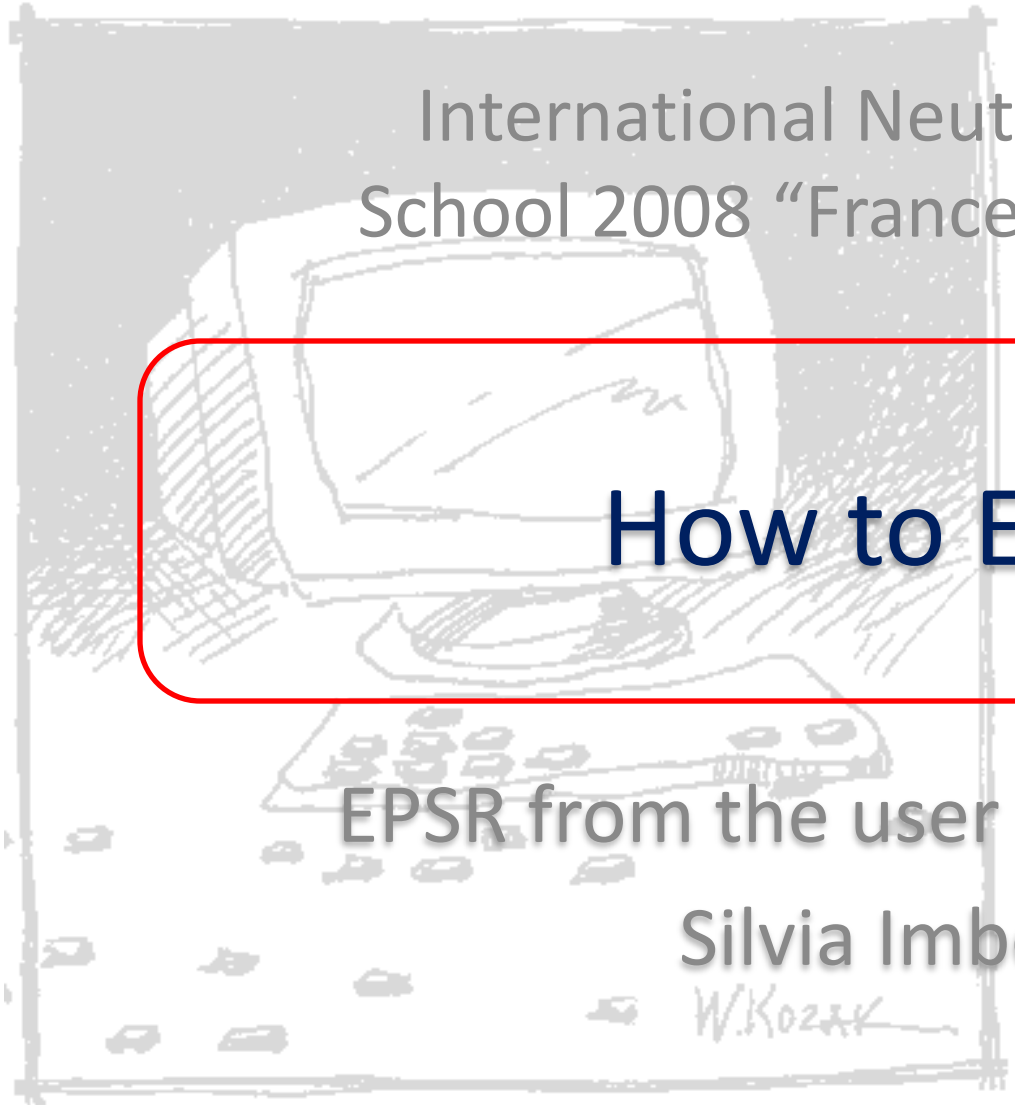


International Neutron Scattering School 2008 “Francesco Paolo Ricci”

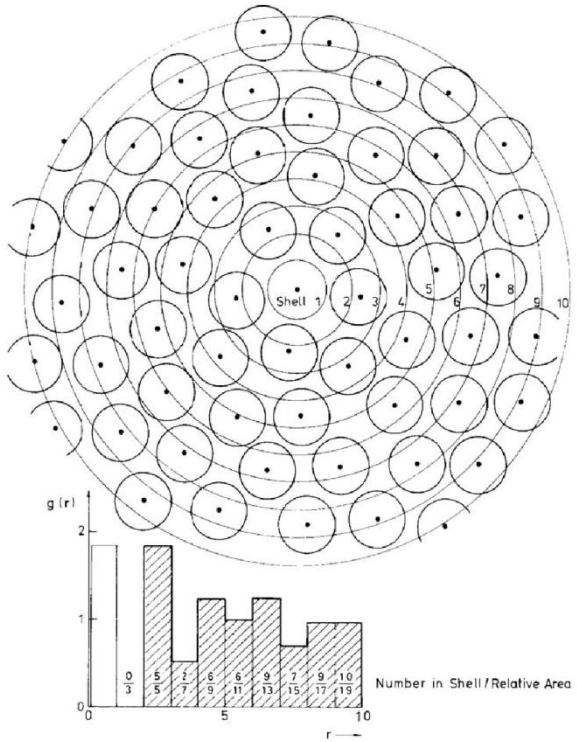
How to EPSR

EPSR from the user point of view

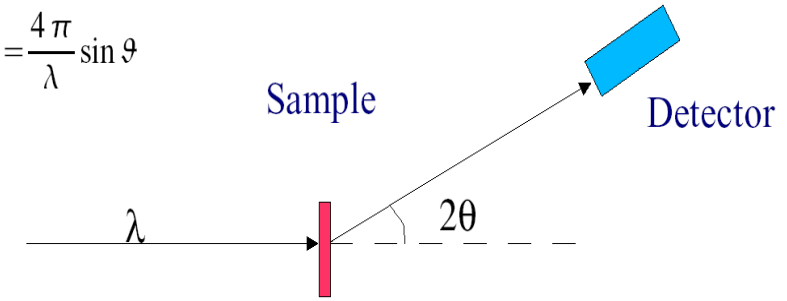
Silvia Imberti

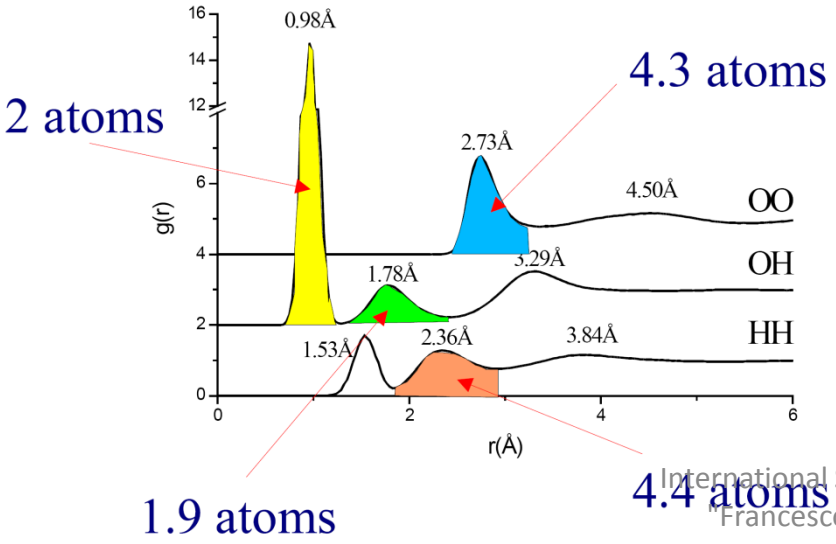
Science & Technology Facilities Council
ISIS

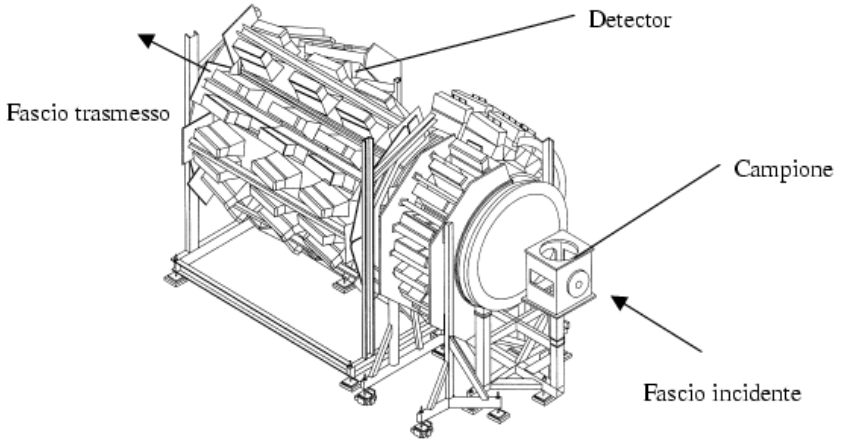
The Neutron Diffraction Experiment

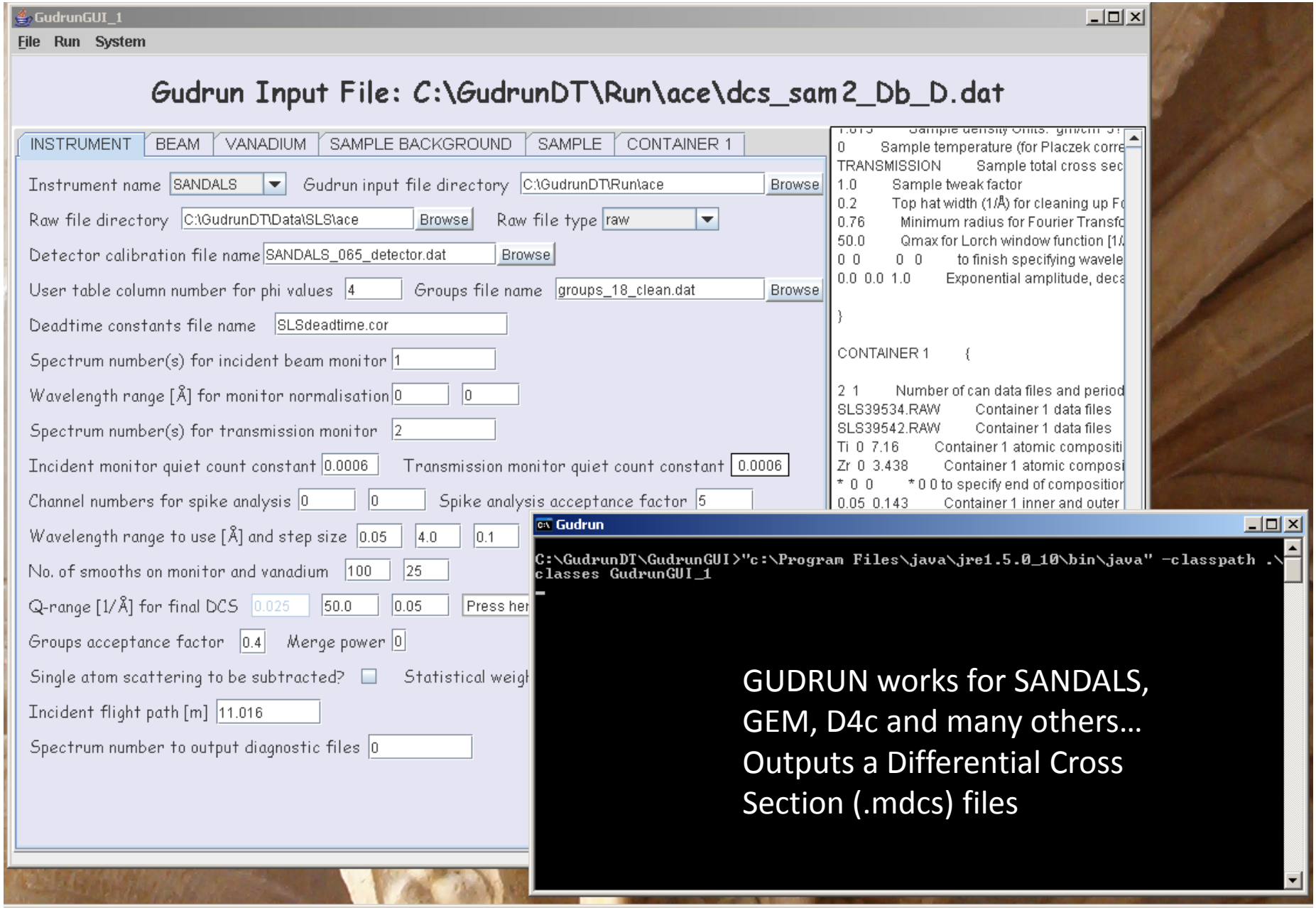


$$Q = \frac{4\pi}{\lambda}\sin\vartheta$$



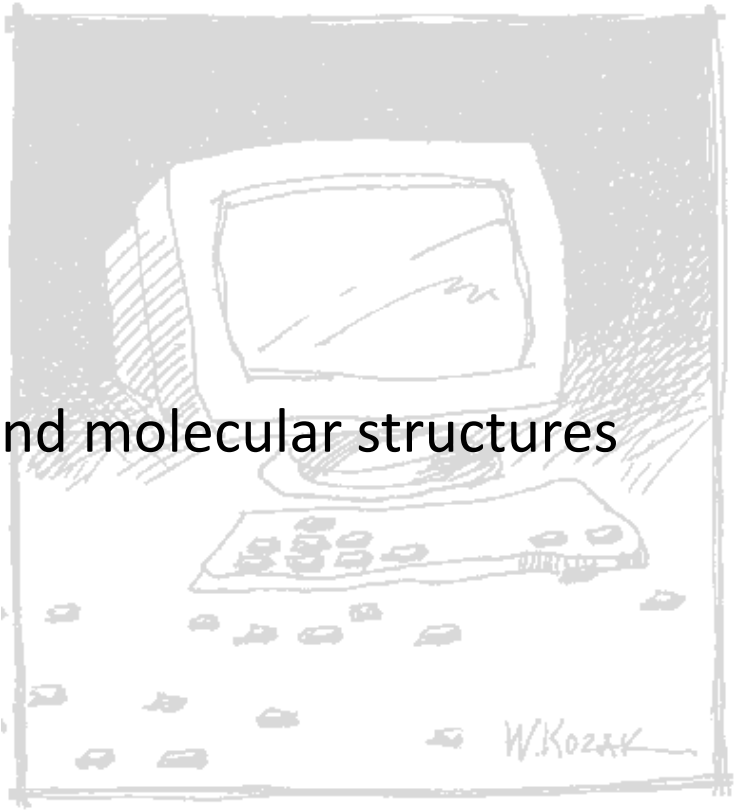





GudrunGUI_1
File Run System
Gudrun Input File: C:\GudrunDT\Run\ace\dcs_sam2_Db_D.dat
INSTRUMENT BEAM VANADIUM SAMPLE BACKGROUND SAMPLE CONTAINER 1
Instrument name SANDALS
Gudrun input file directory C:\GudrunDT\Run\ace
Browse
Raw file directory C:\GudrunDT\Data\SLS\ace
Raw file type raw
Detector calibration file name SANDALS_065_detector.dat
User table column number for phi values 4
Groups file name groups_18_clean.dat
Deadtime constants file name SLSdeadtime.cor
Spectrum number(s) for incident beam monitor 1
Wavelength range [Å] for monitor normalisation 0 0
Spectrum number(s) for transmission monitor 2
Incident monitor quiet count constant 0.0006
Transmission monitor quiet count constant 0.0006
Channel numbers for spike analysis 0 0
Spike analysis acceptance factor 5
Wavelength range to use [Å] and step size 0.05 4.0 0.1
No. of smooths on monitor and vanadium 100 25
Q-range [1/Å] for final DCS 0.025 50.0 0.05
Groups acceptance factor 0.4
Merge power 0
Single atom scattering to be subtracted?
Incident flight path [m] 11.016
Spectrum number to output diagnostic files 0
0 Sample temperature (for Placzek corre
TRANSMISSION Sample total cross sec
1.0 Sample tweak factor
0.2 Top hat width (1/Å) for cleaning up F
0.76 Minimum radius for Fourier Transfo
50.0 Qmax for Lorch window function [1/
0 0 0 0 to finish specifying wavele
0.0 0.0 1.0 Exponential amplitude, deca
}
CONTAINER 1 {
2 1 Number of can data files and period
SLS39534.RAW Container 1 data files
SLS39542.RAW Container 1 data files
Ti 0 7.16 Container 1 atomic compositi
Zr 0 3.438 Container 1 atomic composi
* 0 0 * 0 0 to specify end of composition
0.05 0.143 Container 1 inner and outer
Gudrun
C:\GudrunDT\GudrunGUI>"c:\Program Files\java\jre1.5.0_10\bin\java" -classpath .\classes GudrunGUI_1
GUDRUN works for SANDALS, GEM, D4c and many others… Outputs a Differential Cross Section (.mdcs) files

