

Guide 47

Version 1.0

Advanced Fortran 90/95 Programming

This guide provides an introduction to features of the Fortran 90/95 programming language that are not in its predecessor, Fortran 77. It assumes knowledge at the level of ITS Guide 138, An introduction to programming in Fortran 90, and familiarity with a Fortran 90 or Fortran 95 compiler.



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Conventions:

In this document, the following conventions are used:

- A **bold typewriter font** is used to represent the actual characters you type at the keyboard.
- A *slanted typewriter font* is used for items such as filenames which you should replace with particular instances.
- A typewriter font is used for what you see on the screen.
- A **bold font** is used to indicate named keys on the keyboard, for example, **Esc** and **Enter**, represent the keys marked Esc and Enter, respectively.
- Where two keys are separated by a forward slash (as in **Ctrl/B**, for example), press and hold down the first key (**Ctrl**), tap the second (**B**), and then release the first key.
- A **bold font** is also used where a technical term or command name is used in the text.

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1. Introduction

2. The KIND Parameter for Intrinsic Data Types

Fortran 90/95 introduced a mechanism to specify the precsion of the intrinsic data types with the KIND parameter.

2.1 Selecting precision with the KIND parameter

The terms single and double precision floating point numbers are not precisely defined and depend on the computer. Usually double precision values have approximately twice the precision of single precision values. On many computers single precision floating point numbers are stored in 4 bytes (32 bits) with typically 24 bits for the mantissa and 8 bits for the exponent. This is sufficient for about 7 significant decimal digits and an exponent approximately in the range 10^-38 to 10^38. Double precision has then 64 bits with 53 bits usually devoted to the mantissa and 11 bits to the exponent. This is sufficient to give a precision of approximately 16 significant decimal digits and an exponent in the range 10^-308 to 10^308. However on some computer architectures single and double precision values are represented by 64 and 128 bits respectively. Therefore a program that runs properly in single precision on such a computer may need double precision when run on a 32 bit computer.

To make Fortran programs more portable between different computer systems the KIND parameter for intrinsic data types was introduced. Single and double precision real numbers are different kinds of the real data type, specified with a different KIND number. On some systems it indicates the number of bytes of storage for the type, however the standard does not require this. Therefore the KIND number itself is not portable between computer architectures but is used to distinguish between different kind of literal constants by appending it to the value separated by an underscore. For example

INTEGER, PARAMETER :: single = 4 REAL (KIND = single) :: a , b a = 1.2_single , b = 34.56E7_4

If the KIND number for a variable or constant is not specified then it is of the **default** kind and its value depends on the computer platform.

2.1.1 Making precision portable

Since the KIND number is not portable, Fortran provides functions to specify the required precision across platforms. The compiler will then select the smallest value of the KIND parameter that still can represent the requested precision, or otherwise it will fail to compile. In the case of integers the number of digits can be specified with the SELECED_INT_KIND function which has as argument the number of digits (ignoring the sign) and returns a default integer with the minimum KIND number.

Example

To specify an integer type with up to 9 decimal digits the following declarations can be used:

INTEGER, PARAMETER :: long = SELECED_INT_KIND (9) INTEGER (KIND = long) :: n , m

 $n = 1_long$, $m = -10_long$.

The range of values for n and m is thus between -999999999 and +999999999.

The corresponding intrinsic function for real numbers is

SELECTED_REAL_KIND (*p*, *r***)**

which returns the minimum KIND number necessary to store real numbers with a precision of *p* decimal digits and an exponent in the range 10^{-r} to 10^{r} .

Example

INTEGER, PARAMETER :: dble = SELECTED_REAL_KIND (15, 300) REAL (KIND = dble) :: planck_constant = 6.631 * 10 ** -31_dble PRINT *, 'Planck's constant is ', planck_constant

2.1.2 The KIND number of a variable or constant

Fortran 90/95 also provides an intrinsic function to determine the kind number of any variable or constant.

WRITE (*, '("The KIND number for default integer is ", I2) ') KIND (0)

WRITE (*, '("The KIND number for default single precision is", I2) ') KIND (0.0)

WRITE (*, '("The KIND number for default double precision is ", I2) ') KIND (0.0D0)

On most systems this will return the values 4, 4 and 8 respectively which could, but not have to be, the number of bytes used for storage.

2.2 Exercises

1. Write a program that prints the KIND value for default integers, real and double precision numbers on your computer.

2. Write a program to find the largest possible value of the KIND number for integers that your computer allows.

3. Derived Data Types and Pointers

3.1 Derived data types

It is possible to create new data types in Fortran 90/95, alongside the intrinsic data types. These are called derived data types and are build from any number of components. The components can be intrinsic data types and any other derived data types.

This is an example of an object oriented feature, sometimes called abstract data types.

TYPE [::] type-name component-definitions END TYPE [type-name]

Example

TYPE :: Person CHARACTER (LEN = 10) :: name REAL :: age INTEGER :: id END TYPE Person

Declaration of a variable (or object) of the type type-name is as follows

TYPE (type-name) :: var1, var2, ...

Example

TYPE (Person) :: john , mary

Each instance of a derived data type is called a **structure**. Arrays of derived data types can be defined as well,

TYPE (type-name), DIMENSION (dimensions) :: array-name

Example

TYPE (Person), DIMENSION (10) :: people

3.1.1 The component selector

The components of a structure can be accessed with the **component selector**. This consists of the name of the variable (structure) followed by a percentage sign and the component name

var % component

and in the case of an array of a derived type

array-name (subscripts)% component

Example

PRINT*, 'John''s age is ', john%age PRINT*, 'The name of person number 2 is ', people(2)%name

3.1.2 Constructors

These can be used to initialise a structure, that is, its components. When *struct-name* is of derived type *type* then

```
struct-name = type ( component-1 , ... , component-n )
```

Note

- All components of *type* must be present with a value in the argument list.
- The order of the arguments has to be the **same** as the order in which the components are defined in the derived type definition.

