Fortran95 and Fortran2003

Tips and Techniques to Help Build Robust, Maintainable Code

1. Introduction

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Introduction

- The goal of these Fortran seminars is quite simple:
  - Describe Fortran95 features.
  - Introduce Fortran2003 syntax and features.
  - Discuss how can we use these features in our software development to create high quality, robust, maintainable (extensible?) code?

- What is your experience with f95/2003?

- What do you want to know about f95/2003?

Overview

- What we'll be covering this time
  - Kind types
  - Attributes
  - Derived types
  - Array syntax
- Most of these topics are fundamental, so you may already know about them and use them.
- The subject matter isn't covered linearly, particularly with respect to Fortran2003 features and more esoteric Fortran95 usage.
- Please ask questions for clarification.

Kind types

- New intrinsics to allow user to select the “kind” of integer or real variable.
- `SELECTED_INT_KIND(`*I*`)`
  - Return the kind value of the *smallest* integer type that can represent all values -10^I to 10^I
- `SELECTED_REAL_KIND(`*P*`,`*R*`)`
  - Return the kind value of a real data type with decimal precision of *at least P* digits and exponent range greater than *at least R*.
- Note the “*smallest*” and “*at least*” in the definitions. Supported kind types still depend on hardware and software.

Kind types - Integer

- Some examples:

Integer

```
SELECTED_INT_KIND(1)  = 1
SELECTED_INT_KIND(2)  = 1
SELECTED_INT_KIND(3)  = 2
SELECTED_INT_KIND(4)  = 2
SELECTED_INT_KIND(5)  = 4
SELECTED_INT_KIND(6)  = 4
SELECTED_INT_KIND(7)  = 4
SELECTED_INT_KIND(8)  = 4
SELECTED_INT_KIND(9)  = 4
SELECTED_INT_KIND(10) = 8
```

These specify the size of the integer type.

These are the resultant integer *KIND TYPES*.

NOTE: These values are *not* portable. Different compilers may use different values.

Note the repeated kind type values for different sizes. Not all integer representations are available. E.g. $\pm 10^5$ to $\pm 10^9$ values are possible with a single kind type ("long integer").

Kind types - Real

- Some examples:

Real

```
SELECTED_REAL_KIND(1)  = 4
SELECTED_REAL_KIND(2)  = 4
SELECTED_REAL_KIND(3)  = 4
SELECTED_REAL_KIND(4)  = 4
SELECTED_REAL_KIND(5)  = 4
SELECTED_REAL_KIND(6)  = 4
SELECTED_REAL_KIND(7)  = 8
SELECTED_REAL_KIND(8)  = 8
SELECTED_REAL_KIND(9)  = 8
SELECTED_REAL_KIND(10) = 8
```

These specify the decimal precision of the real type.

These are the resultant real *KIND TYPES*.

Again, these values are *not* portable. Different compilers may use different values.

Note the repeated kind type values for different precisions. As with integer types, not all real representations are available. Remember the "*at least*" part of the definition.

Kind types - Portability issues

- You're probably familiar with the f77 extension:

  `INTEGER*4`, or `REAL*8`

  where the "`4`" and "`8`" indicate byte size.
- These are *not* synonymous with the f95 syntax:

  `INTEGER(4)`, or `REAL(8)` ← Do not do this!

  where the "`4`" and "`8`" are kind types. Some compilers use

  `INTEGER(3)`, or `REAL(2)`

  to represent the same types.
- Never use literal constants for kind types.
- Always use parameterised kind types derived from the `SELECTED_*_KIND()` intrinsics.