Empirical Potential Structure Refinement

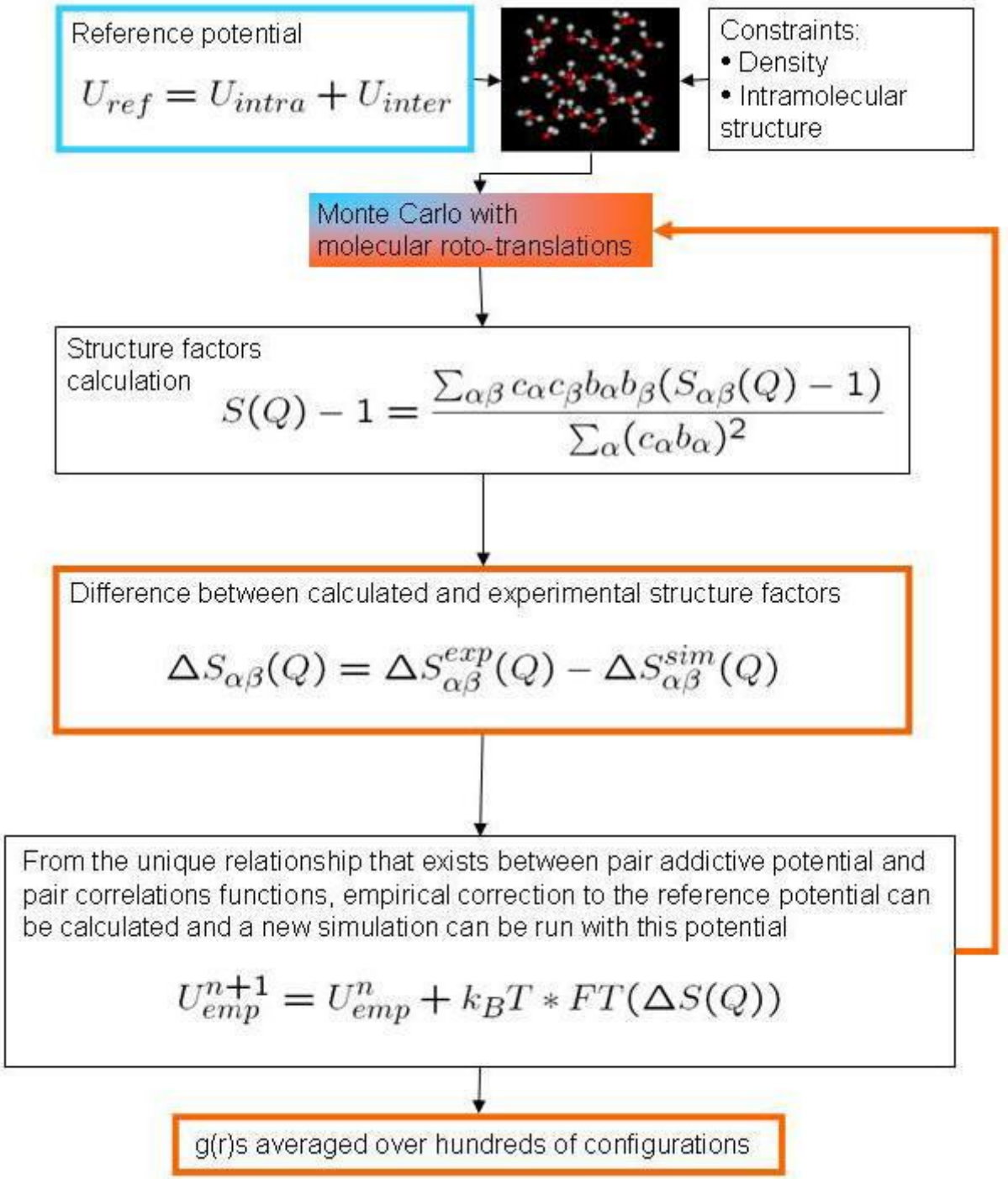
A computational method for building atomic and molecular structural models of disordered materials, such as liquids and glasses, that are consistent with available structural data and known physical/chemical constraints.



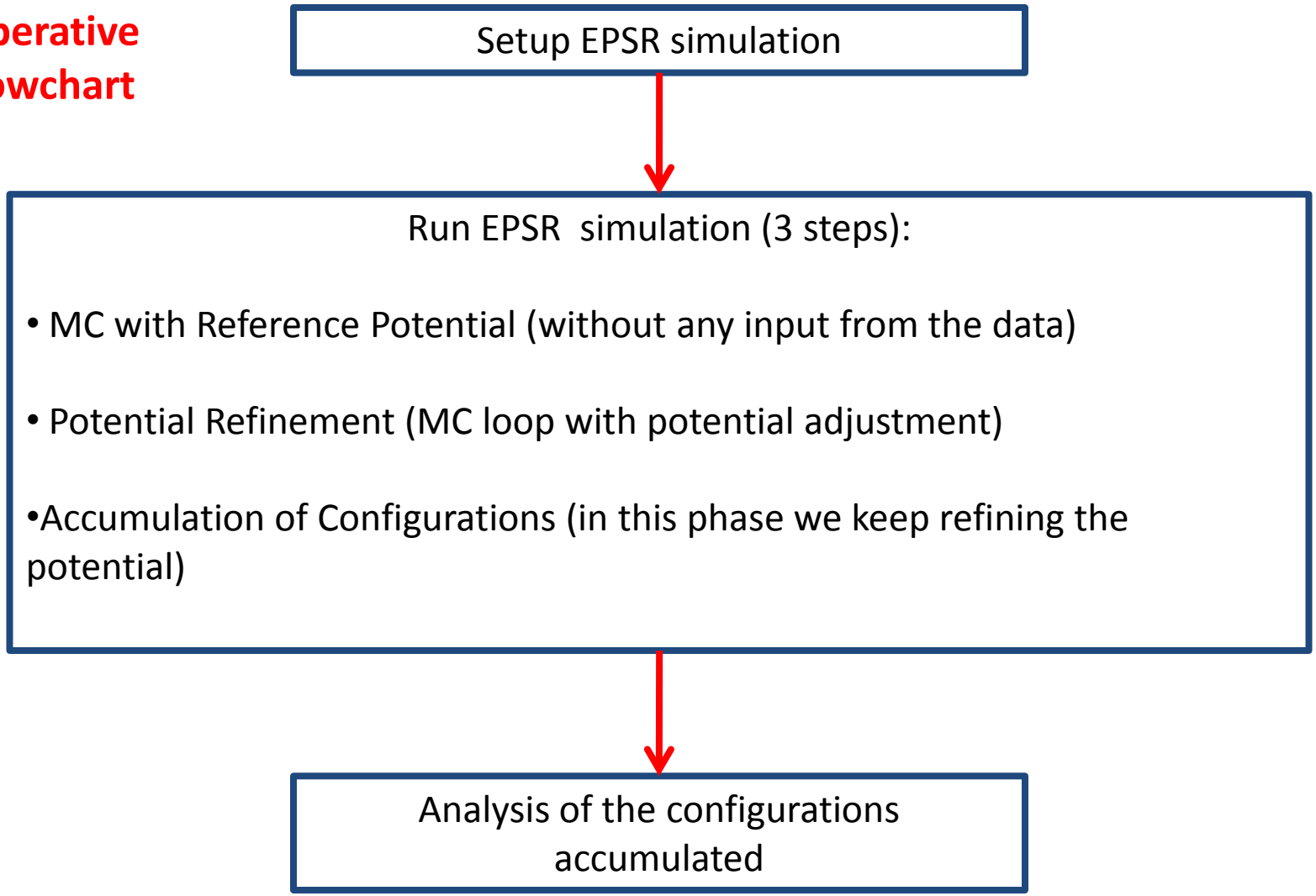
Three main ingredients:
(1) Experimental data
(2) Monte Carlo computer simulation
(3) Known constraints such as density and molecular structures

