計算機およびソフトの準備

- Unix/Linux on PC-Win:**Let's install cygwin**
- （必須ではありませんが，DL-POLYがPC-Win上でも動きます。自分なりにMDのプログラムを変更したりすることも可能ですので，ぜひソースコードからコンパイルして実行ファイルを作ることをおすすめします。また，PCwinとUnixマシーンとの接続にも便利です。cygwinはとてもpopularなsoftwareです。sokolovさんも使ってました。)

- http://www.cygwin.com/

- http://programnet.hp.infoseek.co.jp/coloum/colum.html　第１回から第４回までのインストール，第７回のsshのインストール

- http://journal.mycom.co.jp/special/2002/cygwin/index.html　　ここも参考に。

We need gcc(ver4 more）+ FORTRAN. Please install g95 from the site below

http://www.g95.org/　　<<　cygwin binary is OK.

- You can find the DL-POLY source code(program) at
- d54649@sakura.kudpc.kyoto-u.ac.jp
- /home/d/d54649/DL_POLY
- dl_poly_2.17.tar.gz dl_poly_3.07.tar.gz

How to file-transfer the source code? :sftp command

- **sftp d54649@sakura.kudpc.kyoto-u.ac.jp**
- d54649@sakura.kudpc.kyoto-u.ac.jp's password?: ********** [ask me if you don't know. It is the same passwd to modify new lab HomePage. = MY's nickname+217]
- sftp> **cd DL_POLY**
- sftp>**ls**
- dl_poly_2.17.tar.gz
- dl_poly_3.07.tar.gz
- sftp> **get dl_poly_2.17.tar.gz**
- sftp> **get dl_poly_3.07.tar.gz**
- sftp> **quit**
- your home > **gunzip dl_poly_2.17.tar.gz**
- your home **> tar xvf dl_poly_2.17.tar**
- **以上。 winscp等のソフトでも** file-transfer可能です。

- 研究室内の使用は自由に使っていいアカデミックライセンスを頂いております。研究室外であれば直接W. Smithのサイトhttp://www.cse.scitech.ac.uk/ccg/software/DL_POLY/からregistrationして使用してください。

How to compile the source code (program) to make executable binary file?: in the case of cygwin

- copy DL_POLY/dl_poly_2.17/build/makeWIN to DL_POLY/dl_poly_2.17/srcf90/Makefile
- cd DL_POLY/dl_poly_2.17/srcf90
- type “make cygwin-g95”
- If there is no error, you can find a “executable file” DLPOLY.X in the DL_POLY/dl_poly_2.17/execute directory. Now you can run MD code.
- If it does not work, check the g95 and gcc are installed correctly (or ask someone else. It’s faster!)

- cygwin 補足：PCの容量にもよるがなるべく多くのオプションを選択する。
- makeは必須だがオプションになっている。
  - gcc text.c　で　a.exe　で動くと思います。コマンドはすべて打ち込んでください。
  - x端末が使えるようになるとマウスも使えます。（それ以外の方法でも使えるようです。）
  - DL_POLY.X ができた人は,
  - dl_poly_2.17/data/TEST3/VV　にcd　で移動し
  - 1）cp OUTPUT OUTPUT_keep
  - 2) DLPOLY.X をdl_poly_2.17/execute/DLPOLY.Xからコピーしてください。
  - 3) ./DLPOLY.X
  - でMDが動きます。
  - 内容は　TEST3　- Valinomycin molecule in water. 3837 atoms.です。
  - OUTPUTの最後の方の出力が以下のようになるかチェックください。（OUTPUT_keepとは微妙にちがいますね。？？）
  - ---
  - step　eng_tot　temp_tot　eng_cfg　eng_vdw　eng_cou　eng_bnd　eng_ang　eng_dih　eng_tet
  - time(ps)　eng_pv　temp_rot　vir_cfg　vir_vdw　vir_cou　vir_bnd　vir_ang　vir_con　vir_tet
  - cpu (s)　volume　temp_shl　eng_shl　vir_shl　alpha　beta　gamma　vir_pmf　press
  - ---
  - 500 -9.2499E+03 3.0933E+02 -1.1595E+04 1.9096E+03 -1.3600E+04 0.0000E+00 7.6160E+01 1.9610E+01 0.0000E+00
  - 1.000 -9.0291E+03 3.0816E+02 1.8454E+03 -5.0936E+04 1.4077E+04 0.0000E+00 0.0000E+00 1.8875E+03 0.0000E+00
  - 200.96 3.9370E+04 0.0000E+00 0.0000E+00 0.0000E+00 9.0000E+01 9.0000E+01 9.0000E+01 0.0000E+00 3.6180E-01
  - r.m.s. 3.8947E-01 4.2466E+00 3.1046E+01 6.2081E+01 6.9004E+01 0.0000E+00 5.1895E+00 2.9127E+00 0.0000E+00
  - fluctn. 2.0614E+02 6.6820E+00 6.1084E+02 8.1895E+02 1.2696E+02 0.0000E+00 0.0000E+00 2.7855E+02 0.0000E+00
  - 1.5060E-11 0.0000E+00 0.0000E+00 0.0000E+00 2.6430E-14 2.6430E-14 2.6430E-14 0.0000E+00 3.4955E-01
  - ---
  - これでMDは動きました。あとは入力ファイルの作成です。

