

Introduction to QXMD

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Acknowledgement

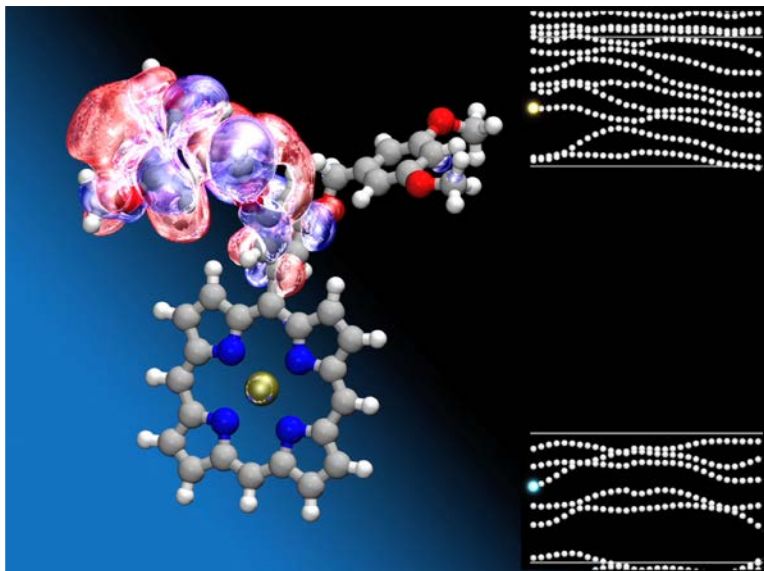
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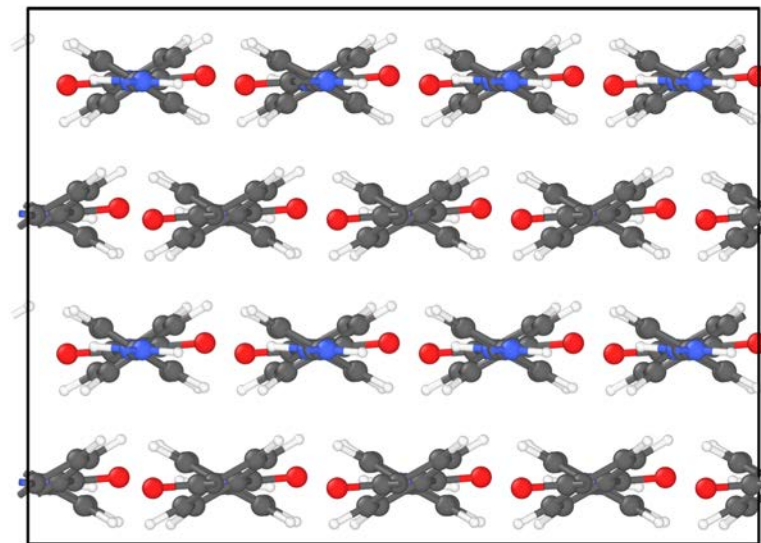
Capabilities

QXMD is scalable parallel quantum molecular dynamics engine.

Non-adiabatic Quantum Molecular Dynamics (NAQMD)

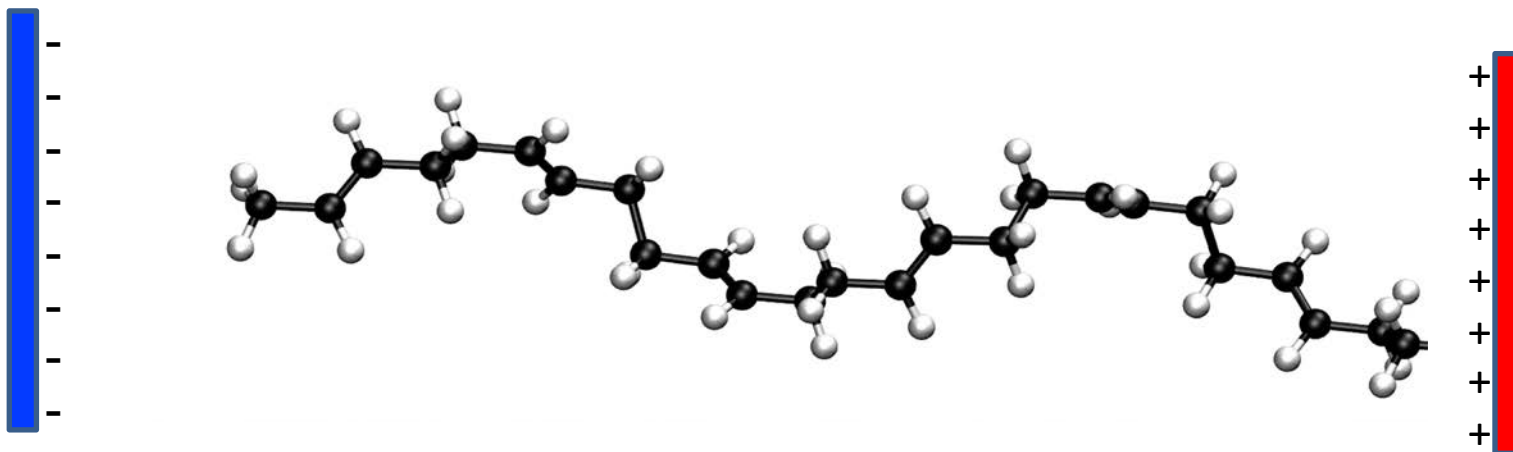


Multiscale Shock theory (MSST)

