Computers in Chemistry – Lecture XI

Prof. Dr. Stephan Irle
Quantum Chemistry Group
Nagoya University

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- Please go to: http://qc.chem.nagoya-u.ac.jp
- Click on “Teaching”
- Click on “PPT” link of “11.1 Lecture XI – File Input/Output in FORTRAN”

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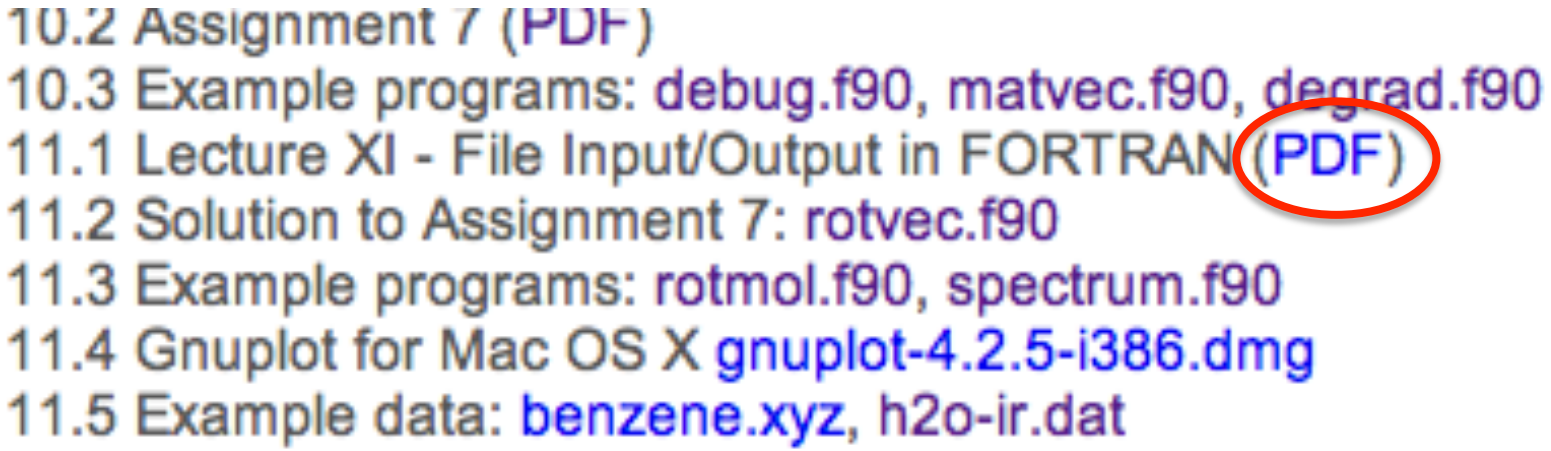


5 – Input/Output

- FORTRAN provides format specifiers for formatted input/output
- For example, the real number 5.0 can be written as “5”, “5.0”, “5.00”, “5.000”, etc.
- Similarly, the real number 5.0 can be written as 5.0*10**0 (=5.0E+00), 0.50*10**1(=0.5E+01), etc.
- The only format specifier we have seen so far is “*”, which is the DEFAULT format specifier.
- The format of a number by which it is printed using the “*” format specifier depends on the compiler and computer type.
- Therefore, it is recommended to use “formatted input/output” whenever possible, however, in this class, the time is insufficient and FORTRAN formatting is actually quite confusing.

5.3 The WRITE and READ Statements I

- The WRITE statement has a more complicated syntax than the PRINT statement, and is more general. It has the form:

```
WRITE (control-list) output-list
```

- The control-list may include items selected from the following:
  - A unit specifier, `UNIT = unit-specifier` or simply `unit-specifier` (the default unit specifier is "`*`", which corresponds to the terminal (-screen))
  - A format specifier, similar as in the PRINT statement, given as: `FMT= format-specifier` or simply `format-specifier` (the default format specifier is "`*`")

5.3 The WRITE and READ Statements II

- The READ statement has the form:

  READ (control-list) input-list

- Same as for the WRITE statement, the control-list for the READ statement may include items selected from the following:
  - A unit specifier, `UNIT = unit-specifier` or simply `unit-specifier` (the default unit specifier is "`*`", which corresponds to the terminal (-screen))
  - A format specifier, similar as in the PRINT statement, given as: `FMT= format-specifier` or simply `format-specifier` (the default format specifier is "`*`")

5.4 File Processing I

- Files on the computer hard disk need to be opened and closed by the FORTRAN program before the data can be read or written.
- Opening files is done using the OPEN statement:

```
OPEN (open-list)
```

- The open-list for the OPEN statement may include items selected from the following:
  - A unit specifier, `UNIT = unit-specifier` or simply `unit-specifier` (Note: the default unit "`*`" does NOT need to be opened)
  - A file specifier, given as: `FILE= character-expression` which can be a character constant or variable. Trailing blanks are ignored
  - A status specifier, given as: `STATUS= character-expression` which can be a character constant or variable as the following 'OLD' (file already exists), 'NEW' (file needs to be created), 'UNKNOWN' (file may or may not yet exist)

5.4 File Processing II

- Closing files is done using the CLOSE statement:

```
CLOSE (close-list)
```

- The close-list for the CLOSE statement may include items selected from the following:
  - A unit specifier, `UNIT = unit-specifier` or simply `unit-specifier` (Note: the default unit "`*`" does NOT need to be opened)
  - A status specifier, given as: `STATUS= character-expression` which can be a character constant or variable as the following 'OLD' (file already exists), 'NEW' (file needs to be created), 'UNKNOWN' (file may or may not yet exist)
  - An ERR = clause, where an integer variable can be obtained regarding the failure (non-zero value) or success (zero value) of the closing.

