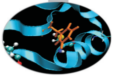
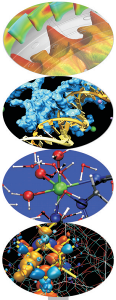


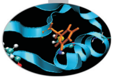
Introduction to Fortran 90

F. Salvadore V. Ruggiero M. Tacconi

CINECA Roma - SCAI Department



Roma, 22-25 January 2013



Part I

A Fortran Survey 1

Program main unit, source formats, comments, declarations and instructions. Fundamental operators, expressions, conditional constructs, loops, functions: arguments passing, intent, interface, intrinsic and external functions. Modules: contains and use. Intrinsic types: integer, real, complex, logical, and parameter. I/O base.

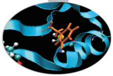
Outline

Formula Translator History

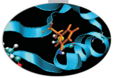
- Developed in the 50s among the earliest high level languages (HLL)
- Widely and rapidly adopted in the area of numerical, scientific, engineering and technical applications
- First standard in 1966: Fortran 66
  - The first of all programming language standards
- Second standard in 1978: Fortran 77
- Third standard in 1991: Fortran 90
  - Adds new, modern features such as structured constructs, array syntax and ADT
  - Extended and revised in 1997: Fortran 95
  - Further extended with published Technical Reports
- Fourth standard in 2004: Fortran 2003
  - Major revision, incorporates TRs, adds many new features (OO!), still not fully supported
- Fifth standard in 2010: Fortran 2008

Fortran General Philosophy

- Strongly oriented to *number crunching*
- Efficient language, highly optimized code
  - Basic data types and operators mapping "naturally" to CPUs
  - Translated by a compiler to machine language
  - Language rules allow for aggressive, automatic optimization
  - Facilities to build new data types from the basic ones
  - Flexible flow control structures mapping the most common numerical computing use cases
- Scientific computing specialized syntax
  - A wealth of math data types and functions available as intrinsics of the language
  - Compact, readable array syntax to operate on many values as a whole



- Why Fortran is bad
  - Current standard embodies four different language versions,...
  - ... all of them still alive in legacy codes
  - Non-numeric computing in Fortran is a real pain
  - There are more C than Fortran programmers
  - GUI and DB accesses are best programmed in C
  - C99 partly addressed numerical computing needs



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- Why Fortran is good
  - Fortran is highly tuned for numerical computation
  - Fortran is older and more “rigid” than C, compilers optimize better
  - Much better than C at managing user defined data types
  - Object-oriented features are now part of the language
  - Provides facilities for interoperability with C and other languages

Our Aims

- Teach you the fundamentals of modern Fortran
- For both reading (old and new) and writing (new) programs
- Showing common idioms
- Illustrating and demonstrating many of the extensions introduced in the more recent standards
- Illustrating best practices
- Blaming bad ones
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Outline

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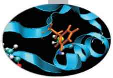
My First Scientific Program in Fortran



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! roots of a 2nd degree equation with real coefficients

program second_degree_eq
  implicit none
  real :: delta
  real :: x1, x2
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  print *,'Solving ax^2+bx+c=0, enter a, b, c:'
  read (*,*) a, b, c

  delta = sqrt(b**2 - 4.0*a*c) ! square root of discriminant
  x1 = -b + delta
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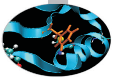

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  - Variable contents
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Comments

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- Best practice: do comment your code!
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  - Tricks
- Best practice: do not over-comment your code!
  - Obvious comments obfuscate code and annoy readers
  - `! square root of discriminant` is a bad example

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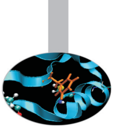

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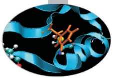

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- Best practice: always mark unit beginning and ending with its type and name
  - Makes your readers (including you) happier

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- Best practice: it is strongly recommended to turn off implicit declarations with **`implicit none`**, at the beginning of each program unit
  - Improves readability and clarity: each variable has its type declared
  - Mistyped names can be caught by the compiler as undeclared variables

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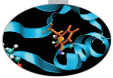

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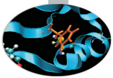

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- `sqrt()` is an intrinsic function returning the square root of its argument
- `x1 = x1 + delta` is a statement assigning the value of expression `x1 + delta` to variable `x1`
- By the way, expressions can be passed as argument to functions, as to `sqrt()`: their value will be computed and passed to the function

Outline

What a Compiler Is

- Fortran lets you write programs in a high-level, human-readable language
- Computer CPUs do not directly understand this language
- You need to translate your code into machine-level instructions for your CPU architecture
- Compilers take care of that translation and generate machine code that can be actually executed by a CPU

What a Compiler Does

- Compilers are sophisticated tools, made up of many components
- When compiler is invoked to generate executable code, three main steps are performed:
  1. parsing of source files, various kinds of analysis and transformations, optimization and *assembly* files creation
  2. machine-code generation and object file creation
     - an object file is an organized collection of all symbols (variables, functions...) used or referenced in the code
  3. linking and executable creation
- Options are provided to execute each step separately, take a look at the manual of your favourite compiler, there's a lot to learn!

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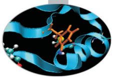

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    An executable file named **`a.out`** (**`a.exe`** under Windows) will be generated

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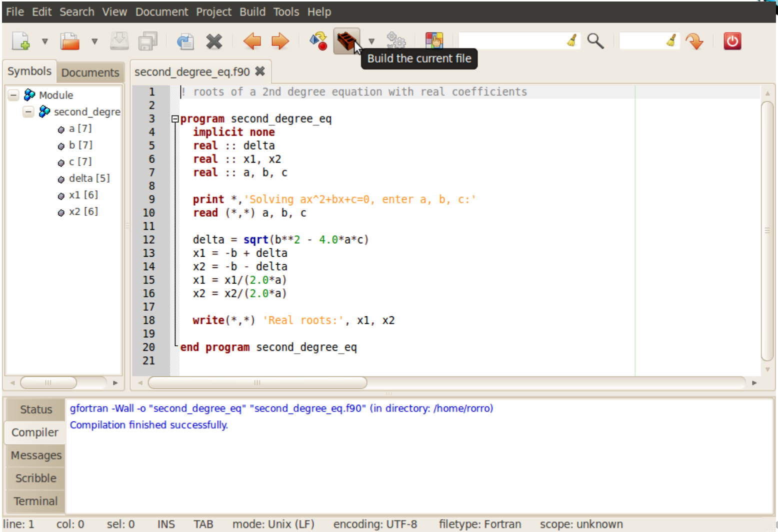
  - Run the program under GNU/Linux with:

```
user@caspur$> ./a.out
```

    or under Windows with:

```
C:\Documents and Settings\user> a.exe
```

Do You Like IDEs? Geany



Hands-on Session #1

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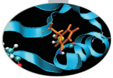
SuperComputing Applications and Innovation

Outline



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- Let's avoid this, by changing from:

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delta = sqrt(b**2 - 4.0*a*c)
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  to:

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delta = b**2 - 4.0*a*c
if (delta < 0.0) then
   stop
end if
delta = sqrt(delta)
```

- Try it now!

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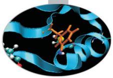
- Try it now!
- Did you check that normal cases still work? Good.

Conditional Statement



- **`if (`***logical-condition***`) then`**
  block of statements
  `end if`
  - Executes *block of statements* only if *logical-condition* is true
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- But let's be more polite by changing from:

```
if (delta < 0.0) then
  stop
endif
```

to:

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if (delta < 0.0) stop 'No real roots!'
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- Try it now!

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- Did you check that normal cases still work? Good.

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if (delta < 0.0) stop 'No real roots!'
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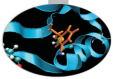
  but this is not that good...

- In general, Fortran disregards white space, but proper indentation visualizes program control flow

SCAI
SuperComputing Applications and Innovation

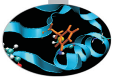
Outline

Let's Refactor Our Program (and Test it!)



```fortran
! roots of a 2nd degree equation with real coefficients

program second_degree_eq
  implicit none
  real :: delta
  real :: rp
  real ::  a, b, c

  print *,'Solving ax^2+bx+c=0, enter a, b, c: '
  read(*,*) a, b, c

  delta = b*b - 4.0*a*c
  if (delta < 0.0) stop 'No real roots!'
  delta = sqrt(delta)/(2.0*a)

  rp = -b/(2.0*a)

  print *,'Real roots: ', rp+delta, rp-delta

end program second_degree_eq
```

And Now Make it More Complex!



```
! roots of a 2nd degree equation with real coefficients

program second_degree_eq
  implicit none
  real :: delta, rp, a, b, c
  logical :: rroots

  print *,'Solving ax^2+bx+c=0, enter a, b, c: '
  read(*,*) a, b, c
  delta = b*b - 4.0*a*c
  rroots = .true.
  if (delta < 0.0) then
    delta = -delta
    rroots = .false.
  end if
  delta = sqrt(delta)/(2.0*a)
  rp = -b/(2.0*a)
  if (rroots) then
    print *, 'Real roots: ', rp+delta, rp-delta
  else
    print *,'Complex roots: ', rp, '+', delta, 'i ', &
             rp, '-', delta, 'i'
  end if
end program second_degree_eq
```

More Types and Choices

- **`logical`** type represents logical values
  - Can be **`.true.`** or **`.false.`**

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SuperComputing Applications and Innovation

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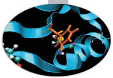
- And Fortran statements cannot exceed one line, unless it ends with an **`&`**

Try it Now!



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                 rp, '-', delta, 'i'
  end if
end program second_degree_eq
```

Let's Make it as Complex as Possible!

```
! roots of a 2nd degree equation with real coefficients

program second_degree_eq
  implicit none
  complex :: delta
  complex :: z1, z2
  real    :: a, b, c

  print *,'Solving ax^2+bx+c=0, enter a, b, c: '
  read(*,*) a, b, c

  delta = b*b - 4.0*a*c
  delta = sqrt(delta)

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- And so do **`read`**, **`write`**, and **`print`**
- **`(1.5, 2.3)`** is *Fortranese* for $1.5 + 2.3\imath$

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    end if
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- Did you check that normal cases still work? Good.

Miscellaneous remarks

- Nested **`if`**s can be a problem
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    ```
    error-message
    stop
    ```
- Best practice: if your program has to fail, always have it fail in a controlled way

Sorting it Out

- Let's give names to **`if`** constructs:

```
no2nd: if (a == 0.0) then
  no1st: if (b == 0.0) then
    no0th: if (c == 0.0) then
             write(0,*) 'A trivial identity!'
           else no0th
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           end if no0th
         else no1st
           write(0,*) 'Too simple problem!'
         end if no1st
         stop
       end if no2nd
```
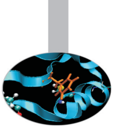

Sorting it Out



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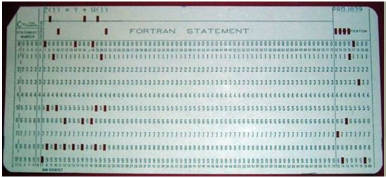
- Names are for readability purposes only, do not enforce pairing rules
- Best practice: always give names to constructs which span many lines of code or are deeply nested

Fortran Code, in the Beginning of Times



- The one on the right, is the statement **`Z(I) = Y + W(I)`**
- The one in the middle, is an IBM punch card reader
- The one on the left, is a complete Fortran source program
- But you'll only encounter these in museums, nowadays

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SuperComputing Applications and Innovation

A Taste of Fortran in the Late 70s

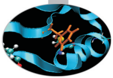
```
C ROOTS OF A 2ND DEGREE EQUATION WITH REAL COEFFICIENTS

      PROGRAM EQ2DEG

      IMPLICIT NONE
      REAL DELTA
      REAL RP
      REAL A, B, C

      PRINT *,'SOLVING AX^2+BX+C=0, ENTER A, B, C: '
      READ(*,*) A, B, C

      DELTA = B*B - 4.0*A*C
      IF (DELTA.LT.0.0) STOP 'NO REAL ROOTS!'
      DELTA = SQRT(DELTA)/(2.0*A)

      RP = -B/(2.0*A)

      PRINT *,'REAL ROOTS: ', RP+DELTA, RP-DELTA

      END
```

Legacy Code: Distinctive Characters

- Code is all capitals
  - First computers had only uppercase letters
- Fixed source form
  - The legacy of punch cards
  - Comment lines must be marked with a `C` or `*` in first column
  - First six columns on each line are reserved for labels and to mark continuation lines
  - Columns after the 72nd are ignored (cause of really nasty bugs!)
- No double colon on variable declarations
  - And no way to initialize a variable at declaration, for that matter
  - More on this later
- And this example is not that different...

SuperComputing Applications and Innovation

A Bottle of Fortran, Vintage Year 1963



```
C        SOLUTION OF QUADRATIC EQUATION
C        (P. 122 OF A FORTRAN PRIMER BY E. ORGANICK)
    1 READ INPUT TAPE 5, 51, ANAME, N
   51 FORMAT(A6,I2)
      WRITE OUTPUT TAPE 6,52, ANAME
   52 FORMAT(1H1,33HROOTS OF QUADRATIC EQUATIONS FROM A6)
      DO 21 I = 1, N
      READ INPUT TAPE 5, 53, A, B, C
   53 FORMAT(3F10.2)
      WRITE OUTPUT TAPE 6,54, I, A, B, C
   54 FORMAT(1H0,8HSET NO. I2/5H A = F8.2,12X,4HB = F8.2,12X,4HC = F8.2)
      IF(A) 10, 7, 10
    7 RLIN = -C/B
      WRITE OUTPUT TAPE 6, 55, RLIN
   55 FORMAT(7H LINEAR,25X,4HX = F10.3)
      GO TO 21
   10 D = B**2 - 4.*A*C
      IF(D) 12, 17, 17
   12 COMPR = -B/(2.*A)
      COMP1 = SQRTF(-D)/(2.*A)
      COMP2= -COMP1
      WRITE OUTPUT TAPE 6, 56, COMPR, COMP1, COMPR, COMP2
   56 FORMAT(8H COMPLEX,21X,7HR(X1)= F10.3,11X,7HI(X1)= F10.3,/1H ,28X,
     17HR(X2)= F10.3,11X,7HI(X2)= F10.3)
   16 GO TO 21
   17 REAL1 = (-B + SQRTF(D))/(2.*A)
      REAL2 = (-B - SQRTF(D))/(2.*A)
   20 WRITE OUTPUT TAPE 6, 57, REAL1, REAL2
   57 FORMAT(6H REAL 25X,5HX1 = F10.3,13X,5HX2 = F10.3)
   21 CONTINUE
      WRITE OUTPUT TAPE 6, 58, ANAME
   58 FORMAT(8H0END OF A6)
      GO TO 1
      END
```

Best Practice: Free Yourself

- Write new code in free source form
  - No limits on beginning of program statements
  - Each line may contain up to 132 default characters
  - Comments can be added at end of line
  - And it comes for free: just give your source file name an `.f90` extension
- Use new language features
  - Like new styles for declarations
  - Or naming of constructs
  - They are more powerful and readable
- We'll focus on modern Fortran programming style
  - Making you aware of differences you are most likely to encounter
  - Look at compiler manuals or reference books to tame very old codes

SuperComputing Applications and Innovation

Outline

A Fortran Program is Made of: I

- Comments
  - Compiler disregards them, but humans do not
  - Please, use them
  - Do not abuse them, please
- Program units
  - One, at least: **`program`**
  - Some of them (functions) are intrinsic to the language
- Variables
  - Named memory location you can store values into
  - Must be declared
- Variables declarations
  - Give name to memory location you can store values into
  - An initial value can be specified

A Fortran Program is Made of: II

- Expressions
  - Compute values to store in variables
  - Compute values to pass to functions and statements
- Statements
  - Units of executable work
  - Whose execution can be controlled by other constructs
- `if` statements and constructs
  - Allow for conditional and alternative execution
  - For both single statements and blocks of

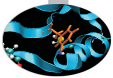
Best Practices

- Use free source form
- `implicit none` statement
  - Turn off implicit declarations
- Use proper indentation
  - Compilers don't care about
  - Readers visualize flow control
- Give names to complex control structures, readers will appreciate
- Do non-regression testing
  - Whenever functionalities are added
  - Whenever you rewrite a code in a different way
- Fail in a controlled way
  - Giving feedback to humans

Outline

Outline

My First Fortran Functions



```
function theta(x) !Heaviside function, useful in DSP
  implicit none
  real :: theta
  real :: x

  theta = 1.0
  if (x < 0.0 ) theta = 0.0
end function theta

function sinc(x) !sinc function as used in DSP
  implicit none
  real :: sinc
  real :: x
  real, parameter :: pi = acos(-1.0)

  x = x*pi
  sinc = 1.0
  if (x /= 0.0) sinc = sin(x)/x
end function sinc

function rect(t, tau) !generalized rectangular function, useful in DSP
  implicit none
  real :: rect
  real :: t, tau
  real :: abs_t, half_tau
  real, external :: theta

  abs_t = abs(t)
  half_tau = 0.5*tau
  rect = 0.5
  if (abs_t /= half_tau) rect = theta(half_tau-abs_t)
end function rect
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  abs_t = abs(t)
  half_tau = 0.5*tau
  rect = 0.5
  if (abs_t /= half_tau) rect = theta(half_tau-abs_t)
end function rect
```
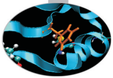

Functions and their Definition

- Functions are program units
  - Function name must be a legal Fortran name
  - Functions specialty is performing computations and returning a value

My First Fortran Functions



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  real :: sinc
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  x = x*pi
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  real :: rect
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Functions and their Definition

- Functions are program units
  - Function name must be a legal Fortran name
  - Functions specialty is performing computations and returning a value
- Type of returned value must be declared
  - In the definition and in each unit calling them
  - Same as a variable declaration
  - Could be declared on the function heading, but it's less flexible and less readable
  - More on this later...

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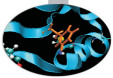
  - Could be declared on the function heading, but it's less flexible and less readable
  - More on this later...
- How to return a value
  - Just assign it to the function name, as if it were a variable
  - But this doesn't force function termination
  - Multiple assignments can be done
  - The last assigned value before function execution is complete will be returned

My First Fortran Functions



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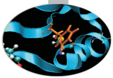

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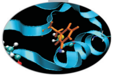

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- What if a dummy argument has the same name of a variable elsewhere in the program?
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- Variables can be defined inside functions
  - Again, they are local, thus completely independent from the rest of the program

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Intrinsic vs. External

- Fortran sports a wealth (over a hundred!) of predefined functions and procedures
- These are termed *intrinsic*
  - **`acos(x)`** returns the arc cosine of x such that $|x| \leq 1$ in the range $0 \leq \arccos(x) \leq \pi$
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- What's this **`external`** keyword?
- It's one of the many attributes you can give to something you define
  - **`external`** tells the compiler **`theta`** is an external (i.e. non intrinsic) function
  - So the compiler is not forced to guess what it is from its use
  - And that way, masters can override intrinsic functions

My First Fortran Functions

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  - I.e. variables that cannot be modified after initialization (compiler will bark if you try)
- In initialization expressions:
  - only constants (possibly other `parameters`) can be used
  - only intrinsic operators or functions are allowed
- Best practice: always give name to constants
  - Particularly if unobvious, like `1.0/137.0`
  - It also helps to centralize updates (well, not for π)

Outline

On To Testing

- Let's put the code in a file named **`dsp.f90`**
- Best practice: always put different groups of related functions in different files
  - Helps to tame complexity
  - You can always pass all source files to the compiler
  - And you'll learn to do better ...

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Hands-on Session #2

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function theta(x) !Heaviside function, useful in DSP
  implicit none
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  theta = 1.0
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```
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  rtheta = theta(i)
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  write(*,*) 'theta(', i, ')= ', rtheta
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end program dsp_test
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Testing DSP Functions

- Let's build our test program putting all together:

```
user@caspur$> gfortran dsp.f90 dsp_test.f90 -o dsp_test
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 Enter i, j, k:
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 theta(  -3.1415927     ) =    0.0000000
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```

- Something is going wrong, isn't it?
  - Seems like one function changed its actual argument!