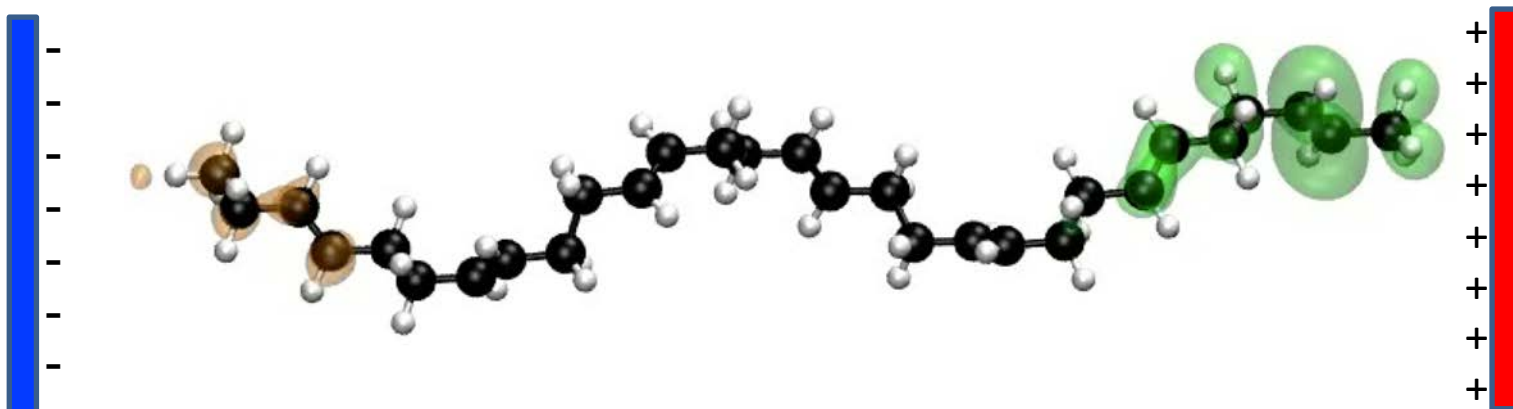


Capabilities

External Electric Field



NAQMD under External Electric Field



Hands On

1- Optimization of Geometry

- Hands-on I: Optimization of water and analysis

2- Non-adiabatic Quantum Molecular Dynamics

- Hands-on II: Excited state dynamics of MoSe_2

Download Slides and Data

https://magics.usc.edu/magics_workshop_downloads/

Download

Download from **MAGICS** website

<https://magics.usc.edu/qxmd/>

Software Download Links

EXECUTABLE



Cray XC_40

ALCF Theta, Cray Intel

Compiler



IBM BG/Q

ALCF Mira, mpiwrapper-xl



USC-HPC

CentOS 7.3, ifort 16.0,

OpenMPI 1.8.8

Documentation download links

PDFs of the installation guide and user manual for QXMD can be downloaded **here**



```
$ cd /staging/magics18/magicsXX/QXMD_session/QXMD
```

Software Package

```
.  
├── Example  
├── LIB  
├── Program  
├── QXMD_Manual_VS.md  
├── README.md  
└── util
```

QXMD Manual in markdown

Examples: Example problem of QXMD

LIB: Psuedopotential

Program: Program executable and input template

util: Utility files for QXMD codes

Directory Structure

```
$ cd Program
```

```
$ ls
```

```
├── IN.PARAM      Input template  
└── qxmdmpi      Executable
```

IN.PARAM: Template input file with complete input settings

```
$ cd ../LIB
```

LIB

```
├── PAW           Projector Augmented wave Pseudopotential  
└── USPP         Ultra soft Pseudopotential
```

```
$ pwd
```

```
/home/rcf-40/magics60/staging/QXMD_session/QXMD/LIB
```

```
$ cd ../Example
```

```
.  
├── 01_Optimization  
├── 02_Adaibatic_MD  
├── 03_ElectricField  
├── 04_MSST  
├── 05_NAQMD  
└── 06_Properties
```

```
$ cd 01_Optimization
```

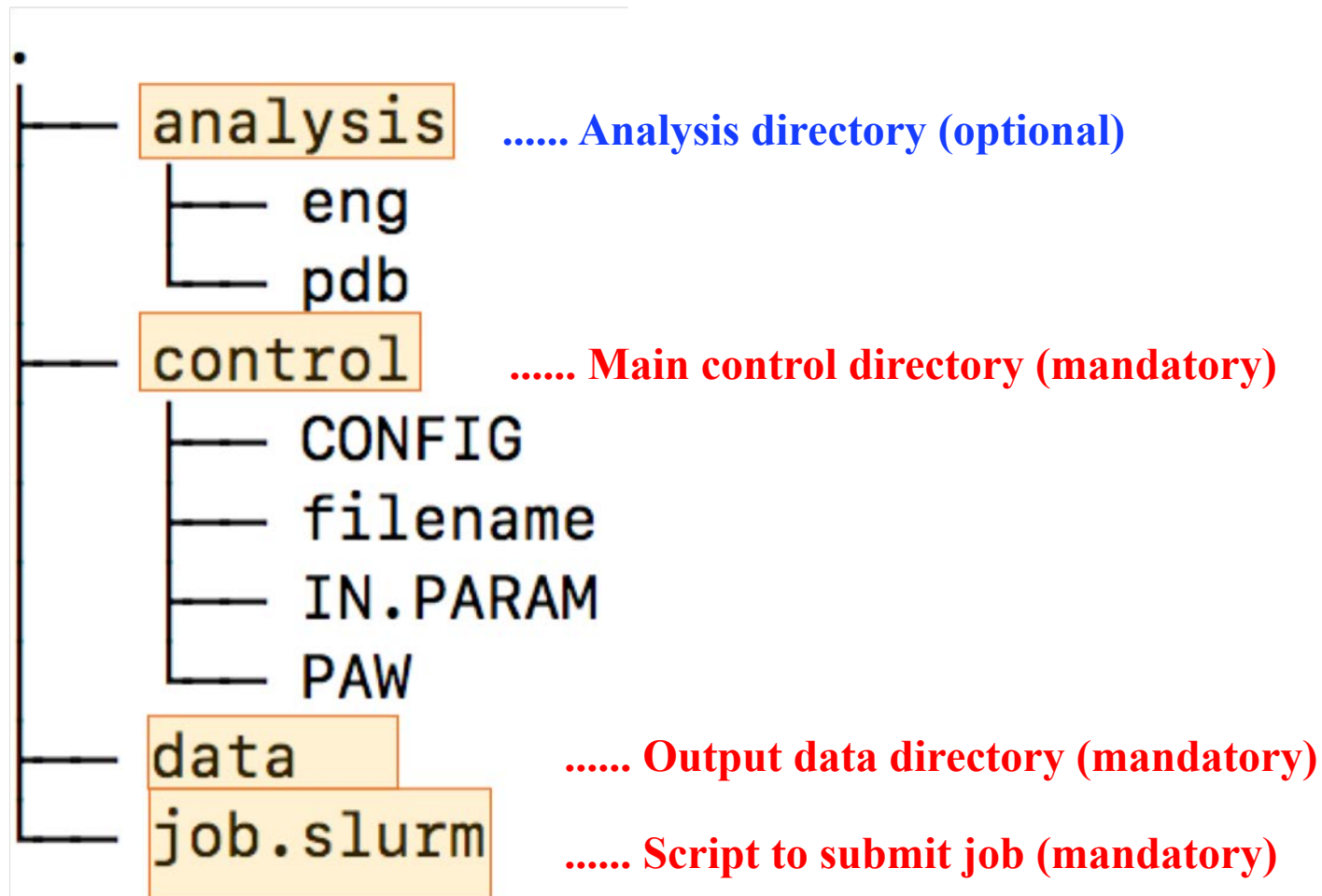
Directory Structure: 01_Optimization

```
$ cd 01_Optimization
```

```
.  
├── 01_Water  
├── 02_MoSe2  
├── 03_WSe2_cell_relax  
└── 04_WSe2_hybrid_relax_restricted
```

