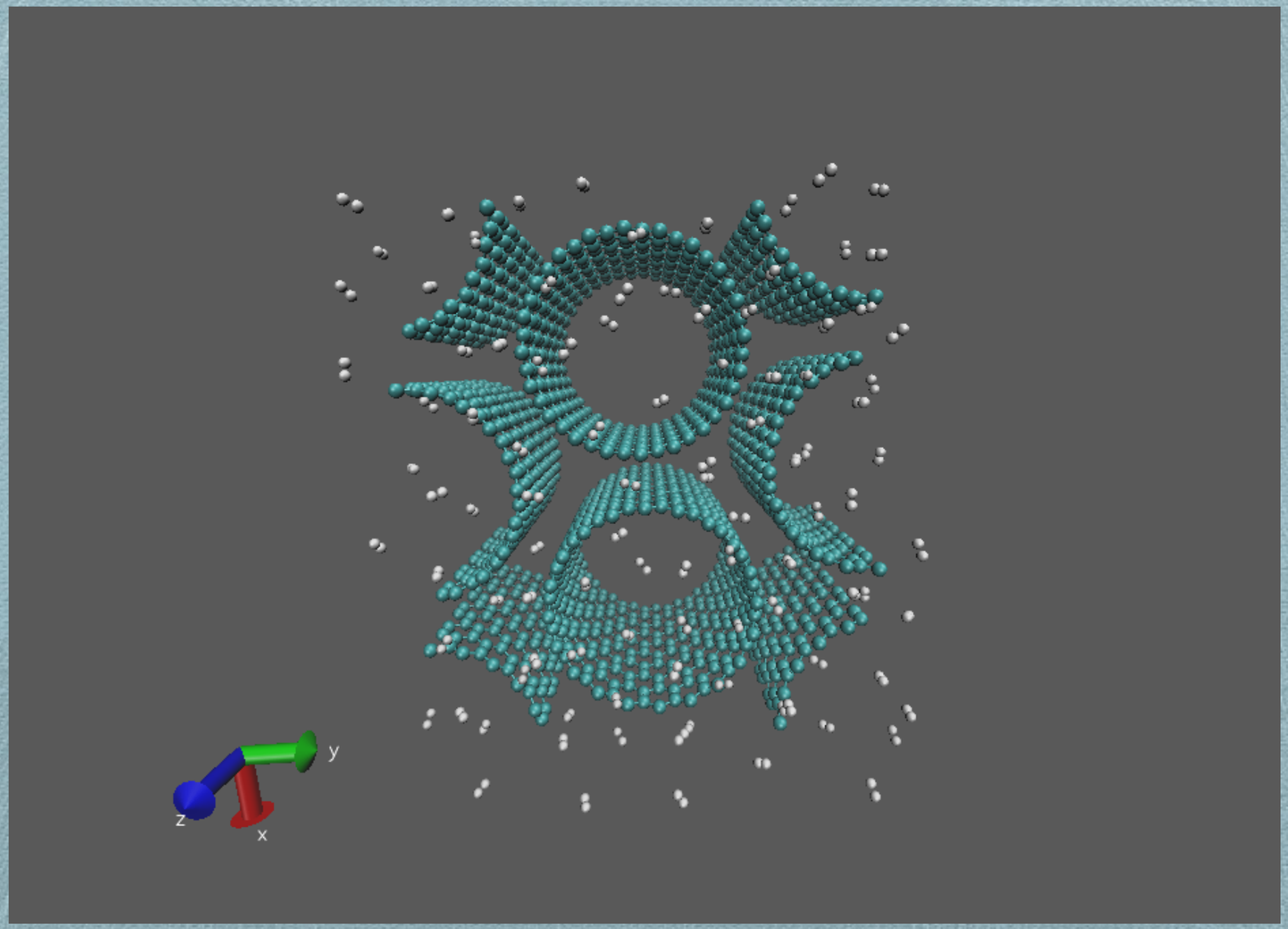


DL_POLY software

The DL_POLY Molecular Simulation Package

General Information

DL_POLY is a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory by I.T. Todorov and W. Smith.

Currently, only one version of the DL_POLY software is available under an STFC licence, DL_POLY_4, and with support provisioned to the UK's academia only. The former DL_POLY_2 version (authored by W. Smith, T.R. Forester and I.T. Todorov) is now transformed intoDL_POLY_CLASSIC and available as open source under the BSD atCCPForge.

DL_POLY_2 (WE will use this version)

- Replicated Data, up to 30,000 atoms
- Full force field and molecular description

