept of an abstract array of processors. The abstract processors may be regarded as an intermediate stage between arrays of data (that depend on the particular program) and the actual physical arrangement of processors that comprise the parallel computing system. The distinction between abstract processors and physical processors is crucial. The programmer will wish to "map" the data arrays onto a set of abstract processors whose configuration is defined within the program. However, the abstract processors may have a different shape to the physical processor array and it is left to the compiler to finish the job by mapping the abstract processors onto the physical processors. The intrinsic functions NUMBER_OF_PROCESSORS and PROCESSORS_SHAPE (Section 15.3) return information about the physical processors: that information could be used by the programmer (or by the program) to decide what arrangement of abstract processors would best suit the problem in hand.

PROCESSORS

The PROCESSORS directive is used to declare one or more abstract arrays of processors, specifying an arbitrary name and a shape for each. The specifications of abstract processors are internal to the program unit in which they are declared. Valid PROCESSORS directives are

!HPF\$ PROCESSORS:: hypercube (16, 16, 16, 16)

!HPF\$ PROCESSORS:: serial (NUMBER_OF_PROCESSORS())

!HPF\$ PROCESSORS:: single

The first of these might be used if the mathematical problem were based on data organized in a fourdimensional hypercubic array and if the programmer envisages that, in theory, the calculations could be efficiently organized on an array of processors having that connectivity. The physical processor array might be different (say, a 256×256 square) but the compiler is left to decide how the hypercube might best be projected onto the square.

In the second example above, the programmer envisages simply a one-dimensional sequence of parallel processing channels, and defines its size by taking the actual number of physical processors. The third example invites the compiler to treat the program as though the program were running on a single-processor computer, giving the processor the name single.

Having declared the names and shapes of the abstract processor arrays, the programmer need no longer be concerned with the physical processors. All the other directives described below deal with the relationships between the data itself and the abstract processors.

DISTRIBUTE

This is the fundamental directive for indicating the relationship between an array of data and an abstract processor array. Like PROCESSORS, it has a syntax not very different from the type declaration statement of Fortran 95: the DISTRIBUTE keyword, followed by some additional specifications, and then a double colon (::), followed finally by a list of the data arrays to which the directive refers. (As with the Fortran type declaration statement there is an alternative notation not using the double colon, but that need not concern us here.)

A very simple DISTRIBUTE directive is in

PROGRAM Lets_Go

!HPF\$ PROCESSORS :: serial (NUMBER_OF_PROCESSORS())

REAL :: x (1000)

!HPF\$ DISTRIBUTE (BLOCK) ONTO serial :: x

Here, the processors are notionally arranged in a row called serial. The data in the array x is distributed between those processors. The keyword BLOCK dictates the mode of that distribution, and just means that x is divided into equal blocks of sequential elements, each block being assigned to one processor. If the number of processors is eight, then x(1:125) will go to the first processor, x(126:250) to the second, x(251: 375) to the third, and so on.

In other words, a BLOCK distribution divides the array into contiguous chunks, one going to each processor, and each processor's chunk has a number of elements equal to

SIZE(array)/NUMBER_OF_PROCESSORS()

The syntax of the DISTRIBUTE directive would allow any number of data arrays to be listed after the double colon, all of them being distributed in the same way across the arrangement of abstract processors, which is named immediately before the double colon.

A variation on the above is to specify the number of data-array elements which are to be mapped onto each processor. The number can be specified in brackets after BLOCK as in

!HPF\$ PROCESSORS :: serial (NUMBER_OF_PROCESSORS())

REAL :: x (1000)

!HPF\$ DISTRIBUTE (BLOCK(200)) ONTO serial :: X

This maps x(1:200) onto the first processor, and so on, using five of the processors by the time all of x's elements have been accounted for. If BLOCK (n) is specified, *n* must not be so small that there are not enough processors to hold all the elements of x with n elements per processor.

Leaving aside for now some complications to do with the dummy arguments of procedures, the general form of the DISTRIBUTE directive is

!HPF\$ DISTRIBUTE (format-list) ONTO processors : array-list

where *processors* is the name of the array of processors, and *array-list* is a list of data arrays (all of the same rank) that are being mapped onto the processor array by this directive. The purpose of *format-list* is to show how the distribution should be made: it is a list of indicators each of which must take one of the following forms:

BLOCK

BLOCK(number-of-elements)

CYCLIC

CYCLIC(number-of-elements)

*

There must be one of these indicators for each dimension of the data arrays. The meanings of BLOCK and of BLOCK (...) have already been mentioned. In the case of, say, a rank-two array, the code

!HPF\$ PROCESSORS :: nodes (8, 4)

INTEGER :: data (1024, 1024)

!HPF\$ DISTRIBUTE (BLOCK, BLOCK) ONTO nodes :: data

would divide the data among the 32 processors by equal partitions of the first index into eight blocks and the second index into four blocks. So, data (1:128, 1:256) would go to one processor, and so on, dividing the square data into the rectangular sections

data (1*128+1:1*128+128, j*256+1: j*256+256)

where i runs from 0 to 7 and j runs from 0 to 3. As in our earlier example, the effect of using BLOCK (...) would be to require each block to span the given number of elements in each direction.

The keyword CYCLIC, in place of BLOCK, means that the array elements along that dimension will be distributed around the processors one by one, like dealing cards. So, adjacent array elements will be distributed to different processors. With

!HPF\$ PROCESSORS :: nodes (8, 4)

INTEGER :: data (1024, 1024)

!HPF\$ DISTRIBUTE (CYCLIC, CYCLIC) ONTO nodes :: data

one processor will receive the elements

data (1:1017:8, 1:1021:4)

and the other 31 will receive similarly separated sets of elements. Specifying CYCLIC (...), with an integer between the brackets distributes the elements not one at a time but two, three or four at a time or whatever the integer is.

The final option mentioned above in a *format-list* is the asterisk (*). This symbol is used to indicate a dimension of the data array that is not to be separated among different processors at all, but should all but kept within one processor. This gives what is called a "degenerate" distribution. For example,

!HPF\$ PROCESSORS :: triad (3)

REAL :: t (6, 3)

!HPF\$ DISTRIBUTE (CYCLIC, *) :: t

will putt(1, 1), t(1, 2), t(1, 3), t(4, 1), t(4, 2), and t(4, 3) onto the first processor; t(2, 1), t(2, 2), t(2, 3), t(5, 1), t(5, 2), and t(5,3) onto the second; and t(3, 1), t(3, 2), t(3, 3), t(6, 1), t(6, 2), and t(6, 3) onto the third. As a further example, consider

!HPF\$ PROCESSORS :: fourfold(4)

REAL :: x(100, 100), y(100, 100), z(100)

!HPF\$ DISTRIBUTE (BLOCK, *) ONTO fourfold :: x

!HPF\$ DISTRIBUTE (*, CYCLIC) ONTO fourfold :: y

!HPF\$ DISTRIBUTE (BLOCK(5)) ONTO fourfold :: 2

This will distribute the array sections x(1:25, 1:100), y(1:100, 1:97:4), z(1:5), z(21:25), z(41:45), z(61:65), and z(81:85) to the first processor, and so on for the other processors.

Besides the syntax above, it is possible for the DISTRIBUTE directive to have its whole format-list replaced by, or preceded by, an asterisk. This has a meaning in relation to the distribution of dummy argument arrays in procedures, and is best discussed in the context of the INHERIT directive on page 294.

ALIGN

We have seen that the PROCESSORS directive defines an array of abstract processors, and the DISTRIBUTE directive states how the elements of data arrays should be distributed amongst them. DISTRIBUTE allows arrays of data to be split into blocks of adjacent elements, or to be dealt cyclically around the processors, or (using *) not to be separated at all but to go to the same processor. With sophisticated combinations of blocking, cycling or degeneracy along different dimensions, high-rank arrays can be distributed in complex ways so as to suit the mathematical logic of the problem and to speed up program execution by minimizing the amount of intercommunication that has to take place between different processors.

However, it could be a tedious and error-prone task to specify distributions separately for all the data arrays in a program. When groups of arrays represent data with similar structures, it is likely to be easier to align them with one another and then to distribute them all onto the processors with one DISTRIBUTE directive. This can be done in HPF with the help of the ALIGN directive, which maps one data array onto another. So, the directives

!HPF\$ DISTRIBUTE (BLOCK, BLOCK) ONTO fourfold :: a

!HPF\$ ALIGN WITH a :: b, c, d, e, f

will have the effect of aligning all six arrays, a-f, with one another and distributing them together across the processor array. In this example the same effect could be achieved just by listing all six arrays at the end of the DISTRIBUTE statement, but in more complicated examples the alignments of b–f with a could differ in detail and would have to be specified by separate ALIGN statements, while the final mapping of all the data onto the processors would still be achieved with the one DISTRIBUTE directive.

Another example of the ALIGN directive is

REAL :: x(1:1000), y(1:1000), z(-499:500)

!HPF\$ PROCESSORS :: singlefile(10)

!HPF\$ DISTRIBUTE (BLOCK) ONTO singleflie :: x

!HPF\$ ALIGN WITH x :: y

!HPF\$ ALIGN WITH x(i+500) :: z(i)

The last line means that the element z(-499) is aligned with x(1), z(-498) with x(2), and so on up to z(500) and x(1000). Notice that alignments and distributions are always made with reference to particular array indices. In this instance it is not sufficient to write

!HPF\$ ALIGN WITH x :: z

because the directive tries to match the arrays index value by index value, not just lining up their total lengths.

The syntax of the ALIGN directive is

!HPF\$ ALIGN WITH target (subscripts) :: array-names &

(dummy-subscripts)

with *array-names* being the names of the arrays being aligned, and *target* the array to which they are being aligned. It is foreseen that the *array-names* will ultimately be distributed onto the processors through *target*, and therefore they are not allowed to appear separately in DISTRIBUTE directives of their own.

The *dummy-subscripts and subscripts in the ALIGN directive are primarily to allow for offsets or unusual mappings between the indices of array-names and target.*

Each dummy-subscript may be either an asterisk(*), a colon (:), or the name of a dummy integer variable (like the i in the example above).

Each *subscript* may be either an asterisk, a *subscript-triplet*, or an *integer-expression*. A *subscript* may refer to a dummy integer variable from the list of *dummy-subscripts*, as in the example of (i+500) given above.

As another example using specification expressions, we could have

REAL :: central(n, n), square(n+2*margin, &

n+2*margin)

!HPF\$ ALIGN WITH square (i+margin, j+margin) :: central (i, j)

We saw that an asterisk may be used in the DISTRIBUTE directive to produce a degenerate distribution, i.e. ensuring that one or more dimensions of an array are not divided between the processors. A similar effect (sometimes called "collapsing" an array) can be achieved by including one or more asterisks among the *dummy-subscripts of* an ALIGN directive.

For example,

!HPF\$ ALIGN WITH targ(i) :: data(i, *)

means that each element of targ has a complete row of data aligned with it. An alternative syntax, using a trivial subscript triplet for data, is

!HPF\$ ALIGN WITH targ(:) :: data(: , *)

Unlike DISTRIBUTE, the ALIGN directive may also be used to replicate an array, or parts of it, by using an asterisk instead of one of the *subscripts* of the *target*. So,

!HPF\$ ALIGN WITH matrixtarget(:, *) :: vector(:)

replicates vector, aligning a copy of it with every column of matrixtarget.

To see how these directives can be used in practice, the example below is a subroutine to multiply together two square matrices as speedily as possible. The processors are imagined to form a 20 x 20 array, but it is the compiler's task to map this abstract processor array onto the physical processors.

SUBROUTINE Square_Matrix_Multiplication (a, b, ab)

REAL, (INTENT, IN) :: a(:, :), b(:, :)

REAL, (INTENT, OUT) :: ab(:, :)

INTEGER :: i, j, n=SIZE(a, DIM=1)

!HPF\$ PROCESSORS grid (20, 20)

!HPF\$ DISTRIBUTE (BLOCK, BLOCK) ONTO grid :: ab

!HPF\$ ALIGN WITH ab(:, *) :: a(:, *)

!HPF\$ ALIGN WITH ab(*,:) :: b(*,:)

FORALL (i=1:n, j=1, n) ab(i,j)=DOT_PRODUCT &

(a(i, :), b(:, j))

END Subroutine Square_Matrix_Multiplication

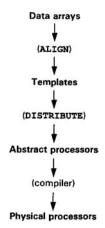


Figure 15.1 A model of the mapping process.

The first ALIGN directive makes n copies (*) of every (:) row of a and broadcasts the copies along (*) the corresponding (:) rows of ab. The second ALIGN makes n copies (*) of every (:) column of b, and puts the copies down (*) the corresponding (:) columns of ab. So, when the FORALL is executed, the processor that is calculating ab (i, j) will have local copies of the elements a (i, k) and b(k, j) for all values (:) of k.

TEMPLATE

Besides aligning data arrays against one another, it can be useful to define a pseudo-array, a "template", against which a variety of data arrays can be sensibly aligned, but without the template occupying any memory space in its own right. The template can then be mapped to the abstract processor array by a DISTRIBUTE directive.

A template can be regarded as allowing for another intermediate stage in the process by which mathematical data arrays are ultimately mapped onto the physical processor array. We can visualize the process like that shown in Figure 15.1:

A template is defined by a special directive, TEMPLATE, with a syntax very similar to that of PROCESSORS. For example,

!HPF\$ TEMPLATE :: chessboard (8,8)

defines a template with the name chessboard. It represents data structured in the form of an 8 X 8 matrix, but it occupies no memory itself. A template can be the *target* of an ALIGN statement, and it can be distributed to the processors like a data array by a DISTRIBUTE directive.

The following code sets up a large square template. It then aligns four smaller data arrays against it, with each data array pushed into one of the four corners of the template.

!HPF\$ TEMPLATE :: square (64, 64)

REAL :: b1(10, 10), br(10, 10), t1(10, 10), tr(10, 10)

ALIGN WITH square (i+54, j):: b1(i, j)

ALIGN WITH square (i+54, j+54):: br(i, j)

ALIGN WITH square (i, j):: t1(i, j)

ALIGN WITH square (i, j+54):: tr(i, j)

INHERIT

The INHERIT directive is used within procedures to ensure that the data represented by a dummy argument will be appropriately mapped.

When a procedure is called, a dummy argument can in fact be handled in any of three distinct ways: "transcriptive", "prescriptive", or "descriptive". The INHERIT directive arises in the first of these, but all three are briefly explained below.

1. Transcriptive mapping means that the distribution of the dummy argument data is "transcribed", i.e. "inherited", from the distribution of the corresponding actual argument data. To achieve this, the procedure must include an INHERIT directive naming the dummy argument or arguments for which this is to happen, as in

SUBROUTINE Jabber (x)

REAL, INTENT (IN OUT) :: X (:,:)

!HPF\$ INHERIT :: x

which means that the assumed-shape argument x takes its distribution, as well as its shape and value, from the actual argument.

Prescriptive mapping occurs when the procedure specifies its own distribution for the dummy argument data, regardless of how the actual argument might have been distributed, as in

SUBROUTINE Hiho (a)

REAL, INTENT (IN OUT) :: a(16, 16)

!HPF\$ PROCESSORS :: procs (32, 32)

!HPF\$ DISTRIBUTE (BLOCK, BLOCK) ONTO procs :: a

If this happens to match the mapping of the actual argument in the calling program, well and good. If the mapping in the calling program was different, then the argument data will be implicitly remapped on entry to Hiho and will be implicitly remapped again on re-entry to the calling program.

3. Descriptive mapping simply consists of specifying within the procedure that the argument data will have a certain distribution, with the requirement that the actual argument must conform to that. This is achieved with a special asterisk notation: in a DISTRIBUTE directive, an asterisk must immediately precede the distribution format:

SUBROUTINE Silver_Lining (q)

REAL, INTENT (IN OUT) :: q (16, 16)

!HPF\$ PROCESSORS :: procs (32, 32)

!HPF\$ DISTRIBUTE *(BLOCK, BLOCK) ONTO procs :: q

The asterisk means that the mapping is assumed from the calling program, although it is specified here anyway. If the actual and dummy arguments have distributions that do not match, it is regarded as an error, unless the procedure has an explicit interface. Interfaces may include HPF directives as well as ordinary Fortran declarative statements. If there is an explicit interface, the compiler will be able to ensure that data array remapping occurs.

REDISTRIBUTE, REALIGN and DYNAMIC

The REDISTRIBUTE and REALIGN directives have much the same syntax as the DISTRIBUTE and ALIGN directives, but they allow the redistribution (or realignment) at execution time of data that has already been distributed or aligned. REDISTRIBUTE and REALIGN can be regarded as executable versions of the corresponding declarative directives.

However, in order for a data array to be realigned or redistributed while the program is executing, i. e. "dynamically", it must have originally been declared to have the HPF attribute DYNAMIC. This can be done with a special declarative directive whose syntax is similar to that of PROCESSORS or TEMPLATE, e.g.

!HPF\$ DYNAMIC :: arrayname

Procedures for data mapping

HPF includes a library of procedures known as HPF_LIBRARY that was mentioned in Section 15.3. Most of the functions described in that section are part of HPF_LIBRARY. In addition, HPF_LIBRARY has procedures that are intended to facilitate the aligning and distributing of data arrays. These procedures are:

- GRADE_UP (array, *dim*), a function that produces an integer array which is a permutation of the indices of array. The permuted indices are such as to re-order the elements of array in ascending order of their values.
- GRADE_DOWN (array, dim) does the same as GRADE_UP, but sorts the elements of array in descending order.
- HPF_ALIGNMENT (alignee, *lb*, *ub*, *stride*, *axis_map*, *identity_map*, *dynamic*, ncoppies) is an inquiry subroutine associated with the ALIGN directive. It returns information about the alignment of alignee. It can be used to return integer arrays containing the lower bounds (lb), upper bounds (ub) and strides (stride) governing the correspondence between the dimensions of the alignee and its alignment target. The *axis_map* argument is normally an array containing successive integers (1, 2, 3,...) but in a permuted order to indicate if the dimensions of the alignee were permuted when it was aligned to its target. If there is a "collapsed" (i.e. "degenerate") dimension, then that dimension is indicated by a zero value in *axis_map*. The identity_map argument is a scalar logical variable used simply to indicate if the alignee was aligned in an identical fashion onto a target of the same shape, and dynamic likewise indicates if the alignee has

the DYNAMIC attribute, i.e. can be realigned dynamically. Finally, the scalar integer *ncopies* is the number of copies that were made of each element of the alignee if replication was involved in the alignment.

- HPF_TEMPLATE (alignee, *templ at e_rank, lb*, ub, *axia_type, saxis_info, number_aligned*, dynamic) is an inquiry subroutine that can largely be understood with reference to HPF_ALIGNMENT. HPF_TEMPLATE also gives information about the alignment of alignee, but it assumes that the alignment was to a template and it gives the information relating to that template. The *axis-type* argument is a character array indicating whether each dimension of the alignee is aligned in a "NORMAL", "REPLICATED" or "SINGLE" way to the template. If "NORMAL", *axis_info* is an array saying which dimension of the template is aligned to which dimension of the alignee. If "REPLICATED", *axis_info* is like *ncopies* for this particular dimension. The "SINGLE" value means that, in this dimension, the alignee is mapped to just one coordinate of the template, in which case *axis_info* says which one.
- HPF_DISTRIBUTION (distributee, axis_type, axis_info, processors_rank, processors_shape) is a subroutine whose usage follows the same pattern as HPF_ALIGNMENT and HPF_TEMPLATE. It is concerned with the ultimate distribution of the *distributee* array onto an abstract processor array. The *axia_type* argument is a character array, as in HPF_TEMPLATE, but the values that may be returned are "BLOCK", "CYCLIC" and "COLLAPSED". In the first two cases, *axis_ info* will contain block sizes (i.e. the integers in brackets after BLOCK or CYCLE in a DISTRIBUTE directive).

15.5

Extrinsic procedures

All the procedures so far described in this chapter, whether written by the programmer or provided as part of HPF, can be imagined to be executed globally for the whole of the computer. Although the computer may consist of a number of parallel processors, and the data may be divided among them, any ordinary procedure is executed centrally and controls all the processors. This is an aspect of the SIMD (single instruction, multiple data) paradigm on which HPF is based.

In reality, however, and depending on the computer's architecture, a compiled procedure may be replicated and executed separately on the different processors. This might already happen behind the scenes, so to speak, under the compiler's control, e.g. for Fortran's simple intrinsic procedures. HPF gives the programmer an explicit method of writing procedures that are to be executed separately on different processors. They are said to be "local" procedures.

Local procedures are one of a new class of procedures called, in HPF terminology, "extrinsic" procedures. If extrinsic procedures are to be called from an HPF program, they must have an explicit interface, and they are defined by specifying EXTRINSIC in that interface. The interface to an extrinsic function is of the form:

INTERFACE

EXTRINSIC (HPF_LOCAL) FUNCTION...

END FUNCTION...

END INTERFACE

The keyword HPF_LOCAL, in brackets, indicates what sort of extrinsic function is being used. As the term suggests, an HPF_LOCAL extrinsic function is written in the HPF language and is a local function in the sense explained above, i.e. it will execute locally and independently on individual processors.

There may be other sorts of extrinsic procedures. For example, the syntax is intended to serve as a way of interfacing HPF to programs written in the language C, in which case we might have

EXTRINSIC (C) FUNCTION

The sorts of extrinsic procedures supported by different implementations of HPF will vary. There is no guarantee that EXTRINSIC (C) will actually work on a particular installation. However, any HPF-conforming system should allow for local procedures with the HPF_LOCAL keyword.

An extrinsic local procedure, in HPF, may look superficially like any other HPF procedure, but when such a procedure is written there are a number of obvious constraints arising from the local nature of its execution. It should work with local data, i.e. data that has been distributed to the particular processor, although one should bear in mind that ALIGN directives in the main program may replicate any array data that needs to be broadcast to all the processors. Scalar arguments will be automatically broadcast to all the processors. An extrinsic function interface may specify global arrays as arguments, but each locally-running copy of it will only have access to a section of it that is distributed to one processor, and the dummy arguments must have assumed shape. Local procedures cannot gain access to global data through modules. Local procedures may invoke other local procedures, but not non-extrinsic ("global") HPF procedures. Extrinsic local procedures are not allowed to be recursive and should be pure, although the syntax above does not allow for the PURE keyword.

An extrinsic local procedure cannot be invoked from a FORALL construct or from within an INDEPENDENT loop, because in those circumstances it is already expected that execution will take place in parallel on separate processors—in a way, FORALL and INDEPENDENT already go part-way (compiler permitting) towards doing the job of local procedures.

The processors are synchronized before a local procedure is invoked, and re-synchronized on return from all the processors. If the local procedure is a scalar-valued function, the values returned from all the processors should be the same, except that the global version of the procedure may be declared to be a vector with one element corresponding to the value returned by each processor.