Example

```
john = Person ( 'Jones', 21, 7 ); mary = Person ( 'Famous', 18, 9 )
people ( 5 ) = Person ( 'Bloggs', 45, 3045 )
people ( 6 ) = john
```

3.2 Pointers

3.2.1 The pointer attribute

Pointers are special kinds of variables (objects) that can be made to refer to other variables (of the same type) or other pointers (of the same type). Storage for pointers is defined by assignment to a target or with the ALLOCATE statement (Sect).

assignin

p => t where t is a target attribute makes p an alias of t

provide information where an object can be found. They are used to allocate unnamed storage and to pass arrays by reference in subprograms.

Pointers can be considered as variables that have certain variables as values. This requires the declaration of the pointer and the target attribute. The type of the objects that can a pointer can point at has to be stated in its

declaration. Pointer objects are declared with the POINTER attribute

```
type , POINTER :: ptr [, ptr ]
type , DIMENSION ( : [, ; ] ) , POINTER :: ptr [, ptr ]
```

where *ptr* is a pointer to scalars and arrays respectively. Alternatively, a POINTER statement can be used, after the object has been declared:

type :: *ptr* [, *ptr*] **POINTER** :: *ptr* [, *ptr*]

Note:

- *type* can be a structure (derived type).
- If the pointer is an array then only the rank has to be declared and the bounds are taken from the array that it points at.

3.2.2 The target attribute

A variable can be become a target for a pointer by adding the TARGET attribute on declaration

```
type , TARGET :: ptr [, ptr ]
type , DIMENSION ( shape ) , TARGET :: ptr [, ptr ]
```

Targets can only be associated with pointers of the same type. Note that other pointers do not need the target attribute.

Summary:

- Pointers can only be assigned to variables that have the TARGET attribute or to other pointers. If the pointer is an array its rank must match the rank of the target.
- Once a pointer is associated with a target then the pointer can be used in the same way as the target (in expressions), it is an alias for the target
- A pointer cannot be specified in a DATA, EQUIVALENCE, or NAMELIST statement.

3.2.3 The pointer assignment operator (=>)

The pointer assignment operator associates a pointer with a target

pointer => target

where *pointer* can be the name of a pointer or a structure component that is a pointer and *target* can be the name of a variable with the TARGET attribute or a reference to a pointer-valued function.

In all these cases the type of the pointer must match that of the target.

3.2.4 The NULLIFY statement

A pointer can be made to point at nothing with the NULLIFY statement **NULLIFY** (*var* [, *var*]...)

Example

REAL, POINTER :: temperature REAL, POINTER, DIMENSION (:) :: position, velocity REAL, POINTER, DIMENSION (:, :) :: potential CHARACTER, POINTER :: name

NULLIFY (temperature, position, velocity, potential, name)

3.2.5 Association status of a pointer

Pointers have an association status. For example if a pointer points to an object it is called associated. The association status can be one of the following:

- **undefined**: This is the initial association status on declaration of a pointer in Fortran 90. This is an undesirable state as there is no way to test for it. This can be avoided in Fortran 95 where a pointer can be disassociated on initialization with the NULL () intrinsic function.
- associated: The pointer points to a target or unnamed object.

 disassociated: The pointer does not point at any object. In Fortran90 this status can be achieved with a NULLIFY statement applied to an undefined pointer. Fortran95 has an intrinsic function NULL () for this purpose.

To determine whether a pointer is associated with a particular target the intrinsic function

ASSOCIATED (pointer [, target])

returns a logical value with the following meaning:

- If only *pointer* appears, the result is true if it is currently associated with any target; otherwise, the result is false.
- If *target* also appears and is a target variable, the result is true if *pointer* is currently associated with *target*; otherwise, the result is false.
- If *target* is a pointer, the result is true if both *pointer* and *target* are currently associated with the same target; otherwise, the result is false. (If either *pointer* or *target* is disassociated, the result is false.)

Example Illustration of the difference between ordinary assignment (=) and pointer assignment (=>)

```
REAL, TARGET :: a, b
  REAL, POINTER :: p1, p2
  NULLIFY(p1, p2) ! Fortran 90 ???????
! some values
  a = 1.1
  b = 3.2
  PRINT*, 'a = ', a, 'b = ', b ! gives a = 1.1 b = 3.2
  p1 => a
  p2 => b
  PRINT*, 'p1 = ', p1, ' p2 = ', p2, ' p1 + p2 = ', p1 + p2 ! Note: Can print pointers just as
variables!
  ! gives p1 = 1.1 p2 = 3.2 p1 + p2 = 4.3
  p2 = p1 ! p2 still points to b!
  PRINT*, 'p1 = ', p1, ' p2 = ', p2 ! gives p1 = 1.1 p2 =1.1
PRINT*, 'a = ', a, ' b = ', b ! gives a = 1.1 b =1.1
  ! b has been overwritten !
  a = -4.5
  b = 6.7
  ! p1 still points to a, p2 to b
  PRINT*, 'p1 = ', p1, ' p2 = ', p2 ! gives p1 = -4.5 p2 = 6.7
  p2 => p1
  PRINT*, 'a = ', a, 'b = ', b ! not changed
  PRINT*, 'p1 = ', p1, ' p2 = ', p2 ! gives p1 = -4.5 p2 = -4.5
Example
  TYPE POINT
     REAL :: x
     REAL :: y
  END TYPE
  TYPE(POINT), TARGET :: a, b, c
  TYPE(POINT), POINTER :: pa, pb, pc
  TYPE(POINT), DIMENSION(3) :: tri1 = (/ POINT(1.0, -2.0), POINT(-3.0, 4.0), &
                                    POINT(5.0, -6.0) /)
```

TYPE(POINT), DIMENSION(3), TARGET :: tri2 TYPE(POINT), DIMENSION(:), POINTER :: ptri ! assumed shape!

REAL :: x1, y1, x2, y2, x3, y3 REAL, TARGET :: x4, y4 REAL, POINTER :: ptr

NULLIFY(pa, pb, pc, ptri, ptr) ! Fortran 90

x1 = 1.0; y1 = -2.0 x2 = -3.0; y2 = 4.0 x3 = 5.0; y3 = -6.0 PRINT*, 'Area is ', area_coords(x1, y1, x2, y2, x3, y3) x4 = x1; y4 = y1 ptr => a

4. Array Features and Operations

4.1 Arrays of intrinsic type

In various areas vectors and matrices are required. Fortran provides for these compound variables the array type. An array of an intrinsic type is declared with the dimension attribute following the type of the array elements. An array can have up to 7 dimensions.