TEST3 benchmark

Valinomycin molecule in water. 3837 atoms, 1 ps simulation

	CPU time
IBM Power5+ (fermi.ehcc.kyoto-u.ac.jp)	270 s
SGI Origin(化研origin.scl.kyoto-u.ac.jp)	500 s
Intel Itanium2 (landau.ehcc.kyoto-u.ac.jp)	230 s
Intel Pentium4 (YK machine, 416 3GHz, NN machine 2.8GHz)	755, 610, 702 s
Intel CeleronM (YY machine)	1108 s
Intel 2x2.66GHz Dual Core Xeon(MY machine)	201 s (2CPUs?)

☞fastest

Intel Core 2 Duo 2.66GHz (room 416)	377 s (2CPUs?)

- Now you can run MD calculation. Congratulations!!

- In this occasion you can see the 3 input files CONTROL, FIELD, CONFIG at dl_poly_2.17/data/TEST3/VV

- We should make these 3 files **without error**!! (remember "Garbage in Garbage out!)

- For example, in ***CONTROL*** file, you may ask
- What means VV (integrator velocity Verlet?
- What means "ensemble nvt hoover 0.5"? What is the unit 0.5?
- What means "cutoff" or "rvdw cutoff"?

- How can we make forcefield in ***FIELD***?

- How can we make simulation cell size and atomic positions, velocity, force in ***CONFIG***?

- **You can see all of the meaning in the DL_POLY USER Manual Chap4, from the information you can make them from scratch, and can do MD simulation by yourself. But I strongly recommend that you should understand the meaning of these before you will jump in the MD simulation.**