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State Your Intent!

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function theta(x) !Heaviside function, useful in DSP
  implicit none
  real :: theta
  real, intent(in) :: x

  theta = 1.0
  if (x < 0.0 ) theta = 0.0
end function theta

function sinc(x) !sinc function as used in DSP
  implicit none
  real :: sinc
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  x = x*pi
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dsp.f90:16.2:

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- Got a compiler error message? Good!

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  - **`intent(inout)`** (default) for those you plan to do both

My First Fortran Functions Fixed!

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  implicit none
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Testing DSP Function the Last Time

- Way much better!

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user@caspur$> ./dsp_test
 Enter i, j, k:
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- Now comment out **`real :: i, j, k`** in **`dsp_test.f90`**, recompile and rerun

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- Now comment out **`real :: i, j, k`** in **`dsp_test.f90`**, recompile and rerun
- Now add **`implicit none`** to **`dsp_test.f90`** and do it again

Outline

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- Try to pass **`integer`** variables as actual arguments to **`theta()`**, **`sinc()`**, and **`rect()`**

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- Got some surprising behavior?
- Our testing program doesn't know enough about external functions it is calling
  - It is knowledgeable about return types
  - It is totally ignorant about argument types
- We can make it aware using **`interface`** blocks

Explicit Interface

```
program dsp

  implicit none

  real :: i,j,k

  real, external :: theta, sinc, rect







  print *, 'Enter i, j, k:'
  read(*,*) i, j, k

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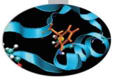
end program dsp
```

Explicit Interface



```
program dsp

  implicit none

  real :: i,j,k

  interface
    function theta(x)
      real :: theta, x
    end function theta
  end interface

  interface
    function sinc(x)
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    end function sinc
  end interface

  interface
    function rect(t, tau)
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    end function rect
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end program dsp
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Ignorance is Evil

- Try to pass **`integer`** variables as actual arguments to **`theta()`**, **`sinc()`**, and **`rect()`**
- Got some surprising behavior?
- Our testing program doesn't know enough about external functions it is calling
  - It is knowledgeable about return types
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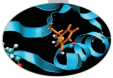

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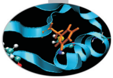

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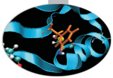
  - Or, if your life is too short for typing, copy and paste it
  - But life is too short to modify interfaces spread around 56 program units
  - Good, but still error prone, no better way?

`use` Modules, Instead!

- Modules are the Fortran way to complete and robust management of sets of related routines and more

My First Module



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module dsp
  implicit none
contains
  function theta(x) !Heaviside function, useful in DSP
    real :: theta
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    theta = 1.0
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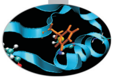

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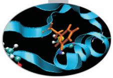

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- But there is a lot more to say about modules

Modules Give You Fine Control

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- or maybe both:
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Managing Wrong Arguments

```
function rect(t, tau)
  implicit none
  real :: rect
  real, intent(in) :: t, tau
  real :: abs_t, half_tau

  abs_t = abs(t)
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```

- What if `rect()` is passed a negative argument for `tau`?
  - Wrong results
- Taking the absolute value of `tau` it's a possibility
- But not a good one, because:
  - a negative rectangle width is nonsensical
  - probably flags a mistake in the calling code
  - and a zero rectangle width is also a problem

Failing Predictably

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function rect(t, tau)
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- A known approach...
- but too rude!
  - No clue at the argument value
  - No clue at which call to **`rect()`** was wrong
  - And stopping a program in a procedure, called by another procedure, called by another procedure, ..., is widely reputed bad programming practice

A Better Approach

```
module dsp
  implicit none
  integer :: dsp_info
  integer, parameter :: DSPERR_DOMAIN = 1
contains
  function theta(x) !Heaviside function, useful in DSP
! code as in previous examples...
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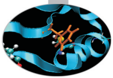

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- And they will be accessible to all program units using it
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  - For variables hosting integer numerical values
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- And yes, **`return`** forces function execution to terminate and return to calling unit

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- Note: even if Fortran ignores case, constants are often highlighted using all capitals

A Widely Used Approach

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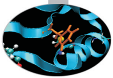

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SuperComputing Applications and Innovation

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```

- But this is annoying when the arguments are guaranteed to be correct
  - **info** can be given the **optional** attribute
  - and omitted when you feel it's safe: **rect(x, 5.0)**

Making Argument Optionals

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module dsp
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  integer, parameter :: DSPERR_DOMAIN = 1
contains

! ...

  function rect(t, tau, info) !generalized rectangular function, useful in DSP
    real :: rect
    real, intent(in) :: t, tau
    integer, intent(out), optional :: info
    real :: abs_t, half_tau

    if (present(info)) info = 0
    if (tau <= 0.0) then
      if (present(info)) info = DSPERR_DOMAIN
      rect = 0.0
      return
    end if

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! ...

  function rect(t, tau, info) !generalized rectangular function, useful in DSP
    real :: rect
    real, intent(in) :: t, tau
    integer, intent(out), optional :: info
    real :: abs_t, half_tau

    if (present(info)) info = 0
    if (tau <= 0.0) then
      if (present(info)) info = DSPERR_DOMAIN
      rect = 0.0
      return
    end if

    abs_t = abs(t)
    half_tau = 0.5*tau
    rect = 0.5
    if (abs_t /= half_tau) rect = theta(half_tau-abs_t)
  end function rect
end module dsp
```

Total Robustness

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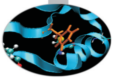
Total Robustness



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- Best strategy: return a NaN and set **`dsp_info`** in these bad cases
  - And do it also for non positive values of **`tau`**
  - But then the floating point environment configuration should be checked, proper floating point exceptions set...
- Being absolutely robust is difficult
  - Too advanced stuff to cover in this course
  - But not an excuse, some robustness is better than none
  - It’s a process to do in steps
  - Always comment in your code bad cases you don’t cover yet!

Outline

- Introduction
- Fortran Basics
- More Fortran Basics
  - My First Fortran Functions
  - Making it Correct
  - Making it Robust
  - Copying with Legacy
  - Wrapping it Up 2
- Integer Types and Iterating
- More on Compiling and Linking
- Homeworks

A Glimpse to Fortran 77

```
FUNCTION SINC(X)
  IMPLICIT NONE
  REAL SINC, X, XPI
  REAL PI
  PARAMETER (PI = 3.1415926)

  XPI = X*PI
  SINC = 1.0
  IF (XPI .NE. 0.0) SINC = SIN(XPI)/XPI
END

FUNCTION RECT(T, TAU)
  IMPLICIT NONE
  REAL RECT, T, TAU
  REAL ABS_T, HALF_TAU
  REAL THETA
  EXTERNAL THETA
  INTEGER DSPINFO
  COMMON /DSP/ DSPINFO

  IF (TAU .LE. 0.0) THEN
    DSPINFO = 1
    RECT = 0.0;
    RETURN
  END IF

  ABS_T = ABS(T)
  HALF_TAU = 0.5*TAU
  RECT = 0.5
  IF (ABS_T .NE. HALF_TAU) RECT = THETA(HALF_TAU-ABS_T)
END
```

Many Things are Missing

- Strange looking relational operators
- No attributes
  - Declarations spread over many lines, error prone
- No initialization expressions
  - You had to type in the actual number
- No **`intent`** i.e. no defense from subtle bugs
- No **`interface`**

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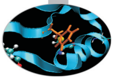

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- No easy way to share variables among program units
  - To share you had to use **`common`** statements
  - And type in variable types and **`common`** statements in each unit
  - And the smallest mistake can turn into a nightmare
- Bottom line:
  - Is **`common`** good or bad? The jury is still out
  - We'll not cover them, but you'll encounter them
  - Read the fine print, or better switch to modules, they are way much better

Refurbishing Old Code

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  - Tested and tried

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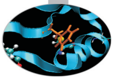
Refurbishing Old Code



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  - Tested and tried
- But no interface
  - Thus no compiler checks when you call it
  - And rewriting a working code in modern language is soooo dangerous...
- Modules come to rescue
  - They don't need to include the actual code
  - But they can publish an interface for code which is elsewhere
  - And then you can use the module in calling program units

Wrapping Old Code in a Module

```
module dspmod

  implicit none

  interface
    function theta(x)
      real :: theta
      real, intent(in) ::x
    end function theta
  end interface

  interface
    function sinc(x)
      real :: sinc
      real, intent(in) :: x
    end function sinc
  end interface

  interface
    function rect(t, tau)
      real :: rect
      real, intent(in) :: t, tau
    end function rect
  end interface

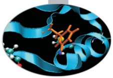
end module dspmod
```

Outline

We Did Progress!

- A program can be subdivided in more source files
- Functions and their arguments
- Arguments are passed to functions by reference
- `intent` attribute is precious to prevent subtle bugs
- Intrinsic and external procedures are two different things
- `parameter` variables
- Explicit interfaces
- Modules allow complete management of procedures
- Modules allow access to variables from many program units
- Modules can be used to make proper use of legacy, reliable codes

Best Practices



- Always name constants
- Test every function you write
  - Writing specialized programs to do it
- Use language support and compiler to catch mistakes
- Use explicit interfaces
- Use modules
- Describe all attributes of a variable at declaration
- Anticipate causes of problems
  - Find a rational way to react
  - Fail predictably and in a user friendly way
  - Robustness it’s a long way to do in steps
  - Comment in your code issues still to address

SuperComputing Applications and Innovation

Outline

Introduction

Fortran Basics

More Fortran Basics

Integer Types and Iterating
- Play it Again, Please
- Testing and Fixing it
- Hitting Limits
- Wider Integer Types
- How Bad it Used to Be
- Wrapping it Up 3

More on Compiling and Linking

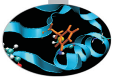
Homeworks

Greatest Common Divisor

- Euclid's Algorithm
  1. Take two integers a and b
  2. Let $r \leftarrow a \mod b$
  3. Let $a \leftarrow b$
  4. Let $b \leftarrow r$
  5. If b is not zero, go back to step 2
  6. a is the GCD

- Let's implement it and learn some more Fortran

GCD & LCM



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module number_theory
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contains
  function gcd(a, b) ! Greatest Common Divisor
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    gcd = a
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  function lcm(a, b) ! Least Common Multiple
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    lcm = a*b/gcd(a,b)
  end function lcm
end module number_theory
```

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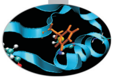

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The Integer Type

- As we said, **`integer`** means that a value is an integer
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SuperComputing Applications and Innovation

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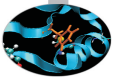

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  - And works for real values too, or values of any type, for that matter
  - More on this later
- Want to know more?
  - Intrinsic function **`huge(0)`** returns the greatest positive value an **`integer`** can assume
  - Again, we'll be back at this

Outline

GCD & LCM

```
module number_theory
  implicit none
contains
  function gcd(a, b) ! Greatest Common Divisor
    integer :: gcd
    integer, intent(in) :: a, b
    integer :: gb, t

    gcd = a
    gb = b

    do
      t = mod(gcd,gb)
      gcd = gb
      if (t == 0) exit
      gb = t
    end do
  end function gcd

  function lcm(a, b) ! Least Common Multiple
    integer :: lcm
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    lcm = a*b/gcd(a,b)
  end function lcm
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Iterating with **`do ... end do`**

- **`do`**
  block of statements
  `end do`

  1. Executes again and again the *block of statements*
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- In this specific example:
  - the code following `end do` is the end of the function
  - thus, we could use `return` instead of `exit`, which is legal,
  - but generally regarded bad practice
- Best practice: do not bail out of a function from inside a loop, particularly a long one
  ```

Outline

Hands-on Session #3

- Put the code in file `numbertheory.f90`
- Write a program to test both `gcd()` and `lcm()` on a pair of integer numbers
- Test it:
  - with pairs of small positive integers
  - with the following pairs: 15, 18; -15, 18; 15, -18; -15, -18; 0, 15; 15, 0; 0, 0

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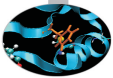
- Test it:
  - with pairs of small positive integers
  - with the following pairs: 15, 18; -15, 18; 15, -18; -15, -18; 0, 15; 15, 0; 0, 0
- In some cases, we get wrong results or runtime errors
  - Euclid's algorithm is only defined for positive integers

Let's Generalize to the Whole Integer Set

- gcd(*a*, *b*) is non negative, even if *a* or *b* is less than zero
  - Taking the absolute value of **`a`** and **`b`** using **`abs()`** will do

GCD & LCM: Dealing with 0 and Negatives



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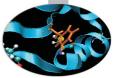

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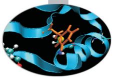

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  - and with the pair: 1000000, 1000000

Outline

Beware of Type Ranges

- `a*b/gcd(a,b)` same as `(a*b)/gcd(a,b)`

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SuperComputing Applications and Innovation

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GCD & LCM: Preventing Overflow

```
module number_theory
  implicit none
contains
  function gcd(a, b) ! Greatest Common Divisor
    integer :: gcd
    integer, intent(in) :: a, b
    integer :: gb, t

    gcd = abs(a)
    gb = abs(b)

    if (a == 0) gcd = gb
    if (a == 0 .or. b == 0) return

    do
      t = mod(gcd,gb)
      gcd = gb
      if (t == 0) exit
      gb = t
    end do
  end function gcd

  function lcm(a, b) ! Least Common Multiple
    integer :: lcm
    integer, intent(in) :: a, b

    if (a == 0 .and. b == 0) then
      lcm = 0 ; return
    end if

    lcm = a*(b/gcd(a,b))
  end function lcm
end module number_theory
```

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  - on the following pairs: 15, 18; -15, 18; 15, -18; -15, -18; 0, 15; 15, 0; 0, 0
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  - with the pair: 1000000, 1000000
  - and let's test also with: 1000000, 1000001

Outline

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- `selected_int_kind(n)`:
  - returns a *kind type parameter* corresponding to an internal representation capable to host the value 10^{n}
  - or `-1` if none is wide enough
- `integer` accepts an optional *kind type parameter*
  - `integer(kind=selected_int_kind(9)) :: di` usually makes `di` a 32 bits wide variable
  - `integer(kind=selected_int_kind(18)) :: wi` makes `wi` a 64 bits wide variable
  - `integer(selected_int_kind(18)) :: wi` will also do

GCD & LCM: Let's Make Kind Explicit

```fortran
module number_theory
  implicit none
contains
  function gcd9(a, b) ! Greatest Common Divisor
    integer(selected_int_kind(9)) :: gcd9
    integer(selected_int_kind(9)), intent(in) :: a, b
    integer(selected_int_kind(9)) :: gb, t

    gcd9 = abs(a)
    gb = abs(b)

    if (a == 0) gcd9 = gb
    if (a == 0 .or. b == 0) return

    do
      t = mod(gcd9,gb)
      gcd9 = gb
      if (t == 0) exit
      gb = t
    end do
  end function gcd9

  function lcm9(a, b) ! Least Common Multiple
    integer(selected_int_kind(9)) :: lcm9
    integer(selected_int_kind(9)), intent(in) :: a, b

    if (a == 0 .and. b == 0) then
      lcm9 = 0 ; return
    end if

    lcm9 = a*(b/gcd9(a,b))
  end function lcm9
end module number_theory
```

Being More General and Generic

- And let's add support for a wider integer range

GCD & LCM: Let’s Add Headroom

```fortran
! add right after: end function lcm9

  function gcd18(a, b) ! Greatest Common Divisor
    integer(selected_int_kind(18)) :: gcd18
    integer(selected_int_kind(18)), intent(in) :: a, b
    integer(selected_int_kind(18)) :: gb, t

    gcd18 = abs(a)
    gb = abs(b)

    if (a == 0) gcd18 = gb
    if (a == 0 .or. b == 0) return

    do
      t = mod(gcd18,gb)
      gcd18 = gb
      if (t == 0) exit
      gb = t
    end do
  end function gcd18

  function lcm18(a, b) ! Least Common Multiple
    integer(selected_int_kind(18)) :: lcm18
    integer(selected_int_kind(18)), intent(in) :: a, b

    if (a == 0 .and. b == 0) then
      lcm18 = 0 ; return
    end if

    lcm18 = a*(b/gcd18(a,b))
  end function lcm18
```

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- Wait!
  - Now we have to remember to call the right function, depending on the integer kind
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  - **`interface`** blocks come to rescue

GCD & LCM: Making it Generic

```
module number_theory
  implicit none

  private gcd9, lcm9, gcd18, lcm18

  interface gcd
    module procedure gcd9, gcd18
  end interface

  interface lcm
    module procedure lcm9, lcm18
  end interface

contains

function gcd9(a, b) ! Greatest Common Divisor
! code as before
end function gcd9

function lcm9(a,b) ! Least Common Multiple
! code as before
end function lcm9

function gcd18(a, b) ! Greatest Common Divisor
! code as before
end function gcd18

function lcm18(a,b) ! Least Common Multiple
! code as before
end function lcm18

end module number_theory
```

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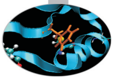

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contains

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end module number_theory
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SuperComputing Applications and Innovation

Outline

Introduction

Fortran Basics

More Fortran Basics

Integer Types and Iterating
- Play it Again, Please
- Testing and Fixing it
- Hitting Limits
- Wider Integer Types
- How Bad it Used to Be
- Wrapping it Up 3

More on Compiling and Linking

Homeworks

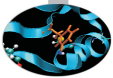
Dusty Decks