The general format is

type , DIMENSION (index_range [, index_range]...) :: array_name

type :: array_name (index_range [, index_range]...)

General rules:

- the subscript range is specified by a lower and upper bound
- the lower bound is optional and the default value is 1
- the rank of an array is the number of dimensions
- the number of elements along a dimension is the extent in that dimension
- the shape of an array is the sequence of extents
- the size of an array is the total number of elements (the product of the extents for all dimensions)

Example:

REAL, DIMENSION (10):: a REAL :: b (5, 3)

4.2 Array Elements and array subscripts

Array elements are addressed with the array name followed by the indices or subscripts in brackets, for example a (2).

Each array element is a scalar and the usual operations for scalar variables apply, as for example in the expression

2.0 * a (2) + a (3) * b (2, 3)

Elements of an array are referenced by subscripts,

- the number of subscripts must equal the rank and
- each subscript must lay within the range for that dimension.

4.3 Array Sections

These are subsets of arrays, specified by replacing one or more array subscripts with.

An array section of an array is a subset of the elements of the array and defined by replacing one or more subscripts by a subset in the form of a **subscript triplet** or a **vector subscript**. An array section is itself an array and all the usual rules for arrays apply. The rank of an array section is the same as the rank of the array or smaller.

4.3.1 Subscript triplet

These have the form subscript-1 : subscript-2 : stride This works much like an implied DO loop. Example REAL :: a (3, 5), b (2, 2), c (5) The array a has the structure a(1,1) a(1,2) a(1,3) a(1,4) a(1,5) a(2,1) a(2,2) a(2,3) a(2,4) a(2,5)a(3,1) a(3,2) a(3,3) a(3,4) a(3,5)Then the array section a (1:2,2:4:2) can be assigned to array b which is conformable b = a(1:2,2:4:2)The array b has the elements a(1,2) a(1,4) a(2,2) a(2,4) An array section with rank one is c = a(2, :)

Example

INTEGER :: i REAL :: a (10) = (/ (REAL(i), i = 1, 10)/) PRINT*, a a (2:10:2) = a (1:9:2) PRINT*, a

4.3.2 Vector subscript

A vector subscript is a rank one integer array where the elements are the subscripts that specify the array section. For example to access the elements a(1, 2), a(2, 2), a(1, 4) and a(2, 4) you can use INTEGER :: p = (/2, 4/) and set B = a((/1, 2/), p)

4.4 Intrinsic Inquiry Functions for Arrays

There are number of intrinsic functions that can be used to inquire about the general properties of a given array, namely its rank, extents etc.

SIZE (array-name [, dim])

This function returns a default integer which is the number of elements (the size) of the array if the dimension number *dim* is absent, or, the extent of the array along dimension *dim* if it is present.

- Returns a default INTEGER
- dim is an optional integer, if it is absent its values is assumed to be one
- If dim is present it must be a valid dimension of array.

Information about the shape of an array can be found with some intrinsic functions.

Example

SIZE (a) returns 10, SIZE (b) returns 15 whereas SIZE (b, 2) returns 3.

SHAPE (array-name)

returns a one dimensional array of default integers with extent (= size) equal to the rank of *array-name* and the elements give the extent of *array-name* in each dimension

Example

REAL :: s1(1), s2(2)s1(1) = SHAPE(a)! gives the array s1 with one element and value s1(1) equal to 10.

 $s_2 = SHAPE(b)$ returns the rank-one array s2 with elements 5 and 3.

LBOUND (*array-name* [, *dim*]) when the dimension dim is absent returns a rank-one default integer array holding the lower bound for the dimensions when dim is present returns a default integer with as value the lower bound for the dimension

UBOUND (*array--name* [, *dim*]) as for LBOUND except it returns upper bounds. UBOUND (*array-name*, *dimension*) *type*, DIMNSION (*range*):: *array* INTEGER, OPTIONAL :: dim

RESHAPE (array, shape, pad, order)

Elements of an array are specified by subscripts the number of subscripts must equal the rank each subscript must lay within the range for that dimension

4.5 Array constructors

Array constructors can be used to initialize or assign values to a whole array or array section. The values are given as a list between the delimiter pair (/ and /) as

(I value-list I)

where value in *value-list* is either an expression or an implied DO loop. The values in the list are used in array element order and define a rank one array. The implied DO loops may be nested.

Example

```
REAL :: a ( 5 ) , b ( 3 )
a = (/ 1.0, 2.0, 3.0, 4.0, 5.0 /)
PRINT*, a
b = (/ ( REAL( i ), i = 1, 3 ) /)
PRINT*, b
```

An array of rank greater than one can be constructed with the intrinsic function RESHAPE.

Example

```
REAL :: a ( 3, 5 )
INTEGER :: i, j
a = RESHAPE ( (/ ( REAL( i ), i = 1, 15 ) /), (/ 3, 5 /) )
PRINT*, ( ( a( i , j ) , j = 1, SIZE( a, 2 ) ), i = 1, SIZE( a, 1 )
```

The first argument of the RESHAPE function is the array that has to be reshaped; the second argument specifies that the set of 15 real numbers are stored as an array with 3 rows and 5 columns.

Array constructors can also be used with constant objects of derived type in the value list.

4.6 Array Initialization and array constants

Just as with scalar variables it is possible to initialize arrays during declaration and to define constant arrays. This can be done with an array constructor or with a whole array assignment. Fortran 77 has the DATA statement for initialization of arrays

Example

INTEGER, PARAMETER :: three = 3 INTEGER :: I, j REAL :: b (three) = (/ (REAL(i), i = 1, three) /) REAL, PARAMETER :: a (5) = (/ 1.0, 2.0, 3.0, 4.0, 5.0 /) REAL, PARAMETER :: c(5, 6) = 1.0 ! all elements initialized to 1.0 REAL :: d (-3 : 3 , 10) DATA ((d (i , j) , I = -3 , 3), j = 1, 10) / 70 * 1.0 /

4.7 Whole Array Operations

In order to simplify code arithmetic operations on arrays can be written symbolically in the same fashion as mathematical expressions. This also reduces the risk of coding errors but a more important reason is that the compiler can optimize the order in which the underlying scalar operations on the array elements are executed on the target computer architecture.