Applications of FORTRAN to Chemistry I

- Today, we will discuss two applications that involve both programming with arrays and File Input/Output (I/O).
- First example: rotation of a planar molecule (example: benzene) around the z-axis
- Second example: simulation of an IR spectrum by statistical broadening of computed vibrational frequencies and IR intensities of the water molecule

Applications of FORTRAN to Chemistry II

- Rotation of a planar molecule (oriented in the xy-plane) around the z-axis
- "xyz format": very popular format to specify molecular geometries
- Format:
  - 1st line: Number of atoms (NATOMS)
  - 2nd line: a title of 80 characters
  - 3rd to 2+NATOMS line: for each atom in the molecule, the specification of the chemical element, followed by x, y, z coordinates in units of Å (Ångstrom).

Applications of FORTRAN to Chemistry III

- Example: benzene.xyz (download from http://qc.chem.nagoya-u.ac.jp/teaching)

```
12
Benzene
C                  0.000000    1.396490    0.000000
C                 -1.209396    0.698245    0.000000
C                 -1.209396   -0.698245    0.000000
C                  0.000000   -1.396490    0.000000
C                  1.209396   -0.698245    0.000000
C                  1.209396    0.698245    0.000000
H                  0.000000    2.483191    0.000000
H                 -2.150506    1.241595    0.000000
H                 -2.150506   -1.241595    0.000000
H                  0.000000   -2.483191    0.000000
H                  2.150506   -1.241595    0.000000
H                  2.150506    1.241595    0.000000
```

X-coordinate Y-coordinate Z-coordinate

Applications of FORTRAN to Chemistry IV

- Rotation of the molecule around the z-axis can be performed by the following rotation matrix:

$$A = \begin{bmatrix} \cos\theta & \sin(\theta) & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Applications of FORTRAN to Chemistry V

- The rotated Cartesian coordinates of an atom in the planar molecule is given by the following matrix-vector product:

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix}$$

- This rotation has to be carried out for all atoms in the molecule.
- Download program “rotmol.f90” from http://qc.chem.nagoya-u.ac.jp/teaching), compile, and test using the “benzene.xyz” example

Applications of FORTRAN to Chemistry VI

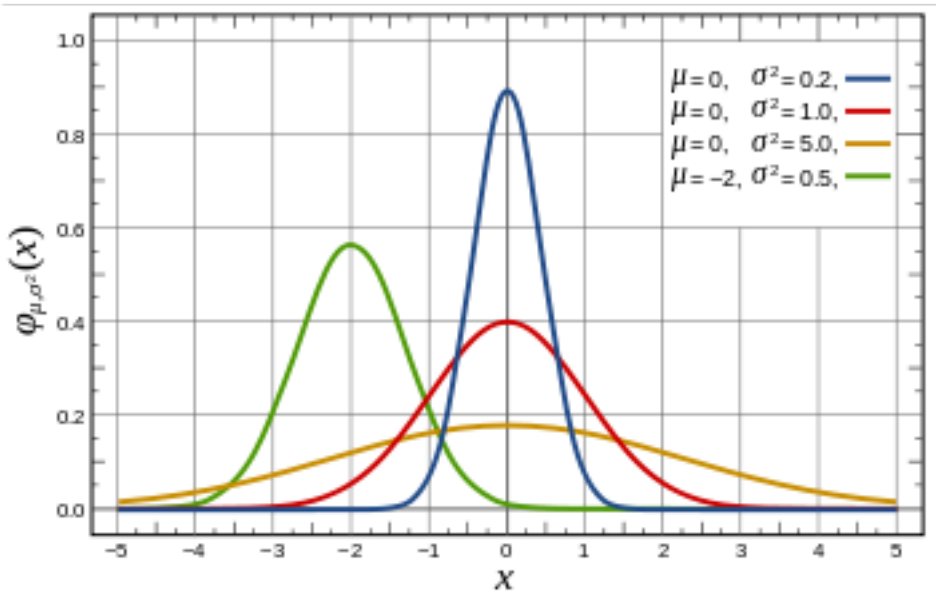
- Second example: Simulation of an IR spectrum.
- Example: IR spectrum of water.
- Sample data: Download “h2o-ir.dat” from http://qc.chem.nagoya-u.ac.jp/teaching:

1713.0153	75.7994
3727.3732	1.6952
3849.4717	19.3975

Applications of FORTRAN to Chemistry VII

- We wish to include thermal/solution effects. We include statistical changes in the vibrational frequencies by assuming a Gaussian normal distribution:

$$f(x) = e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$



Source: wikipedia

Applications of FORTRAN to Chemistry VIII

- Download program “spectrum.f90” from http://qc.chem.nagoya-u.ac.jp/teaching), compile, and test using the “h2o-ir.dat” example
- Plot the spectra for various choices of σ using the GNUPLOT software, also available on http://qc.chem.nagoya-u.ac.jp/teaching
- This concludes today’s lecture.