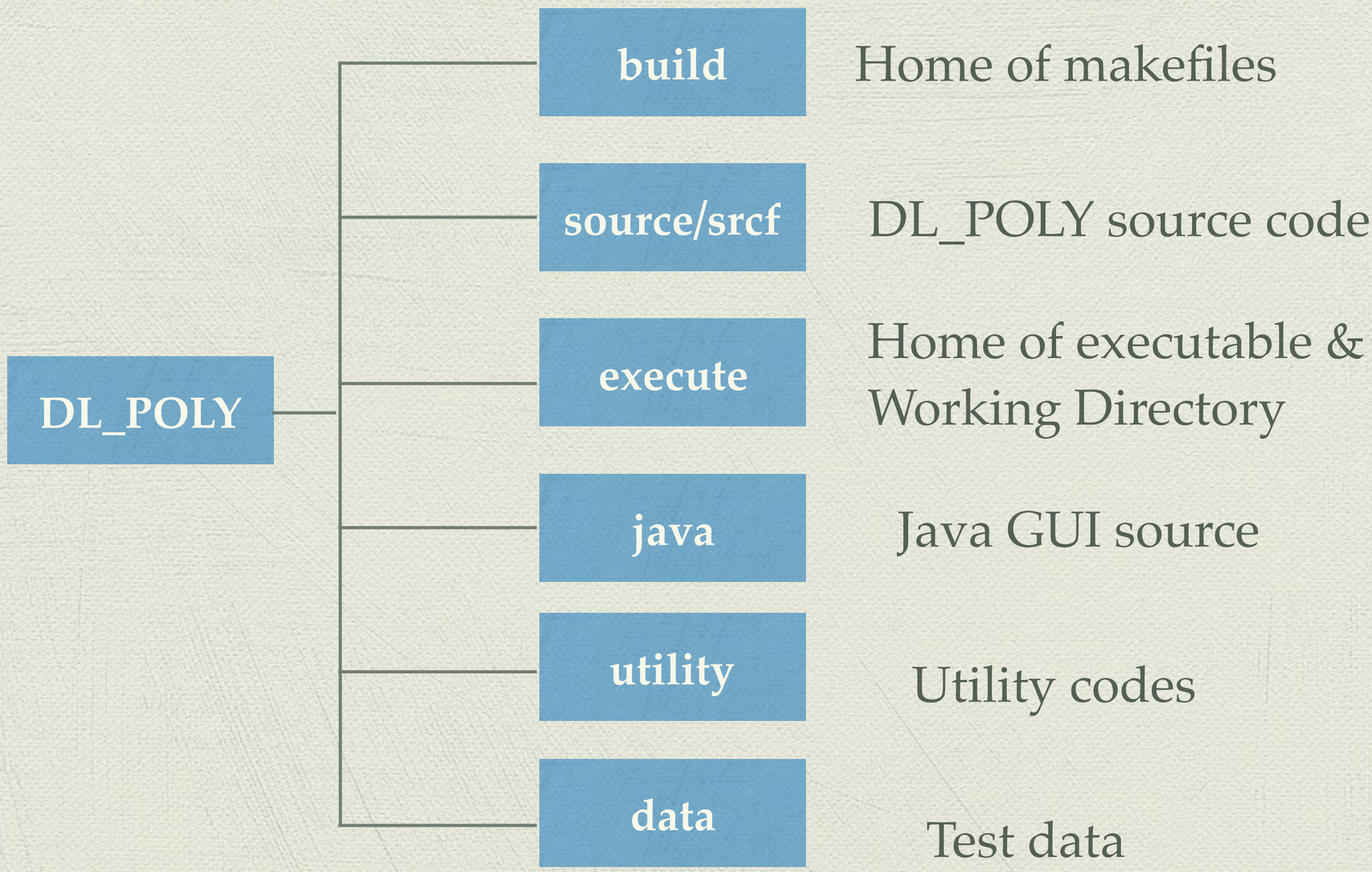
DL_POLY_3

-Domain Decomposition, up to 1,000,000 atoms
-Full force field but no rigid body description.