Array expressions and assignment

An array expression may be assigned to an array of the same shape. Such an assignment is done on an element by element basis.

To be able to operate on an array element by element the two arrays must have the same shape.

Two arrays are called **conformable** if they have the same shape. A scalar is conformable with any array.

Note: The correspondence is by position in the extent of each dimension, not by subscript value. For example, the two arrays declared as

REAL, DIMENSION :: a(-2:2, 3), b(5,3)

are conformable.

Example: A system of N point particles in 3D space is described by position and velocity vectors and interact through a mutual potential field. The data declarations to describe this are

INTEGER :: N = 100 ! Initialised here to some value.

REAL, DIMENSION :: r (3, N), v (3, N), F (3, N, N) INTEGER :: i, j

! some operations: ! add postion of particle 1 and 2: SUM = R(:, 1) + R(:, 2) The distance between particles i and j is

d (:) = r (:, i) - r (:, j) d = SQRT ((r (:, i) - r (:, j)) ** 2)

Often the velocity of a particle is approximated by a finite difference. If $r_old(:, i)$ and $r_new(:, i)$ are the position vectors of particle i at times t1 and t2 respectively then its average velocity vector may be approximated by the expression

v_average (:, i) = (r_new (:,i) - r_old (:, i))/ (t2 - t1)

In fact this can be written as a whole array operations for all particles:

v_average (:,:) = (r_new (:,:) - r_old (:, :))/ (t2 - t1)

However whole array multiplication is not what might be expected.

Example The Inner product of two vectors.

```
REAL :: x ( 3 ), y (3 ), prod( 3 )
REAL :: sum
prod = x * y
sum = SUM ( x * y )
```

The product of the arrays x and y is evaluated on an element by element basis and assigned to prod with elements prod (i) = x (i) * y (i). The intrinsic SUM function returns the sum of the elements of prod.

4.8 Arrays as subscripts of other arrays

The range of an array can also be defined with a rank-one integer array INTEGER, DIMENSION :: odd (5) = (/ (i, i= 1, 9, 2) /), even (5) = (/ (i, i= 2, 10, 2) /) ! same as odd = (/ 1, 3, 5, 7, 9 /); even = (/ 2, 4, 6, 8, 10 /) REAL :: a (10) a (odd) = 1.0 a (even) = - 1.0 PRINT*, a

The range of an array can also be defined with a rank-one integer array

```
INTEGER, DIMENSION :: odd (5) = (/ (i, i= 1, 9, 2) /), even (5) = (/ (i, i= 2, 10, 2) /)

! same as odd = (/ 1, 3, 5, 7, 9 /); even = (/ 2, 4, 6, 8, 10 /)

REAL, DIMENSION :: a (10), b (10, 10)

a (odd) = 1.0

a (even) = - 1.0

! this creates a 'checker board' pattern of one and zeros

b (odd, even) = 1.0

b (even, odd) = 0.0

! also

a = b (1, even)

b (even, odd) = 1.0 - b (odd, even)
```

4.9 Array expressions, elemental array operations and assignment

Arithmetic operations on arrays can be written symbolically in the same fashion as mathematically. This also reduces the risk of coding errors but more importantly reason is that the compiler can optimize the order in which the scalar operations are executed as it sees fit for the target computer architecture. This includes addition, subtraction, multiplication, division and exponentiation An array expression may be assigned to an array of the same shape. Such an assignment is done on an element by element basis.

The scalar arithmetic operations of addition, subtraction, multiplication, division and exponentiation can be generalized to arrays. These are called elemental operations because they work on an element by element basis. For example

REAL :: a (3, 5), b (3, 5)

The sum is an array expression with elements a (i, j) + b (i, j) with 1 <= i <= 3 and 1 <= j <= 5.

To be able to operate on two arrays on an element by element basis they both must have the same shape.

Two arrays are called **conformable** if they have the same shape. A scalar is conformable with any array.

Note: The correspondence is by position in the extent in each dimension, not by subscript value. For example the two arrays a (5, 6) and b (-2:2, 0:5) have the same shape although their lower and upper bound values differ.

Note: Whole array multiplication and division are not what might be expected. For example the multiplication of two square matrices a and b (rank 2 arrays with same extent in each dimension) would not form a product with the usual rule of matrix multiplication. Instead the result would be a square matrix with elements a (i, j) * b (i, j).

4.10 Elemental Intrinsic Functions

Most intrinsic functions for scalars can also be applied to arrays. The intrinsic function will be applied on an element by element basis. Usually the same result could be obtained by applying the intrinsic functions inside a series of nested DO loops.

Example: b = SIN (a) c = ABS (a + SQRT (b)) This requires a , b and c all having the same shape.

- elemental, each element is operated on in the same way
- singel operation to the whole array, e.g. the sum of all elements
- operations on indvidual elements
- match certain conditions

4.11 Mask arrays

These are arrays of LOGICAL type and are used to select a subset of array elements for which the correponding mask array element is true. This is usefull in whole array operations when an operation should only be applied array elements that satisfy some condition. For example

```
INTEGER :: i
REAL :: a ( 5 ) = (/ ( (-1.0)**i, i = 0, 4 ) /)
LOGICAL :: lg ( SIZE ( a ) )
PRINT*, a
lg = a > 0.0
PRINT*, lg
```

4.12 Transformational Intrinsic Functions for numeric arrays

The following intrinsic functions have an array of numeric type as argument and some optional arguments to control the behaviour of the function.

- They all return a scalar result of the same type as the array.
- If the dimension dim is present then the function will be applied only to the elements in that dimension.
- If the LOGICAL array mask is present then it must be conformable to array and the function will be applied only to those elements for which the corresponding element of the mask array is true.