One principal output:
A 3-dimensional structural model

Logic flowchart



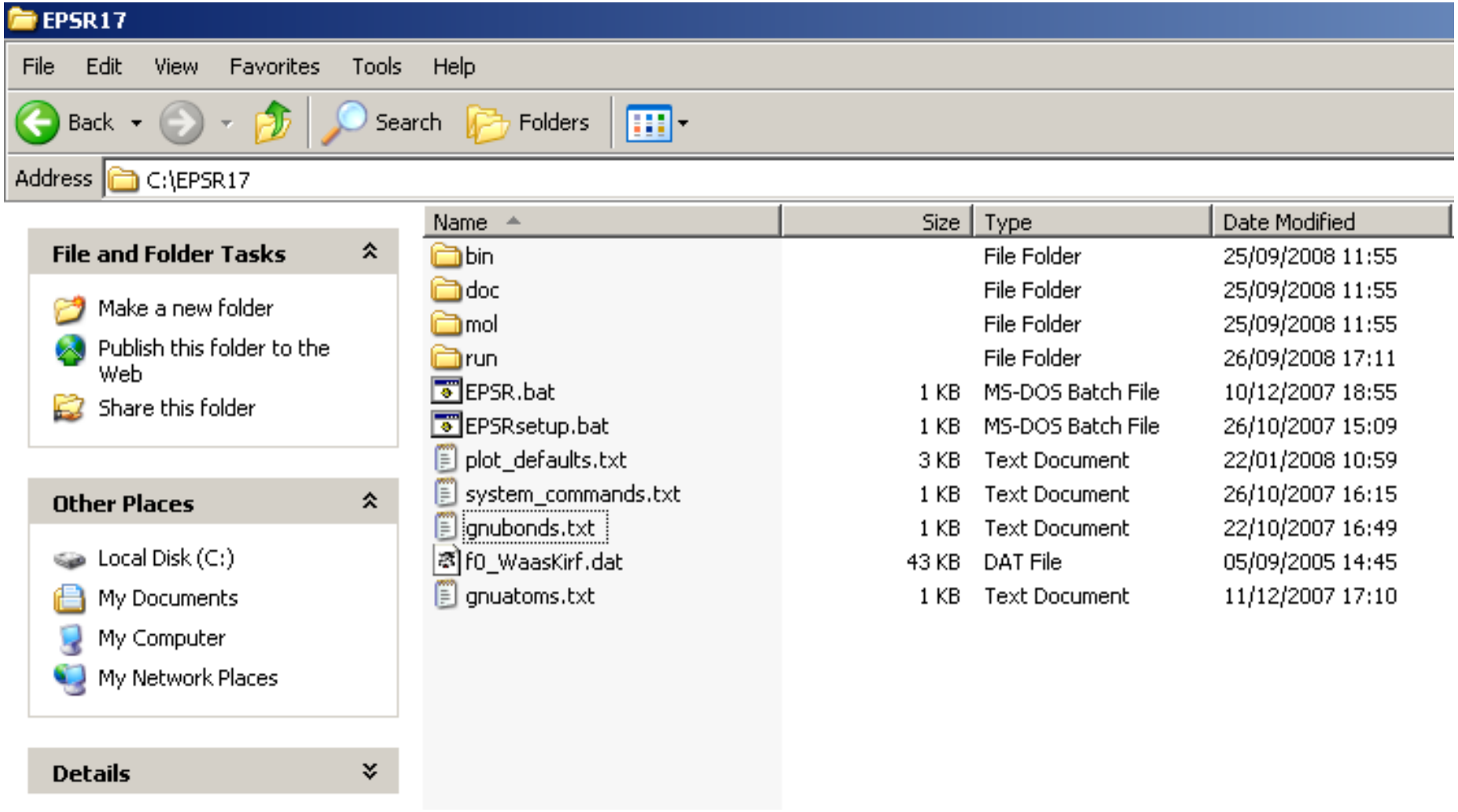
Operative flowchart



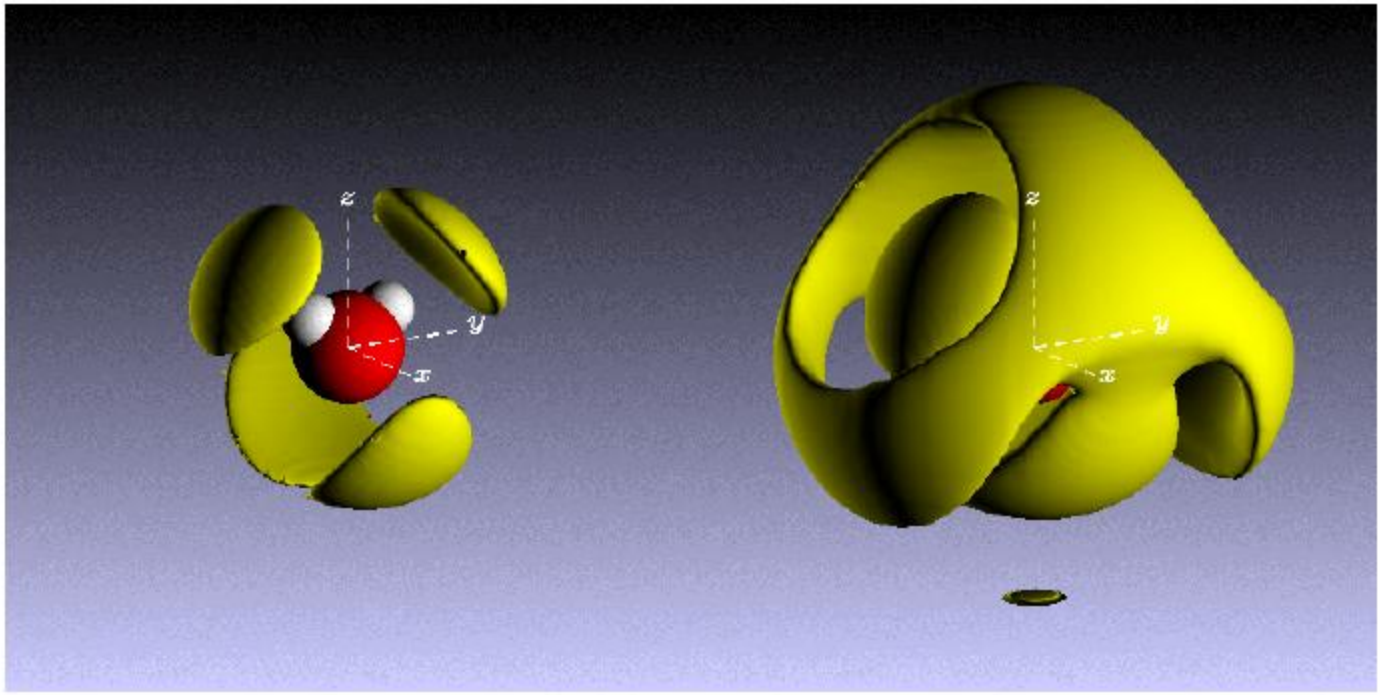
Getting started…

1) Google “EPSR neutron”

2) Download program, manual and examples from www.isis.rl.ac.uk\disorderedmaterials in C:\



- EPSRshell



A User's Guide

by

Alan K Soper

Read at least the first 3 chapters…

Then jump to the exercises or even to your own data…

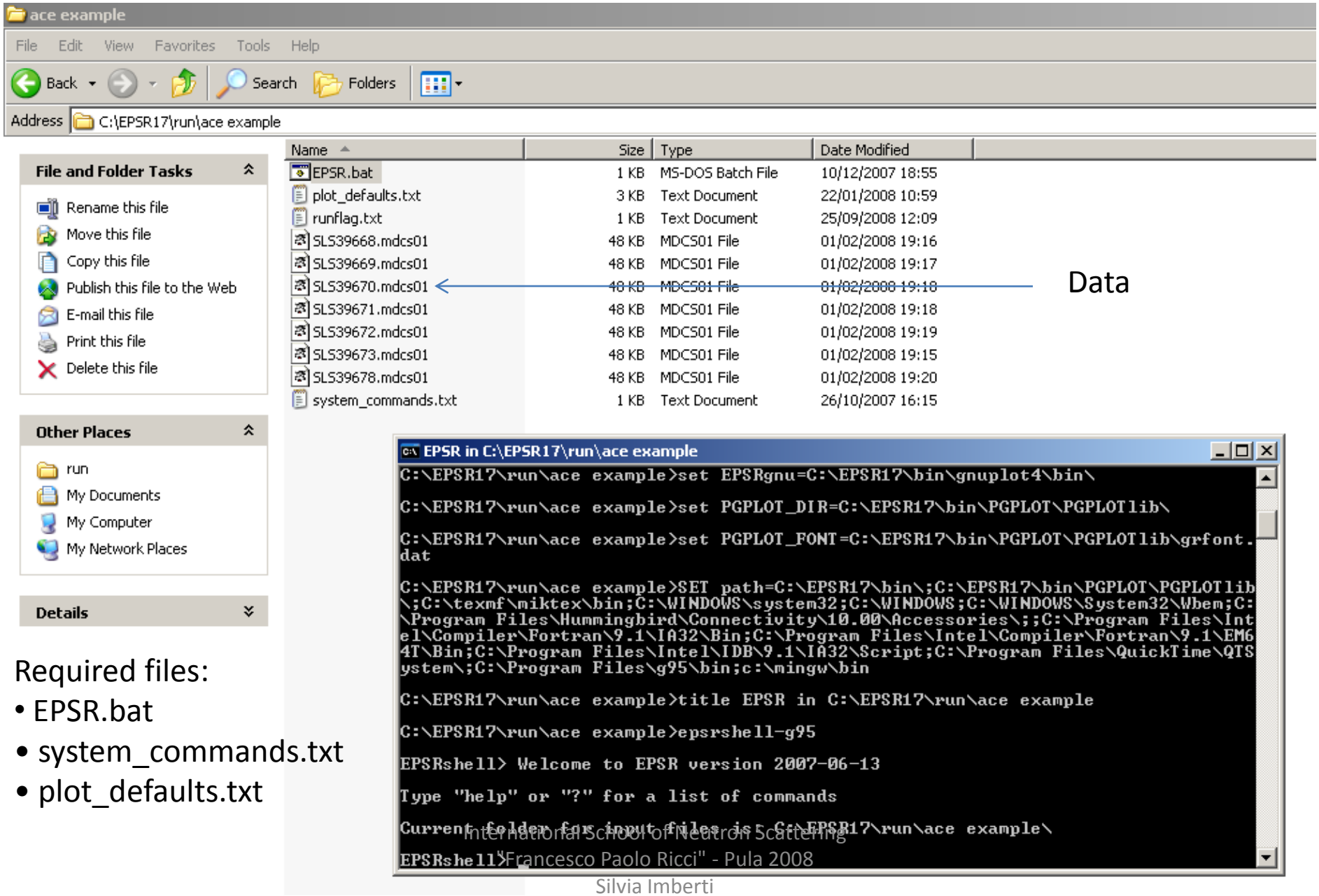
9. Appendices

9.1. Files you need to run EPSRshell
9.2. Example of system_commands.txt
9.3. Setting up EPSR to run under Windows

8. Some examples and exercises

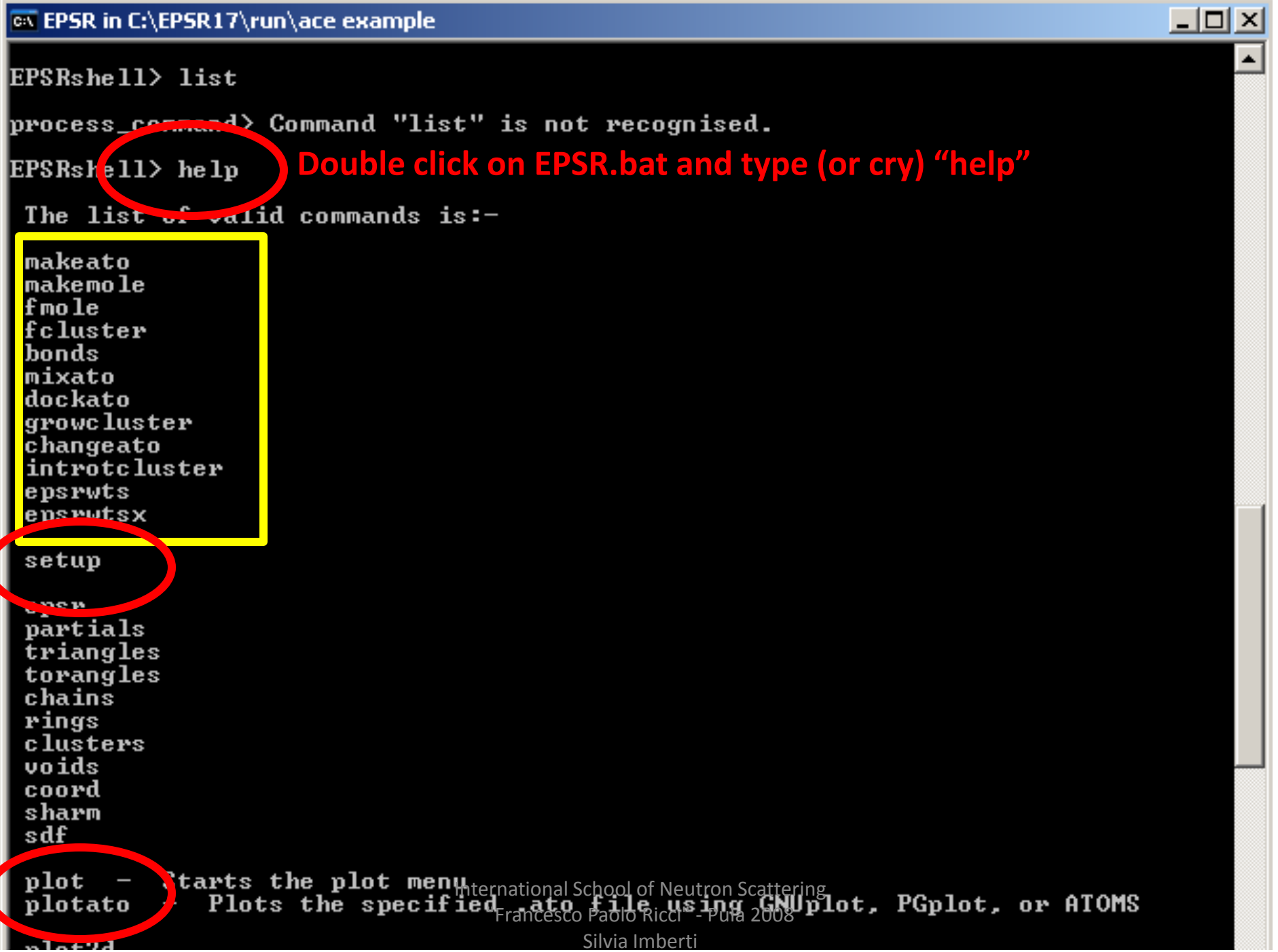
8.1. Single component Lennard-Jonesium.
8.2. Two component charged Lennard-Jonesium – NaCl.
8.3. Amorphous silica
8.4. Water.
8.5. Methanol.
8.6. Benzene.
8.7. Plot the spatial density function for methanol
8.8. Now try it with your own datasets!

Setup a working folder…



Required files:

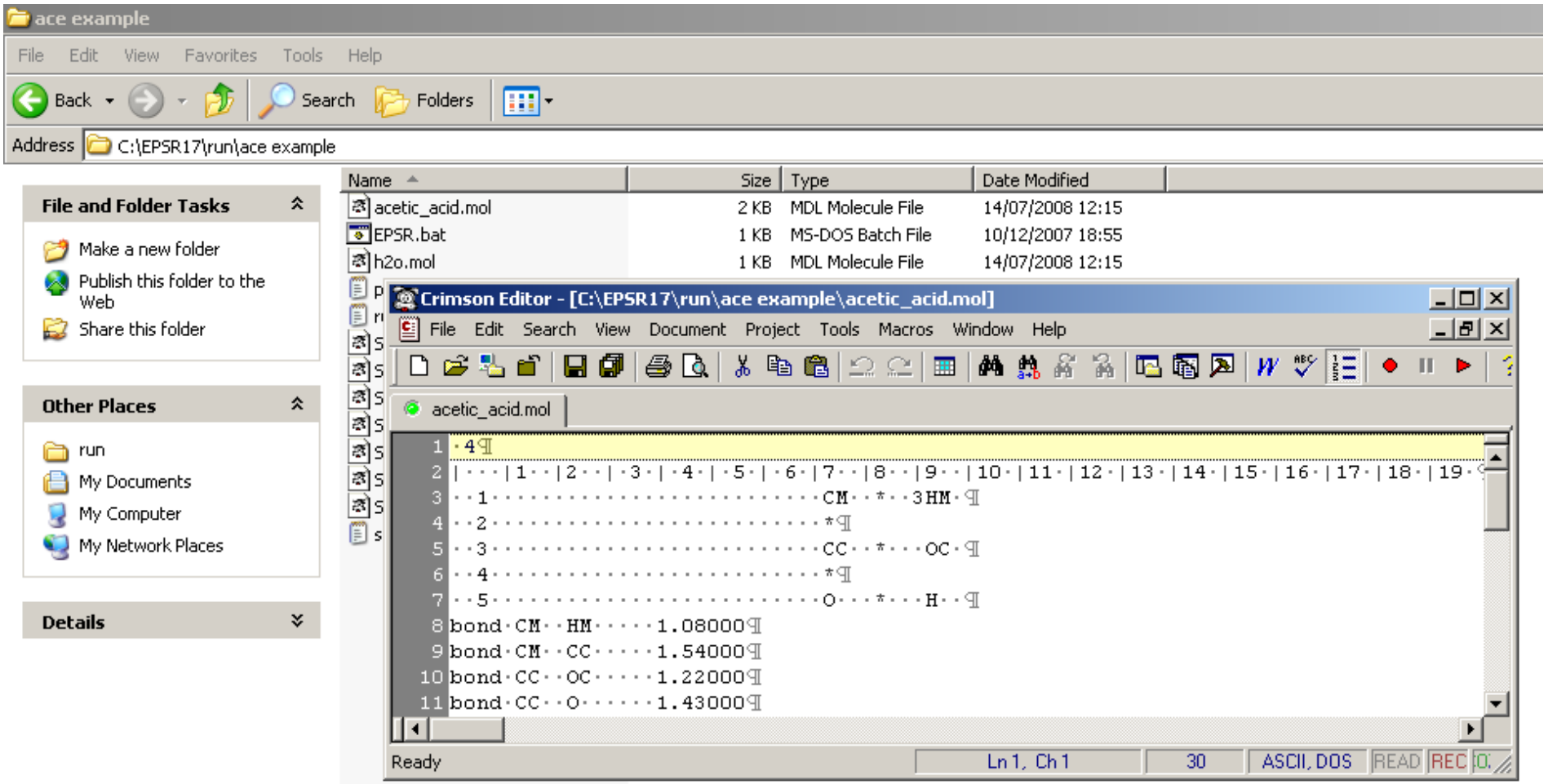
- EPSR.bat
- system_commands.txt
- plot_defaults.txt