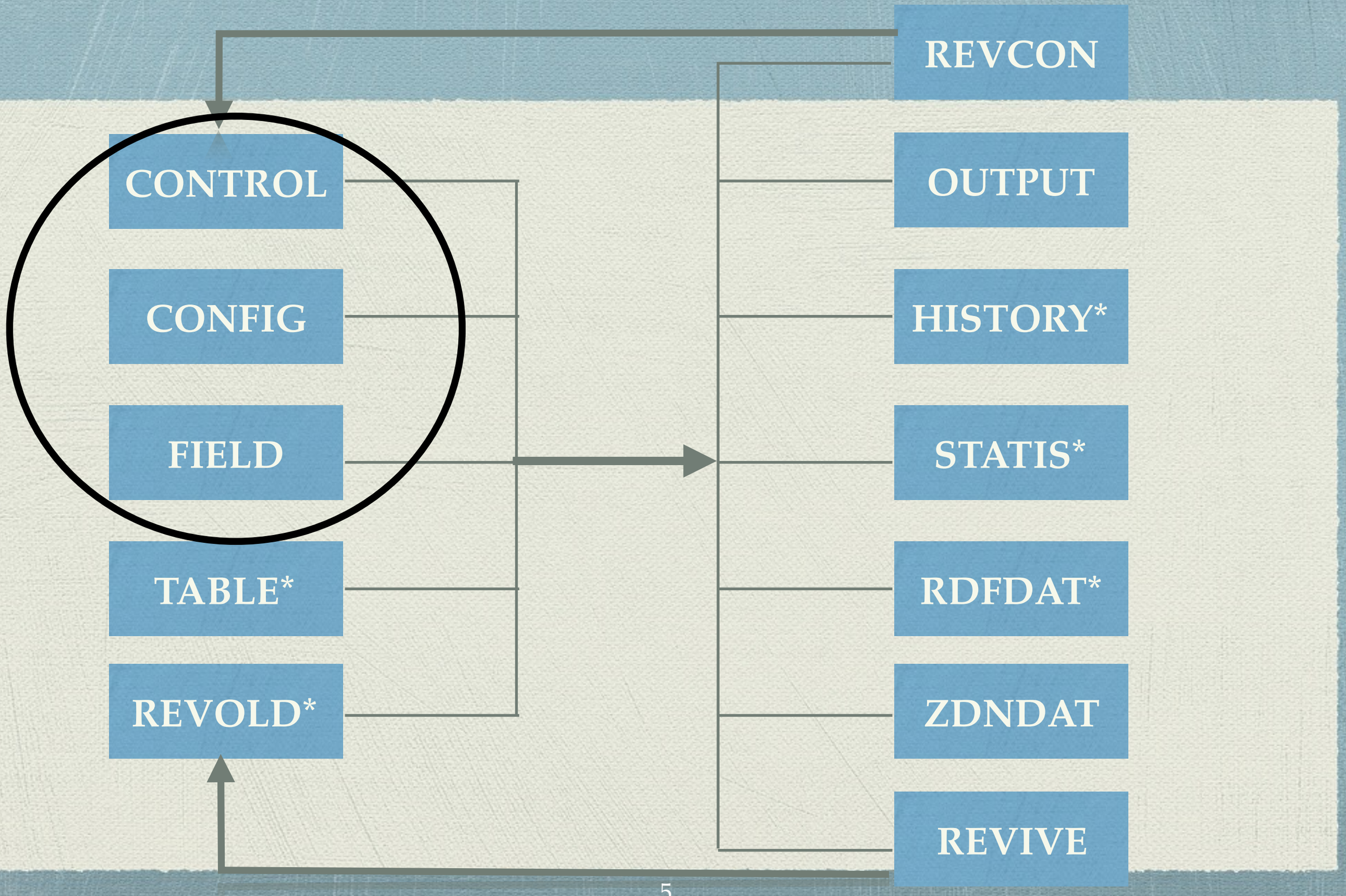
DL_POLY_4

- Code design is based on the principles of portability, maintenance, transparency and user verification. The code architecture adopts the Fortran90 modularisation in a C/C++ header style manner, where concepts and functionality are separated in a functional way by modules. The code routines relate to features/actions by their file names, which often relate to module names.

DL_POLY Directories



DL_POLY I/O files



DL_POLY units

Internally DL_POLY uses atomic scale units:

- Mass - mass of H atom (D) [Daltons]
- Charge - charge on proton (e)
- Length - Angstroms (A)
- Time - picoseconds (ps)
- Force - D A ps-2
- Energy - D A2 ps-2

[comment: pressure is expressed in k-atm for I/O]

CONTROL file

Simulation control

- Free Format
- Mandatory
- Driven by **keywords**:

keyword [options] {data}

e.g.:

ensemble NPT Hoover 1.0 8.0

CONTROL — Edited

```
SODIUM ION IN SPC WATER (NVE)


temperature  300.0
ensemble nve
pressure          0.0010
steps           5000
equilibration   1000
scale           10
print           100
stack           100
stats           100
rdf             10

timestep        0.0010
cutoff            9.9500
rvdw cutoff       9.9500
delr width      0.5
ewald precision 1.e-5
traj nstraj  1001 istraj 500 keytraj 0
quaternion tolerance  1.0000E-05
print rdf

job time        999999.0
close time      20.0

finish
```

CONFIG — Edited

```
simulation of Na+ with 255 water molecules
         0         1
        20.66340857          0.00000000          0.00000000
         0.00000000         20.66340857          0.00000000
         0.00000000          0.00000000         20.66340857
Na+               1
         0.00000000          0.00000000          0.00000000
OW                2
       -10.15250063         -9.97256123         -7.11750873
HW                3
       -10.32737963         -9.03542706         -7.41950611
HW                4
         9.99395787        -10.15521124         -6.28120308
OW                5
       -10.26935347         -0.19189945          7.16862889
HW                6
       -10.15319013         -1.17329854          7.01575994
HW                7
         9.45243227         -0.00760127          7.45038692
OW                8
       -10.31715314         -0.78059530          1.53668527
HW                9
         9.76995246         -0.06589264          1.14035268
HW               10
        -9.38576598         -0.43407821          1.64825784
OW               11
       -10.21477353          4.11064203         -2.27055456
HW               12
         9.64258730          3.97625568         -2.84695209
HW               13
        -9.42517662          4.32350110         -2.84608413
OW               14
        -9.90790253         -2.06607378         -2.09045693
HW               15
        -9.52154168         -2.94486569         -1.81035658
HW               16
        -9.16725034         -1.42050195         -2.27667615
OW               17
        -9.86839354          7.15368352         -8.41578964
```

Title line

CONFIG Key

Periodic Boundary key

boundary coordinates XYZ

atom name

atom index

atom's coordinates

Table 4.5: CONFIG file key (record 2)

levcfg	meaning
0	Coordinates included in file
1	Coordinates and velocities included in file
2	Coordinates, velocities and forces included in file

Table 4.6: Periodic boundary key (record 2)

imcon	meaning
0	no periodic boundaries
1	cubic boundary conditions
2	orthorhombic boundary conditions
3	parallelepiped boundary conditions
4	truncated octahedral boundary conditions
5	rhombic dodecahedral boundary conditions
6	x-y parallelogram boundary conditions with no periodicity in the z direction
7	hexagonal prism boundary conditions