Kind types - the Module

```
MODULE Type_Kinds
  ! No implicit typing
  IMPLICIT NONE
  ! Explicit visibility declaration
  PRIVATE
  PUBLIC :: Byte, Short, Long
  PUBLIC :: Single, Double
  PUBLIC :: ik, rk
  ! Integer kinds
  INTEGER, PARAMETER :: Byte  = SELECTED_INT_KIND(1) ! Byte
  INTEGER, PARAMETER :: Short = SELECTED_INT_KIND(4) ! Short
  INTEGER, PARAMETER :: Long  = SELECTED_INT_KIND(8) ! Long
  ! Floating point kinds
  INTEGER, PARAMETER :: Single = SELECTED_REAL_KIND(6)  ! Single
  INTEGER, PARAMETER :: Double = SELECTED_REAL_KIND(15) ! Double
  ! Generic kinds
  INTEGER, PARAMETER :: ik = Long   ! Generic integer kind
  INTEGER, PARAMETER :: rk = Double ! Generic real kind
END MODULE Type_Kinds
```

Always do this!

Self-documentation!

Use of generic kind types makes precision changes easier.

Kind types – USE*ing the Module*

```
PROGRAM Display_Type_Kinds
  ! Use the module
  USE Type_Kinds
  ! No implicit typing
  IMPLICIT NONE
  ! Declare variables
  INTEGER(Byte)  :: bi
  INTEGER(Short) :: si
  INTEGER(Long)  :: li
  REAL(Single) :: sr
  REAL(Double) :: dr
  WRITE(*,'("Huge(bi)=",i10,5x,i10)')HUGE(bi),10_Byte**1 - 1
  WRITE(*,'("Huge(si)=",i10,5x,i10)')HUGE(si),10_Short**4 - 1
  WRITE(*,'("Huge(li)=",i10,5x,i10)')HUGE(li),10_Long**8 - 1
  WRITE(*,'("Prec,Range(sr)=",i5,1x,i5)')PRECISION(sr),RANGE(sr)
  WRITE(*,'("Prec,Range(dr)=",i5,1x,i5)')PRECISION(dr),RANGE(dr)
END PROGRAM Display_Type_Kinds
```

How to use modules in your code.

How to declare variables of different kinds.

New intrinsics to inquire about a datatype: **HUGE(), PRECISION(), RANGE()**.

Kind types – USE*ing the Module*

```
PROGRAM Display_Type_Kinds
  ! Use the module
  USE Type_Kinds
  ! No implicit typing
  IMPLICIT NONE
  ! Declare variables
  INTEGER(Byte)  :: bi
  INTEGER(Short) :: si
  INTEGER(Long)  :: li
  REAL(Single) :: sr
  REAL(Double) :: dr
  WRITE(*,'("Huge(bi)=",i10,5x,i10)')HUGE(bi),10_Byte**1 - 1
  WRITE(*,'("Huge(si)=",i10,5x,i10)')HUGE(si),10_Short**4 - 1
  WRITE(*,'("Huge(li)=",i10,5x,i10)')HUGE(li),10_Long**8 - 1
  WRITE(*,'("Prec,Range(sr)=",i5,1x,i5)')PRECISION(sr),RANGE(sr)
  WRITE(*,'("Prec,Range(dr)=",i5,1x,i5)')PRECISION(dr),RANGE(dr)
END PROGRAM Display_Type_Kinds
```

```
Huge(bi)=        127          9
Huge(si)=      32767       9999
Huge(li)=2147483647   99999999
```

This is how you type literal constants

```
Prec,Range(sr)=    6    37
Prec,Range(dr)=   15   307
```

Kind types - Literal constants(1)

- Always use the kind type when defining and assigning real literal constants. If we have a double precision kind type "dp",

```
REAL(dp), PARAMETER :: MW_DRYAIR = 28.9648_dp

REAL(dp) :: g_per_g, g_per_kg
g_per_g = 1.0e-03_dp * g_per_kg
```

- The "_dp" suffix on the literal constants ensures the constant has the same precision as its data type. Doing something like,

```
g_per_kg = 8.754
```

assigns a *single* precision constant to a *double* precision variable. To be consistent, do

```
g_per_kg = 8.754_dp
```

Kind types - Literal constants(2)

```
PROGRAM Display_Literals
  USE Type_Kinds
  IMPLICIT NONE
  REAL(Double) :: var1, var2, var3
  var1 = 10.0_Double
  var2 =  3.1415927         * var1
  var3 =  3.1415927_Double * var1
  WRITE(*,'("var2 = ",f19.15)')var2
  WRITE(*,'("var3 = ",f19.15)')var3
END PROGRAM Display_Literals
```

The difference is one literal is typed, the other is not

```
$:~/Fortran/Type_Kinds $ gfortran -c Type_Kinds.f90
$:~/Fortran/Type_Kinds $ gfortran Display_Literals.f90
$:~/Fortran/Type_Kinds $ a.out
var2 =  31.415927410125732
var3 =  31.415927000000000
```

The precision of the result is dependent on the precision of the literal, regardless of all the type declarations.