15.6 HPF local procedures

Although a local procedure is executed separately on a number of processors, it is necessarily written in a single "extrinsic" version, and it might therefore be thought that it must execute in exactly the same fashion on every processor, apart from differences in the values of the data arrays. It might also be thought that a local procedure can obtain no information at all about the global situation. But this is not so: HPF provides a

number of special procedures that can be used to give useful and processor-specific information to a local procedure.

- MY_PROCESSOR() is an argument-free function returning an integer identifying the local physical processor. All the processors are imagined to be numbered in sequence (1, 2, 3,...).
- LOCAL_BLKCNT (array, dim, proc) returns the number of blocks of elements from array, along the dimension *dim*, that are distributed to the processor numbered proc.
- LOCAL_LINDEX (array, dim, proc) and LOCAL_UINDEX (array, dim, proc) return the lower and upper index values of elements from array, in the dimension indicated, that are distributed to the processor numbered proc.

These procedures obviously enable a local procedure, running on a single processor, to find out which processor it is and to establish which bits of the global data arrays have been distributed to it.

The procedures HPF_ALIGNMENT, HPF_TEMPLATE and HPF_DISTRIBUTION, already described in Section 15.4, will also work when called from local procedures. However, their results will be different—when called locally, they are interpreted in terms of the local data arrays on the particular processor. To give the same global information when called from local procedures, three new procedures have been defined. They, and the others below, are part of a procedure library known as HPF_LOCAL_LIBRARY:

- GLOBAL_ALIGNMENT (array,...) is the Same as HPF_ALIGNMENT but gives the global information when called locally.
- GLOBAL_DISTRIBUTION (array,...) is like HPF_DISTRIBUTION.
- GLOBAL_TEMPLATE (array,...) is like HPF_TEMPLATE.
- GLOBAL_LBOUND (array, *dim*) is a function that takes as its array argument the local (dummy) name of an array, and its value is the lower index bound (in the dimension indicated) of the corresponding whole actual array.
- GLOBAL_UBOUND (array, dim) is similar to GLOBAL_LBOUND, but returning a lower bound. If dim is absent, GLOBAL_LBOUND and GLOBAL_ UBOUND are array-valued, spanning the dimensions of *array*.
- GLOBAL_SHAPE (source), where source is a dummy argument, tells the local procedure the shape of the global array of which *source* is a part.
- GLOBAL_SIZE (array, dim) is similar to GLOBAL_SHAPE, but will return the extent of the global array along the specified dimension.
- ABSTRACT_TO_PHYSICAL (array, index, proc) and PHYSICAL_TO_ ABSTRACT (array, proc, index) are subroutines giving the correspondence between a physical processor (see MY_PROCESSOR above), an abstract processor (identified by its indices in the array given in a PROCESSORS directive), and data that has been distributed to a particular processor (array being its dummy argument name in a local procedure). ABSTRACT_TO_PHYSICAL yields the *proc* identifier, the other two arguments having INTENT (IN) . PHYSICAL_TO_ABSTRACT yields the abstract processor's index, the other two arguments having INTENT (IN).
- LOCAL_TO_GLOBAL (array, 1_index, g_index) and GLOBAL_TO_ LOCAL (array, g_index, 1_index, local, ncopies, procs) are subroutines to convert local indices to global indices, and *vice versa*, for an element of the array argument whose local dummy name is array. In GLOBAL_TO_LOCAL, the argument local is a logical flag saying whether the specified global element is within the local array, and *ncopies* and *procs* will say how many copies there are on other processors if it was replicated.

15.7 Final summary

Work is already being done in preparation for a major revision of Fortran for early next century (Fortran 2000), but the real future of Fortran probably lies in the line of research and development that is represented by HPF. It has no serious competitor as a *de facto* standard language for the advanced parallelprocessing computers on which leading-edge scientific research now depends. Since advanced computer systems are now as important to science as new devices for collecting or measuring physical data, HPF is central to the future of many different scientific disciplines. Enjoy using it!

APPENDIX A Input and output

Fortran's READ and WRITE statements were introduced in a simple form early in this book so that statements could be written that would pass data from or to the processor's default input or output (i/o) devices. It has been assumed that these default devices are a keyboard and a screen and that the format of the data takes a simple form. Appendix A. 1 describes the READ and WRITE statements more fully, and also a second output statement, PRINT. The rules of straightforward "list-directed" i/o and "unformatted" i/o are also explained in detail, as are NAMELIST groups.

The full details of Fortran's data edit descriptors and device control descriptors are listed in Appendix A. 2, and finally a number of specialized filehandling procedures are covered in Appendix A. 3.

The i/o procedures GET, PUT and PUT_LINE, for reading and writing variable-length character strings, are to be found in Appendix C.

The details of i/o are relegated to this appendix because Fortran is not primarily a language for data acquisition, data display, or file handling. Although Fortran's i/o facilities are powerful and extensive, computer users today are more likely to use other tools for these purposes. A programmer who tries to use Fortran for anything more than the most straightforward kinds of i/o is probably using the wrong tool for the job. Fortran's i/o facilities date back to a time when black-and-white fixed-font text printers were essentially the only way of producing output for direct human consumption. This history has left its mark not only on the Fortran language but, more generally, on the ASCII character set itself: the bell character was once the only way of getting a computer to make an intentional sound and the underscore exists because originally one of the very few methods of highlighting text was by underlining it, i.e. by writing the text, then backspacing, and then writing a line of underscores. That is now of interest only to historians of technology.

A.1

Data transfer

A.1.1

READ, WRITE and other statements

The READ and WRITE statements are essential for any program that is to communicate with the outside world. READ and WRITE are the Fortran "data transfer statements", by which information is transferred from or to any external medium (keyboard, screen, disk files, printers, or whatever).

The information is usually expected to take the form of a sequence of characters (possibly including special control characters), and in this case the data is said to be in "formatted" i/o records. So far we have

always used formatted i/o, and most of this chapter will be devoted to formatted data. However, there is such a thing as "unformatted" i/o, which will be explained in Section A.1.5.

As we shall see, reading and writing data can be a complex and sophisticated task for the programmer. As a general rule it is advisable for those parts of a program that deal with i/o statements to be organized into dedicated subroutines, and they could be kept in a special module. It is usually bad programming practice to scatter data transfer statements across subroutines whose primary functions are something else. Grouping i/o statements together also simplifies matters if the program ever needs to be modified for use on a processor with a different set of i/o devices.

The general forms of the data transfer statement are

READ (UNIT=..., FMT=...,) input-item-list

and

WRITE (UNIT=..., FMT=...,) output-item-list

except that FMT may be replaced by NML in the special case of namelist formatting, which will be described in Section A.1.6.

READ or WRITE indicates, obviously, the direction of data transfer. UNIT= is normally followed by a unit number that is an integer (or a scalar integervalued expression) indicating which i/o unit is to be used. The idea is that different numbers will point to different devices. The available devices will be system-dependent. More details about i/o units are given in Appendix A.3. Fortunately, to simplify matters the default i/o devices can be selected by inserting an asterisk in place of the unit number.

The FMT keyword gives a "format specifier" that will normally be a character expression or character variable as described in Appendix A.2. However, there is a simple kind of default formatting, "list-directed" formatting, which is invoked by putting an asterisk as the format specifier. List-directed formatting, which in fact we have used so far in this book, is described in more detail in Sections A.1.3 and A.1.4.

Between the brackets following READ or WRITE there may in fact be a fairly lengthy list of control specifications in addition to UNIT= and FMT=. The additional control specifications are optional, and will arise mostly in connection with reading and writing magnetic disk files and tapes. The control specifications in the brackets can appear in any order, being identified by the keywords UNIT, FMT, and others. However, the keyword UNIT is unnecessary if this specification comes first, and the FMT keyword is unnecessary if this specification follows second; hence READ(*,*) is equivalent to READ(UNIT=*, FMT=*).

The PRINT statement and abbreviated READ statement

A statement

PRINT f, ...

where f is any format specifier (including, possibly, *) can be used as an alternative to

WRITE (UNIT=*, FMT=f)

Also, it is possible to replace the statement

READ (UNIT=*,FMT=f)

by

READ f,

A.1.2

I/O item lists

The data transfer statement, after the bracketed set of control specifications, has a list of input items or output items. Items for input, in a READ statement, must be represented by the names of variables and, if the statement is successful, those variables will thereby be assigned values. In principle, the items may be of any type or dimension, with just one or two technical exceptions mentioned below. Examples of input lists are:

namestring x, y, z bstring(1:5), bstring(7:7) address%postcode

address

kounts, (milliamps(j), j=1, kounts)

Here, namestring could be one string of characters or could be an array of strings, as long as it has been previously declared as such. When an i/o list contains an array or an array section, it is as though the elements were specified one after another in array element order. However, it is not possible to input data into an assumed-size array.

In the second example above, x, y and z could be three real numbers, but if they have been declared as (say) complex numbers then the equivalent of six real numbers will be input. The third example illustrates that input characters may be assigned to sections of strings. Also, a single derived-type structure-component can be read (address%postcode), as can a complete data structure (address), but input and output statements are not allowed with derived-type structures containing pointer components. The final example shows how the "implicit-Do" notation can be used to control an i/o list: here we have one integer (kounts) followed by that number of further integers, namely milliamps(1), milliamps(2),..., up to milliamps(kounts). The integer variable j is an arbitrarily-named dummy index. This example is equivalent to

kounts, milliamps(1:kounts)

However, something like

```
(milliamps(i), j=1,milliamps(1))
```

would not be allowed as you cannot read a variable and also utilize it within the same item of an i/o list.

Any of the above could equally well appear as output item lists in a WRITE statement as long as the variables have previously assigned values. An output item list may also contain constants and expressions, such as:

```
"There is no further data available to you"
"Date: ", nday, " ", months(nmonth)," ", nyear+2000–
&100*INT(nyear/50)
"Sines:", (SIN(theta(i)), i=1, 99, 2)
((rmass(i), Prob(rmass(i), errbar(i), rm(i), nalgo), &
i=1, 22), nalgo=1, 3)
```

The second of these consists of a character string constant, an integer variable, another character constant (the blank), an element of a character string array, another blank, and an integer expression that depends on the integer variable nyear and invokes the function INT. The third example outputs the values of the sines of alternate members of the array theta. Implied DO loops in i/o may be nested, as illustrated in the final example, and in a WRITE statement there is no reason why an external function (e.g. Prob above) should not appear.

By using arrays or derived types, very large amounts of data can be handled by short and elegant statements. For example, the statement

WRITE (UNIT=laserprinter, FMT=memo) document

could do a great deal of work, all the complications being expressed elsewhere in the definitions of memo and document.

A.1.3

List-directed input

The FMT control specification will be explained in more detail in Appendix A.2, but it is often sufficient to use what is called "list-directed" formatting, invoked by inserting an asterisk (FMT=*). With list-directed formatting, the input or output format is determined by the nature of the i/o item list alone.

Bear in mind that list-directed formatting (like all forms of i/o formatting in Fortran) amounts to a conversion between internal Fortran data and a sequence of characters used by an external device. On input, a sequence of characters is converted into Fortran data objects (real, logical, character or whatever) and on output the conversion goes the other way.

If a single integer number is to be input, then the input format will be simply the number expressed in ordinary decimal form, e.g.

and this is also a valid input format for a real number that happens to have no fractional part. Remember that here we are not talking about Fortran statements but about the form of data input (e.g. through a keyboard) to the processor as it runs the program. For a real number having a fractional part, a decimal point may be used:

365.242

For convenience with numbers of very large or very small magnitude, a multiplying power often may be indicated by putting the exponent after the letter E immediately following the number: examples are:

2.997925E8 2.997925E+8 6.626176E-34 365242E-3

of which the first two are equivalent to one another and the last is exactly equivalent to the example in the previous paragraph. If a complex number is to be input, then its real and imaginary parts are enclosed together in brackets; valid forms of complex numbers are:

(0, 1)

.

(–0.5, 1.73205)

(41975.9, 3.7E6)

If a series of numbers is input, their types must match the names listed in the READ statement and the numbers can be separated by commas. For example, the Fortran code

INTEGER :: k; REAL :: days, root3

COMPLEX :: omega, zero

READ (UNIT=*, FMT=*) k, days, root3, omega, zero

will be satisfied by the input data

365, 365242E-3, 1.73205, (-0.5, 1.73205), (0, 0)

Blanks alongside a comma are not significant and may be omitted, as in the data

365, 365242E-3, 1.73205, (-0.5, 1.73205), (0, 0)

but one or more blanks may be used (outside a complex number) as separators by themselves instead of commas:

365 365242E-3 1.73205 (-0.5, 1.73205) (0, 0)

An "end of record" (i.e. the enter or return key on a keyboard) normally has the effect of a blank and so this may be used as a separator or a terminator: so all the above examples should be understood as having the return key pressed after the final character of the line. It is possible for every item to appear on a separate line:

365 365242E–3 1.73205 (–0.5, 1.73205) (0, 0)

Arrays of numbers, or derived data types formed out of numbers, may be input in the same way. If we have

```
INTEGER :: nwars(6)
```

.

READ (UNIT=*, FMT=*) nwars

then the data may be put in as

1914, 1918, 1939, 1945, 1998, 2007

If the input data is of type logical, it is sufficient if it consists of letters T (for TRUE) and/or F (for FALSE) separated like numbers by blanks or commas, e.g. for seven logical items we may have

T, F, F, F, T, T, F

or

TFFFTTF

but the T or F may be immediately preceded by a decimal point, and other arbitrary characters may follow it before the next separator, so

TRUE FALSE FALSE FALSE TRUE TRUE FALSE

and

.T.F.F.F.T.T.F

and also

.

.TRUE. .FALSE. .FALSE. .FALSE. .TRUE. .TRUE. .FALSE.

are all equivalent valid input formats.

Things can be a little more complicated if character constants are to be input. A pair of statements like

CHARACTER(20) :: title, forename, surname

READ (UNIT=*, FMT=*) title, forename, surname

will be satisfied by the input

Bishop Thomas Finnegan

because the blanks (which could equally well be commas) will act as separators between the three character strings. However, ambiguities could arise if the strings themselves are supposed to contain blanks or commas (or slashes). To get over this, it is possible to use double or single quotes when a character string is input, just as we do when specifying a character constant in Fortran itself. In other words,

"Bishop" "Thomas" "Finnegan"

will have exactly the same effect as the previous example, and

"Air Vice-Marshal" "Howard" "Tudor Jones"

will correctly include the spaces in the first and third items. The usual rules for character string constants apply: a double quote may appear as part of a string delimited by single quotes (apostrophes); a single quote may occur as part of a string delimited by double quotes; a doubled double quote can be used to represent a

(single) double quote within a string delimited by double quotes; and a doubled single quote can be used to represent a (single) single quote within a string delimited by single quotes. A string delimited by either single or double quotes may run from one record (i.e. one line) to the next, as long as the end-of-record does not appear between doubled (single or double) quotes within the string.

If this seems complicated, remember that when character input is contained within one line, does not involve any blanks, slashes, or commas, and does not start with a quote or apostrophe, then there is no need for it to be enclosed in quotes (single or double) at all.

It remains to be said that, with list-directed character string input, an input string longer than that declared for the list item will be truncated from the right; if it is shorter, the list item will be padded out with blanks to the right. This is just the same as happens in character assignment statements when strings of different length are equated.

Whatever the type of the input data, null values can be input by having no characters between successive commas, e.g. for six integers of which only the first four are actually input

1914, 1918, 1939, 1945, , ,

or, if the line is ended by pressing enter/return, we can have

1914, 1918, 1939, 1945, ,

Remember that a blank is purely cosmetic when it is next to a comma. In the above example, the first four integers are specified but the last two are not altered within the program: a null value does not change anything and an undefined value will remain undefined. A null value is not equivalent to a zero or (for character data) a blank. If items in an input list have been preset to certain values by assignment statements before the READ statement, null inputs will leave the preset values unchanged.

It is sometimes convenient to input a series of identical values. This can be done by a "multiplier", or "repeat specification", as in

3*0 3*1 3 5 5*1 3*F 7*Yes

which is equivalent to the collection of integer, logical and character string inputs

00011135TTTTTFFF Yes Yes Yes Yes Yes Yes Yes

In general, if the form r* (where r is an unsigned positive integer) immediately precedes any input value, the value is regarded as having been input r times. (For this reason, a character string being input naked, i.e. not enclosed in quotes or parentheses, may not begin with numeric digits followed by an asterisk.) If the r* is immediately followed by a blank, then a series of r null values is understood, e.g.

1914 1918 1939 1945 2*

or

1914, 1918, 1939, 1945, 2*

are equivalent to the example given earlier. At the end of a list, another way of inputting null values is with a slash as in

1914 1918 1939 1945/

The slash always terminates the execution of a list-directed input statement, with null values for any remaining items, unless of course the slash is part of a character string delimited by quotes or apostrophes.

A.1.4 List-directed output

A statement such as

WRITE (UNIT=*, FMT=*) o/p item list

will output the values of the listed items according to a simple convention similar to that which we have seen for list-directed input. Integer numbers appear in the obvious format, and logical items appear as T or as F. Real numbers appear in decimal form, if necessary with an exponent (i.e. an E suffix and power of ten) if they are very large or very small: the number of decimal places given, and the exact criterion for using the exponent notation, are processor-dependent. Complex numbers will be in parentheses, with a comma between the real and imaginary parts. Integer, real and complex data items will be separated by commas and/or blanks, but character strings will normally appear without separators or surrounding quotes or apostrophes.

A.1.5

Unformatted i/o

Formatted i/o, in Fortran, involves some sort of transformation between data as it is stored internally in the processor and data as it is stored or displayed externally. Whatever the internal form, the external form can always be regarded as a sequence of characters divided into records. The "records" may simply be lines, as on a printed page, and the characters will almost always be separate bytes coded according to a convention such as ASCII.

Unformatted i/o, by contrast, involves no conversion of the structure of the data: it is transferred to or from the external medium in the same form that it has within the processor. The internal form is a technical matter and Fortran does not care about the details of it. In general, unformatted records can only be read by the same processor, or the same type of processor, that wrote them: general portability between processors cannot be assumed.

The advantage of unformatted i/o is that it is likely to be faster and more efficient than formatted i/o, and it is easier for the programmer because no format specification or namelist specification is needed.

In practice, unformatted i/o does not arise in Fortran with data coming from a keyboard or going to a display device such as a screen or printer. It can arise if, say, data is being dumped onto a tape for periodic backup purposes, or if data needs to be transferred between disk files.

Unformatted i/o is achieved simply by omitting the FMT specifier in an i/o statement.

To be on the safe side, especially where derived-type data structures are concerned, unformatted data should be written and read with similar data item lists. If Decay_Modes is a data structure (not involving pointers), and if disk99 is the number of a disk unit, then we could have

WRITE (UNIT=disk99, REC=1) Decay_Modes

READ (UNIT=disk99,REC=1) Decay_Modes

These statements could be used to store the data temporarily outside the processor's memory. The meaning of REC will be mentioned in Appendix A.3.

A.1.6

Namelists

A data transfer statement such as

READ (UNIT=..., NML=..., ...)

provides a concise method of reading (or writing, in the case of a WRITE statement) a set of data the structure of which is defined elsewhere in a special kind of statement, a NAMELIST statement. Because the NAMELIST statement gathers data together under a collective group name, there is no need to specify an i/ o list in this data transfer statement. Neither is it necessary to have a format specifier. When namelists are used for input or output, the data is given in the input or output records in a standard annotated form described below. Namelist output is especially convenient as a way of dumping out data when a program is being debugged.

The NAMELIST statement is a specification statement with the syntax

NAMELIST / group-name / group-object-list

where group-name is a name constructed according to the usual Fortran rules. The *group-object-list* is simply a list of the names of variables. These variables can be of a mixture of types, including arrays and derived types, but they must have been declared (or be implicitly defined) previous to the NAMELIST statement. Examples are

NAMELIST /Years/ nwars, nfloods, nfamines

NAMELIST /Person/ title, forename, surname

NAMELIST /Coordinates/ x, y, z

A single NAMELIST statement can include more than one group, as in

NAMELIST /Months/ birthmonths, deathmonths &

/Years/ nbirthyears, ndeathyears

and one group can be continued later on a second or successive NAMELIST statement, e.g.

NAMELIST /Person/ bmonth, dmonth, nbyears, ndyears

would append four more items to the group /Person/ defined in the earlier example. There is no reason why the same item of data should not crop up in two or more different namelist groups.

The sets of data in the above examples could be input or output by statements like

```
READ (UNIT=*, NML=Years)
```

WRITE (UNIT=*, NML=Person)

or

READ (UNIT=*, NML=Coordinates)

but note that group names cannot be manipulated or switched about by assignment statements: group names can only occur in NAMELIST, READ or WRITE statements and they cannot be passed as arguments of procedures. In some respects a namelist group is similar to a derived-type data structure, but derived types can be manipulated and assigned with much more flexibility.

If we return to the example above, the statement

READ (UNIT=*, NML=Coordinates)

will invoke the input of three real numbers, thereby assigning values to the variables x, y and z. The input must take a form like

&Coordinates x=3.8, y=-6.6, z=0 /

i.e. on a keyboard the user must type an ampersand followed by the group name, then a blank (or a number of blanks), then a series of values. Each value must be specified by the name of a group member followed by an equals sign followed by the value itself. The group members need not all be specified, nor need they be in the original order; so we could input

&Coordinates y=0.332, x=4.9 /

in which case the value of z would not be changed. The value specifications are separated from one another by commas and/or one or more blanks, and the set must be terminated with a slash. The values themselves must be specified according to the same rules as for list-directed input, described earlier in this chapter, except that character input must always be enclosed in quotes or apostrophes, as in

&Security Keyword="Carthaginian" /

Array elements may be specified. We could have, for example,

LOGICAL :: leaps(2000) NAMELIST /Calendrical/ leaps leaps=false READ (UNIT=*, NML=Calendrical)

with the actual input

&Calendrical leaps(4:2000:4) = 500*T /

so the program presets as false all members of a logical array called leaps and at execution time the user sets every fourth member to be true. The great advantage of namelist input is that the program user can decide at execution time to change any selection of variables as long as their names have been included in the namelist group.

It is much more straightforward to use namelists for output rather than input, since with output the program user does not need to remember any names or syntax. A statement like

WRITE (UNIT=*, NML=Coordinates)

could output the following data:

&COORDINATES X=4.9, Y=0.332, Z=0.0 /

Fortran 95 Feature not in Fortran 90

On input, namelist data can have, following one or more name/value pairs, an exclamation mark followed by comment as in

&Calendrical leaps(4:2000:4) = 500*T /! i/p record 21

A.2 Data editing and formatting

A.2.1

Introducing formats

So far we have only considered data transfer statements in which the format of the data is determined by default conventions according to the nature of the data, i.e. "list-directed" formatting with FMT=*. However, for complete flexibility the programmer can control the format through the FMT specifier. The

FMT specifier should take the form of a character expression. Below, most of our examples will refer to WRITE statements, but the same rules generally apply to READ.