DL_POLY Force Field

$$
\begin{aligned}
U(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N) \;=\; & \sum_{i_{bond}=1}^{N_{bond}} U_{bond}(i_{bond}, \underline{r}_a, \underline{r}_b) \\
& + \sum_{i_{angle}=1}^{N_{angle}} U_{angle}(i_{angle}, \underline{r}_a, \underline{r}_b, \underline{r}_c) \\
& + \sum_{i_{dihed}=1}^{N_{dihed}} U_{dihed}(i_{dihed}, \underline{r}_a, \underline{r}_b, \underline{r}_c, \underline{r}_d) \\
& + \sum_{i_{inv}=1}^{N_{inv}} U_{inv}(i_{inv}, \underline{r}_a, \underline{r}_b, \underline{r}_c, \underline{r}_d) \\
& + \sum_{i=1}^{N-1} \sum_{j>i}^{N} U_{pair}(i, j, |\underline{r}_i - \underline{r}_j|) \\
& + \sum_{i=1}^{N-2} \sum_{j>i}^{N-1} \sum_{k>j}^{N} U_{3\_body}(i, j, k, \underline{r}_i, \underline{r}_j, \underline{r}_k) \\
& + \sum_{i=1}^{N-1} \sum_{j>i}^{N} U_{Tersoff}(i, j, \underline{r}_i, \underline{r}_j, \underline{R}^N) \\
& + \sum_{i=1}^{N-3} \sum_{j>i}^{N-2} \sum_{k>j}^{N-1} \sum_{n>k}^{N} U_{4\_body}(i, j, k, n, \underline{r}_i, \underline{r}_j, \underline{r}_k, \underline{r}_n) \\
& + \sum_{i=1}^{N} U_{Metal}(i, \underline{r}_i, \underline{R}^N) \\
& + \sum_{i=1}^{N} U_{extn}(i, \underline{r}_i, \underline{v}_i)
\end{aligned}
$$

FIELD file

Force Field specification

- Mandatory
- Fixed format:

-Integers I5

-Reals F12

-Names A8

-Keywords A4

- Maps on to CONFIG file structure
- The FIELD file must be closed with the directive :

close

FIELD — Edited

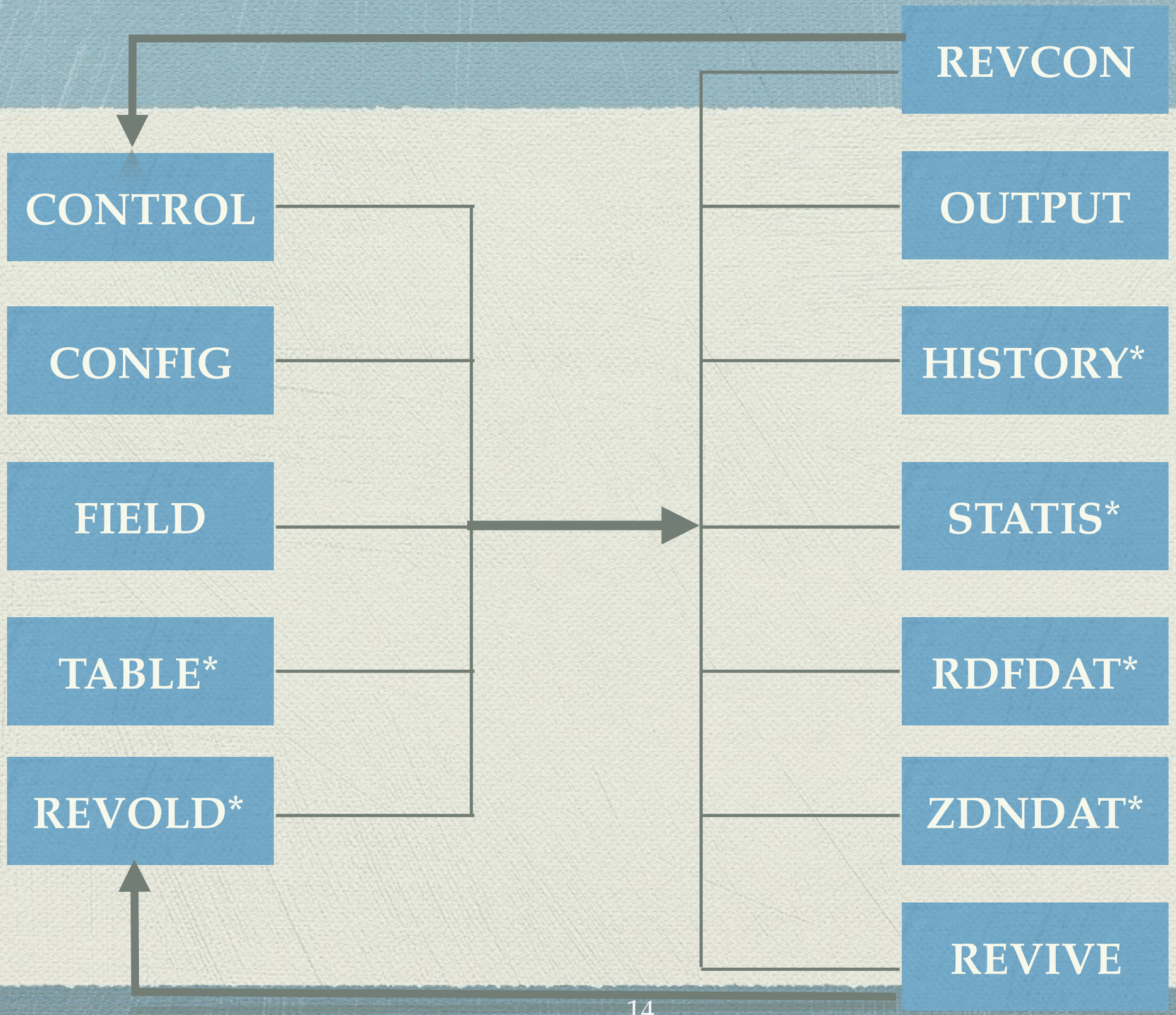
```
SODIUM ION IN SPC WATER (NVE)

UNITS kcal
MOLECULAR TYPES 2
SODIUM ION
NUMMOLS 1
ATOMS 1
Na+            22.9898          1.00     1
FINISH
SPC WATER
NUMMOLS 253
ATOMS 3
OW             15.9994    -0.82000       1
HW              1.0080     0.41000       2
RIGID 1
     3     1     2     3
FINISH
VDW 2
OW       OW        LJ     0.16000000  3.19600000
OW       Na+        LJ     0.14422205  2.77300000
CLOSE
```