```
      FUNCTION GCD18(A, B)
        INTEGER*8 GCD18, A, B
        INTEGER*8 GB, T

        GCD18 = A
        GB = B

1       T = MOD(GCD18,GB)
        GCD18 = GB
        IF (T .EQ. 0) GO TO 2
        GB = T
        GO TO 1

2       CONTINUE
      END

      FUNCTION LCM18(A, B)
        INTEGER*8 LCM18, A, B
        INTEGER*8 GCD18
        EXTERNAL GCD18

        LCM18 = A*B/GCD18(A,B)
      END
```

A Limited Language with Many Dialects

- No structured endless loops
  - Labels and `GO TO`s where used instead
- `CONTINUE` was a no-op
  - Used to mark destination of jumps
  - No comment
- `INTEGER*8` was used to declare an 8 bytes integer variable
  - Absolutely non standard
  - As are `INTEGER*1`, `INTEGER*2`, `INTEGER*4`, `REAL*4`, `REAL*8`, `COMPLEX*8`, `COMPLEX*16`
- Many dialects
  - Many proprietary extensions used to be developed
  - And then copied among vendors for compatibility reasons
  - Many extensions were eventually standardized
  - But not all of them!
  - They still lurk around, and can be tempting: resist!

Outline



Introduction

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Homeworks

More Types and Flow Control

- There are many integer types
  - With implementation dependent ranges
  - Selectable by kind type parameters
  - Whose limits can be devised using **`huge()`** or **`range()`**
- Library functions have generic names, good for most types
- And you can write your own generic interfaces
- Behavior on integer overflow is implementation defined
  - Some control is possible using parentheses
- Blocks of statements can be iterated forever...
  - ... and **`exit`** gets off the roundabout
- Logical conditions can be combined using **`.or.`** and **`.and.`** operators

Best Practices

- Do not rely on type sizes, they are implementation dependent
- Do not leave a function from inside a loop
- Think of intermediate results in expressions: they can overflow or underflow
- Be consistent with Fortran approach
  - E.g. writing generic interfaces
  - Even if it costs more work
  - Even if it costs learning more Fortran
  - Once again, you can do it in steps
  - You'll appreciate it in the future
- Hide implementation details as much as possible
  - You'll never regret
- Resist the temptation of old Fortran or non standard extensions
  - Will pay back in the future

Outline

Introduction

Fortran Basics

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Homeworks

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- If given earlier ...
- Something is an error if not in Fortran 95 standard
  - Use `-std=f95` to force reference standard

Building a Program

Creating an executable from source files is in general a three phase process:

- pre-processing:
  - each source file is read by the pre-processor
    - substitute (**`#define`**) MACROs
    - insert code by **`#include`** statements
    - insert or delete code evaluating **`#ifdef`**, **`#if`** ...
- compiling:
  - each source file is translated into an object code file
    - an object code file is an organised collection of symbols, referring to variables and functions defined or used in the source file
- linking:
  - object files should be combined together to build a single executable program
  - every symbol should be resolved
    - symbols can be defined in your object files
    - or available in other object code (external libraries)

Compiling with GNU gfortran

- When you give the command:

```
user@caspur$> gfortran dsp.f90 dsp_test.f90
```

SuperComputing Applications and Innovation

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```
user@caspur$> gfortran -E -cpp dsp.f90
user@caspur$> gfortran -E -cpp dsp_test.f90
```

  - **`-E -cpp`** option, tells **`gfortran`** to stop after pre-process
  - Simply calls **`cpp`** (automatically invoked if the file extension is **`F90`**)
  - Output sent to standard output

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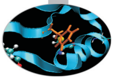
```

  - **-E -cpp** option, tells **gfortran** to stop after pre-process
  - Simply calls **cpp** (automatically invoked if the file extension is **F90**)
  - Output sent to standard output
- Compiling sources

```
user@caspur$> gfortran -c dsp.f90
user@caspur$> gfortran -c dsp_test.f90
```

  - **-c** option tells **gfortran** to only compile the source
  - An object file **.o** is produced from each source file

Linking with GNU gfortran



- Linking object files together

```
user@caspur$> gfortran dsp.o dsp_test.o
```

- To resolve symbols defined in external libraries, specify:
  - which libraries to use (**-l** option)
  - in which directories they are (**-L** option)
- How to link the library **libdsp.a** in **/mypath**

```
user@caspur$> gfortran file1.o file2.o -L/mypath -ldsp
```

- How to create and link the DSP library:

```
user@caspur$> gfortran -c dsp.f90
ar curv libdsp.a dsp.o
ranlib libdsp.a
gfortran test_dsp.f90 -L. -ldsp
```

  - **ar** create the archive **libdsp.a** containing **dsp.o**
  - **ranlib** generate index to archive
- To include file like **.mod**, specify
  - in which directories they are (**-I** option)

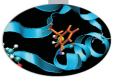
Outline

Homework I

- Write a program that reads an integer value **`limit`** and prints the first **`limit`** prime numbers
  - Use the GCD function to identify those numbers
  - After testing the basic version, handle negative **`limit`** values: print an error message and attempt to read the value again

Homework II

- Write a module containing a function that takes an integer **n** as input, and returns the **n-th** element of the Fibonacci series **fn**
- Hint:
  - $F_0 = 0$
  - $F_1 = 1$
  - $F_n = F_{n-1} + F_{n-2}$
- Write a main program to test your function
  - Read **n** from standard input
  - Try with **n=2, 10, 40, 46, 48, ...**
  - What's the greatest **n** := **maxn**, for which **fn** is representable by a default integer? (**huge** can help to find it out)
  - Use this information to handle too large values of **n** in your function:
  - If **n** > **maxn** print an error message and return -1



Part II

A Fortran Survey 2

Passing functions as arguments of procedurs. Conditional and numerical loops. Managing the precision, conversions, overflow, underflow, Inf e NaN. Expressions and subexpressions with mixed types. Types, operators and logical expressions. Type character and intrinsic functions for strings. Subroutine. Array. Default constructor for arrays and implicit loops. Assumed-shape array and automatic object. Expressions with arrays and conformity.

Outline

Caveat Emptor

The code in this section is meant for didactical purposes only.

It is deliberately naive: focus is on language aspects, not on precision or accuracy.

As a consequence, it is prone to numerical problems.

Outline

- More Flow Control
  - Numerical Integration
  - Wrapping it Up 4
- Fortran Intrinsic Types, Variables and Math
- Arrays

Numerical Integration

- Let's use the trapezoidal rule to estimate $\int_a^b f(x)\,dx$
- Dividing the interval $[a, b]$ into n equal sized slices, it boils down to:
$\int_a^b f(x)\,dx \approx \frac{b-a}{n}\left(\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{n-1} f\left(a + k\frac{b-a}{n}\right)\right)$
- And to make it more juicy, let's make a succession of estimates, doubling n each time, until the estimate seems stable

Double Steps

```
module integrals
  implicit none
contains
  function trap_int(a,b,f,tol)        ! recursive approximation of integral
    real :: trap_int                  ! by trapezoidal rule
    real, intent(in) :: a, b, tol     ! integration interval and tolerance
    interface
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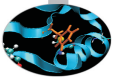
Double Steps



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Function Arguments

- Yes, a function can be passed as an argument to another function!
- Simply pass the name on call, like this:

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g = trap_int(-pi, pi, sinc, 0.0001)
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- And then the function can be called using the dummy argument name
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  - I.e. reuse the same routine to integrate different functions in the same program

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SuperComputing Applications and Innovation

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- Integer and real values can be mixed in expressions
  - As well as values of same type but different kind
  - And the right thing will be done
  - Which is: when two values of different type/kind meet each other at a binary operator, the one with smaller numeric range is converted to the other

SuperComputing Applications and Innovation

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Iterating with `do while ... end do`

- **`do while (`***logical-condition***`)`**
  block of statements
  `end do`
  1. Evaluates *logical-condition*
  2. If *logical-condition* is false, goes to 5
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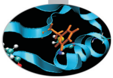
  2. Particularly for nested loops
- Best practices:
  1. use names to mark loops when they are long or belong to a deep nest
  2. NEVER, NEVER permit your code to loop forever for some inputs

Double Steps



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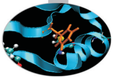

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Hands-on Session #1

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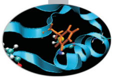
Time to Put it at Work



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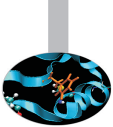

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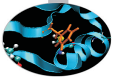
  - What if some arguments take a ... value?

Good Ol' Fortran

- Procedure arguments and mixed-mode expressions were already there

Good Ol' Fortran



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      do 10, i=1,10,3
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- **`do while`**, **`exit`**, **`end do`** weren't there...
  - ... at least in the standard...
  - but are often found in codes, as dialect extensions.

SuperComputing Applications and Innovation

Outline

- More Flow Control
  - Numerical Integration
  - Wrapping it Up 4
- Fortran Intrinsic Types, Variables and Math
- Arrays

Forward Steps

- More flow control
  - Procedure arguments
  - `do while`
  - Counted `do`
- Mixed-mode expressions
- Name your loops
  - Particularly if long or nested
  - Particularly if you `exit` them
  - But don't do it for short ones
- Prevent any loop from running forever for some program inputs

Outline

More Flow Control

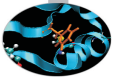
Fortran Intrinsic Types, Variables and Math
- Integer Types
- Floating Types
- Expressions
- Arithmetic Conversions
- More Intrinsic Types

Arrays

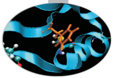
Data

- Computing == manipulating data and calculating results
  - Data are manipulated using internal, binary formats
  - Data are kept in memory locations and CPU registers
- Fortran doesn't make assumptions on internal data representations
  - And tries to abstract
  - Most CPU are similar but all have peculiarities
  - Some details depend on the specific executing (a.k.a. target) hardware architecture and software implementation
  - Fortran provides facilities to translate between internal formats and human readable ones
- Fortran allows programmers to:
  - think in terms of data types and named containers
  - disregard details on actual memory locations and data movements

Fortran is a Strongly Typed Language



- Each literal constant has a type
  - Dictates internal representation of the data value
- Each variable has a type
  - Dictates content internal representation and amount of memory
  - Type must be specified in a declaration before use
  - Unless you are so naive to rely on implicit declaration
- Each expression has a type
  - And subexpressions have too
  - Depends on operators and their arguments
- Each function has a type
  - That is the type of the returned value
  - Specified in function interface
- Procedure arguments have types
  - I.e. type of arguments to be passed in calls
  - Specified in procedure interface
  - If the compiler doesn't know the interface, it will blindly pass whatever you provide



More Flow Control

Fortran Intrinsic Types, Variables and Math

- Integer Types
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Arrays

Integer Types (as on most CPUs)

Type	Sign	Usual `huge()`	Usual Width (bits)	Usual Size (bytes)
`integer(selected_int_kind(2))`	+/-	127	8	1
`integer(selected_int_kind(5))`	+/-	32767	16	2

`integer`
`integer(kind(0))`
`integer(selected_int_kind(9))`
	+/-	2147483647	32	4

`integer(selected_int_kind(18))`	+/-	9223372036854775807	64	8

- **`selected_int_kind(n)`** returns the least type able to host 10^n
- **`selected_int_kind(n)`** returns -1 if no suitable type is available
- New platform/compiler? Always check maximum headroom with **`huge()`** or **`range()`**
- As we said, on most platforms **`kind()`** returns the byte size, but it's not standard

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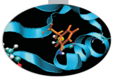

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- Remember:
  - do not write **`spokes = bycicles*2*36`**
  - **`integer, parameter :: SpokesPerWheel = 36`**
  - code will be more readable, and you'll be ready for easy changes

`integer` Math

Function	Returns
`abs(i)`	$\|i\|$
`sign(i,j)`	$\|i\|$ if $j \geq 0$, $-\|i\|$ otherwise
`dim(i,j)`	if $i > j$ returns $i - j$ else returns 0
`mod(i,j)`	Remainder function $i - \texttt{int}(i/j) \times j$
`modulo(i,j)`	Modulo function $i - \texttt{floor}(i/j) \times j$
`min(i,j[, ...])`	$\min\{i, j[, ...]\}$
`max(i,j[, ...])`	$\max\{i, j[, ...]\}$

- Use like: `a = abs(b+i) + c`
- More functions are available to manipulate values
  - E.g. for bit manipulations on binary computers
  - We'll not cover them in this course, you can learn more about if you need to
- They can be found under different names (e.g. `iabs()`): these are relics from the past

Floating Types (as on most CPUs)

Type	Usual `huge()`	Usual Width (bits)	Usual Size (bytes)

`real`
`real(kind(0.0))`
`real(selected_real_kind(6))`
	3.40282347e38	32	4

`double precision`
`real(kind(0.0d0))`
`real(selected_real_kind(15))`
	1.7976931348623157e308	64	8

`real(selected_real_kind(18))`	> 1.2e4932	80 or 128	10 or 16

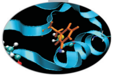
`complex`
`complex(kind(0.0))`
`complex(selected_real_kind(6))`
	NA	NA	8

`complex(kind(0.0d0))` `complex(selected_real_kind(15))`	NA	NA	16
`complex(selected_real_kind(18))`	NA	NA	20 or 32

- In practice, always in IEEE Standard binary format, but not a Standard requirement
- **`selected_real_kind()`** gets number of significant decimal digits, plus a second optional argument for exponent range, returns negative result if no suitable type is available
- **`tiny()`** returns smallest positive value
- New platform/compiler? Always check maximum headroom with **`huge()`** or **`range()`**

SuperComputing Applications and Innovation

`real` Literal Constants



- Need something to distinguish them from integers
  - Decimal notation: **`1.0`**, **`-17.`**, **`.125`**, **`0.22`**
  - Exponential decimal notation: **`2e19`** (2×10^{19}), **`-123.4e9`** (-1.234×10^{11}), **`.72e-6`** (7.2×10^{-7})

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- By default, `kind(0.0)`
- Unless you specify it
  - For double precision only:

```
-1.23456d5
```

  - For all kinds:

```
integer, parameter :: r8=selected_real_kind(15)
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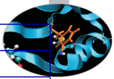
  - For all kinds:

    ```
    integer, parameter :: r8=selected_real_kind(15)
    -123456.0_r8
    ```

- Remember:
  - do not write `charge = protons*1.602176487E-19`
  - `real,parameter::UnitCharge=1.602176487E-19`
  - it will come handier when more precise measurements will be available

`real` Math



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`sign(x,y)`	$\vert\mathbf{x}\vert$ if $\mathbf{y} \geq 0$, $-\vert\mathbf{x}\vert$ otherwise
`dim(x,y)`	if $\mathbf{x} > \mathbf{y}$ returns $\mathbf{x} - \mathbf{y}$ else returns 0
`mod(x,y)`	Remainder function $\mathbf{x} - \mathtt{int}(\mathbf{x}/\mathbf{y}) \times \mathbf{y}$
`modulo(x,y)`	Modulo function $\mathbf{x} - \mathtt{floor}(\mathbf{x}/\mathbf{y}) \times \mathbf{y}$
`aint(x)`[2], `int(x)`[1,2]	if $\mathbf{x} > 0$ returns $\lfloor\mathbf{x}\rfloor$ else returns $\lceil\mathbf{x}\rceil$
`anint(x)`[2], `nint(x)`[1,2]	nearest integer to **x**
`floor(x)`[1,2], `ceiling(x)`[1,2]	$\lfloor\mathbf{x}\rfloor$, $\lceil\mathbf{x}\rceil$
`fraction(x)`	fractional part of **x**
`nearest(x,s)`	next representable value to **x**, in direction given by the sign of **s**
`spacing(x)`	absolute spacing of numbers near **x**
`max(x,y[, ...])`	$\max\{\mathbf{x}, \mathbf{y}[, ...]\}$
`min(x,y[, ...])`	$\min\{\mathbf{x}, \mathbf{y}[, ...]\}$
1. Result is of integer type 2. Accept an optional argument for kind type of the result	

- They can be found under different names (e.g. `dabs()`): these are relics from the past
- More functions are available to manipulate values
  - Mostly in the spirit of IEEE Floating Point Standard
  - We'll not cover them in this course, but encourage you to learn more about

`real` Higher Math

Functions	Compute
`sqrt(x)`	$\sqrt{\mathbf{x}}$
`sin(x)`, `cos(x)`, `tan(x)`, `asin(x)`, `acos(x)`, `atan(x)`	Trigonometric functions
`atan2(x, y)`	Arc tangent in $(-\pi, \pi]$
`exp(x)`, `log(x)`, `log10(x)`	$e^{\mathbf{x}}$, $\log_e \mathbf{x}$, $\log_{10} \mathbf{x}$
`sinh(x)`, `cosh(x)`, `tanh(x)`	Hyperbolic functions

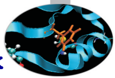
- Again, they can be found under different names (e.g. `dcos()`): these are relics from the past

`complex` Math

Functions	Compute
`abs(z)`,	$\lvert\mathbf{z}\rvert$,
`aimag(z)`	imaginary part of **`z`**,
`real(z)` [1]	real part of **`z`**
`cmplx(x,y)` [1]	converts from real to complex
`conj(z)`	Complex conjugate of **`z`**
`sqrt(z)`	$\sqrt{\mathbf{z}}$
`sin(z)`, **`cos(z)`**	sine and cosine
`exp(z)`, **`log(z)`**	$e^{\mathbf{z}}$, $\log_e \mathbf{z}$
1. Accept an optional argument for kind type of the result	

- Once again, they can be found under different names (e.g. **`cabs()`**): again, these are relics from the past

Hands-on Session #2



- The intrinsic function **`precision (x)`** for real or complex **`x`** returns the number of significant decimal digits.
- Write a **`module`** which defines the **`kind`** constant for single, double and quadruple real precision

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module real_kinds
   integer, parameter :: sp = kind(1.0)
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end module real_kinds
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- To gain confidence: write a small program to print out **`range`** and **`huge`** values for these kinds
- Something going wrong?
- GNU Fortran compiler, up to release 4.5, lacks support for the quad-precision
- If you are using, Linux load the GNU compiler version 4.6 and try again:
  `module load gcc`

Let's Be *Generic*

- Use the **`real_kinds`** module to rewrite **`dsp`** module functions to support both single and double precision
- And make all of them generic procedures
- Modify your test program to see exercise the new **`dsp`** module

Outline

More Flow Control

Fortran Intrinsic Types, Variables and Math
- Integer Types
- Floating Types
- Expressions
- Arithmetic Conversions
- More Intrinsic Types

Arrays

Arithmetic Expressions and Assignment

- Binary operators `+`, `-`, `*` (multiplication) and `/` have the usual meaning and behavior
- And so do unary operators – and `+`
- Precedence
  - `-a*b + c/d` same as `((-a)*b) + (c/d)`
  - `-a + b` same as `(-a) + b`
- Associativity of binary ones is from left to right
  - `a + b + c` same as `(a + b) + c`
  - `a*b/c*d` same as `((a*b)/c)*d`
- Explicit `(` and `)` override precedence and associativity
- `**` is the exponentiation operator
- Assignment: `=`
  - Assigns the value of expression on right hand side to a variable on the left hand side
  - Prior to first assignment, a variable content is *undefined*

Hitting Limits

- All types are limited in range
- What about:
  - `huge(0) + 1`? (too big)
  - `-huge(0.0)*3.0`? (too negative)
- Technically speaking, this is an arithmetic *overflow*
- And division by zero is a problem too
- For integer types, the Standard says:
  - behavior and results are unpredictable
  - i.e. up to the implementation
- For real types, it also depends on the floating point environment
  - i.e. how behavior is configured for those cases
  - you could get `-huge(0.0)`, or a `NaN`, or `-Inf`
- Best practice: NEVER rely on behaviors observed with a specific architecture and/or compiler

Order of Subexpressions Evaluation

- Just imagine both functions **`foo(x,y)`** and **`bar(x,y)`** modify their actual arguments, or do I/O

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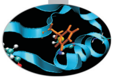

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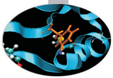

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- Ditto for order of evaluation of function arguments!
- NEVER! NEVER write code that relies on order of evaluation of subexpressions, or actual arguments!

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    ```
    a = b*2 + 1_i8
    ```
    multiplication will overflow too
  - while:

    ```
    a = b*2_i8 + 1
    ```
    is OK

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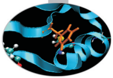

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- A 32 bits **`real`** has fewer digits of precision than a 32 bits **`integer`**
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- The result of a conversion could actually be smaller than expected!

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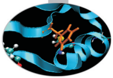
  - Only convert values, not type of variables you assign to
- Do not abuse them
  - Make codes unreadable
  - Could be evidence of design mistakes
  - Or that your Fortran needs a refresh

Outline

Being `logical`



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SCAI SuperComputing Applications and Innovation

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  - `==` (equal), `/=` (not equal), `>`, `<`, `>=`, `<=`
  - or, in ancient Fortran, `.eq.`, `.ne.`, `.gt.`, `.lt.`, `.ge.`, `.le.`
- Logical expressions
  - `.not.` is unary NOT, `.and.` and `.or.` are binary AND and OR respectively, `.eqv.` is logical equivalence (`.true.` if operands both `.true.` or both `.false.`)
  - `.not. a .and. b .or. a .and. .not. b` means `((.not.a).and.b).or.(a.and.(.not.b))`
  - In doubt, add parentheses, but be sober

More Logic

- Logical friends from **`ieee_arithmetic`** module (simply **`use`** it)
  - **`ieee_is_finite(`*`x`*`)`**: **`.true.`** if argument value is finite
  - **`ieee_is_nan(`*`x`*`)`**: **`.true.`** if argument value is **`NaN`**
  - **`ieee_unordered(`*`x`*`, `*`y`*`)`**: **`.true.`** if at least one among ***x*** and ***y*** is **`NaN`**

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  - `ieee_is_finite(x)`: `.true.` if argument value is finite
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- As usual, order of subexpressions evaluation is implementation dependent

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- As usual, order of subexpressions evaluation is implementation dependent
- But it's worse:
  - if **`test()`** is a function returning a logical type value
  - and **`a`** is **`.true.`**
  - and **`b`** is **`.false.`**
  - implementation is free (but not forced!) to not call **`test()`** at all in **`a.or.test(x)`** and **`b.and.test(x)`**
  - Again, do not rely on expressions side effects

character

- Fortran is not that good at manipulating text
- But it has some **`character`**:
  - **`character :: c`** defines a variable holding a single character, like **`'f'`**
  - **`character(len=80) :: s1, s2, s3`** defines three variables holding strings of up to 80 characters, like **`'Fortran 2003'`**
- There are character expressions, like:
  - **`s3(1:40) = s1(1:20)//s2(21:40)`**
    which assigns to first half of **`s3`** the first quarter of **`s1`** and second quarter of **`s2`**
- On assignment of a character expression to a longer variable, blank filling will take place
- On assignment of a character expression to a shorter variable, truncation will happen

String Manipulation

Function	Returns
`len(s)`	string length
`len_trim(s)`	string length with trailing blanks ignored
`trim(s)`	string with trailing blanks removed
`repeat(s, n)`	string made of **n** copies of **s**
`adjustl(s)`	move leading blanks to trailing position
`adjustr(s)`	move trailing blanks to leading position
`lge(s1,s2)`, `lgt(s1,s2)`, `lle(s1,s2)`, `llt(s1,s2)`	string comparisons
`index(s,subs)`	starting position of **subs** in **s**, 0 if not found
`scan(s,set)`	first position in **s** of a character matching **set**, 0 if none found
`verify(s,set)`	first position in **s** of a character not matching **set**, 0 if all match
`achar(i)`	character with ASCII code **i**
`iachar(c)`	ASCII code of character **c**

- Our advice:
  - For most practical purposes, use I/O statements to manipulate strings as internal files (more on this later)
  - If you are really serious about textual data, learn more
  - Or switch to a different language

Outline

More Flow Control

Fortran Intrinsic Types, Variables and Math

Arrays
- Smoothing Signals
- A More Compact Notation

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In Place Smoothing of a Periodic Signal

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module smoothing
  implicit none
contains
  subroutine smooth(v, k)
    real,intent(inout) :: v(:)
    integer,intent(in) :: k
    integer  :: n, l, i, j
    real :: work(size(v))

    n=size(v)
    l = 2*k +1
    work = 0.0
    do i=1,n
       do j=i-k,i+k
          work(i) = work(i) + v(1+mod(n-1+j, n))
       enddo
    enddo
    v = work/l
  end subroutine smooth
end module smoothing

program test_smooth
  use smoothing
  implicit none
  integer, parameter :: n=10
  integer :: i, k
  real    :: x(n)

  k = 2
  x = (/ (real(mod(i,n/2)), i=1,n) /)
  if ( k > n) stop 'More smoothing points than array elements'
  call smooth(x,k)
  write(*,*) x
end program test_smooth
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```

Subroutines

- Subroutines are procedures, like functions, except they do not return any value
- They are invoked by:
  `call subroutine-name(argument-list)`
- Like functions, they have *dummy* arguments that will be associated to *actual* arguments at call time
- Unlike functions, they can not be used inside expressions
- Their use is to be preferred to functions when:
  - actual arguments must be modified
  - more than one result needs to be returned

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Arrays

- **`real :: x(n)`**
  - Declares an array named **`x`**
  - A collection of variables of the same type (elements), laid out contiguously in memory
  - **`i`**-th element can be accessed with **`x(i)`**
  - **`n`** must be an integer expression whose value must be known at declaration time

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- What's that **`x = (/.../)`** ?
  - **`(/.../)`** is an array constructor
  - I.e. a sequence of values forming an array
  - Assigned to array in a single statement
  - **`(`*`expression`*`, `*`index`*`=`*`initial`*`, `*`final`*`)`** evaluates ***`expression`*** for each value of ***`index`*** as in a do-loop (hence is termed *implied do-loop*)

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Subroutines and Arrays

- Arrays can be passed as arguments to procedures
- How can subroutine *smooth* know the size of the actual argument passed as **`v`**?
  - **`real :: v(:)`** states that size of **`v`** will be that of the actual argument
  - **`v`** is termed an *assumed-shape* array
  - This only works if the subroutine has explicit interface
- Otherwise, you can still use the good ol' way:

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subroutine smooth(v,k,n)
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```
subroutine smooth(v,k,n)
  integer n
  real v(n)
  ...
```