Suppose there is just one object in the i/o item list, and we are writing its value onto the standard output device:

WRITE (UNIT=*, FMT=format1) datum

Before the execution of this statement, format 1 (which is an arbitrary name) must have been assigned a character value, e.g. by

format1 = "(110)"

Here, quotes are present because the variable format1 is being set to the character constant

(I10)

and this character constant is known as the "format specification". The parentheses are a feature of the syntax needed for any format specification. Inside the parentheses we have in this example the single "edit descriptor"

I10

and this means that the output item is an integer and can occupy up to ten spaces, i.e. the specification allows for an integer of up to ten digits to be printed or displayed, or nine digits with a minus sign. In other words, datum should be an integer not greater than 9999999999 and not less than –9999999999. If datum were going to be a real number, we would need something like

format1 = "(F10.4)"

The edit descriptor F10. 4 means that datum is real (the F stands for "floating point"), that a total of ten spaces are allowed, and that the value will be shown rounded to four decimal places. For example, if datum is equal to 22.0/7 then the above will display four blanks followed by

3.1429

In general a format specification takes the form of a bracketed list of edit descriptors, where the total number of edit descriptors should normally match the number of data items in the i/o item list. For example, for a series of three real numbers and one integer we could have the format specification

(F10.4, F10.4, F10.4, 110)

and the blanks between the edit descriptors are not significant. To abbreviate things, there is a simple notation for repeating identical edit descriptors: the number of them is put immediately before the letter F or I, so the above example is equivalent to

(3F10.4, 110)

Repetitions may be nested using brackets, i.e. we could have something like

(3(2I10, F10.4))

which is an abbreviation for

(I10, I10, F10.4, I10, I10, F10.4, I10, I10, F10.4)

and this would present the nine numbers side by side over 90 spaces. Here is a more complete example:

```
REAL :: volume(3), weight(3)
```

INTEGER :: number(3)

.

-

format99 = "(3I6,6F8.3)"

WRITE (*, FMT=format99) number, weight, volume

So far only the simplest edit descriptors have been mentioned for integer and real-number data (I and F editing). There are in addition many other types of edit descriptor in Fortran. In practice, format specifications often consist of long lists of edit descriptors of different sorts. They fall into three classes, namely:

(a) data edit descriptors;(b) character string edit descriptors; and(c) control edit descriptors.

These will be explained in turn in the sections following.

In addition we could say that there is a fourth class (d) consisting only of the null edit descriptor where there is nothing between the brackets, as in

WRITE(*, FMT="()")

which has the effect of writing an empty record (or, on input, skipping over a record). So the statement

READ (*, FMT="()")

should just pause the execution of the program until the return key is pressed.

A.2.2

Data edit descriptors and character edit descriptors

The letters I and F discussed above are special cases of "data edit descriptors" Data edit descriptors guide the input or output of the data items listed at the end of the READ or WRITE statement. Each edit descriptor starts with a letter depending on the nature of the data and how it is to be edited. The possible initial letters are listed below.

I Integer data (decimal form) B Integer data (binary form) 0 Integer data (octal form) Integer data (hexadecimal form) Z F Real or complex data (simple decimal form) Е Real or complex data (exponential notation) L Logical data Α Character data G Generalized editing (for data of any type).

For I editing, as we have seen, the letter I is followed immediately by an integer specifying the total number of character positions used to display the data item. For example, on input, 16 will read a decimal integer from a field of six characters, i.e. with up to six digits or five digits and a sign. On output, 16 will display an integer in a field six characters wide, if necessary with leading blanks. B, o and z editing is very similar to I editing except that the integer is displayed or stored in binary, octal or hexadecimal form. For example, B10 will edit an integer in binary form up to a maximum value of 1111111111, i.e. (in decimal) up to 1023.

Note that binary, octal and hexadecimal editing have nothing to do with how the integers are stored within the processor's memory. The descriptors I, B, o and z would all apply to data of the same Fortran integer type. The editing simply determines the external display or storage format.

For output with I, B, O and Z editing it is possible to display leading zeros so that each data item has a certain specified minimum number (m) of digits. This is done by adding the integer m after a decimal point, e.g. the descriptor 4I10.8 might display

00079451 00175600 10905502 0000000

given the data 79451, 175600, 10905502, and 0. So, the general forms of integer edit descriptors are Iw, Iw.m, Bw, Bw.m, Ow, Ow.m, Zw, and Zw.m, where w is the total field width and m is used to arrange leading zeros. Obviously m, if present, cannot exceed w.

The integers w and m, and similar elements of the other edit descriptors mentioned below, must appear in Fortran as actual integers and not as variables or expressions.

An F edit descriptor is used for real-number data (or two of them could be used for a complex number). The general form is Fw.d, where w is an integer giving the total field width. On output, there will be a decimal point in the appropriate position followed by d places of decimals. On input, if there is a decimal point, d could mean that the final d digits are interpreted as the fractional part of the number, but if a decimal point appears explicitly in the input stream then the value of d is irrelevant. Also on input (but not output) the actual data item may include an exponent as described under E editing below.

E editing has exactly the same effect as F editing for input. E7.0 and F7.0 will both take a real number from a field seven characters wide. On output, however, E editing writes the data in exponential notation, i.e. with a power of ten so that very large or very small numbers can be represented compactly. This is best illustrated by examples: the edit descriptor E10.4 could display numbers in the form

-.5000+009 (meaning -500 million)
-.3408-015 (-0.34×10⁻¹⁵)
.1000+129 (10¹²⁸)
.1000+000 (0.1)
.0000+000 (0)

So, the number appears as an optional sign followed by a decimal fraction less than 1 but not less than 0.1, followed after a + or - sign by a power of ten (exponent) which determines the magnitude of the number. In these examples up to three digits are allowed for the exponent, but if necessary more can be allowed by an extension to the edit descriptor: the general form is Ew.dEe, and e gives the maximum number of digits in the exponent (default three). The above examples are therefore equivalent to E10.4E3.

There is a further elaboration of E editing, relevant for output, known as EN ("engineering")editing. The general form ENw.d will display a real number across a field of w characters in exponent notation but with the exponent being always a multiple of three. To do this the number appears first in the range from 1 to 999 with a fractional part specified to d places of decimals. With EN12.4 the number of seconds in a year would appear as 31.5360+006, and half a millionth would appear as 500.0000–009. The extended form ENw. dEe extends the possible magnitude of the exponent as mentioned in the previous paragraph.

Finally, there is a another variation known as ES editing (general forms ESw. d and ESw. dEe) which is like E editing but displays one significant figure before the decimal point. With ES12.4, therefore, the last example would appear as 5.0000–007.

L editing is for transmitting data of logical type. The letter L is followed by an integer giving the number of character positions taken up by the data item. The item is represented, on output, by a right-justified letter T or F representing the values .TRUE. or .FALSE. respectively. The edit descriptor 8L4 could produce the output

TTFTFFFF

On input, the T (or F) may be preceded by a decimal point and may be followed by other characters, as in the case of list-directed input. Thus, forms like .T, .T., TRUE and .TRUE, would all be acceptable inputs as long as the field width is adequate.

For data of character type the A edit descriptor is used. (This is not quite the same thing as a "character edit descriptor" that will be explained at the end of this section.) The letter A can be followed by an (integer) field width, and that number of characters are directly transferred in or out.

Character editing is particularly simple because we are, in effect, doing the trivial job of converting a character string into a character string, whereas all the other data edit descriptors have to carry out a conversion between a character string and some other data type. The letter A need not be followed by a field width: if it is not, the length of the string is taken to be the length of the corresponding data item as listed in the READ or WRITE statement. If a field width is specified and is not equal to the length of the corresponding list item, then characters may be lost or padding blanks may be inserted, so it is generally best just to use the descriptor A by itself to transfer a character string of any length.

As an alternative to all the data edit descriptors mentioned so far in this section, G ("generalized") editing can be used for data of any type. A descriptor of the form Gw.d or Gw.dEe will output a real number in exactly the same way as Ew.d or Ew.dEe. If the data is of integer, logical or character type, the d and e parameters are ignored, and Gw.d (or Gw.dEe) is equivalent to an Iw, Lw or Aw descriptor.

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The possibility of specifying zero field width has been introduced for IBOZ-and F descriptors, with the meaning of the *minimum* field needed to accommodate whatever data there is. It is possible to have a double zero, e.g. with F0.0 meaning that as many digits are displayed as are necessary to show the actual data item.

Hollerith data: a Fortran 90 Feature excluded from Fortran 95

For formatted output there is another type of edit descriptor, nH, for writing a specific string of characters. Such a string is sometimes called "Hollerith" data. The descriptor **nH**... causes the output of a string of n characters immediately following the letter **H**. So, **8HOVERFLOW** is equivalent to 'OVERFLOW' and **8HMartin's** is equivalent to 'Martin' 's'.

Hollerith editing is outmoded and unnecessary and should be avoided in new programs. It has been eliminated from the Fortran 95 standard.

A "character string edit descriptor" is a kind of descriptor that, technically, is not a data edit descriptor because it does not correspond to an item in an i/o item list and therefore does not transfer a data object. A character string edit descriptor is simply a character constant, specified explicitly between quotes or apostrophes, and is used only with a WRITE statement to output a fixed set of characters. For example,

"The result is"

is a character string edit descriptor, and could be included within a format specification like

presentation="('The result is ', F10.4, ' •, A)"

to guide the output statement

WRITE(*, FMT=presentation) result, units

In fact this format specification actually has two character string edit descriptors, the second containing only a blank character to write a space between the number result and the word units.

It is always possible to use character data instead of a character string edit descriptor. Instead of

```
f = "('Execution terminating.')"
```

```
WRITE(*, FMT=f)
```

we could have

f ="(A)"

signoff="Execution terminating."

WRITE(*, FMT=f) signoff

Bear in mind that character variables must be declared and must have defined lengths, so in the above examples f and signoff must have previously appeared in CHARACTER type declaration statements. This could of course be avoided by having simply

WRITE(*, FMT="(•Execution terminating•)")

and remember that the need to count characters can be avoided by statements like

CHARACTER(*) :: f = "('Execution terminating.')"

. .

WRITE(*, FMT=f)

The FORMAT statement:

The format specifier in an i/o statement need not only be a character expression or an asterisk. It may alternatively be a statement label (Chapter 14). In that case the labelled statement must be of a special kind, a FORMAT statement, which gives the format specifier. For example,

101 FORMAT (3(8X,F12.4))

WRITE (UNIT=3, FMT=101) a, b, c

is equivalent to

CHARACTER;*) :: f101="(3(8X, F12.4))"

WRITE (UNIT=3, FMT=f101) a, b, c

It is also possible to have the name of an integer variable as a format specifier, but the variable must be assigned (by an ASSIGN statement) to the label of a FORMAT statement.

A.2.3

Control edit descriptors

Control edit descriptors, as their name suggests, are useful to control i/o devices but they do not themselves refer to individual i/o data items. Fortran's control edit descriptors are listed below:

Tn.	Tabulate to character position n in the i/o record
TLn	Tabulate n characters to the left
TRn	Tabulate n characters to the right
nx	Skip forward n characters
/	Skip to start of next record
:	Stop i/o immediately if the i/o list is finished
S	Plus signs optional (numeric output only)
SP	Plus signs written (numeric output only)
SS	Plus signs omitted (numeric output only)
BN	Ignore blanks (numeric input only)
BZ	Treat blanks as zeros (numeric input only)
kP	Scale numbers by 10 ^k

With the first four of these, n is a positive integer that must be specified explicitly. For example, T1 will move to the first character of the current record. With printed output,

WRITE (UNIT=iprint, FMT="(3(T1, A))") word, word, word

will write the word word in bold (three times superimposed) at the beginning of the line. Note that TL (leftward tabulation) cannot move further left than the beginning of the record. TRn and nx are equivalent to one another. On output, TR1 and 1X are both equivalent to the character string edit descriptor containing one blank (" ").

The slash (/) skips to the start of the next record, and may be preceded by an integer greater than one if it is to be repeated. So,

WRITE (UNIT=iprint, FMT="(6/)")

leaves six blank lines. Slash editing (or format reversion, mentioned below) is used whenever one i/o statement is to transfer more than one record. For example,

WRITE (UNIT=mtape, FMT="(50(A,/))") strings

writes 50 records (followed by a final empty record) if there are 50 elements in the array strings.

The colon (:) is useful if it is not known in advance how long the i/o item list will be. So if keynumbers is an array of any size, but not greater than 100,

WRITE (*, FMT="(:,'keynumbers ',/,T10,100(16,:,/,T10))") &

keynumbers

will output all the elements of keynumbers but will not execute the / and T10 after the final element. The first colon means that nothing at all is written if keynumbers is a size-zero array. The same effect could be achieved with

WRITE (*, FMT="(:,'keynumbers ',100(/,T10,I6))" &

keynumbers

Usually, if a format specification allows for more data items than are actually present in the i/o list, the statement terminates only when an unfulfillable data edit descriptor is encountered, and this may mean that some unnecessary control or character string edit descriptors are executed.

Incidentally, if a format specification allows for fewer data items than are present in the i/o list, then a process known as "reversion" occurs and the processor runs through the format specification (or the last bracketed section of it) again as often as necessary. So in fact,

WRITE (*, FMT="(:, 'keynumbers', /, (T10, I6))") keynumbers

would work just like the example above, irrespective of the size of the array keynumbers. When a format specification involves nested brackets, format reversion only goes back over the edit descriptors within the current level brackets, so in the above example it is (T10, I6) that is repeated, not the whole format specification. Reversion always involves moving forward to the next i/o record, so we have (T10, I6) and not (/, T10, I6) in the above example. Simpler examples of format reversion are

WRITE (UNIT=mtape, FMT="(A)") strings

READ (UNIT= mtape, FMT="(A)") strings

both of which will transfer as many records (each interpreted as a single character string) as there are elements in the character array strings.

When numbers are output, positive numbers may or may not be preceded by plus signs. The *S*, SP and SS descriptors control this. SP means that subsequent positive numbers written by the WRITE statement will have plus signs, *SS* means that the plus signs will be omitted, and S lets the processor decide. BN and BZ refer to the interpretation of non-leading blanks in numeric input. BN means that they will be ignored, i.e. it does not matter if the digits of a number are interspersed with blanks or followed by blanks. BZ means that blanks in or after a number are treated as zeros.

The kP descriptor is for use in conjunction with F editing. The number k must be an integer, interpreted as a power of ten, and with subsequent F editing (without exponent) real and complex data items are scaled up (for output) or down (for input) by that factor.

A.2.4 Exercises A.2

A. Which of the following are valid format specifications? And which are valid edit descriptors? 2.1

(i) "(F10.4)"	(ii) (F10.4)	(iii) F10.4
(iv) 8(F10.4)	(v) 8F10.4	(vi) (8F10.4)
(vii) ((F10.4))	(viii) (F10.6, I8)	(ix) ()
(x) "3()"		

A. Write a format specification to output a four-digit integer, followed by three real numbers, all neatly

- 2.2 spaced out over an 80-column line. Assume that the real numbers do not exceed a value of 1000.0 and must be specified to two decimal places.
- A. Write a WRITE statement, incorporating the format specification, to output an integer variable called n
- 2.3 in decimal, binary and octal form on one line, the three forms suitably separated with blanks. Assume that n does not exceed (in decimal) 99.
- A2. What is the output from:

4

(i) WRITE (*, ''(2L2, 2X)'') (/ .TRUE. , (.FALSE., k=1, 3) /)

- (ii) WRITE (*, "(A4, :, TR1)") "Cause", "of", "death"
- (iii) WRITE (*, ''(2F7.4)'') SQRT(2.0), SQRT(3.0)
- (iv) WRITE (*, "(B6, 1X, I6.6)") 40, 40*40
- (v) WRITE (*, "(2E12.4)") SQRT(2.0), 40.0*40.0
- (vi) WRITE (*, "('FA', L1, 'E')") 2+2<5

A. Write a WRITE statement to produce the output

2.5

TERMINATION

(i.e. underlined and with spaces between the letters) given a character string called caption such that

caption = "TERMINATION"

A.3 File handling

A3.1

Units, files and records

Little has been said so far about the nature of input and output devices. The following sections cover a number of ways in which it is possible to control i/ o devices and files. The statements concerned are OPEN, CLOSE, BACKSPACE, ENDFILE, REWIND and INQUIRE. Also, we will mention here a number of special control specifications that can be used with the READ and WRITE statements.

Terms such as "unit", "file" and "record", although often used loosely, have precise technical meanings. A "record" is to be understood simply as a sequence of data items, usually in the form of characters. A record may have any length, and if it is a sequence of characters then the "length" is defined simply as the number of characters in it.

For example, a single line of printed characters is usually regarded as a "record". A sequence of characters from a keyboard would usually constitute a single input record. In general a record does not have to end with any particular kind of character, even though the end of a record may be indicated to Fortran by pressing the enter or return key (keyboard input) or by the slash (/) edit descriptor.

There are two types of "file", external and internal. "Internal" files are explained in Section 9.5. An "external" file is a set of data having a physical existence external to the program. It is rarely necessary to work with internal files, and so the word "file" is usually used by itself to refer to an external file. For example, you might say that a magnetic tape contains a "file" of data.

A file may consist of any number of records (including zero!) and may have, as its final record, a special "endfile record". The word "file" is usually used to refer to a durable set of machine-readable data, as opposed to something ephemeral like a screen display or the tapping of a keyboard. As we shall see, a file can have a name in Fortran. Most commonly, files are stored on magnetic media, i.e. disks or tapes. Some processors may store files on other media such as optical discs or in special areas of memory ("RAM disks").

An important distinction must be made between "sequential access" and "direct access" files. A sequential-access file has a beginning and an end, and the data items must be read or written in sequence. When such a file is first opened it will be positioned at the beginning. As a general rule, sequential-access files consist of "formatted" records, i.e. each record consists of a sequence of characters. "Unformatted" records (Section A. 1.5), on the other hand, are most often of direct-access type.

Historically, the concept of sequential access arose from the use of magnetic tapes: obviously a magnetic tape has to be wound from one end to the other, although backspacing and rewinding are possible. By contrast, a direct-access file corresponds to something like a magnetic disk where any part of the file can be reached very quickly.

It is assumed that a direct-access file is divided into records, and that any record can be read or written independently of the others. However, it is not possible to dive into the middle of a record: each record must be read or written from the first character. For reference purposes, the records of a direct-access file are numbered, but the numbering need not correspond to physical positions on the surface of the disk. The physical layout of data on a disk is a matter for the operating system, not for Fortran, and a sophisticated system may switch records about in complicated ways to optimize the utilization of space on the disk. In a direct-access file the records must all have the same length and they must be numbered: otherwise the operating system would have to be inordinately complicated. The record numbers must be positive integers. In the case of a direct-access file there is no such thing as an "endfile record".

A sequential-access file, such as a file on a magnetic tape, can have records of varying lengths. Unless otherwise specified (and we shall see soon how these things are specified) all files are assumed by Fortran to be sequential-access files. The keyboard, for example, is treated like a sequential-access file, since the records must be input in a particular order—the real-time order— and the records may vary in length. It is possible for a sequential-access file to have zero length.

A possible feature of a sequential-access file is "non-advancing" i/o, as opposed to the usual "advancing" i/o. Usually, a WRITE or READ statement will transfer data to or from an exact number of records. Even if a READ statement only looks at the data in the first part of a record, nevertheless the unit will have physically passed over the whole of the record. So, between two i/o statements a file will always be

positioned between two records. If you want to examine two parts of a record separately, you must either read the record twice (using BACKSPACE, Section A.3.3) or you must read the whole thing once and store in memory the information that you are not ready to analyze. "Non-advancing" i/o offers an alternative: you can read or write a record on a character-by-character basis, executing i/o statements several times as you move through one record. This is called "non-advancing" because the file does not advance automatically to the end of the record after a READ or WRITE, which is the usual procedure.

In Fortran, external files are associated with "units". A "unit" is an i/o device, such as a printer, a tape drive, a barcode reader, or whatever. The definition of a unit is quite independent of the particular data that happen to be flowing through it. A processor will have access to a range of different units, usually numbered by different non-negative integers, except that a standard input device and a standard output device may be referred to by asterisks.

It must be remembered that a "unit" is not the same thing as a "file". A unit is a channel by which the processor may access a file.

A.3.2

Opening and closing files

In the earlier part of this book, READ and WRITE were the only types of i/o statement mentioned. It could be imagined that the input device was the keyboard and the output device was a VDU or perhaps a printer. There was no need to do any more than READ or WRITE to transfer the data, and distinctions between, say, direct-access and sequential-access files did not arise. In general, however, it is not possible to READ or WRITE a file without first executing a special setting-up statement, OPEN. The OPEN statement is used to connect a file to a numbered unit and to decide certain options. It is most commonly used with magnetic tape or disk files. The syntax is simply

OPEN (connection-specification-list)

where connection-specification-list is a selection of specifications, separated by commas, of the sort

UNIT =	the unit number (compulsory!)
IOSTAT =	for error-checking
FILE =	to specify the file's name
STATUS =	new file or old?
ACCESS =	SEQUENTIAL Or DIRECT
FORM =	FORMATTED or UNFORMATTED
RECL =	record length
BLANK =	NULL Or ZERO
POSITION =	ASIS, REWIND Or APPEND
ACTION =	READ, WRITE Or READWRITE
DELIM =	APOSTROPHE, QUOTE Or NONE
PAD =	YES or NO

None of these may appear more than once in the same OPEN statement. They need not all be present, but there must be a UNIT specifier. In many cases an OPEN statement will only involve a small number of the possible options. A typical OPEN statement might be

OPEN (UNIT=6, IOSTAT=ncheck, FILE="april.dat", &

STATUS="NEW", ACCESS="DIRECT", &

FORM="FORMATTED", RECL=512)

What do the specifiers mean? Taking them in the order listed above, each is discussed at more length below.

• UNIT This specifier must be set to an integer expression. It would be quite possible to have, say,

OPEN (UNIT= ndisk1,....)

with *ndisk1* being an integer to be specified as a parameter at the start of the program. The particular meanings of the unit numbers will be processor-dependent. It is not possible to have UNIT=* in an OPEN statement, i.e. opening the processor's default i/o unit.

- IOSTAT This supplies the name of a scalar integer variable that, on execution of the statement, will be given either:
 - 1. a positive value if an error condition is encountered;
 - 2. negative values if an end-of-file or an end-of-record condition is encountered; or
 - 3. the value zero otherwise.

