THE UNIVERSITY of MANCHESTER

Fortran 90

A Conversion Course for Fortran 77 Programmers

OHP Overviews

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Edition 3.0 July 1995

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Acknowledgements

These slides were developed using the Manchester Computing Centre Fortran 90 course as a basis, which was compiled by:

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- ❑ G S Noland

We are grateful to Dr. A C Marshall from the University of Liverpool and Michael Hennecke from the University of Karlsruhe for their very useful comments.

Thanks to system group at MCC, especially Miss L J Savage, for supporting the Fortran 90 compilers at MCC.

Contents

Introduction

Introduction

Topics

- History
- Objectives
- Major new features
- Other new features
- Availability of compilers
- References
- Resource list
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- Coding convention

History

- 1957 IBM Fortran
- 1966 Fortran 66 standard
- 1978 Fortran 77 standard
- 1991 Fortran 90 standard

Objectives

- Language evolution
  - Obsolescent features
- Standardise vendor extensions
  - Portability
- Modernise the language
  - Ease-of-use improvements through new features such as free source form and derived types
  - Space conservation of a program with dynamic memory allocation
  - Modularisation through defining collections called modules
  - Numerical portability through selected precision

Objectives

- Provide data parallel capability
  - Parallel array operations for better use of vector and parallel processors
- Compatibility with Fortran 77
  - Fortran 77 is a subset of Fortran 90
- Improve safety
  - Reduce risk of errors in standard code
- Standard conformance
  - Compiler must report non standard code and obsolescent features

Major new features

- Array processing
- Dynamic memory allocation
- Modules
- Procedures:
  - Optional/Keyword Parameters
  - Internal Procedures
  - Recursive Procedures
- Pointers

Other new features

- Source form
- Specifications/IMPLICIT NONE
- Parameterised data types (KIND)
- Derived types and operator overloading
- Control structures
- New intrinsic functions
- New I/O features

Obsolescent features

May be removed at the next major revision:

- Arithmetic IF
- REAL and DOUBLE precision DO variables and control expressions
- Shared DO termination, and DO termination on a statement other than on a CONTINUE or an END DO statement
- ASSIGN and assigned GO TO statements
- Assigned FORMAT specifiers
- Branching to END IF from outside IF block
- Alternate RETURN
- PAUSE statement
- H edit descriptor

Availability

Fortran 90 compilers

- **Cray CF90** - YMP (EL98), vectorising and autotasking, but limited messages and some intrinsics not tuned
- **DEC Fortran 90** - DEC OSF/1 AXP, including HPF extensions
- **EPC Fortran 90** - SPARC Solaris 1X and 2X, IBM RS/6000, Intel 3/486, Motorola 88000
- **IBM XLF V3** - RISC System 6000
- **Lahey LF90** - for DOS, Windows
- **Microway** - DOS, OS/2, Unix

Availability

Fortran 90 compilers

- ❑ **NA Software F90+** - 386/486, Sparc, T800, T9000
- ❑ **NAG f90** - Variety of Unix platforms, and VAX VMS. Uses C as intermediate language
- ❑ **Pacific Sierra VAST-90** - Uses F77 as intermediate language
- ❑ **Parasoft** - Uses F77 as intermediate language
- ❑ **Salford FTN90** - PC implementation of NAG f90, direct generation of object code

References

- ❑ Information Technology - Programming Languages - Fortran

  on-line or paper, the official standard, ISO/IEC 1539:1991 or ANSI x3.198-1992
- ❑ Fortran 90 Handbook
  Complete ANSI/ISO Reference

  J C Adams et. al., McGraw-Hill, 1992
- ❑ Programmer's Guide to Fortran 90

  2nd edition, W S Brainerd et. al., Unicomp, 1994
- ❑ Fortran 90

  M Counihan, Pitman, 1991
- ❑ Fortran 90 Programming

  T M R Ellis et. al., Wesley, 1994

References

- ❑ Fortran 90 for Scientists and Engineers

  B D Hahn, Edward Arnold, 1994
- ❑ Migrating to Fortran 90

  J Kerrigan, O'Reilly and Associates, 1993
- ❑ Fortran 90 Explained

  M Metcalf & J Ried, Oxford University Press, 1992
- ❑ Programming in Fortran 90

  J S Morgan & J L Schonfelder, Alfred Waller Ltd., 1993
- ❑ Programming in Fortran 90

  I M Smith, Wiley

Resource list

The compiled resource list is available on WWW:

http://www.hpctec.mcc.ac.uk/hpctec/courses/Fortran90/resource.html

which has links to:

- ❑ Fortran market
- ❑ Fortran 90 FAQ
- ❑ Tutorials and articles available on WWW
- ❑ NAG Fortran 90 software repository
- ❑ Fortran 90/HPF email discussion group
- ❑ Fortran newsgroup in Netnews/Usenet

Fortran 90 at MCC

- ❑ Cray EL98

  Compile with f90
- ❑ NAG f90 on Cray CS6400

  Compile with f90
- ❑ Salford FTN90 on fileserver MCC.FS1

  Compile and run with ftn90/lgo
- ❑ IBM

  Compile with xlf90 (Note default code generated for ibmb, ibmc, ibmd, NOT ibma)

Coding convention

Recommended by NAG and others

- ❑ Put all Fortran 90 keywords and intrinsic function names in upper case, everything else in lower case
- ❑ Indent by 2 columns in the body of program units and INTERFACE blocks, DO-loops, IF-blocks, CASE-blocks etc.
- ❑ Always include the name of a program, a subroutine and a function on its END statement
- ❑ In USE statements, use the ONLY clause to document explicitly all entities which are actually accessed from that module
- ❑ In CALL statement and function references, always use argument keywords for optional arguments

Sources
Types
Control Structures

Sources, types and control structures

Topics

- ❑ Source form
- ❑ Specifications
- ❑ IMPLICIT NONE
- ❑ Kind values
- ❑ Derived types
- ❑ Control structures

Source form

Free source form

- Lines up to 132 characters
- Lowercase letters permitted
- Names up to 31 characters (including underscore)
- Semicolon to separate multiple statements on one line
- Comments may follow exclamation (!)
- Ampersand (&) is a continuation symbol
- Character set includes + < > ; ! ? % - “ &
- New relational operators: ‘<’, ‘<=’, ‘==’, ‘/=’, ‘>=’, ‘>’

Source form

Example

```
PROGRAM free_source_form
! Long names with underscores

   ! No special columns
   IMPLICIT NONE

   ! upper and lower case letters
   REAL :: tx, ty, tz          ! trailing comment

   ! Multiple statements per line
   tx = 1.0; ty = 2.0; tz = tx * ty;

   ! Continuation on line to be continued
   PRINT *, &
        tx, ty, tz

END PROGRAM free_source_form
```


Specifications

type [[,*attribute*]... ::] entity list

- *type* can be INTEGER, REAL, COMPLEX, LOGICAL or CHARACTER with optional kind value:
  - INTEGER [(KIND=] kind-value)]
  - CHARACTER ([actual parameter list])

    ([LEN=] len-value and/or [KIND=] kind-value)
  - TYPE (type name)
- *attribute* can be

  PARAMETER, PUBLIC, PRIVATE, ALLOCATABLE, POINTER, TARGET, INTENT(inout), DIMENSION (extent-list), OPTIONAL, SAVE, EXTERNAL, INTRINSIC
- Can initialise variables in specifications

Specifications

Examples

```
! Integer variables:
INTEGER :: ia, ib

! Parameters:
INTEGER, PARAMETER :: n=100, m=1000

! Initialisation of variables:
REAL :: a = 2.61828, b = 3.14159

! Character variable of length 8:
CHARACTER (LEN = 8) :: ch

! Integer array with negative lower bound:
INTEGER, DIMENSION(-3:5, 7) :: ia

! Integer array using default dimension:
INTEGER,DIMENSION(-3:5, 7) :: ia, ib, ic(5, 5)
```

IMPLICIT NONE

- In Fortran 77, implicit typing permitted use of undeclared variables. This has been the cause of many programming errors.
- IMPLICIT NONE forces you to declare all variables.
- IMPLICIT NONE may be preceded in a program unit only by USE and FORMAT statements (see Order of statements).

Kind values

- 5 intrinsic types: REAL, INTEGER, COMPLEX, CHARACTER, LOGICAL
- Each type has an associated non negative integer value called the KIND type parameter
- Useful feature for writing portable code requiring specified precision
- A processor must support at least 2 kinds for REAL and COMPLEX, and 1 for INTEGER, LOGICAL and CHARACTER
- Many intrinsics for enquiring about and setting kind values

Kind values

REAL

```
REAL (KIND = wp) :: ra                    ! or
REAL(wp) :: ra
```

- Declare a real variable, ra, whose precision is determined by the value of the kind parameter, wp
- Kind values are system dependent
- An 8 byte (64 bit) real variable usually has kind value 8 or 2
- A 4 byte (32 bit) real variable usually has kind value 4 or 1
- Literal constants set with kind value:

```
const = 1.0_wp
```


Kind values

REAL

- Simplest example is to replace DOUBLE PRECISION:

```
INTEGER, PARAMETER :: idp = KIND(1.0D0)
REAL (KIND = idp) :: ra
```

ra is declared as ‘double precision’, but this is system dependent.

- To declare real in system independent way, specify kind value associated with precision and exponent range required:

```
INTEGER, PARAMETER :: &
    i10 = SELECTED_REAL_KIND(10, 200)
REAL (KIND = i10) :: a, b, c
```

a, b and c have at least 10 decimal digits of precision and the exponent range 200.