- How can subroutine *smooth* declare a local array matching in size the actual argument?
  - **size(v)** returns the number of elements (size) of **v**
  - **real :: work(size(v))** gives **work** same size as **v**
  - **work** is termed an *automatic object*

WARNING: NO BOUNDS CHECKING!

- In Fortran, there is no bounds checking on array access
- And it is possible for something like this to happen

```
real :: a(10)
...
do i=-100,100
  a(i) = i
end do
```

- If you are lucky, you'll get a runtime error, otherwise you'll corrupt surrounding memory areas, with really puzzling behavior
- Once upon a long ago, it used to be a 'feature':

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subroutine smooth(v,k,n)
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- Use compiler options to enable runtime detection of out of bounds accesses
  - But execution is incredibly slowed down
  - Just a debugging tool, do not use it in production

Hands-on Session #3

- The intrinsic subroutine **cpu_time()** is used to time code regions

```
real :: t1, t2
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call cpu_time(t1)
  ...                   ! code to be timed
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- Yes: once **`work(1)`** is computed, we can compute

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work(2) = work(1)+v(1+mod(n+k, n))-v(1+mod(n-1-k, n))
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  and so on

SCAI SuperComputing Applications and Innovation

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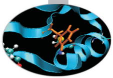

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  and so on
- Try it now!

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Same Smoothing in a Different Idiom

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module smoothing
  implicit none
contains

  subroutine smoothinplace(v, k)
    implicit none
    real,intent(inout) :: v(:)
    integer,intent(in) :: k
    real               :: work(-k+1:size(v)+k)
    integer :: i, j, l, n

    n=size(v)
    l = 2*k +1
    work(1:n) = v
    work(-k+1:0) = v(n-k+1:n)
    work(n+1:n+k) = v(1:k)

    do j=1, k
      v = v + work(1-j:n-j) + work(1+j:n+j)
    end do
    v = v/l

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SuperComputing Applications and Innovation

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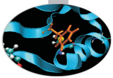

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    `work(n+1:n+k)` selects...
- Arrays and array sections are assigned to by = in a natural manner (more on this later)

Same Smoothing in a Different Idiom

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  implicit none
contains

  subroutine smoothinplace(v, k)
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    real,intent(inout) :: v(:)
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    v = v/l

  end subroutine smoothinplace

end module smoothing
```

Array Expressions

- Arrays and array sections may be
  - referenced and used in expressions
  - passed as arguments to procedures

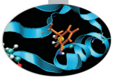
```
do j=1, k
  v = v + work(1-j:n-j) + work(1+j:n+j)
end do
```

- Without array expressions, this code would look like:

```
do j=1, k
  do i=1, n
    v(i) = v(i) + work(i-j) + work(i+j)
  end do
end do
```

- In an array expression, result must not depend in any way on the order of evaluation of elements
- You should think of array expressions as if all elements were computed at the same time

In Good Shape

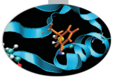


- The size of a one-dimensional array is its *shape*
- Arithmetic operators act on arrays element by element
- Binary operators combine pairs of corresponding elements from the operands
- With binary operators and assignments, you must use *conformable*, i.e. identically shaped, arrays
- Except for scalar values (not variables!), that match any shape, as if they were replicated

```
real, dimension(4) :: u, v, w
real :: t(1), s
t = s ! it's right
s = t ! it's wrong
w = (u-v)**2 ! it's right
w = s*u+v+2.3 ! it's OK
w = u+v(1:2)  ! it's wrong
```

- By the way, **`dimension`** attribute lets you specify bounds and dimensions for a list of identical arrays

Hands-on Session #4: RNG



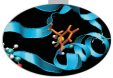
- Intrinsic subroutine **`random_number(x)`** returns pseudo-random numbers uniformly distributed in $[0, 1)$ interval
  - Takes an argument of type **`real`**, that can be either a scalar or an array
  - Returns one random number if ***x*** is a scalar
  - Returns an array of random numbers if ***x*** is an array
- Is **`random_number()`** as uniform as advertised? Let's check...

Let's Build An Histogram

- Write a program that:
  1. reads an integer **`niter`** from standard input
  2. generates **`niter`** random numbers in interval $[0, 10)$
  3. builds an histogram and computes their average
  4. Prints out results

- To build the histogram:
  1. Initialize to 0s an array **`hist`** of 20 **`integer`**s to hold the bin count, then, at each iteration:
  2. generate a random number
  3. find out the bin it belongs to (i.e. its index in the array **`hist`**)
  4. intrinsic **`ceiling(x)`** function helps: it returns $\lceil \mathbf{x} \rceil$
  5. increment the corresponding array element and compute the percentages
  6. accumulate the sum of the random numbers to compute the average value

Hands-on Session #5



- A prime number is a natural number which has only two distinct natural divisors: 1 and itself
- Find all primes less than or equal to a given n by Eratosthenes' algorithm:
  1. create a list of consecutive integers from 2 to n
  2. let be $p \leftarrow 2$ the first prime
  3. strike from the list all multiples of p up to n
  4. let $p \leftarrow$ next number still in the list after p
  5. if $2p < n$, get back to step 3
  6. all remaining numbers in the list are primes

  Try it now!

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  Try it now!

- How could you spare iterations?
- How could you spare memory?

Part III

Array Syntax and I/O

Multidimensional arrays, array-syntax, array-value function, temporary array, shape, data, reshape, constant array and elemental procedure. Costructs where, forall, array reduction. Advanced I/O: formats and descriptors, I/O to/from file, namelist, internal file, unformatted I/O, positioning instructions, stream access. Managing errors.

Outline

- Array Syntax
  - More dimensions
  - Not a Panacea
  - Arrays of Constants
  - Elemental Procedures
  - More Array Syntax
- Input/Output

Outline

Matrix Averaging

```
function avgk(v, k)

  implicit none

  real,intent(in) :: v(:,:)
  integer,intent(in) :: k
  real :: avgk(size(v,1)/k,size(v,2)/k)

  integer  :: i, j, n, m

  n = (size(v,1)/k)*k
  m = (size(v,2)/k)*k

  avgk = 0.0

  do j=1, k
    do i=1, k
      avgk = avgk + v(i:n:k,j:m:k)
    end do
  end do

  avgk = avgk/k**2

end function avgk
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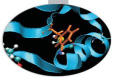
More Dimensions



- Arrays may have up to 7 dimensions
- Lower bounds default to 1, but you can specify them as for one-dimensional arrays, like in **`q(-k:k,11:20)`**
- Elements are referenced by a list of indices: **`v(1,1)`**
- The sequence of extents of an array is termed its *shape*, e.g. if **`a`** is **`real :: a(3,2:5)`** then:
  - **`shape(a)`** returns the array of extents **`(/3,4/)`**
  - whereas **`size(a)`** returns **`12`**
- Multidimensional (i.e. rank>1) arrays and array sections may be involved in array expressions
- As in the case of rank 1 arrays, they must be conformable when needed:
  `avgk(1:3,:) = avgk(5:9,:)` is wrong

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Array-Valued Functions

- Yes, a function may return an array
  - And can be used in array expressions
  - Its type is defined like any automatic object
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- An explicit interface is mandatory in the calling program
- **`size(`*`array,dim`*`)`** returns the integer extent of ***`array`*** along dimension ***`dim`***
- Number of dimensions (a.k.a. rank) is mandatory in assumed shape arrays

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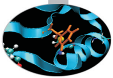
Pay Attention to Conformability



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- Compile time detection of non conformable operands only works in a few cases
- Again, use compiler options for runtime bounds checking
- Again, very slow, only tolerable in debugging

Lower-Triangular Linear System

- Good ol' style:

```
do i=1,n
  x(i) = b(i) / a(i,i)
  do j=i+1,n
    b(j) = b(j) - A(j,i)*x(i)
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enddo
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- In modern idiom:

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- What happens for **`i==n`**?
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  - No operation is performed

Picking Up Array Elements

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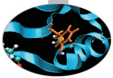

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  - and `size(b)` returns 10

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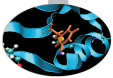
- Array syntax can be very compact and elegant
- But temporary copies may impact performance, use your compiler options to spot them

Outline

Trace



```
function trace(matrix)
implicit none
real, intent(in) :: matrix(:,:)
real :: trace
integer :: i
integer :: dim(2)

dim = shape(matrix)
trace = 0.0
if (dim(1) /= dim(2)) return

do i=1,dim(1)
   trace = trace + matrix(i,i)
enddo
end function trace
```

- Not all operations on arrays can easily be expressed in array syntax
- Do you remember `shape()`? It returns an array whose elements are the extents of its argument

Optimized Array Smoothing

```
subroutine smooth(v, k)
  implicit none
  real,intent(inout) :: v(:)
  integer,intent(in) :: k
  integer  :: n, l, i, j
  real :: work(size(v))

  n=size(v)
  l = 2*k +1
  work(1) = 0.0
  do j=1-k,1+k
    work(1) = work(1) + v(1+mod(n-1+j, n))
  enddo
  do i=2,n
    work(i)=work(i-1)+v(1+mod(n-1+i+k, n))-v(1+mod(n-2+i-k, n))
  enddo
  v = work/l
end subroutine smooth
```

- The above code does the smoothing with minimal operations count
- And cannot be expressed at all in array syntax
- This is a quite common situation: optimal algorithms operating on arrays often sports dependencies in elements evaluations and updates

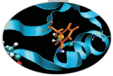
Outline

Array Syntax

- More dimensions
- Not a Panacea
- Arrays of Constants
- Elemental Procedures
- More Array Syntax

Input/Output

Tables of Coefficients



```
! Polinomial approximation of J0(x) for -3<=x<=3
! See Abramowitz&Stegun for details

function j0(x)
  implicit none
  real :: j0
  real, intent(in) :: x

  integer, parameter :: order = 6
  real, parameter, dimension(0:order) :: coeff = &
    (/ 1.0000000, &
      -2.2499997, &
       1.2656208, &
      -0.3163866, &
       0.0444479, &
      -0.0039444, &
       0.0002100 /)
  real :: xo3sq
  integer :: i

  xo3sq = (x/3.0)**2
  j0 = coeff(order)

! horner method
  do i=order, 1, -1
    j0 = j0*xo3sq + coeff(i-1)
  end do
end function j0
```

`parameter` Arrays

- **`parameter`** arrays are very good at storing tables of:
  - polynomial coefficients
  - physical measurements
  - function values at discrete points

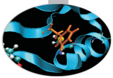
- In the past, **`data`** statements were used:

```
data coeff /1.0,-2.2499997,1.2656208,-0.3163866, &
            0.0444479,-0.0039444,0.0002100/
```

- **`data`** statements:
  - are very versatile
  - very difficult to decipher
  - and tend to float away from variable declaration
- Use initialization instead

Outline

Arrays Swap



```
program array_swap

  implicit none
  integer :: i, j
  real    :: a(0:10,10), b(11,10)









  a=reshape( (/ (i*0.1, i=1,110) /), (/11,10/) )
  b=reshape( (/ ((i*j+i, i=1,11), j=1,10) /), (/11,10/) )
  call swap(a,b)

end program array_swap


subroutine swap(a,b)

  implicit none

  real, intent(inout) :: a(:,:),b(:,:)
  real, dimension(size(a,1),size(a,2)) :: tmp

  tmp = a
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SuperComputing Applications and Innovation

Arrays Swap

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- **`reshape(`*`source`*`,`*`new_shape`*`)`** returns an array with shape given by the rank one integer array ***`new_shape`***, and elements taken from ***`source`*** in array element order

Arrays Swap

```
program array_swap

  implicit none
  integer :: i, j
  real    :: a(0:10,10), b(11,10)

  interface
    subroutine swap(a,b)
      real, intent(inout)        :: a(:,:), b(:,:)
      real, dimension(size(a,1),size(a,2))  :: tmp
    end subroutine swap
  end interface


  a=reshape( (/ (i*0.1, i=1,110) /), (/11,10/) )
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- But life can be simpler...