In fact only case 1 or case 3 may occur as a result of the OPEN statement, but it will be seen that the IOSTAT specifier can also be used with other statements such as READ and WRITE and then case 2 may arise. In case 2, the end-of-file condition can only be relevant to a sequential sequential secess file, and the end-of-record condition can only be relevant to a sequential-access file with non-advancing i/o. With a direct-access file, case 2 is never relevant.

- FILE This specifier lets the programmer state a name for the file as a scalar character expression. It is not always needed: for example, magnetic tape files or printers do not usually have names. However, processors usually require disk files to be named. To read an existing file from a disk, it will be necessary to know its name and, to write a new file, a name must be supplied. The convention for constructing names will depend on the processor. It is possible to specify the filename either as a constant expression (like "april.dat") or through the name of a variable.
- STATUS This is a character string (or a character expression) that must be either "OLD", "NEW", "SCRATCH", "REPLACE", or "UNKNOWN". OLD means that a named file already exists, NEW means that it does not yet exist, and REPLACE creates a fresh file and deletes any old file of the same name. SCRATCH is used for a file that has not been given a name, creating a "scratch" file for temporary use as the program executes: a scratch file is deleted when the program terminates or when a

CLOSE statement (below) is executed for the unit. The UNKNOWN option, which is the default if STATUS is omitted, simply means that the status is processordependent.

For STATUS, and for the other specifiers below which call for character expressions, there is no distinction between upper and lower case and any trailing blanks will be ignored.

- ACCESS This is a character expression which is equivalent to either "SEQUENTIAL" or "DIRECT", specifying whether this is a sequential access or direct-access file. The default is SEQUENTIAL.
- FORM This specifier determines whether the file is formatted or unformatted, and it must be a character expression equal to "FORMATTED" or to "UNFORMATTED". The default is FORMATTED for a sequential-access file, or UNFORMATTED in the case of direct access.
- ZRECL This specifier, which is set to an integer expression, gives the record length. For formatted records this means the number of characters in a record. In the direct-access case, RECL is the length of every record, and must be specified. In the sequential-access case records may be of variable length and RECL is taken to be the maximum record length: it may be omitted, in which case a processor-dependent default value takes effect.
- BLANK A specifier applicable to formatted input files, which is set to a character expression equal to either "NULL" or "ZERO", the former being the default. NULL means that blanks are ignored in numeric data (except that a whole field of blanks is treated as a zero) and ZERO means that blanks are treated as zeros.
- POSITION This is a character expression equal to "REWIND", "APPEND" or "ASIS", and it can be specified in the case of an existing sequential-access file. It determines whether the file will be positioned at its start or at its end. REWIND positions it at the start, and APPEND at the end. The ASIS option, which is the default, leaves the file positioned wherever it was.
- ACTION This permits the file to be restricted to read-only or writeonly use. ACTION may have the character values "READ", "WRITE" or "READWRITE". The first two are self-explanatory. READWRITE, the default, permits both reading and writing to take place on this file.
- DELIM This may have one of the character values "APOSTROPHE", "QUOTE" or "NONE", and it has a significance in relation to list-directed or namelist character-string data output. It specifies whether character strings will be displayed between apostrophes (single quotes), between quotes (double quotes), or without any delimiters.
- **PAD** This is a character expression equal to "YES" or "NO". It determines whether or not a formatted input record should be padded out with blanks if it is shorter than expected. If NO, the record's length must match what the READ statement demands. The default is YES.

The list of specifiers above may seem long and confusing at first sight, but in practice the OPEN statement is not difficult to use. A simple procedure is:

- 1. Specify the UNIT number. This will depend on the particular configuration of the processor being used.
- 2. Does the unit refer to a sequential-access file, such as a printer or a tape drive? Or is it a direct-access file such as a disk file? If the latter, skip to step 5. For sequential access, continue with step 3. If you do not know, there is an intrinsic function INQUIRE that can tell you (Section A.3.5).
- 3. If direct access is not specified, files are taken by default to be sequential access. And, unless otherwise specified, sequential-access files are taken by default to be formatted. Formatted sequential-access records may vary in length, but there will be a processor-dependent maximum record length. The INQUIRE function can tell you the processor's maximum record length.

- 4. The specifiers BLANK, DELIM and PAD, which are for formatted records, are not of great interest. They can almost always be omitted. The optional POSITION specifier, for a sequential file, is an opportunity to position the file at its starting point ("REWIND", equivalent to the REWIND statement) or at its end ("APPEND"). Skip to step 6.
- 5. For direct access, specify ACCESS="DIRECT". A direct-access file is taken by default to be unformatted. For direct access, it is necessary to specify the record length using the RECL specifier.
- 6. A file-name may be given using the FILE specifier, but a file name is usually only needed in the case of direct-access disk files. The specifiers STATUS and ACCESS may be useful for protecting files from being inadvertently overwritten. Remember that when STATUS ="SCRATCH", the file should not have a name.
- 7. The IOSTAT specifier is not compulsory but should be included if the code is to be watertight.

Here are a few examples of OPEN statements:

OPEN (UNIT=7, ACCESS="DIRECT", RECL=128, &

FILE='studentgrades.dat', ACTION=READ)

OPEN (UNIT=14, POSITION="APPEND", &

IOSTAT=k_error_unit_14)

OPEN (UNIT=ndiskb, ACCESS="DIRECT", &

RECL=nrecs, FILE=fstring)

OPEN (UNIT=4, ACCESS="DIRECT", &

RECL=idata_unit(4), STATUS="SCRATCH")

After a file has been opened, records may be written or read and other operations may be performed as described below. Finally, the CLOSE statement may be used to disconnect the file from a unit. The syntax is similar to that for OPEN:

CLOSE (specification list)

but the specification list for CLOSE is taken from

UNIT=	the unit number (compulsory!)
IOSTAT=	for error-checking, as for OPEN
STATUS =	KEEP or DELETE?

The optional STATUS specifier may be set either to "KEEP" or "DELETE". In the latter case, the file will be deleted when CLOSE is executed. Note that a file opened with STATUS="SCRATCH" is always deleted on closure anyway. The default STATUS is "KEEP".

Some examples of CLOSE statements are:

CLOSE(UNIT=6, IOSTAT=ncheck)

DO k=1,6; CLOSE(k); END DO

CLOSE(UNIT=14, IOSTAT=k_error_unit_14)

CLOSE(UNIT=ndiskb, STATUS="DELETE")

A.3.3 BACKSPACE, ENDFILE and REWIND

These are the "file positioning statements" and their functions should be clear from their names. They are applicable only to sequential-access files, and in particular magnetic tapes. The syntax can be illustrated by the BACKSPACE statement, which takes the form

BACKSPACE (UNIT=..., IOSTAT=...)

where the UNIT specifier is compulsory and IOSTAT is as usual optional. UNIT and IOSTAT have the same meanings as for the OPEN statement. BACKSPACE moves the file back to the start of the previous record if there is one. The REWIND statement moves the file back to the start of the first record. ENDFILE writes an endfile record. However, an endfile record will be written automatically after a CLOSE statement or simply if a program terminates normally after writing on the file has taken place.

A.3.4

I/O control specifications

So far READ and WRITE statements have been considered of the form

READ (UNIT=..., FMT=...,) input-item-list

and

WRITE (UNIT=..., FMT=...,) output-item-list

and for namelist groups NML has been explained as an alternative to FMT. If the data is unformatted, neither FMT nor NML will be present. The following additional specifiers may be included:

IOSTAT=	as for OPEN
REC=	record number
ADVANCE=	advancing or nonadvancing i/o
SIZE=	number of characters to be read

If IOSTAT is present it allows the program to detect an i/o error or the end of a record or of a file as was described for the OPEN statement earlier.

- REC If REC is present the file must be of direct-access type and REC specifies the number of the record that is to be written or read. Records in a direct-access file do not have to be written or read in any particular order (that is what direct access means, of course) and so the i/o statement has to include the record number. If REC is not present the file is of sequential-access type.
- ADVANCE This is an option available when formatted sequential files are being written or read. The default option, ADVANCE="YES", the most common situation, simply means that the i/o statement will read or write one record, moving the file from the start of one record to the start of the next: it is not possible to read or write a fraction of a record and stop part way through. The option ADVANCE="NO" means that "non advancing" i/o will take place, i.e. the file does not automatically advance to the start of the subsequent record. The effect of this is to make it possible to read or write a record piece by piece. Individual characters can be transferred, the exact number of them depending on the format specification and the i/o item list.
- SIZE In the case of a READ statement, with formatted sequential non-advancing input, the SIZE specifier may be used to give the name of an integer variable that will yield, after the statement has been executed, the number of characters transferred.

Some examples of i/o statements are:

WRITE (UNIT=*, FMT=format, IOSTAT=icheck) (title(k), &

data(:,k), k=1,6)

READ (UNIT=4, REC=1) dump

READ (UNIT=11, FMT=f4, ADVANCE="NO", SIZE=nchars) string

READ (*, FMT="(A1)", ADVANCE="NO") char

The last of these reads a single character from the keyboard. Because ADVANCE= "NO" the statement is not expecting to input a complete record and therefore the data is transferred without any need for the return or enter key to be pressed.

A.3.5 INOUIRE

Some of the statements mentioned above, especially OPEN, may require a knowledge of the detailed properties of the i/o unit being referred to. However, the Fortran programmer does not have to look up all these details in the processor's user guide: there is a statement called INQUIRE which permits the program, at execution time, to find out most of the necessary information automatically. In fact INQUIRE can yield a bewilderingly large array of information. The statement's syntax is simple enough:

INQUIRE (specification-list)

In many respects the *specification-list* is similar to what we have already seen for OPEN and other statements above. The specification list for INQUIRE must include either UNIT=... or FILE=..., but not both, specifying either a unit number or a filename. If a unit is specified, we have what is said to be the "inquire by unit" form of the statement. If a filename is given, it is "inquire by file". (There is a third possibility, "inquire by output list", mentioned at the end of this section.)

With "inquire by unit", the keyword UNIT= may be omitted if the unit specifier is the first in the list, i.e.

INQUIRE (3, EXIST=being_3)

is a permissible statement to check the existence of unit 3. In any INQUIRE statement the unit number must be specified by an integer expression, not by an asterisk, and consequently the default i/o devices cannot be referred to.

After UNIT or FILE, other items in the specification list are of the usual form

SPECIFIER=variable-name

and depending on the specifier the variable may be of integer, character or logical type. The possible specifiers are listed below, and they are all optional, but none of them may appear more than once in the statement. The variables named must all be scalars. They will be given values when the statement is executed.

IOSTAT=	as for OPEN
EXIST =	does the unit/file exist?
OPENED =	file and unit connected?
NUMBER =	what is the unit number?
NAMED =	does the file have a name?
ACCESS =	as for OPEN
SEQUENTIAL = .	can this be sequentially accessed?
DIRECT =	can this be directly accessed?
FORM =	as for OPEN
FORMATTED = UNFORMATTED = RECL = NEXTREC = BLANK = POSITION = ACTION = READ = WRITE = READWRITE = DELIM = PAD =	is formatted i/o possible? is unformatted i/o possible? maximum record length number of next record as for OPEN as for OPEN can the file be read? can the file be read? can the file be written? are reading and writing both allowed? as for OPEN as for OPEN as for OPEN

It should be stressed that all the specifiers in the above list are for the program to obtain information from the processor, not to supply information to it. For example, the ACCESS specifier here is working in the opposite direction to that in the OPEN statement.

Except for those already explained earlier, more details of the above specifiers are given below:

- EXIST This specifies a logical variable that will be true if the file, or unit, exists, and false otherwise.
- OPENED This is also a logical variable. In an "inquire by file" statement it is true if the named file is connected to a unit. In "inquire by unit" it is true if the unit has a file attached.
- NUMBER In an "inquire by file" statement, this is an integer equal to the file's unit number. If the file cannot be found it is set to -1.
- NAMED In "inquire by unit", this logical variable says whether or not there is a named file at this unit.
- SEQUENTIAL This will be a character string equal to "YES" if the file/ unit can be used in sequentialaccess mode, and "NO" if it can only be used in direct access. The processor may answer "UNKNOWN"!
- DIRECT This is similar to SEQUENTIAL. A character string is set to "YES" if the file/unit may be used in direct-access mode, and to "NO" if it may not.
- FORMATTED This is a character string equal to "YES" if formatted records are possible, and "NO" if it is restricted to unformatted use.
- UNFORMATTED The opposite of FORMATTED: "YES" means that unformatted i/o is possible, "NO" means that i/o must be formatted.
- RECL This specifies an integer, the processor's maximum record length for this file/unit. This cannot be exceeded by the RECL specified for the same unit in an OPEN statement.
- NEXTREC When a direct-access file is being written or read, it can be useful to know the number of the next record. The integer specified by NEXTREC is one greater than the number of the last record, or is equal to 1 if none have yet been written or read.
- READ This is a character string set to "YES" if the file/unit may be read from, and "NO" otherwise.
- WRITE This is equal to "YES" if writing is possible, and "NO" if it is not. For example, this specifier will give "NO" if the unit is a keyboard, because a keyboard is an input device. You cannot write onto a keyboard!
- READWRITE "YES" is given if, and only if, the file/unit can be used both for reading and writing.

INQUIRE is an extremely useful statement because it can be used to interrogate a processor and yield information on the basis of which other i/o statements can be constructed to make the best use of the facilities available to the processor. INQUIRE is the key to writing good, portable and crashproof i/o code. A few examples of INQUIRE statements are

INQUIRE (UNIT=laser_printer, RECL=linelength)

INQUIRE (UNIT=3, IOSTAT=j, FORM=sform)

INQUIRE (FILE=scratch_disk_output, NEXTREC=k)

The following subroutine could be used to set up and read a named disk file:

SUBROUTINE Peruse (filename, nrec)

USE Data, ONLY: input => stringbank

CHARACTER(*), INTENT (IN) :: filename

INTEGER, INTENT (IN) :: nreo

INTEGER :: n_unit, icheck

LOGICAL :: q

INQUIRE (FILE=filename, IOSTAT=icheck, EXIST=q, &.

NUMBER=n_unit)

File: IF (icheck/=0) THEN

filename="FAULTY"

ELSE

Existence: IF (.NOT.q) THEN

filename="NOTFOUND"

ELSE

OPEN (UNIT=n_unit, IOSTAT=icheck, &

FILE=filename, ACCESS="DIRECT")

Opening: IF (icheck/=0) THEN

filename="ERROR1"

ELSE

READ (UNIT=n_unit, REC=nrec, IOSTAT=icheck) input

IF (icheck/=0) filename="ERROR2"

ENDIF Opening

ENDIF Existence

ENDIF File

END SUBROUTINE Peruse

So far two forms of the INQUIRE statement have been described: "inquire by unit" and "inquire by file". A third form uses the syntax

INQUIRE (IOLENGTH=integer) output-list

where integer is the name of a scalar integer variable and output-list is a list of data such as could appear in a WRITE statement. The purpose of this statement is to ascertain the record length that the processor would require to output the data with an unformatted WRITE statement. The integer variable specified by IOLENGTH will be set to the necessary record length, and could then be used to open an output file with records of sufficient length, as in

INQUIRE (IOLENGTH=n) stringbank

OPEN (UNIT=k, ACCESS="DIRECT", RECL=n, STATUS="SCRATCH")

WRITE (UNIT=k, REC=1, IOSTAT=nasty) stringbank

The ERR, END and EOR specifiers

In the OPEN, CLOSE, READ, WRITE, BACKSPACE, ENDFILE, REWIND and INQUIRE i/o statements the list of specifications may include ERR=... with the number of a statement label being given. The effect is to transfer control to a statement with that label if there is an error as the i/o statement executes.

Similarly, in a READ statement there can be an END=... specification giving the label of a statement to which control passes if the end of the file is encountered.

There can also be an EOR=... specification in a READ or WRITE statement being used for nonadvancing i/o. Control then passes to the labelled statement if the end of the record is reached.

A.3.6

Exercises A.3

A. Write OPEN statements: 3.1

- (i) To open a magnetic tape scratch file on unit 7.
- (ii) To open a magnetic tape file on unit 3, positioning it at the end of the file so that more data can be appended.
- (iii) To open a direct-access disk file called s_sheet_45 on unit 2, the record length being 256. Then write a CLOSE statement to close the file and discard it.

A. Write statements to:

3.2

(i) Write the 20 elements of an array called datasave as 20 records in an unformatted file on unit 5. (Use a DO loop.)

- (ii) Read the first 10 characters of a record on unit 1, without advancing further through the record. The 10 characters are to be interpreted as two five-digit integers,
- (iii) Inquire which of the units 1 to 10 exist on the processor, and which may be used for unformatted i/o. (Use a DO loop.)
- (iv) Inquire whether a file called temper a is attached to a unit, and what the number of the unit is.

APPENDIX B Bits

Besides Fortran's intrinsic data types (INTEGER, REAL, COMPLEX, CHARACTER and LOGICAL) it is possible to manipulate data in the form of individual binary bits. Bits are similar in some ways to LOGICAL data, in that both are restricted to two possible values, called .FALSE, or .TRUE, for LOGICAL and 0 or 1 for a bit. However, lengthy sequences of binary data can be handled much more naturally and flexibly as bits than in LOGICAL form. Bits are packed within data of integer type, and stored in memory much more economically than LOGICAL data.

To handle bits, Fortran provides the intrinsic functions BIT_SIZE, IBSET, IBCLR, IBITS, ISHFT, NOT, IAND, IOR, and IEOR, and the subroutine MVBITS. These procedures manipulate sets of bits that have to be declared as data of integer type.

B.1

Inside integers

A non-negative integer *i* may be regarded as a sequence of "bits" or binary digits w_k as in

$$i = \sum_{k} w_{k} 2^{k} = w_{0} + 2w_{1} + 4w_{2} + 8w_{3} + \dots$$

with the sum running from k=0 to a value s=1, where s is the number of bits. This formula can be taken to relate an integer *i* to the sequence of bits w_0, w_1, \dots, w_{s-l} .

It is important to know how many bits can be contained in each integer, i.e. what is the processor's value of s, and this is given by a special inquiry function BIT_SIZE(I). The argument I is any integer. The statement

numbits=BIT_SIZE(1)

will therefore tell the program the number of bits per integer on the processor being used. Typically this might be 32 or 64.

The function BTEST (I, POS) looks into the integer I and tests whether the bit in position POS is 0 or 1. The argument POS corresponds to the index k in the equation above, and so it must be an integer in the range from 0 to s-1. BTEST itself has logical value, i.e. BTEST (I=64, pos=k) has the value .TRUE. if and only if k=6.

BTEST is an elemental intrinsic function, as are the other bit functions mentioned below, and may therefore have an array as argument and result. Taking POS as an array, on a 32-bit processor, we could have

INTEGER :: ibitstring; LOGICAL :: bdigits(32)

bdigits=BTEST (l=ibitstring, POS=(/ (i, i=0,31) /))

converting ibitstring (an integer corresponding to a sequence of 32 bits) into the logical array bdigits.

The functions IBSET(I, POS) and IBCLR(I, POS) are used to reset individual bits within the integer I, the result being the modified version of I. IBSET sets the bit in position POS equal to 1 (if that is not already its value) and IBCLR clears the bit to 0. If POS were an array spanning the whole of the integer I, as in the previous example, then IBCLR would clear all the bits in I to zero.

There is a function IBITS(I, IPOS, LEN) which forms a new integer by picking out a subset of the bits within I, i.e. a number LEN of bits starting at position POS. The result IBITS is obtained by right-justifying the chosen bits and setting the others to 0. So, for example, IBITS (I=munch, POS=0, LEN=8) picks out the first byte from munch, and IBITS(I=munch, POS=8, LEN=8) picks out the second byte. When using IBITS, the sum of POS and LEN cannot exceed the total number of bits in I that would be given by the function **BIT SIZE.**

B.2 Bit logic

To carry out logical operations on bits there are the intrinsic functions NOT(I), IAND(I, J), IOR(I, J), and IEOR(I, J). The first of these simply yields the complement of I, i.e. NOT (17) =238 on an eight-bit machine. The other functions have two arguments and form the logical "and", "or", and "exclusive or" combinations on a bit-by-bit basis. So, if

$$i = \sum_{k} w_k 2^k$$
 and $j = \sum_{k} y_k 2^k$
the *ws* and *ys* being binary digits, then

$$\operatorname{NOT}(\mathbf{i}) = \sum_{k} (1 - w_k) 2^k$$

$$\operatorname{IAND}(\mathbf{i}, \mathbf{j}) = \sum_{k} w_k y_k 2^k$$

$$\operatorname{IOR}(\mathbf{i}, \mathbf{j}) = \sum_{k} (w_k + y_k - w_k y_k) 2^k$$
and
$$\operatorname{IEOR}(\mathbf{i}, \mathbf{j}) = \sum_{k} (w_k + y_k - 2w_k y_k) 2^k$$

There are two intrinsic functions to shift the bits around within an integer. ISHFT(I,SHIFT) shifts the bits within I by a number of places given by SHIFT. They go left if SHIFT is positive, and right if SHIFT is

negative, and bits that fall off the end are lost, while places vacated at the other end are filled with zeros. Another function, ISHFTC(I, SHIFT) does a circular shift so that bits pushed off one end of I appear at the other end. In fact, ISHFTC may have a third argument, SIZE, in which case the circular shift occurs only among the SIZE bits at the right. So, SHFTC(I=90, SHIFT=-2, SIZE=8) just operates on the first byte of I and has the value 150.

Finally, there is an intrinsic elemental subroutine called MVBITS (FROM, FROMPOS, LEN, TO, TOPOS) which will do the job of taking a sequence of bits (of length LEN) from the integer FROM (starting with bit position FROMPOS) and copying it into the integer TO (starting at position TOPOS). The statement

CALL MVBITS(FROM=source, FROMPOS=0, LEN=16, TO=dest, &

TOPOS=16)

uses the first two bytes of source to replace the third and fourth bytes of dest.

B.3 A warning

In Fortran, when we use the intrinsic procedures described above, bits are assumed to be packed into nonnegative integers according to the equation at the beginning of Appendix B.1. That equation is fundamental to the working of the procedures. However, variables of integer type in Fortran are not normally represented according to that equation but according to another, processor-dependent, scheme that must of course allow for negative as well as positive numbers.

In other words, the basic equation is valid only in the context of the bit manipulation procedures. If a bitpattern is set up according to that equation, the value of the integer i will not necessarily be the same as the value we would get if the same bit-pattern were interpreted for the purposes of ordinary Fortran integer arithmetic. In fact if ibitstring defines a string of bits by that equation, then its value when regarded as a 32digit binary number is given by

intval = SUM (MERGE (&

TSOURCE=(/(2**k, k=0, 31)/), &

FSOURCE =(/(0, k=0, 31)/), &

MASK=BTEST(I=ibitstring, POS=(/(i, i=0, 31)/))))

and this is not necessarily equal to ibitstring's value when regarded as being of Fortran's integer type!