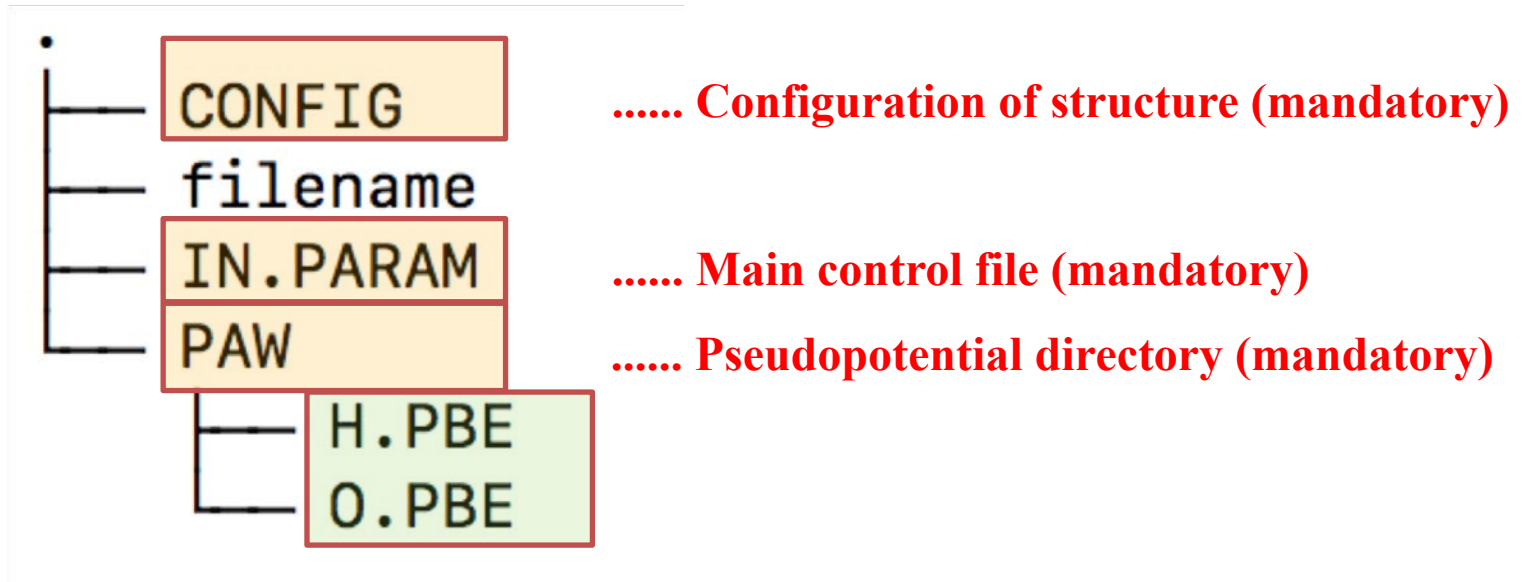
```
$ cd 01_Water
```

Directory Structure



```
$ cd control
```

Directory Structure-Control



PAW directory should be replaced with **USPP** for ultra soft Pseudopotential

Control Directory

control/PAW/

PAW directory must contain potential file for each atom used in

Example: For H₂O, we have H.PBE and O.PBE

control/CONFIG

```
$ less CONFIG
```

This file contains ionic positions either in fractional coordinate or real coordinate

Example:

Fractional

```
3
1 0.853 0.625 0.321
1 0.836 0.670 0.415
.....
```

Unitless

Real

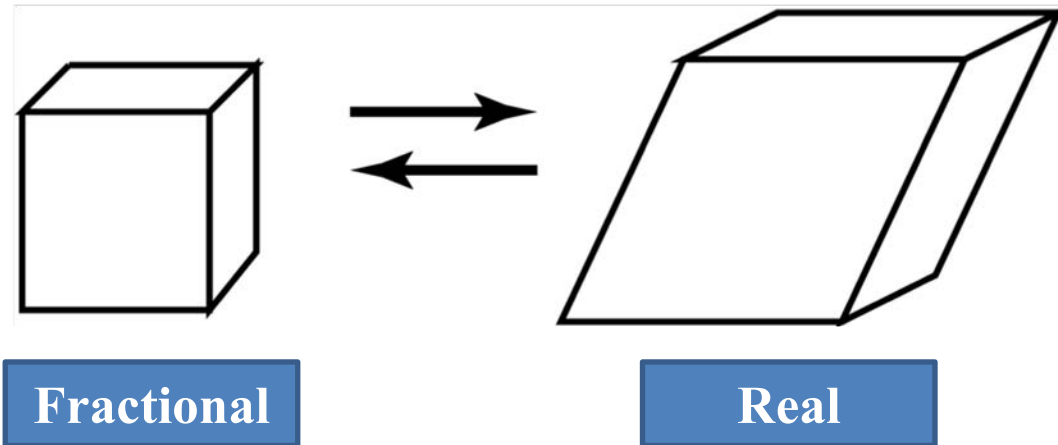
```
3
1 0.000 0.000 0.0
2 1.757 -0.586 0.0
.....
```

Units are Å or bohr

CONFIG

control/CONFIG

Both fractional or real can be given as input



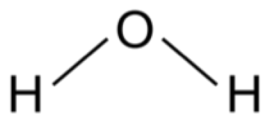
CONFIG (Water/MoSe₂)

control/CONFIG

Real

```
3
1    0.000  0.000  0.0
2    1.757 -0.586  0.0
.....
```

Units are Å or bohr

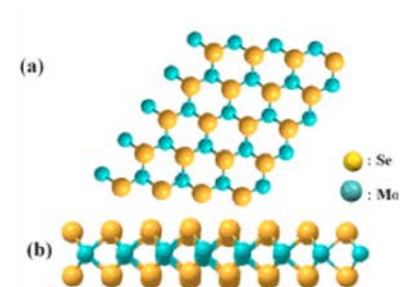


Water:

O- 1
H- 2

MoSe₂

Mo- 1
Se - 2



IN.PARAM

```
$ less IN.PARAM
```

control/IN.PARAM

Main control file

A Template is provided with your program

Control file is divided into several sections. Each section start with its ***\$SECTION_NAME** and ends with ***end**.

Example

```
*parallel      :  
(QM-nodes)    :  
  1 1 1       : (npx, npy, npz)  
(k-points)    :  
  1           : (npk)  
(MD-nodes)    :  
  1 1 1       : (md_npx, md_npy, md_npz)  
*end          :
```

Input File: Enable/Disable calculation

Enabling section

Each section name **must start with 1 column** of the file to enable

Disabling section

To disable set **false** at the sub-section (How).

Other option is to entirely delete the section. If it's required program will take a default value.