EPSR in C:\EPSR17\run\ace example
EPSRshell> list
process_command> Command "list" is not recognised.
EPSRshell> help
Double click on EPSR.bat and type (or cry) “help”
The list of valid commands is:-
makeato
makemole
fmole
fcluster
bonds
mixato
dockato
growcluster
changeato
introtcluster
epsrwts
epsrwtsx
setup
partials
triangles
torangles
chains
rings
clusters
voids
coord
sharm
sdf
plot - Starts the plot menu
plotato - Plots the specified .ato file using GNUplot, PGplot, or ATOMS

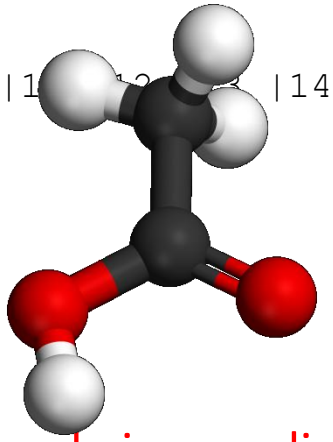
Setup a simulation box…

4. Preparing for an EPSR simulation.

4.1. Building the .**ATO** file – single atom molecules – **makeato**.
4.2. Making a molecule – **makeato.**
4.3. Making a molecule, role of the template file – **makemole**.
4.4. Running **fmole** to generate molecular coordinates.
4.5. Calculating intra-molecular atomic distances - **bonds**.
4.6. Modifying, mixing, growing, randomising the .**ato** file – **changeato, mixato, growcluster, introtcluster**.
4.7. Running **fcluster** to generate an initial configuration of molecules.
4.8. Building complex molecules and structures – **dockato.**


ace example
File Edit View Favorites Tools Help
Back Search Folders
Address C:\EPSR17\run\ace example
File and Folder Tasks
Make a new folder
Publish this folder to the Web
Share this folder
Other Places
run
My Documents
My Computer
My Network Places
Details
Name Size Type Date Modified
acetic_acid.mol 2 KB MDL Molecule File 14/07/2008 12:15
EPSR.bat 1 KB MS-DOS Batch File 10/12/2007 18:55
h2o.mol 1 KB MDL Molecule File 14/07/2008 12:15
Crimson Editor - [C:\EPSR17\run\ace example\acetic_acid.mol]
File Edit Search View Document Project Tools Macros Window Help
acetic_acid.mol
4
1 CM * 3 HM
2 *
3 CC * OC
4 *
5 O * H
bond CM HM 1.08000
bond CM CC 1.54000
bond CC OC 1.22000
bond CC O 1.43000
Ready
Ln 1, Ch 1
30
ASCII, DOS
READ
REC

```
 4
|    |1   |2   | 3 | 4 | 5 | 6 |7   |8   |9   |10 |11  |12  |13  |14 |15 |16 |17 |18 |19
  1                              CM   *   3HM
  2                              *
  3                              CC   *    OC
  4                              *
  5                              O    *    H
```



```
bond CM   HM      1.08000
bond CM   CC      1.54000
bond CC   OC      1.22000
bond CC   O       1.43000
bond O    H       0.96000
angle HM   CM   HM    109.28000
angle HM   CM   CC    109.28000
angle CM   CC   OC    120.00000
angle OC   CC   O     120.00000
angle CM   CC   O     120.00000
angle CC   O    H     104.50000
rot    5    1
```

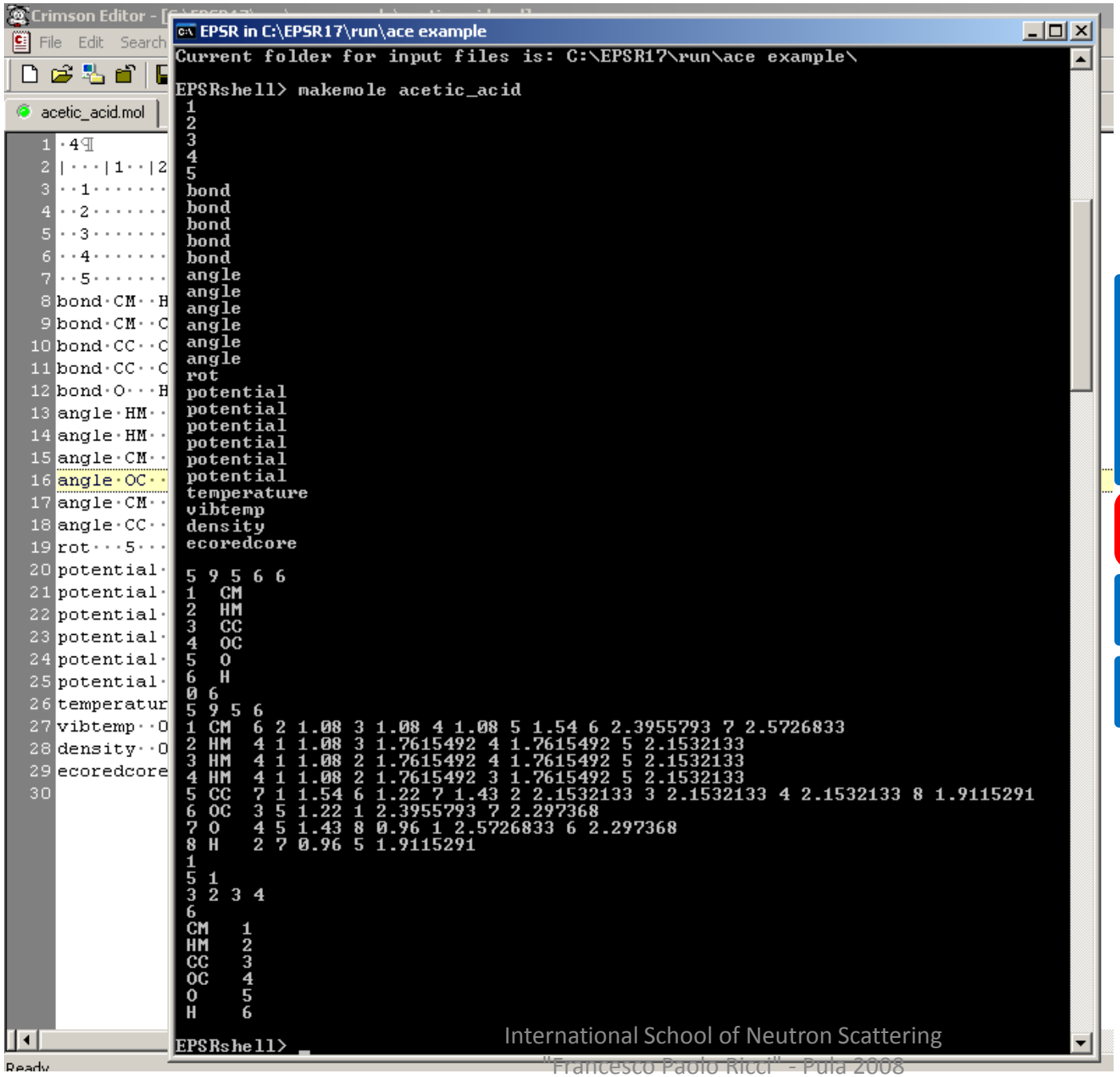
- If the molecule is complicated, I usually download the .pdb file, read it with (for example) Jmol and copy bonds, angles and dihedral angles
- We might think of having EPSR to read directly a .pdb file at some point…

```
potential CM    0.39000E+00  0.37000E+01  0.12000E+02  0.00000E+00 C
potential HM    0.65000E-01  0.18000E+01  0.20000E+01  0.00000E+00 H
potential CC    0.39000E+00  0.37000E+01  0.12000E+02  0.29700E+00 C
potential OC    0.58500E+00  0.30830E+01  0.16000E+02 -0.72800E+00 O
potential O     0.58500E+00  0.30830E+01  0.16000E+02 -0.72800E+00 O
potential H     0.00000E+00  0.00000E+00  0.20000E+01  0.43100E+00 H
temperature  0.300000E+03
vibtemp  0.650000E+02
density  0.100200E+00
ecoredcore     1.00000     3.00000
```

```
 4
|   |1  |2  | 3 | 4 | 5 | 6 |7  |8  |9  |10 |11 |12 |13 |14 |15 |16 |17 |18 |19
  1                           CM  *  3HM
  2                           *
  3                           CC  *   OC
  4                           *
  5                           O   *   H
bond CM  HM     1.08000
bond CM  CC     1.54000
bond CC  OC     1.22000
bond CC  O      1.43000
bond O   H      0.96000
angle HM  CM  HM   109.28000
angle HM  CM  CC   109.28000
angle CM  CC  OC   120.00000
angle OC  CC  O    120.00000
angle CM  CC  O    120.00000
angle CC  O   H    104.50000
rot   5   1
potential CM   0.39000E+00  0.37000E+01  0.12000E+02  0.00000E+00 C
potential HM   0.65000E-01  0.18000E+01  0.20000E+01  0.00000E+00 H
potential CC   0.39000E+00  0.37000E+01  0.12000E+02  0.29700E+00 C
potential OC   0.58500E+00  0.30830E+01  0.16000E+02 -0.72800E+00 O
potential O    0.58500E+00  0.30830E+01  0.16000E+02 -0.72800E+00 O
potential H    0.00000E+00  0.00000E+00  0.20000E+01  0.43100E+00 H
temperature  0.300000E+03
vibtemp  0.650000E+02
density  0.100200E+00
ecoredcore    1.00000    3.00000
```

The Lennard Jones potential and charges can searched in the literature and particularly useful are the following references:

(……)



Create a **.mol** file for each molecule you want to put into the box

makemole

.atm file

.ato file

Crimson Editor

File Edit Search View Document Project Tools Macros Window Help

acetic_acid.mol | acetic_acid.atm | acetic_acid.ato

C:\EPSR17\run\ace example\acetic_acid.ato

```
     1  0.430600E+01  0.300000E+03
   0.000E+00  0.100E+00  0.100E+01  0.100E+01  0.100E-01  0.650E+02
   8  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00     1
 CM          1
  0.00000E+00  0.00000E+00  0.00000E+00
  6    2 0.108E+01    3 0.108E+01    4 0.108E+01    5 0.154E+01    6 0.240E+01
    7 0.257E+01
 HM          2
  0.00000E+00  0.00000E+00  0.00000E+00
  4    1 0.108E+01    3 0.176E+01    4 0.176E+01    5 0.215E+01
 HM          3
```

C:\EPSR17\run\ace example\acetic_acid.atm

```
 4
|   |1  |2  |  3  |  4  |  5  |  6  |7  |8  |9  |10 |11 |12 |13 |14 |15 |16 |17 |18 |19
  1                            1   *  32
  2                            *
  3                            5   *   6
  4                            *
  5                            7   *   8
```

C:\EPSR17\run\ace example\acetic_acid.mol

```
 4
|   |1  |2  |  3  |  4  |  5  |  6  |7  |8  |9  |10 |11 |12 |13 |14 |15 |16 |17 |18 |19
  1                            CM  *  3HM
  2                            *
  3                            CC  *   OC
  4                            *
  5                            O   *   H
bond CM  HM     1.08000
```

Crimson Editor - [C:\EPSR17\run\ace example\acetic_acid.ato]

File Edit Search View Document Project Tools Macros Window Help

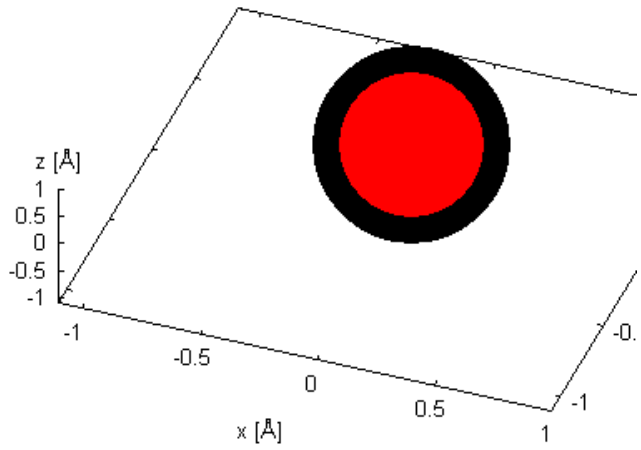
acetic_acid.mol | acetic_acid.atm | acetic_acid.ato

```
     1  0.430600E+01  0.300000E+03
     8  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00     1
 CM          1
  0.00000E+00  0.00000E+00  0.00000E+00
  6    2 0.108E+01    3 0.108E+01    4 0.108E+01    5 0.154E+01    6 0.240E+01
    7 0.257E+01
 HM          2
  0.00000E+00  0.00000E+00  0.00000E+00
  4    1 0.108E+01    3 0.176E+01    4 0.176E+01    5 0.215E+01
 HM          3
  0.00000E+00  0.00000E+00  0.00000E+00
  4    1 0.108E+01    2 0.176E+01    4 0.176E+01    5 0.215E+01
 HM          4
  0.00000E+00  0.00000E+00  0.00000E+00
  4    1 0.108E+01    2 0.176E+01    3 0.176E+01    5 0.215E+01
 CC          5
  0.00000E+00  0.00000E+00  0.00000E+00
  7    1 0.154E+01    6 0.122E+01    7 0.143E+01    2 0.215E+01    3 0.215E+01
    4 0.215E+01    8 0.191E+01
 OC          6
  0.00000E+00  0.00000E+00  0.00000E+00
  3    5 0.122E+01    1 0.240E+01    7 0.230E+01
 O           7
  0.00000E+00  0.00000E+00  0.00000E+00
  4    5 0.143E+01    8 0.960E+00    1 0.257E+01    6 0.230E+01
 H           8
  0.00000E+00  0.00000E+00  0.00000E+00
  2    7 0.960E+00    5 0.191E+01
    1
 ROT
    5    1
    3    2    3    4
```