Kind values

INTEGER

- Integers usually have 16, 32 or 64 bit
- 16 bit integer normally permits
  -32768 < i < 32767
- Kind values for each supported type
- To declare integer in system independent way, specify kind value associated with range of integers required:

```
...
INTEGER, PARAMETER :: &
    i8 = SELECTED_INT_KIND(8)
INTEGER (KIND = i8) :: ia, ib, ic
...
```

ia, ib and ic can have values between -10^8 and $+10^8$ **at least (**if permitted by processor**)**.

Kind values

Intrinsics

```
INTEGER, PARAMETER :: &
    i8 = SELECTED_INT_KIND(8)
INTEGER (KIND = i8) :: ia
PRINT *, HUGE(ia), KIND(ia)
```

This will print the largest integer available for this integer type (2147483674), and its kind value.

```
INTEGER, PARAMETER :: &
    i10 = SELECTED_REAL_KIND(10, 200)
REAL (KIND = i10) :: a
PRINT *, RANGE(a), PRECISION(a), KIND(a)
```

This will print the exponent range, the decimal digits of precision and the kind value of a.

Derived types

- Defined by user
- Can include different intrinsic types and other derived types
- Components accessed using percent (%)
- Only assignment operator (=) is defined for derived types
- Can (re)define operators - see later operator overloading

Derived types

Examples

- Define the form of derived type

```
TYPE vreg
    CHARACTER (LEN = 1) :: year
    INTEGER :: number
    CHARACTER (LEN = 3) :: place
END TYPE vreg
```

- Create the structures of that type

```
TYPE (vreg) :: mycar1, mycar2
```

- Assigned by a derived type constant

```
mycar1 = vreg('L', 240, 'VPX')
```

- Use % to select a component of that type

```
mycar2%year = 'R'
```

Derived types

Examples

- Arrays of derived types:

```
TYPE (vreg), DIMENSION (n) :: mycars
```

- Derived type including derived type:

```
TYPE household
    CHARACTER (LEN = 30) :: name
    CHARACTER (LEN = 50) :: address
    TYPE (vreg) :: car
END TYPE household

TYPE (household) :: myhouse

myhouse%car%year = 'R'
```


Control structures

- Three block constructs
  - IF
  - DO
  - CASE
- All can be nested
- All may have construct names to help readability or to increase flexibility

Control structure

IF

- General form

```
[name:]IF (logical expression) THEN
            block
        [ELSE IF (logical expression) THEN [name]
            block]...
        [ELSE [name]
            block]
        END IF [name]
```

- Example

```
selection:  IF (i < 0) THEN
                CALL negative
            ELSE IF (i == 0) THEN selection
                CALL zero
            ELSE selection
                CALL positive
            END IF selection
```


Control structures

DO loops

- General form

  [name:] DO [*control clause*]
  block
  END DO [name]

- *control clause* may be:
  - an iteration control clause

    count = initial, final [,inc]

  - a WHILE control clause

    WHILE (logical expression)

  - or nothing (no control clause at all)

Control structures

DO loops

- Iteration control clause:

```
rows: DO i = 1, n
cols:    DO j = 1, m
            a(i, j) = i + j
         END DO cols
      END DO rows
```

- WHILE control clause:

```
true:  DO WHILE (i <= 100)
          ...
          body of loop
          ...
       END DO true
```


Control structures

DO loops

- Use of EXIT and CYCLE:
  - exit from loop with EXIT
  - transfer to END DO with CYCLE
  - EXIT and CYCLE apply to inner loop by default but can refer to specific, named loop

```
outer: DO i = 1, n
middle:  DO j = 1, m
inner:     DO k = 1, l
             IF (a(i,j,k) < 0.0) EXIT outer ! leave loops
             IF (j == 5) CYCLE middle    ! set j = 6
             IF (i == 5) CYCLE           ! skip rest of inner
             ...
           END DO inner
         END DO middle
      END DO outer
```


Control structures

DO loops

- No control clause:

```
DO
   READ (*, *) x
   IF (x < 0) EXIT
   y = SQRT(x)
   ...
END DO
```

Notice that this form can have the same effect as a DO WHILE loop.

Control structures

CASE construct

- Structured way of selecting different options, dependent on value of single expression
- Replacement for
  - computed GOTO
  - or IF ... THEN ... ELSE IF ... END IF constructs

Control structures

CASE construct

- General form:

```
[name:]  SELECT CASE (expression)
            [CASE (selector) [name]
                block]
                ...
         END SELECT [name]
```

- *expression* - character, logical or integer
- *selector* - DEFAULT, or one or more values of same type as expression:
  - single value
  - range of values separated by : (character or integer only), upper or lower value may be absent
  - list of values or ranges

Control structures

CASE construct

- Example

```
colour: SELECT CASE (ch)
          CASE ('C', 'D', 'G':'M')
            colour = 'red'
          CASE ('X':)
            colour = 'green'
          CASE DEFAULT
            colour = 'blue'
        END SELECT colour
```


Procedures and Modules

Procedures and modules

Topics

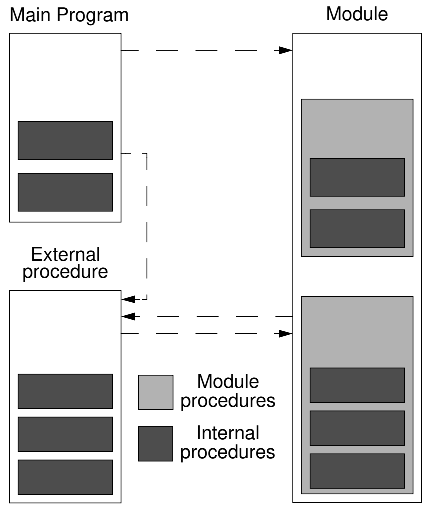
- Program units
- Procedures
- INTERFACE blocks
- Internal procedures
- Procedure arguments
- RESULT clause for functions
- Array-valued functions
- Recursive procedures

Procedures and modules

Topics

- ❑ Generic procedures
- ❑ Modules
- ❑ Overloading operators
- ❑ Defining operators
- ❑ Assignment overloading
- ❑ Scope
- ❑ Program structure

Program units



Main program

- ❑ Form:

```
PROGRAM name
    [specification statements]
    [executable statements]
    ...
END [PROGRAM [name]]
```

- ❑ Example:

```
     PROGRAM test
         ...
         ...
!    END
!    END PROGRAM
     END PROGRAM test
```


Procedures

Functions and subroutines

- ❑ Structurally, procedures may be:
  - ■ External - self contained (not necessarily Fortran)
  - ■ Internal - inside a program unit
  - ■ Module - member of a module
- ❑ Fortran 77 has only external procedures

External procedures

Form

```
SUBROUTINE name ( dummy-argument-list )
    [specification-statements]
    [executable-statements]
    ...
END [SUBROUTINE [name]]
```

or

```
FUNCTION name ( dummy-argument-list )
    [specification-statements]
    [executable-statements]
    ...
END [FUNCTION [name]]
```


Internal procedures

- Each program unit can contain internal procedures
- Internal procedures are collected together at the end of a program unit and preceded by a CONTAINS statement
- Same form as external procedures except that the word SUBROUTINE/FUNCTION must be present on the END statement
- Variables defined in the program unit remain defined in the internal procedures, unless redefined there
- Nesting of internal procedures is not permitted

Internal procedures

Example

```
PROGRAM main

    IMPLICIT NONE
    REAL :: a, b, c
    REAL :: mainsum

    ...

    mainsum = add( )
    ...

CONTAINS

    FUNCTION add ( )
        REAL :: add      ! a,b,c defined in 'main'
        add = a + b + c
    END FUNCTION add
    ...

END PROGRAM main
```


INTERFACE blocks

Explicit vs implicit

- If an ‘explicit’ interface for a procedure is provided, compiler can check argument inconsistency
- Module and internal procedures have an ‘explicit’ interface by default
- External procedures have an ‘implicit’ interface by default
- INTERFACE block can be used to specify an ‘explicit’ interface for external procedures
- Always use INTERFACE block in the calling program unit for external procedures

INTERFACE blocks

Form

- General form:

```
INTERFACE
    interface_body
    ...
END INTERFACE
```

where *interface_body* is an exact copy of the subprogram specification, its dummy argument specifications and its END statement

- Example

```
INTERFACE
    REAL FUNCTION func(x)
        REAL, INTENT(IN) :: x
    END FUNCTION func
END INTERFACE
```


Procedure arguments

INTENT

- Argument intent - can specify whether an argument is for:
  - input (IN),
  - output (OUT)
  - or both (INOUT)
- Examples

```
INTEGER, INTENT(IN) :: in_only

REAL, INTENT(OUT) :: out_only

INTEGER, INTENT(INOUT) :: both_in_out
```


Procedure arguments

Keyword arguments

- Example

```
REAL FUNCTION area (start, finish, tol)
    IMPLICIT NONE
    REAL, INTENT(IN) :: start, finish, tol
    ...
END FUNCTION area
```

- Call with:

```
a = area(0.0, 100.0, 0.01)

b = area(start = 0.0, tol = 0.01, finish = 100.0)

c = area(0.0, finish = 100.0, tol = 0.01)
```

- Once a keyword is used, all the rest must use keywords

Procedure arguments

Optional arguments

- Example

```
REAL FUNCTION area (start, finish, tol)
    IMPLICIT NONE
    REAL, INTENT(IN), OPTIONAL ::      &
        start, finish, tol
    ...
END FUNCTION area
```

- Call with:

```
a = area(0.0, 100.0, 0.01)

b = area(start=0.0, finish=100.0, tol=0.01)

c = area(0.0)

d = area(0.0, tol=0.01)
```