The following subroutine is an example of how a "non-advancing" input statement could be used to read a stream of bits. Since there is no requirement for format conversion, character-type editing is used, and one character at a time is input. It is assumed that one character represents one byte (eight bits) and that four characters (32 bits) can be stored in the "integer" ibitstring. The subroutine reads 32 bits, but with null bytes if there is an end-of-file, an end-of-record or an input error.

SUBROUTINE Instream (ibitstring, n_unit, icheck)

INTEGER :: ibitstring, n_unit, icheck=0

CHARACTER :: char(4), cnull=ACHAR(0)

DO k=1, 4

READ (UNIT=n_unit, FMT="(A)", &

ADVANCE="NO", IOSTAT=icheck) char(k)

IF (icheck==0) CYCLE

char(k)=cnull

EXIT

END DO

ibitstring=TRANSFER(SOURCE= char(1)//char(2)//char(3)&

//char(4), MOLD=1)

END SUBROUTINE Instream

The TRANSFER function here is taking a concatenation of four characters (32 bits) and designating it as the "integer" ibitstring so that it could subsequently be used in the context of the intrinsic bit manipulation functions. The arithmetical value of ibitstring is irrelevant.

APPENDIX C ISO_VARYING_STRINGS

Full details are given in this appendix of the data type VARYING_STRING, a standard modular extension to the Fortran language. The rationale and structure of the type are explained, and the operators and intrinsic procedures that can operate on it. After some examples of its use, there is a brief critique of the **ISO VARYING STRINGS module.**

C.1

Rationale

Since the publication of the Fortran 90 language by the International Standards Organization (ISO), an auxiliary standard has been accepted and published that adds a new data type to the language. The new data type is called VARYING_STRING. It allows for character strings of variable length to be manipulated, instead of just the fixed-length strings allowed with data of type **CHARACTER**.

Of course CHARACTER-type strings can be of any length, but the length of any particular variable of CHARACTER type must be declared in a type declaration statement and cannot subsequently be altered. The use of a specification expression, or an asterisk in the case of a procedure's dummy argument, provides only very limited leeway with the length of a character string. It has long been felt that this is an irksome restriction and that Fortran should allow character strings to have lengths that can vary dynamically as a program runs. The VARYING_STRING data type now provides this. When a VARYING_STRING variable is declared, the number of characters in the string is not, and indeed cannot be, specified. The programmer may write programs manipulating character strings without ever having to worry about their lengths.

Since VARYING_STRING data is an extension to Fortran, and not yet a required part of the language, the necessary facilities are in a module that is optional to the programmer. The module is called ISO_VARYING_STRINGS, and any program unit that is to have access to it must include the statement

USE ISO_VARYING_STRINGS

This module contains the definition of the VARYING_STRING data type together with a number of functions and subroutines that can be used to manipulate VARYING_STRING data. The names of these functions and subroutines are standardized and are given below.

ISO does not specify exactly how the module ISO_VARYING_STRINGS should be written. In principle, it could be written in a language other than Fortran and it need not be the same on all processors. The ISO standard only specifies what the module must do, not how it should do it. The situation is similar to

that for Fortran compilers. However, ISO_VARYING_STRINGS can in fact be written in Fortran 90. In a version written by J.L. Schonfelder, the VARYING_STRING type is defined by code equivalent to

TYPE VARYING_STRING

PRIVATE

CHARACTER(1), POINTER :: chars(:)

END TYPE VARYING_STRING

which is to say that it is implemented as a pointer to a rank-one deferred-shape array, each element of that array being a single character. However, the user need not know these details and should not make any presumptions about the internal structure of the type.

C.2 The VARYING_STRING data type

Like any user-defined derived type, a variable of VARYING_STRING type must be declared by a type definition statement such as

TYPE (VARYING_STRING) :: forenames(2), surname, &

qualifications(:)

This example also serves to illustrate that, like other data types, VARYING_STRING variables may be scalars or arrays, including assumed-shape arrays. The array qualifications represents an arbitrary number of character strings, each having arbitrary (and differing) numbers of characters.

The internal structure of VARYING_STRING data is PRIVATE to the ISO_VARYING_STRINGS module. Structure components (using the % notation) cannot therefore be used, and neither should structure constructors such as

surname=VARYING_STRING ((/"S","m","i","t","h"/))

because no assumptions should be made about the layout of the components of the data.

In principle the programmer could ascertain the structure of VARYING_STRING data by reading the code of the local implentation of the ISO_VARYING_STRINGS module or by using the TRANSFER function, but it would not be wise to assume that a VARYING_STRING argument can be used with TRANSFER and it is best avoided for the sake of program portability. However, this is no handicap: a range of procedures is provided to facilitate the use of VARYING_STRING data much more elegantly than with structure components and structure constructors. Some of these procedures extend the meanings of the intrinsic Fortran operators for assignment, concatenation and comparison so that they can be applied to VARYING_STRING data. Others are extensions of existing intrinsic procedures (such as LEN) normally only applicable to CHARACTER data. Additionally, there are some completely new procedures specifically for working with VARYING_STRING data.

C.3

Operators

The assignment operator (=) can be used between data of VARYING_STRING and CHARACTER types. Given, for example, the declarations

TYPE (VARYING_STRING) :: V, w

CHARACTERS) :: C

then the assignment operator (=) can be used between VARYING_STRING and CHARACTER data in statements such as

v = w

v = c c = v

If the variable on the left is of VARYING_STRING type (the first two cases above) then it takes on the length of the expression on the right whether that is itself VARYING_STRING (v=w) or CHARACTER (v=c). In the third case above (c=v), the string v will be either truncated or padded with blanks to yield the correct length for the CHARACTER string on the left. Note that the successive statements

c = v

v = **c**

will have the effect of truncating or padding v to the length of c (i.e. to six characters in this example). VARYING_STRING data can therefore be constructed with assignments such as

v="Smith"

The concatenation operator (//) can also be applied to VARYING_STRING data. With the above examples, the concatenations v//w, v//c and c//v are all legal and are expressions of VARYING_STRING type.

The comparison operators ==, /=, <, <=, > and >= (and their equivalent forms .EQ., etc.) can also be applied to VARYING_STRING data or to combinations of VARYING_STRING and CHARACTER data. The results are logical expressions having the same meanings as if the operators were applied to CHARACTER data.

However, with VARYING_STRING data all these operators are defined only for scalars. They cannot be used on arrays of variable-length strings. To concatenate arrays of such strings, for example, it would be necessary to construct a more complicated expression such as

(/ (v(i)//w(i), i=1, SIZE(v)) /)

Here, with v and w being arrays of VARYING_STRING type, v (i) and w {i) are elements of the arrays and are therefore scalars. The concatenation v(i)// w(i) is therefore valid and it is a scalar expression of VARYING_STRING type. The array constructor (/.../) yields an array of VARYING_STRING type equal in size to v, here assumed equal in size also to w.

C.4 Extensions of intrinsic procedures

The module ISO_VARYING_STRINGS contains procedures that allow the following functions to be called with scalar arguments of VARYING_STRING type. In the descriptions below, v and w represent VARYING_STRING variables or expressions and c represents a CHARACTER variable or expression. In this list, italicized arguments are optional.

- LEN(V) Returns the length of the string (integer valued)
- CHAR(v, *length*) Carries out type conversion, VARYING_STRING to CHARACTER. If the optional integer argument *length* is absent, CHAR is returned as a CHARACTER string containing the same characters, and having the same length, as v. If *length* is present, v is truncated or padded to make CHAR the specified length.
- ICHAR(V) As for the intrinsic function ICHAR(C), the argument must have length 1 and the result (an integer) is the position of that character in a processor-dependent sequence.
- IACHAR(V) As ICHAR(v) above, but with the result being based on the ASCII character numbering sequence.
- TRIM(v) Removes trailing blanks from v.
- LEN_TRIM(v) Ascertains the number of characters in v not counting trailing blanks.
- ADJUSTL (v) Replaces leading blanks by trailing blanks.
- ADJUSTR(v) Replaces trailing blanks by leading blanks.
- REPEAT (v, ncopies) ncopies must be a non-negative integer, and the function value is v//v//v...v//v, being that number of copies of v concatenated together.
- LLT(v, w) A logical function corresponding to that for CHARACTER data. The result is . TRUE . if v is "logically less than" w. This function also works with arguments of mixed VARYING_STRING and CHARACTER types, i.e. for LLT(v, c) and for LLT(c, v).
- LLE(v, w) Analogous to LLT.
- LGE(v, w) Analogous to LLT.
- LGT(v, w) Analogous to LLT.
- INDEX (v, w, *back*) Returns an integer which is zero if w is not a substring of v but otherwise is the starting position (or the first starting position, if there is more than one) of the substring w in v. If the optional logical argument *back* is present and is true, then the function picks out the last such starting position if there is more than one occurrence of the substring w in v. Like LLT, this function also works if one of its string arguments is of CHARACTER type.
- SCAN(v, w, *back*) Like INDEX above, but finding the position in v of any single character from w if v contains such a character.
- VERIFY (v, w, back) Like INDEX above, but finding the position in v of a character that is *not* among those comprising w. VERIFY is zero if all the characters in v are also to be found in w.

C.5

New procedures for VARYING_STRING data

The procedures below do not correspond to existing intrinsic functions. Again, v and w are VARYING_STRING scalars and italicized arguments are optional.

VAR_STR(c)

An inverse to CHAR, this function takes a string of CHARACTER type as argument and returns the corresponding string of VARYING_STRING type.

GET(unit, v, set, separator, maxlen, iostat)

The subroutines GET, PUT, and PUT_LINE are very important innovations in Fortran because they provide for the first time a simple and modern alternative to the old-established set of i/o procedures READ, WRITE and PRINT. I/o procedures have to be provided as part of the ISO_VARYING_STRINGS package because otherwise it would be impossible to read or write VARYING_STRING data without first converting it to another type. A VARYING_STRING variable may not appear in a READ, WRITE or PRINT statement because the internal structure of such a variable (i.e. how the characters are laid out) is not specified by the ISO standard and will be found to be PRIVATE to the **ISO_VARYING_STRINGS module.**

GET has one argument which must be present (v ofVARYING_STRING type) and five arguments which are optional.

GET causes a sequence of characters to be read from the input unit number specified by the integer unit, or from the standard input device (normally a keyboard) if the argument unit is not present. The characters read are placed in the string v.

The input stream can be terminated by the occurrence of any one of the termination characters specified by comprising the string *set*, which may be of either CHARACTER or VARYING_STRING type. If *set* is present, there may also be an argument *separator* which would be of VARYING_STRING type and would be returned to indicate which character from *set* was actually encountered if indeed input had been halted in that way (and would be a zero-length string if it had not). Alternatively, input may be halted not by encountering a special character but when a certain specified maximum number of characters, maxlen, have been read from the input record.

If the argument *maxlen* is not present, the input stream will be terminated at the end of the current input record or file. The integer argument *iostat* can be used to check what happened: it will be returned with a negative value if an end-of-file is reached, with a different negative value if an end-of-record is reached, as zero if the record has not been read to its end, or with a positive value if some sort of reading error has occurred. The argument separator, if present, would be returned as a zero-length string.

A subsequent call to the GET subroutine will continue with the reading of the current record (if it had not reached its end) or will start on the next record.

Although most of GET'S arguments are optional, there should be no confusion between them: unit is present if the first argument is an integer, then comes the string v, if there is a second string it is *set*, and if there is a third string it is *separator*. Then, a second integer argument will be maiden, and a third will be *iostat*. You cannot have *separator* without *set*, and you cannot have *iostat* without maxlen.

Although GET is designed for VARYING_STRING data, it can also be used for data of other types by performing a type conversion to CHARACTER data (using CHAR) and then, if necessary, to another data

type by using the TRANSFER function or by writing and reading an auxiliary internal file. Similar comments apply to the PUT and PUT_LINE subroutines described below.

GET, PUT, and PUT_LINE read and write formatted sequential files, but unfortunately (since the unit number must be an argument of integer type) not internal files.

PUT(unit, v, iostat)

This is a subroutine that is an inverse of GET in the sense that it writes a string of characters v to an external file which, if not the default output unit, is specified by the unit number unit. If there is a current record, the string is appended to it, but otherwise a new record is started. The argument *iostat*, if present, is returned zero or positive according to whether the writing operation was successful or led to an error condition.

PUT_LINE(unit, v, iostat)

This subroutine is very similar to PUT except that, when the string v has been written, the output record is terminated and the file is moved to the start of a subsequent record. With screen output, PUT_LINE would move to the start of the next line after writing v, while PUT would stay on the same line unless it had reached the end of it.

INSERT(v, istart, w)

The argument istart being an integer, this function inserts the string w into the string v immediately before the character at position istart within v. If istart is less than 1, w is inserted at the beginning as if istart=1. If istart is greater than LEN(v), w is appended to v. INSERT is a function whose value is of VARYING_STRING type. It makes no difference if one or both of v and u are of CHARACTER type instead of VARYING_STRING.

REPLACE(v, *istart*, *ifinish*, *target*, w, *every*, *back*)

This function may replace one or more substrings within v by copies of the string w. If the second argument is an integer, it is *istart* and this represents the position in v before which w will be inserted. If the third argument is an integer it is *i finish*, and w replaces the characters from position *istart* going rightward to position *ifinish* in v. However, if *i finish* is less than *istart* or greater than the length of v, then the string w is simply added at the beginning or end of v without any deletion of characters.

If *ifinish* is absent, w replaces its own length's-worth of v's characters (or whatever number remain, if fewer) going rightward from position *istart*. If *istart* is less than 1 it is treated as if it were equal to 1, and if it is greater than the length of v then w is simply appended to v.

Alternatively, if REPLACE'S second argument is a string, the string is *target* and the function looks for occurrences of *target* within v, searching from right to left. The first occurrence of *target* within v, if there is one, will be replaced by a copy of w. If the argument w is followed by a true logical argument, *every*, then all distinct occurrences of *target* are replaced by copies of w. A second logical argument, *back*, may follow *every*, and if *back* is true then the search for *target* is carried out from right to left through v.

The REPLACE function can therefore work in either of two modes according to whether the replaced string is identified by its position (if *istart* is present) or by its content (if target is present). The logical

arguments *every* and *back* may only be present if target is present, and *ifinish may* only be present if *istart* is.

As in the case of the INSERT function, the string arguments in REPLACE may be of either character type but the result is always of VARYING_STRING type. Examples are:

REPLACE("aaaa", "aa", "b") is equal to VAR_STR("baa")

REPLACE("aaaa", "aa", "b",.TRUE.) is equal to VAR_STR("bb")

REPLACE("aaaa", "aa", "b", .FALSE., .TRUE.) is equal to

VAR_STR("aab")

REPLACE("aa", "a", "bb", .TRUE.) is equal to VAR_STR("bbbb")

REMOVE(v, *istart*, *ifinish*)

REMOVE (v) removes all the characters from v, leaving a zero-length string.

REMOVE (v, istart) removes all the characters from v starting from position *istart, istart* being an integer. The function's result is what is left.

If the integer *ifinish* is not less than *istart*, then REMOVE (v, *istart*, *ifinish*) will remove from v the characters from position *istart* to position *ifinish*. If *ifinish* is less than *istart*, no characters are removed.

The argument v may be of either character type. An example is:

REMOVE(text, LEN(text))

which cuts off the last character of text.

EXTRACT(v, istart, ifinish)

This function yields the substring of v that would be removed if the REMOVE function were called with the same arguments. Examples are:

EXTRACT(text, LEN(text))

which gives the final character of text, and

EXTRACT(text, 2)

which cuts off the first character of text, i.e. extracts the rest of text, from the second character on.

SPLIT(v, w, set, separator, back)

This is a subroutine which runs through v looking for the occurrence of a character from among those specified by being members of the string set. When such a character is found (or at the end of v if none is), the characters that were to the left of it form the string w and only those to the right of it are retained in v. If *separator* is present, and a character from set was encountered, *separator* is returned with that character.

The logical argument *back*, if present and true, causes the search for a character from set to be carried out from right to left through v. In this case v will remain with the leftmost part, and w the rightmost part, of the original v.

The arguments v, w and separator must be of VARYING_STRINGtype; set may alternatively be of CHARACTER type.

An example is as follows: after

Type (VARYING_STRING) :: title, name

the code fragment

title = "Alexander the Great"

CALL SPLIT(title, name, " ")

has the same effect as

title = "the Great"

name = "Alexander"

but

title = "Alexander the Great"

CALL SPLIT(title, name, " ")

has the same effect as

title = " "

name = "Alexander the Great"

because in the latter case set contains no characters, and therefore no character from set is encountered in v (i.e. in title), and therefore all the characters from v are decanted into w (i.e. into name).

C.6 Programs using ISO_VARYING_STRINGS

As a very simple example of the use of the VARYING_STRING data type, the following program reads text from the keyboard word by word, assuming that words are separated either by blanks or by the end of a line. The words are then displayed on the screen, one to a line. The program stops when the word terminate is typed.

PROGRAM Wordfinder

USE ISO_VARYING_STRINGS

TYPE (VARYING_STRING) :: word

! Set up a string containing the non-alphabetic characters:

CHARACTER(*), PARAMETER :: &

set = "'!""£\$%&*()_-+={}[]:~;'#<>?,./\\¬^1234567890"

! Read the words

Words: DO

! Read in one word

CALL GET (word, "")

! Remove any non-alphabetic characters

Characters: DO

ipos=SCAN(word, set); IF (ipos==0) EXIT Characters

word=REMOVE(word, ipos)

END DO Characters

! If appropriate, display the word on screen

IF (word=="terminate") EXIT Words

IF (word/=" ") CALL PUT_LINE (word)

END DO Words

END PROGRAM Wordfinder

The program below does much the same job, but it reads characters one at a time from the keyboard and forms words by concatenating sequences of adjacent alphabetic characters.

PROGRAM Wordfinder_II

USE ISO_VARYING_STRINGS

TYPE (VARYING_STRING) :: word, onekey

! Set up strings containing the alphabetic characters:

CHARACTER(26), PARAMETER :: &

uppercase = "ABCDEFGHIJKLMNOPRSTUVWXYZ", &

lowercase = "abcdefghijkInmopgrstuvwxyz"

! Read the words

Words: DO

! Read in one word

word = " "

Word: DO

! Read in one keystroke

CALL GET (onekey, 1)

! A blank ends a word

IF (onekey==" ".OR.onekey=="") EXIT Words

! Note that a null input may arise at the end of a

! record

! It is assumed that no word is split between two

! records

! Replace any upper-case letter by its lower-case

equivalent

ipos=VERIFY (uppercase, onekey)

IF (ipos/=0) onekey = EXTRACT (lowercase, ipos, ipos)

! Ignore non-alphabetic characters

ipos=VERIFY (lowercase, onekey)

IF (ipos==0) CYCLE Words

word = word//onekey

END DO Words

! If appropriate, display the word on screen

IF (word=="terminate") EXIT Words

IF (word/="") CALL PUT_LINE (word)

END DO Words

END PROGRAM Wordfinder_II

Arguably, Wordf inder_II is a better-designed program than Wordf inder because (a) it reads the data in character by character in the first place, while Wordf inder reads complete words and then has to scan through them; and (b) Wordf inder_II checks positively that characters are alphabetic, instead of depending on a possibly incomplete list of non-alphabetic characters. Both programs are somewhat inelegant in using both character data types: with ISO_VARYING_STRINGS being used, there is a case for not using CHARACTER-type data at all (except to specify constants such as ""). Also, both programs fail to check against i/o errors by utilizing the iostat argument of GET and **PUT_LINE.**

The following example shows a way of implementing a derived data type in Fortran to represent sets of discrete objects. The sets can be of any size, and the problem of modelling them can be simplified and solved economically using **ISO_VARYING_STRINGS** as a tool.

MODULE Sets

! This module defines a new data type, "Set", together

! with a number of associated operators and procedures.

! An entity of type Set is a finite set of unordered

! distinct elements. Since a set may have any number of

! elements, this module is coded with the help of the

! VARYING_STRING type defined in ISO_VARYING_STRINGS.

! Internally, a set will be represented by an ordered

! sequence of positive integers separated by commas, e.g.

!

! 2,5,17,18,19,572,1024

```
!
!
but coded as a VARYING_STRING data object
!
!
VAR_STR("2,5,17,18,19,572,1024")
!
!
together with an integer that is the number of
!
! elements in the set.
```

! It is assumed that integers will be used as set-member
! identifiers, i.e. each potential member of a set can
! be uniquely identified by an integer label. Each
! member may also involve further data. For example, if
! the sets are the members of different golf clubs then
! their names and addresses, handicaps, etc. will have to
! be stored somewhere. The association between a
! member's identification number and that data is not
! the concern of this module. This module merely
! manipulates sets of identification numbers.

!

USE ISO_VARYING_STRINGS

! Enables VARYING_STRING type to be utilized.

PRIVATE

! Entities within this module will normally be

! inaccessible outside it.

TYPE Set

PRIVATE

! The components are private even if Set itself is

! made public.

TYPE (VARYING_STRING) :: stringset

INTEGER :: multiplicity

END TYPE Set

PUBLIC :: Set, Construct, Union

! These entities are to be accessible outside the

! module.

CONTAINS

! Module procedures are as follows:

FUNCTION Construct (integers)

! Constructs a set out of the array of integers provided

! as argument.

TYPE (Set) :: Construct, temporary

INTEGER, INTENT (IN) :: integers(:)

TYPE (VARYING_STRING) :: build

CHARACTER(100) :: internal_file

! Identification numbers may have up to 100 digits.

CHARACTER(100) :: item

! Sets may have up to 100 members

INTEGER :: itemp1 (SIZE(integers)), &

itemp2(SIZE(integers)), number, n

! First, order the integers and eliminate duplicates.