SUM (*array* [, DIM = *dim*]) returns the sum of the elements of a numeric type array and zero if its size is zero

PRODUCT (*array* [, DIM = *dim*]) returns the sum of the elements of a numeric type array and zero if its size is zero

MAXVAL (array [, DIM = dim]) returns the maximum value

MINVAL (*array* [, DIM = *dim*] [, MASK = *mask*]) returns the minimum value

MAXLOC (*array* [, MASK = *mask*]) returns a rank-one with the rank of *array* as size and the subscripts of the maximum value as elements

MINLOC(*array* [, MASK = *mask*]) as MAXLOC except for the minimum value

DOT_PRODUCT

gives the sum of all products of corresponding elements as in a (i, j) * b (i, j) with $1 \le i \le 10$, $1 \le j \le 20$

Example

REAL, DIMENSION (5):: a = (/ 1.2, -0.3, 0.0, 1E-5, 1.6E3 /)REAL :: min INTEGER :: loc (SIZE (SHAPE (a))) ! find the smallest positive number in this array and its index PRINT*, a > 0.0min = MINVAL (a, a > 0.0) loc = MINLOC (a, a > 0.0) PRINT*, min, loc, a (loc (1))

single argument case

have an array as argument and some optional arguments to control the behaviour of the function return a scalr result

```
ALL ( mask [, dim])
```

ANY (*mask* [, *dim*])

in the following mask is of type logical, it can also be an expression

ALL(mask, dim)

ANY(mask, dim)

Returns a logical array

Example:

If A(1:10, -4:4) is a REAL array then ANY(A(:,:) < 0.0) will return .TRUE. if any array elements are negative, otherwise .FALSE.

If a set of 10 files have to be opened and the STATUS value returned for each file is stored in a vector IOSVECTOR(10) then ANY(IOSVECTOR(:) /= 0) will return .TRUE. if there was an error for at least one file.

COUNT (*mask* [, DIM = *dim*]) default integer the number of elements of mask that are .TRUE. *mask* a LOGICAL array

SUM (*array* [, DIM = *dim*]) returns the sum of the elements of a numeric type array and zero if its size is zero

PRODUCT (*array* [, DIM = *dim*]) returns the sum of the elements of a numeric type array and zero if its size is zero

MAXVAL (array [, DIM = dim]) returns

MINVAL (array [, DIM = dim] [, MASK = mask]) returns

CEILING(array) integer elemental fnx array of type real, returns scalar of type integer, which is the least integer greater than or equal to array FLOOR(array) returns the greatest default??? integer less than or equal to array

Arithmetic operations on elements of a single matrix

SUM(array, dim, mask) type[, DIMENSION(:[,:])] :: array INTEGER, OPTIONAL :: dim

PRODUCT(

Operations on multiple arrays

MERGE(*truearray*,*falsearray*,*maskarray*) All arguments must have the same shape, the return type is of that shape. *maskArray* is logical

MERGE(*true*, *false*, *mask*)

elemental function true and false are of same type and shape return type is same type and shape as parameters true and false mask is type logical and same shape as true and false Example: INTEGER, DIMENSION :: A(10) = / 0,1, 2, 3,4, 5, 6,7 ,8 ,9/ A(:) = MERGE(0, A(:), A(:) > 5) ! sets all array values greater than 5 to zero:

matrix transpose

4.13 The WHERE construct

```
[ name : ] WHERE ( mask-expr )
array-assignment
ELSEWHERE
array-assignment
END WHERE
```

Example

```
INTEGER :: i

REAL :: a (5) = (/ ((-1.0 * (i + 1)) ** i, i = 0, 4) /)

REAL :: b (5)

PRINT*, a

WHERE (a >= 0.0)

b = SQRT (a)

ELSE WHERE

b = SQRT (-a)

END WHERE

PRINT*, b
```

4.14 Exercices

- 1) Find the rank of an array using intrinsic functions.
- 2) Write a program that reads two vectors of length 3 and calculates the inner product.
- 3) Write a program for the example in section
- 4) Write a program that processes students' exam marks. Every student who scores more than 50% has passed the exam. Use arrays and array constructors to record the students' names, their marks and whether they have passed. Calculate the total number who have passed, the average mark, and identify the person with the top mark. Display the arrays in a vertical layout, e.g.

Student:	Mark:		Pass?
Fred	64		Р
Susie	57		Р
Tom	49		
Anita	71		Р
Peter	37		
No. of passes =		3	
Average mark =		55.6	
Prize awarded to		Anita	

5. Dynamic Storage Allocation

5.1 About Dynamic memory

The rules for allocating storage are very similar for array variables and pointer variables. The main differences are in the fact that pointers are associated with **unnamed** storage (that is storage not assigned to an allocatable variable) and the allocation status intermixes with the association status.

Also, all pointers are implicitly ALLOCATABLE whereas variables need that attribute.

5.1.1 Dynamic Storage for Arrays

Often the size of an array is only known after data has been read or as the result of some calculation.

Allocatable arrays are arrays whose rank is declared but the extent (bounds) in each dimension is determined at runtime (dynamically). An array that is not a dummy argument of a procedure or the return value of an array valued function. (later)

5.1.2 The ALLOCATABLE attribute and statement

Use of the ALLOCATABLE attribute in the declaration of an array specifies the array as allocatable.

The formal notation is:

type, **DIMENSION(** *shape* **)**, **ALLOCATABLE**, [**SAVE**]:: *array_name*, [*array_name*] ...

type, ALLOCATABLE, [SAVE]:: array_name(shape), [array_name(shape)] ...

This is an example of a deferred-shape array as the actual shape will be defined until storage is allocated. The initial allocation status of such an array is "not currently allocated". Allocatable arrays are useful to save large arrays between procedure calls.

5.1.3 The ALLOCATE statement

This is defined with the ALLOCATE statement and keyword

ALLOCATE (array-name (shape) [array_name (shape)] ... [, STAT = status])

array-name is the name of an array, but which cannot be a structure component.

INTEGER status

must not be allocated in the same ALLOCATE statement as where it is used.

If the STAT = statement is absent and the ALLOCATE produces an error then the program will terminate with an error.

