PH502: Scientific Programming Concepts

Irish Centre for High End Computing (ICHEC)

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Overview

- Here we shall continue to discuss global variables and the FORTRAN equivalent.
- Finally we shall take a look at some of the predefined functions.

Global Variables

- In C, a variable that are defined outside any programming unit is called a **global variable**.
- These global variables are defined over the whole set of programming units.

```c
#define MAXSIZE 100000
double array1[MAXSIZE]; float  array2[MAXSIZE];
float root2 = 1.4142136;
float function1(float x);
double function2(int i, int j);

int main(void) {
   ....
}
float function1(float x) {
  ....
}
double function2(int i, int j) {
  ....
}
```

Fortran Modules

- FORTRAN modules are special programming units that contain definitions, prototypes and even function/subroutines.
- More than one can be generated and named. Modules are then included in each programming unit which requires them.

```fortran
module mod1
  real (kind=4), parameter :: root2 = 1.4142136
  integer (kind=4), parameter :: maxdim = 100000
end module mod1

module mod2
   interface
     function xxx(x)
        real (kind=4) :: xxx,x
     end function xxx
     subroutine yyy(a,b,c)
        real (kind=8), dimension(5,5) :: a,b,c
     end subroutine yyy
   end interface
end module mod2
```

Modules (Use)

```fortran
program MyProg
   use mod1
   use mod2
!  Stuff in program unit
end program MyProg

subroutine yyy(a,b,c)
   use mod1
! Stuff in subroutine
end subroutine yyy

real (kind=4) :: function xxx(x)
! Cannot have "use mod2" here
! because contains prototype
!    Stuff in function
end function xxx
```

Modules (Use): without 'interface'

```fortran
program MyProg
   use mod1
   use mod2
! Stuff in program unit
end program MyProg
module mod1
  real (kind=4), parameter :: root2 = 1.4142136
  integer (kind=4), parameter :: maxdim = 100000
end module mod1
module mod2
    contains
    function xxx(x)
       real (kind=4) :: xxx,x
       ! stuff in function
    end function xxx
    subroutine yyy(a,b,c)
       real (kind=8), dimension(5,5) :: a,b,c
       ! stuff in subroutine
    end subroutine yyy
end module mod2
```

Intrinsic Functions

- To make life easier for a programmer, intrinsic functions are available.
- The functions below take a single *double* argument and return a *double* value. Note that the trigonometric functions work with radians.

Function	Description
abs(x)	absolute value (FORTRAN)
fabs(x)	absolute value for (C)
cos(x), acos(x)	cosine and arccosine
exp(x)	e^x
log(x), log10(x)	natural, base 10 log
sin(x), asin(x)	sine and arcsine
sqrt(x)	square root
tan(x), atan(x)	tan and arctan

Summary

- This week we discussed:
  1. array variables,
  2. code blocks (functions and subroutines),
  3. as a consequence variables have a scope,
  4. lastly global variables and intrinsics.