Elemental Arrays Swap

```
program array_swap
  implicit none
  integer :: i, j
  real    :: a(0:10,10), b(11,10)

  interface
    elemental subroutine swap(a,b)
      real, intent(inout)  :: a, b
      real                 :: tmp
    end subroutine swap
  end interface

a = reshape( (/ (i*0.1, i=1,110) /), (/11,10/) )
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```

Elemental Procedures

- Elemental procedures are applied element-wise to arrays (like most intrinsic arithmetic operators and mathematical functions)

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  - If a function, it shall not have side effects of sort (not even **`stop`**!)
  - If a subroutine, side effects shall be restricted to **`intent(out)`** and **`intent(inout)`** arguments
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  - And some more constraints ensure the different procedure calls can be safely executed in any order
- An explicit interface is mandatory
  - It must specify the procedure as **`elemental`**
  - It must specify **`intent()`** attribute for all arguments

Outline

- Array Syntax
  - More dimensions
  - Not a Panacea
  - Arrays of Constants
  - Elemental Procedures
  - More Array Syntax
- Input/Output

Masks and `where`

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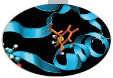

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- **where** constructs can be nested and given a name

Say it With `forall`s

- `forall` allows writing array assignments which cannot be expressed with array expressions:

```
forall(i = 1:n) a(i,i) = x(i)**2
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forall(i = 1:n, j = 1:n, y(i,j)/=0.) x(j,i) = 1.0/y(i,j)
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- In its construct form, it looks like:

```
forall(i = 2:n-1, j = 2:n-1)
  a(i,j) = a(i,j-1) + a(i,j+1) + a(i-1,j) + a(i+1,j)
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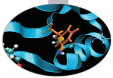

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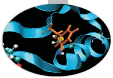

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Laplace Equation in Three Idioms

- Using `do` loops (dependencies! loop order is crucial)

```
do j=2,n-1
  do i=2,n-1
    T(i,j) = ( T(i-1,j) + T(i+1,j) + &
                           T(i,j-1) + T(i,j+1) )/4.0
  enddo
enddo
```

Laplace Equation in Three Idioms

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  do i=2,n-1
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  enddo
enddo
```

- Using array syntax (compiler enforces correct semantics)

```
T(2:n-1,2:n-1) = ( T(1:n-2,2:n-1) + T(3:n,2:n-1) &
                     + T(2:n-1,1:n-2) + T(2:n-1,3:n) )/4.0
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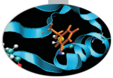
                     + T(2:n-1,1:n-2) + T(2:n-1,3:n) )/4.0
```

- Using **forall** (ditto, but more readable)

```
forall (i=2:n-1, j=2:n-1)
  T(i,j) = ( T(i-1,j) + T(i+1,j) + &
                       T(i,j-1) + T(i,j+1) )/4.0
end forall
```

Bilateral Filter



```
integer, parameter :: maxn=768, maxm=939, R=3
real, parameter :: sd=10.0, sr=10.0
real, parameter :: sd22=2.0*sd**2, sr22=2.0*sr**2
integer :: i,j,m,n
real :: B(maxn,maxm), A(maxn,maxm)
real :: zsum,z
real, dimension(-R:R,-R:R), parameter :: z0=&
   reshape((/ ((exp(-(m**2 + n**2)/sr22), m=-R, R), n=-R,R) /), (/ 2*R+1, 2*R+1 /))
...
B =0.0
do i=1,maxn
  do j=1,maxm
    zsum = 0.0
    do m= -R,R
      if (i+m >= 1 .and. i+m <= maxn) then
        do n = -R,R
          if(j+n >= 1 .and. j+n <= maxm) then
            z = exp(-(A(i+m,j+n)-A(i,j))**2/sd22)*z0(m,n)
            zsum = zsum + z
            B(i,j) = B(i,j) + z*A(i+m,j+n)
          end if
        end do
      end if
    end do
    B(i,j) = B(i,j)/zsum
  end do
end do
```

Bilateral Filter Using `forall`

```
integer, parameter :: maxn=768, maxm=939, R=3
real, parameter :: sd=10.0, sr=10.0
real, parameter :: sd22=2.0*sd**2, sr22=2.0*sr**2
integer :: i,j,m,n
real :: B(maxn,maxm), A(maxn,maxm)
real :: z(-R:R,-R:R), aw(-R:R,-R:R)
real, dimension(-R:R,-R:R), parameter :: z0=&
   reshape((/ ((exp(-(m**2 + n**2)/sr22), m=-R, R), n=-R,R) /), (/ 2*R+1, 2*R+1 /))
...
do i=1,maxn          ! These two cannot be changed into forall
  do j=1,maxm        ! Why?
    z = 0.0
    forall (m=max(1,i-R):min(maxn,i+R))
      forall (n=max(1,j-R):min(maxm,j+R))
        aw(m-i,n-j) = A(m,n)
        z(m-i,n-j) = exp(-(aw(m-i,n-j)-A(i,j))**2/sd22)*z0(m-i,n-j)
      end forall
    end forall
    B(i,j) = sum(z*aw)/sum(z)
  end do
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```

Bilateral Filter Using **forall**

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...
do i=1,maxn        ! These two cannot be changed into forall
  do j=1,maxm      ! Why?
    z = 0.0        ! Because this happens at every iteration, it's a dependency!
    forall (m=max(1,i-R):min(maxn,i+R))
      forall (n=max(1,j-R):min(maxm,j+R))
        aw(m-i,n-j) = A(m,n)
        z(m-i,n-j) = exp(-(aw(m-i,n-j)-A(i,j))**2/sd22)*z0(m-i,n-j)
      end forall
    end forall
    B(i,j) = sum(z*aw)/sum(z)
  end do
end do
```

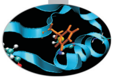
Array Reductions

- Reductions squeeze an array to a scalar
  - `all(mask)` returns true if all the elements of mask are true
  - `any(mask)` returns true if any of the elements of mask are true
  - `count(mask)` returns the number of `.true.` elements in mask
  - `maxval(array)` returns the maximum value of array
  - `minval(array)` returns the minimum value of array
  - `sum(array)` returns the sum of the elements of array
  - `product(array)` returns the product of the elements of array
- Or to an array of rank reduced by one, if you specify an optional dimension to perform reduction along, like in `sum(a(:,:,:), dim=2)`

More Array Little Helpers

- More functions, good to know:
  - **`maxloc()`** and **`minloc()`** return locations of maximum and minimum value respectively
  - **`cshift()`** performs a *circular* shift along an array dimension
  - **`eoshift()`** perform a *end-off* shift along an array dimension
  - **`spread()`** increases by one the rank of an array expression
  - **`pack()`** selects elements from an array according to a mask and packs them in a rank-1 array
  - And **`unpack()`** does the reverse
- But too much detail to cover in this introduction, look for them on your compiler documentation, and experiment

Matrix Algebra



- Vector and matrix multiplication functions
  - `dot_product(vector_a, vector_b)`
  - `matmul(matrix_a, matrix_b)`
- But the BLAS libraries are around
  - Widely used
  - Highly optimized implementations available
- Outstanding compilers include special purpose, optimized BLAS version for those calls
- Good compilers do not include BLAS, but give option to link them for those calls
- Average compilers do not shine for those calls
- Our advice: install a reputably good BLAS version and use it
- There is more to matrix algebra than matrix multiplies and vector products

SCAI SuperComputing Applications and Innovation

Hands-on Session #1

- Re-write the Sieve of Eratosthenes algorithm using array syntax

Outline

Array Syntax

Input/Output

- Formatted I/O
- File I/O
- Namelist
- Internal Files
- Unformatted I/O
- Robust I/O

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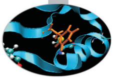
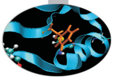
Formatted I/O



- Data are manipulated in internal (usually binary) format
- Fortran Standard leaves internal format details up to the implementation
- Formatted I/O translates internal representation of variables into human readable format
- Best practices:
  - Use formatted I/O just for small amount of data meant to be read by humans
  - Beware: human readable representation may cause problems because of rounding or not enough digits
  - Do not use I/O inside heavy computations: inhibits some code optimizations, and significantly affects performance

Iterative search for the Golden Ratio



```
program golden_ratio
! experiments with the golden ratio iterative relation
  implicit none
  integer, parameter :: rk = kind(1.0d0)
  real(rk) :: phi, phi_old
  real(rk) :: phi_start, tol
  integer :: i, max_iter

  write(*,*) 'Enter start value, tol, max iterations'
  read(*,*) phi_start, tol, max_iter

  phi_old = phi_start
  do i=1,max_iter
    phi = 1.0d0/phi_old + 1.0d0
    if (abs(phi - phi_old) < tol) exit
    phi_old = phi
  end do

  write(*,100) 'Start value:',phi_start
  write(*,100) 'Tolerance:',tol
  write(*,'(2(A," ",I11,"  "))') 'Ended at iteration:', i, 'of', max_iter
  write(*,100) 'Final value:',phi

100 format(A," ",F13.10)
end program golden_ratio
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Iterative search for the Golden Ratio

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```
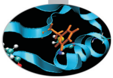

CINECA

List Directed I/O



- The easiest way to do formatted I/O
- Specified using *
- Values are translated according to their types
- In the order they are listed on I/O statements
- No-nonsense, implementation dependent format
- Often outputs more digits than you actually care of
- Best practices:
  - Use it for terminal input
  - Use it for input of white-space separated values
  - Use it for quick output
  - Not suitable for rigid tabular formats

Explicit formats

- Put you in total control of what is read/written

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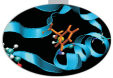
Explicit **`formats`**



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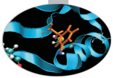

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  - Like in **`5I3`**, which will convert 5 **`integer`** values
  - Like in **`2(I3,F7.4)`**, which will convert 2 pairs, each made of an **`integer`** and a **`real`** value

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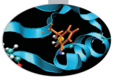
Explicit **`format`s**



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  - Like in **`2(I3,F7.4)`**, which will convert 2 pairs, each made of an **`integer`** and a **`real`** value
- Formats must be specified on I/O statements
  - As a literal string, usually in single quotes
  - As a character expression
  - As a numeric label of a **`format`** statement in the same program unit (traditionally, before its end), reusable in many statements

Edit Descriptors: `characters` and `integers`

- `A` is used to translate `character` values
  - `A` will emit the value as is
  - `A10` will emit 10 characters, truncating the value if longer, right justifying it if shorter
  - Beware: leading white-space skipped on input
  - Beware: `A10` and `10A` mean very different things!

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  - Beware: **`A10`** and **`10A`** mean very different things!
- **`I`** is used to translate **`integer`** values
  - **`I6`** will emit up to 6 characters (sign included!), right justified with blanks
  - **`I6.3`** will emit 6 characters (sign included!), containing at least 3 (possibly zero) digits, right justified with blanks
  - Beware: again, **`I10`** and **`10I`** mean very different things!

Edit Descriptors: `reals`

- **`F`** can be used to translate **`real`** values
  - **`F8.3`** will emit up to 8 characters (sign and decimal point included!) in total, with 3 decimal digits (possibly zero), right justified with blanks
  - Beware: if **`F6.2`** is specified in input, and **`-12345`** is met, the value -123.45 will be read in!
  - Beware: if **`F6.2`** is specified in input, and **`-1.234`** is met, the value -1.234 will be read in anyhow!
- Beware of rounding: internal representation could have more precision than specified in edit descriptors

More Edit Descriptors for `reals`

- **`E`** (or **`D`**) can also be used to translate **`real`** values
  - Exponential form is used (mantissa in the [0,1) range)
  - Values $|x| < 10^{99}$, as -1.5372×10^{98}, will be converted like: **`-.15372E+99`**
  - Values $|x| \geq 10^{99}$, as -1.5372×10^{99}, will be converted like: **`-.15372+100`**
  - **`E15.7`** will emit up to 15 characters (sign, decimal point, and exponent field included!), with 7 decimal mantissa digits (possibly zero), right justified with blanks
  - Ditto for **`E15.7E4`**, except that 4 digits will be used for exponent
  - Again, input is more liberal

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  - Ditto for **E15.7E4**, except that 4 digits will be used for exponent
  - Again, input is more liberal
- And more can be used to the same purpose
  - Like **EN** (engineering notation), same as **E**, with exponent always multiple of 3
  - Like **G**, which uses the most suitable between **F** and **E**, depending on the value magnitude

Even More Edit Descriptors

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  - Forces a new line on output
  - Skips to next line on input

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  - **SP** forces following numeric conversions to emit a leading **+** character for positive values
  - **SS** restores the default (sign is suppressed for positive values)

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- And more... browse your compiler manuals

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  - First one for real part, second one for imaginary part
- Arrays are indexed collections of elements
  - Thus a proper edit descriptor must be provided for each element
  - And if elements are of `complex`, or derived types, see above

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Iterative Matrix Inversion

```
program iterative_inversion
! experiments with matrix iterative inversion
  implicit none
  real, dimension(4,4) :: a, x, x_old, x_start
  real :: tol, err
  integer :: i, max_iter

  write(*,*) 'Enter 4x4 matrix to invert'
  read(*,*) a
  write(*,*) 'Enter 4x4 start matrix'
  read(*,*) x_start
  write(*,*) 'Enter tol, max iterations'
  read(*,*) tol, max_iter

  x_old = x_start
  do i=1,max_iter
    x = 2.0*x_old - matmul(x_old,matmul(a,x_old))
    err = maxval(abs(x - x_old))
    if (err < tol) exit
    x_old = x
  end do

  write(*,'("Matrix to invert:")')
  write(*,100) a
  write(*,'(/,"Start matrix:")')
  write(*,100) x_start
  write(*,'(/,A," ",E15.7)') 'Tolerance:',tol
  write(*,'(/,2(A," ",I11,"  "))') 'Ended at iteration:', i, 'of', max_iter
  write(*,'("Final matrix:")')
  write(*,100) x

100 format(4(E15.7," "))
end program iterative_inversion
```

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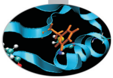

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  - The field is filled with asterisks (i.e. `*`)
- What if a type mismatch happens between an item to read/write and its corresponding edit descriptor?
  - Your fault, you are in for a runtime, implementation defined surprise!

Hands-on Session #2

- Play with `golden.f90` and `itinv.f90`:
  - trying good and bad inputs
  - giving less or more inputs than needed
  - changing format descriptors

Outline

Array Syntax

Input/Output

- Formatted I/O
- File I/O
- Namelist
- Internal Files
- Unformatted I/O
- Robust I/O

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! experiments with the golden ratio iterative relation
  implicit none
  integer, parameter :: rk = kind(1.0d0)
  real(rk) :: phi, phi_old
  real(rk) :: phi_start, tol
  integer :: i, max_iter

  open(11,FILE='golden.in',STATUS='old')
  read(11,*) phi_start, tol, max_iter
  close(11)

  phi_old = phi_start
  do i=1,max_iter
    phi = 1.0d0/phi_old + 1.0d0
    if (abs(phi - phi_old) < tol) exit
    phi_old = phi
  end do

  open(12,FILE='golden.out')
  write(12,100) 'Start value:',phi_start
  write(12,100) 'Tolerance:',tol
  write(12,'(2(A,"  ",I11,"   "))') 'Ended at iteration:', i, 'of', max_iter
  write(12,100) 'Final value:',phi
  close(12)

100 format(A," ",F13.10)
end program golden_ratio
```

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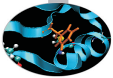

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`open`ing a File for I/O

`open(`*`u`*`,FILE=`*`file_name`*`[,`*`option`*`][,`*`option`*`][...])`

- ***u*** is an integer, positive expression specifying a *file handle*

opening a File for I/O

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- *file handle* is then used as first argument to **`read`** and **`write`**

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  - For error messages, **0** is commonly used, but **error_unit** from **iso_fortran_env** module is portable

Some **open** Options

- **ACTION=*act*** specifies allowed actions
  - use **'read'** to only read
  - use **'write'** to only write
  - use **'readwrite'** (the default) to allow both

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- **STATUS=*st*** tells how to behave wrt. file existence:
  - use **'old'** to open a file that must already exist
  - use **'new'** to open a file that must not exist
  - use **'replace'** to open a new file, even if one already exists
  - use **'unknown'** (the default) to leave it up to the implementation (in all cases we know of, this means **'replace'**)

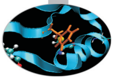
Some `open` Options

- **`ACTION=`*`act`*** specifies allowed actions
  - use **`'read'`** to only read
  - use **`'write'`** to only write
  - use **`'readwrite'`** (the default) to allow both

- **`STATUS=`*`st`*** tells how to behave wrt. file existence:
  - use **`'old'`** to open a file that must already exist
  - use **`'new'`** to open a file that must not exist
  - use **`'replace'`** to open a new file, even if one already exists
  - use **`'unknown'`** (the default) to leave it up to the implementation (in all cases we know of, this means **`'replace'`**)

- **`POSITION=`*`pos`*** tells where to start I/O on an existing file
  - use **`'rewind'`** (the default) to start at beginning of file
  - use **`'append'`** to start at end of file

Iterative search for the Golden Ratio



```
program golden_ratio
! experiments with the golden ratio iterative relation
  implicit none
  integer, parameter :: rk = kind(1.0d0)
  real(rk) :: phi, phi_old
  real(rk) :: phi_start, tol
  integer :: i, max_iter

  open(11,FILE='golden.in',STATUS='old')
  read(11,*) phi_start, tol, max_iter
  close(11)

  phi_old = phi_start
  do i=1,max_iter
    phi = 1.0d0/phi_old + 1.0d0
    if (abs(phi - phi_old) < tol) exit
    phi_old = phi
  end do

  open(12,FILE='golden.out')
  write(12,100) 'Start value:',phi_start
  write(12,100) 'Tolerance:',tol
  write(12,'(2(A," ",I11,"  "))') 'Ended at iteration:', i, 'of', max_iter
  write(12,100) 'Final value:',phi
  close(12)

100 format(A," ",F13.10)
end program golden_ratio
```

How to `close` a File

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close(u[,STATUS=st])
```

- **`close`** completes all pending I/O operations and disassociates the file from the unit

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- ***st*** tells what to do with the file after closing it
  - use **`'keep'`** to preserve the file (it's the default)
  - use **`'delete'`** to remove it (good for files used for temporary storage)

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SuperComputing Applications and Innovation

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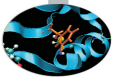

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- File content is structured, self-describing, order independent, comments are allowed:

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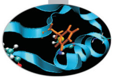

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- Items can be added to a namelist in different statements, but code like this easily misleads readers (and you read your own codes, don't you?)
- Use them to make input robust, in output mostly good for debugging

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  integer :: i, max_iter, test_no
  character(15) :: outfilename

  namelist /golden_inputs/ phi_start, tol, max_iter, test_no

  test_no = 1
  open(11,FILE='golden.in',STATUS='old')
  read(11,golden_inputs)
  close(11)

  phi_old = phi_start
  do i=1,max_iter
    phi = 1.0d0/phi_old + 1.0d0
    if (abs(phi - phi_old) < tol) exit
    phi_old = phi
  end do

  write(outfilename,'("golden",I5.5,".out")') test_no
  open(12,FILE=outfilename)
  write(12,100) 'Start value:',phi_start
  write(12,100) 'Tolerance:',tol
  write(12,'(2(A," ",I11,"  "))') 'Ended at iteration:', i, 'of', max_iter
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  - dynamically assemble complex I/O formats, depending on actual data
  - prepare complex labels for plot data formats
  - build commands to be sent to hardware devices
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  - dynamically assemble complex I/O formats, depending on actual data
  - prepare complex labels for plot data formats
  - build commands to be sent to hardware devices
  - ...

- Reading from internal files can be useful to read complex inputs
  - You have a textual input file sporting different formats
  - And the right format depends on actual data in the file
  - Just read each line in a **`character`** variable, suitably sized
  - Pick the suitable format
  - And use it to read from the variable itself

Hands-on Session #3

- Play with **`goldenfile.f90`**, **`goldenfnl.f90`**, and **`goldeniio.f90`**:
  - writing input files
  - writing good and bad data in input files
  - giving input files wrong file names

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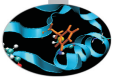
Unformatted I/O

- Formatted I/O is good, but:
  - internal data format is much more compact
  - and roundoff may happen, making recovery of original values impossible
  - and conversion takes time

Iterative Matrix Inversion



```
program iterative_inversion
! experiments with matrix iterative inversion
  implicit none
  real, dimension(4,4) :: a, x, x_old, x_start
  real :: tol, err
  integer :: i, max_iter

  open(21,FILE='input.dat',FORM='unformatted',STATUS='old')
  read(21) a
  read(21) x_start
  read(21) tol,max_iter
  close(21)

  x_old = x_start
  do i=1,max_iter
    x = 2.0*x_old - matmul(x_old,matmul(a,x_old))
    err = maxval(abs(x - x_old))
    if (err < tol) exit
    x_old = x
  end do

  open(22,FILE='itinv.dat',FORM='unformatted')
  write(22) a
  write(22) x_start
  write(22) tol,max_iter
  write(22) i
  write(22) x
  close(22)

end program iterative_inversion
```

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end program iterative_inversion
```

Unformatted I/O

- Formatted I/O is good, but:
  - internal data format is much more compact
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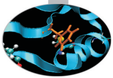
- Unformatted I/O is used to store and recover data in internal representation
  - Just give **`FORM='unformatted'`** option when opening the file
  - And omit format in **`read`** and **`write`** statements

Unformatted I/O



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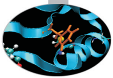
- Unformatted I/O is used to store and recover data in internal representation
  - Just give **`FORM='unformatted'`** option when opening the file
  - And omit format in **`read`** and **`write`** statements
- Unformatted I/O is performed on a *record* basis
  - In unformatted mode, each **`write`** writes a *record*
  - As we'll see, this allows walking your files backward and forward
  - But has interesting consequences, as more than your data is written to your file...