Attributes

- Attributes are properties that can be specified for an object (variable, argument, function, etc)
- There are 12 attributes in Fortran95. Fortran2003 adds 5 more.
- Some attributes in Fortran95 are carried over from FORTRAN77 statements
  - `DIMENSION`, `EXTERNAL`, `INTRINSIC`, `PARAMETER`, and `SAVE`
- We'll look at some "old" attributes but using new syntax, and then cover new attributes.

Attributes - "Old"

- **PARAMETER**. FORTRAN77 syntax:

```
INTEGER N
PARAMETER (N=10)
```

Fortran95 syntax:

```
INTEGER, PARAMETER :: N=10
```

Double colon required for inline attribute specification

- **SAVE**. Same syntax change as for parameters:

```
INTEGER, SAVE :: my_int
```

Important: *initialisation implies save*!

```
INTEGER :: my_int = 0
```

Required for initialisation

This declaration is equivalent to:

```
INTEGER, SAVE :: my_int = 0
```

Attributes - Allocatable(1)

- **ALLOCATABLE**. Fortran finally has dynamic storage allocation! Type declaration example,

```
REAL, ALLOCATABLE :: x(:,:)
```

Deferred shape specifies rank.

  – Allocation via the `ALLOCATE` statement…

```
ALLOCATE(x(N,N),STAT=alloc_stat)
```

Allocation error if ≠ 0. Please use.

  – …and deallocation via the obvious,

```
DEALLOCATE(x,STAT=alloc_stat)
```

Fortran95 standard stipulates that local allocatable arrays are deallocated upon exit.

Fortran90 does not!

Attributes - Allocatable(2)

- An allocatable array has both a *definition* status and an *allocation* status.
  - Definition status is the same as for other objects and depends on whether the object has had its value established. In general, objects start their lives in an undefined state.
  - Allocation status lets you know whether an allocatable array is or is not allocated. This can be determined with a new intrinsic function like so,

```
IF (ALLOCATED(x)) THEN…
```

The allocation status of an allocatable array is *never* undefined.

Remember this!

Attributes - Target

- **`TARGET`**. Indicates the variable (or argument) can be pointed to by a Fortran pointer. Type declaration example,

```
REAL, TARGET :: x(N,N), y(N)
```

- Why require this?
  - To provide compilers with information that can be utilised to produce efficient code.
  - Also makes clear the intent of the programmer that the variables/arguments in question can be aliased.

- You cannot access a variable/argument via a pointer unless it has the `TARGET` attribute.

Attributes - Pointer(1)

- **`POINTER`**. Now easier to shoot oneself in the foot in Fortran too! (Just kidding).

- Fundamental differences between Fortran pointers and those of other languages.
  - There is no mechanism for indicating that a pointer to one data type is to be treated as if it were a pointer to different data type.
  - No generic pointer type.
  - No pointer arithmetic.

Attributes - Pointer(2)

- Type declaration example,

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

This is *very* important. You should always do this!

Fortran90 does not have this capability!

  – `ptr` can *only* point to rank-1 real arrays, e.g.

```
REAL, TARGET :: x(N,N), y(N)
ptr=>x(:,1)
ptr=>y
```

  – Can also allocate new space directly, e.g.

```
ALLOCATE(ptr(N),STAT=alloc_stat)
```

Attributes - Pointer(3)

- Similar to allocatables, a pointer has both a *definition* status and an *association* status.
  - Association status lets you know whether a pointer is or is not associated with a target. This can be determined with a new intrinsic function like so,

```
IF (ASSOCIATED(ptr)) THEN…
```

- Unless you initialise the pointer, the association status is *undefined*.