The STAT return values are:

0 indicates success.

> 0 indicates a system dependent runtime error.

Example

REAL, ALLOCATABLE :: a(:), b(:) INTEGER :: err ALLOCATE(a(1:10), b(1:10), STAT=err) ! should test for err /= 0 here

If more than one array, dimensions cannot depend on each other: ALLOCATE(a(1:10), b(SIZE(a)), STAT=err)

Note: It is not allowed to allocate an array that is already in the allocated state and this will generate a run time error. (See)

5.1.4 The allocation status of an array and the ALLOCATED function

It is always possible to use the intrinsic **logical** function ALLOCATED to check the allocation status of an array.

ALLOCATED (array_name)

This function will return true if the array is allocated, otherwise false.

5.1.5 De-allocating storage of an array

Once an allocatable array is no longer required the allocated memory should be released to the heap. This is to ensure that no unused memory will be held by the program.

This is called de-allocating the array and the DEALLOCATE statement is the counterpart of the ALLOCATE statement. Once the array has been deallocated any data in it is no longer accessible

DEALLOCATE (array_name (shape) [array_name (shape)] ... [, STAT = status])

Again the STAT = clause is optional.

5.1.6 Variable-sized arrays as component of a structure

It is not allowed to declare an array allocatable if it is a component of a structure. In this case an array pointer must be used, see Section .

5.1.7 Dynamic Storage Allocation for Pointers

As was explained in the beginning of this chapter, pointers are by default allocatable and this applies to any type of pointer. A number of examples are given below. This reflects the various structures of the storage allocated.

REAL, POINTER :: temperature REAL, POINTER, DIMENSION (:) :: position, velocity REAL, POINTER, DIMENSION (:, :) :: potential CHARACTER, POINTER :: name

Example

NULLIFY (temperature, position, velocity, potential, name)

An object pointer can be allocated storage with the ALLOCATE statement

ALLOCATE (pointer [(shape)], [pointer (shape)] ... [, STAT = status])

In the case of the above declarations one could have

ALLOCATE (temperature, position (3), velocity (3), potential (2, 3), name (8))

temperature = 18.0 position = (1.5, -0.2, 1.4E8) velocity =

De-allocation is done similar to allocatable arrays

DEALLOCATE (pointer [, pointer] ... [, **STAT** = status])

An error will be flagged if a pointer is deallocated in the following situations

- if the pointer has undefined association status.
- a pointer whose target was not created by allocation.
- if it is associated with an allocatable array.
- it the pointer is associated with a component of an object.

The usefulness of the STAT clause is to prevent trying to deallocate a pointer which is associated with a not allocated target.

Example

REAL, TARGET :: x = 10 REAL, POINTER :: p NULLIFY (p) p => x PRINT*, p DEALLOCATE (p)! This will cause a run time error!

The absence of the STAT parameter will cause a runtime error.

Allocating and de-allocating storage for a pointer also affects the association status.

If the pointer is de-allocated, the association status of any other pointer associated with the same target (or component of the target) becomes undefined.

Example

integer, parameter :: dimensions = 3 integer status real, pointer :: ptr_vector(:)

allocate(ptr_vector(dimensions), status) ! use ptr_vector deallocate()

5.2 Mixing pointers and arrays

The allocate and de-allocate statements can contain both pointers and arrays as arguments.

5.3 Exercises

1) Write a procedure where the user can enter an integer to allocate an array. Use the UNIX/Linux time command to plot the time required to allocate increasing amount of memory.

2) Are the following statements valid? ALLOCATE (a (SIZE (B),) ALLOCATE (a (n), b (SIZE (a))

6. Program Units, Subprograms and Modules

A program unit is contained in a program source file that can be compiled separately. They are self contained and in principle the compiler does not need any further information to compile the file as an independent unit. There are three kinds of program units:

- main program can contain internal subprograms
- external subprogram can contain internal subprograms
- module

can contain module and internal subprograms

Functionality that is internal to the module can be "hidden" and therefore be changed without need to alter any program that uses the module.

6.1 Fortran Procedures: Functions and Subroutines

Fortran 90/95 introduced a new concept of subroutines and functions as compared to Fortran 77. To distinguish these from the old version a distinction is now made between external and internal subprograms.

The internal subprograms correspond to the Fortran 77 subroutines and functions whereas the external subprograms act as container of multiple internal subprograms.

A subprogram defines one or more procedures. A procedure is either a function, which returns a value, or a subroutine which does not return a value but can return values through its argument list.

Functions have the advantage that they can be used in expressions. An external subprogram is neither part of the main program nor part of a module.

Internal subprograms are defined inside the main program, any external subprogram or any module. In this case its definition is placed inside a CONTAINS section of the program unit. An internal subprogram can only be invoked from within the program unit where it is defined.

Internal subprograms are convenient because they allow to break up a large (external) subprogram into smaller logical units (the internal subprograms) without the need of introducing additional (external) subprograms that would be accessible by other external subprograms. This is in line with exposing functionality to other units only when they need it.

Note: External procedures require an interface, see the section on modules (Section).

6.1.1 The INTENT attribute of procedure arguments

Procedure arguments have an INTENT attribute

INTENT (intent)

This can only be used for dummy arguments and helps to improve correctness and aids in maintaining the code as incorrect use will give a compilation error. Values of intent are:

IN a dummy argument with this attribute cannot be changed in the procedure. The actual argument has to be defined

OUT the dummy argument returns information from the procedure and must be given a value in the procedure. The actual argument does not have to be defined.

INOUT both IN and OUT values apply. The actual variable has to be defined

on entry and has to be modified by the procedure.

Note: The dummy arguments of a function should always be given the INTENT(IN) attribute as the function returns a result .

6.2 A comparison of the structure of the three kinds of program units.

main program (one instance only)	module	external
		subprogram
[PROGRAM program_name]	MODULE module_name	(external)
[specification_statements]	[specification_statements]	procedure(s)
[executable statements]	[CONTAINS	
[CONTAINS	module subprogram(s)	
internal-subprogram(s)	END [MODULE [module name]]	
END [PROGRAM [program_name]]		

Notes:

The PROGRAM program_name is optional but is recommended for clarity.