Mandatory Input: Parallel

```
*parallel           :  
(QM-nodes)          :  
  1 1 1             : (npx, npy, npz)  
(k-points)          :  
  1                  : (npk)  
(MD-nodes)          :  
  1 1 1             : (md_npx, md_npy, md_npz)  
*end               :
```

QM-Nodes: Parallelization over band

K-points: Parallelization over k-points

MD-nodes: Used for QM/MM calculation

Mandatory Input: restart/PAW

```
*start           :  
(on/off)         :  
.false.          : (lstart) .true. = restart  
*end           :
```

Set **.true.** , if you would like to restart your job from previous file.
QM_\$file must be present to restart a job.

Mandatory Input: restart/PAW

```
*start           :  
(on/off)         :  
.false.          : (lstart) .true. = restart  
*end           :
```

Set **.true.** , if you would like to restart your job from previous file.
QM_\$file must be present to restart a job.

```
*PAW             :  
(on/off)         :  
.true.           : (lpaw) .true. = PAW method  
: .false. = pseudopotential method  
*end
```

.true. Projected Augmented Wave method
.false. pseudopotential method

Mandatory Input: Exchange Correlation

```
*approximation for Exc      :  
(approximation)              :  
    2                        : 1:LDA, 2:GGA(PBE)  
(DFT-D)                      :  
.true.                        :(ldftd)  
*end
```

Approximation

LDA	1
GGA	2
GGA(RPBE)	3
GGA(revPBE)	4
vdW-DF	5
vdW-DF2	6

Empirical Correction

DFT-D	vdW interaction
DFT-U	Mean field Hubbard model

HSE function can be used by turning on range separated function

Mandatory Input: SCF

```
*SCF iteration      :  
(global iteration)  :  
    100  
(tolerance)        :  
    3.0d-08         : (tolerance for total energy)  
    5.0d-08         : (tolerance for average residual)  
*end
```

SCF: Self consistent field

Tolerance are relative change between two successive run. Units are in a.u.

Mandatory Input: Molecular Dynamics

***molecular dynamics** :
(method) :
1 : (ifmd)

Method

Debug	0
Optimization	1
NVE	2
NVT	3
NPT	4
MSST	10

Mandatory Input: Molecular Dynamics

***molecular dynamics** :
(method) :
1 : (ifmd)

Method

Debug	0
Optimization	1
NVE	2
NVT	3
NPT	4
MSST	10

(time step) :
0.1d0 1000 : (dtmd, nstop) time
step, total step

Time step is in a. u.

Mandatory Input: Molecular Dynamics

(temperature)	: only for real dynamics (NVE-, NVT-, NPT-MD)
300.d0	: (treq) temperature in [K]
(check temperature)	:
.false.	: (liscalc) .true. = Do it !
25	: (iscnum) total number of temperature check
20	: (iscstp) skip step

If check temperature is true: First 500 step will have velocity scaling. Since we have set it to false, no velocity scaling will be done

iscnum=Total number of scaling performed

iscstp= scale every iscstp step

Mandatory Input: Molecular Dynamics

(temperature) : only for real dynamics (NVE-, NVT-, NPT-MD)
300.d0 : (treq) temperature in [K]
(check temperature) :
.false. : (liscalc) .true. = Do it !
25 : (iscnum) number of temperature check
20 : (iscstp) skip step

(optimization) : only for structural optimization (ifmd == 1)
2 : (ioptmze)

Method

Do not optimize coordinate	-1
Conjugate gradient	0
Projected Velocity Verlet	1
Quasi Newton Method	2

Mandatory Input: Molecular dynamics

(stabilizer for quasi-Newton) :

0.1d0 : (gammamin)

:

(clear Hessian)

:

0 : (ibfgsclear) clear Hessian every ibfgsclear step

(tolerance)

: tolerance (ifmd == 1)

1.d-07

: (tol_energy) energy/atom in [a.u.]

5.d-04

: (tol_force) max. force in [a.u.]

***end**

:

Tolerance is in the unit of Hartree and Hartree/bohr

Mandatory Input: Supercell/Cutoff Energy

```
*supercell           :  
(unit of length)      :  
(ang)                 : (bohr) or (ang)  
                        :  
(lengths & angles)    :  
7.00d0, 7.00d0, 5.0d0 : lengths of cell vectors  
90.000, 90.000, 90.000 : angles between cell vec. in [deg.]  
*end
```

Mandatory Input: Supercell/Cutoff Energy

```
*supercell           :  
(unit of length)      :  
(ang)                 : (bohr) or (ang)  
                        :  
(lengths & angles)    :  
7.00d0, 7.00d0, 5.0d0 : lengths of cell vectors  
90.000, 90.000, 90.000 : angles between cell vec. in [deg.]  
*end
```

```
*planewaves         :  
(unit of cutoff energy) :  
(ry)                  : (ry) or (hr) or (ev)  
(for wavefunctions)    :  
30.0                   : (ecut)  
(for electron density) :  
250.0                  : (ecutdens)  
(for soft part of density) :  
70.0                   : (ecutsoft)  
*end                 :
```

Mandatory Input: Electronic Band

*electronic bands	:
(occupied bands)	:
8	: (noband) No. of occupied bands
(empty bands)	:
2	: (neband) No. of empty bands
	: total No.= noband + neband
(broadening)	:
3 500.d0	: (lfermi) = 1:nonmetallic, 2:Fermi, 3:Gaussian,
*end	:

$$\text{Min occupied bands} = \frac{\text{No. of electron}}{2} \times 1.1$$

$$\text{Water} = \frac{8}{2} \times 1.1 = 4.4 \cong 5$$

Empty band= 1-20

Unit of smearing is Kelvin

Mandatory Input: atom

```

*atoms          :
(species)       :
  2             : (ntype) No. of atomic species
=====
(atomic number) :
  8.0           : (zatom)
(pseudopotential) :
uspp            : kbpp .or. uspp .or. vand
(nonlocal potential) :
.true. 1.5d0 1.25d0 0.8d0 : (lking) .true. = on, (rking, gkgmax, gkgexct)
(local potential) :
.false. 1.5d0 1.15d0 0.8d0 : (llking) .true. = on, (rlking, glkgmax, glkgexct)
(partial core correction) :
.true. 1.4d0      : (lpcc) .true. = on, (r_cut) in [a.u.]
.true. 1.1d0 1.15d0 0.8d0 : (lpking) .true. = on, (rpking, gpkgmax, gpkgexct)
                    : smoothing parameters
                    :

```

Mandatory Input: atom

(unit of length)	: only for positions
(ang)	: (bohr) or (ang)
	:
(position file)	: Ignored, if (nhk) > 0.
'control/input.config'	:
2	: 1:scaled, 2:real coordinates
1	: (keyword)
	:
(fix positions)	:
.false.	: (lfixion) .true. = fix atomic position
	:
(end)	:
*end	