Procedure arguments

PRESENT

- Example

```
REAL FUNCTION area (start, finish, tol)
   IMPLICIT NONE
   REAL, INTENT(IN), OPTIONAL ::     &
      start, finish, tol
   REAL :: ttol
   ...
   IF ( PRESENT(tol) ) THEN
      ttol = tol
   ELSE
      ttol = 0.01
   END IF
   ...
END FUNCTION area
```

- Use intrinsic function PRESENT to check for presence of argument

Procedure arguments

Derived type

Procedure arguments can be of derived type if:

- the procedure is internal to the program unit in which the derived type is defined
- or the derived type is defined in a module which is accessible from the procedure

Procedure arguments

Procedures as arguments

- In Fortran 77, a procedure argument is declared as EXTERNAL
- In Fortran 90, the procedure that is passed as argument must be an external or a module procedure
- Internal procedures are not permitted
- For external procedure, you are recommended to supply an INTERFACE block in the calling program unit
- A module procedure has an explicit interface by default

Procedure arguments

Procedures as arguments

- Example

The calling program unit:

```
...
INTERFACE
   REAL FUNCTION func(x, y)
      REAL, INTENT(IN) :: x, y
   END FUNCTION func
END INTERFACE
...
CALL area(func, start, finish, tol)
```

The external function:

```
REAL FUNCTION func(x, y)
   IMPLICIT NONE
   REAL, INTENT(IN) :: x, y
   ...
END FUNCTION func
```

RESULT clause for functions

- Functions can have a result clause:

```
FUNCTION add (a, b, c) RESULT (sum_abc)
    IMPLICIT NONE
    REAL, INTENT(IN) :: a, b, c
    REAL :: sum_abc
    sum_abc = a + b + c
END FUNCTION add
```

- Result clause required for recursive functions which call themselves directly

Array-valued functions

- In Fortran 90 functions may have an array-valued result:

```
FUNCTION add_vec (a, b, n)

    IMPLICIT NONE
    INTEGER, INTENT(IN) :: n
    REAL, DIMENSION (n), INTENT(IN) :: a, b
    REAL, DIMENSION (n) :: add_vec
    INTEGER :: i

    DO i = 1, n
        add_vec(i) = a(i) + b(i)
    END DO

END FUNCTION add_vec
```


Recursive procedures

- Procedures may be called recursively:
  - either A calls B calls A, or
  - A calls A directly (RESULT clause required).
- Must be defined as recursive procedure:

```
RECURSIVE FUNCTION fact(n) RESULT(res)
    IMPLICIT NONE
    INTEGER, INTENT(IN) :: n
    INTEGER :: res
    IF (n == 1) THEN
        res = 1
    ELSE
        res = n * fact(n - 1)
    END IF
END FUNCTION fact
```


Generic procedures

- Can define your own generic procedures
- Need distinct procedures for specific type of arguments and a ‘generic interface’:

```
INTERFACE generic_name
    specific_interface_body
    specific_interface_body
    ...
END INTERFACE
```

- Each distinct procedure can be invoked using the generic name, depending on the type of arguments
- Generic procedures with derived type of arguments require Modules - see later

Generic procedures

Example

- Two distinct external subroutines for REAL and INTEGER types:

```
SUBROUTINE swapreal (a, b)
    IMPLICIT NONE
    REAL, INTENT(INOUT) :: a, b
    REAL :: temp
    temp = a; a = b; b = temp
END SUBROUTINE swapreal

SUBROUTINE swapint (a, b)
    IMPLICIT NONE
    INTEGER, INTENT(INOUT) :: a, b
    INTEGER :: temp
    temp = a; a = b; b = temp
END SUBROUTINE swapint
```


Generic procedures

Example

- Generic interface:

```
INTERFACE swap            ! generic name
    SUBROUTINE swapreal (a, b)
        REAL, INTENT(INOUT) :: a, b
    END SUBROUTINE swapreal
    SUBROUTINE swapint (a, b)
        INTEGER, INTENT(INOUT) :: a, b
    END SUBROUTINE swapint
END INTERFACE
```

- Invoke with:

```
CALL swap(x, y)
```


Modules

- Very powerful facility with many applications in terms of program structure
- Method of sharing data and/or procedures to different program units
- Very useful role for definitions of types and associated operators
- Form:

```
MODULE module-name
    [specification-stmts]
    [executable-stmts]
[CONTAINS
    module procedures]
END [MODULE [module-name]]
```

- Accessed via the USE statement

Modules

Global data

- Global if used in main program or with SAVE attribute (substitute for COMMON)

```
MODULE globals
    REAL, SAVE :: a, b, c
    INTEGER, SAVE :: i, j, k
END MODULE globals
```

- Examples of the USE statements:

```
USE globals
! allows all variables in the module to be accessed

USE globals, ONLY : a, c
! allows only variables a and c to be accessed

USE globals, r => a , s => b
! allows a, b and c to be accessed with local
! variables r, s and c
```

Modules

Module procedures

- ❑ Modules may contain procedures that can be accessed by other program units
- ❑ Same form as external procedure except:
  - ■ Procedures must follow a CONTAINS statement
  - ■ The END statement must have SUBROUTINE or FUNCTION specified.
- ❑ Particularly useful for a collection of derived types and associated operations

Modules

Module procedures

Example to 'add' variables with derived type:

```
MODULE point_module
   TYPE point
      REAL :: x, y
   END TYPE point
CONTAINS
   FUNCTION addpoints (p, q)
      TYPE (point), INTENT(IN) :: p, q
      TYPE (point) :: addpoints
      addpoints%x = p%x + q%x
      addpoints%y = p%y + q%y
   END FUNCTION addpoints
END MODULE point_module
```

A program unit would contain:

```
USE point_module
TYPE (point) :: px, py, pz
...
pz = addpoints(px, py)
```


Modules

Generic procedures

- ❑ Using modules allows arguments of derived type and hence generic procedures with derived types

Modules

Generic procedures

- ❑ Example with derived type:

```
MODULE genswap
   IMPLICIT NONE
   TYPE point
      REAL :: x, y
   END TYPE point
   INTERFACE swap        ! generic interface
      MODULE PROCEDURE swapreal, &
         swapint, swaplog, swappoint
   END INTERFACE
CONTAINS
   SUBROUTINE swappoint (a, b)
      TYPE (point), INTENT(INOUT) :: a, b
      TYPE (point) :: temp
      temp = a; a = b; b = temp
   END SUBROUTINE swappoint
   ...          ! swapint, swapreal, swaplog
                ! procedures are defined here
END MODULE genswap
```

Modules

Public and private objects

- By default all objects in a module are available to a program unit which includes the USE statement
- Can restrict the use of certain objects to the guest program
- May wish to update module subroutines at any time, keeping the purpose and interface the same, but changing the meaning of specific variables
- Achieved via PRIVATE attribute or PRIVATE statement:

```
INTEGER, PRIVATE :: keep, out
```


Overloading operators

- Can extend the meaning of an intrinsic operator to apply to additional data types - operator overloading
- Need an INTERFACE block with the form

```
INTERFACE OPERATOR (intrinsic_operator)
   interface_body
END INTERFACE
```

- Example - define ‘+’ for character variables to concatenate two strings ignoring any trailing blanks

Overloading operators

Example

```
MODULE operator_overloading
   IMPLICIT NONE
   ...
   INTERFACE OPERATOR (+)
      MODULE PROCEDURE concat
   END INTERFACE
   ...
CONTAINS
   FUNCTION concat(cha, chb)
      CHARACTER (LEN=*), INTENT(IN) ::&
         cha, chb
      CHARACTER (LEN=LEN_TRIM(cha) +&
         LEN_TRIM(chb)) :: concat
      concat = TRIM(cha) // TRIM(chb)
   END FUNCTION concat
   ...
END MODULE operator_overloading
```

Now the expression ‘cha + chb’ is meaningful

Defining operators

- Can define new operators - especially useful for user defined types
- Operator name must have a ‘.’ at the beginning and end
- Need to define the operation via a function which has one or two non-optional arguments with INTENT(IN)
- Example - find the straight line distance between two derived type ‘points’

```
PROGRAM main
   IMPLICIT NONE
   USE distance_module
   TYPE (point) :: p1, p2
   REAL :: distance
   ...
   distance = p1 .dist. p2
   ...
END PROGRAM main
```

Defining operators

Example

```
MODULE distance_module
   IMPLICIT NONE
   TYPE point
      REAL :: x, y
   END TYPE point
   ...
   INTERFACE OPERATOR (.dist.)
      MODULE PROCEDURE calcdist
   END INTERFACE
   ...
CONTAINS
   ...
   REAL FUNCTION calcdist (px, py)
      TYPE (point), INTENT(IN) :: px, py
      calcdist = SQRT ((px%x-py%x)**2 &
         + (px%y-py%y)**2 )
   END FUNCTION calcdist
   ...
END MODULE distance_module
```


Assignment overloading

- When using derived data types, may need to extend the meaning of assignment (=) to new data types:

```
REAL :: ax
TYPE (point) :: px
...
ax = px       ! type point assigned to type real
...           ! not valid until defined
```

- Need to define the assignment via a subroutine with two non-optional arguments, the first having INTENT(OUT) or INTENT(INOUT), the second having INTENT(IN) and create an interface assignment block:

```
INTERFACE ASSIGNMENT (=)
   subroutine interface body
END INTERFACE
```


Assignment overloading

Example

```
MODULE assignoverload_module
   IMPLICIT NONE
   ...
   TYPE point
      REAL :: x, y
   END TYPE point
   ...
   INTERFACE ASSIGNMENT (=)
      MODULE PROCEDURE assign_point
   END INTERFACE
   ...
CONTAINS
   SUBROUTINE assign_point(ax, px)
      REAL, INTENT(OUT) :: ax
      TYPE (point), INTENT(IN) :: px
      ax = MAX(px%x, px%y)
   END SUBROUTINE assign_point
   ...
END MODULE assignoverload_module
```


Assignment overloading

Example

The program unit might include:

```
...
USE assignoverload_mod
...
REAL :: ax
TYPE (point) :: px
...
ax = px    ! Type point to type real now defined
...
```

Scope

Scoping unit

The scope of a named entity or label is the set of non-overlapping scoping units where that name or label may be used unambiguously.