There is exactly one main program in a complete program

The compiler will only go as far as the END statement and during execution this will cause termination of the program, so no STOP is required.

External subprogram defines an external procedure.

A module can contain module subprograms which define module procedures.

External procedure / Module procedure has the structure:		
SUBROUTINE name [(argumentlist)] ret-type FUNCTION name (argumentlist)		
[spec-stmnts]		
[exe-stmnts]		
[CONTAINS		
internal-subprogram(s)]		

Note:

FUNCTION or SUBROUTINE must be present in the END statement for a module procedure (the last statement in a module is END MODULE)

Internal subprogram has the structure:		
SUBROUTINE (name	ret-type FUNCTION name (argumentlist)	
argumentlist)		
[specification_statements]		

6.3 Modules

Modules are usually defined in their own source file. After compilation there will be a special object file with .mod extension.

Modules are used for:

- sharing definitions of derived data types
- global access to variables and derived types, control which variables and internal subprograms can be accessed by users of the module, therefore provides data hiding

- providing an explicit interface for external procedures
- defining new operators
- · extending the meaning of intrinsic operators and assignment
- defining internal procedures (module procedures)
- defining generic procedures

6.3.1 Definition of a module

Example:

This module declares and initializes a number of variables that can be accessed by any subprogram that has the the USE statement. MODULE global_data IMPLICIT NONE INTEGER, PARAMETER :: N = 500 REAL, DIMENSION (N):: XAR, YAR REAL :: XINIT = 1.0 END MODULE global_data

A program that requires access to these variables can USE the module: PROGRAM use_global_data USE global_data IMPLICIT NONE PRINT*, N END PROGRAM

Note: If the variable N would also be declared in PROGRAM use_global_data then a compiler error would result. With the USE statement all the variables in this example of a MODULE are automatically also accessible in the program.

6.3.2 USE of a module

USE association makes the entities of a module available to a program unit.

USE module_name provides access to all public named data objects derived types interface blocks procedures

Note: The USE statement must **precede** the IMPLICIT NONE statement and any other specification statements.

Example: It makes sense to combine the definition of the POINT type and the area function in a module like this:

```
MODULE points_2D_mod

IMPLICIT NONE

TYPE POINT

REAL :: x

REAL :: y

END TYPE

CONTAINS

FUNCTION area_points(p1, p2, p3)

REAL :: area_points

TYPE(POINT), INTENT(IN) :: p1, p2, p3

area_points = 0.5 * ABS( p2%y * (p3%x - p1%x) + p1%y * (p2%x - p3%x) + &

p3%y*(p1%x-p2%x))
```

END FUNCTION area_points END MODULE ! To use this module one could write a program like PROGRAM points_2D USE points_2D_mod IMPLICIT NONE TYPE(POINT) :: a, b, c a = POINT(1.0, -2.0) b = POINT(1.0, -2.0) b = POINT(-3.0, 4.0) c = POINT(5.0, -6.0) PRINT*, 'Area is ', area_points(a, b, c) END PROGRAM

6.4 Overloading the build-in operators

Similar to whole array operators where the usual arithmetic operator have been extended to work on arrays, it is possible to extend these operators also to arbitrary data types. For example, it is possible to extend the addition operator (+) to variables of the TYPE POINT that were defined in a previous example. Each point in the plane can be considered the endpoint of a vector with begin point in the origin. In that case the + operator for two POINTs could mean the usual vector addition, giving the endpoint of the sum vector.

The assignment operator (=) can also be extended to arbitrary types, which would be useful in the POINT example to assign the endpoint of the vector sum to another POINT.

This mechanism of giving a different meaning to the intrinsic operators is called operator overloading. The compiler can decide from the type of the operands (the context) what definition of the operator is intended.

Overloading is done with specific interface blocks.

Example:

```
MODULE points 2D mod
IMPLICIT NONE
  TYPE POINT
    REAL :: x
    REAL :: y
  END TYPE
  ! overloaded assignment operator (=)
  INTERFACE ASSIGNMENT (=) ! interface ASSIGNMENT block
    MODULE PROCEDURE assign
  END INTERFACE
  ! overloaded operator (+)
  INTERFACE OPERATOR (+) ! interface OPERATOR block
    MODULE PROCEDURE add
  END INTERFACE
CONTAINS
  SUBROUTINE assign(lhs, rhs)
  TYPE(POINT), INTENT(OUT) :: Ihs
  TYPE(POINT), INTENT(IN) :: rhs
    ! here you have to fill in what you want this procedure to do
  END SUBROUTINE
  ! overloaded + operator
  TYPE(POINT) FUNCTION add(pt1, pt2)
  TYPE(POINT), INTENT(IN) :: pt1, pt2
    ! here you have to fill in what you want this procedure to do
  END FUNCTION
END MODULE
```

Exercise: Copy the above example in a file and fill in the bodies of the assignment and addition operators. The write a main program that declares some points and does some addition and assignment operators. Also add

some more overloaded operators, e.g. subtraction of two vectors. With what would functionality could you overload the * operator for two POINTs?

6.5 Generic Procedures

Previously it was shown that a generic intrinsic function like SIN can be applied to both scalar and array arguments of any intrinsic type. It is also possible to apply this to user defined procedures, and make them into a single generic name but allowing different types of arguments.

Example:

Returning to the example of calculating the area of a triangle in 2D, there were a number of functions available for this purpose but each had a different name, e.g. area_coords(x1, y1, x2, y2, x3, y3), area_points(a, b, c) and area_triangle(triangle) depending on the argument types. In the next example a generic interface block is used to define the generic function area which covers all the different types of arguments, including the derived types.