- In this case, it is *illegal* to query the association status of the pointer.

Attributes - Pointer(4)

- Important: a pointer with no initialisation,
  `REAL, POINTER :: ptr(:)=>NULL()`
  means its association status is *undefined*.

Always do this!

- In this case, testing its association status is *illegal*,
  `IF (ASSOCIATED(ptr)) THEN…`

- You should either initialise in the declaration as shown before, or immediately after by using
  `NULLIFY(ptr)` [Fortran90/95/2003]
  or
  `ptr=>NULL()` [Fortran95/2003 *only*]

Attributes - Intent

- **INTENT**. Allows programmer to explicitly state whether subprogram arguments are input, output, or both. Good self-documentation.

- Subprogram example,

```
SUBROUTINE mysub(a,b,x,y)
   REAL, INTENT(IN)      :: a,b
   REAL, INTENT(IN OUT) :: x
   REAL, INTENT(OUT)     :: y
```

  - You cannot change the value of the "`a`" and "`b`" dummy arguments in `mysub()`.
  - Any value the actual argument "`y`" had prior to calling `mysub()` is lost - assignment is expected.

Attributes - Optional(1)

- **OPTIONAL**. Allows programmer to specify dummy arguments as optional.

- Subprogram example,

```
SUBROUTINE mysub(a,b,x,c)
   REAL,                INTENT(IN)  :: a,b
   REAL,                INTENT(OUT) :: x
   REAL, OPTIONAL, INTENT(IN)  :: c
```

  – You can test if the actual argument was passed using a new intrinsic,

```
IF (PRESENT(c)) THEN…
```

Attributes - Optional(2)

- There is no mechanism for specifying a default value for an omitted argument. Use a local variable,

```
SUBROUTINE mysub(…other arguments…,c)
  REAL, OPTIONAL, INTENT(IN)  :: c
  REAL :: c_local
  …
  IF (PRESENT(c)) THEN
    c_local = c
  ELSE
    c_local = default value
 END IF
```

Attributes - Optional(3)

- Recommended to use keyword arguments in calls to distinguish mandatory and optional arguments,

```
CALL mysub(a,b,x,c=c)
```

  If the convention is adopted, then the calling statement indicates which arguments are optional.

- Explicit interface is required.
  - Use of optional attribute for dummy argument.
  - Use of keyword form in passing actual arguments

  We'll cover interfaces later on.

Attributes - Accessibility

- These attributes control accessibility of entities (type definitions, variables, procedures, parameters) and are inherently related to the use of modules so I'll only mention them briefly - we'll look more closely at them when we cover modules.

- **`PUBLIC`**. The default. Declares module entities are accessible outside the module via use association.

- **`PRIVATE`**. Prevents access of entities outside a module by use association.

Attributes - Fortran2003

- **`ASYNCHRONOUS`**. Specifies a variable may be used in asynchronous I/O. Used to facilitate compiler optimisation.
- **`BIND(C)`**. Pertains to interoperability with the C language.
- **`PROTECTED`**. Allows a module variable to be visible (i.e. not private), but not definable outside the module.
- **`VALUE`**. Specifies a form of argument association for dummy arguments.
- **`VOLATILE`**. Specifies a variable may be used or modified by means not specified in the program. E.g. if some other program modifies shared memory.

Derived Types

- More commonly known as structures. Also referred to as user defined types.
- Defined within a `TYPE…END TYPE` construct.
- May contain any combination of intrinsic or derived type components.
- Limitations on component attributes:
  - Only `POINTER` or `DIMENSION` attributes allowed.
  - Fortran2003 (or TR15881 compliant) compiler allows the `ALLOCATABLE` attribute.
- Fortran2003 also greatly increases the utility of derived types for OOP. We'll cover those changes in a later seminar.