A scoping unit is one of the following:

- ❑ a derived type definition,
- ❑ a procedure interface body, excluding any derived-type definitions and interface bodies contained within it, or
- ❑ a program unit or an internal procedure, excluding derived-type definitions, interface bodies, and subprograms contained within it.

Scope

Labels and names

- ❑ The scope of a label is a main program or a procedure, excluding any internal procedures contained within it
- ❑ Entities declared in different scoping unit are always different
- ❑ Within a scoping unit, each named entity must have a distinct name, with the exception of generic names of procedures
- ❑ The names of program units are global, so each must distinct from the others and from any of the local entities of the program unit
- ❑ The scope of a name declared in a module extends to any program units that USE the module

Scope

Example

```
MODULE scope1                        ! scope 1
...                                  ! scope 1
CONTAINS                             ! scope 1
   SUBROUTINE scope2                 ! scope 2
      TYPE scope3                    ! scope 3
         ...                         ! scope 3
      END TYPE                       ! scope 3
      INTERFACE                      ! scope 3
      ...                            ! scope 4
      END INTERFACE                  ! scope 3
      REAL x, y                      ! scope 2
100   ...                            ! scope 2
   CONTAINS                          ! scope 2
         FUNCTION scope5(...)        ! scope 5
            REAL y                   ! scope 5
            y = x + 1.0              ! scope 5
100         ...                      ! scope 5
         END FUNCTION scope5         ! scope 5
   END SUBROUTINE scope2             ! scope 2
END MODULE scope1                    ! scope 1
```


Program structure

Order of statements

<table>
<tr><td colspan="3">PROGRAM, FUNCTION, SUBROUTINE,
or MODULE Statement</td></tr>
<tr><td colspan="3">USE Statements</td></tr>
<tr><td rowspan="4">FORMAT Statements</td><td colspan="2">IMPLICIT NONE Statement</td></tr>
<tr><td>PARAMETER Statements</td><td>IMPLICIT Statements</td></tr>
<tr><td>PARAMETER and DATA Statements</td><td>Derived-type Definitions,
Interface Blocks,
Type Declaration Statements,
and Specification Statements</td></tr>
<tr><td colspan="2">Executable Statements</td></tr>
<tr><td colspan="3">CONTAINS Statement</td></tr>
<tr><td colspan="3">Internal Subprograms
or Module Subprograms</td></tr>
<tr><td colspan="3">END Statement</td></tr>
</table>

Program structure

When to use INTERFACE blocks

When a module/external procedure is called:

- Which defines or overloads an operator, or the assignment
- Using a generic name

Additionally, when an external procedure:

- Is called with keyword/optional argument
- Is an array-valued/pointer function or a character function which is neither a constant nor assumed length
- Has a dummy argument which is an assumed-shape array, a pointer/target
- Is a dummy or actual argument (not mandatory but recommended)

Program structure

Summary

Fortran 77 style:

- Main program with external procedures, possibly in a library.
- No explicit interfaces, so argument inconsistencies are not checked by compiler.

Simple Fortran 90:

- Main program with internal procedures.
- Interfaces are ‘explicit’, so argument inconsistencies are trapped by compiler.

Program structure

Summary

Fortran 90 with modules:

- Main program and module(s) containing interfaces and possibly specifications, and external procedures (possibly precompiled libraries).

  A Fortran 90 version of the Fortran 77 style - with interfaces to permit compiler checking of argument inconsistencies.

- Main program and module(s) containing specifications, interfaces and procedures.

  No external procedures.

  Expected for sophisticated Fortran 90 programs.

Array Processing

Array processing

Topics

- ❑ Terminology
- ❑ Specifications
- ❑ Whole array operations
- ❑ WHERE statement and construct
- ❑ Elemental intrinsic procedures
- ❑ Array sections
- ❑ Element location versus subscript

Array processing

Topics

- ❑ Zero-sized arrays
- ❑ Array assignment
- ❑ Array constructors
- ❑ Allocatable arrays
- ❑ Automatic arrays
- ❑ Assumed shape arrays
- ❑ Array intrinsic procedures

Terminology

- ❑ Rank

  Number of dimensions
- ❑ Extent

  Number of elements in a dimension
- ❑ Shape

  Vector of extents
- ❑ Size

  Product of extents
- ❑ Conformance

  Same shape

Terminology

Example

```
...
REAL, DIMENSION :: a(-3:4, 7)
REAL, DIMENSION :: b(8, 2:8)
INTEGER :: c
REAL, DIMENSION :: d(8, 1:8)
...
```

- ❑ a has
  - rank 2
  - extents 8 and 7
  - shape (/ 8, 7 /)
  - size 56
- ❑ a is conformable with b & c, but not with d

Specifications

type [[,DIMENSION (*extent-list*)] [,*attribute*]... ::] *entity-list*

where:

- *type* - INTRINSIC or derived type
- DIMENSION - Optional, but required to define default dimensions
- (*extent-list*) - Gives array dimension:
  - Integer constant
  - integer expression using dummy arguments or constants.
  - : if array is allocatable or assumed shape.
- *attribute* - as given earlier
- *entity-list* - list of array names optionally with dimensions and initial values.

Specifications

Example

- Two dimensions:

```
REAL, DIMENSION(-3:4, 7) :: ra, rb
```

- Initialisation:

```
INTEGER, DIMENSION (3) :: ia = (/ 1, 2, 3 /), &
    ib = (/ (i, i = 1, 3) /)
```

- Automatic arrays:

```
LOGICAL, DIMENSION (SIZE(loga)) :: logb
```

  where loga is a dummy array argument
- These are all explicit shape arrays

Specifications

Example

- Allocatable arrays (deferred shape):

```
REAL, DIMENSION (:, :), ALLOCATABLE :: a, b
```

  Dimensions are defined in subsequent ALLOCATE statement.
- Assumed shape arrays:

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

  Dimensions taken from actual arguments in calling routine.

Whole array operations

- Arrays for whole array operation must be conformable
- Evaluate element by element, i.e., expressions evaluated before assignment
- Scalars broadcast
- Functions may be array valued

Whole array operations

Example

- Fortran 77:

```
REAL a(20), b(20), c(20)
...
DO 10 i = 1, 20
    a(i) = 0.0
10  CONTINUE
...
DO 20 i = 1, 20
    a(i) = a(i) / 3.1 + b(i) * SQRT(c(i))
20 CONTINUE
```

- Fortran 90:

```
REAL, DIMENSION (20) :: a, b, c
...
a = 0.0
...
a = a / 3.1 + b * SQRT(c)
```


Whole array operations

Example

- Fortran 77:

```
REAL a(5, 5), b(5, 5), c(5, 5)
...
DO 20 i = 1, 5
    DO 10 j = 1, 5
        c(j, i) = a(j, i) * b(j, i)
10      CONTINUE
20  CONTINUE
```

- Fortran 90:

```
REAL, DIMENSION (5, 5) :: a, b, c
...
c = a * b
```


Whole array operations

Example

Find the maximum value less than 1000 in a three dimensional array:

- Fortran 77 requires triple DO loop and IF statements
- Fortran 90:

```
REAL, DIMENSION (10, 10, 10) :: a
amax = MAXVAL(a, MASK = (a < 1000))
```

Find average value > 3000 in an array:

- Fortran 77 requires DO loops and IF statements
- Fortran 90:

```
av = SUM(a, MASK = (a > 3000)) / &
    COUNT(MASK=(a> 3000))
```


Elemental intrinsic procedures

- Elemental procedures specified for scalar arguments
  - May also be applied to conforming array arguments
  - As if applied to each element separately.
- Example

```
! To find square root of all elements of array, a
a = SQRT(a)

! To find the string length excluding trailing blanks
! for all elements of a character array, ch
length = LEN_TRIM(ch)
```

WHERE statement

- Form:

  WHERE (*logical-array-expr*) *array-assignment*

- Assignment if logical condition is true

```
REAL DIMENSION (5, 5) :: ra, rb
...
WHERE (rb > 0.0) ra = ra / rb
```

- Note mask (rb > 0.0) must conform with LHS ra

WHERE construct

- Form:

  WHERE (*logical-array-expr*)
  array-assignments
  END WHERE

  WHERE (*logical-array-expr*)
  array-assignments
  ELSEWHERE
  array-assignments
  END WHERE

- Example

```
REAL DIMENSION (5, 5) :: ra, rb
...
WHERE (rb > 0.0)
   ra = ra / rb
ELSEWHERE
   ra = 0.0
END WHERE
```


Array sections

A subarray, called a section, of an array may be referenced by specifying a range of subscripts, either:

- A simple subscript

  a (2, 3, 1) ! single array element

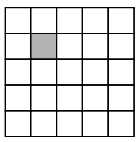
- A subscript triplet
  - [lower bound]:[upper bound] [:stride]
  - defaults to declared bounds and stride 1
- A vector subscript

Array sections

Example

REAL, DIMENSION (5, 5) :: ra

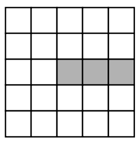
ra(2, 2) (=ra(2:2:1, 2:2:1))



Array Element

Shape (/ 1 /)

ra(3, 3:5)



Sub-row

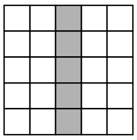
Shape (/ 3 /)