EPSR in C:\EPSR17\run\ace_example

```
EPSRshell> plotato

Filename: acetic_acid.ato? (Type y to accept, u to go back, e to exit) y

minitc> Following molecule types found:-

   1 CM   0.10000E+01  0.10000E-01

minitc> Following molecule types found:-

   1 CM  acetic_aci  0.10000E+01  0.10000E-01
 3.7291057 4.306
 no. of molecules to read =      1     8     8     6  0.430600E+01
 79.840294 0.10020003
 Atomic fraction  1 =  0.12500E+00
 Atomic fraction  2 =  0.37500E+00
 Atomic fraction  3 =  0.12500E+00
 Atomic fraction  4 =  0.12500E+00
 Atomic fraction  5 =  0.12500E+00
 Atomic fraction  6 =  0.12500E+00
 no. of molecules to read =      1     8     6    21

plotato> Decide what kind of output you want:-

 1 = GNUplot
 2 = PGplot
 3 = ATOMS

plotato> ? 1

plotato> Specify whether to plot all molecules (1)

or several, centred about one particular molecule (2): 1
 1 8

plotato>   6 components available for plotting:-
   1 CM
   2 HM
   3 CC
   4 OC
   5 O
   6 H

plotato> Give number of components to plot, and component numbers: 6 1 2 3 4 5 6


plotato> Number of classes read from gnuatoms.txt =    13

plotato> Following atom classes will be plotted:-
   1 C
   2 H
   3 O

plotato> Min and max of plot =  -0.100000E+01  0.100000E+01

plotato> For each new bond: type two atom symbols,
 minimum and maximum lengths of bond, and radius of bond.
 Type 0 0 0 0 0 to end bond input or ste 0 0 0 0 for stereo pairs.

 plotato> ? 0 0 0 0 0

 plotato> Total number of bonds read in =  17

 plotato> Give overall scale factor on atom sizes: 1

 plotato> Give plot rotation about x and y (deg): 20 20
```

gnuplot graph



view: 20.0000, 20.0000 scale: 1.00000, 1.00000

7:18
7:18
7:18
7:18
7:18
7:18

cattering
2008

Setup a simulation box flowchart:

Create a **.mol** file for each molecule you want to put into the box

makemole

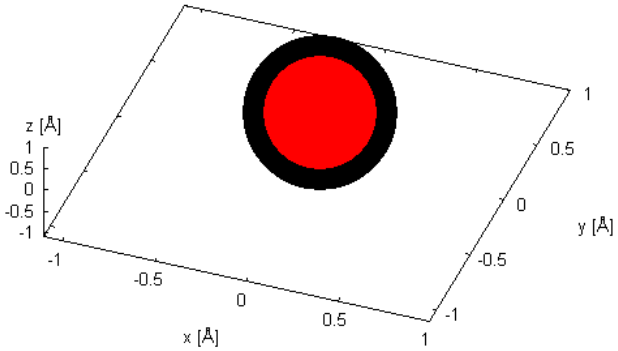
.atm file

.ato file

fmole

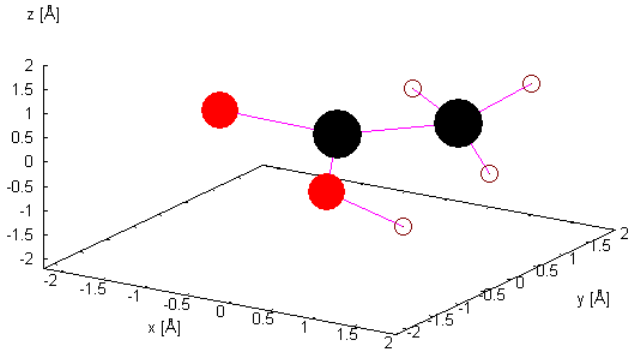
.ato file

plotato



view: 20.0000, 20.0000 scale: 1.00000, 1.00000

plotato



view: 59.0000, 32.0000 scale: 1.00000, 1.00000

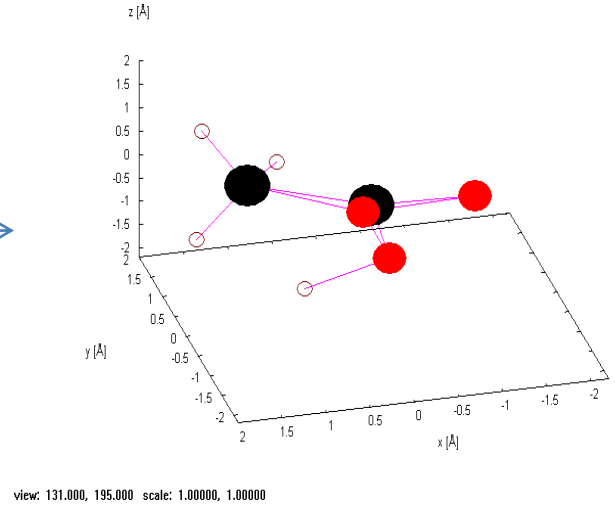
Density and relative composition of the system

.ato file

mixato

.ato file

plotato



WARNING! ROT groups defined BUT step size is ZERO!

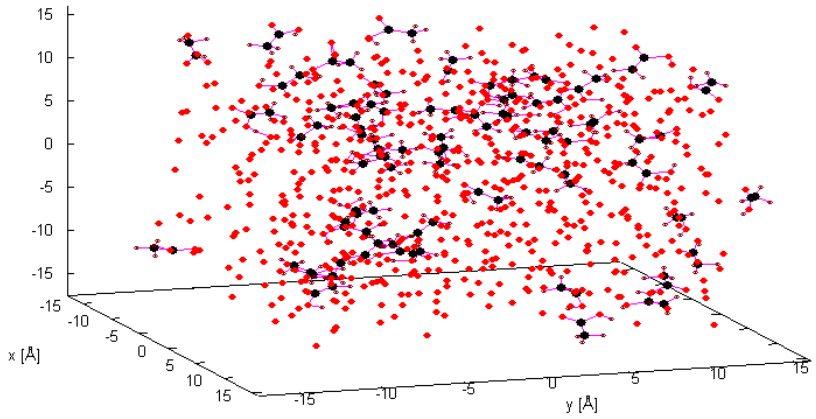
changeato (stepri=1)

introtcluster

fcluster

.ato file

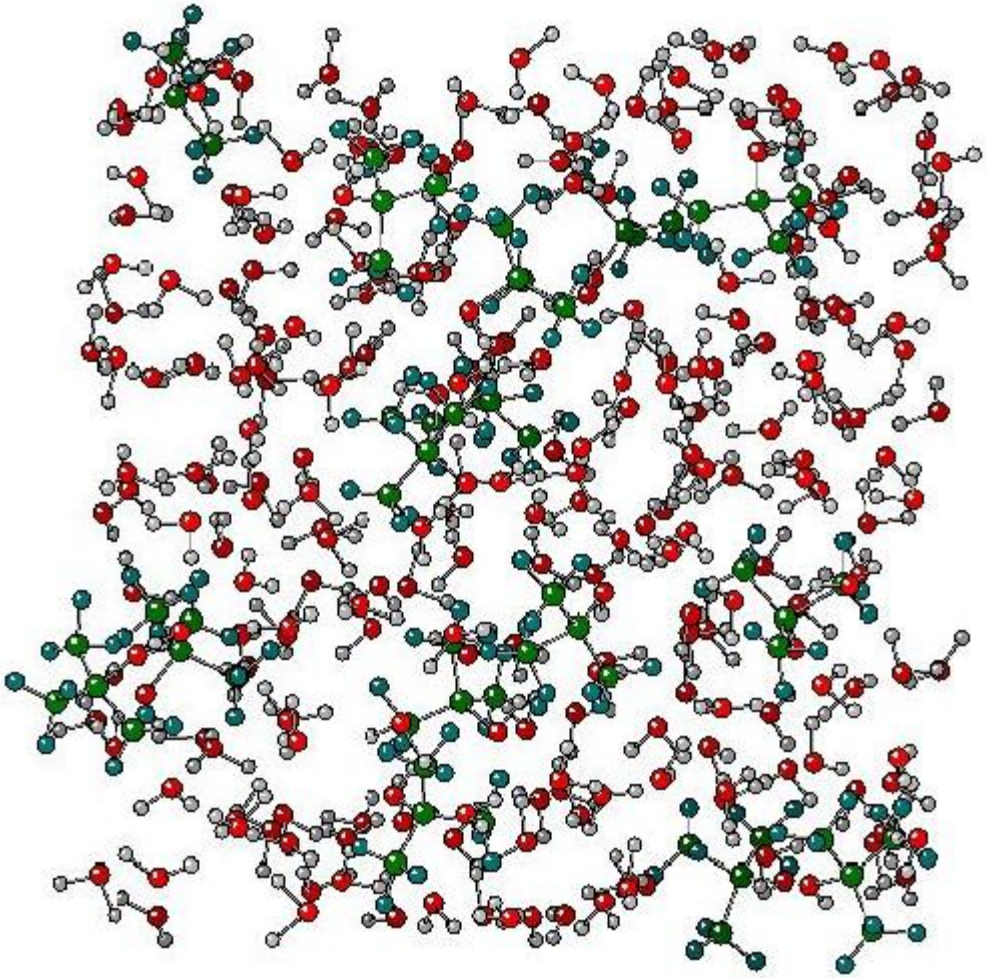
plotato

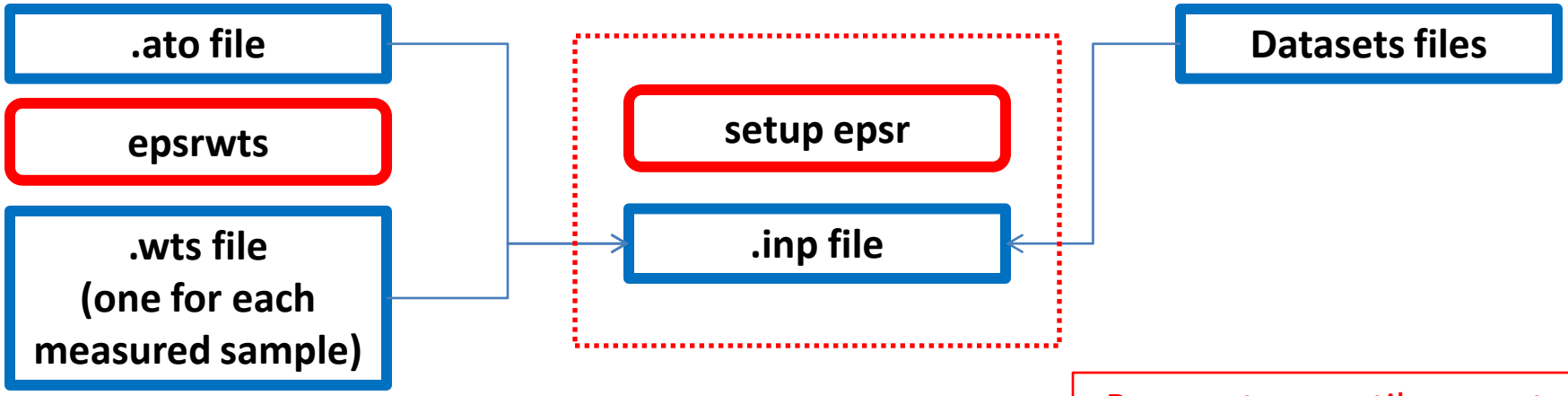


A box of atoms and molecules:

Cubic box of side length L/Å
A store of atomic coordinates:
Constraints on first and second neighbour distances within specific groups of atoms are one means by which it is possible to define molecules and maintain their shapes.

Key parameters for the box are:
(1) The density of atoms
(2) The total energy, U
(3) The total pressure



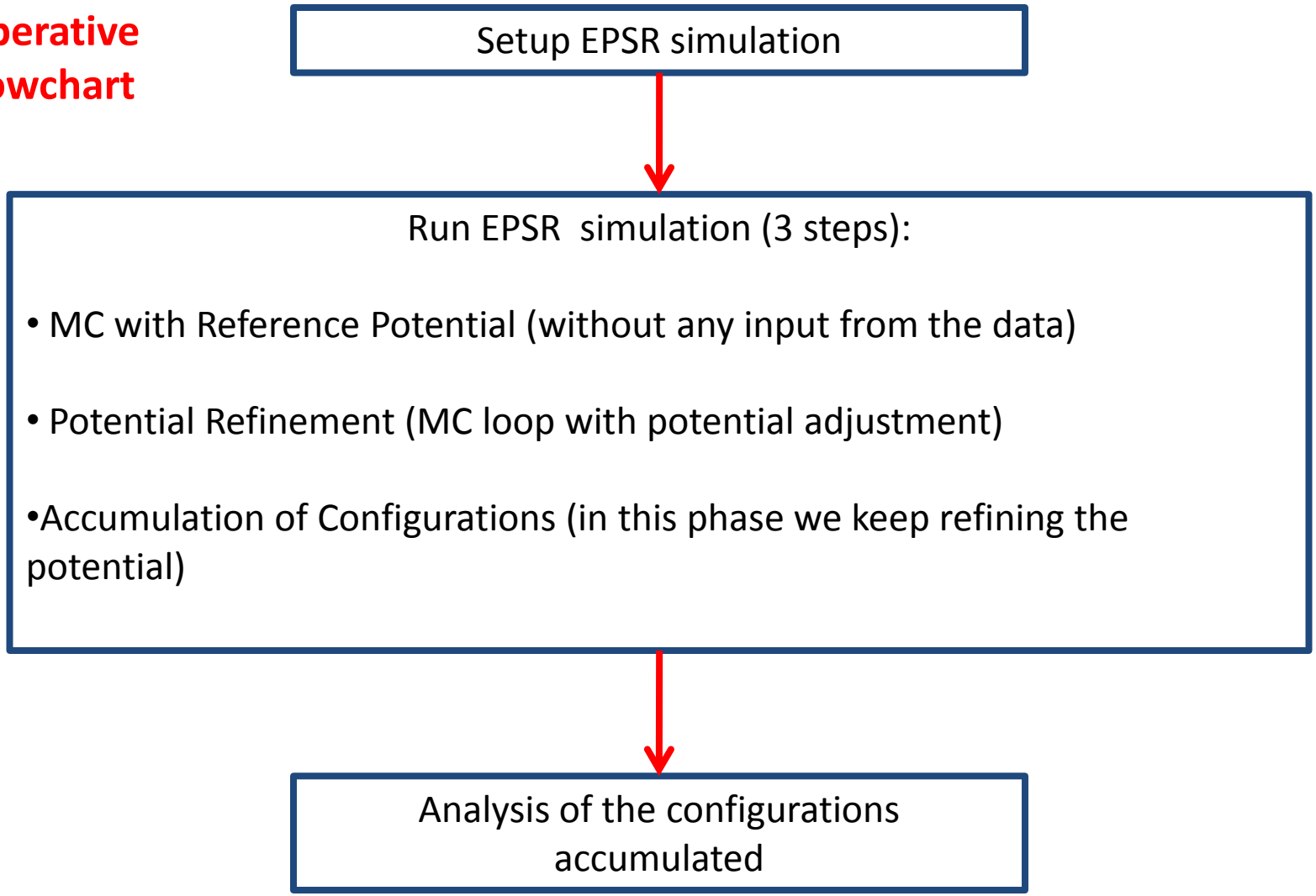



```
EPSRshell> setup epsr
setup_input_file> File class: "epsr"; file extension:

File Not Found

 No files of extension ".EPSR.inp" found in directory                    \"

 No files selected...

 Type the required filename with extension: ace

setup_input_file> Full filename = C:\EPSR17\run\ace_example\ace.EPSR.inp

setup_input_file> Problems with specified input file: ace.EPSR.inp

   - will use default values

Setup epsr>
```