Derived Types - Simple Example

Give your type a name. Note: my personal style is to append "_type" so I know it's a derived type name.

```
TYPE :: whereami_type
   REAL(rk) :: lat
   REAL(rk) :: lon
   REAL(rk) :: alt
   TYPE(date_type) :: date
   CHARACTER(80) :: location
END TYPE whereami_type
```

The components

Other derived types can be components

Naming the END TYPE is not mandatory, but recommended (e.g. if you have scripts for creating documentation)

Derived Types - Assignment(1)

- Can assign to a derived type two ways:
  - Regular assignment

```
TYPE(whereami_type) :: x
x%lat = 38.89_rk
x%lon = 77.02_rk
x%alt = 6.1_rk
x%date%year  = 2008
x%date%month = 12
x%date%day   = 4
x%location = “Washington, DC”
```

Structure components are referenced recursively.

The component selector is “%”. Many other languages use “.” Why not Fortran? Think about `.AND.`, `.OR.`, `.NOT.`, etc.

Derived Types - Assignment(2)

– Structure constructors

```
x = whereami_type(38.89_rk,&
                  77.02_rk,&
                  6.1_rk,&
                  date_type(2008,12,4),&
                  "Washington, DC")
```

The derived type name

The sequence of component values. Must agree in number and order.

An embedded constructor.

Derived Types - Parameters

- A structure constructor is how you specify a derived type parameter,

```
TYPE(whereami_type), PARAMETER :: x = &
  whereami_type(38.89_rk,&
                77.02_rk,&
                6.1_rk,&
                date_type(2008,12,4),&
                “Washington, DC”)
```

Derived Types - Default Init(1)

- Default initialisation of our simple structure,

```
TYPE :: whereami_type
  REAL(rk) :: lat = -999.0_rk
  REAL(rk) :: lon = -999.0_rk
  REAL(rk) :: alt = -999.0_rk
  CHARACTER(80) :: location = “”
  TYPE(date_type) :: date = date_type(0,0,0)
END TYPE whereami_type
```

Note that this initialisation overrides any default initialisation in the `date_type` definition. The “highest level” initialisation wins.

Derived Types - Default Init(2)

- Warning #1. Keep dummy argument `INTENT` in mind.
  - Let's say we had a subroutine interface like so

```
SUBROUTINE get_map(x)
  TYPE(whereami_type), INTENT(OUT) :: x
```

  - Everytime `get_map()` is called, `x` is reinitialised to its default value because of the `INTENT(OUT)` attribute of the dummy argument.
  - For arrays, or large structures, this can be expensive. Not dangerous, just expensive.

Derived Types - Default Init(3)

- Warning #2. Keep dummy argument `INTENT` in mind. (Sound familiar?)
  - Let's say we have the derived type

```
TYPE :: ptr_type
  REAL(rk), POINTER :: p(:)=>NULL()
END TYPE ptr_type
```

  - And let's allocate an instance,

```
TYPE(ptr_type) :: ptr
ALLOCATE(ptr%p(100000))
```

  - And let's use it in this subroutine,

```
SUBROUTINE futz_ptr(ptr)
  TYPE(ptr_type), INTENT(OUT) :: ptr
```

  - What will happen?

`ptr` is reinitialised, so our allocated memory is no longer reachable.

Memory leak!

Derived Types - Example 2

```
TYPE :: CRTM_Atmosphere_type
  ! Dimension values
  INTEGER :: n
  INTEGER :: n
  INTEGER :: n
  INTEGER :: n
  ! Number of
  INTEGER :: n
  ! Climatolog
  INTEGER :: C
  ! Absorber I
  INTEGER, POI
  INTEGER, POI
  ! Profile LE
  REAL(fp), PO
  REAL(fp), POINTE
  REAL(fp), POINTE
  REAL(fp), POINTER :: Absorber(:,:)      => NULL()  ! K x J
  ! Clouds associated with each profile
  TYPE(CRTM_Cloud_type),  POINTER :: Cloud(:)   => NULL()  ! Nc
  ! Aerosols associated with each profile
  TYPE(CRTM_Aerosol_type), POINTER :: Aerosol(:) => NULL()  ! Na
END TYPE CRTM_Atmosphere_type
```

```
TYPE :: CRTM_Cloud_type
  ! Dimension values
  INTEGER :: n_Layers   = 0  ! K dimension
EN
```

```
TYPE :: CRTM_Aerosol_type
  ! Dimensions
  INTEGER :: n_Layers   = 0  ! K dimension
  ! Number of added layers
  INTEGER :: n_Added_Layers = 0
  ! Aerosol type
  INTEGER :: Type = NO_AEROSOL
  ! Aerosol state variables
  REAL(fp), POINTER :: Effective_Radius(:) => NULL() ! K
  REAL(fp), POINTER :: Concentration(:)    => NULL() ! K
END TYPE CRTM_Aerosol_type
```