Array sections

Example

REAL, DIMENSION (5, 5) :: ra

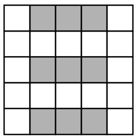
ra(:, 3)



Whole column

Shape (/ 5 /)

ra(1::2, 2:4)



Stride 2

Shape (/ 3, 3 /)

Vector subscripts

- 1D integer array used as array subscript

  (/ 3, 2, 12, 2, 1 /)

- Example

```
...
REAL, DIMENSION :: ra(6), rb(3)

INTEGER, DIMENSION (3) :: iv

iv = (/ 1, 3, 5 /)          ! rank 1 integer expression

ra = (/ 1.2, 3.4, 3.0, 11.2, 1.0, 3.7 /)

rb = ra(iv)                 ! iv is the vector subscript
    ! = (/ ra(1), ra(3), ra(5) /)
    ! = (/ 1.2, 3.0, 1.0 /)
...
```


Vector subscripts

- Vector subscript can be on LHS of expression

```
iv = (/ 1, 3, 5 /)
ra(iv) = (/ 1.2, 3.4, 5.6 /)
    ! = ra( (/ 1, 3, 5 /) ) = (/ 1.2, 3.4, 5.6 /)
```

- Must not repeat values of elements on LHS (many to one)

```
iv = (/ 1, 3, 1 /)
ra(iv) = (/ 1.2, 3.4, 5.6 /)     ! not permitted
    ! = ra((/ 1, 3, 1 /)) = (/ 1.2, 3.4, 5.6 /)

iv = (/ 1, 3, 5 /)
ra(iv) = (/ 1.2, 3.4, 5.6 /)     ! permitted
```


Array assignment

- Operands must be conformable
- Example

```
REAL, DIMENSION (5, 5) :: ra, rb, rc
INTEGER :: id

...

ra = rb + rc * id           ! Shape(/ 5, 5 /)

ra(3:5, 3:4) = rb(1::2, 3:5:2) + rc(1:3, 1:2)
! Shape(/ 3, 2 /)

ra(:, 1) = rb(:, 1) + rb(:, 2) + rb(:, 3)
! Shape(/ 5 /)
```

Beware of recursion

The following code:

```
DO i=2,n
   x(i) = x(i) + x(i-1)                    (1)
END DO
```

is not the same as:

```
x(2:n) = x(2:n) + x(1:n-1)                 (2)
```

- In (1):

```
x(i) = x(i) + x(i-1) + x(i-2) + ... + x(1)
```

- Fortran 90 equivalent:

```
x(2:n) = (/ (SUM(x(1:i)), i = 2, n) /)
```


Element location versus subscript

MAXLOC/MINLOC returns the max/min element location instead of subscript:

```
REAL, DIMENSION (1:8) :: ra
REAL, DIMENSION (-3:4) :: rb
INTEGER, DIMENSION (1) :: locmax1, locmax2
REAL :: max1, max2
ra = (/ 1.2, 3.4, 5.4, 11.2, 1.0, 3.7, 1.0, 1.0/)
rb = ra

! To find the location of max value
locmax1 = MAXLOC(ra)              ! = (/ 4 /)
locmax2 = MAXLOC(rb)              ! = (/ 4 /)

! To find maximum value from the location
max1 = ra(locmax1(1))
! OK, because ra defined with 1 as lower bound

max2 = rb(LBOUND(rb) + locmax2(1) - 1)
! general form required when lower bound ≠ 1
```


Zero-sized arrays

- When lower bound exceeds upper bound, array has size zero
- Valid providing normal rules are followed
- In particular, must be conformable (if one is zero-sized, all must be)
- Useful at boundaries - code does not need to treat boundaries in a special way:

```
INTEGER, PARAMETER :: n = 10
REAL, DIMENSION (n, n) :: a
REAL, DIMENSION (n) :: b, x
...
DO i = 1, n
   x(i) = b(i) / a(i, i)
   b(i+1:n) = b(i+1:n) - a(i+1:n, i) * x(i)
   ! zero-sized when i = n
END DO
```


Array constructor

- Construction of rank 1 array:

```
REAL, DIMENSION (6) :: a, b(6,6)
a = (/ array-constructor-value-list /)
```

where *array-constructor-value-list* can be:

- `(/ 1.2, 3.4, 3.0, 11.2, 1.0, 3.7 /)`
- `(/ b(i,2:4), b(1:5:2, i+3) /)`
  `! = (/ b(i,2),b(i,3),b(i,4),b(1,i+3),b(3,i+3), b(5,i+3) /)`
- `(/ (1.0 / REAL(i), i = 1, 6) /)`
  `!=(/1.0/1.0,1.0/2.0,1.0/3.0,1.0/4.0,1.0/5.0,1.0/6.0/)`
- `(/ ((i + j, i = 1, 3), j = 1, 2) /)`
  `! = (/ 2, 3, 4, 3, 4, 5 /)`

Array constructor

- Transfer to rank > 1 array via RESHAPE function:

  RESHAPE(SOURCE, SHAPE [,PAD] [,ORDER])

- Note that the size of SHAPE must be a constant
- Example:

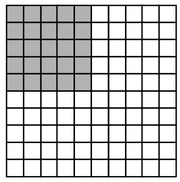
```
REAL, DIMENSION (3, 2) :: ra
ra = RESHAPE( (/ ((i + j, i = 1, 3), j = 1, 2) /), &
    SHAPE = (/ 3, 2 /) )
```

```
2  3
3  4      Shape(/ 3, 2 /)
4  5
```


Array arguments 1

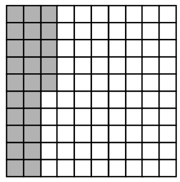
Fortran 77 (wrong)

```
PROGRAM array
PARAMETER (n = 10)
REAL a(n, n)
...
READ (*, *) n1
CALL sub(a, n1, res)
...
END
```



main program (n1 = 5)
25 elements wanted

```
SUBROUTINE sub(a, n1, res)
REAL a(n1, n1)
REAL work(10, 10)
...
res = a(...)
...
END
```

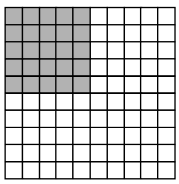


sub
25 elements passed

Array arguments 2

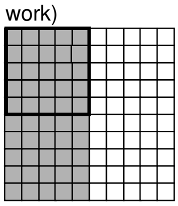
Fortran 77 (right)

```
PROGRAM array
PARAMETER (n = 10)
REAL a(n, n)
REAL work(n, n)
...
READ (*, *) n1
CALL sub(a, n, n1, res, work)
...
END
```



main program (n1 = 5)
25 elements wanted

```
SUBROUTINE sub(a, n, n1, res, work)
REAL a(n, n1)
REAL work(n1, n1)
...
res = a(...)
...
END
```



sub
50 elements passed

Dynamic arrays

- Fortran 77
  - static (fixed) memory allocation
- Fortran 90
  - allocate and deallocate storage as required via **allocatable arrays**
  - allow local arrays in a procedure to have different size and shape every time the procedure is invoked via **automatic arrays**
  - reduce overall storage requirement
  - simplify subroutine arguments

Allocatable arrays

- A deferred shape array which is declared with the ALLOCATABLE attribute
  - ALLOCATE(allocate_object_list [, STAT= status])
  - DEALLOCATE(allocate_obj_list [, STAT= status])
  - When STAT= is present, status = 0 (success) or status > 0 (error). When STAT= is not present and an error occurs, the program excution aborts
- Example:

```
...
REAL, DIMENSION (:, :), ALLOCATABLE :: ra
INTEGER :: status
READ (*, *) nsize1, nsize2
ALLOCATE (ra(nsize1, nsize2), STAT = status)
IF (status > 0) STOP 'Fail to allocate meomry'
...
IF (ALLOCATED(ra)) DEALLOCATE (ra)
...
```


Automatic arrays

- An explicit shape array in a procedure, whose bounds are provided when the procedure is invoked via:
  - dummy arguments
  - variables defined by use or host associations
- Automatic array must not appear in SAVE or NAMELIST statement, nor be initialised in type declaration
- Be aware that Fortran 90 provides no mechanism for checking whether there is sufficient memory for automatic arrays. If there is not, the outcome is unpredictable - the program will probably abort

Automatic arrays

Example

- Example 1: Bounds of automatic arrays depend on dummy arguments

```
SUBROUTINE sub(n, a)
   IMPLICIT NONE
   INTEGER :: n
   REAL, DIMENSION(n, n) :: a
   REAL, DIMENSION (n, n) :: work1
   REAL, DIMENSION (SIZE(a, 1)) :: work2
   ...
END SUBROUTINE sub
```

- Example 2: Bounds of an automatic array is defined by the global variable in a module

Automatic arrays

Example

```
MODULE auto_mod
   IMPLICIT NONE
   INTEGER :: n
CONTAINS
   SUBROUTINE sub
      REAL, DIMENSION(n) :: w
      WRITE (*, *) 'Bounds and size of a: ', &
         LBOUND(w), UBOUND(w), SIZE(w)
   END SUBROUTINE sub
END MODULE auto_mod

PROGRAM auto_arrays
! automatic arrays using modules instead of
! procedure dummy arguments
   USE auto_mod
   IMPLICIT NONE
   n = 10
   CALL sub
END PROGRAM auto_arrays
```

Array arguments 3

Fortran 90 dynamic arrays

```
PROGRAM array
    IMPLICIT NONE
    REAL, ALLOCATABLE, DIMENSION (:, :) :: a
    ...
    READ (*, *) n1
    ALLOCATE (a(n1, n1), STAT = alloc_stat)
    IF (alloc_stat /= 0) THEN
        ! ... error processing code ...
    END IF
    CALL sub(a, n1, res)
    DEALLOCATE(a)
    ...
CONTAINS
    SUBROUTINE sub(a, n1, res)
        REAL, DIMENSION (n1, n1) :: a
        REAL, DIMENSION(n1, n1) :: work
        ...
        res = a(...)
        ...
    END SUBROUTINE sub
END PROGRAM array
```