- Press return until you get to the line you want to modify
- Press “u” if you want to go back
- Press “e” for save and exit

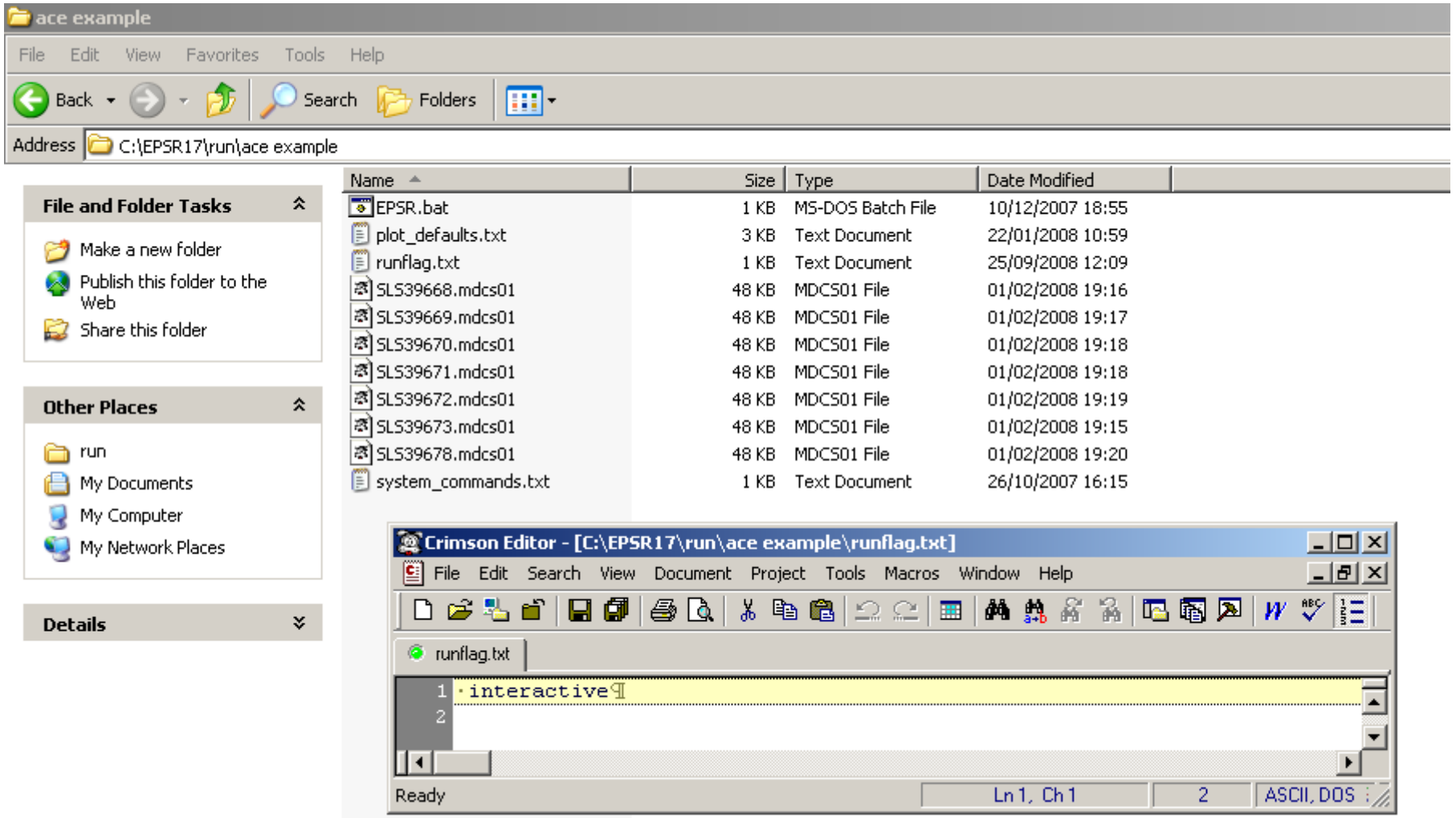
```
ace.EPSR                Title of this file
feedback    0.9                 Confidence factor - should be < 1. [0.8]
potfac      1.0                 1.0 to enable potential refinement, 0.0 to inhibit
ereq        10.00000                 Overall requested energy amplitude - overrules efilereq
sizefactor  1.0                 Multiplying factor for box dimension. [1.0]
nq          400                 Number of Q values. [400]
qstep       0.05                 Size of Q step [1/A]. [0.05]
ireset      0                 Sets the Empirical Potential to zero
iinit       0                 Sets accumulators to zero. Recalculates r and Q. [1]
ntimes      5                 Number of MC cycles between potential refinements. [5]
niter       1                 Number of potential refinements before exitting. [1]
nsumt       7487                 Number of iterations already accumulated. [-1 with reset]
intra       100                 Number of molecule moves between molecule shakes. [100]
inter       5                 Number of iterations in running averages. [5]
rho         0.09979964                 Atomic number density - will be derived from .ato file
cellst      0.03                 Size of r step [A]. [0.03]
fwhm        0.0                 Resolution width - Q independent term. [0.0]
fwhmq       0.02                 Resolution width - Q dependent term. [0.02 for SLS]
nsmoop      1                 1 means background subtraction is ON, 0 means OFF
fnameato    ace.ato                 Name of .ato file
fnamepcof   ace.pcof                 Name of potential coefficients file.
qmin        0.7                 Minimum value of Q used for potential fits. [0.05]
ndata       7                 Number of data files to be fit by EPSR

data   1

datafile    SLS39668.mdcs01                 Name of data file to be fit
wtsfile     ace2dbdtot.wts                 Name of weights file for this data set
nrtype      5                 Data type - see User Manual for more details
rshmin      0.7                 Minimum radius [A] - used for background subtraction
szeros      0.0                 Zero limit - 0 means use first data point for Q=0
tweak       1.0                 Scaling factor for this data set. [1.0]
efilereq    1.0                 Requested energy amplitude for this data set [1.0]

data   2 etc etc……
```

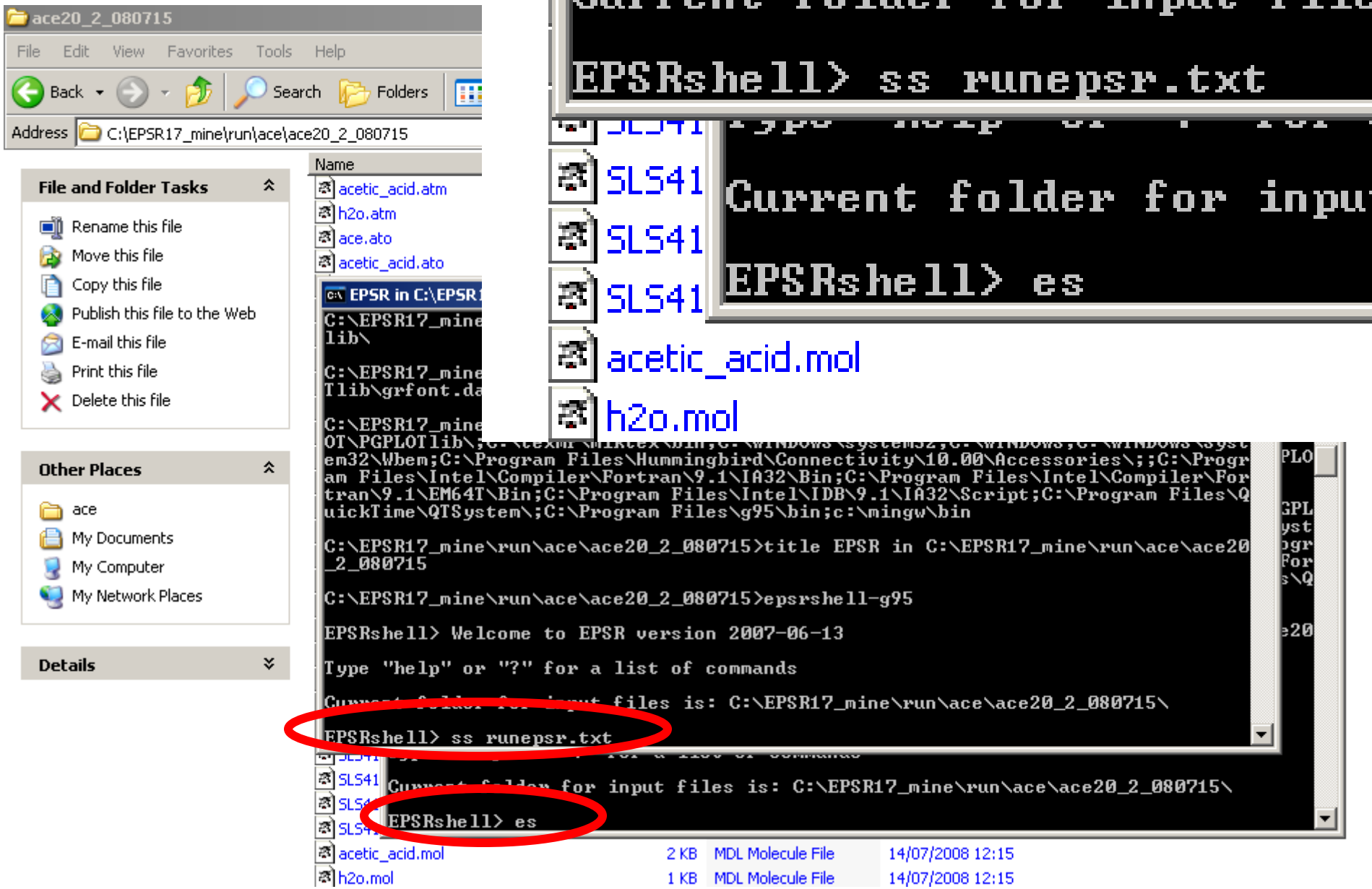
Operative flowchart

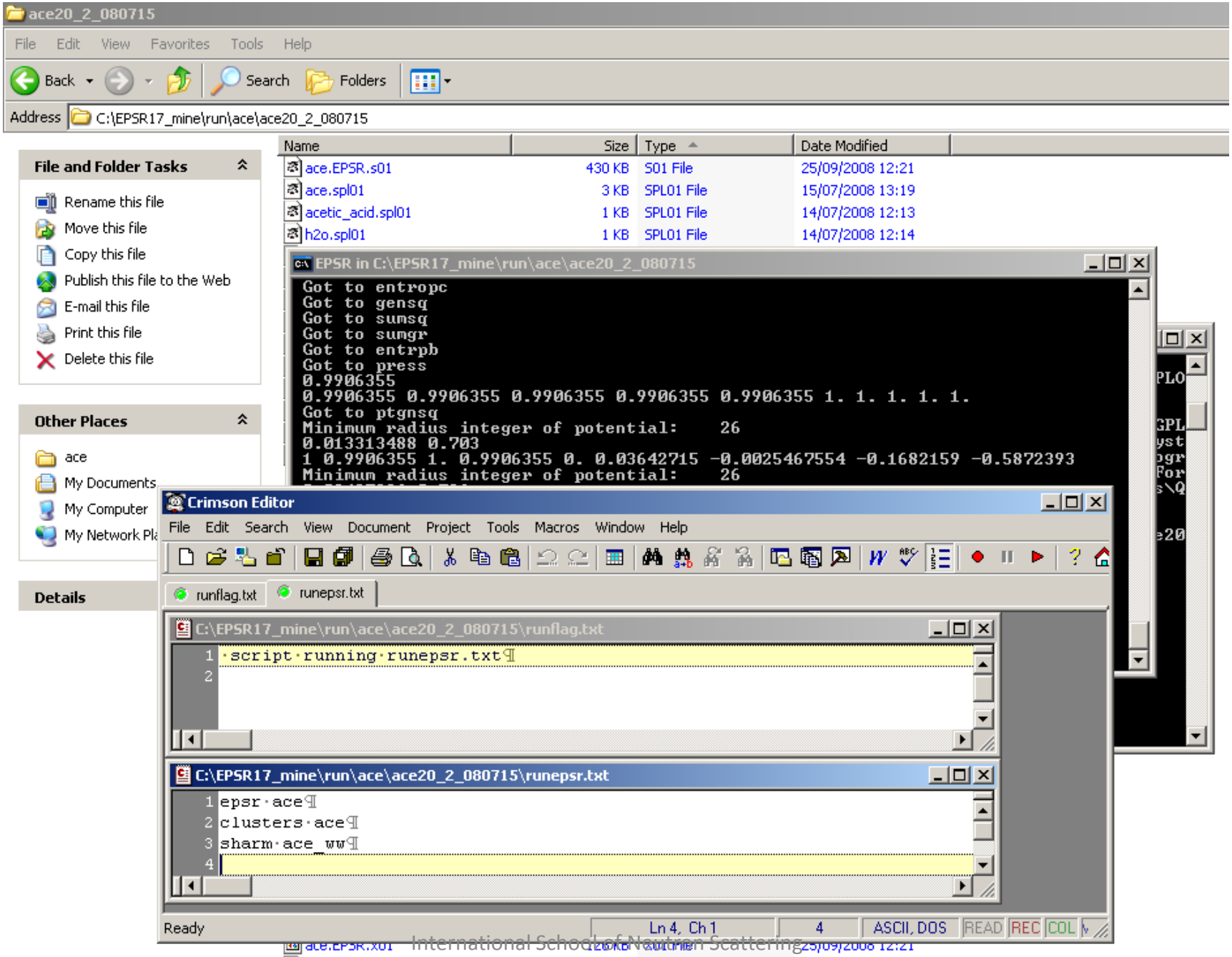


```
ace.EPSR                Title of this file
feedback    0.9             Confidence factor - should be < 1. [0.8]
potfac      1.0             1.0 to enable potential refinement, 0.0 to inhibit
ereq        10.00000            Overall requested energy amplitude - overrules efilereq
sizefactor  1.0             Multiplying factor for box dimension. [1.0]
nq          400             Number of Q values. [400]
qstep       0.05             Size of Q step [1/A]. [0.05]
ireset      0               Sets the Empirical Potential to zero
iinit       0               Sets accumulators to zero. Recalculates r and Q. [1]
ntimes      5               Number of MC cycles between potential refinements. [5]
niter       1               Number of potential refinements before exitting. [1]
nsumt       7487             Number of iterations already accumulated. [-1 with reset]
intra       100              Number of molecule moves between molecule shakes. [100]
inter       5               Number of iterations in running averages. [5]
rho         0.09979964              Atomic number density - will be derived from .ato file
cellst      0.03             Size of r step [A]. [0.03]
fwhm        0.0              Resolution width - Q independent term. [0.0]
fwhmq       0.02                                                 t term. [0.02 for SLS]
nsmoop      1                                                    s ON, 0 means OFF
fnameato    ace.ato
fnamepcof   ace.pcof                                             cients file.
qmin        0.7                                                  otential fits. [0.05]
ndata       7                                                    by EPSR

data   1

datafile    SLS39668.mdcs01             Name of data file to be fit
wtsfile     ace2dbdtot.wts              Name of weights file for this data set
nrtype      5               Data type - see User Manual for more details
rshmin      0.7              Minimum radius [A] - used for background subtraction
szeros      0.0              Zero limit - 0 means use first data point for Q=0
tweak       1.0              Scaling factor for this data set. [1.0]
efilereq    1.0              Requested energy amplitude for this data set [1.0]

data   2 etc etc.....
```