Hands-on Session #4

- Modify **`itinv.f90`** to perform unformatted I/O
- To test it, you'll need an additional program:
  - taking text input from keyboard or initializing all needed data
  - to write a good unformatted input file for the new version of **`itinv.f90`**

As you are at it...



- Try different ways to output the results:
  - element-wise

```
do j=1,n
  do i=1,n
    write(79) a(i,j)
  end do
end do
```

  - column-wise, using an implied do-loop:

```
do j=1,n
  write(79) (a(i,j), i=1,n)   ! a(:,j) will also do
end do
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  - with two implied do-loops:

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write(79) ((a(i,j), i=1,n), j=1,n)
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- Can you spot the difference?

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write(79) ((a(i,j), i=1,n), j=1,n)
```

- Can you spot the difference?
- Not a big issue for 4×4 matrices, but think of a $256 \times 256 \times 1024$ grid!

File Positioning

- **`read`** always advance to next record, even if you read only part of the record (or possibly nothing)
- **`backspace(`*`u`*`)`** moves position for subsequent I/Os to the record preceding the current one
- **`rewind(`*`u`*`)`** moves position for subsequent I/Os to file beginning
- To allow positioning back and forth, a four bytes record marker is added in 32 bit mode (eight bytes in 64 bit mode) before and after each record
- Best practice: write data in whole blocks

Fortran 2003: Stream Access I/O

- Record markers added in unformatted I/O make exchanging data with other programs (notably C ones) troublesome
- **`open(unit,...,ACCESS='stream',...)`** is a new method to access external files
- No record markers are written before or after a **`write`**
  - Thus, advancing or backspacing over records is not possible
  - But required position may be specified by:

```
write(unit,POS=position) x
read(unit,POS=position) y
```

- Best practice: if you are really serious about data exchanges, across different programs and systems, use libraries like HDF5, VTK, CGNS

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I/O Errors and Mishaps

- You may happen to:
  - Try to open a new file, when one with same name already exists
  - Look for an existing file, which is missing
  - Encounter an unexpected end of record in a **`read`**
  - Encounter an unexpected end of file while reading
  - Run out of disk space while writing
  - Try writing to a read-only file
  - ...

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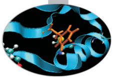
  - ...
- And get an unfriendly runtime error
- Or you may need to open a file in a library you are writing
  - And use a unit already opened in a calling program
  - The previously opened unit is automatically closed
  - With surprising consequences on program behavior

Managing I/O Errors



- All I/O statements accept an **`IOSTAT=`*`ios`*** option
  - ***`ios`*** must be an integer variable of default kind
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  - Set to negative values on end of file or record (in Fortran 2003, **`iostat_end`** and **`iostat_eor`** respectively, from **`iso_fortran_env`** module)
  - Set to positive values on error
  - Execution will not stop
- Use it to identify the issue, and recover or fail gracefully

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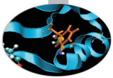

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- Use it to identify the issue, and recover or fail gracefully

- All I/O statements accept an **`ERR=`*`err-label`*** option
  - ***`err-label`*** is a statement label in the same program unit
  - Flow control jumps to ***`err-label`*** in case of error
- Use it to centralize error management and recovery
- Together with **`iostat`**, of course

In Doubt? **`inquire`**!

- Let's assume **`ans`** is a logical variable, **`k`** is an integer variable, and **`s`** is a character variable of suitable length

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- **`inquire(FILE='input.dat',EXIST=ans)`** will set **`ans`** to **`.true.`** if file **`input.dat`** exists

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- `inquire(FILE='input.dat',EXIST=ans)` will set `ans` to `.true.` if file `input.dat` exists
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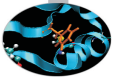
- **`inquire(15,OPENED=ans)`** will set **`ans`** to **`.true.`** if a file is already opened on unit **`15`**

In Doubt? **inquire**!



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- `inquire(FILE='input.dat',NUMBER=k)` will set **k** to **−1** if file **input.dat** is not opened, to connected unit otherwise

More Doubts? `inquire` More!

- `inquire(15,FORM=s)` will set `s` to `'FORMATTED'` or `'UNFORMATTED'` if unit 15 is connected for formatted or unformatted I/O respectively, to `'UNDEFINED'` otherwise

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- **`inquire(15,FORM=s)`** will set **`s`** to **`'FORMATTED'`** or **`'UNFORMATTED'`** if unit 15 is connected for formatted or unformatted I/O respectively, to **`'UNDEFINED'`** otherwise
- **`inquire(15,ACTION=s)`** will set **`s`** to **`'READ'`** or **`'WRITE'`** or **`'READWRITE'`**, depending on what actions are allowed on unit 15, to **`'UNDEFINED'`** if unconnected

More Doubts? **`inquire`** More!

- **`inquire(15,FORM=s)`** will set **`s`** to **`'FORMATTED'`** or **`'UNFORMATTED'`** if unit 15 is connected for formatted or unformatted I/O respectively, to **`'UNDEFINED'`** otherwise
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- **`inquire(15,FORM=s)`** will set **`s`** to **`'FORMATTED'`** or **`'UNFORMATTED'`** if unit 15 is connected for formatted or unformatted I/O respectively, to **`'UNDEFINED'`** otherwise
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- **`inquire(IOLENGTH=k)`** ***`output-list`*** will set **`k`** to the number of processor dependent units (bytes, in practice) occupied by an unformatted write of ***`output-list`***
- And many more variations, look to manuals
- Of course, **`IOSTAT`** and **`ERR`** can be useful on **`inquire`** too

Hands-on Session #5

- Write a program that:
  - reads an ‘arbitrarily’ long column of real numbers from an ASCII file
  - prints maximum, minimum, average of the numbers
  - and prints the $\lfloor n/2 \rfloor$-th row where n is the length of the column

Part IV

Derived Types and Memory Management

Derived types, operators overloading, parametric types and inheritance. Memory management, dynamic allocation and memory heap. Pointers. C and Fortran interoperability.

SuperComputing Applications and Innovation

Outline

Extending the Language

- Derived Types
- Operators Overloading
- Parameterized Types
- Extending Types, and Much More

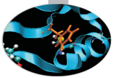
Managing Memory

Conclusions

Outline

- Extending the Language
  - Derived Types
  - Operators Overloading
  - Parameterized Types
  - Extending Types, and Much More
- Managing Memory
- Conclusions

User Defined Types



- Fortran allows programmers to add new types, built as assemblies of existing ones

```
type position
  real :: x, y, z
end type position

type velocity
  real :: x, y, z
end type velocity
```

- Components in different derived types may have the same name (not a surprise!)
- `type(position) :: r` declares a variable of type `position`
- Components of a derived type can be accessed like this: `r%y = 0.0`

Growing Types from Types

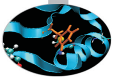
- Derived types are not second class citizens
- Thus derived types (also termed *structures*) can be assembled from other derived types too

```
type particle
  type(position) :: r
  type(velocity) :: v
  real :: mass
end type particle

type atom
  type(position) :: r
  type(velocity) :: v
  real :: mass ! In atomic units
  integer :: an ! Atomic number
end type atom
```

- `type(particle) :: p` declares a variable of type `particle`
- Components of a component of a variable can be accessed like this: `p%v%z = 0.0`

Structures In Action



```
type(atom) :: h1, h2, he

h1%r = position(0.0, 0.0, 0.0)
h1%v = velocity(1.0, -1.0, 0.0)
h1%mass = 1.00794
h1%an = 1 ! Assigns atomic number

h2 = h1 ! Intrinsic assignment

he = atom(position(1.0, 0.0, -1.0), h2%v, 4.002602, 2)
```

- Derived type name can be used to construct values of the type
- Unsurprisingly, `velocity()` is termed a *constructor*
- Values passed as argument to constructors must be ordered as in type definition
- Assignment is intrinsically available

Formatted I/O of Derived Types

- Derived types boil down (possibly recursively) to collections of intrinsic types
- And behavior is coherent with I/O of complex values and arrays
- All single intrinsic type (sub)components will be processed in sequence
- If you want control of the conversion:
  - a proper edit descriptor must be provided for each component
  - in same order as components are declared in type declaration
- Fortran 2003 introduces the `DT` edit descriptor to give users total control

Outline

Same Name, Different Personality

- Binary operator **+** can be used to add:

Same Name, Different Personality

- Binary operator **+** can be used to add:
  - a pair of integer values

Same Name, Different Personality

- Binary operator **+** can be used to add:
  - a pair of integer values
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- Binary operator **+** can be used to add:
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  - a pair of real values
  - a pair of complex values

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- Binary operator **+** can be used to add:
  - a pair of integer values
  - a pair of real values
  - a pair of complex values
  - two integer values of different kinds

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  - two integer values of different kinds
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  - two real values of different kinds
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  - an integer and a real value

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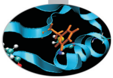

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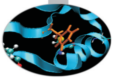

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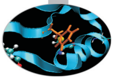
- It's like the meaning of **+** is 'overloaded'
  - Different machine code is generated depending on operand types
- And ditto for **–**, `*`, `/`, `>`, `>=`, ...

Bringing Abstractions Further



Wouldn't it be nice to have arithmetic operators work on structures?

```
interface operator(-)
  function subvel(p1, p2)
    type(velocity), intent(in) :: p1, p2
    type(velocity) :: subvel
  end function
end interface operator(-)

interface operator(-)
  function chsvel(p)
    type(velocity), intent(in) :: p
    type(velocity) :: chsvel
  end function
end interface operator(-)

function subvel(p1, p2)
  implicit none
  type(velocity), intent(in) :: p1, p2
  type(velocity) :: subvel
  subvel%x = p1%x-p2%x; subvel%y = p1%y-p2%y; subvel%z = p1%z-p2%z
end function subvel

function chsvel(p)
  implicit none
  type(velocity), intent(in) :: p
  type(velocity) :: chsvel
  chsvel%x = -p%x; chsvel%y = -p%y; chsvel%z = -p%z
end function chsvel
```

Changing Rules as We Need

- We are fitting an infinite space into a finite box with periodic boundary conditions
- Wouldn't it be nice to define our operators with custom functionality?

```
interface operator(+)
  function addpos(p1, p2)
    type(position), intent(in) :: p1, p2
    type(position) :: addpos
  end function
end interface operator(+)

function addpos(p1, p2) ! Adds positions with periodic boundary conditions
  implicit none
  type(position), intent(in) :: p1, p2
  type(position) :: addpos
  real,parameter :: boxwidth = 128.0

  addpos%x = modulo(p1%x+p2%x, boxwidth)
  addpos%y = modulo(p1%y+p2%y, boxwidth)
  addpos%z = modulo(p1%z+p2%z, boxwidth)
end function addpos
```

Operator Overloading

- **`interface operator(`*`op-name`*`)`** lets you overload *op-name* with a generic procedure
  - Arguments must be **`intent(in)`** and can be either one or two
  - *op-name* may be an intrinsic operator, or a **`.`*`new_name`*`.`**

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- Now velocities may be added as intrinsic arithmetic types
- And defining subtraction is an easy job
- Positions may be added as usual intrinsic variables and boundary conditions are automatically imposed

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- Now velocities may be added as intrinsic arithmetic types
- And defining subtraction is an easy job
- Positions may be added as usual intrinsic variables and boundary conditions are automatically imposed

- Time for a module

A Module Centered on Derived Types

```
module periodic_box
  implicit none
  real, private, parameter :: boxwidth = 128.0
  private addpos, addvel, chsvel, subvel, subpos

  type position
    real :: x, y, z
  end type position

  type velocity
    real :: x, y, z
  end type velocity

  interface operator(+)
    module procedure addpos
    module procedure addvel
  end interface operator(+)
! ...
contains
  function addpos(p1, p2) ! Adds positions with periodic boundary conditions on x
    type(position), intent(in) :: p1, p2
    type(position) :: addpos
    addpos%x = modulo(p1%x+p2%x, boxwidth)
    addpos%y = modulo(p1%y+p2%y, boxwidth)
    addpos%z = modulo(p1%z+p2%z, boxwidth)
  end function addpos

  function addvel
    !...
  end function addvel
! ...
end module periodic_box
```

Structuring Structures

- Again, modules are the best way of grouping related stuff
- Again, with modules and module procedures we don't need to write interface blocks
- Modules let us hide implementation details
- Best practice: put structure definitions and related functions and operators in modules
  - Anyway, they will be used together
  - When dealing with nested types with many related functions, a hierarchy of modules would probably help
  - Because, of course, you can `use` modules in a module

Hands-on Session #1

- Write a module that defines:
  - A new type *vector* made up of three real components
  - Operator `.cross.` for cross product
  - Operator **+** to sum two `vectors`
- Write a program to test your module

```
program test_class_vector
  use class_vector

  implicit none

  type(vector) :: v, w, z

  v=vector(1.d0,0.d0,0.d0)
  w=vector(0.d0,1.d0,0.d0)
  z=vector(0.d0,0.d0,1.d0)

  write(*,*) v+w.cross.z

end program test_class_vector
```

- Definition of cross product:

$$a \times b = (a_2 b_3 - a_3 b_2)\hat{i} + (a_3 b_1 - a_1 b_3)\hat{j} + (a_1 b_2 - a_2 b_1)\hat{k}$$

- Then extend operators to have them work with array of vectors: it's elementary!

A Possible Solution

```
module class_vector

contains

end module class_vector
```

A Possible Solution

```
module class_vector
  implicit none

contains

end module class_vector
```

A Possible Solution

```
module class_vector
  implicit none
  type vector
    real(kind(1.d0)) :: x
    real(kind(1.d0)) :: y
    real(kind(1.d0)) :: z
  end type vector










contains
















end module class_vector
```

SuperComputing Applications and Innovation

A Possible Solution

```
module class_vector
  implicit none
  type vector
    real(kind(1.d0)) :: x
    real(kind(1.d0)) :: y
    real(kind(1.d0)) :: z
  end type vector

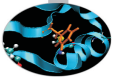
  interface operator(.cross.)
    module procedure cross_prod
  end interface

contains

  function cross_prod(a,b)
    type(vector) :: cross_prod
    type(vector), intent(in) :: a, b
    cross_prod%x = a%y * b%z - a%z * b%y
    cross_prod%y = a%z * b%x - a%x * b%z
    cross_prod%z = a%x * b%y - a%y * b%x
  end function cross_prod

end module class_vector
```

A Possible Solution



```
module class_vector
  implicit none
  type vector
    real(kind(1.d0)) :: x
    real(kind(1.d0)) :: y
    real(kind(1.d0)) :: z
  end type vector

  interface operator(.cross.)
    module procedure cross_prod
  end interface

  interface operator(+)
    module procedure vec_sum
  end interface

contains

  function cross_prod(a,b)
    type(vector) :: cross_prod
    type(vector), intent(in) :: a, b
    cross_prod%x = a%y * b%z - a%z * b%y
    cross_prod%y = a%z * b%x - a%x * b%z
    cross_prod%z = a%x * b%y - a%y * b%x
  end function cross_prod

  function vec_sum(a,b)
    type(vector) :: vec_sum
    type(vector), intent(in) :: a, b
    vec_sum%x = a%x + b%x
    vec_sum%y = a%y + b%y
    vec_sum%z = a%z + b%z
  end function vec_sum
end module class_vector
```

A Possible Solution

```
module class_vector
  implicit none
  type vector
    real(kind(1.d0)) :: x
    real(kind(1.d0)) :: y
    real(kind(1.d0)) :: z
  end type vector

  interface operator(.cross.)
    module procedure cross_prod
  end interface

  interface operator(+)
    module procedure vec_sum
  end interface

contains

  elemental function cross_prod(a,b)
    type(vector) :: cross_prod
    type(vector), intent(in) :: a, b
    cross_prod%x = a%y * b%z - a%z * b%y
    cross_prod%y = a%z * b%x - a%x * b%z
    cross_prod%z = a%x * b%y - a%y * b%x
  end function cross_prod

  elemental function vec_sum(a,b)
    type(vector) :: vec_sum
    type(vector), intent(in) :: a, b
    vec_sum%x = a%x + b%x
    vec_sum%y = a%y + b%y
    vec_sum%z = a%z + b%z
  end function vec_sum
end module class_vector
```

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- Derived Types
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- Extending Types, and Much More

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Conclusions

Making It wider

- What if we wanted different **kinds** of **points**?
- This is a possibility:

```
type point
  real( selected_real_kind(5) ) :: x, y, z
end type point

type widepoint
  real( selected_real_kind(12) ) :: x, y, z
end type widepoint
```

- But not very elegant, nor easy to manage

Fortran 2003 Adds Parameterized Types

- In Fortran 2003, types may have kind type parameters:

```
type point(point_kind)
  integer, kind :: point_kind = kind(0.0)
  real(point_kind) :: x, y, z
end type point

type(point(point_kind=kind(0.0))) :: apoint
type(point) :: anotherpoint
type(point(selected_real_kind(12))) :: awiderpoint
```

- **kind** states that this type parameter behaves as a kind
- And it works as **kind** does for intrinsic types

More Derived Type Parameters

- Structures may have array components

```
type segments(point_kind)
  integer, kind :: point_kind = kind(0.0)
  type(point(point_kind)), dimension(100) :: start_point
  type(point(point_kind)), dimension(100) :: end_point
end type segments
```

- Our **`segments`** type looks a bit rigid, doesn't it?
- Derived type parameters come to rescue:

```
type segments(point_kind, n)
  integer, kind :: point_kind = kind(0.0)
  integer, len :: n
  type(point(point_kind)), dimension(n) :: start_point
  type(point(point_kind)), dimension(n) :: end_point
end type segments

type(segments(n=100)) :: ahundredsegments
type(segments(n=1000)) :: athousandsegments
```

- Warning: compilers support still lags behind, your mileage may vary

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Objects

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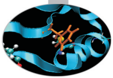
Objects



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  - But they are conceptually (and dimensionally!) different things
- And **`particle`**, and **`atom`** share identical components
  - And a **`ion`** would simply add a **`charge`** component
- Wouldn't it be nice to 'inherit' from one type to another?
  - Yeah, and easier to manage, too!
  - And this is what CS priests call *Object-Oriented* programming, and is so trendy!

Fortran 2003 **extends** Derived Types

```
type point
  real :: x, y, z
end type point

type, extends(point) :: position
end type position

type, extends(point) :: velocity
end type velocity

type  particle
  type(position) :: r
  type(velocity) :: v
  real :: mass
end type particle

type, extends(particle) :: atom
  integer :: an ! atomic number
end type atom

type, extends(atom) :: ion
  integer :: charge ! in units of elementary charge
end type ion
```

- **extends** means that the new type has the same components, and possibly more
- Now we still have to write procedures and operators, don't we?