Derived Types - Example 3

```
TYPE :: CRTM_CSVariables_type
  PRIVATE
  ! The interpolation data
  TYPE(CSinterp_type) :: csi(MA
  ! The interpolation result
  REAL(fp), DIMENSION(MAX_N_LAY
  REAL(fp), DIMENSION(MAX_N_LAY
  REAL(fp), DIMENSION(MAX_N_LAY
  REAL(fp), DIMENSION(0:MAX_N_L
                      MAX_N_PHA
                      MAX_N_LAY
```

```
TYPE :: CSinterp_type
  ! The interpolating polynomia
  TYPE(LPoly_type) :: wlp, xlp,
  ! The LUT interpolation indic
  INTEGER :: i1, i2, j1, j2, k1
  ! The LUT interpolation boundary check
  LOGICAL :: f_outbound, r_outbound, t_outbound
  ! The interpolation input
  REAL(fp) :: f_int, r_int, t_int
  ! The data to be interpolated
  REAL(fp) :: f(NPTS), r(NPTS), t(NPTS)
END TYPE CSinterp_type
```

```
TYPE :: LPoly_type
  INTEGER :: Order=ORDER
  INTEGER :: nPts =NPOLY_PTS
  ! Left and right side polynomials
  REAL(fp) :: lp_left(NPOLY_PTS)  = ZERO
  REAL(fp) :: lp_right(NPOLY_PTS) = ZERO
  ! Left and right side weighting factors
  REAL(fp) :: w_left  = ZERO
  REAL(fp) :: w_right = ZERO
  ! Polynomial numerator differences
  REAL(fp) :: dxi_left(NPOLY_PTS)  = ZERO
  REAL(fp) :: dxi_right(NPOLY_PTS) = ZERO
  ! Polynomial denominator differences
  REAL(fp) :: dx_left(NPOLY_PTS)  = ZERO
  REAL(fp) :: dx_right(NPOLY_PTS) = ZERO
END TYPE LPoly_type
```

Array Syntax (1)

- Array syntax has been available since Fortran90. Many powerful, and convenient, features.

- Array constructors.

```
REAL :: x(4)=(/3.7,4.6,7.2,6.9/)
```
[f90/95/2003]

```
INTEGER :: j(N)=[(i*2,i=1,N)]
```
[f2003 only]

- Subscript triplets specify array sections.
  - Backwards access, `j(N:1:-1)`
  - Every other element, `j(1:N:2)`
  - Elements are optional, `j(4:N-3),j(4:),j(:N-1)`

- Vector Subscripts.

  If `k=(/7,4,10/)`, then `j(k)≡(/14,8,20/)`

Array Syntax (2)

- This is a pet peeve of mine. Given an array,

  ```
  REAL :: x(N)
  ```

  that will be assigned a value, some people recommend,

  ```
  x(:)=1.0
  ```

  rather than

  ```
  x=1.0
  ```

  with the idea that the "`(:)`" indicates to readers that "`x`" is an array.
- But, `x(:)` is an array section, an expression, derived from the actual array, `x`.
- 99.99% of the time it probably doesn't matter, but just remember they are not the same thing.