For fix position **.true.**, create a **new atom ID** and set fix position true

Some Optional Input: dump

```
*dump charge density      :  
(on/off)                   :  
  .true.                   : (ldpchg) .true. = Do it !  
(skip step)                : only for molecular dynamics  
  5                         : (nskip_dpchg)  
(output area)              : output area for charge density  
  1.0  0.0                 : x_min & x_max  
  1.0  0.0                 : y_min & y_max  
  1.0  0.0                 : z_min & z_max  
*end                      :  
  
*dump wavefunctions      :  
(on/off)                   :  
  .true.                   : (ldpwav) .true. = Do it !  
(bands)                    :  
  79, 85                   : (ibstt1,ibstt2) band index ( 0, 0 -> all bands)  
(skip step)                : only for molecular dynamics  
  5                         : (nskip_dpwav)  
*end                      :
```

If ($x_{\min} > x_{\max}$) dump charge density for whole space

Some optional Input: On the fly results

```
*stress calculation                : only for bulk calculations
(on/off)                          :
.true.                            : (lstress) .true. = Do it !
(skip step)                       : only for molecular dynamics
5                                 : (nskip_stress)
*end                               :
                                   :
*atomic charge                    :
(on/off)                          :
.true.                            : (lintchg) .true. = Do it !
(skip step)                       : only for molecular dynamics
5                                 : (nskip_intchg)
*end                               :
```

Example:01

```
$ pwd
```

```
../QXMD/Example/01_Optimization/01_water/control
```

```
$ cd ..  
$ mkdir data  
$ sbatch job.slurm
```

```
$ squeue -u magicsXX
```

Replace magicsXX with your magics account number

Example:01

```
$ cd data
```

QM_cds
QM_cell
QM_eig
QM_hrt
QM_ion
QM_pcds
QM_peig
MD_mts0
MD_Tocontinue

Restart file. Required for continuing a job

Example:01

```
$ cd data
```

```
.  
├── md_box.d  
├── md_cel.d  
├── md_eng.d  
├── md_frc.d  
├── md_ion.d  
├── md_log  
├── md_spc.d  
├── qm_box.d  
├── qm_cel.d  
├── qm_eig.d  
├── qm_eng.d  
├── qm_fer.d  
├── qm_frc.d  
├── qm_ion.d  
├── qm_log  
└── qm_zan.d
```

Output files:qm_ion.d

Output files: qm_ion.d

```
$ less qm_ion.d
```

```
# Atomic scaled coordinates
```

Comment

```
0 2 1 2
```

```
1.0000000E-01
```

```
4.28571 4.28571 7.00000 5.71429 4.28571 6.80000 3.00000 4.28571 6.80000
```

```
1 2 1 2
```

```
1.0000000E-01
```

```
4.29596 4.28571 7.00366 5.71100 4.28571 6.79902 2.99305 4.28571 6.79732
```

```
2 2 1 2
```

Output files:qm_ion.d

Atomic scaled coordinates

0	2	1	2
---	---	---	---

1.0000000E-01

4.28571 4.28571 7.00000 5.71429 4.28571 6.80000 3.00000 4.28571 6.80000

1	2	1	2
---	---	---	---

1.0000000E-01

4.29596 4.28571 7.00366 5.71100 4.28571 6.79902 2.99305 4.28571 6.79732

2	2	1	2
---	---	---	---

Step number, No of atom type, Atom type 1, Atom type 2

Output files:qm_ion.d

```
# Atomic scaled coordinates
      0      2      1      2
1.0000000E-01
4.28571 4.28571 7.00000 5.71429 4.28571 6.80000 3.00000 4.28571 6.80000
      1      2      1      2
1.0000000E-01
4.29596 4.28571 7.00366 5.71100 4.28571 6.79902 2.99305 4.28571 6.79732
      2      2      1      2
```

Scaling factor for position of each atoms

Output files:qm_ion.d

```
# Atomic scaled coordinates
```

```
0      2      1      2
```

```
1.0000000E-01
```

```
4.28571 4.28571 7.00000 5.71429 4.28571 6.80000 3.00000 4.28571 6.80000
```

```
1      2      1      2
```

```
1.0000000E-01
```

```
4.29596 4.28571 7.00366 5.71100 4.28571 6.79902 2.99305 4.28571 6.79732
```

```
2      2      1      2
```

Coordinate of each atom laid out in x, y, z

Output files:qm_ion.d

```
$ less qm_box.d
```

# supercell (FFT cell) vectors (lengths & angles)						Comment
#	L_1	L_2	L_3	angle(2-3)	angle(3-1)	angle(1-2)
0	1.3228082E+01	1.3228082E+01	9.4486299E+00	90.000000	90.000000	90.000000

Box length in bohr (a.u.)

```
$ press q to exit
```

```
$ pwd
```

../QXMD/Example/01_Optimization/01_water/data

Visualizing Energy convergence

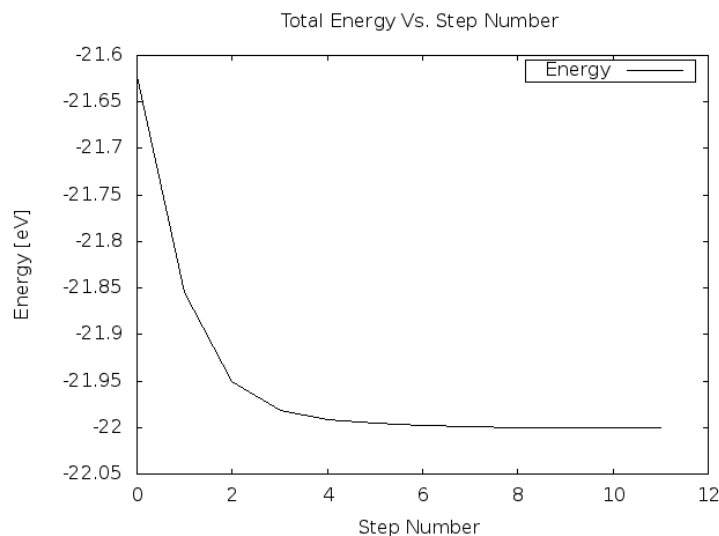
Go to “eng” analysis directory

```
$ cd ../analysis/eng
```

Run a GNUplot script to generate figure. You can choose any other line plotting software to generate same figure

```
$ gnuplot plot_eng.gnu
```

This will generate a file named “eng.png”. Bring it on your computer using filezilla/SCP and visualize.