Force Field

Table 4.12: Definition of pair potential functions and variables

key	potential type	Variables (1-5)					functional form
12-6	12-6	A	B				$U(r) = \left(\frac{A}{r^{12}}\right) - \left(\frac{B}{r^6}\right)$
lj	Lennard-Jones	ϵ	σ				$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right]$
nm	n-m	E_o	n	m	r_0		$U(r) = \frac{E_o}{(n-m)}\left[m\left(\frac{r_o}{r}\right)^n - n\left(\frac{r_o}{r}\right)^m\right]$
buck	Buckingham	A	ρ	C			$U(r) = A\ \exp\left(-\frac{r}{\rho}\right) - \frac{C}{r^6}$
bhm	Born-Huggins -Meyer	A	B	σ	C	D	$U(r) = A\ \exp[B(\sigma - r)] - \frac{C}{r^6} - \frac{D}{r^8}$
hbnd	12-10 H-bond	A	B				$U(r) = \left(\frac{A}{r^{12}}\right) - \left(\frac{B}{r^{10}}\right)$
snm	Shifted force† n-m [31]	E_o	n	m	r_0	r_c‡	$U(r) = \frac{\alpha E_o}{(n-m)}\times \left[m\beta^n\left\{\left(\frac{r_o}{r}\right)^n - \left(\frac{1}{\gamma}\right)^n\right\} - n\beta^m\left\{\left(\frac{r_o}{r}\right)^m - \left(\frac{1}{\gamma}\right)^m\right\}\right] + \frac{nm\alpha E_o}{(n-m)}\left(\frac{r-\gamma r_o}{\gamma r_o}\right)\left\{\left(\frac{\beta}{\gamma}\right)^n - \left(\frac{\beta}{\gamma}\right)^m\right\}$
mors	Morse	E_0	r_0	k			$U(r) = E_0[\{1 - \exp(-k(r - r_0))\}^2 - 1]$
wca	WCA	ϵ	σ				$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] + \epsilon \quad (r < \sigma * 2^{1/6})$
tab	Tabulation						tabulated potential

OUTPUT FILES



REVCON file

```
H2 molecules on top of a SWNT bundle
         2          3       1000    0.5000000000E-04
     45.000000000000       0.000000000000       0.000000000000
      0.000000000000      45.000000000000       0.000000000000
      0.000000000000       0.000000000000      30.000000000000
C                    1
    -15.09884631         -22.00032798          5.086660519
  0.859667148368       0.146971003561       0.963422589934
  -649.004587529       -46.4490706042       -675.267158221
C                    2
    -15.30660399         -20.78235711          5.783967062
  0.433169181626E-01 -0.102580080322       0.246048629462
   1070.57597729        692.373445210        1033.43846028
C                    3
    -15.48719868         -19.55871122          5.087011186
  0.876870694758       0.238924334567       1.00383492338
  -496.132870939       -582.707254650       -580.333429662
C                    4
    -16.06019231         -18.46348550          5.783321095
  0.120941978747      -0.100649343386       0.744393817757
   1115.05103836        335.163238222        1671.17734862
C                    5
    -16.60790184         -17.35578131          5.086637415
  0.856856767794       0.475934669789       1.04461812814
  -568.691221306       -395.707510151       -585.832480517
C                    6
    -17.49405887         -16.49485150          5.784050000
 -0.344040064838       0.357268287824       0.430078780983
```

OUTPUT File

Provides Job Summary (mandatory!)

- Formatted to be human readable
- Contents:
  - Summary of input data
  - Instantaneous thermodynamic data at selected intervals
  - Rolling averages of thermodynamic data
  - Statistical averages
  - Final configuration
  - Radial distribution data
  - Estimated mean-square displacements
- Plus:
  - Timing data
  - Error reports

```
run terminating. elapsed cpu time =       373.030, job time =    999999.000, close time =        20.000


run terminated after    5000 steps. final averages calculated over    4000 steps.

-------------------------------------------------------------------------------------------------------------------

    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

-------------------------------------------------------------------------------------------------------------------
    5000 -1.3228E+03  3.0697E+02 -1.7858E+03  1.5093E+02 -1.9367E+03  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   5.000 -1.2889E+03  3.0955E+02  3.5757E+02 -6.3959E+03  1.9365E+03  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  373.05  8.8228E+03  0.0000E+00  0.0000E+00  0.0000E+00  9.0000E+01  9.0000E+01  9.0000E+01  0.0000E+00  2.6303E-01

 r.m.s.   3.8114E-02  8.7215E+00  1.3169E+01  1.8824E+01  2.5238E+01  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
fluctn.   6.0859E+01  1.3320E+01  1.8337E+02  2.5903E+02  2.5326E+01  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
          1.4672E-11  0.0000E+00  0.0000E+00  0.0000E+00  1.5842E-13  1.5842E-13  1.5842E-13  0.0000E+00  4.7298E-01
-------------------------------------------------------------------------------------------------------------------


 Approximate 3D Diffusion  coefficients (10^-9 m^2 / s)

 atom         D
 Na+       1.7938E+00
 OW        1.2759E+01
 HW        1.2986E+01


     Average pressure tensor                                          r.m.s. fluctuations
```

RDFDAT file

This is a formatted file containing em Radial Distribution Function (RDF) data. Its contents are as follows:

record 1

`cfgname`	character (A80)	configuration name

record 2

`ntpvdw`	integer (i10)	number of RDFs in file
`mxrdf`	integer (i10)	number of data points in each RDF

There follow the data for each individual RDF i.e. *ntpvdw* times. The data supplied are as follows:

first record

`atname 1`	character (A8)	first atom name
`atname 2`	character (A8)	second atom name

following records (*mxrdf* records)

`radius`	real (e14)	interatomic distance (A)
`g(r)`	real (e14)	RDF at given radius.

