Computers in Chemistry – Lecture IV

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Get this lecture online

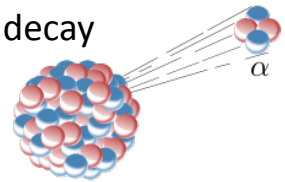
- Please go to: http://qc.chem.nagoya-u.ac.jp
- Click on "Teaching" (English website only, sorry!)
- Click on "PPT" link of "4.1 Lecture IV – Programming and problem solving"

  userid: qcguest, password: qcigf!

3.2 Assignment 3 (PDF)
3.3 Example programs: hello.c hello.f
4.1 Lecture IV - Programming and problem solving (PDF)
4.2 Assignment 4 (PDF)
4.3 Part of Chapter 1 by NL (English) (Japanese)
4.4 Example program: fig1-8.f90 (Radioactive Decay)

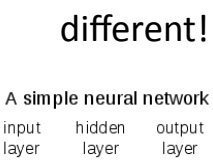
Today's Lecture

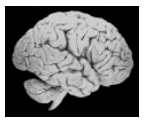
- The "art" of programming and problem solving
- Five steps of program development
- A specific example: radioactive decay
- Flow charts
- Key concepts in FORTRAN 90



The "art" of programming

- Human brain and computer is ***radically*** different!





Not digital: fuzzy logic (continuous spectrum within [0,1])

Digital: binary logic (only "off"=0 and "on"=1 state)

Five Steps of Program Development I

- Step 1: Problem Analysis and Specification
- Step 2: Data Organization and Algorithm Design
- Step 3: Program Coding (the act of writing a program)
- Step 4: Compilation, execution and testing
- Step 5: Program maintenance

Five Steps of Program Development II

- Step 1: Problem Analysis and Specification

Example Problem (from NL page 6, check English or Japanese PDF files):

How much Polonium 210 (most widely available isotope) remains after 180 days if 10 milligrams were available initially? Note that the half-life of Polonium 210 is ~140 days.

Five Steps of Program Development III

Step 1 (continued): Analyze the problem and formulate a specification of it.

Input: what information is given

Output: what information must be produced to solve the problem

Input: initial amount of ^{210}Po, half-life, time-period

Output: Amount remaining

Five Steps of Program Development IV

Step 2: Data Organization and Algorithm Design

Determine how to organize and store the data in the problem

Develop procedures to process the data and produce the required output. These procedures are called algorithms

Example for Data Organization:

Input variables: 1) InitialAmount, 2) HalfLife, 3) Time

Output variable: AmountRemaining

Five Steps of Program Development V

Step 2 (continued): Data Organization and Algorithm Design

Algorithm Design: What needs to be done?

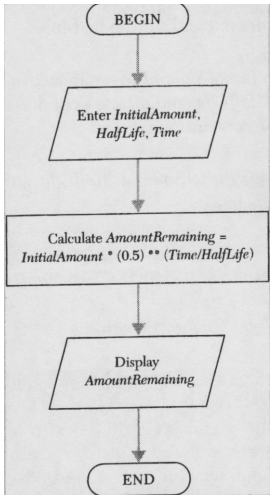
1. Get values for InitialAmount, HalfLife, and Time
2. Compute the value of AmountRemaining using a mathematical formula
3. Display AmountRemaining

Five Steps of Program Development VI

Step 2 (continued): Data Organization and Algorithm Design

Express this by a **flow chart:**

1. Get values for InitialAmount, HalfLife, and Time
2. Compute the value of AmountRemaining using a mathematical formula
3. Display AmountRemaining



Five Steps of Program Development VII

Step 3: Program Coding (writing)

Usually, we use an editor to write a file that contains the program, such as “pico” (see lecture III)

In this case, get the program from QC website (Ctrl-Click and save):

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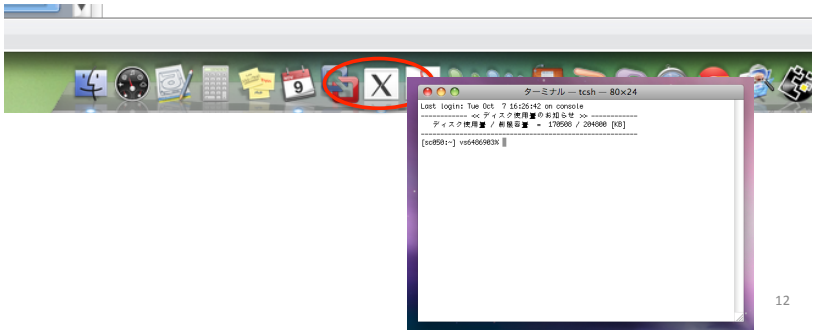
Five Steps of Program Development VIII

Step 3 (continued): Program Coding (writing)

Check that the program exists on your home directory ($HOME):

Login to X-windows, which opens a terminal



Five Steps of Program Development IX

Step 3 (continued): Program Coding (writing)

Type “ls”: check that the program fig1-8.f90 exists in your directory.

Type “pico fig1-8.f90” which opens the pico editor with your file. If you are happy with this file, exit pico by <Ctrl-X>

Five Steps of Program Development IX

Step 4: Compilation, execution, and testing

Compile: Type “gfortran –o fig1-8.x fig1-8.f90” – this should produce no output if everything was successful.

Execute: Type “./fig1-8.x”

You will see:

```
Enter initial amount (mg) of substance, its half-life (days)<
and time (days) at which to find amount remaining:
```


Five Steps of Program Development X

Step 4 (continued): Compilation, execution, and testing

Enter answers and you will see:

```
 10, 140, 180
Amount remaining =   4.101677     mg
```

Play with the input and output. For instance, the half-time of Cs 137 is ~30.2 years = 11023 days

This concludes today’s lecture.