! Duplicated entries are replaced by negatives.

itemp1 = integers

n = 0

number = SIZE(integers)

Order: DO i = 1, number

max=MAXLOC(itemp1)

itemp2(number+1-i) = itemp1 (max)

itemp1 (max) = -1

END DO Order

Duplicates: DO i = 2, number

IF (itemp2(i)==itemp2(i-1)) itemp2(i) = -1

END DO Duplicates

build= VAR_STR("")

IF (number/=0) THEN

```
DO i = 1, number
```

IF (itemp2(i)<0) CYCLE

n = n+1

WRITE (internal_file, "(I100)") itemp2(i)

READ (internal_file, "(A100)") item

build = build // TRIM(ADJUSTL(item))

build = build // ","

END DO

END IF

temporary%stringset = Remove (build, LEN(build))

temporary%multiplicity = number

Construct = temporary

END FUNCTION Construct

FUNCTION Union (s1, s2)

! Returns the union of the two sets s1 and s2

TYPE (Set) :: Union

TYPE (Set), INTENT (IN) :: S1, S2

VARYING_STRING :: contents1, contents2

CHARACTER(100) :: internal_file

CHARACTER(100) :: item

INTEGER :: integers1(s1%multiplicity), &

integers2 (s2%multiplicity)

INTEGER:: number1, numbers, icount1, icount2, icount3, &

numbers_full_3, more

INTEGER :: integers3(s1%multiplicity + s2%multiplicity)

Trivial: IF (s1%multiplicity==0) THEN

Union = s2

ELSE IF (s2%multiplicity==0) THEN

Union = s1

ELSE

! unpack s1 and s2

contents1 = s1%stringset

number 1 = s1%multiplicity

DO i = 1, number1

CALL SPLIT(contents1, item, ",")

WRITE (internal_file, "(A100)") item

READ (internal_file, "(I100)") integers1(i)

END DO

contents2 = s2%stringset

number2 = s2%multiplicity

DO i = 1, number2

CALL SPLIT(contents2, item, ",")

WRITE (internal_file, "(A100)") item

READ (internal_file, "(I100)") integers2(i)

END DO

! Now combine integers1 with integers2 and construct

! Union

Pairs: DO

icount1 = 1

icount2 = 1

icount3 = 1

IF (integers1(icount1)<integers2(icount2)) THEN

integersB(icount3) = integers1(icount1)

icount1 = icount1 + 1

icount3 = icount3 + 1

ELSE IF (integers1(icount1)>integers2(icount2)) THEN

```
integers3(icount3) = integers2(icount2)
```

icount2 = icount2 + 1

icount3 = icount3 + 1

```
ELSE IF (integers1(icount1)==integers2(icount2)) &
```

THEN

```
integers3(icount3) = integers2(icount2)
```

```
icount1=icount1+1
```

```
icount2=icount2+1
```

```
icount3=icount3+1
```

END IF

```
IF(icount1>number1.OR.icount2>number2) EXIT Pairs
```

END DO Pairs

```
IF (icount1==(number1+1) .AND.icount2==(number2+1)) &
```

THEN

```
! Enough of integers3 has been filled and
```

```
numbers_full_3=icount3-1
```

```
ELSE IF (icount1>number1) THEN
```

```
! fill out integers3 with the remainder of integers2
```

more=number2-icount2+1

integers3(icount3:icount3+more-1) = &

integers2(icount2:number2)

numbers_full_3 = icount3+more-1

ELSE IF(icount2>number2) THEN

! Fill out integers3 with the remainder of integers1

more=number1-icount1+1

integers3(icount3:icount3+more-1)=&

integers1(icount1:number1)

numbers_full_3 = icount3+more-1

END IF

Union = Construct (integers3(1:numbers_full_3))

END IF Trivial

END FUNCTION Union

END MODULE Sets

C.7 Deficiencies of ISO VARYING STRINGS

Although the VARYING_STRING data type is *a* great improvement on the CHARACTER type, it is interesting to notice that the specification of ISO_VARYING_STRINGS is a compromise designed to allow the module to be written in Fortran. So, VARYING_STRING is a derived type like any other, albeit with its internal structure hidden (to avoid inadvertent name clashes) by PRIVATE statements within the module.

Consequently, ISO_VARYING_STRINGS has one or two disadvantages. It is not possible to write constants of VARYING_STRING type. So, a statement like

word = ""

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(from the example program Wordf inder_n above) involves the implicit use of CHARACTER data because "" is a CHARACTER constant. To avoid implicit or unexpected type conversions, VARYING_STRING constants should ideally be written using VAR_STR, e.g. in the form

VAR_STR("abcdefghij klmnopqrst")

The procedures listed in this appendix are strictly speaking module procedures, not intrinsic procedures or external procedures. Functions like LEN and CHAR are therefore classed as module procedures when their arguments are of one type but are intrinsic procedures with another type. This could conceivably make a difference to code which uses the INTRINSIC statement. Functions such as CHAR and IACHAR are elemental as intrinsic functions, but not as they are extended by ISO_VARYING_STRINGS. Also, the assignment operator cannot be used elementally with VARYING_STRING arrays. So, VARYING_STRING arrays be manipulated as easily as CHARACTER arrays.

Another disadvantage of ISO_VARYING_STRINGS arises because the natural way for the module to work is by using ALLOCATE statements with array pointers to allocate sufficient memory space to hold the strings. However, there is then no easy way of deallocating the space when the corresponding variable is no longer needed. For example, on return from a subroutine that uses large arrays of non-saved local data of

VARYING_STRING and CHARACTER types, the space taken up by the CHARACTER arrays will in principle be released, but the space taken up by the VARYING_STRING arrays would not be deallocated and therefore could not be used to store any other data while the program is running. So, ISO_VARYING_STRINGS is likely to be wasteful of computer memory, at least if it is written using array pointers in Fortran 90 (see the comment at the end of Section 12.1 concerning automatic deallocation in Fortran 95).

These remarks are not intended to discourage the use of ISO_VARYING_ STRINGS, merely to make it clear that VARYING_STRING is a derived type and has the same limitations of any other derived type defined in Fortran. If, in a future version of the language, VARYING_STRING is adopted as an additional intrinsic type, then a good feature will have evolved into an excellent one -which is what the evolutionary philosophy of Fortran is all about.

APPENDIX D Fortran 95's new features: summary

The new features of Fortran 95, which were not present in Fortran 90, are summarized below:

D.1 FORALL (Section 6.5)

FORALL statements and FORALL constructs can be regarded as like DO loops but without the time sequence implied in DO. FORALL is intended to allow for parallel execution. Examples of the FORALL statement are

FORALL (i=1:n, i/=13) square(i, i) = backdiag(n-i)

FORALL (j=1:n-1, Test(r(j))==.TRUE.), r(j) = Fun(r(j)) &

+ Fun(r(j+1))

In FORALL assignments, the right-hand sides are all calculated before any of the left-hand sides are changed. Any procedures that arise, like Test and Fun above, must be pure (see Appendix D.5).

D.2 Enhancements to WHERE (Sections 4.9 and 6.6)

WHERE statements and constructs may now be nested within one another and within FORALL constructs. In a WHERE construct, masks may be applied not only to the WHERE statement itself but also to ELSE WHERE statements.

D.3 Initialization of pointers (Sections 8.7 and 13.1)

Variables which are pointers may be initialized with the NULL function (see Appendix D.8).

D.4

Default initialization of derived types (Section 12.5)

Data of derived type may be initialized within the derived type definition. This default initialization applies to all variables of the type and can be over-ridden for individual variables by initialization of the usual sort in type declaration statements. For example,

TYPE Default_zero_real

REAL :: r=0.0

END TYPE

defines a new type of real variable which, unlike REAL, is always automatically initialized to zero.

D.5 Pure procedures (Section 11.2)

A pure function calculates its value but does not alter the values of its arguments or of any other variables accessible from outside it. A pure subroutine may affect the values of INTENT (IN OUT) or INTENT (our) arguments.

Pure functions may be used in specification expressions (Section 11.9).

D.6

Elemental procedures (Section 11.3)

Elemental procedures are pure procedures which are defined in terms of scalar arguments but which may be referenced elementally in array assignments. So, in Fortran 95, the programmer may write procedures, like the intrinsic elemental procedures, that can be called with scalar or array arguments.

D.7

Automatic deallocation of allocatable arrays (Section 12.1)

To avoid memory loss, allocatable arrays (unless declared with the SAVE attribute) will be automatically deallocated on return from the procedure in which they occur.

D.8

New and enhanced intrinsic procedures (Appendix F)

- MINLOC and MAXLOC These functions have been extended so that their arguments correspond to those of MINVAL and MAXVAL.
- CEILING and FLOOR These may now be called with a KIND keyword.
- NULL This is a new function that evaluates to a disassociated pointer.
- SIGN This function may distinguish between positive and negative zero if the processor supports the distinction.

• CPU_TIME This new intrinsic subroutine may, in the case of parallel processing, return an array giving the timings of the individual processors.

D.9

Newly obsolescent features

Computed GO TO, statement functions, DATA interspersed with executable statements, assumed character length functions (which can be receded as subroutines), fixed-form source code, and assumed-size arrays have been added to the official list of Fortran's obsolescent features.

They join the rarely-used features that were declared to be obsolescent in Fortran 90, i.e. the arithmetic IF, a syntax for returning from a procedure to a particular labelled statement, and some irregular ways of terminating DO loops.

D.10

Deletions from Fortran 90

Fortran 95 deletes some of the features that were labelled as obsolescent in the Fortran 90 standard, i.e. PAUSE, ASSIGN, assigned GO TO, real indices for DO loops, branching to an END IF from an outer block, assigned integers as FORMAT specifications, and H editing.

With the advent of user-written elemental subroutines (Appendix D.6) defined assignment statements (in WHERE) are now restricted to being elemental.

APPENDIX E Fortran 95 statements

This appendix is in two parts. Appendix E. 1 lists a "core" of Fortran 95 statements whose usage is recommended. Appendix E.2 lists statements that, although neither illegal nor officially obsolescent, are not recommended. The distinction between "recommended" and "non-recommended" statements is a matter of opinion, and sometimes merely style, on which Fortran specialists have differing views.

E.1 Recommended statements

- Scoping unit boundaries
- Program unit control statements

USE

INTERFACE

MODULE PROCEDURE

END INTERFACE

CONTAINS

CALL

EXTERNAL PRIVATE

INTRINSIC PUBLIC

• Type declaration statements

REAL	INTEGER
LOGICAL	CHARACTER
Com any management statements	

COMPLEX TYPE (...)

Memory management statements

ALLOCATE

DEALLOCATE

Pointer assignment Assignment statement Execution control stat	t (=)	NULLIFY	
SELECT CASE CASE END SELECT		IF ELSE IF ELSE END IF	DO DO WHILE CYCLE EXIT END DO
WHERE ELSE WHERE END WHERE Input/output statemen	ts	FORALL END FORALL	STOP
OPEN CLOSE Pseudo-statements	READ WRITE	BACKSPACE REWIND	INQUIRE ENDFILE
INCLUDE		Comment line (!)	
Alphabetical list			
ALLOCATE Assignment statem BACKSPACE CALL CASE CHARACTER CLOSE COMMENT COMPLEX CONTAINS CYCLE DEALLOCATE DO ELEMENTAL FU ELSE ELSE IF ELSE WHERE END DO END FORALL END IF END INTERFACE	NCTION BROUTINE	 Dynamically allocates memory to arrays or to pointers Gives a value to a variable. Moves an i/o file back by one record. Invokes a subroutine. Specifies a range of values for a CASE expression. Declares data of character type. Closes an i/o unit. For program annotation. Declares data of complex type. Heads a set of module procedures. Jump to the bottom of a DO loop. Deallocates a pointer or an allocatable array. Starts an elemental function Starts an elemental subroutine Heads the final catch-all block within an IF construct. Heads an alternative block within a WHERE construct End of a FORALL construct. End of an IF construct. 	

END EUNCTION	End of a function submus around
END FUNCTION	End of a function subprogram.
END MODULE	End of a module.
END PROGRAM	End of the main program.
END SELECT	End of a CASE selection construct.
END SUBROUTINE	End of a subroutine.
END TYPE	End of a derived type definition block.
END WHERE	End of a WHERE construct.
ENDFILE	Writes an end-of-file record.
EXIT	Jump out of a DO loop.
EXTERNAL	Declares that a name refers to a procedure.
FORALL	Heads a FORALL construct or FORALL statement.
FUNCTION	Starts a function subprogram.
IF	Conditional statement.
IFTHEN	Heads a block of conditional statements
INCLUDE	Inserts a file of additional Fortran statements.
INQUIRE	I/o unit general status inquiry.
INTEGER	Declares data of integer type.
INTERFACE	Start of an interface block.
INTRINSIC	Declares that a name is that of an intrinsic function.
LOGICAL	Declares data of logical type.
MODULE	Starts a module.
MODULE PROCEDURE	Declares names of module procedures.
NULLIFY	Disassociates a pointer.
OPEN	Opens an i/o unit or file.
Pointer Assignment (=>)	Points a pointer to a target.
PRIVATE	Bars access of data from outside the module.
PROGRAM	Starts the main program.
PUBLIC	Permits access of data from outside the module.
PURE FUNCTION	Starts a pure function.
PURE SUBROUTINE	Starts a pure subroutine.
READ	Causes data to be input.
REAL	Declares data of real type.
RECURSIVE FUNCTION	Starts a function which may refer to itself.
RECURSIVE SUBROUTINE	Starts a subroutine which may call itself.
REWIND	Go back to the first record of an i/o file.
SELECT CASE	Starts a CASE construct.
STOP	Halts execution immediately.
SUBROUTINE	Starts a subroutine.
Type declaration ()	The general data-declaration statement.
TYPE (<i>Typename</i>)	Declares data of a specified derived type.
TYPE Typename	Starts a derived type definition block.
USE	Summons the contents of a module.
WHERE	Heads a WHERE statement or a WHERE construct.
WRITE	Causes data to be output.
WRITE	Causes data to be output.

E.2 Non-recommended statements

E.2.1

Miscellaneous statements

The following are discouraged either because they are regarded as linguistically obsolescent (e.g. the arithmetic IF), or because they have been superseded by newer Fortran syntax (e.g. data modules have superseded COMMON), or because of inelegance.

Arithmetic IF A switchable GO TO choosing between three labelled statements.

ASSIGN	Assigns a statement label to an integer variable.
Assigned GO TO	A GO TO with a variable statement label.
BLOCK DATA	Introduces a block data subprogram.
COMMON	Declares data to be accessible from more than one program unit.
Computed GO TO	A switchable GO TO, specifying several labelled statements.
CONTINUE	A dummy statement, to carry a label.
DATA	Gives values to variables
DOUBLE PRECISION	Type declaration statement for the obsolete DOUBLE PRECISION type.
END	Terminates a program unit (use suffixed ENDS instead).
END BLOCK DATA	End of a BLOCK DATA unit.
ENTRY	Alternative entry point to a procedure.
EQUIVALENCE	Declares more than one name for the same area of memory.
FORMAT	A labelled statement containing an i/o format specification.
GO TO	Jump to another statement.
IMPLICIT	Changes the initial-letter data type convention.
IMPLICIT NONE	Withdraws the initial-letter data type convention.
NAMELIST	Specifies data to be included in a NAMELIST group.
PAUSE	Causes program execution to pause.
PRINT	Writes data to a default output unit.
RETURN	Alternative point of exit from a procedure.
SEQUENCE	Declare sets of data to be stored sequentially in memory.
Statement function	A form of one-line internal function.

E.2.2

Attribute specification statements

In spite of the initial-letter convention which allows REAL and INTEGER variables to be used without the need for a type declaration statement (TDS), it is recommended that virtually all data (and function names) should be declared in TDSs. Consequently, the following statements are unnecessary because these attributes can be specified within the TDS for the data involved.

ALLOCATABLE	Declares an array to be allocatable.
DIMENSION	Declares data to be arrays of a specified shape.

INTENT	Declares dummy argument data to be incoming/outgoing.
OPTIONAL	Declares a dummy argument to be optional.
PARAMETER	Declares a named constant.
POINTER	Declares a data item to be a pointer.
SAVE	Declares subprogram data to be retained on return.

TARGETDeclare that a data item may be the target of a pointer.

E.2.3

Type-specific function statements

It is best to avoid altogether the variants of the FUNCTION statement which have a prefix indicating the type of the function's result. The type should instead be specified by a type declaration statement after a FUNCTION statement. So, the only prefixes used before the FUNCTION keyword should be **ELEMENTAL, PURE, or RECURSIVE.**

APPENDIX F Fortran 95 intrinsic procedures

This appendix lists all the Fortran 95 intrinsic procedures. It does not include the functions defined in ISO_VARYING_STRINGS (Appendix C) or in High Performance Fortran (Chapter 15). In Appendix F. 1 "specific" (as opposed to generic) function names are not listed: the different specific names, whose use is not recommended, are listed in Appendix F.2.

F.1 Recommended intrinsic procedures

"Intrinsic" procedures are one of the six or seven classes of procedures in Fortran:

- Intrinsic procedures
- External procedures
- Module procedures
- Dummy procedures (no independent existence)
- Extrinsic procedures (HPF only)
- Internal procedures
- · Statement functions

and are themselves divided into four sub-classes:

- Elemental functions
- Inquiry functions
- Transformational functions
- Subroutines

Of these, the elemental functions are most numerous and are used mainly for manipulating data and making standard calculations. They have the feature that they may be used with either scalar or array arguments, correspondingly returning either scalar or array values.

Elemental functions

 Numeric fund 	ctions:			
ABS	ANINT	CONJG	MAX	MODULO

AIMAG	CEILING	FLOOR	MIN	MINT
AINT	CMPLX	INT	MOD	REAL
 Mathematical func 	ctions:			
ACOS	ATAN2	EXP	SIN	TAN
ASIN	COS	LOG	SINK	TANH
ATAN	COSH	LOG10	SQRT	
Character function	is:			
ACHAR	IACHAR	LEN_TRIM	LLE	SCAN
ADJUSTL	INDEX	LGE	LLT	TRIM
ADJUSTR	LEN	LGT	REPEAT	VERIFY
 Logical function: 				
LOGICAL				
• Bit manipulation f	unctions:			
IAND	IBITS	IEOR	ISHFT	BTEST
IBCLR	IBSET	IOR	ISHFTC	NOT
• Floating-point mar	nipulation functions:			
EXPONENT	RRSPACING	FRACTION	NEAREST	SCALE
SPACING	SETEXPONENT			
 Vector and matrix 	multiplication functions:			
MATMUL	DOTPRODUCT			

Inquiry functions

- Argument presence inquiry function: **PRESENT**
- Character inquiry function: LEN
- Kind inquiry functions: **KIND**
- Numeric inquiry functions:
- Bit inquiry function:

BIT_SIZE

• Array inquiry functions:

LBOUND UBOUND SHAPE SIZE ALLOCATED

• Pointer inquiry function: ASSOCIATED

Transformational functions

• Character functions:

REPEAT TRIM

• Kind functions:

SELECTED INTEGER KIND SELECTED REAL KIND

• Transfer function:

TRANSFER

• Array reduction functions:

ALL ANY MINVAL PRODUCT

COUNT SUM

MAXVAL

• Array construction functions:

MERGE PACK SPREAD UNPACK

- Array reshape function: RESHAPE
- Array manipulation functions:

EOSHIFT CSHIFT TRANSPOSE

• Array location functions:

MINLOC MAXLOC

• Pointer function: NULL (Fortran 95)

Intrinsic subroutines

- Bit-copying: **MVBITS**
- Timekeeping:

DATE AND TIME **CPU TIME (Fortran 95)**

SYSTEM CLOCK

• Random numbers:

RANDOM RANDOMSEED

Alphabetical list

All the intrinsic procedures are listed below (but see also Appendix F.2). After each procedure name there is a bracketed list of arguments. All the arguments of all the intrinsic procedures have keywords, and it is by the keywords that they are indicated here (but in lower case, contrary to our usual convention for quoting keywords). Optional arguments are italicized. In some complex cases, the descriptions are followed by references to sections in this book where more details are given.

It should noticed that all trigonometric functions, and their inverses, refer to angles in radians. To indicate data types, the following abbreviations are made:

I=Integer
C=Character

R=Real S=Character string

Z=Complex L=Logical

Where no data type is indicated, the type is irrelevant. A number of procedures (ALLOCATED, ASSOCIATED, CSHIFT, EOSHIFT, MERGE, NULL, PACK, PRESENT, **RESHAPE, SOURCE, SIZE, SPREAD, TRANSFER, TRANSPOSE and UBOUND) may** have arguments of any type, not excluding derived types. The PRESENT function, moreover, may have a dummy procedure name as argument.

F.2

Non-recommended procedures

Strictly speaking this section deals not with non-recommended procedures but non-recommended procedure *names*. The list below (p. 375) gives several type-specific names for functions that exist (and are listed in Appendix F.1) under different generic names. The names below are not essential since the functions can always be invoked through the generic names in Appendix F. 1 (see Section 5.8).

In addition, the "double precision" functions DBLE and DPROD have been included in this list: they are unnecessary since the old double precision data type is not recommended.

Argument and result types follow the abbreviations listed at the start of Appendix F.1, with the addition of D for double precision data.

Name	Argument type	Result type (for functions)	
ABS(a)	R, I or z	R or I	Absolute value
ACHAR(i)	Ι	с	ASCII character
ACOS (x)	R	R	Inverse cosine, $\cos^{-1}(x)$
ADJUSTL (string)	С	С	Replace leading blanks by trailing blanks
ADJUSTR(string)	С	С	Replace trailing blanks by leading blanks.
AIMAG(z)	Ζ	R	Imaginary part
AINT(a, <i>kind</i>)	R	R	Truncate to a whole number by removing fractional part AINT(-a) = -AINT(a)
ALL (mask, dim)	L, I	L	True if all elements of mask (or all elements along dimension dim) are true (Section 5.7)
ALLOCATED (array)		L	True if array is allocated
ANINT(a, kind)	R	R	Nearest whole number
ANY (mask, <i>dim</i>)	L, I	L	True if any element of mask (or any element along dimension dim) is true. (Section 5.7)
ASIN(x)	R	R	Inverse sine, $\sin^{-1}(x)$
ASSOCIATED (pointer, <i>target</i>)		L	Is pointer associated with target?
ATAN(x)	R	R	Inverse tangent, $tan^{-1}(x)$
ATAN2 (y, x)	R, R	R	Inverse tangent, $\tan^{-1}(y/x)$, but in the range $(-\pi, +\pi)$ reflecting the signs of both <i>x</i> and <i>y</i> . Other inverse

Fortran 96 intrinsic procedure

Name	Argument type	Result type (for functions)	
			trigonometrical functions have results in the range $(-1/2\pi, +1/2\pi)$
BIT_SIZE(i)	Ι	Ι	Number of bits in an integer. (Appendix B.1)
BTEST(i, pos)	Ι	L	Tests the bit in position pos within the integer I. (Appendix B.2)
CEILING (a, <i>kind</i>)	R	Ι	The integer equal to a or immediately above it in the positive direction. The kind parameter is a <i>Fortran 95 feature</i> <i>not in Fortran 90</i> .
CHAR(i, kind)	Ι	С	The character in the ith position in the processor's sequence.
CMPLX(x, y, kind)	I/R/Z, I/R, I	Ζ	Constructs (or changes the kind of) the complex number $x+iy$.
CONJG(z)	Z	Z	Complex conjugate, z^* .
COS(x)	R or z	R or z	Real or complex cosine, $cos(x)$.
COSH(x)	R	R	Hyperbolic cosine, cosh(x).
COUNT (mask, dim)	L, I	I	Number of true elements of mask, or the number along dimension dim. (Section 5.7)
Name	Argument type	Result type (for functions)	
CPU_TIME (t ime)	R	Subroutine	A measure of the processor time in seconds. The result is a scalar in standard Fortran 95, but a parallel processor might return an array of times. This is <i>a</i> <i>Fortran 95 intrinsic procedure absent in</i> <i>Fortran 90.</i>
CSHIFT (array, dim, shift)		As array	Performs circular shift of elements of array. (Section 5.7)
DATE_AND_TIME(all, coun	nt, msecond, secor	ıd, minute, hour, day, month	, year, zone)
	IS	Subroutine	Timekeeping subroutine. (Section 5.1)
DIGITS (x)	I or R	Ι	Number of significant digits in a number of x's type and kind.
DIM(x, y)	IS or RS	I or R	MAX(x - y, y - x)
	I, R, z or L	I, R, z or L	Vector product.
DOTPRODUCT (vector_a, vector_b)	1, IX, Z 01 L	1, R, 2 01 L	L L
		As array	Shifts off elements of an array. (Section 5.7)
vector_b)			Shifts off elements of an array.
vector_b) EOSHIFT(array, dim, shift, bo	oundary)	As array	Shifts off elements of an array. (Section 5.7)
vector_b) EOSHIFT(array, dim, shift, <i>bo</i> EPSILON(x)	pundary) R	As array R	Shifts off elements of an array. (Section 5.7) A very small positive number.