Summary

- What we've looked at
  - Kind types and how to use them.
  - Attributes in type definitions.
  - Derived type definitions.
  - Quick look at array syntax.
- What to do with this information?
  - Apply it to new code (if it ain't broke…), or
  - Refactor old code (let me tell you about unit testing…)
- Was the information useful? What would you like to see in any future Fortran seminars? Volunteers?
  - Let me know: `paul.vandelst@noaa.gov`

Next Time

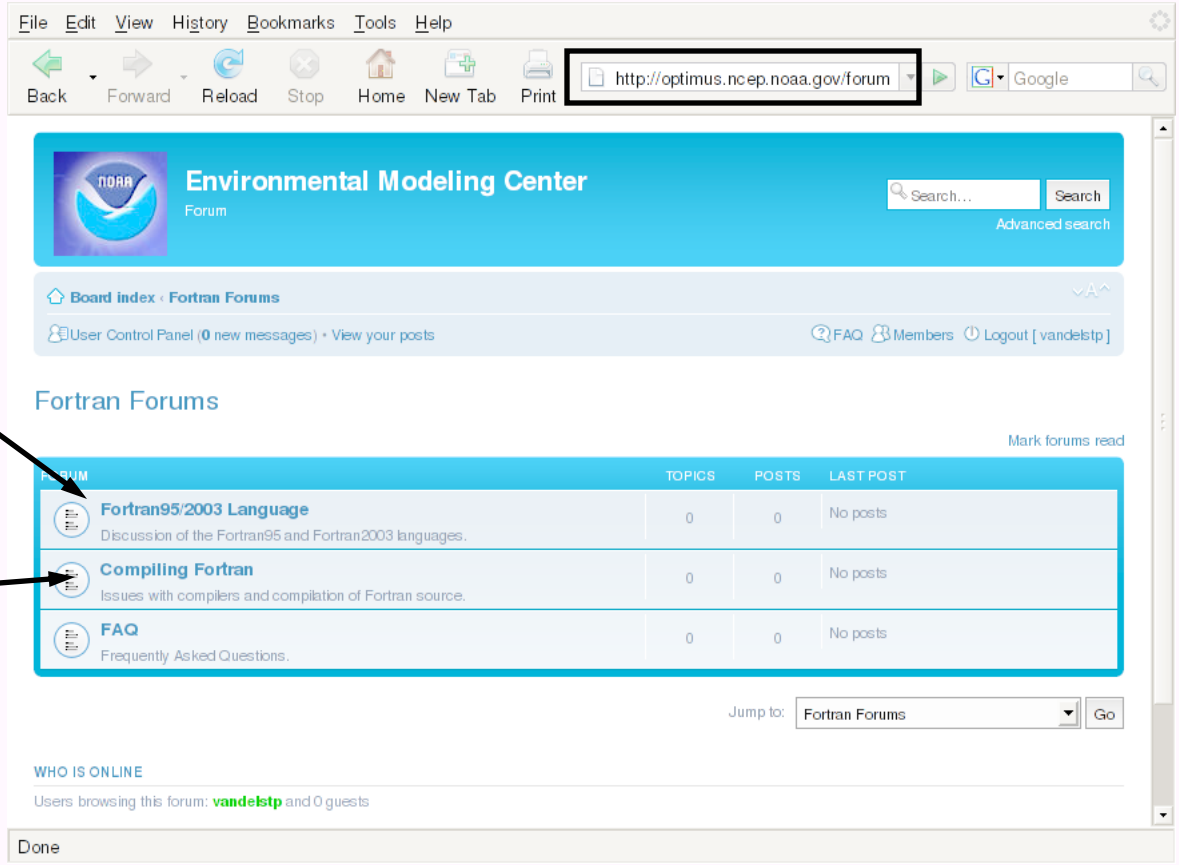
- Concept of scope
- Interfaces
  - Difference between explicit and implicit interfaces
- Modules
  - Create your own generic procedures
  - Create your own operators
- Block constructs
- Input and output processing

Where to Get More Information

- EMC Fortran Forum. Post questions, and/or discoveries. It's not too helpful for non-NCEP folks without VPN so maybe setup similar on library website?

Forum for language issues.

Forum for compiler and compilation issues.



Where to Get More Information

- Many online guides.
  - Google is your friend.
- `comp.lang.fortran` newsgroup.
  - Many members of the current and past standards committee, and some compiler vendors, frequent it.
- Books!
  - The ones below I use almost daily.