Analysis

Go to data directory

```
$ cd ../pdb
```

Compile program

```
$ ifort toPDBcell.f -o toPDBcell
```

Run Program

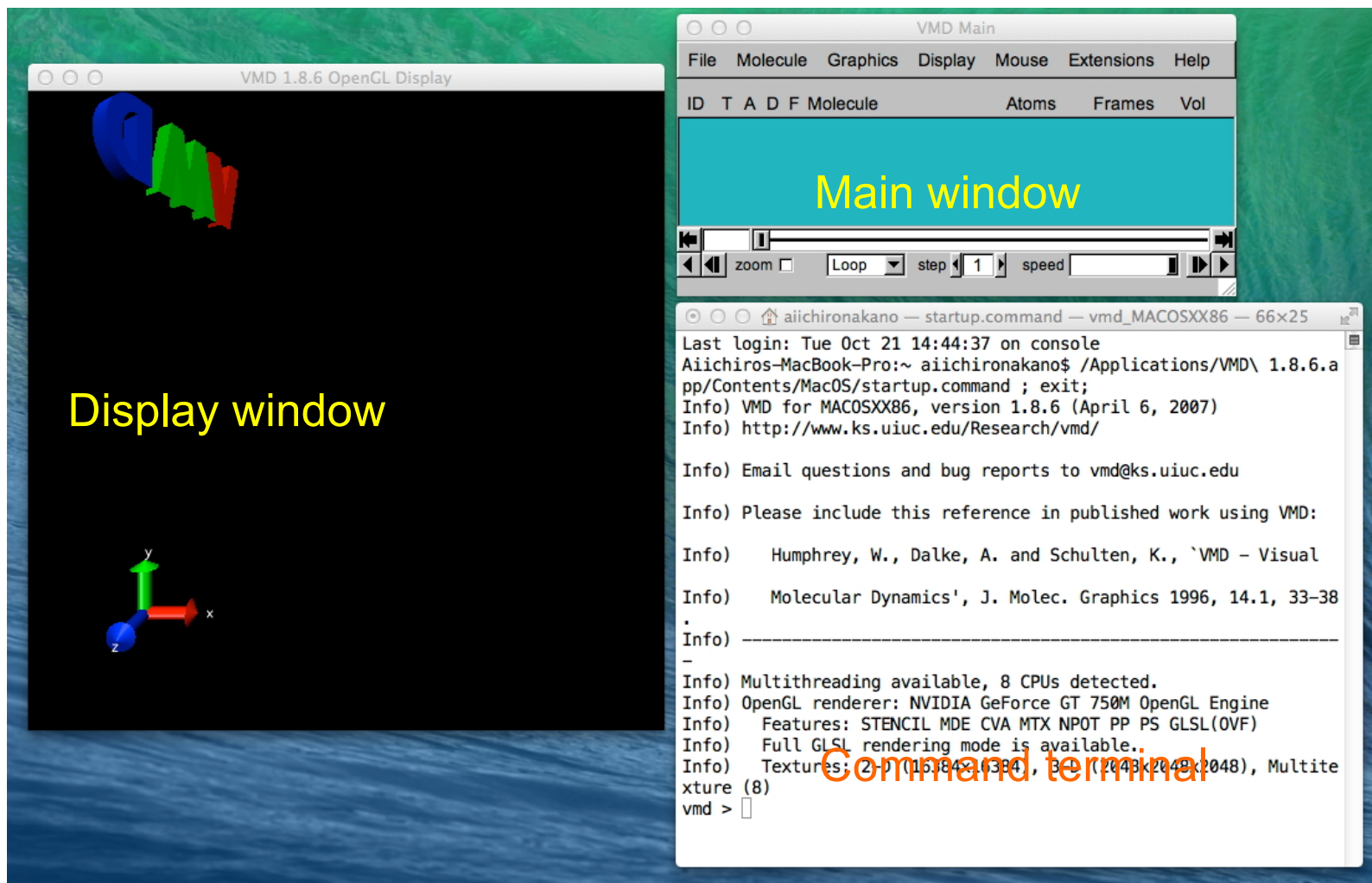
```
$ ./toPDBcell -d ../../data
```

```
open :  
../../data/qm_ion.d  
  
open :  
../../data/qm_box.d  
  
open :  
../../data/md_spc.d
```

```
0  
1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12
```