Note the RDFDAT file is optional and appears when the **print rdf** option is specified in the CONTROL file.

RDFDAT — Modificato

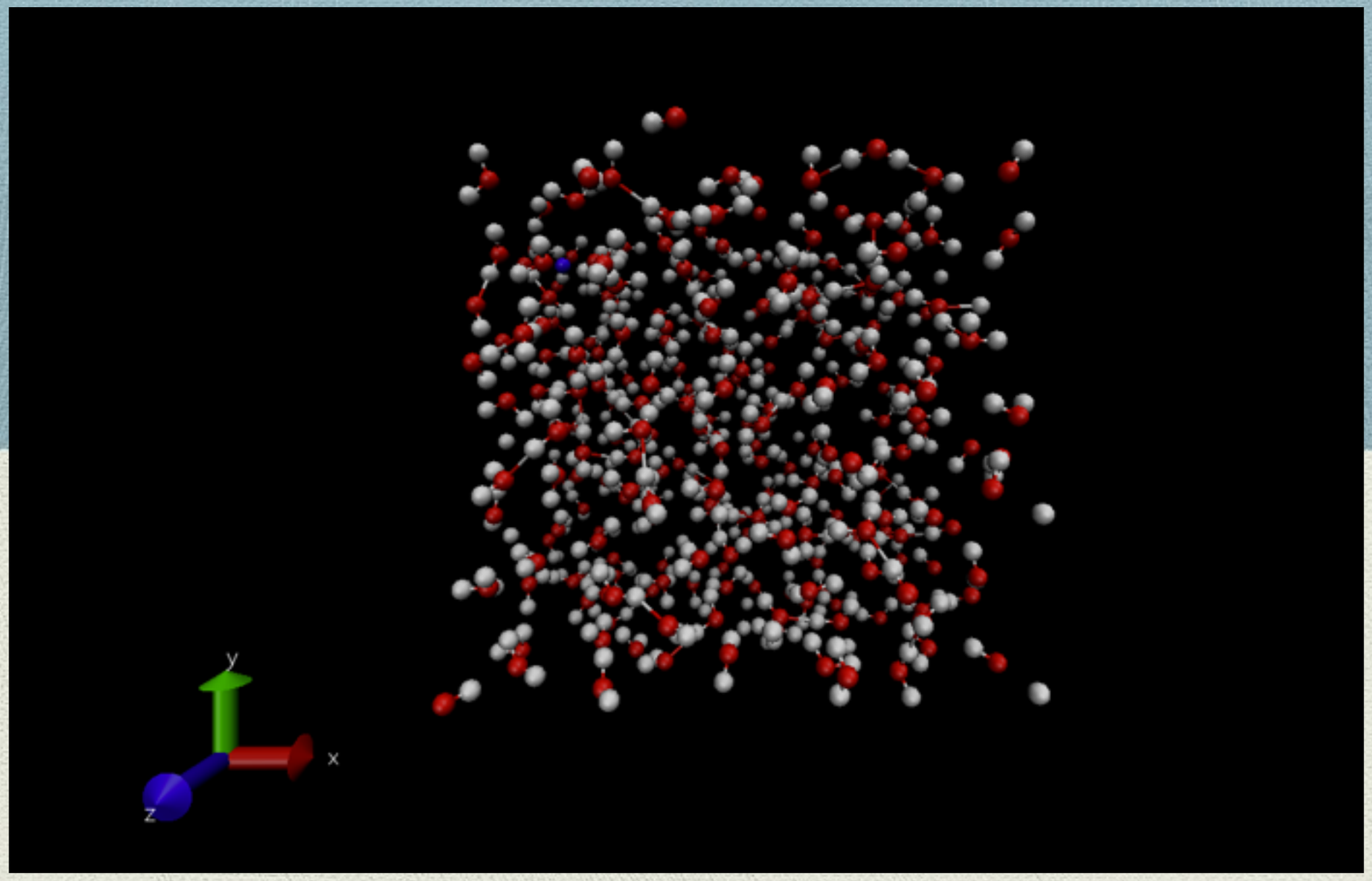
```
simulation of Na+ with 253 water molecules
          6       199
Na+     Na+
  2.500000E-02  0.000000E+00
  7.500000E-02  0.000000E+00
  1.250000E-01  0.000000E+00
  1.750000E-01  0.000000E+00
  2.250000E-01  0.000000E+00
  2.750000E-01  0.000000E+00
  3.250000E-01  0.000000E+00
  3.750000E-01  0.000000E+00
  4.250000E-01  0.000000E+00
  4.750000E-01  0.000000E+00
  5.250000E-01  0.000000E+00
  5.750000E-01  0.000000E+00
  6.250000E-01  0.000000E+00
  6.750000E-01  0.000000E+00
  7.250000E-01  0.000000E+00
  7.750000E-01  0.000000E+00
  8.250000E-01  0.000000E+00
  8.750000E-01  0.000000E+00
  9.250000E-01  0.000000E+00
  9.750000E-01  0.000000E+00
  1.025000E+00  0.000000E+00
  1.075000E+00  0.000000E+00
  1.125000E+00  0.000000E+00
  1.175000E+00  0.000000E+00
  1.225000E+00  0.000000E+00
  1.275000E+00  0.000000E+00
  1.325000E+00  0.000000E+00
  1.375000E+00  0.000000E+00
  1.425000E+00  0.000000E+00
  1.475000E+00  0.000000E+00
```