Assumed shape arrays

- Shape of actual and dummy arguments must agree
- Fortran 77: pass array dimensions as arguments
- Fortran 90: not necessary to pass array dimensions
  - Assumed shape array uses dimension of actual arguments
  - Can specify lower bound
  - Explicit interface required, so must provide an INTERFACE block if using an external procedure

Assumed shape arrays

Example

```
...                              ! calling program unit
INTERFACE
    SUBROUTINE sub (ra, rb, rc)
        REAL, DIMENSION (:, :) :: ra, rb
        REAL, DIMENSION (0:, 2:) :: rc
    END SUBROUTINE sub
END INTERFACE
REAL, DIMENSION (0:9,10) :: ra ! Shape (/ 10, 10 /)
...
CALL sub(ra, ra(0:4, 2:6), ra(0:4, 2:6))
...

SUBROUTINE sub(ra, rb, rc)         ! External
    REAL, DIMENSION (:, :) :: ra    ! Shape (/10, 10/)
    REAL, DIMENSION (:, :) :: rb    ! Shape (/ 5, 5 /)
    ! = REAL, DIMENSION (1:5, 1:5) :: rb
    REAL, DIMENSION (0:, 2:) :: rc ! Shape (/ 5, 5 /)
    ! = REAL, DIMENSION (0:4, 2:6) :: rc
    ...
END SUBROUTINE sub
```


Array arguments 4

Fortran 90: allocatable, automatic, and assumed shape

```
PROGRAM array
    IMPLICIT NONE
    REAL, ALLOCATABLE, DIMENSION(:, :) :: a
    ...
    READ (*, *) n1
    ALLOCATE ( a(n1, n1) )          ! allocatable
    CALL sub(a, res)
    DEALLOCATE(a)
    ...
CONTAINS
    SUBROUTINE sub(a, res)
    REAL, DIMENSION (:, :) :: a     ! assumed shape
    REAL, DIMENSION (SIZE(a, 1),SIZE(a, 2)) :: work
                                    ! automatic
    ...
    res = a(...)
    ...
    END SUBROUTINE sub
END PROGRAM array
```

Array intrinsic functions

List

- Reduction:

  ALL(MASK[,DIM])
  ANY(MASK[,DIM])
  COUNT(MASK[,DIM])
  MAXVAL(ARRAY[,DIM][,MASK])
  MINVAL(ARRAY[,DIM][,MASK])
  PRODUCT(ARRAY[,DIM][,MASK])
  SUM(ARRAY[,DIM][,MASK])

- Inquiry:

  ALLOCATED(ARRAY)
  LBOUND(ARRAY[,DIM])
  SHAPE(SOURCE)
  SIZE(ARRAY[,DIM])
  UBOUND(ARRAY[,DIM])

Array intrinsic functions

List

- Construction:

  MERGE(TSOURCE,FSOURCE,MASK)
  PACK(ARRAY,MASK[,VECTOR])
  UNPACK(VECTOR,MASK,FIELD)
  SPREAD(SOURCE,DIM,NCOPIES)

- Reshape:

  RESHAPE(SOURCE,SHAPE[,PAD][,ORDER]

- Array Location:

  MAXLOC(ARRAY[,MASK])
  MINLOC(ARRAY[,MASK])

Array intrinsic functions

List

- Array manipulation:

  CSHIFT(ARRAY,SHIFT[,DIM])
  EOSHIFT(ARRAY,SHIFT[,BOUND-ARY][,DIM])
  TRANSPOSE(MATRIX)

- Vector and matrix arithmetic:

  DOT_PRODUCT(VECTOR_A,VECTOR_B)
  MATMUL(MATRIX_A, MATRIX_B)

Array intrinsic functions

Example

Three students take four exams. The results are stored in an INTEGER array:

	85	76	90	60
score(1:3,1:4) =	71	45	50	80
	66	45	21	55

- Largest score:

  MAXVAL (score) ! = 90

- Largest score for each student:

  MAXVAL (score, DIM = 2)
  ! = (/ 90, 80, 66 /)

Array intrinsic functions

Example

- Student with largest score:

```
MAXLOC (MAXVAL (score, DIM = 2))
! = MAXLOC((/ 90, 80, 66 /)) = (/ 1 /)
```

- Average score:

```
average = SUM (score) / SIZE (score)    ! = 62
! average is an INTEGER variable
```

- Number of scores above average:

```
above = score > average
! above(3, 4) is a LOGICAL array
!                    T  T  T  F
! above =            T  F  F  T
!                    T  F  F  F
n_gt_average = COUNT (above)     ! = 6
! n_gt_average is an INTEGER variable
```


Array intrinsic functions

Example

- Pack all scores above the average:

```
...
INTEGER, ALLOCATABLE, DIMENSION (:) :: &
    score_gt_average
...
ALLOCATE (score_gt_average(n_gt_average))
scores_gt_average = PACK (score, above)
! = (/ 85, 71, 66, 76, 90, 80 /)
```

- Did any student always score above the average?

```
ANY (ALL (above, DIM = 2))     ! = .FALSE.
```

- Did all students score above the average on any of the tests?

```
ANY (ALL (above, DIM = 1))     ! = .TRUE.
```


Array example

Conjugate gradient algorithm

```
PROGRAM conjugate_gradients

    IMPLICIT NONE
    INTEGER :: iters, its, n
    LOGICAL :: converged
    REAL :: tol, up, alpha, beta
    REAL, ALLOCATABLE :: a(:,:), b(:), x(:), r(:), &
        u(:), p(:), xnew(:)

    READ (*,*) n, tol, its
    ALLOCATE ( a(n,n), b(n), x(n), r(n), u(n), &
        p(n), xnew(n) )

    OPEN (10, FILE='data')
    READ (10,*) a
    READ (10,*) b

    x = 1.0
    r = b - MATMUL(a,x)
    p = r
```


Array example (contd)

```
    iters = 0

    DO
        iters = iters + 1
        u = MATMUL(a, p)
        up = DOT_PRODUCT(r, r)
        alpha = up / DOT_PRODUCT(p, u)
        xnew = x + p * alpha
        r = r - u * alpha
        beta = DOT_PRODUCT(r, r) / up
        p = r + p * beta
        converged = ( MAXVAL(ABS(xnew-x)) / &
            MAXVAL(ABS(x)) < tol )
        x = xnew
        IF (converged .OR. iters == its) EXIT
    END DO

    WRITE (*,*) iters
    WRITE (*,*) x

END PROGRAM conjugate_gradients
```

Pointers

Pointers

Topics

- ❑ What is a pointer
- ❑ Specifications
- ❑ Pointer assignment
- ❑ Pointer status
- ❑ Dynamic storage
- ❑ Pointer arguments
- ❑ Pointer functions
- ❑ Arrays of pointer
- ❑ Linked list

What is a pointer?

A pointer variable has the POINTER attribute and may point to:

- ❑ Another data object of the same type, which has the TARGET attribute, or
- ❑ An area of dynamically allocated memory

The use of pointers provides:

- ❑ A more flexible alternative to allocatable arrays
- ❑ The tool to create and manipulate linked lists and other dynamic data structures

Specifications

type [[,*attribute*]... ::] list of variables

- ❑ Where *attribute* includes:
  - ■ POINTER for a pointer variable, or
  - ■ TARGET for a target variable
- ❑ The type, type parameters and rank of a pointer must be the same as the type and rank of any target to which it is pointing
- ❑ If a pointer is an array pointer, only the rank, not the shape, need be defined

```
REAL, DIMENSION(20), POINTER :: p   ! illegal

REAL, DIMENSION(:), POINTER :: p    ! legal
```

Pointer assignment

=>

```
REAL, POINTER :: p1, p2
REAL, TARGET :: t1 = 3.4, t2 = 4.5
p1 => t1
PRINT *, t1, p1              ! all 3.4
p2 => t2
PRINT *, t2, p2              ! all 4.5
```


```
p2 => p1
PRINT *, t1, p1, p2          ! all 3.4
```


```
t1 = 5.2
PRINT *, t1, p1, p2          ! all 5.2
```


Pointer assignment

Vs ordinary assignment

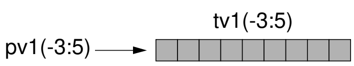
```
REAL, POINTER :: p1, p2
REAL, TARGET :: t1 = 3.4, t2 = 4.5
p1 => t1
PRINT *, t1, p1              ! all 3.4
p2 => t2
PRINT *, t2, p2              ! all 4.5
```


```
p2 = p1                      ! Equivalent to t2 = t1
                             ! So p1 = p2 = t1 = t2 = 3.4
PRINT *, t1, t2, p1, p2 ! all 3.4
```

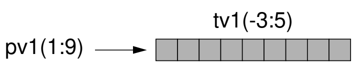
Pointer assignment

Array pointers

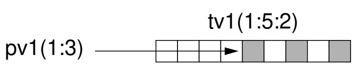
```
REAL, DIMENSION (:), POINTER :: pv1
REAL, DIMENSION (-3:5), TARGET :: tv1
pv1 => tv1              ! pv1 aliased to tv1
```




```
pv1 => tv1(:)           ! pv1 points to tv1 with
                        ! section subscript
```



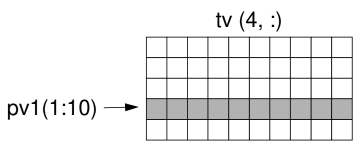

```
pv1 => tv1(1:5:2)       ! pv1 points to a section of
                        ! tv1 with subscript triplet
```