Example: (Continued from previous) MODULE points_2D_mod IMPLICIT NONE

TYPE POINT

REAL :: x, y

END TYPE

! interface blocks for overloaded assignment and addition operators here ! generic interface for the area function

INTERFACE area

MODULE PROCEDURE area_coords MODULE PROCEDURE area_points MODULE PROCEDURE area_triangle END INTERFACE

CONTAINS

! overloaded functions for assignment and addition operators here

REAL FUNCTION area_coords(x1, y1, x2, y2, x3, y3) RESULT(area) REAL, INTENT(IN) :: x1, y1, x2, y2, x3, y3 area = 0.5 * ABS(y2 * (x3 - x1) + y1 * (x2 - x3) + y3*(x1-x2)) END FUNCTION area_coords ! and similar for area_points and area_triangle here END MODULE

6.6 Summary

- A module may contain USE statements itself to access other modules.
- A module but must not access itself directly or indicrectly through a chain of USE statements.
- The standard does not require ordering of modules for compilation. However many compilers require this. Eg if the file mod_a.f90 defines MODULE mod_a and USEs MODULE mod_b, which is defined in mod_b.f90 then often mod_b.f90 has to be compiled before mod_a.f90.

6.7 An extended example

Example 1 PROGRAM points ! in the plane described by x and y coordinates IMPLICIT NONE REAL,EXTERNAL :: area coords ! a function to calculate the area of a triangle REAL :: x1, y1, x2, y2, x3, y3

x1 = 1.0 ; y1 = -2.0 x2 = -3.0 ; y2 = 4.0 x3 = 5.0 ; y3 = -6.0

PRINT*, 'Area is ', area_coords(x1, y1, x2, y2, x3, y3) END PROGRAM

FUNCTION area_coords(x1, y1, x2, y2, x3, y3) REAL :: area_coords REAL, INTENT(IN) :: x1, y1, x2, y2, x3, y3 area_coords = 0.5 * ABS(y2 * (x3 - x1) + y1 * (x2 - x3) + y3*(x1-x2)) END FUNCTION area_coords

Example 2

```
PROGRAM points ! in the plane described by x and y coordinates
IMPLICIT NONE
REAL,EXTERNAL :: area_coords ! a function to calculate the area of a triangle
```

TYPE POINT REAL :: x REAL :: y END TYPE

TYPE(POINT) :: a, b, c

REAL :: x1, y1, x2, y2, x3, y3

x1 = 1.0 ; y1 = -2.0 x2 = -3.0 ; y2 = 4.0 x3 = 5.0 ; y3 = -6.0

a = POINT(1.0, -2.0) b = POINT(-3.0, 4.0) c = POINT(x3, y3)

```
PRINT*, 'Area is ', area_coords(x1, y1, x2, y2, x3, y3)

PRINT*, 'Area is ', area_points(a, b, c)

CONTAINS

FUNCTION area_points(p1, p2, p3)

REAL :: area_points

TYPE(POINT), INTENT(IN) :: p1, p2, p3

area_points = 0.5 * ABS( p2%y * (p3%x - p1%x) + p1%y * (p2%x - p3%x) + &

p3%y*(p1%x-p2%x))

END FUNCTION area_points

END PROGRAM
```

```
FUNCTION area_coords(x1, y1, x2, y2, x3, y3)

REAL :: area_coords

REAL, INTENT(IN) :: x1, y1, x2, y2, x3, y3

area_coords = 0.5 * ABS( y2 * (x3 - x1) + y1 * (x2 - x3) + y3*(x1-x2))

END FUNCTION area_coords
```

Example 3

PROGRAM points IMPLICIT NONE ! Instead of an external statement for the function area_coords !REAL,EXTERNAL :: area_coords ! use an INTERFACE block INTERFACE FUNCTION area_coords(x1, y1, x2, y2, x3, y3) REAL :: area_coords REAL, INTENT(IN) :: x1, y1, x2, y2, x3, y3 END FUNCTION area_coords

```
END INTERFACE
  TYPE POINT
    REAL :: x
    REAL :: y
  END TYPE
  TYPE(POINT) :: a, b, c
  TYPE(POINT), DIMENSION(3) :: triangle
  REAL :: x1, y1, x2, y2, x3, y3
  x1 = 1.0 ; y1 = -2.0
  x2 = -3.0 ; y2 = 4.0
  x3 = 5.0; y3 = -6.0
  a = POINT(1.0, -2.0)
  b = POINT(-3.0, 4.0)
  c = POINT(x3, y3)
  triangle(1) = a
  triangle(2) = POINT(x2, y2)
  triangle(3) = c
  PRINT*, 'Area is ', area_coords(x1, y1, x2, y2, x3, y3)
PRINT*, 'Area is ', area_points(a, b, c)
  PRINT*, 'Area is ', area_triangle(triangle)
CONTAINS
  FUNCTION area points(p1, p2, p3)
  REAL :: area points
  TYPE(POINT), INTENT(IN) :: p1, p2, p3
    area_points = 0.5 * ABS( p2%y * (p3%x - p1%x) + p1%y * (p2%x - p3%x) + &
                         p3%y*(p1%x-p2%x))
  END FUNCTION area points
  FUNCTION area_triangle(t)
  REAL :: area triangle
  TYPE(POINT), DIMENSION(3) :: t
    area_triangle = &
              area_coords(t(1)%x, t(1)%y, t(2)%x, t(2)%y, t(3)%x, t(3)%y)
  END FUNCTION area triangle
```

END PROGRAM

```
! External procedure
FUNCTION area_coords(x1, y1, x2, y2, x3, y3)
REAL :: area_coords
REAL, INTENT(IN) :: x1, y1, x2, y2, x3, y3
area_coords = 0.5 * ABS( y2 * (x3 - x1) + y1 * (x2 - x3) + y3*(x1-x2))
END FUNCTION area coords
```

Note: In the above examples the triangle array is assigned a POINT object, e.g. triangle(1) = a. The assign operator (=) for the type POINT has not yet been defined here, therefore the components of the left hand side are simply copied to the components of the right hand side, e.g. triangle(1) % x = a % x etc. This is called a shallow copy. Although this straight copy does not cause problems here, more care must be taken with a structure that has one or more pointers as component.

6.8 Exercises

- 1. Fill in the missing code for area_points and area_triangle.
- 2. Copy the example of Section 6.4 in a file and complete the bodies of the assignment and addition operators. Write a main program that declares some POINTs and does some addition and assignment operatins. Also add some more overloaded operators, e.g. subtraction of two vectors. With what would functionality could you overload the * operator for two POINTs?