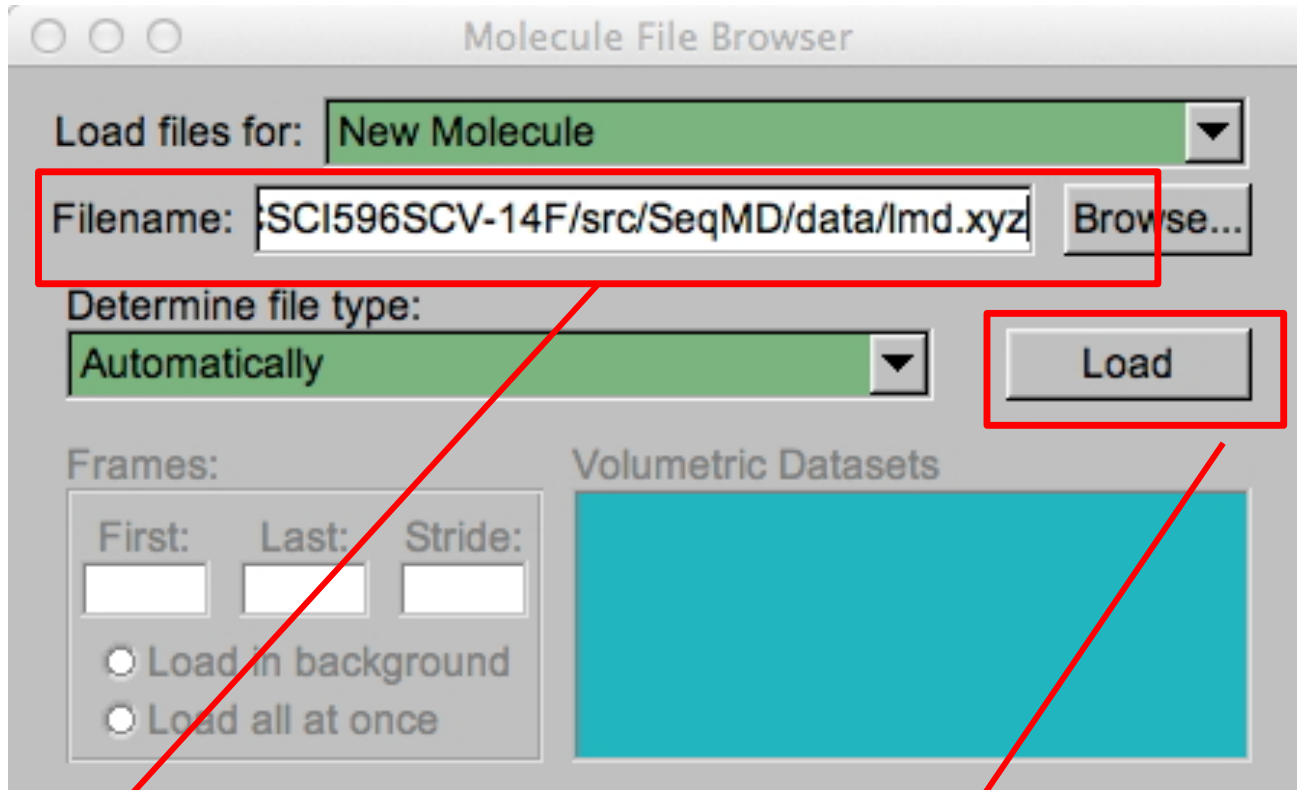
Start VMD

- It will open 3 windows



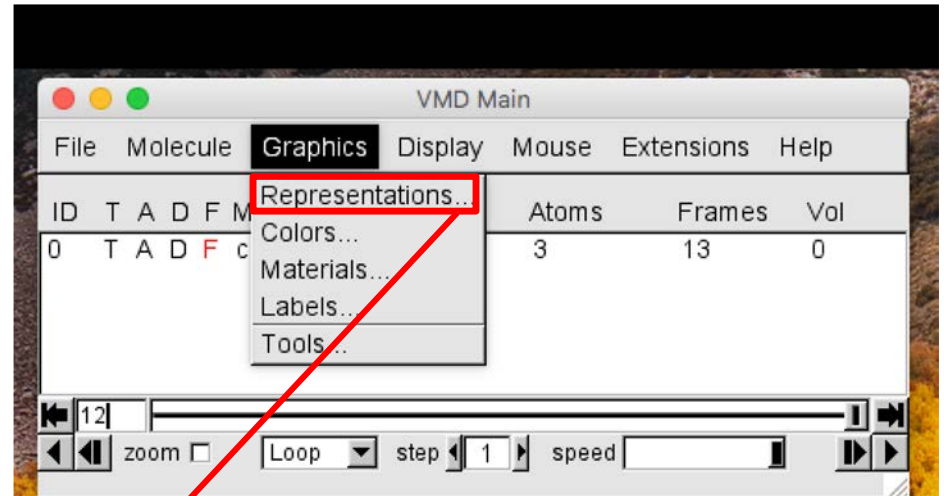
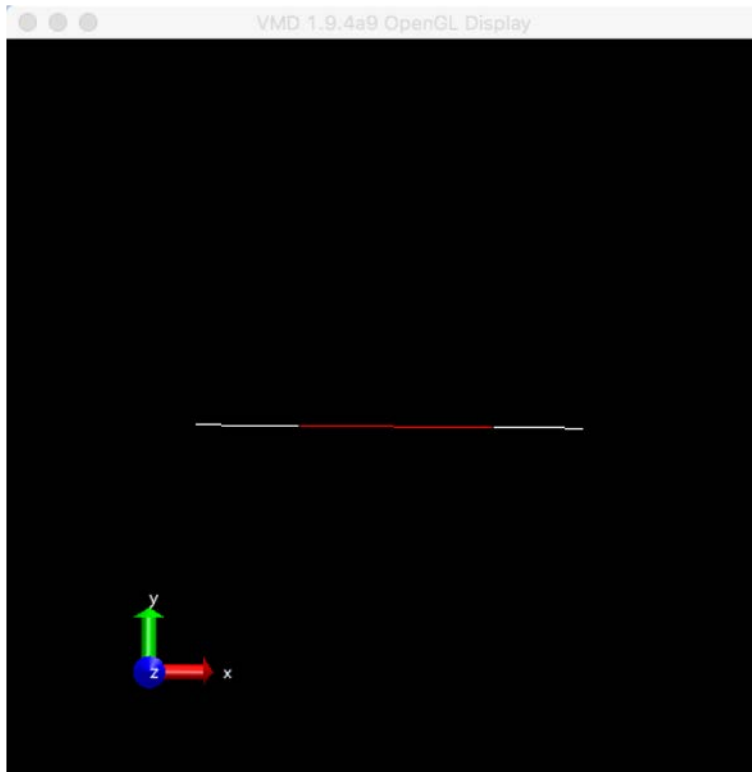
Load the MD-Trajectory PDB File

- In the File menu in the VMD main window, select New Molecule; the following new window will open.



- Drag and drop the PDB file you have created in the Filename field (or press the browse button to locate the file).
Click the Load button to load the file.