Now we are ready to run the simulation, and the main commands are given from the .inp file


ace example
File Edit View Favorites Tools Help
Back Search Folders
Address C:\EPSR17\run\ace example
File and Folder Tasks
Make a new folder
Publish this folder to the Web
Share this folder
Other Places
run
My Documents
My Computer
My Network Places
Details
Name Size Type Date Modified
EPSR.bat 1 KB MS-DOS Batch File 10/12/2007 18:55
plot_defaults.txt 3 KB Text Document 22/01/2008 10:59
runflag.txt 1 KB Text Document 25/09/2008 12:09
SLS39668.mdcs01 48 KB MDCS01 File 01/02/2008 19:16
SLS39669.mdcs01 48 KB MDCS01 File 01/02/2008 19:17
SLS39670.mdcs01 48 KB MDCS01 File 01/02/2008 19:18
SLS39671.mdcs01 48 KB MDCS01 File 01/02/2008 19:18
SLS39672.mdcs01 48 KB MDCS01 File 01/02/2008 19:19
SLS39673.mdcs01 48 KB MDCS01 File 01/02/2008 19:15
SLS39678.mdcs01 48 KB MDCS01 File 01/02/2008 19:20
system_commands.txt 1 KB Text Document 26/10/2007 16:15
Crimson Editor - [C:\EPSR17\run\ace example\runflag.txt]
File Edit Search View Document Project Tools Macros Window Help
runflag.txt
1 interactive
2
Ready
Ln 1, Ch 1
2
ASCII, DOS


ace20_2_080715
File Edit View Favorites Tools Help
Back Search Folders
Address C:\EPSR17_mine\run\ace\ace20_2_080715
File and Folder Tasks
Rename this file
Move this file
Copy this file
Publish this file to the Web
E-mail this file
Print this file
Delete this file
Other Places
ace
My Documents
My Computer
My Network Places
Details
Name
acetic_acid.atm
h2o.atm
ace.ato
acetic_acid.ato
EPSR in C:\EPSR
C:\EPSR17_mine\run\ace\ace20_2_080715>title EPSR in C:\EPSR17_mine\run\ace\ace20_2_080715
C:\EPSR17_mine\run\ace\ace20_2_080715>epsrshell-g95
EPSRshell> Welcome to EPSR version 2007-06-13
Type "help" or "?" for a list of commands
EPSRshell> ss runepsr.txt
EPSRshell> es
SLS41
SLS41
SLS41
acetic_acid.mol
h2o.mol
2 KB MDL Molecule File 14/07/2008 12:15
1 KB MDL Molecule File 14/07/2008 12:15
Current folder for input file
EPSRshell> ss runepsr.txt
Current folder for inpu
EPSRshell> es
acetic_acid.mol
h2o.mol


ace20_2_080715
File Edit View Favorites Tools Help
Back Search Folders
Address C:\EPSR17_mine\run\ace\ace20_2_080715
File and Folder Tasks
Rename this file
Move this file
Copy this file
Publish this file to the Web
E-mail this file
Print this file
Delete this file
Other Places
ace
My Documents
My Computer
My Network Pl
Details
Name Size Type Date Modified
ace.EPSR.s01 430 KB S01 File 25/09/2008 12:21
ace.spl01 3 KB SPL01 File 15/07/2008 13:19
acetic_acid.spl01 1 KB SPL01 File 14/07/2008 12:13
h2o.spl01 1 KB SPL01 File 14/07/2008 12:14
EPSR in C:\EPSR17_mine\run\ace\ace20_2_080715
Got to entropc
Got to gensq
Got to sumsq
Got to sumgr
Got to entrpb
Got to press
0.9906355
0.9906355 0.9906355 0.9906355 0.9906355 0.9906355 1. 1. 1. 1. 1.
Got to ptgnsq
Minimum radius integer of potential: 26
0.013313488 0.703
1 0.9906355 1. 0.9906355 0. 0.03642715 -0.0025467554 -0.1682159 -0.5872393
Minimum radius integer of potential: 26
Crimson Editor
File Edit Search View Document Project Tools Macros Window Help
runflag.txt runepsr.txt
C:\EPSR17_mine\run\ace\ace20_2_080715\runflag.txt
1 script running runepsr.txt
2
C:\EPSR17_mine\run\ace\ace20_2_080715\runepsr.txt
1 epsr ace
2 clusters ace
3 sharm ace_ww
4
Ready
Ln 4, Ch 1
4
ASCII, DOS
READ REC COL
ace.EPSR.y01 826 KB Y01 File 25/09/2008 12:21
ace.EPSR.z01 826 KB Z01 File 25/09/2008 12:21

A “push the button” approach to EPSR

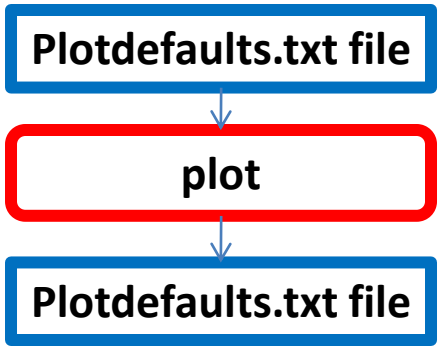
ON

OFF

	IRESET	NSMOOP &POTFAC	EREQ	IINIT	NSUMT
Starting point	1	0	0	1	-1
MC with Reference Potential	0	0	0	0	-1
MC with Potential Refinement	0	1	10, 20, 50, 100……	0	-1
MC with Accumulation of configurations	0	1		0	0
	Resets the empirical potential	Switches on the potential	Controls the amplitude of the empirical potential	Resets the accumulated distributions	Number of configuratio ns accumulated

How do you decide when to push the button?

```
plot> l
plot> Available plot types are:-
   1  - EPSR S(Q) fit
   2  - EPSR S(Q) fit and difference
   3  - EPSR S(Q) fit and data
   4  - EPSR S_intra(Q)
   5  - EPSR F(Q) fit
   6  - EPSR F(Q) fit and difference
   7  - EPSR F(Q) fit and data
   8  - EPSR site-site g(r)
   9  - EPSR site-site g(r) fit and data
  10  - EPSR g_intra(r) fit
  11  - EPSR f(r) fit
  12  - EPSR f(r) fit and data
  13  - EPSR empirical potentials
  14  - EPSR energy
  15  - EPSR pressure
  16  - SHARM coefficients
  17  - Cluster size distribution
  18  - Torsional angle distribution
  19  - EPSR R-factor
  20  - PARTIALS g(r)
  21  - EPSR g(r) and N(r)
  22  - Triangles
  23  - Coordination No.
  24  - Chains
  25  - R-factor v. Abs. Energy
  (…)
```



- f ace

sets the filename

- p 14

selects plot type and plots it

- b 1 2 9

selects columns to plot (luckily columns have also a name in the file)

- xmin, xmax, ymin, ymax, ydel…..

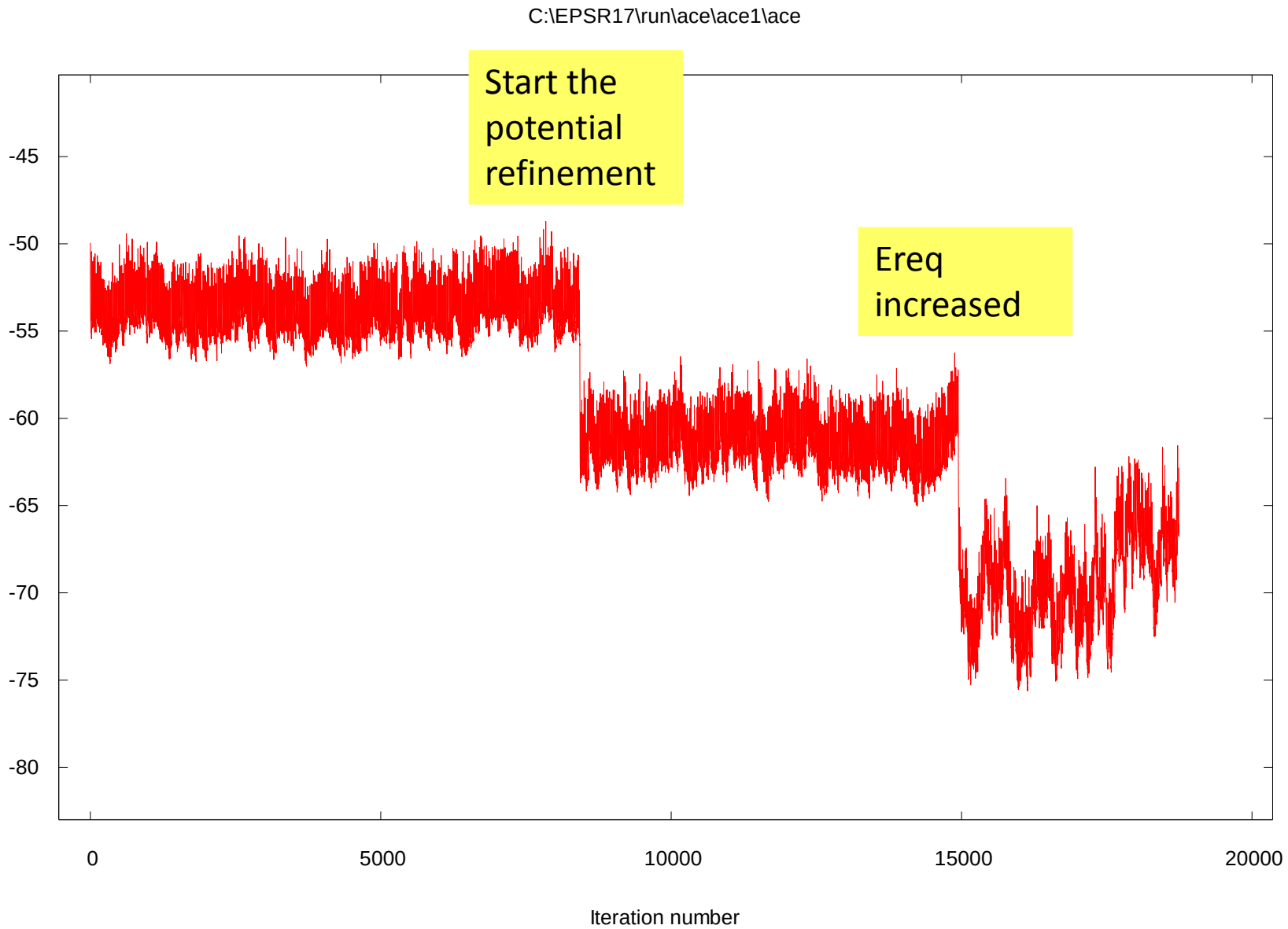
sets range for plot

- e

exits and asks you if you want to save

•<CR>

skips to the next


C:\EPSR17\run\ace\ace1\ace
Start the potential refinement
Ereq increased
-45
-50
-55
-60
-65
-70
-75
-80
0
5000
10000
15000
20000
Iteration number

Reviewing the output

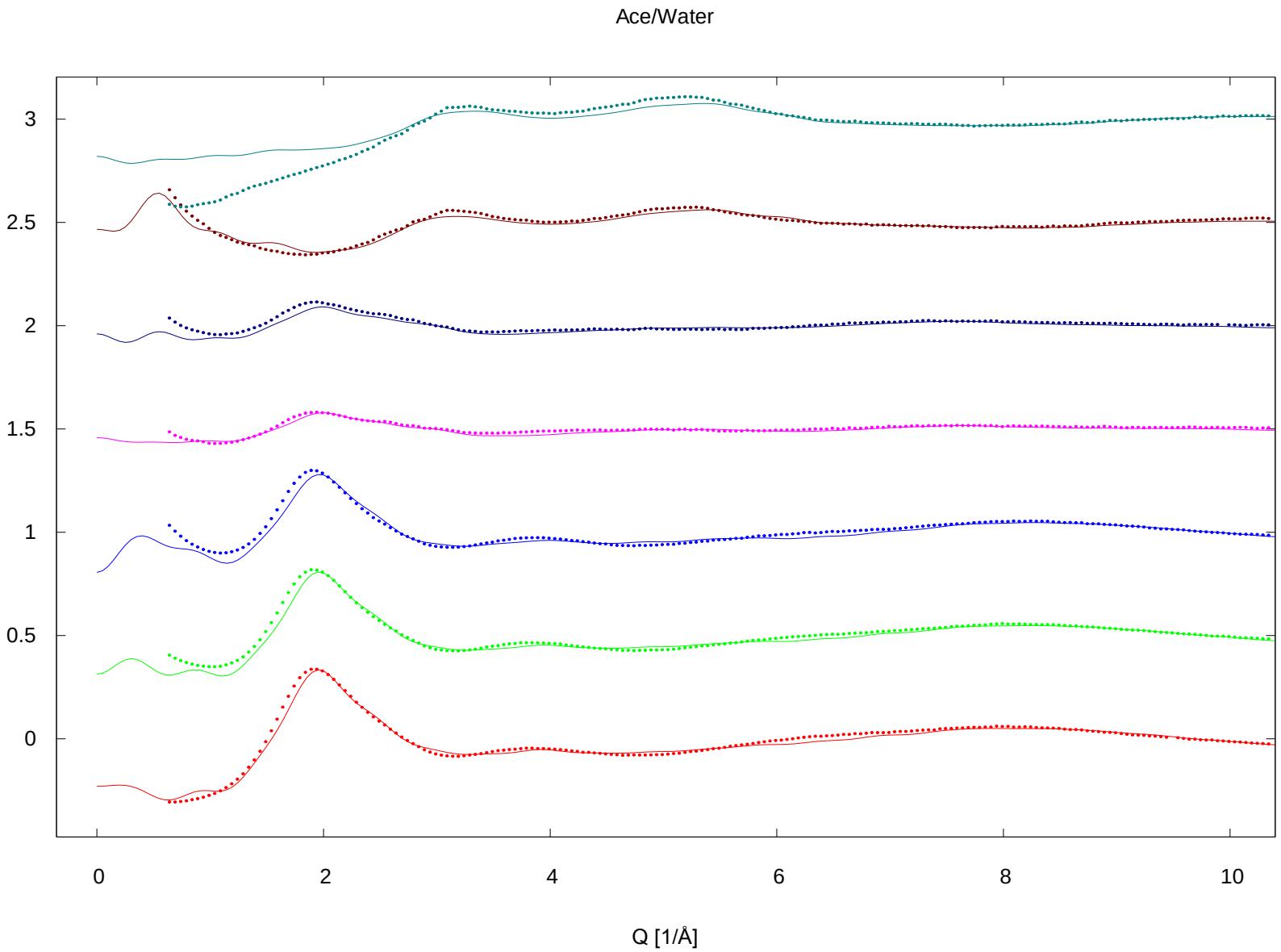
```
plot> l
plot> Available plot types are:-
   1  - EPSR S(Q) fit
   2  - EPSR S(Q) fit and difference
   3  - EPSR S(Q) fit and data
   4  - EPSR S_intra(Q)
   5  - EPSR F(Q) fit
   6  - EPSR F(Q) fit and difference
   7  - EPSR F(Q) fit and data
   8  - EPSR site-site g(r)
   9  - EPSR site-site g(r) fit and data
  10  - EPSR g_intra(r) fit
  11  - EPSR f(r) fit
  12  - EPSR f(r) fit and data
  13  - EPSR empirical potentials
  14  - EPSR energy
```

