Computers in Chemistry – Lecture IX

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Get this lecture online

- Please go to: http://qc.chem.nagoya-u.ac.jp
- Click on “Teaching”
- Click on “PPT” link of “9.1 Lecture IX – Subroutines and Arrays in FORTRAN”
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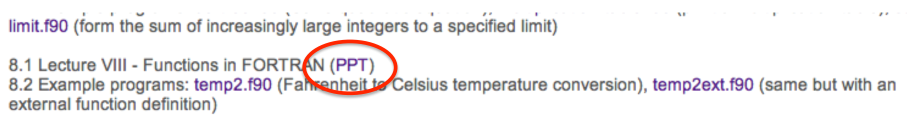


limit.f90 (form the sum of increasingly large integers to a specified limit)

8.1 Lecture VIII - Functions in FORTRAN (PPT)
8.2 Example programs: temp2.f90 (Fahrenheit to Celsius temperature conversion), temp2ext.f90 (same but with an external function definition)

7.1 Subroutines I

- Programming with Subroutines
- Program units designed to perform particular tasks under the control of some other program unit.
- Look like FUNCTIONS *but do not return a value.*
- FORTRAN 90 allows three types of subroutines: internal, module, and external subroutines
- May not return a value to all, or may return more than one value modified in the argument-list.
- A function is referenced by its name alone, whereas a subroutine is referenced by a CALL statement

7.1 Subroutines II

- The form of a subroutine subprogram is:

```
subroutine heading
Specification part
Execution part
END SUBROUTINE statement
```

- Like functions, the subroutine can be contained in the same or a different .f90 file. For simplicity, we will only consider the case where one .f90 source code file contains both **program** and **subroutine(s)**.

7.1 Subroutines III

- Subroutine heading is a SUBROUTINE statement of the form:

```
SUBROUTINE subroutine-name (formal-argument-list)
```

- Or, for a recursive subroutine,

```
RECURSIVE SUBROUTINE subroutine-name (formal-argument-list)
```

- "subroutine-name" is a legal Fortran identifier, "formal-argument-list" is an identifier or list (possibly empty, in which case **we do not need "()"**) of identifiers separated by commas.
- A subroutine is referenced in the program by a CALL statement of the form:

```
CALL subroutine-name (actual-argument-list)
```

- Subroutines can contain CALL statements themselves. However, they cannot call themselves unless they are specified as a "recursive" subroutine (see previous page).

7.1 Subroutines IV

- Variables in the "formal-argument-list" are called "**formal**" or "**dummy arguments**" and are used to pass information to the function subprogram.
- Note: Different program languages have different default ways of passing information from the main program to the subprogram.
- FORTRAN: "pass-by-reference" (use a memory pointer)
- C/C++ and Java: "pass-by-value" (the value cannot be changed by the subprogram)

7.1 Subroutines V

- Specfication part of a subroutine has the same form as that of a regular program. It must declare:

  The type of each formal argument appearing in the "list-of-arguments" as well as variables that appear in the subroutine
- The execution part of a function subprogram is similar to a regular program, but unlike a function **it does NOT require a statement:**

```
function-name = expression
```

- The last statement of a function subprogram should be:

```
END SUBROUTINE subroutine-name
```


7.1 Subroutines VI

- Example: download a program to convert temperature from Fahrenheit to Celsius units, this time using an external subroutine, temp3.f90, and compile and run it in an X-Windows terminal by:
- cd Downloads
- gfortran –o temp3.x temp3.f90
- ./temp3.x

7.1 Subroutines VII

- Sample run:

```
$ ./temp3.x
 Enter temperature in Fahrenheit:
32
   32.00000     is equivalent to   0.000000     in Celsius
 More tmperatures to convert (Y/N)?
y
[stephan@hawk ~]$ ./temp3.x
 Enter temperature in Fahrenheit:
32
   32.00000     is equivalent to   0.000000     in Celsius
 More tmperatures to convert (Y/N)?
Y
 Enter temperature in Fahrenheit:
212
   212.0000     is equivalent to   100.0000     in Celsius
 More tmperatures to convert (Y/N)?
Y
 Enter temperature in Fahrenheit:
-22.5
  -22.50000     is equivalent to  -30.27778     in Celsius
 More tmperatures to convert (Y/N)?
```


8.1 Arrays I

- An array is a **data structure**
- Arrays can be 1-dimensional (vector), 2-dimensional (matrix), or multi-dimensional

```
REAL, DIMENSION(2) :: Vector, Rotated_Vector
REAL, DIMENSION(2,2) :: Rotation_Matrix
```

- Arrays are often used in vector calculus, linear algebra, data processing, etc.
- Ideal for computation, especially in combination with counter-controlled DO loops

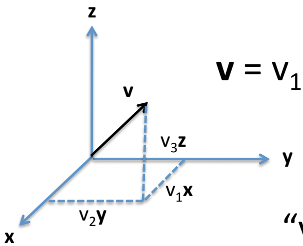
8.1 Arrays II

- A vector needs to be defined in a space. Typically, this is three-dimensional Euclidean space $\mathbf{R}^3$ where the three base vectors are orthogonal on each other (form 90° angles with each other):

$$\mathbf{x} = \begin{bmatrix}1\\0\\0\end{bmatrix} \quad \mathbf{y} = \begin{bmatrix}0\\1\\0\end{bmatrix} \quad \mathbf{z} = \begin{bmatrix}0\\0\\1\end{bmatrix}$$

8.1 Arrays III

- Then, any vector **v** in $\mathbf{R}^3$ can be mathematically expressed as a *linear combination* of these three vectors:

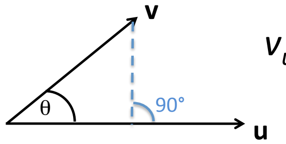


$$\mathbf{v} = v_1 \bullet \mathbf{x} + v_2 \bullet \mathbf{y} + v_3 \bullet \mathbf{z} = \begin{bmatrix}v_1\\v_2\\v_3\end{bmatrix}$$

a, b, c are called "vector coefficients"

8.1 Arrays IV

- A scalar projection v_u of a vector **v** on another vector **u** is given by:



$v_u = |v| \bullet \cos\theta$

- A scalar product between two vectors corresponds to their "inner product":

  $v \bullet u = |v| \bullet |u| \bullet \cos\theta$.

8.1 Arrays V

- In two dimensions, the scalar ("dot") product is given by:

  $\mathbf{v \bullet u} = v_1 * u_1 + v_2 * u_2 = |u| * |v| * \cos\theta$

- **Properties of the scalar ("dot") product:**

  a) If the two vectors are "orthogonal" (form 90° angles), their scalar product is 0!

  b) If the two vectors are identical (form 0° angles), their scalar product is the square of its magnitude, $|\mathbf{v}|^2$

8.1 Arrays VI

- Task: Write a program that reads two 2-dimensional vectors **v** and **u**, and then calculates and prints their scalar product.
- Note: Please try to use a subroutine to compute the scalar product for any two vectors.
- **Good luck. This concludes today's lecture.**