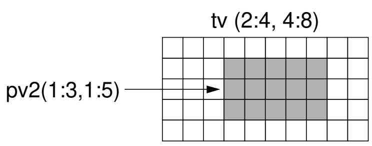
Pointer assignment

Array pointers

```
REAL, DIMENSION (:), POINTER :: pv1
REAL, DIMENSION (:, :), POINTER :: pv2
REAL, DIMENSION (5, 10), TARGET :: tv
pv1 => tv(4, :)       ! pv1 aliased to the 4th row of tv
```




```
pv2 => tv(2:4, 4:8)
```



Pointer status

- Undefined - As at start of program
- Null - Not the alias of any data object

  Must not reference undefined pointer, so set to null with NULLIFY statement
- Associated - The alias of a data object

  The status can be tested by ASSOCIATED intrinsic function, for example:

```
REAL, POINTER :: p              ! p undefined
REAL, TARGET :: t
PRINT *, ASSOCIATED (p)         ! not valid
NULLIFY (p)
PRINT *, ASSOCIATED (p)         ! .FALSE.
p => t
PRINT *, ASSOCIATED (p)         ! .TRUE.
```


Dynamic storage

ALLOCATE and DEALLOCATE

- Can allocate storage for a pointer to create an un-named variable or array of specified size with implied target attribute:

```
REAL, POINTER :: p
REAL, DIMENSION (:, :), POINTER :: pv
INTEGER :: m, n
...
ALLOCATE (p, pv(m, n))
```

- Can release storage when no longer required:

```
DEALLOCATE (pv)     ! pv is in null status
```

- Before assignment like p = 3.4 is made, p must be associated with its target via ALLOCATE, or aliased with target via pointer assignment statement

Dynamic storage

Danger!

- Dangling pointer

```
REAL, POINTER :: p1, p2
ALLOCATE (p1)
p1 = 3.4
p2 => p1
...
DEALLOCATE (p1)
```

- Unreferenced storage

```
REAL, DIMENSION(:), POINTER :: p
...
ALLOCATE(p(1000))
...
NULLIFY(p)  ! nullify p without first deallocating it
```


Pointer arguments

- Pointers, whether allocated or not, are allowed to be procedure arguments (allocatable arrays can not be dummy arguments and only allocated allocatable arrays can be actual argument)
- If a procedure has a pointer or target dummy argument, the interface to the procedure must be explicit
- If a dummy argument is a pointer, then the actual argument must be a pointer with the same type, type parameter and rank
- A pointer dummy argument can not have the intent attribute
- If the actual argument is a pointer but the dummy argument is not, the dummy argument becomes associated with the target of the pointer

Pointer arguments

Example

```
...                       ! calling program unit
INTERFACE                 ! do not forget interface
  SUBROUTINE sub2(b)
    REAL, DIMENSION(:, :), POINTER :: b
  END SUBROUTINE sub2
END INTERFACE
REAL, DIMENSION(:, :), POINTER :: p
...
ALLOCATE (p(50, 50))
CALL sub1(p)              ! both sub1 and sub2
CALL sub2(p)              ! are external procedures
...

SUBROUTINE sub1(a)        ! a is not a pointer
  REAL, DIMENSION(:, :) :: a
  ...
END SUBROUTINE sub1

SUBROUTINE sub2(b)        ! b is a pointer
  REAL, DIMENSION(:, :), POINTER :: b
  ...
END SUBROUTINE sub2
```


Pointer functions

- A function result may also have the POINTER attribute
- Useful if the result size depends on calculations performed in the function
- The result can be used in an expression, but must be associated with a defined target
- The interface to a pointer function must be explicit

Pointer functions

Example

```
...
IMPLICIT NONE
INTEGER, DIMENSION(100) :: x
INTEGER, DIMENSION(:), POINTER :: p
...
p => gtzero(x)
...
CONTAINS
  ! function to get all values .gt. 0 from a
  FUNCTION gtzero(a)
    INTEGER, DIMENSION(:), POINTER :: gtzero
    INTEGER, DIMENSION(:) :: a
    INTEGER :: n
    ...     ! find the number of values .gt. 0, n
    ALLOCATE (gtzero(n))
    ...     ! put the found values into gtzero
  END FUNCTION gtzero
  ...
END
```


Arrays of pointers

- An array of pointers can not be declared directly:

```
REAL, DIMENSION(20), POINTER :: p   ! illegal
```

- An array of pointers can be simulated by means of a derived type having a pointer component:

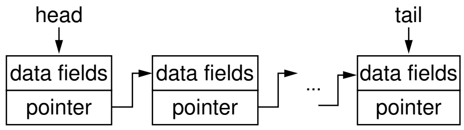
```
TYPE real_pointer
   REAL, DIMENSION(:), POINTER :: p
END TYPE real_pointer
TYPE(real_pointer), DIMENSION(100) :: a
INTEGER :: i
...
! possible to refer to the ith pointer by a(i)%p
DO i = 1, 100
   ALLOCATE (a(i)%p(i))
END DO
```

Linked list

- A pointer component of a derived type can point at an object of the same type; this enables a linked list to be created

```
TYPE node
   INTEGER :: value                   ! data field
   TYPE (node), POINTER :: next   ! pointer field
END TYPE node
```

- A linked list typically consists of objects of a derived type containing fields for the data plus a field that is a pointer to the next object of the same type in the list



Linked list

- In a linked list, the connected objects
  - Are not necessarily stored contiguously
  - Can be created dynamically at execution time
  - May be inserted at any position in the list
  - May be removed dynamically
- The size of a list may grow to an arbitrary size as a program is executing
- Trees or other dynamic data structures can be constructed in a similar way

Linked list

Example

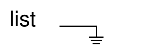
```
...
TYPE node
   INTEGER :: value                   ! data field
   TYPE (node), POINTER :: next   ! pointer field
END TYPE node

INTEGER :: num
TYPE (node), POINTER :: list, current

NULLIFY(list)           ! initially nullify list (empty)

DO
   READ *, num          ! read num from keyboard
   IF (num == 0) EXIT      ! until 0 is entered
   ALLOCATE(current)       ! create new node
   current%value = num
   current%next => list    ! point to previous one
   list => current         ! update head of list
END DO
...
```


Linked list

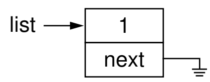
Example

If, for example, the values 1, 2, 3 are entered in that order, the list looks like (progressively):

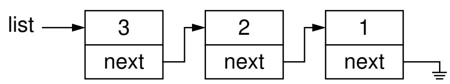
- After NULLIFY(list)



- After the first num is read



- After all 3 numbers are read



New I/O Features

New I/O features

Topics

- ❑ Non-advancing I/O
- ❑ INQUIRE by I/O list
- ❑ NAMELIST
- ❑ New edit descriptors
- ❑ New statement specifiers

Non-advancing I/O

- ❑ Each READ or WRITE normally involves full records
- ❑ Non-advancing I/O permits READ or WRITE without advancing position to new record
- ❑ ADVANCE='NO' specifier:

```
WRITE(*, '("Input size?")', ADVANCE='NO')
READ(*, '(I5)') n
```

- ❑ Non-advancing I/O not applicable with list directed I/O

INQUIRE by I/O list

```
INQUIRE (IOLENGTH=length) output-list
```

- ❑ To determine the length of an unformatted output item list
- ❑ May be used as value of RECL specifier in subsequent OPEN statement
- ❑ Example:

```
INTEGER :: rec_len
...
INQUIRE (IOLENGTH = rec_len) name, title, &
    age, address, tel
...
OPEN (UNIT = 1, FILE = 'test', RECL = rec_len, &
    FORM = 'UNFORMATTED')
...
WRITE(1) name, title, age, address, tel
...
```

NAMELIST

- Gather set of variables into group to simplify I/O
- General form of NAMELIST statement:

  NAMELIST /namelist-group-name/ variable-list

- Use namelist-group-name as format instead of io-list on READ and WRITE
- Input record has specific format:

  &namelist-group-name var2=x, var1=y, var3=z/

- Variables optional and order unimportant

NAMELIST

Example

```
...
INTEGER :: size = 2
CHARACTER (LEN = 4) :: &
    colour(3) = (/ ' red', 'pink', 'blue' /)
NAMELIST /clothes/ size, colour
WRITE(*, NML = clothes)
...
```

outputs:

```
&CLOTHES SIZE = 2, COLOUR =  redpinkblue/
```


New edit descriptors

- EN - (Engineering) Same as E but exponent divisible by 3, value before decimal point between 1 and 1000
- ES - (Scientific) Same as E but value before decimal point is between 1 and 10
- B - Binary
- O - Octal
- Z - Hexadecimal
- G - Generalised edit descriptor now applicable for all intrinsic types

New edit descriptors

Example

To compare the differences among E, EN, ES and G edit descriptors:

```
PROGRAM e_en_es_g_compare
   IMPLICIT NONE
   REAL, DIMENSION(4) :: &
       x=(/1.234, -0.5, 0.00678, 98765.4/)
   PRINT '(4E14.3/4EN14.3/4ES14.3/4G14.3)',&
       x, x, x, x
END PROGRAM e_en_es_g_compare
```

Output:

```
0.123E+01     -0.500E+00  0.678E-02   0.988E+05
1.234E+00  -500.000E-03  6.780E-03  98.765E+03
1.234E+00     -5.000E-01  6.780E-03   9.877E+04
1.234            -0.500        0.678E-02   0.988E+05
```