Name	Argument type	Result type (for functions)	
			negative). The kind argument is a <i>Fortran 95 feature not present in Fortran 90.</i>
FRACTION (x)	R	R	"Fractional" part of the internal representation of x. (Section 5.8)
HUGE(X)	I or R	I or R	Largest representable positive number of x's type and kind.
IACHAR(C)	c	Ι	ASCII code number of the character c.
IAND(i, j)	IS	Ι	Bit-by-bit logical intersection of i with j. (Appendix B.2)
IBCLR(i, pos)	IS	Ι	Sets to zero the bit in position pos within i, returning the modified value of i. (Appendix B.1)
IBITS(i, pos, len)	IS	Ι	Forms an integer from a sequence of len bits, starting from position pos, within i. (Appendix B.1)
IBSET(i, pos)	IS	Ι	Like IBCLR, but sets the bit to 1. (Appendix B.1)
ICHAR(C)	С	Ι	Processor's sequence number for the character c.
IEOR(i, j)	IS	Ι	Exclusive OR between the bits within i and j. (Appendix B.2)
INDEX (string, substring, <i>back</i>)	C, C, L	Ι	Starting position of substring within string. (Section 8.2)
INT(a, <i>kind</i>)	I, R or z	Ι	Converts to (or changes the kind of) an integer, reducing a real number (or the real part of a complex number) to the nearest integer of lower magnitude.

Name	Argument type	Result type (for functions)	
IOR(i, j)	IS	Ι	Inclusive OR between the bits within i and j. (Section B.2)
ISHFT(i, shift)	IS	Ι	Shift the bits within i by shift places. (Appendix B.2)
ISHFTC(i, shift, <i>size</i>)	IS	Ι	Perform a circular shift, by shift places, on i (or on the size rightmost bits of i). (Appendix B.2)
KIND(X)	Intrinsic	Ι	Kind parameter of x.
LBOUND(array, dim)	dim=I	Ι	Lower bound(s) of an array . (Section 12.2)
LEN(string)	С	Ι	Number of character in a string (or in any element of string, if it is an array).
LEN_TRIM(string)	С	Ι	Number of characters in string, disregarding trailing blanks. Note that although LEN is an inquiry function, LEN_TRIM is an elemental function.

Name	Argument type	Result type (for functions)	
			Although both may have array arguments, only LEN_TRIM may have an array value.
LGE(string_a, string_b)	cs	L	True if string_a is "lexically greater than or equal to" string_b in terms of ASCII code sequences. (Section 8.2)
LGT(string_a, string_b)	CS	L	"Lexically greater than". See LGE and Section 8.2.
LLE(string a, string_b)	cs	L	"Lexically less than or equal to". See LGE and Section 8.2.
LLT(string_a, string_b)	cs	L	"Lexically less than". See LGE and Section 8.2.
LOG(x)	R or z	R or z	Natural logarithm of x. If real, $x > 0$, and if complex, $X = 0$.
LOGICAL (1, kind)	L, I	L	Converts between kinds of logical values.
LOGIC (x)	R	R	Logarithm to base 10, i.e. $\log_{10}(x)$, for $x > 0$.
MATMUL (matrix_a, matrix_b)	I, R, Z or L	I, R, z or L	Matrix multiplication of two same-type matrices. (Section 5.7)
MAX(a1, a2, <i>a3</i> ,)	I or R	I or R	The maximum value from among the arguments. There is no maximum number of arguments, but all must be of the same type and kind.
MAXEXPONENT(x)	R	Ι	Maximum "exponent" in the internal representation of <i>x</i> . (Section 5.8)
MAXLOC(array, dim, mask)	I or R, L	Ι	Location of the maximum-valued element within array. (Section 5.7). The argument dim is a Fortran 95 feature absent in Fortran 90.
MAXVAL(array, dim, <i>mask</i>)	I or R, I, L	IorR	The maximum value from among elements of array. (Section 5.7)
MERGE (tsource, f source, mask)	mask=L	As tsource and f source	Pick elements from tsource or from f source according to the value of mask. (Section 5.7)

Name	Argument type	Result type (for functions)	
MIN(a1, a2, a3,)	I or R	I or R	Like MAX, but minimum.
MINEXPONENT(x)	R	Ι	Minimum exponent in the internal representation of x. (Section 5.8)
MINLOC(array, <i>dim, mask</i>)	I or R, I, L	Ι	Like MAXLOC, but minimum. <i>The argument dim is a Fortran 95 feature not present in Fortran 90</i> ,
MINVAL(array, dim, mask)	I or R, I, L	I or R	Like MAXVAL, but minimum.
MOD (a, p)	Both I or R	I or R	Remainder when a is divided by p. (Section 5.3)

Name	Argument type	Result type (for functions)	
MODULO (a, p)	Both I or R	I or R	a modulo p. (Section 5.3)
MVBITS (from, frompos, len, to, topos)	IS	Subroutine	Takes a sequence of bits from within the integer from and copies it into part of the integer to. (Appendix B.2). Exceptionally for Fortran, the dummy arguments to and from may be associated with the same actual arguments.
NEAREST (x, 8)	R, R	R	Finds the closest other representable number to x in the direction indicated by the sign of s .
NINT(a, <i>kind</i>)	R, I	Ι	Nearest integer to a. (Section 5.3)
NOT(i)	Ι	Ι	Bit-by-bit logical complement of i. (Appendix B.2)
NULL (mold)			A disassociated pointer of the same type and kind as mold. If mold is absent, the type must be determined from the context in which NULL is called. NULL <i>is a</i> <i>Fortran 95 intrinsic function absent in</i> <i>Fortran 90.</i>
An example of NULL:			
REAL, POINTER :: point	er_a, pointer_b, &	a pointer_z => NULL()	The first call to NULL needs no argument because it is to initialise a pointer (pointer_z) of declared type.
INTEGER, POINTER :: i_p pointer_a => NULL() CALL Genroute (w, x, NUL CALL Genroute (y, z, NUL)	L (pointer b))		The second call also needs no argument because pointer_a is of pre-declared type. In the third and fourth cases, Genroute is imagined to be a generic subroutine name whose third argument could be a pointer of any type. So, NULL is given arguments of which the types (but not the associated values) will determine the specific procedures that will be entered.

Name	Argument type	Result type (for functions)	
PACK (array, mask, vector)	mask=L	As array	Takes elements from array, for which mask is true, in array element order, to form a rank-one array. (Section 5.7)
PRECISION(x)	Ror Z	Ι	Decimal precision (i.e. number of significant decimal places) provided for numbers of x's type and kind. (Section 5.4)
PRESENT (a)		L	Whether the dummy argument called a is present as an actual argument.
PRODUCT (array, <i>dim</i> , <i>mask</i>)	I/R/Z, I, L	I/R/Z	Multiplies the elements of array for which mask is true along the

Name	Argument type	Result type (for functions)	
			dimension dim. A zero-sized array has PRODUCT=1. (Section 5.7)
RADIX (x)	I or R	Ι	The numerical base for representing numbers of x's type and kind. (Section 5.8)
RANDOM (harvest)	R	Subroutine	Returns a random number in the range 0 harvest < 1 .
RANDOMSEED(size, <i>put</i> , <i>get</i>)	IS	Subroutine	Initializes random number generator. (Section 5.6)
RANGE (x)	I, R or z	Ι	Order of magnitude of the largest representable number of x's type and kind. (Section 5.4.
REAL (a, kind)	I/R/Z, I	R	Converts to real type, or between kinds of real type. (Section 5.3)
REPEAT (string, ncopies)	C, I	С	Concatenates ncopies copies of string.
RESHAPE (source, shape, <i>pad, order</i>)	shape and order=I	As shape	Changes the shape of array. (Section 9.1)
RRSPACING(x)	R	R	Inverse of the spacing between representable real numbers. (Section 5.8)
SCALE (x, i)	R, I	R	Scales up x by the ith power of the internal representation base. (Section 5.8)
SCAN(string, set, back)	C, C, L	Ι	Scans through string looking for characters from set. (Section 8.2)
SELECTED_INTEGER_KI ND (r)	Ι	Ι	The smallest kind parameter needed for an integer to have R decimal digits.
SELECTED_REAL_KIND (p, r)	IS	Ι	The smallest kind parameter needed for a real number to have a precision of P digits and a magnitude of R powers of ten. (Section 5.4)

Name	Argument type	Result type (for functions)	
SETEXPONENT(x, i)	R, I	R	In terms of its internal representation, set x's exponent to <i>i</i> . (Section 5.8)
SHAPE (source)		Ι	The shape (as a vector of integers) of the array source. Source may not be an assumed-size array.
SIGN (a, b)	Both I or R	I or R	Changes the sign of a to that of b. Fortran 95 feature not in Fortran 90: if the processor distinguishes between "positive" and "negative" representions of zero, then the SIGN function may distinguish between them in the argument b.

Name	Argument type	Result type (for functions)		
SIN(x)	R or z	Same as x	Sin(x)	
SINH(X)	R	R	Sinh(x)	
SIZE (array , <i>dim</i>)	dim=I	Ι	Number of elements in array, or its extent along the dimth dimension.	
SPACING(x)	R	R	Spacing between adjacent representable numbers in the vicinity of x.	
SPREAD (source, dim, ncopies)	dim and ncopies = I	As source	Replicates (ncopies times) the dimth dimension of source, thereby increasing the rank by 1. (Section 5.7)	
SQRT(x)	R or z	As x	Square root of $x (x 0)$.	
SUM (array, <i>dim, mask</i>)	I/R/Z, I	As array	Adds the elements of array for which mask is true along the dimension dim. (Section 5.7)	
SYSTEM CLOCK (count, <i>count_rate,</i> count_max)	IS	Subroutine	Counts clock ticks. (Section 5.6)	
TAN(x)	R	R	tan(x)	
TANH(x)	R	R	tanh(x)	
TINY(x)	R	R	Tiniest possible positive (non-zero) representable number.	
TRANSFER (source, mold, <i>size</i>)	size=I	As mold	Changes the type interpretation of what is physically stored in source. (Section 9.5)	
TRANSPOSE (matrix)		As matrix	The transpose of matrix.	
TRIM (string)	С	С	Removes trailing blanks from string.	
UBOUND (array, dim)	dim= <i>I</i>	Ι	Upper bound of array's index in the dimth dimension (or in all dimensions). (Section 12.2)	
UNPACK (vector, mask, field)	mask=L	As vector	Distributes the elements of a rank- one array. (Section 5.7)	
VERIFY (string, set, <i>back</i>)	C, C, I	Ι	Checks in string for the characters contained in set. (Section 8.2)	

Name	Generic name	Argument type	Result type
ALOG(x)	LOG	R	R
ALOG10(x)	LOG 10	R	R
AMAX0(a1, a2, a3,)	REAL (MAX)	IS	R
AMAX1(a1, a2, a3,)	MAX	RS	R
AMIN0(a1, a2, a3,)	REAL(MIN)	IS	R
AMIN1(a1, a2, a3,)	MIN	RS	R
AMOD(a, p)	MOD	R, R	R
CABS (a)	ABS	Z	R

Name	Generic name	Argument type	Result type
CCOS(x)	COS	Ζ	Z
CEXP(x)	EXP	Z	Z
CLOG(X)	LOG	Z	Ζ
CSIN(x)	SIN	Z	Ζ
CSQRT(x)	SQRT	Z	Ζ
DABS(X)	ABS	D	D
DACOS(x)	ACOS	D	D
DASIN(X)	ASIN	D	D
DATAN(x)	ATAN	D	D
DATAN2(y, x)	ATAN2	D, D	D
DBLE(a)	DBLE	I, R or z	D
DCOS(X)	COS	D	D
DCOSH(X)	COSH	D	D
DDIM(x, y)	DIM	D, D	D
DEXP(X)	EXP	D	D
DINT(a)	AINT	D	D
DLOG(x)	LOG	D	D
DLOG10(x)	LOG 10	D	D
DMAX1(a1, a2, a3,)	MAX	DS	D
DMIN1(a1, a2, a3,)	MIN	DS	D
DMOD(a, p)	MOD	D, P	D
DNINT(a)	ANINT	D	I
DPROD (x, y)	DPROD	R, R	D
DSIGN(a, b)	SIGN	D, D	D
DSIN(x)	SIN	D	D
DSINH(X)	SINK	D	D
DSQRT (x)	SQRT	D	D
DTAN(x)	TAN	D	D
DTANH(x)	TANH	D	D
FLOAT (a)	REAL	Ι	R
ABS(a)	ABS	Ι	Ι
DIM(x, y)	DIM	I, I	I
IDINT(a)	INT	D	I
IDNINT(a)	NINT	D	I
(FIX(a)	INT	R	I
ISIGN(a, b)	SIGN	I, I	I
MAX0(a1, a2, a3,)	MAX	IS	I
MAX1(a1, a2, a3,)	INT(MAX)	Rs	I
MIN0(a1, a2, a3,)	MIN	IS	I
MIN1(a1, a2, a3,)	INT (MIN)	Rs	Ι

386 APPENDIX F: FORTRAN 95 INTRINSIC PROCEDURES

Name	Generic name	Argument type	Result type
SNGL(a)	REAL	D	R

APPENDIX G Answers to selected exercises

Chapter 2

2.A A, ,, ,, ,, , and > are in the Fortran character set.

1

2.A

2

(i) 6561

- (ii) 6/12 is evaluated first, and because it is an integer expression it is truncated to zero. Answer: 4
- (iii) 2**(-1) is evaluated first, and being an integer it is truncated to zero. Since you cannot divide by zero the expression is illegal,
- (iv) Exponentiations go right-to-left. Answer: 512
- (v) Because divisions of integers give results that are truncated to integers, the answer is 1
- (vi) 32
- (vii 3
 -)
- (vii 2048.0
- i)
- (ix) 1.0
- (x) 1.0

2.A

3

- (i) (a+b+c+d+e)/5.0 (ii) ((a**2+b**2+c**2)/3.0)**0.5 (iii) 100.0*b/(a+b+c+d+e)
- (iv) (a*b)**0.5

2.A **PROGRAM Larger**

5

REAL : : a, b, x

WRITE (*,*) "Input two numbers: " READ (*,*) a., b x=a IF (a<b) THEN x=b END IF WRITE (*,*) "The larger number is ", x END PROGRAM Larger

Using a function introduced later, five lines of the above could be abbreviated to

WRITE (*,*) "The larger number is ", M&x(a,b)

2.B The valid names are aramaic, zhq5, p998530, top_mark, and (having no more than 31 characters) 1 state_population_estimate_1997. Others are invalid because the currency symbol, the apostrophe and the blank space are not allowed as parts of names, and although a name may include digits it may not start with a digit.

```
PROGRAM Quad
WRITE (*,*) "Input the coefficients of the quadratic: "
READ (*,*) a, b, c
d = b**2 - 4.0*a*c
IF (d<0) THEN; WRITE (*,*) "Solutions are unreal"
ELSE; d=SQRT(d)
```

e=(-b+d)/(2.0*a); f=(-b-d)/(2.0*a)

WRITE (*,*) "The solutions are: ", e, ${\rm f}{\rm t}$

END IF

2.B

3

END PROGRAM Quad

3.A 1		
(i) (ii) (iii) (iv) (v) (v)	-2 0 -2 520	
3.A 2		
(ii) (iii) (iii) (iv) (v)	0.666 24000.0 10.0 27E8 101E-7 IE-16	
3.A 3		
(ii) (iii) (iii) (iv) (v) (v) (v) (v) (v) (v) (v) (v) (v) (–9.0 5.8 –7.111	
3.A 4	PROGRAM Lsd	
	REAL :: x, bob,	
	INTEGER :: ipounds, ishillings, ioldpence	
	WRITE (*,*) "Input a sum in pounds and pence, expressed &	
&as a decimal number"		
READ (*,*) x ; ipounds = INT(x)		

bob = 20.0*(x-ipounds) ; ishillings = INT(bob)

ioldpence = NINTCL2 . 0* (bob-ishillings))

WRITE (*,*) "The equivalent in pounds, shillings and &

& old pence is f", ipounds," ",ishillings,"s &

& ",ioldpence,"d"

END PROGRAM Lsd

3.B

```
1
```

- (i) Illegal (a number must include a digit)
- (ii) Real
- (iii) Real
- (iv) Integer
- (v) Real
- (vi) Integer
- (vii Illegal (a real number must have a digit in the "significand" preceding the exponent letter)
- (vii Character (with no relationship to the ACHAR function!)
- i)
- (ix) Illegal (embedded blank not allowed)
- (x) Illegal (commas not allowed within numbers)
- (xi) Character
- (xii This is a legal expression but not a legal constant
-)
- (xii Real
 - i)
- (xi Real
- v)
- (xv Character
-)
- (xv Real, of kind big
- i)
- (xv Complex
- ii)
- (xv Integer
- iii)
- (xi Illegal (There must be an "exponent" after the E)
- (x)
- (xx Integer (Fortran specifies no maximum number of digits)
-)

3.B

- 2
 - (i) **REAL : : power 1, power 2, creeper**
 - (ii) INTEGER :: kappa, kappa_prime
 - (iii) **REAL(KIND=3) :: finetune**
 - (iv) CHARACTERS) :: v, w

3.B 3.B 3 cl = z**power

```
c2 = (-ABS(cI), 0.0)
```

c3 = CONJG(cI)

When a complex number is raised to a complex power, say $x^{**}y$, the result is equivalent to EXP ($y^{*}LOG(x)$). The LOG of a complex number is the principal value with imaginary part in the range $+\pi$. In the above example LOG (z), i.e. LOG (-2, 0),has the value (LOG(2), π) and so c1 is set approximately equal to (1.09, 0.63), i.e. with magnitude 1.26 and argument $\pi/3$ radians. Then, c2 is set to (-1.26, 0) and finally c3 issetto (1.09, -0.63).

3.B

5

- (i) The order of operator precedence is such that .NOT. is evaluated first, and then .NEQV. and .EQV. are evaluated left-to-right. The answer is **.TRUE..**
- (ii) This expression is equivalent to that in (i) above, whatever the values of the variables. Answer: .TRUE..
- (iii) .FALSE.
- (iv) .TRUE.

3.B (ABS(nl-n2)-ABS(rol-m2))>=ABS(k)

6

```
3.B PROGRAM Stringy
```

7

CHARACTER(12) :: first, second, check = "satisfactory"

WRITE (*,*) "Type in two strings each of 12 characters"

READ (*,*) first, second

IF (second==check) THEN

WRITE (*,*) first

ELSE

WRITE (*,*) second, " is unsatisfactory"

END IF

END PROGRAM Stringy

3.B PROGRAM Trapezium REAL :: a, b, c, d REAL :: areal=0.0, area2=0.0, areasgl=0.0, areasq2=0. 8 0 WRITE (*,*) "Input the lengths of the sides of a trapezium & & in cyclic order" READ (*,*) a, b, c, d IF (a==C.AND.b==d) THEN WRITE (*,*) "That is a parallelogram" ELSE ! We don't know which pair of sides are parallel IF (d/=b) areasql = ((a**2-c**2)**2/(d-b)**2 fc + a**2 + c**2 - (d-b)**2) * (b+d)**2/16.0 IF (a/=c) areasq2=((b**2-d**2)**2/(a-c)**2 & + b**2+d**2 - (a-c)**2) * (a+c)**2/16.0 IF (areasql>0.0) areal = SQRT(areasq1) IF (areasq2>0.0) area2 = SQRT(areasq2) IF (areal==0.0.AND.area2==0.0) WRITE (*,*) & "That is not a real trapezium" IF (areal==0.0.NEQV.area2=-=0.0) WRITE (*,*) & "The area is ", areal+area2 IF (areal/=0.0.AND.area2/=0.0) WRITE (*,*) & "Possible values for the area are ", areal," and ", area2 END IF END PROGRAM Trapezium

Chapter 4

```
4.A
  1
(ii) INTEGER :: n(60)=(/(-1, i=1,30), (1, i-1,30)/)
(iii) REAL :: powers (10) = (/(3.14159265358**m, m=1,10)/)
4.B
  1
    (i) "at"
   (ii) "mull"
   (iii) "g"
   (iv) "wat"
4.B
  2
    (i) CHARACTER!0) :: null
   (ii) CHARACTER(24) :: s1, s2, s3
   (iii) CHARACTER(*) : : me = "Eisenstein"
   (iv) CHARACTER, PARAMETER :: bs = ACKARO2)
4.B
```

3

```
(ii) CHARACTER :: c(11) = (/("abracadabra"(1:k), k=1,11)/)
4.B REAL :: pl(10), p2(10), greatness(10) COMPLEX :: z(10) READ (*,*) pi READ (*,*) p2 z =
  4 CMPLX(p1,p2) greatness = abs(z) WRITE (*,*) z(MAXLOC(greatness))
4.B
  5
    (i) (/"light", "trick"/)
   (iii) (/"hazel", "witch"/)
   (v) (/"t"/)
   (ii) (/"beach", "shore"/)
   (iv) (/"gh", "ic"/)
4.B
         .
  7
         •
         .
         REAL :: x(n), y(n), z(n), r(n), theta(n), phi(n)
         •
         .
         -
         r = SQRT(x^{**}2 + y^{**}2 + z^{**}2)
         theta = ACOS(z/r)
         phi = ATAN2(y, x)
         max = MAXLOC(r)
         WRITE(*,*) "The point nearest to the origin is at:"
         WRITE(*,*) " r = ", r(max)
         WRITE(*,*) " theta = ", theta(max)
         WRITE(*,*) " phi = ", phi(max)
         •
```

.

```
4.B WHERE (MOD(n,2)==0) n = n/2
```

4.B **PROGRAM Stringpull**

```
9
```

8

CHARACTER(20) :: string

CHARACTER :: blank = " ", asterisk = "*"

LOGICAL :: trailers= .TRUE.