HISTORY file (trajectory)

HISTORY — Edited

```
simulation of Na+ with 255 water molecules
         0         1       760
timestep      1001       760         0         1    0.001000
   20.66       0.000       0.000
   0.000       20.66       0.000
   0.000       0.000       20.66
Na+               1   22.989800    1.000000
  9.1681E-01  3.2364E-01  2.3074E-01
OW                2   15.999400   -0.820000
  1.0139E+01 -8.8741E+00 -8.8571E+00
HW                3    1.008000    0.410000
 -1.0171E+01 -8.1800E+00 -9.4843E+00
HW                4    1.008000    0.410000
  9.2106E+00 -8.6293E+00 -8.5774E+00
OW                5   15.999400   -0.820000
 -1.0082E+01 -9.3288E-01  7.3081E+00
HW                6    1.008000    0.410000
 -1.0043E+01 -1.6756E+00  6.6397E+00
HW                7    1.008000    0.410000
 -1.0307E+01 -1.3061E+00  8.2082E+00
OW                8   15.999400   -0.820000
 -9.9376E+00 -6.2781E-01  1.9036E+00
HW                9    1.008000    0.410000
 -9.9417E+00  2.4813E-01  1.4212E+00
HW               10    1.008000    0.410000
 -9.1973E+00 -6.3466E-01  2.5758E+00
OW               11   15.999400   -0.820000
  8.9901E+00  4.7811E+00 -2.3611E+00
HW               12    1.008000    0.410000
  8.0374E+00  4.7941E+00 -2.6647E+00
HW               13    1.008000    0.410000
  9.3034E+00  5.7180E+00 -2.2061E+00
OW               14   15.999400   -0.820000
 -8.9136E+00 -1.3990E+00 -2.5510E+00
HW               15    1.008000    0.410000
 -9.8831E+00 -1.5612E+00 -2.3671E+00
HW               16    1.008000    0.410000
```

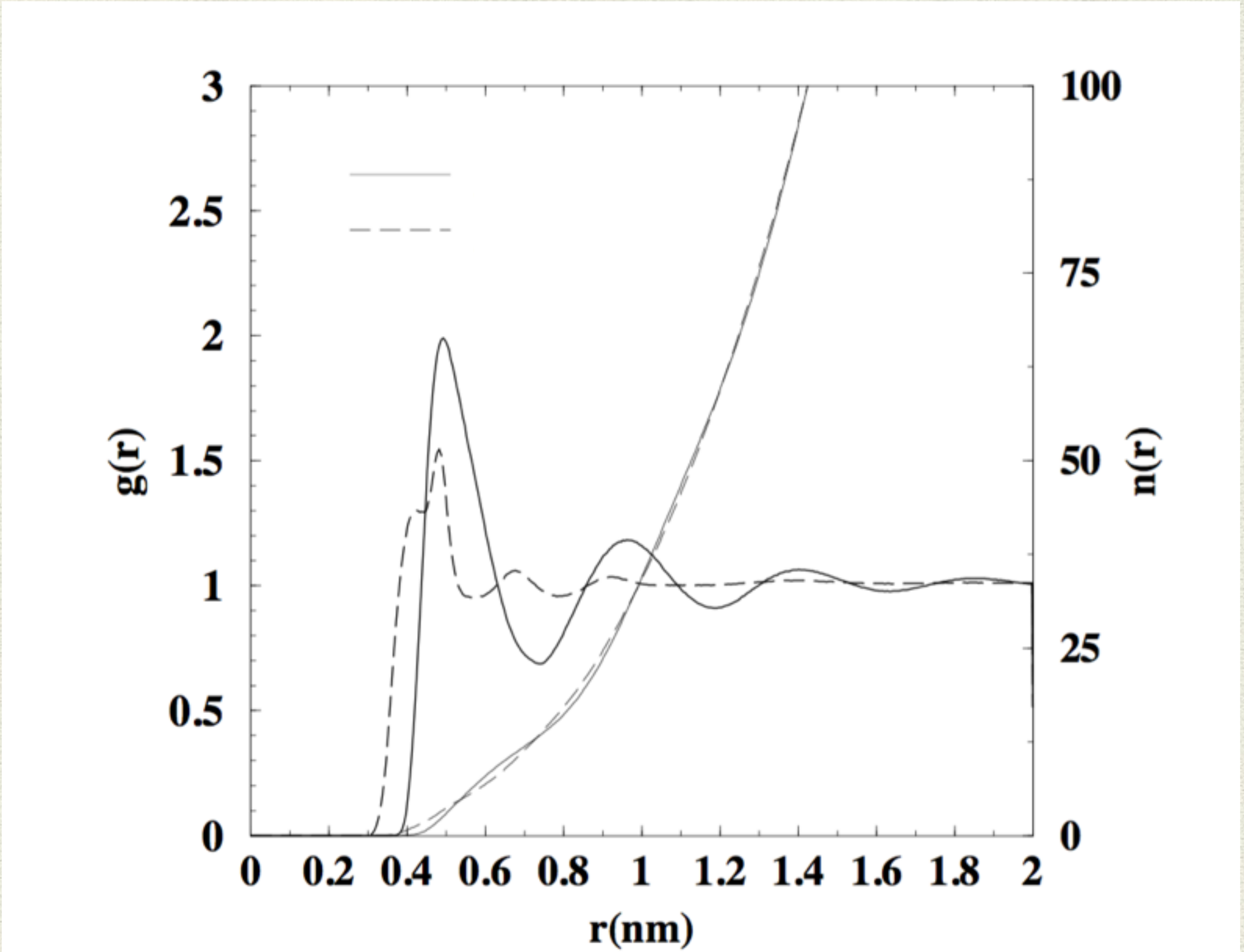
hands-on
Solvation Na^+



Exercise: solvation of M^+ in water (rigid and flexible)