New statement specifiers

- INQUIRE

POSITION	=	'ASIS'	'REWIND'	'APPEND'
ACTION	=	'READ'	'WRITE'	'READWRITE'
DELIM	=	'APOSTROPHE'	'QUOTE'	'NONE'
PAD	=	'YES'	'NO'	
READWRITE	=)			
READ	=)	'YES'	'NO'	'UNKNOWN'
WRITE	=)			

- OPEN

  POSITION, ACTION, DELIM, PAD are same as above
  STATUS = 'REPLACE'

- READ/WRITE

  NML = namelist_name
  ADVANCE = 'YES' 'NO'

- READ

  EOR = label SIZE = character_count

Intrinsic Procedures

Intrinsic procedures

Topics

- Rich set with four categories
- List of new intrinsic procedures

Intrinsic procedures

Four categories

- Elemental procedures

  A set of functions and one sub-routine, specified for scalar arguments, but applicable for conforming array arguments,

- Inquiry functions

  Return properties of principal arguments that do not depend on their values

- Transformational functions

  usually have array arguments and an array result whose elements depend on many of the elements of the arguments

- Nonelemental subroutines

New intrinsic procedures

Elemental functions:

- ❑ Numeric
  - CEILING (A)
  - FLOOR (A)
  - MODULO (A, P)
- ❑ Character
  - ACHAR (I)
  - ADJUSTL (STRING)
  - ADJUSTR (STRING)
  - IACHAR (C)
  - INDEX (STRING, SUBSTRING [, BACK])
  - LEN_TRIM (STRING)
  - SCAN (STRING, SET [, BACK])
  - VERIFY (STRING, SET [, BACK])

New intrinsic procedures

- ❑ Bit manipulation
  - BTEST (I, POS)
  - IAND (I, J)
  - IBCLR (I, POS)
  - IBITS (I, POS, LEN)
  - IBSET (I, POS)
  - IEOR (I, J)
  - IOR (I, J)
  - ISHFT (I, SHIFT)
  - ISHFTC (I, SHIFT [, SIZE])
  - NOT (I)
- ❑ Kind
  - SELECTED_INT_KIND (R)
  - SELECTED_REAL_KIND (P,R)

New intrinsic procedures

- ❑ Floating point manipulation
  - EXPONENT (X)
  - FRACTION (X)
  - NEAREST (X, S)
  - RRSPACING (X)
  - SCALE (X, I)
  - SET_EXPONENT (X, I)
  - SPACING (X)
- ❑ Logical:
  - LOGICAL (L [,KIND])

Elemental subroutine:

- MVBITS (FROM, FROMPOS, LEN, TO, TOPOS)

New intrinsic procedures

Inquiry functions:

- PRESENT (A)
- ASSOCIATED (POINTER [,TARGET])
- KIND (X)
- BIT_SIZE (I)

- ❑ Numeric
  - DIGITS (X)
  - EPSILON (X)
  - HUGE (X)
  - MAXEXPONENT (X)
  - MINEXPONENT (X)
  - PRECISION (X)
  - RADIX (X)
  - TINY (X)

New intrinsic procedures

Transformational functions:

- REPEAT (STRING, NCOPIES)
- TRIM (STRING)
- TRANSFER (SOURCE, MOLD [, SIZE])

Non elemental intrinsic subroutines:

- DATE_AND_TIME ([DATE][,TIME][,ZONE][VALUES])
- SYSTEM_CLOCK ([COUNT][,COUNT_RATE][COUNT_MAX])
- RANDOM_NUMBER (HARVEST)
- RANDOM_SEED ([SIZE] [,PUT] [,GET])

Array intrinsic procedures:

- See section on array processing

Redundant Features

Redundant features

Topics

- ❑ Obsolescent features
- ❑ Other redundant features
- ❑ Redundant features are divided into 5 groups:
  - Source form
  - Data
  - Control
  - Procedures
  - Input/Output

Redundant features

Source form

- ❑ Fixed source form

  Use new free source form instead
- ❑ INCLUDE line

  Use modules instead

Redundant features

Data

- DOUBLE PRECISION data type

  Superseded by the concept of parameterised data types for numerical **portability**

- Implicit typing and IMPLICIT statement

  Use IMPLICT NONE statement always

- Old form of type declaration statements e.g.: REAL list of real variables

  Use the new form with a double colon (::) between the type and the list of variables

- PARAMETER, DIMENSION and other attribute statements

  Use of the attribute forms, rather than the statement forms

Redundant features

Data

- DATA statement

  Not needed as variables may be initialised in a type statement except for octal, hexadecimal and array section initialisations

- Assumed-size arrays as dummy arrays

  Superseded by the assumed-shape arrays

- COMMON blocks and BLOCK DATA

  Use of modules obviates the need for them

- EQUIVALENCE statement

  The introduction of modules, dynamic storage allocation, pointers, and the intrinsic function TRANSFER makes its use unnecessary

- SEQUENCE attribute

  Should never be used

Redundant features

Control

- Obsolescent features
  - **Arithmetic IF statement**
  - **Shared DO termination, and DO termination on a statement other than on a CONTINUE or an END DO statement**
  - **REAL and DOUBLE precision DO variables and control expressions**
  - **ASSIGN and assigned GO TO statements**
  - **Branching to END IF from outside IF block**

  Can be replaced by IF statement, IF, DO and CASE control constructs, and EXIT and CYCLE statements

  - **Alternate RETURN**
  - **PAUSE statement**

  The above listed should never be used in new or revised programs.

Redundant features

Control

- Labels

  The use of labels are rarely necessary with the introduction of modern control constructs and the character string format specifications

- CONTINUE statement to end DO loop

  Can be replaced by using DO construct, EXIT and CYCLE statements

- GO TO and computed GO TO statements

  IF, DO and CASE constructs, EXIT and CYCLE statements should be used instead

- DO WHILE logical-expression statement

  Can replaced by DO loop construct and EXIT statement

Redundant features

Procedures

- Intrinsic functions with specific names for different data types

  Superseded by generic versions (note: a specific name is required only when an intrinsic function is being used as an actual argument)

- ENTRY statement

  Can be replaced by internal procedures and modules

- Statement functions

  Superseded by the concept of internal procedures

- External procedures and EXTERNAL statement

  Putting procedures either in a module or another program unit as internal procedures makes things much easier that it really is not necessary to use external procedures in any new or revised programs

Redundant features

Input/Output

- Obsolescent features

  - **Assigned FORMAT specifiers,** should be replaced by the character string format specifications
  - **H edit descriptor**, should be replaced by the character constant edit descriptor A

- FORMAT statement

  The same effect can be achieved by assigning the format specification to a character string

- ERR=, END=, and EOR= specifiers

  Each of these conditions are recommended to be checked by using the IOSTAT= specifier

- NAMELIST input/output

  Is an extremely poorly designed feature and best not to use it unless absolutely necessary

Redundant features

Input/Output

- D edit descriptor

  Superseded by the E edit descriptor

- BN and BZ edit descriptors

  The BLANK specifier provides a better way to deal with the problem

- P edit descriptor

  Can lead to confusion and is best to avoid

- G edit descriptor

  Using I, E, EN, ES, F, L, or A edit descriptors can provide some checking whether the data types are all corrected

- X edit descriptor

  This position edit descriptor is the same as TR

Further Development

Fortran 95

- Corrections to Fortran 90
- FORALL

```
FORALL (i = 1:n, j = 1:n, y(i, j) /= 0 .AND. i /= j) &
    x(i, j) = 1.0 / y(i, j)

FORALL (i = 1:n)
    a(i, i) = i
    b(i) = i*I
END FORALL
```

- PURE attribute - make PURE procedures safe for use in FORALL statement
- CPU time - CALL CPU_TIME(t1)
- Also allocatable dummy arguments and results

Fortran 95

- Nested WHERE

```
WHERE (mask1)
    ...
    WHERE (mask2)
        ...
    ELSEWHERE
        ...
    ENDWHERE
ELSEWHERE
    ...
ENDWHERE
```

- Initial pointer or type default status

```
REAL, POINTER :: p(:) => NULL()

TYPE string
    CHARACTER, POINTER :: ch(:) => NULL()
ENDTYPE
```


Further development

With FORTRAN 90 barely out of cradle, why are there already efforts to enhance it?

- The limelight of HPC research has recently shifted away from vector computers and towards parallel and “massive” parallel computers
- Fortran 90 may be suitable for HPC on conventional and vector computers, but it does not include features to obtain the best performance on parallel systems.
- Demands for such features has led to the development of two de facto standards:
    - High Performance Fortran (HPF)
    - Message Passing Interface (MPI)

HPF

Goals

HPF provides a set of language extensions to Fortran 90 to support:

- Data parallel programming
- Top performance on MIMD and SIMD computers with non-uniform memory access
- Code tuning for various architectures
- Minimal deviation from other standards
- Define open interfaces to other languages

HPF

What is in it

- ❑ Compiler directives for data alignment and distribution
- ❑ Concurrent execution features using the FORALL statement
- ❑ A number of intrinsic functions to enquire about machine specific details
- ❑ A number of extrinsic functions which provide an escape mechanism from HPF
- ❑ A library of routines to support global operations

MPI

What

Message Passing Interface is a proposed standard for:

- ❑ Explicit message passing
- ❑ Application programs
- ❑ MIMD distributed memory concurrent computers
- ❑ Workstation networks

MPI

Why

- ❑ Portability and ease-of-use
- ❑ Time right for standard
- ❑ Library construction
- ❑ Prerequisite for development of concurrent software industry
- ❑ Provides hardware vendors with well-defined set of routines that they must implement efficiently

MAN T&EC

The Manchester and North HPC
Training and Education Centre

Fortran 90 (Edition 3.0)

OHP Overviews Comment Sheet

Please send comments you have on any of the Fortran 90 materials to:

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