Fortran 2003 Object Oriented Full Glory

- Fortran 2003 adds *type bound procedures* (a.k.a. *methods* in OO jargon)
  - Which are sorts of ’code components’ of a type
  - And are inherited when it is extended

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- Unfortunately (or maybe fortunately) we'll not cover this stuff, because:
  - compilers support lags way behind
  - and OO programming is not that easy
  - get your type hierarchy wrong, and you'll bitterly regret
- OO programming is not a matter of good coding, but of thoughtful and thorough design

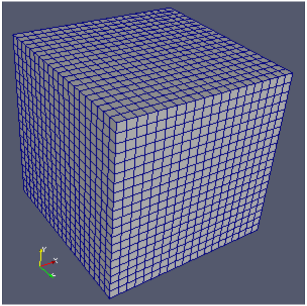
Outline

Extending the Language

Managing Memory
- Dynamic Memory Allocation
- Fortran Pointers
- Bridging the Gap with C
- Sketchy Ideas on Data Structures

Conclusions

A PDE Problem



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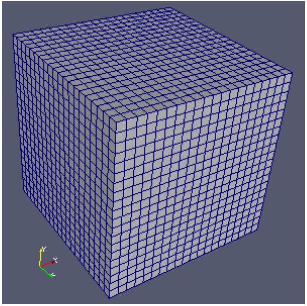

- Let's imagine we have to solve a PDE
- On a dense, Cartesian, uniform grid
  - Mesh axes are parallel to coordinate ones
  - Steps along each direction have the same size
  - And we have some discretization schemes in time and space to solve for variables at each point

A Rigid Solution

```
integer, parameter :: NX = 200
integer, parameter :: NY = 450
integer, parameter :: NZ = 320

integer, parameter :: rk = selected_real_kind(12)

real(rk) :: deltax ! Grid steps
real(rk) :: deltay
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real(rk) ::  u(NX,NY,NZ)
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  - A slow process, for big programs
  - And error prone, as we may forget about

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- But it has annoying consequences
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  - A slow process, for big programs
  - And error prone, as we may forget about
- Couldn't we size data structures according to user input?

SuperComputing Applications and Innovation

A Recurrent Issue

- ```
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  ```
  or
  ```
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  Which one is best?
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  - The latter brings in cache all values related to a grid point as soon as one component is accessed
- We lean to the former
  - As in most numerical schemes, values of the same field in neighboring grid points are accessed together
  ```

Looking for Flexibility

```
subroutine my_pde_solver(nx, ny, nz)
  integer, intent(in) :: nx, ny, nz

  integer, parameter :: rk = selected_real_kind(12)
  real(rk):: deltax, deltay, deltaz ! Grid steps

  real(rk) ::  u(nx,ny,nz)
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```

- We could think of declaring automatic arrays inside a subroutine
- This is unwise
  - Automatic arrays are usually allocated on the process stack
  - Which is a precious resource
  - And limited in most system configurations

A Bad, Old, Common approach

```
program pde_solve
  parameter (MAXNX=400, MAXNY=400, MAXNZ=400)
  parameter (MAXSIZE=MAXNX*MAXNX*MAXNZ)

  real*8 u(MAXSIZE),v(MAXSIZE),w(MAXSIZE),p(MAXSIZE)

  common u,v,w,p
! ...
  call my_pde_solver(nx,ny,nz,u,v,w,p)
! ...
end

subroutine my_pde_solver(nx,ny,nz,u,v,w,p)
  real*8 u(nx,ny,nz),v(nx,ny,nz),w(nx,ny,nz),p(nx,ny,nz)
!...
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- We could give a different shape to dummy arguments

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- But this only works if interface is implicit
  - Which is dangerous

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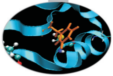
- We could give a different shape to dummy arguments
- But this only works if interface is implicit
  - Which is dangerous
- Maximum problem size still program limited: **`nx*ny*nz`** must be less than **`MAXSIZE`**

Removing Limitations



- Being program limited is annoying

- It's much better to accommodate to any user specified problem size
  - Right, as long as there is enough memory
  - But if memory is not enough, not our fault
  - It's computer or user's fault

- And there are many complex kinds of computations
  - Those in which memory need cannot be foreseen in advance
  - Those in which arrays do not fit
  - Those in which very complex data structures are needed

Outline

Enter Allocatable Arrays

```
integer, parameter :: rk = selected_real_kind(12)

real(rk), dimension(:,:,:), allocatable ::  u,v,w,p

allocate(u(nx,ny,nz),v(nx,ny,nz),w(nx,ny,nz),p(nx,ny,nz))
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- When allocatable arrays are declared, only their rank is specified (**`dimension(:,:,:)`**)

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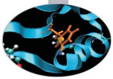

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  - But if **`STAT=`*`integer_var`*** is specified, ***`integer_var`*** is set to zero on success and to a positive value on failure, and execution doesn't stop
- Best practice: use **`STAT=`** and, on failure, provide information to users before terminating execution

Freeing Memory

- Where all these 'dynamic allocated memory' comes from?
  - From an internal area, often termed "*memory heap*"
  - When that is exhausted, OS is asked to give the process more memory
  - And if OS is short of memory, or some configuration limit is exhausted...

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- Best practice: always deallocate when you are done with an allocatable array

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  - In some cases (error recovery) use logical **`allocated()`** function to check
- Mistaking allocatables for a substitute to procedure automatic arrays
  - Dynamic allocation incurs costs
  - Only worth for big arrays that would not fit program stack

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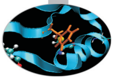

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- Sometimes, you need to have allocatable components in a derived type
- These were added in Fortran 2003
- But some compilers may still lag in this respect
- But Fortran has one more feature to be used to this aim
- And it is also useful to build complex, dynamic data structures

Outline

Enter Fortran Pointers

- Fortran pointers are aliases to other objects
- Declared like regular variables, with attribute **`pointer`**
- Associated to actual objects with pointer assignment **`=>`**
- To be associated with a pointer, variables must have the **`target`** attribute
  - But compilers are often liberal (sloppy?) on this
- Disassociated by actual objects with **`nullify`** statement or by pointer assignment of **`null()`**

```
real, dimension(:,:,:), pointer :: r

real, target :: a(5,15,6), b(3,22,7)

r => a
! now r is an alias of a
nullify(r)

r => b
! now r is an alias of b
r => null()
```

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type atom_list
  type(atom) :: a
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  which comes in handy to define complex data structures, like lists
- Pointers may also alias subobjects

```
real, dimension(:,:,:), pointer :: r
type(velocity), pointer :: v
real, target :: a(5,15,6)
type(atom), target ::  oneatom

r => a(2:4,1:10,3:6) ! r(1,1,1) aliases a(2,1,3)
                     ! r(3,10,4) aliases a(4,10,6)
v => oneatom%velocity
```

Allocating Pointers

- If you allocate a pointer, an unnamed object of the pointee type is created, and associated with the pointer itself

```
real, dimension(:,:,:), pointer :: r
type(atom_list), pointer :: first

allocate(r(5,15,6))
! now r refers an unnamed array allocated on the heap

allocate(first)
! now first refers to an unnamed type(atom_list) variable,
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- You can deallocate the pointee by specifying the pointer in a **`deallocate`** statement
- This gives you a workaround if your compiler doesn't support allocatable structure components
  - Just add a suitable pointer component
  - And allocate it

BIG Mistakes with Pointers

- Referencing an undefined pointer (strange things may happen, it may also seem to work)
  - Good practice: initialize pointers to **`null()`**

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```
real, dimension(:,:), pointer :: r, p
!...
allocate(r(n,m))
p => r
! ...
deallocate(r)
p(k,l) = p(k,l)+1
```

  Now you'll be in troubles with **`p`**, with really strange behavior

Hands-on Session #2: Laplace Equation

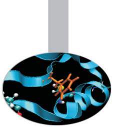
- Discretization on Cartesian 2D grid with Dirichelet Boundary Conditions

$$
\begin{cases}
f(x_{i+1,j}) + f(x_{i-1,j}) - 2f(x_{i,j}) + & \\
f(x_{i,j+1}) + f(x_{i,j-1}) - 2f(x_{i,j}) = 0 & \forall x_{i,j} \in (a,b)^2 \\
f(x_{i,j}) = \alpha(x_{i,j}) & \forall x_{i,j} \in \partial[a,b]^2
\end{cases}
$$

- Iterative advancement using Jacobi method

$$
\begin{cases}
f_{n+1}(x_{i,j}) = \frac{1}{4}[& f_n(x_{i+1,j}) + f_n(x_{i-1,j}) + & \\
 & f_n(x_{i,j+1}) + f_n(x_{i,j-1}) \quad] & \forall n > 0 \\
f_0(x_{i,j}) = 0 & \forall x_{i,j} \in (a,b)^2 & \\
f_n(x_{i,j}) = \alpha(x_{i,j}) & \forall x_{i,j} \in \partial[a,b]^2, & \forall n > 0
\end{cases}
$$

Laplace: static implementation



```
program laplace
   implicit none
   integer, parameter :: dp=kind(1.d0), n = 100
   integer            :: maxIter = 100000, i, j, iter = 0
   real(dp), dimension(0:n+1,0:n+1) :: T, Tnew
   real(dp)           :: tol = 1.d-4, var = 1.d0, top = 100.d0
   T(0:n,0:n) = 0.d0
   T(n+1,1:n) = (/ (i, i=1,n) /) * (top / (n+1))
   T(1:n,n+1) = (/ (i, i=1,n) /) * (top / (n+1))
   do while (var > tol .and. iter <= maxIter)
      iter = iter + 1;   var = 0.d0
      do j = 1, n
         do i = 1, n
            Tnew(i,j) = 0.25d0*( T(i-1,j) + T(i+1,j) + &
                                 T(i,j-1) + T(i,j+1) )
            var = max(var, abs( Tnew(i,j) - T(i,j) ))
         end do
      end do
      if (mod(iter,100)==0) &
        write(*,"(a,i8,e12.4)") ' iter, variation:', iter, var
      T(1:n,1:n) = Tnew(1:n,1:n)
      end do
   end do
end program laplace
```

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   integer             :: maxIter = 100000, i, j, iter = 0
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   real(dp)            :: tol = 1.d-4, var = 1.d0, top = 100.d0
   T(0:n,0:n) = 0.d0
   T(n+1,1:n) = (/ (i, i=1,n) /) * (top / (n+1))
   T(1:n,n+1) = (/ (i, i=1,n) /) * (top / (n+1))
   do while (var > tol .and. iter <= maxIter)
      iter = iter + 1;   var = 0.d0
      do j = 1, n
         do i = 1, n
            Tnew(i,j) = 0.25d0*( T(i-1,j) + T(i+1,j) + &
                                 T(i,j-1) + T(i,j+1) )
            var = max(var, abs( Tnew(i,j) - T(i,j) ))
         end do
      end do
      if (mod(iter,100)==0) &
        write(*,"(a,i8,e12.4)") ' iter, variation:', iter, var
      T(1:n,1:n) = Tnew(1:n,1:n)
      end do
   end do
end program laplace
```

Hands-on Session #2

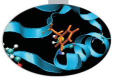
- Modify the code using advanced Fortran features:
  - array syntax
  - allocatable arrays
  - pointer arrays

- Try to list pros and cons of each approach

Laplace in Array-*syntax*

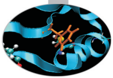
```
program laplace
   implicit none
   integer, parameter :: dp=kind(1.d0), n = 100
   integer            :: maxIter = 100000, i, j, iter = 0
   real(dp), dimension(0:n+1,0:n+1) :: T, Tnew
   real(dp)           :: tol = 1.d-4, var = 1.d0, top = 100.d0
   T(0:n,0:n)  = 0.d0
   T(n+1,1:n)  = (/ (i, i=1,n) /) * (top / (n+1))
   T(1:n,n+1)  = (/ (i, i=1,n) /) * (top / (n+1))
   do while (var > tol .and. iter <= maxIter)
      iter = iter + 1
      Tnew(1:n,1:n) = 0.25d0*( T(0:n-1,1:n) + T(2:n+1,1:n) + &
                               T(1:n,0:n-1) + T(1:n,2:n+1) )
      var =  maxval(abs( Tnew(1:n,1:n) - T(1:n,1:n) ))
      T(1:n,1:n) = Tnew(1:n,1:n)
      if (mod(iter,100)==0) write(*,"(a,i8,e12.4)") &
                     ' iter, variation:', iter, var
   end do
end program laplace
```

Laplace: dynamic allocation



```
program laplace
   implicit none
   integer, parameter :: dp=kind(1.d0)
   integer            :: n, maxIter, i, j, iter = 0
   real (dp), dimension(:,:), allocatable :: T, Tnew
   real (dp)          :: tol, var = 1.d0, top = 100.d0
   write(*,*) 'Enter mesh size, max iterations and tollerance:'
   read(*,*)  n, maxIter, tol
   allocate (T(0:n+1,0:n+1), Tnew(0:n+1,0:n+1))
   call init_and_set_bc(T, top, 'linear')
   do while (var > tol .and. iter <= maxIter)
      iter = iter + 1
      Tnew(1:n,1:n) = 0.25d0 * ( T(0:n-1,1:n) + &
         T(2:n+1,1:n) + T(1:n,0:n-1) + T(1:n,2:n+1) )
      var =  maxval(abs( Tnew(1:n,1:n) - T(1:n,1:n) ))
      T(1:n,1:n) = Tnew(1:n,1:n)
      if( mod(iter,100) == 0 ) write(*,"(a,i8,e12.4)") &
         ' iter, variation:', iter, var
   end do
   deallocate(T,Tnew)
end program laplace
```

Laplace: pointer implementation



```
program laplace
   implicit none
   integer, parameter :: dp=kind(1.d0)
   integer            :: n, maxIter, i, j, iter = 0
   real (dp), dimension(:,:), pointer :: T, Tnew, Tmp=>null()
   real (dp)          :: tol, var = 1.d0, top = 100.d0
   write(*,*) 'Enter mesh size, max iterations and tollerance:'
   read(*,*)  n, maxIter, tol
   allocate (T(0:n+1,0:n+1), Tnew(0:n+1,0:n+1))
   call init_and_set_bc(T, top, 'linear')
   Tnew = T
   do while (var > tol .and. iter <= maxIter)
      iter = iter + 1
      Tnew(1:n,1:n) = 0.25d0 * ( T(0:n-1,1:n) + &
         T(2:n+1,1:n) + T(1:n,0:n-1) + T(1:n,2:n+1) )
      var =  maxval(abs( Tnew(1:n,1:n) - T(1:n,1:n) ))
      Tmp =>T; T =>Tnew; Tnew => Tmp;
      if( mod(iter,100) == 0 ) write(*,"(a,i8,e12.4)") &
         ' iter, variation:', iter, var
   end do
   deallocate (T, Tnew)
   nullify(Tmp)
end program laplace
```

Homework

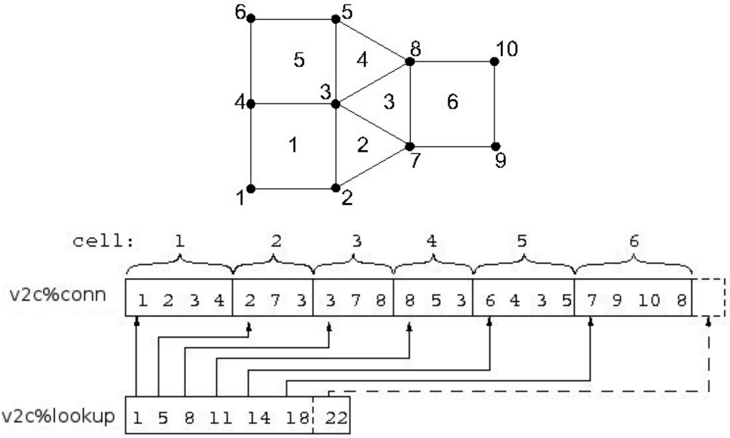
- Re-write a program that:
  - reads an ‘arbitrarily’ long column of real numbers from an ASCII file
  - copy the values to a suitably allocated array
  - prints maximum, minimum, average of the numbers
  - and prints the $\lfloor n/2 \rfloor$-th row where n is the length of the column

  avoiding the constraint of the declaration of a static maximal array, e.g. a(1000)
- Use allocatables: you need to read the file twice
- Use pointers, first store the values in a linked list and then copy them to an allocatable array
  - How to spare memory?

Compressed Sparse Row Format

- The `class_connectivity` implements the CSR format

Compressed Sparse Row Format



class_connectivity Module

```
module class_connectivity

  implicit none

  type connectivity
     integer, allocatable :: lookup(:)
     integer, allocatable :: conn(:)
  end type connectivity

end module class_connectivity
```

Compressed Sparse Row Format

- The `class_connectivity` implements the CSR format
- Array extents are unknown at compile time, so components must be allocatable

Compressed Sparse Row Format

- The **`class_connectivity`** implements the CSR format
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- Let's hide implementation details so that:
  - changes to the data structure will not affect codes using our class
  - provided that we don't change interfaces

Encapsulation

```
module class_connectivity

  implicit none

  type connectivity
     private
     integer, allocatable :: lookup(:)
     integer, allocatable :: conn(:)
  end type connectivity

contains
...
```

Compressed Sparse Row Format

- The **`class_connectivity`** implements the CSR format
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- Now we need *methods* to initialize and access our data:

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  - a constructor to allocate components

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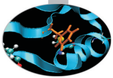

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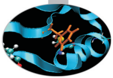
- Now we need *methods* to initialize and access our data:
  - a constructor to allocate components
  - a setter to assign vertices of the *i*-th cell

Constructor and Destructor

```
...
contains

   subroutine alloc_conn(a2b,nel,nconn)
    type(connectivity), intent(inout) :: a2b
    integer, intent(in) :: nel, nconn
    integer :: info

    allocate(a2b%lookup(nel+1), a2b%conn(nconn), stat=info)
    if(info /= 0) then
       write(0,100)
       stop
    end if
    a2b%lookup(1) = 1

100 format(' ERROR! Memory allocation failure in ALLOC_CONN')
  end subroutine alloc_conn

  subroutine free_conn(a2b)
    type(connectivity), intent(inout) :: a2b
    !
    integer :: info(2)

    info = 0
    if (allocated(a2b%lookup)) deallocate(a2b%lookup,stat=info(1))
    if (allocated(a2b%conn))   deallocate(a2b%conn,stat=info(2))
    if(any(info /= 0)) then
       write(0,100)
       stop
    end if

100 format(' ERROR! Memory deallocation failure in FREE_CONN')
  end subroutine free_conn
...
```

Setter and Getter



```
...
  subroutine set_ith_conn(a2b,i,ith_conn)
    type(connectivity), intent(inout) :: a2b
    integer, intent(in) :: i
    integer, intent(in) :: ith_conn(:)
    !
    integer :: i1, i2


    i1 = a2b%lookup(i)
    i2 = i1 + size(ith_conn) - 1

    a2b%conn(i1:i2) = ith_conn(:)

    a2b%lookup(i+1) = i2 + 1
  end subroutine set_ith_conn

  subroutine get_ith_conn(ith_conn,a2b,i)
    integer, allocatable:: ith_conn(:)
    type(connectivity), intent(in), target :: a2b
    integer, intent(in) :: i
    !
    integer :: i1, i2, n

    if (allocated(ith_conn)) deallocate(ith_conn)

    i1 = a2b%lookup(i)
    i2 = a2b%lookup(i+1) - 1
    n=i2-i1+1
    allocate(ith_conn(n))
    ith_conn = a2b%conn(i1:i2)
  end subroutine get_ith_conn

end module class_connectivity
```