4.1 The INPUT files

simulation cell, atomic position

simulation control variables such as temperature

force field

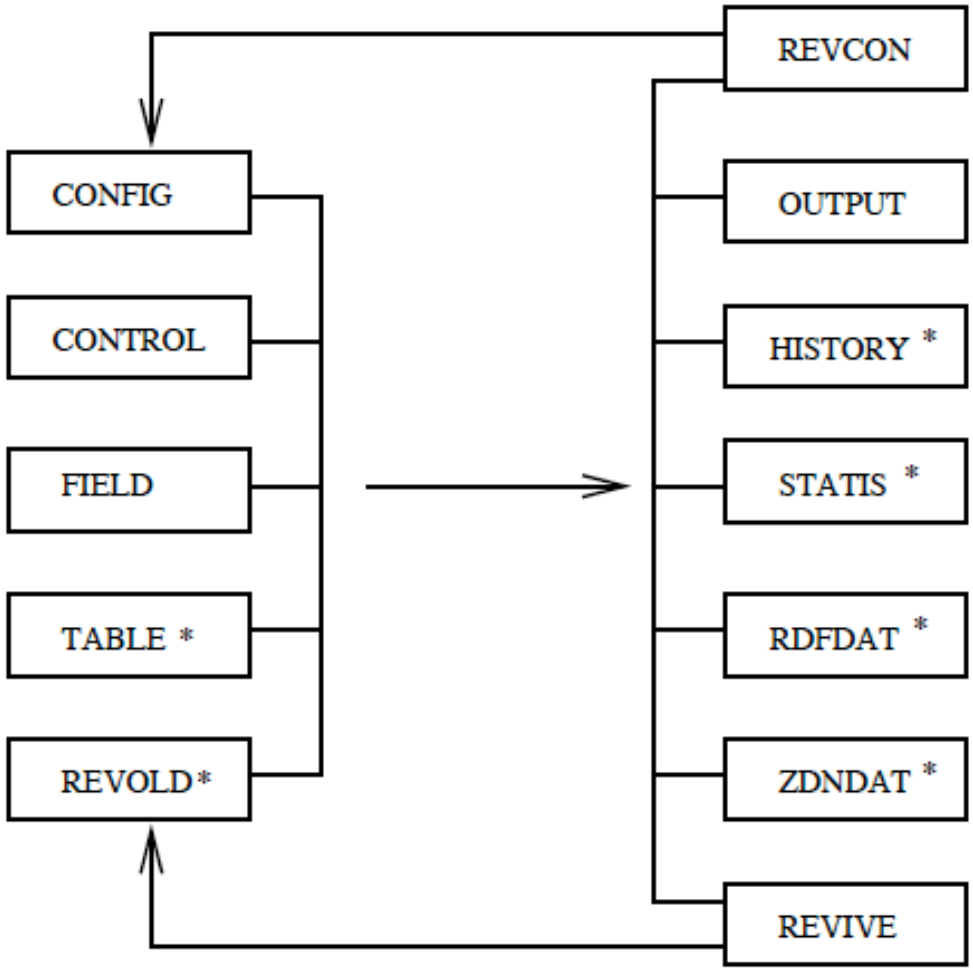

Figure 4.1: DL_POLY_2 input (left) and output (right) files. Note: files marked with an asterisk are non-mandatory.

DL_POLY_2 requires six input files named CONTROL, CONFIG, FIELD, TABLE, TABEAM and REVOLD. The first three files are mandatory, while TABLE and TABEAM are used only to input certain kinds of pair potential, and are not always required. REVOLD is required only if the job represents a continuation of a previous job. In the following sections we describe the form and content of these files.

TEST3: CONTROL

```
DL_POLY TEST CASE 3:Valinomycin in water

integrator velocity verlet
temperature      310.00
pressure         0.0000
ensemble nvt hoover 0.5

steps              500
equilibration      100
multiple step      1
restart scale
scale              1
print              1
stack              100
stats              5

timestep         0.0020
cutoff           12.000
delr width       1.2000
rvdw cutoff      10.000
shift
shake tolerance  1.0E-8
quaternion tolerance  1.0E-5

job time             6000.00
close time           100.00

finish
```

FIELD

```
DL_POLY TEST CASE 3:Valinomycin in water : forcefield
UNITS kcal
molecular types  2
Valinomycin
nummols 1
atoms 168     mass       charge    rept
   CT       12.0100     0.2820    3
   C        12.0100     0.4670    3
   CT       12.0100    -0.0183    3
   CT       12.0100    -0.1390    6
   CT       12.0100    -0.1495    3
   CT       12.0100    -0.0183    3
   CT       12.0100    -0.0730    2
   CT       12.0100    -0.1390    5
   CT       12.0100    -0.0730    1
   CT       12.0100    -0.1390    1
   CT       12.0100    -0.0183    3
   CT       12.0100    -0.1390    6
   C        12.0100     0.6920    3
   CT       12.0100     0.2720    3
   C        12.0100     0.4770    3
   CT       12.0100    -0.0730    3
   C        12.0100     0.6920    3
   H         1.0080     0.2110    2
   HC        1.0080    -0.0090    3
   HC        1.0080     0.0370    3
   HC        1.0080     0.0473   18
   HC        1.0080     0.0580    9
   HC        1.0080     0.0370    3
   HC        1.0080     0.0580    2

.......
```

CONFIG

```
DL_POLY TEST CASE 3:Valinomycin in water : structure
         2         4     53968     .2000000000E-02
      42.8612871524        .0000000000        .0000000000
        .0000000000      42.8612871524        .0000000000
        .0000000000        .0000000000      42.8612871524
CT              1
    -5.367652772       -4.974650238       -5.990217152
    -3.753414027       -2.997453843        4.469020573
    -4347.618322        785.7157385        1473.633382
CT              2
     3.003781357       -2.113965206       -9.072751563
    -.1064779764       -7.995944387       -2.124247219
    -7659.821296        7084.040034        1636.186068
CT              3
     .6161357221       -.7620477643        .2241570309
     .7626881371       -3.230043534        .5300852274
     672.8034938       -5115.436464        1472.292984
C               4
    -4.576445424       -6.095700053       -6.560959051
    -6.435542296       -2.986174745        .6915005257
    -11128.04339        313.0420425       -6860.330915
C               5
     4.017562150       -2.837127352       -8.279575916
     1.956722880       -2.753762280        .6392392670E-01
    -8757.712215        5604.322459        1079.930166
C               6
     .7083687555       -2.226753838        .7166232424
     2.665657890       -2.667111059        1.859027677
    -2433.464352       -3213.498004        7581.488044

........
```

In the next correspondence, I will explain
system with Ar atoms (gas, liquid, solid)

interatomic force only
vdW origin
periodic boundary condition
cut-off
minimum image convention
initial positions, velocity
equation of motion: Verlet, Leapfrog, Velocity Verlet

DL-POLY source code, unit, input files