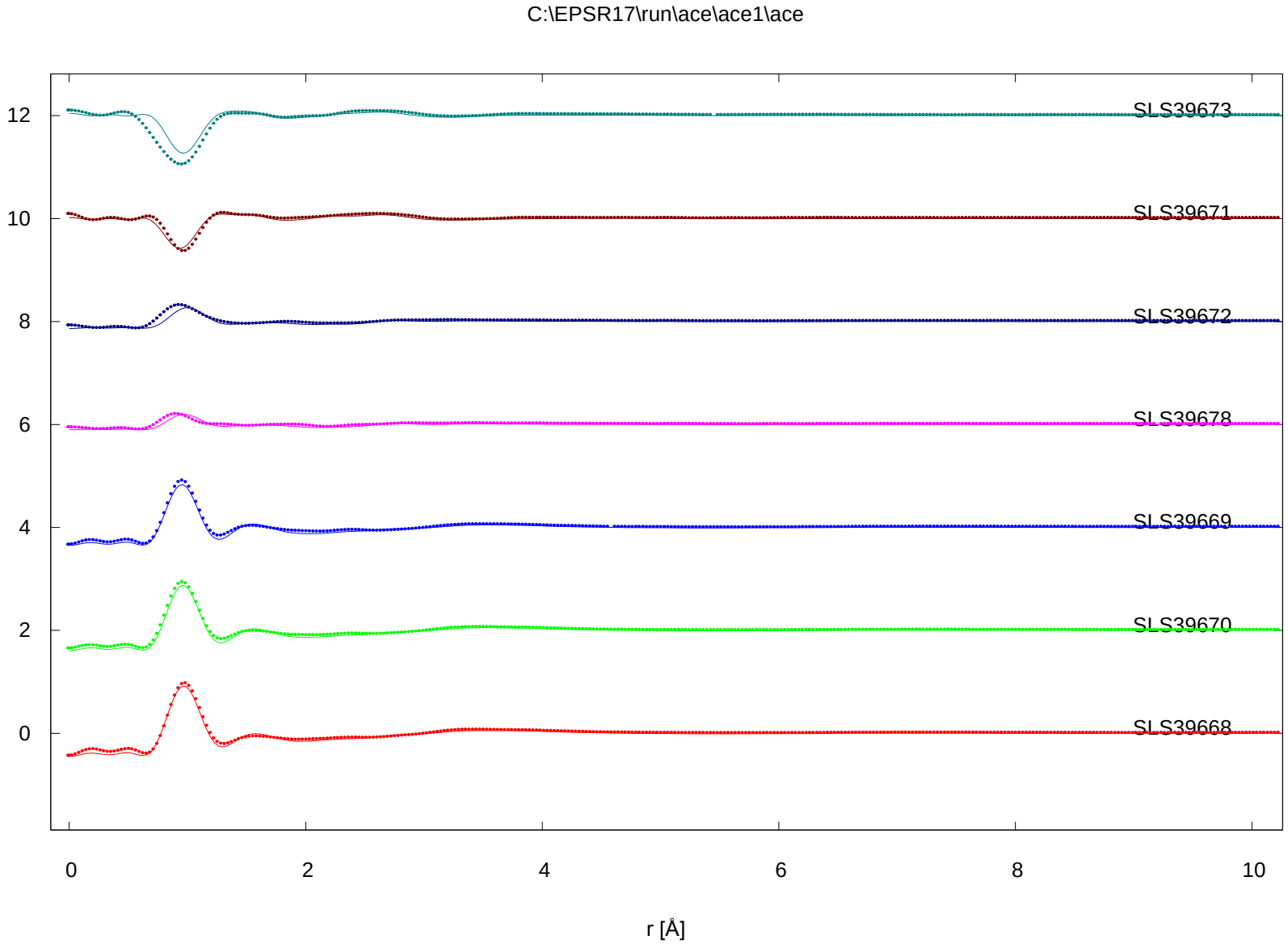
	Q			r			
	SIM	**DATA**	**DIFF**	**SIM**	**DATA**	**POT**	**COORD**
Totals	5-6-7	7	6	11 – 12	12		
Partials Intramol.	1 - 2 - 3	3	2	8 – 9 -21	9	13	21 -23
Partials Intermol.	4		10				

(Much needed)
Table of output file extensions

<filename>.<program>.<filetype>
<filename>.**EPSR.<filetype>**

	Q			r			
	SIM	**DATA**	**DIFF**	**SIM**	**DATA**	**POT**	**COORD**
Totals	.U01	.T01 (mdcs)	.V01	.X01	.W01 (mgor)		
Partials Intramol.	.F01	.Q01	.D01	.G01	.R01	.P01	.Z01
Partials Intermol.	.S01		.Y01				


Ace/Water
3
2.5
2
1.5
1
0.5
0
0
2
4
6
8
10
Q [1/Å]


C:\EPSR17\run\ace\ace1\ace
SLS39673
SLS39671
SLS39672
SLS39678
SLS39669
SLS39670
SLS39668
12
10
8
6
4
2
0
0
2
4
6
8
10
r [Å]

When you are happy with the fit it's time to go and have a look at the results…

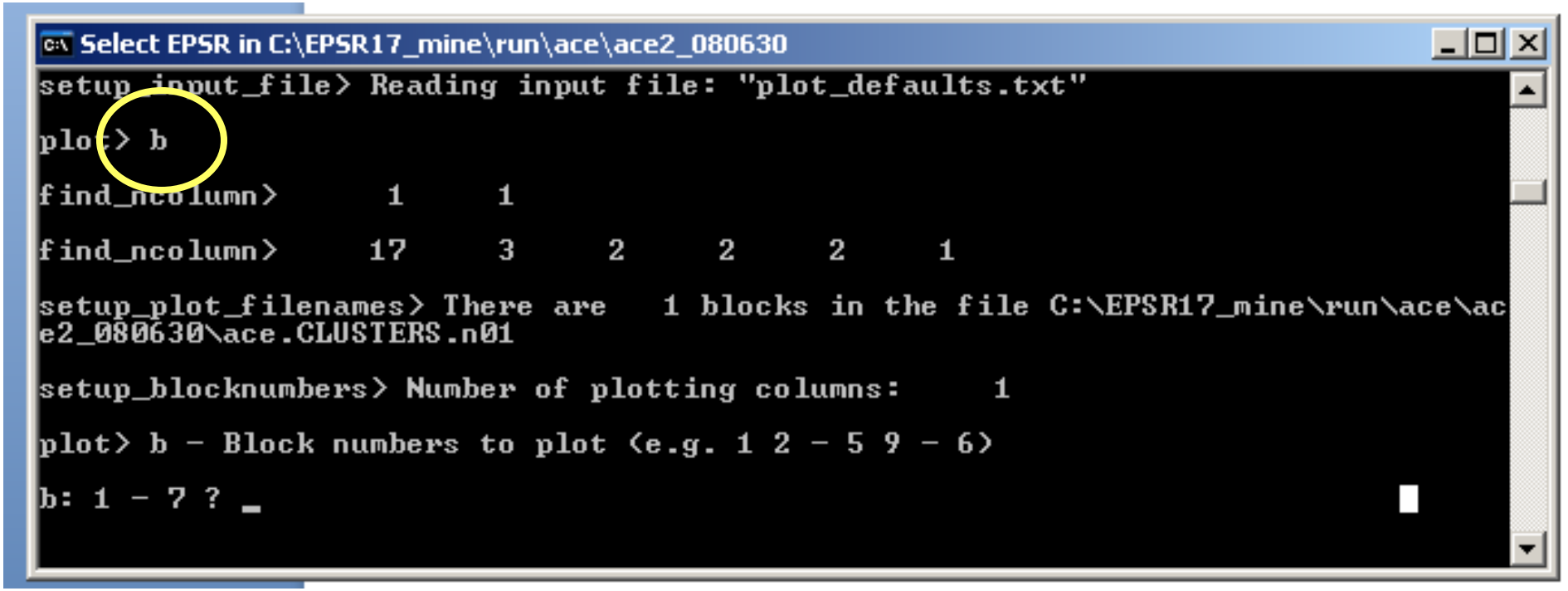
Put the atoms in the same order as they appear at the end of your .ato file

	OW	HW	CM	HM	CC	OC	O	H
OW	1	2	3	4	5	6	7	8
HW		9	10	11	12	13	14	15
CM			16	17	18	19	20	21
HM				22	23	24	25	26
CC					27	28	29	30
OC						31	32	33
O							34	35
H								36

It helps you thinking what you want to visualize:

- solvent-solvent, solute-solute and solute-solvent correlations separately
- Hydrophilic-philic, phobic-phobic, philic-phobic
- OO, OH, HH to compare with pure water….
- ……

p 9 (partials)



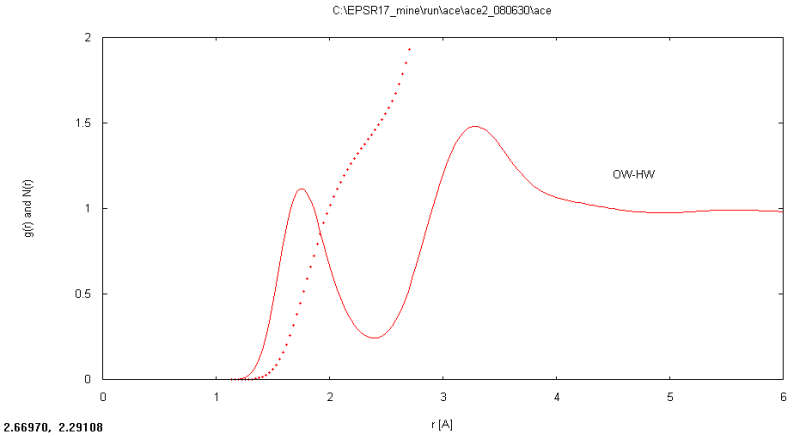
ace.EPSR.g01

# r	OW-OW		OW-HW		OW-CM etc etc	
0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00
0.7500000E-02	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00
0.3000000E-01	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00
0.6000000E-01	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00

p 21 (partials and coord numbers)

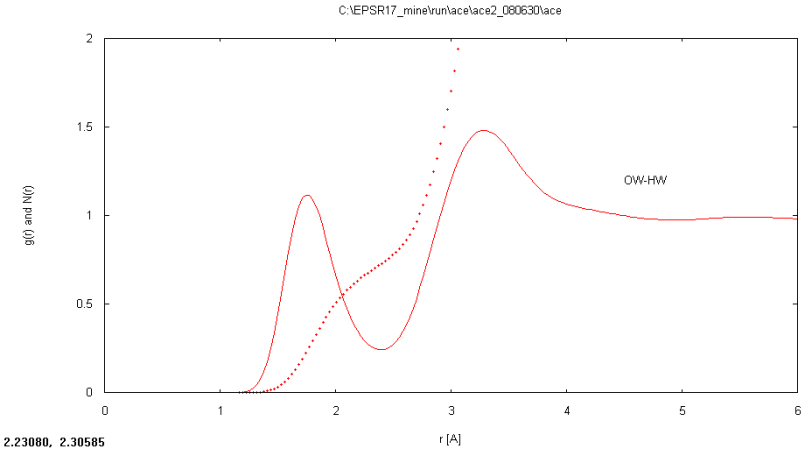
OW-HW

```
b 2 (no. of partial)
boffset 2 2
(second column of ace.EPSR.g01,
second column of ace.EPSR.z01)
```



HW-OW (careful because the label doesn't change in the actual plot)

```
b 2
boffset 2 3
(second column of ace.EPSR.g01,
third column of ace.EPSR.z01)
```



ace.EPSR.z01

```
#     r                OW-HW              HW-OW
  0.0000000E+00  0.0000000E+00  0.0000000E+00
  0.7500000E-02  0.0000000E+00  0.0000000E+00
  0.3000000E-01  0.0000000E+00  0.0000000E+00
  0.6000000E-01  0.0000000E+00  0.0000000E+00
```

Useful references

- ***Computer Simulation of Liquids, M.P.Allen and D.J.Tildesley, (1987) Oxford*** University Press, Oxford and New York
- ***Empirical Potential Monte Carlo simulation of fluid structure*** A.K.Soper, Chemical Physics, **202, (1996) 295-306**
- ***The radial distribution functions of water and ice from 220 to 673K and at pressures up to 400MPa*** A.K.Soper, Chemical Physics, **258, (2000) 121-137**
- ***Tests of the empirical potential structure refinement method and a new method of application to neutron diffraction data on water*** A.K.Soper, Molecular Physics, **99 (2001) 1503-1516**
- ***Partial structure factors from disordered materials diffraction data: An approach using empirical potential structure refinement*** A.K.Soper, Physical Review B, **72, (2005) 104204**

www.isis.rl.ac.uk\disorderedmaterials for latest EPSR release, manual, further references and updates

Advertisement:

silvia.imberti@stfc.ac.uk for submitting a proposal on SANDALS or other information

Deadline for proposals submission 16th October & 16th April