- $M^+ = Na^+ / K^+$
- H_2O= 253 molecules
- Solvation of M^+ in a box with water using a LJ and a SPC water model

RDF



- create the system , add water to the cation, visualise the system with VMD—> CONFIG

- look the CONTROL and FIELD File and adjust it if necessary

- use the script to run the job “script.sh”

- hands-on 2:

  - create FIELD, CONFIG files to use the ILJ potential

  - modified FIELD file to use the flexible water with

- cp from /tmp in hscw the tar file **test_noelia.tar** to $HOME

Table 4.7: Chemical bond potentials

key	potential type	Variables (1-4)				functional form
harm **-hrm**	Harmonic	k	r_0			$U(r) = \frac{1}{2}k(r - r_0)^2$
mors **-mrs**	Morse	E_0	r_0	k		$U(r) = E_0[\{1 - \exp(-k(r - r_0))\}^2 - 1]$
12-6 **-126**	12-6	A	B			$U(r) = \left(\frac{A}{r^{12}}\right) - \left(\frac{B}{r^6}\right)$
rhrm **-rhm**	Restraint	k	r_0	r_c		$U(r) = \frac{1}{2}k(r - r_0)^2 \quad \lvert r - r_0\rvert \le r_c$ $U(r) = \frac{1}{2}kr_c^2 + kr_c(\lvert r - r_0\rvert - r_c) \quad \lvert r - r_0\rvert > r_c$
quar **-qur**	Quartic	k	r_0	k'	k''	$U(r) = \frac{k}{2}(r - r_0)^2 + \frac{k'}{3}(r - r_0)^3 + \frac{k''}{4}(r - r_0)^4$
buck **-bck**	Buckingham	A	ρ	C		$U(r) = Aexp(-r/\rho) - C/r^6$
fene **-bck**	FENE	k	R_o	Δ		$U(r_{ij}) = -0.5\ k\ R_o^2\ ln\left[1 - \left(\frac{r_{ij} - \Delta}{R_o}\right)^2\right]$

Table 4.8: Valence Angle potentials

key	potential type	Parameters p_1-p_4				functional form†
harm **-hrm**	Harmonic	k	θ_0			$U(\theta) = \frac{k}{2}(\theta - \theta_0)^2$
quar **-qur**	Quartic	k	θ_0	k'	k''	$U(\theta) = \frac{k}{2}(\theta - \theta_0)^2 + \frac{k'}{3}(\theta - \theta_0)^3 + \frac{k''}{4}(\theta - \theta_0)^4$
thrm **-thm**	Truncated harmonic	k	θ_0	ρ		$U(\theta) = \frac{k}{2}(\theta - \theta_0)^2 \exp[-(r_{ij}^8 + r_{ik}^8)/\rho^8]$
shrm **-shm**	Screened harmonic	k	θ_0	ρ_1	ρ_2	$U(\theta) = \frac{k}{2}(\theta - \theta_0)^2 \exp[-(r_{ij}/\rho_1 + r_{ik}/\rho_2)]$
bvs1 **-bv1**	Screened Vessal[28]	k	θ_0	ρ_1	ρ_2	$U(\theta) = \frac{k}{8(\theta-\theta_0)^2}\left\{[(\theta_0 - \pi)^2 - (\theta - \pi)^2]^2\right\}$ $\exp[-(r_{ij}/\rho_1 + r_{ik}/\rho_2)]$
bvs2 **-bv2**	Truncated Vessal[29]	k	θ_0	a	ρ	$U(\theta) = k[\theta^a(\theta - \theta_0)^2(\theta + \theta_0 - 2\pi)^2 - \frac{a}{2}\pi^{a-1}$ $(\theta - \theta_0)^2(\pi - \theta_0)^3] \exp[-(r_{ij}^8 + r_{ik}^8)/\rho^8]$
hcos **-hcs**	Harmonic Cosine	k	θ_0			$U(\theta) = \frac{k}{2}(cos(\theta) - cos(\theta_0))^2$
cos **-cos**	Cosine	A	δ	m		$U(\theta) = A[1 + cos(m\theta - \delta)]$
mmsb **-msb**	MM Stretch-bend	A	θ_0	d_{ab}	d_{ac}	$U(\theta) = A(\theta - \theta_0)(r_{ab} - d_{ab})(r_{ac} - d_{ac})$
stst **-sts**	Compass stretch-stretch	A	d_{ab}	d_{ac}		$U_{bac} = A(r_{ab} - d_{ab})(r_{ac} - d_{ac})$
stbe **-stb**	Compass stretch-bend	A	θ_0	d_{ab}		$U_{bac} = A(\theta - \theta_0)(r_{ab} - d_{ab})$
cmps **-cmp**	Compass all terms	A $p_5 = d_{ab}$	B	C $p_6 = d_{ac}$	θ_0	$U_{bac} = A(r_{ab} - d_{ab})(r_{ac} - d_{ac}) + (\theta - \theta_0)*$ $(B(r_{ab} - d_{ab}) + C(r_{ac} - d_{ac}))$

†θ is the a-b-c angle.