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- Write module procedures to:

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  - *destruct* object of **`class_connectivity`** type when no longer needed

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  - a setter to assign vertices of the *i*-th cell
- Write module procedures to:
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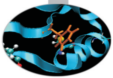
  - retrieve vertices values of the *i*-th cell (getter)

Compressed Sparse Row Format



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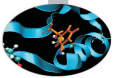
- Write module procedures to:
  - *destruct* object of **`class_connectivity`** type when no longer needed
  - retrieve vertices values of the *i*-th cell (getter)
- Then, for the sake of performance:
  - Write a module procedure returning a pointer to the vertices of *i*-th cell

Constructor and Destructor

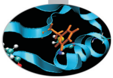
```fortran
...
contains

   subroutine alloc_conn(a2b,nel,nconn)
    type(connectivity), intent(inout) :: a2b
    integer, intent(in) :: nel, nconn
    integer :: info

    allocate(a2b%lookup(nel+1), a2b%conn(nconn), stat=info)
    if(info /= 0) then
       write(0,100)
       stop
    end if
    a2b%lookup(1) = 1

100 format(' ERROR! Memory allocation failure in ALLOC_CONN')
  end subroutine alloc_conn

  subroutine free_conn(a2b)
    type(connectivity), intent(inout) :: a2b
    !
    integer :: info(2)

    info = 0
    if (allocated(a2b%lookup)) deallocate(a2b%lookup,stat=info(1))
    if (allocated(a2b%conn))   deallocate(a2b%conn,stat=info(2))
    if(any(info /= 0)) then
       write(0,100)
       stop
    end if

100 format(' ERROR! Memory deallocation failure in FREE_CONN')
  end subroutine free_conn
...
```

Setter and Getter



```
...
  subroutine set_ith_conn(a2b,i,ith_conn)
    type(connectivity), intent(inout) :: a2b
    integer, intent(in) :: i
    integer, intent(in) :: ith_conn(:)
    !
    integer :: i1, i2


    i1 = a2b%lookup(i)
    i2 = i1 + size(ith_conn) - 1

    a2b%conn(i1:i2) = ith_conn(:)

    a2b%lookup(i+1) = i2 + 1
  end subroutine set_ith_conn

  subroutine get_ith_conn(ith_conn,a2b,i)
    integer, allocatable:: ith_conn(:)
    type(connectivity), intent(in), target :: a2b
    integer, intent(in) :: i
    !
    integer :: i1, i2, n

    if (allocated(ith_conn)) deallocate(ith_conn)

    i1 = a2b%lookup(i)
    i2 = a2b%lookup(i+1) - 1
    n=i2-i1+1
    allocate(ith_conn(n))
    ith_conn = a2b%conn(i1:i2)
  end subroutine get_ith_conn

end module class_connectivity
```

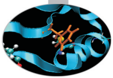
Returning Pointers



```
function ith_conn(a2b,i)
    integer, pointer:: ith_conn(:)
    type(connectivity), intent(in), target :: a2b
    integer, intent(in) :: i
    !
    integer :: i1, i2, n

    i1 = a2b%lookup(i)
    i2 = a2b%lookup(i+1) - 1
    ith_conn => a2b%conn(i1:i2)

  end function ith_conn
```

Outline

Mixing C and Fortran



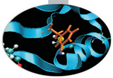
- You may want to call a C function from a Fortran program
- Or call a Fortran procedure from a C program
- And you don't want to translate and re-debug
- Or you can't, as you don't have sources

- You may also want to share global data among C and Fortran program units

- This has been done in the past with non-standard tricks

- Fortran 2003 offers a better, standard way
- Let's look at it in steps

Two Naive Examples



- Imagine you have this C function:

```
double avg_var(int n, const double a[], double *var) {
    double avg = 0.0;
    double avg2 = 0.0;
    for(int i=0;i<n;i++) {
        avg += a[i];
        avg2 += a[i]*a[i];
    }
    avg = avg/n;
    *var = avg2/n - avg*avg;
    return avg;
}
```

and you want to call it from your Fortran code like:

```
avg = avg_var(m,b,var)
```

Two Naive Examples

- Imagine you have this C function:

```
double avg_var(int n, const double a[], double *var) {
    double avg = 0.0;
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    for(int i=0;i<n;i++) {
        avg += a[i];
        avg2 += a[i]*a[i];
    }
    avg = avg/n;
    *var = avg2/n - avg*avg;
    return avg;
}
```

  and you want to call it from your Fortran code like:

```
avg = avg_var(m,b,var)
```

- Ore you have your favorite, thoroughly tested Poisson solver:

```
interface
    subroutine myPoissonSolver(l, m, n, f)
        integer, intent(in) :: l, m, n
        real(kind(1.0D0)), intent(inout) :: f(l,m,n)
    end subroutine myPoissonSolver
end interface
```

  and you want to call it from your C code like:

```
myPoissonSolver(nx, ny, nz, field);
```

A Naive Approach

- We could think that Fortran interfaces and C declarations are enough
- And write, to call C from Fortran:

```
interface
    function avg_var(n, a, var)
        integer, intent(in) :: n
        real(kind(1.0D0)), intent(in) :: a(*)
        real(kind(1.0D0)), intent(out) :: var
        real(kind(1.0D0)) :: avg_var
    end function avg_var
end interface
```

- And to call Fortran from C, add on Fortran side:

```
interface
    subroutine myPoissonSolver(l, m, n, f)
        integer, intent(in) :: l, m, n
        real(kind(1.0D0)), intent(inout) :: f(l,m,n)
    end subroutine myPoissonSolver
end interface
```

  and on the C side, the declaration:

```
void myPoissonSolver(int nx, int ny, int nz, field[nz][ny][nx]);
```

- This is the right track, but still half way from our destination

Thou Shalt Not Mangle Names

- Fortran compilers mangle procedure names
  - All uppercase or all lowercase
  - Compilers may append/prepend one or two _ characters
  - And for module procedures is even worse
  - Used to be sorted out on the C side, in non-portable ways

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- Enter Fortran 2003 **`bind`** attribute

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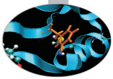
  - Used to be sorted out on the C side, in non-portable ways
- Enter Fortran 2003 **bind** attribute
- For C to Fortran:

```
interface
    function avg_var(n, a, var) bind(c)
        integer, intent(in) :: n
        real(kind(1.0D0)), intent(in) :: a(*)
        real(kind(1.0D0)), intent(out) :: var
        real(kind(1.0D0)) :: avg_var
    end function avg_var
end interface
```

Thou Shalt Not Mangle Names



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- Enter Fortran 2003 **`bind`** attribute
- For C to Fortran:

```
interface
    function avg_var(n, a, var) bind(c)
        integer, intent(in) :: n
        real(kind(1.0D0)), intent(in) :: a(*)
        real(kind(1.0D0)), intent(out) :: var
        real(kind(1.0D0)) :: avg_var
    end function avg_var
end interface
```

- For Fortran to C, Fortran side:

```
interface
    subroutine myPoissonSolver(l, m, n, f) bind(c)
        integer, intent(in) :: l, m, n
        real(kind(1.0D0)), intent(inout) :: f(l,m,n)
    end subroutine myPoissonSolver
end interface
```

and on the C side, the declaration:

```
void myPoissonSolver(int nx, int ny, int nz, field[nz][ny][nx]);
```

Thou Shalt Care for Argument Passing

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  - Under the hood, it's like a C pointer
  - Works for C arrays and pointers to scalar variables
  - But usually scalars are passed by value in C
- Enter Fortran 2003 **`value`** attribute
- For C to Fortran:

```
interface
    function avg_var(n, a, var) bind(c)
        integer, value :: n
        real(kind(1.0D0)), intent(in) :: a(*)
        real(kind(1.0D0)), intent(out) :: var
        real(kind(1.0D0)) :: avg_var
    end function avg_var
end interface
```

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- Enter Fortran 2003 **`value`** attribute
- For C to Fortran:

```
interface
    function avg_var(n, a, var) bind(c)
        integer, value :: n
        real(kind(1.0D0)), intent(in) :: a(*)
        real(kind(1.0D0)), intent(out) :: var
        real(kind(1.0D0)) :: avg_var
    end function avg_var
end interface
```

- For Fortran to C, Fortran side:

```
interface
    subroutine myPoissonSolver(l, m, n, f) bind(c)
        integer, value :: l, m, n
        real(kind(1.0D0)), intent(inout) :: f(l,m,n)
    end subroutine myPoissonSolver
end interface
```

and on the C side, still the declaration:

```
void myPoissonSolver(int nx, int ny, int nz, field[nz][ny][nx]);
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Thou Shalt Care for Data Size and Layout

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```
interface
    function avg_var(n, a, var) bind(c)
        use iso_c_binding
        integer(c_int), value :: n
        real(c_double), intent(in) :: a(*)
        real(c_double), intent(out) :: var
        real(c_double) :: avg_var
    end function avg_var
end interface
```

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        real(c_double) :: avg_var
    end function avg_var
end interface
```

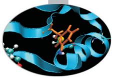
- For Fortran to C, Fortran side:

```
interface
    subroutine myPoissonSolver(l, m, n, f) bind(c)
        use iso_c_binding
        integer(c_int), value :: l, m, n
        real(c_double), intent(inout) :: f(l,m,n)
    end subroutine myPoissonSolver
end interface
```

and on the C side, still the declaration:

```
void myPoissonSolver(int nx, int ny, int nz, field[nz][ny][nx]);
```

More from `iso_c_binding`



- `iso_c_binding` defines named constants holding kind type parameter values for intrinsic types for the platform
- `integer(c_int)` is the kind value corresponding to a C `int`
- Negative values are used for unsupported C types, so the compiler will flag the problem
- A few of them:

Type	Kind	C type
`integer`	`c_int`	`int`
	`c_short`	`short int`
`real`	`c_float`	`float`
	`c_double`	`double`
`complex`	`c_float_complex`	`float _Complex`
	`c_double_complex`	`double _Complex`
`logical`	`c_bool`	`_Bool`
`character`	`c_char`	`char`

- Fortran 2008 adds `c_sizeof()`, check with your compiler!

Mapping Arrays

- Fortran has multidimensional arrays
- C has arrays of arrays (of arrays...)
- Thus the mapping of array indexes to actual data layout in memory is inverted
  - Fortran array **`a(L,M,N)`**
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- Before C99, the leading dimension of an array function parameter could not be specified in C
  - C array parameter `a[]`
  - maps to Fortran assumed size array parameter `a(*)`

- In C99, Variable Length Arrays were introduced
  - C99 array parameter `a[nz][ny][nx]`
  - maps to Fortran array parameter `a(nx,ny,nz)`

Derived Types and Global Data

- **bind** also helps for derived types and global data
- For derived types, each component must be interoperable

Fortran

```fortran
type, bind(c) :: particle
  integer(c_int) :: n
  real(c_float) :: x,y,z
  real(c_float) :: vx,vy,vz
end type particle
```

C

```c
typedef struct particle {
  int n;
  float x,y,z;
  float vx,vy,vz;
} particle;
```

- For module variables or common blocks, use

Fortran

```fortran
integer(c_long), bind(c) :: n

real(c_double) :: m,k
common /com_mk/ m,k
bind(c) :: /com_mk/
```

C

```c
extern long n;

extern struct mk {
  double m, k;
} com_mk;
```

- Note: common blocks become C **structs**

Fortran Pointers vs. C Pointers

- As of argument passing, not a problem
- But Fortran pointers are not interoperable with C
- Fortran pointers sport richer semantics, notably:
  - multidimensional arrays
  - non-contiguous memory areas

- C functions returning a pointer must have **`type(c_ptr)`** type (from **`iso_c_binding`**)
- Ditto for C pointer variables and pointer members of C **`struct`**s:

Fortran

```fortran
type, bind(c) :: block
  integer(c_int) :: n_neighbors
  type(c_ptr) :: neighbors
  type(c_ptr) :: grid
end type block
```

C

```c
typedef struct {
  int n_neighbors;
  int *neighbors;
  mesh *grid;
} block;
```

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  - An optional ***`shape`*** argument like **`(/n/)`** or **`(/l,m,n/)`** gives it a shape for array pointers
- If **`f_proc`** is an interoperable Fortran procedure, **`c_funloc(f_proc)`** returns a valid C pointer (**`type(c_funptr)`**) to it
- **`c_f_procpointer(`*`cfptr`*`,`*`fpptr`*`)`** performs the opposite translation, writing the result in the Fortran procedure pointer ***`fpptr`***

Thou Shalt Compile and Link Properly

- Obviously, C and Fortran sources must be separately compiled and then linked

```
user@caspur$> gcc -c fun_cmd.c
user@caspur$> gfortran -c main_cmd.f90
user@caspur$> gfortran fun_cmd.o main_cmd.o -o main_cmd
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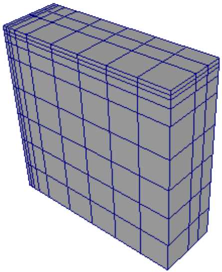
- Easy, if calling C functions from a Fortran program
  - Fortran Runtime Library is usually built on top of C one
- Less so if calling Fortran procedures from a C program
  - Fortran compiler might insert calls to its Runtime Library
- Best practice:

```
user@caspur$> gcc -lgfortran procedures.o main.c
```

- Your mileage may vary, browse your compiler manuals

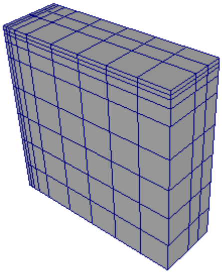
Outline

Nonuniform Grids



- Let's imagine we have to solve a PDE

Nonuniform Grids



- Let's imagine we have to solve a PDE
- On a dense, Cartesian, non uniform grid
  - Mesh axes are parallel to coordinate ones
  - Steps along each direction differ in size from point to point

Keeping Information Together

```
type nonuniform_grid
  integer :: nx, ny, nz
 ! Grid steps
  real(rk), dimension(:), allocatable :: deltax
  real(rk), dimension(:), allocatable :: deltay
  real(rk), dimension(:), allocatable :: deltaz
end type
!...
type(nonuniform_grid) :: my_grid
integer :: alloc_stat
!...
allocate(my_grid%deltax(nx),my_grid%deltay(ny), &
         my_grid%deltaz(nz), STAT=alloc_stat)
if (alloc_stat > 0) then
 ! graceful failure
end if
```

- Related information is best kept together

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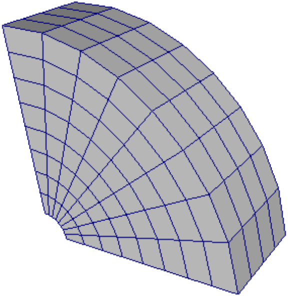
- Use pointer components if your compiler lags behind the standard

Structured Grids in General Form



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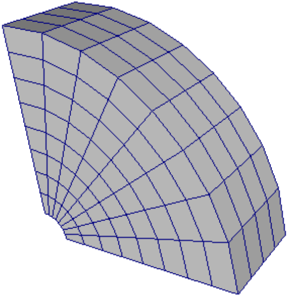
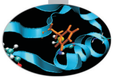


- Let's imagine we have to solve a PDE
- On a dense structured mesh
  - Could be continuously morphed to a Cartesian grid
  - Need to know coordinates of each mesh point

Sketching a Mesh Description



```
type meshpoint
  real(rk) :: x, y, z
end type

type, extends(meshpoint) :: normal
end type

type mesh
  integer :: nx, ny, nz

  type(meshpoint), dimension(:,:,:), allocatable :: coords

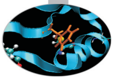
  type(normal), dimension(:,:,:), allocatable :: xnormals
  type(normal), dimension(:,:,:), allocatable :: ynormals
  type(normal), dimension(:,:,:), allocatable :: znormals

  real(rk), dimension(:,:,:), allocatable :: volumes
end type
!...
type(mesh) :: my_mesh

! allocate my_mesh components with extents nx, ny, nz
! immediately checking for failures!
```

- Again, use pointer components if your compiler lags behind the standard

A Recurrent Issue, Again



- ```
  real(rk) ::  x(NX,NY,NZ)
  real(rk) ::  y(NX,NY,NZ)
  real(rk) ::  z(NX,NY,NZ)
  ```

  or

  ```
  type meshpoint
    real(rk) :: x, y, z
  end type

  type(meshpoint), dimension(NX,NY,NZ) :: coords
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  Which one is best?
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  - The latter brings in cache all values related to a grid point as soon as one component is accessed
- Here, we lean to the latter
  - As in most numerical schemes, *x*, *y*, and *z* components of the same mesh point are accessed together
  ```

Multiblock Meshes and More

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  - You want your blocks resolution to adapt to dynamical behavior of PDE solution
  - Which means splitting blocks to substitute part of them with more resolved meshes
- Eventually, you'll need more advanced data structures
  - Like lists
  - Like binary trees, oct-trees, n-ary trees

If You Read Code Like This...

```
type block_item
  type(block), pointer :: this_block

  type(block_item), pointer :: next
end type

!...
   do while (associated(p))
     call advance_block_in_time(p%this_block)
     p => p%next
   end do
```

SuperComputing Applications and Innovation

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   end do
```
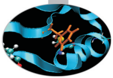

- It is processing a singly-linked list of mesh blocks
- You need to learn more on abstract data structures
- Don’t be afraid, it’s not that difficult

And If You Read Code Like This...

```
type block_tree_node
  type(block), pointer :: this_block

  integer :: children_no
  type(block_tree_node), pointer :: childrens

  type(block_tree_node), pointer :: next_sibling
end type

!...
recursive subroutine tree_advance_in_time(n)
  type(block_tree_node) :: n
  type(block_tree_node), pointer :: p
  integer :: i

  p => n%childrens
  do i=0,n%children_no
    call tree_advance_in_time(p)
    p => p%next_sibling
  end do

  call advance_block_in_time(n%this_block)
end subroutine tree_advance_in_time
```

And If You Read Code Like This...



```fortran
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recursive subroutine tree_advance_in_time(n)
  type(block_tree_node) :: n
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  integer :: i

  p => n%childrens
  do i=0,n%children_no
    call tree_advance_in_time(p)
    p => p%next_sibling
  end do

  call advance_block_in_time(n%this_block)
end subroutine tree_advance_in_time
```

- It is processing a tree of mesh blocks (AMR, probably)
- You need to learn more on abstract data structures
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Outline

Extending the Language

Managing Memory

Conclusions

What We Left Out

- More Fortran practice
  - Time was tight, and that’s your job

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  - Code development management tools
  - Debugging tools
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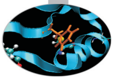
- More Fortran
  - Full object oriented programming
  - Floating point environment
  - Direct I/O
  - Asynchronous I/O
  - Submodules
  - Even more format edit descriptors
  - A few more statements and quite a few intrinsics

Looking for More



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- Fortran 2003 Standard Final Draft
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  `www.ce.uniroma2.it/people/filippone.html`
- Parallel Sparse Basic Linear Algebra Subroutines
  `www.ce.uniroma2.it/psblas/index.html`
- Numerical Engine (for) Multiphysics Operators
  `www.ce.uniroma2.it/nemo/index.html`
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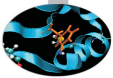

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