READ (*,*) string

DO k=20,1,-1

IF (string(k:k) /= blank) trailers = .FALSE.

```
IF (string(k:k) == blank .AND. .NOT. trailers) &
```

string(k:k) = asterisk

END DO

```
WRITE (*,*) TRIM(string)
```

END PROGRAM Stringpull

Chapter 5

5.A 1

```
(i) PROGRAM Secant
```

REAL :: angle, radians, cosine, sec, c = 57.29577951

WRITE (*,*) "Input the value of an angle in degrees:

READ (*,*) angle

radians = angle / c

cosine = COS(radians)

IF (cosine==0.0) THEN; sec = HUGE(0.0)

ELSE; sec = 1.0/cosine

END IF

WRITE (*,*) "The secant of the angle is ", sec

```
END PROGRAM Secant
```

(ii) • • $\operatorname{arcsinh} = \operatorname{LOG}(x + \operatorname{SQRT}(x^{**}2 + 1))$ • (iii) . . REAL :: logI6, ..., ratio = LOG(16.0) • • log16 = LOG(x) / ratio• • 5.A PROGRAM Interest 2 REAL :: p, r, t, permonth, factor, total INTEGER :: months WRITE (*,*) "Principal: "; READ (*,*) p WRITE (*,*) "Rate: "; READ (*,*) r WRITE (*,*) "Time: "; READ (*,*) t ! If r is the annual interest rate then

! the annual growth factor is 1+r

! So, the monthly growth factor is

```
permonth = EXP(LOG(1.0+r)/12.0)
```

! The number of months is

months = INT(12*t)

! So the principal grows by a factor

factor = permonth ** months

! giving a total sum to the nearest pound

total = NINT(p * factor)

WRITE (*,*) "Final sum: ", total

END PROGRAM InterestCHARACTERO) :: xnname

5.A 4

CALL DATE_AND_TIME (MONTH=m)

IF (m==1) mname == "January"

IF (m==2) mname == "February"

IF (m==3) mname == "March"

IF (m==4) mname == "April"

IF (m==5) mname == "May"

IF (m==6) mname == "June"

IF (m==7) mname == "July"

IF (m==8) mname == "August"

IF (m==9) mname == "September"

IF (m==10) mname == "October"

IF (m==II) mname == "November"

IF (m==12) mname == "December"

WRITE (*, *) "The month is ", TRIM(name)

This can be done much more elegantly using an array of character strings (Chapter 7). 5.A result = LOG((COSH(x), SINK(x)))

- 5.A PROGRAM Smalls
- 8

5

```
REAL :: eps, thoutimes, ntens, epssg
```

eps = EPSILON(0.0)

thoutimes = 1000.0 * eps

ntens = 3 - NINT(LOG10(thoutimes))

! thoutimes is used only to make sure that the

! argument of LOG10 is not too small

WRITE (*,*) "EPSILON has the order of magnitude"

WRITE (*,*) "10**(-", ntens,")"

epssq = eps ** 2

IF (epssq>TINY(0.0)) THEN

WRITE (*,*) "Its square is distinct from zero"

ELSE

```
WRITE (*,*) "Its square is, in effect, zero"
```

END IF

```
END PROGRAM Smalls
5.A IF (a*b<0.0) a=-a
9
5.B MERGE(TSOURCE=.TRUE., FSOURCE=.FALSE., MASK=(n==1))
1
```

Chapter 6

```
6.A SELECT CASE (IACHAR(string(1:1)))
```

```
2
```

CASE(97:121)

string(1:1) = ACHAR(IACHAR(string(1:1)) - 32)

CASE (65: 90)

CONTINUE

CASE(32)

```
string = string(2:)
```

CASE DEFAULT

string(1:1) = "X"

```
END SELECT
```

```
6.A initialcode = IACHAR(string(1:1))
```

```
3
```

```
IF (initialcode >= 97.AND.initialcode <= 121) THEN
```

```
string(1:1) = ACHARtinitialcode - 32)
```

```
ELSE IF (initialcode >= 65.AND.initialcode <= 90) THEN
```

CONTINUE

```
ELSE IF (initialcode == 32) THEN
```

string = string(2:)

ELSE

string(1:1) = "X"

END IF

6.A INTEGER : : n, nsr, ncr

4

REAL :: en, ensr, encr, eps = EFSILON(1.0)

LOGICAL :: square = .FALSE., cube = .FALSE.

```
en = REAL(n); ensr = SQRT(en); encr = en^{**}(1.0/3.0)
```

```
IF (ensr-INT(ensr) < eps) square = .TRUE.
```

```
IF (encr-INT(encr) < eps) cube = .TRUE.
```

```
IF (square.AND..NOT.cube) THEN
```

```
WRITE (*,*) "The number is a perfect square but not a &
```

& perfect cube"

ELSE IF (cube.AND..NOT.square) THEN

WRITE (*,*) "The number is a perfect cube but not a &

& perfect square"

```
END IF
```

.

•

.

```
6.B
1
```

```
DO j = 1, n
```

nfac = 1

nfac = nfac * j

END DO

```
6.B n = LEN(string); number = 0
```

3

DO j = n, 1, -1

number = number + (IACHAR(string(j:j) -48) * 10**(n-j)

END DO

6.B PROGRAM Vowels

6

CHARACTER(30) :: word

CHARACTER :: v(5) = (/"a", "e", "i", "o", "u"/)

READ (*,*) word

DO k = 1, LEN_TRIM(word) DO m = 1, 5 IF (word(k:k) == v(m)) THEN WRITE (*,*) v(m) EXIT END IF END DO END DO END PROGRAM Vowels

6.B

PROGRAM Average

9

REAL :: addin, totin=0.0, endmark=9999999

INTEGER :: numin=0

WRITE (*,*) "Input a series of numbers, and &

&show when you have finished by giving 9999999"

Number: DO

READ (*,*) addin

IF (addin/=endmark) THEN

totin = totin + addin; numin = numin + 1

ELSE; EXIT Number

END IF

END DO Number

WRITE (*,*) "The average is", totin/numin

END PROGRAM Average

Chapter 7

7.A	REAL FUNCTION Sphere (radius)
-----	-------------------------------

REAL :: radius, fourthirdspi = 3.14159265358 * 4.0 / 3.0

Sphere = fourthirdspi * radius * radius * radius

END FUNCTION Sphere COMPLEX FUNCTION Arcsine (z)

7.A 2

1

COMPLEX :: z, eye - (0.0, 1.0)

INTEGER FUNCTION Luck (i)

END FUNCTION Arcsine

Arcsine = -eye * LOG(eye*z + SQRT(1.0 - z*z))

7.A

10

REAL :: x

INTEGER :: n1, n2

Luck = 0

DO

CALL RANDOM(x); n1 = 1 + INT(6.0 * x)

CALL RANDOM(x); n2 = 1 + INT(6.0 * x)

Luck = Luck + n1 + n2; IF (n1 /= n2) EXIT

END DO

7.B

1

REAL :: r1, r2, r3, r(3), ar(3)

SUBROUTINE Order (r1, r2, r3)

END FUNCTION Luck

r = (/r1, r2, r3/)

ar = ABS(r)

r1 = r(MAXLOC(ar))

r3 = r(MINLOC(ar))

 $r^{2} = SUM(r) - r^{1} - r^{3}$

END SUBROUTINE Order

Chapter 8

8.A

1

- (i) 11
- (ii) " "
- (iii) 0
- (iv) 32
- (v) .FALSE.
- (vi) This has a processor-dependent value since the character a is not in the ASCII character set.
- (vii .FALSE.
-) (vii .TRUE.
 - i)

8.A initialcode = IACHAR(x(1:1))

2

IF (initialcode>47.AND.initialcode<58) THEN

 $\mathbf{x} = \mathbf{x}(2: \mathsf{LEN}(\mathbf{x}))$

END IF

Alternatively, the SCAN function does the job in one line: **IF** (SCAN(x(1:1), "0123456789")==1) x=x(2:LEN(x)) 8.A WRITE (*,*) ADJUSTL(x) 3 8.B 1 (i) COMPLEX :: xbanks(30) (ii) LOGICAL, OPTIONAL : : cbeck1, check2, checks (iii) REAL, SAVE :: matrix_name(20, 20), vector_name (45) (iv) INTEGER, PARAMETER :: squares(0:99) = (/(k**2, k=0,99)/) (v) CHARACTER(12) :: julius (:,:) (vi) REAL :: inverse_squares(100) = (/(1.0/REAL(m**2), -& m=1,100)/) (vii CHARACTER(*), PARAMETER :: moniker = "Abigail Sara Lemoine"

```
9.A INTEGER FUNCTION Logpack(data)
```

2

LOGICAL :: data(32)

INTEGER :: i

DO k = 0, 32

IF(.NOT.data(k)) THEN

i = IBCLR(i,k)

ELSE

i = IBSET(i,k)

END IF

END DO

Logpack = i

```
END FUNCTION Logpack
0.A chessboard = RESHAPE(SHAPE=(/8,8/), &
```

```
9.A
4
```

SOURCE=(/six_rows,((/.TRUE.,.FALSE!/), k=1,8)/))

9.A

5

A1

```
(i) (/"a","o","u"/)
(ii) (/"e","i"/)
(iii) (/4, 5/)
(iv) (/"o", "e"/)
(v) (/"ae", "oe","ue"/)
```

Chapter 10

10. MODULE Year

CHARACTER(9):: daynames(7) = &

(/"Monday", "Tuesday", "Wednesday", "Thursday", "Friday", &

&"Saturday", "Sunday"/)

CHARACTER(9):: monthnames(12) = &

(/"January", "February", "March", "April", "May", "June", &

&"July","August","September","October","November", &

&"December"/)

INTEGER:: daynumbers (12) = (/31,28,31,30,31,30,31,31, &

30,31,30,31/)

END MODULE Year

10. MODULE Constants

A2

REAL, PARAMETER :: pi = 2.0 * ASIN(1.0)

REAL, PARAMETER :: e = EXP(1.0)

INTEGER, PARAMETER :: ipow2(20) = (/(2**k, k=1, 20)/)

END MODULE Constants

10. MODULE Sheet

A3

```
CHARACTER(12) :: strings(30, 10)
```

```
CHARACTER :: contents(30,10)
```

! 'contents' is blank if the corresponding cell is empty,

! = "c" if it contains a word

! = "i" if it contains an integer

! = "r" if it contains a real number

CONTAINS

INTEGER FUNCTION Number (irow, icolumn)

INTEGER :: irow, icolumn, n

INTEGER :: ivalue, idefault = 0

IF (contents(irow, icolumn) == "i") THEN

READ (strings(irow, icolumn), "I12") n

Number = n

ELSE

Number = idefault

END IF

END FUNCTION Number

END MODULE Sheet

Chapter 11

11. RECURSIVE REAL FUNCTION Sinpow(n, x1, x2) RESULT (v)

A4

INTEGER :: n

REAL :: x1, x2, value

SELECT CASE (n)

CASE (3:)

value = Sinpow(n-2, x1, x2) * REAL(n-1) / REAL(n)

value = value - SIN(x1)**(n-1) * COS(x1) / REAL(n) &

+ SIN(x2)**(n-1) * COS(x2) / REAL(n)

CASE (2)

value = $0.5^{*}(x1-x2) - 0.25^{*}SIN(2.0^{*}x1) + \&$

0.25*SIN(2.0*x2)

CASE (1)

value = COS(x2) - COS(x1)

END SELECT

v = value

END FUNCTION Sinpow

- 11. FUNCTION Mean (n1, n2, n3, n4, n5, n6, n7, n8, &
- B2

n9, n10, n11, n12)

INTEGER, OPTIONAL : : n1, n2, n3, n4, n5, n6, n7, n8, n9, &

n10, n11, n12

INTEGER :: Mean, nargs, nsum; nargs = 0; nsum = 0

- IF (PRESENT(n1)) THEN; nsum = nsum + n1; nargs = nargs &
- + 1; END IF
- IF (PRESENT(n2)) THEN; nsum = nsum + n2; nargs = nargs &

+ 1; END IF

- IF (PRESENT(n3)) THEN; nsum = nsum + n3; nargs = nargs &
- + 1; END IF
- IF (PRESENT(n4)) THEN; nsum = nsum + n4; nargs = nargs &

+ 1; END IF

IF (PRESENT(n5)) THEN; nsum = nsum + n5; nargs = nargs &

+ 1; END IF

- IF (PRESENT(n6)) THEN; nsum = nsum + n6; nargs = nargs &
- + 1; END IF
- IF (PRESENT(n7)) THEN; nsum = nsum + n7; nargs = nargs &

+ 1; END IF

IF (PRESENT(n8)) THEN; nsum = nsum + n8; nargs = nargs &

+ 1; END IF

IF (PRESENT(n9)) THEN; nsum = nsum + n9; nargs = nargs &

+ 1; END IF

```
IF (PRESENT(n10)) THEN; nsum = nsum + n10; nargs = &
nargs + 1; END IF
IF (PRESENT (n10)) THEN; nsum = nsum + n11; nargs = &
nargs + 1; END IF
IF (PRESENT(n12)) THEN; nsum = nsum + n12; nargs = &
nargs + 1; END IF
Mean = NINT(REAL(nsum)/REAL(nargs))
END FUNCTION Mean
```

The above is not particularly elegant and it requires an interface to be provided. A much more elegant version, not needing an interface, could be written if the argument were an assumed-shape array instead of a set of scalars. This makes a good supplementary exercise! However, the function would then have to be called with an array name or an array constructor as the actual argument, i.e. the function would have to be referenced by a statement like

```
klose = Meant (/5,4,8,6,9/))
```

rather than having Mean (5,4,8,6,9).

```
11. FUNCTION Cross (v1, v2)
```

B3

REAL :: Cross(3), v1(3), v2(3)

REAL, PARAMETER :: x(3) = (/1.0, 0.0, 0.0), &

y(3) = (/0.0, 1.0, 0.0/), z(3) = (/0.0, 0.0, 1.0/)

Cross = x * (v1(2)*v2(3) - v1(3)*v2(2)) &

+ y * (v1(3)*v2(1) - v1(1)*v2(3)) &

+ z * (v1(1)*v2(2) - v1(2)*v2(1))

END FUNCTION Cross

```
FUNCTION Geomean (a, b)
```

11. B5

REAL : : a, b, geo, Geomean

geo = SQRT(ABS(a*b))

IF (a*b < 0.0) geo = -geo

Geomean = geo

END FUNCTION Geomean

INTERFACE OPERATOR (.X.)

REAL FUNCTION Geomean (a, b)

REAL :: a, b

END FUNCTION Geomean

END INTERFACE

11. B9

If a and b are of opposite sign, this function copes by defining a "geometric mean" with a negative value.

SUBROUTINE Rescale (array, average)		
REAL, OPTIONAL, INTENT(IN) :: average		
REAL, INTENT (IN OUT) :: array(:)		
REAL :: factor		
IF (PRESENT(average)) factor = average / SUM(array)		
IF (.NOT.PRESENT(average)) factor = 1.0/SUM(array)		
array = array * factor		
END SUBROUTINE Rescale CHARACTER FUNCTION Pick (string)		
CHARACTER(*) :: string		
INTEGER :: n, k; REAL :: x		
n = LEN(string); CALL RANDOM (x); k = 1 + INT(x*REAL(n))		
Pick = string(k:k)		
END FUNCTION Pick		

Chapter 12

12. A1				
(i)	COMPLEX, ALLOCATABLE : : cmatrix (:, :)			
(ii)	CHARACTER(12), ALLOCATABLE :: rivernames (:) ALLOCATE (cmatrix(4,4))			
(iii)	ALLOCATE (rivernames(200)) IF (ALLOCATED(rivernames)) DEALLOCATE(rivernames)			
	ALLOCATE (rivernames(150))			
12.	ALLOCATE (characters(LEN(string))			
A2 12. A3	characters = (/(string(k:k), k=1, LEN(string))/)			
(ii) ((iii) ((iii) ((iv) ((v) ((vii 1) (vii 4 i) (ix) 3 (x) 2 12.	40000 S			
B1				
(i)	TYPE Species			
	CHARACTER(12) :: name			
	REAL :: weight, extent, height			
	INTEGER :: legs			

LOGICAL :: marine

END TYPE Species

- (ii) TYPE (Species) :: panda, shark, whale, butterfly
- (iii) TYPE (Species) :: big_cats(15)
- (iv) whale = Species("cetus____", 4578.0, 12.71, 2.86, &
 - 0, .TRUE.)
- (v) big_cats(5) = Species("snow_leopard", 46.0, 1.35, 0.69, &

4, .TRUE.)

- (vi) whale%weight = 4287.0
- (v) big_cats(5)%marine = .FALSE.
- 12.

B2

(i) TYPE Person

CHARACTER(40) :: name

INTEGER :: nbirthday(3)

(ii) END TYPE Person TYPE Couple

TYPE (Person) :: husband, wife

INTEGER :: nmarriage(3)

(iii) END TYPE Couple TYPE Family

TYPE (Couple) :: parents

TYPE (Person) :: children(8)

END TYPE Family

robinson%parent s%nmarriage (3)

robinson%parents%wife%name

12. FUNCTION Addition (x, y)

B4

```
TYPE Fuzzy
```

REAL :: evalue ! expectation value

REAL :: error ! statistical error

END TYPE Fuzzy

TYPE (Fuzzy) :: Addition

TYPE (Fuzzy), INTENT(IN) :: x, y

TYPE (Fuzzy) : : a

a = Fuzzy(x%evalue + y%evalue, SQRT(x%error**2 &

+ y%error**2))

Addition = a

END FUNCTION Addition

INTERFACE OPERATOR (+)

FUNCTION Addition (x, y)

TYPE Fuzzy

- REAL :: evalue ! expectation value
- REAL :: error ! statistical error

END TYPE Fuzzy

TYPE (Fuzzy) :: Addition

TYPE (Fuzzy), INTENT(IN):: x, y

END FUNCTION Addition

END INTERFACE

SUBROUTINE Intchar(n, string)

12. B6

INTEGER, INTENT (OUT) :: n

CHARACTER, INTENT (IN) :: string

n=IACHAR(string(1:1))

IF (n<0.OR.n>127) n = 0

END SUBROUTINE Intchar

INTERFACE ASSIGNMENT (=)

SUBROUTINE Intchar(n, string)

INTEGER, INTENT (OUT) :: n

CHARACTER, INTENT (IN) :: string

END SUBROUTINE Intchar

END INTERFACE

Chapter 13

13. FUNCTION Snakehead(vector) RESULT (head)

A2

TYPE (Link), POINTER :: Snakehead, beta, gamma

TYPE (Link), TARGET :: alpha

REAL :: vector(:)

alpha%x = vector(1)

beta => alpha

DO i = 2, SIZE(vector)

ALLOCATE (gamma)

beta%nextlink => gamma

gamma%x = vector(i)

NULLIFY (gamma%nextlink)

beta => gamma

END DO

head => alpha

END FUNCTION Snakehead

Chapter 14

14. WRITE (*,*) &

A8

PACK((/ (i, 1=1,100) /), &

ALL (&

RESHAPE(SHAPE=(/100,100/), &

SOURCE=(/(&

(MOD((MOD(j,100)+1), INT(j/100+1))/=0) &

.OR. (INT(j/100)==0) .OR. ((MOD(j,100)+1)==(INT(j/100)+1)) &

, j = 0, 9999)/) &

), 2 &

) &

Appendix A

A. 2.1

- (i) Technically this is not a format specification, it is a character string that is a format "specifier". But...
- (ii) (F10.4) is a valid format specification. A format specification always includes parentheses around it.
- (iii) F10.4 is a valid edit descriptor, but not a format specification. The point is that a format specification should control all the data that passes when an i/o statement is executed, and in general will contain a list of edit descriptors within parentheses.
- (iv, 8(F10.4) and 8F10.4 are equivalent, representing a set of eight identical edit descriptors.
- v)
- (vi) (8F10.4) is a valid format specification,
- (vii ((F10.4)) is illegal.

)

(vii (F10.6,I8) is a valid format specification.

i)

- (ix) () is a valid format specification, representing an empty i/o list. It could be used to skip over an input record or to write out an empty record. However, the slash edit descriptor (/) is usually used for this purpose,
- (x) "3()" is invalid. For three empty records, the format specifier " (3/) " could be used.

```
A. (8X, I4, 3(13X, F7.2), 8X)
2.2
A. WRITE (*, FMT=" (I2,10X,B7,10X,O3)") n, n, n
2.3
A.
2.4
   (i) T F T F T F
        (This has one blank at the start and two blanks at the end.)
   (ii) Caus of deat
        (no trailing blanks),
  (iii) 1.4142 1.7321
        (one leading blank but no trailing blanks)
  (iv) 101000 001600
   (v) 0.1414E+01 0.1600E+04
        (two leading blanks)
  (vi) FATE
        WRITE (*, FMT=" (A, TL1, '_',:,' ')") (/ (caption(k:k) , k=1,
A.
2.5
        LEN(caption))/)
A.
3.1
   (i) OPEN (UNIT=7, STATUS="SCRATCH")
            OPEN (UNIT=3, STATUS="OLD", POSITION = "APPEND", &
   (ii)
             ACTION="WRITE")
            OPEN (UNIT=2, FILE="s_sheet_45", RECL=256, &
  (iii)
             ACCESS="DIRECT", FORM="FORMATTED")
            CLOSE (UNIT=2, STATUS="DELETE")
A.
```

3.2

(i) INQUIRE (UNIT=5, RECL=max)

OPEN (UNIT=5, FILE="savedata", STATUS="NEW", &

ACCESS="DIRECT", RECL=max)

DO k=1, 20

WRITE (UNIT=5, REC=k) datasave(k)

END DO

.

•

.

(ii) CHARACTERS) :: i1,i2

INTEGER :: k1, k2

READ (UNIT=1, ADVANCE="NO", FMT="(2A5)") i1, 12 READ (i1, FMT="(I5)") k1 READ (i2, FMT="(I5)") k2

This reads ten characters from unit 1, and then reads the strings i1 and i2 as internal files to interpret them as integers.

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