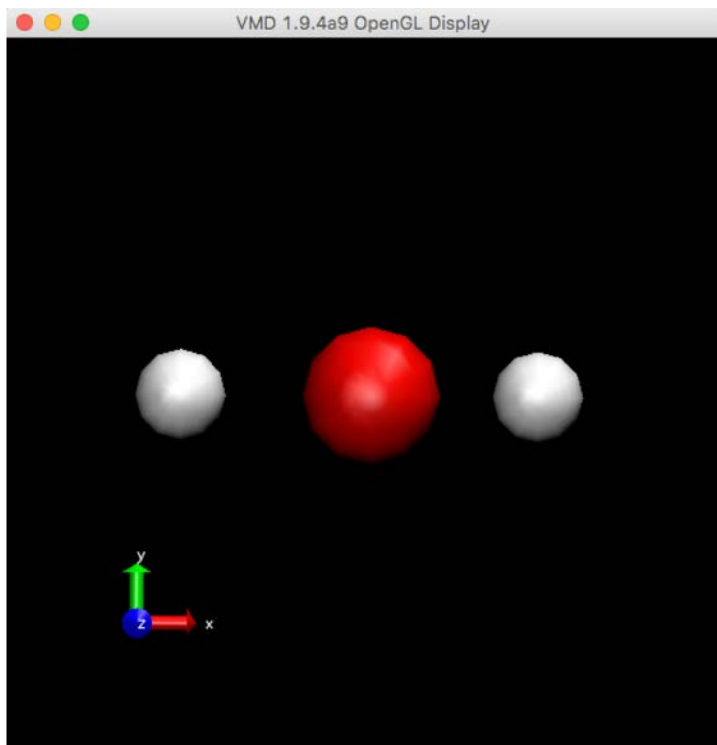
Load the MD-Trajectory PDB File



- Click on Representation to make add different representation of each atoms

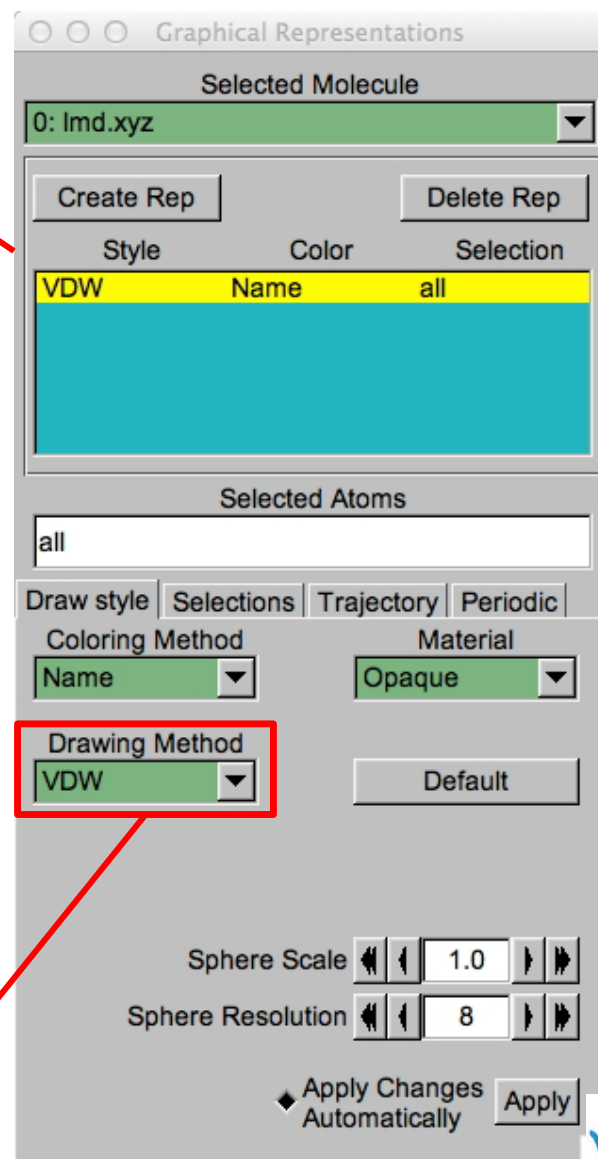
Choose the Graphic Representation

- In the Graphics menu in the VMD main window, select Representations; the following new window will open.



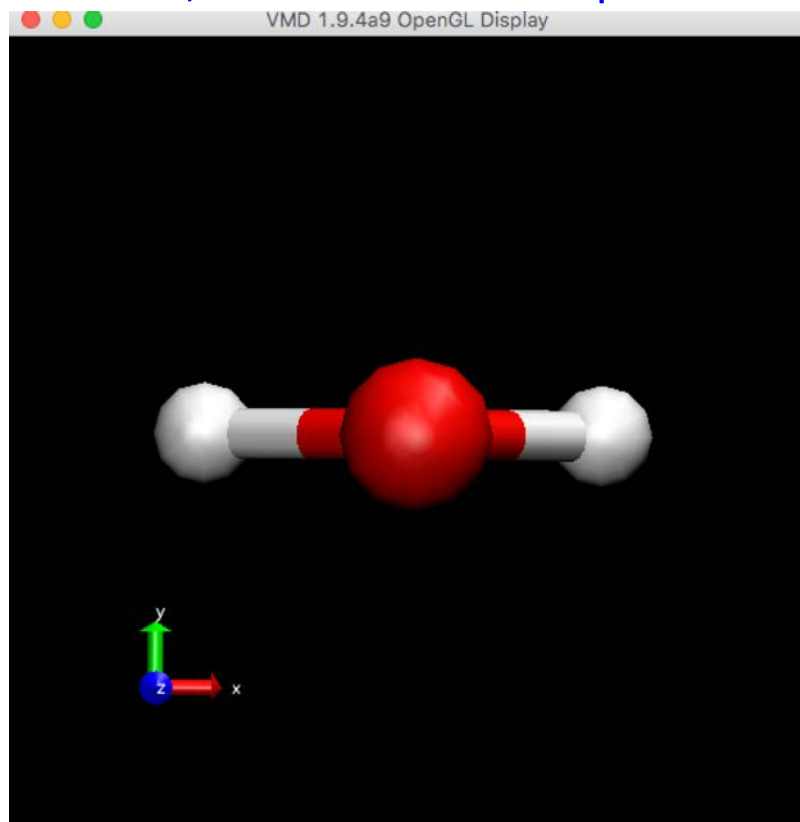
Display now looks like this

- In the Drawing Method menu, choose the VDW (van der Waals radius) representation.



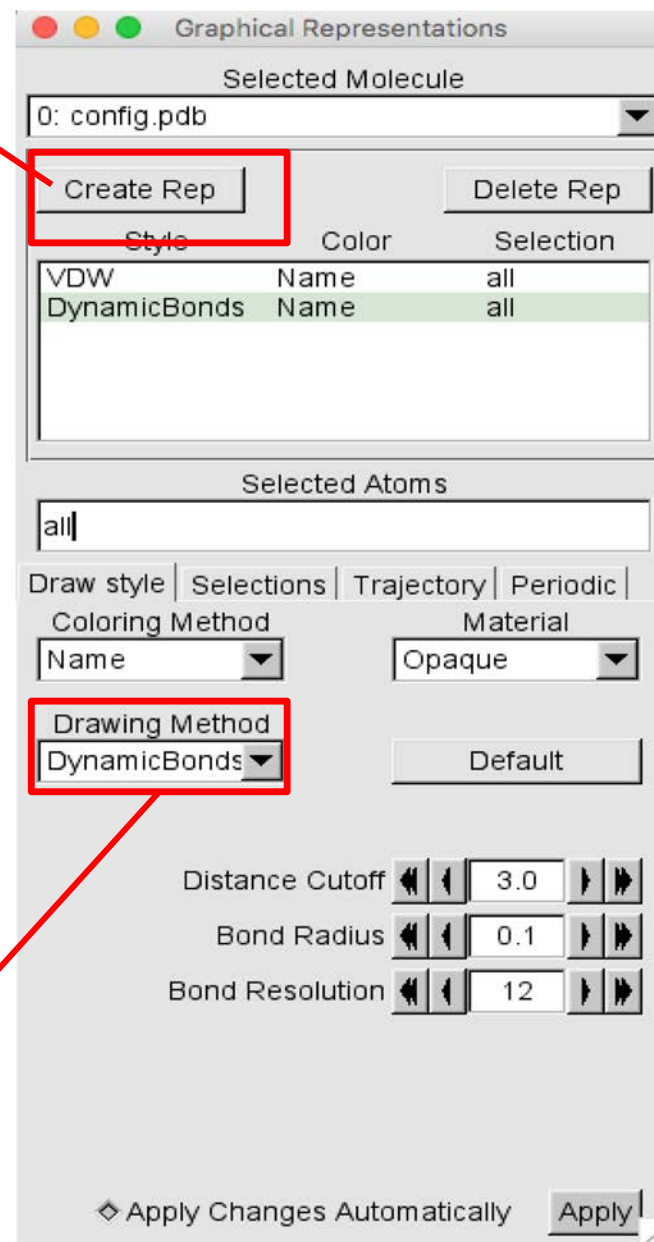
Choose the Graphic Representation

- In the Graphical Representations window; click on Create Rep



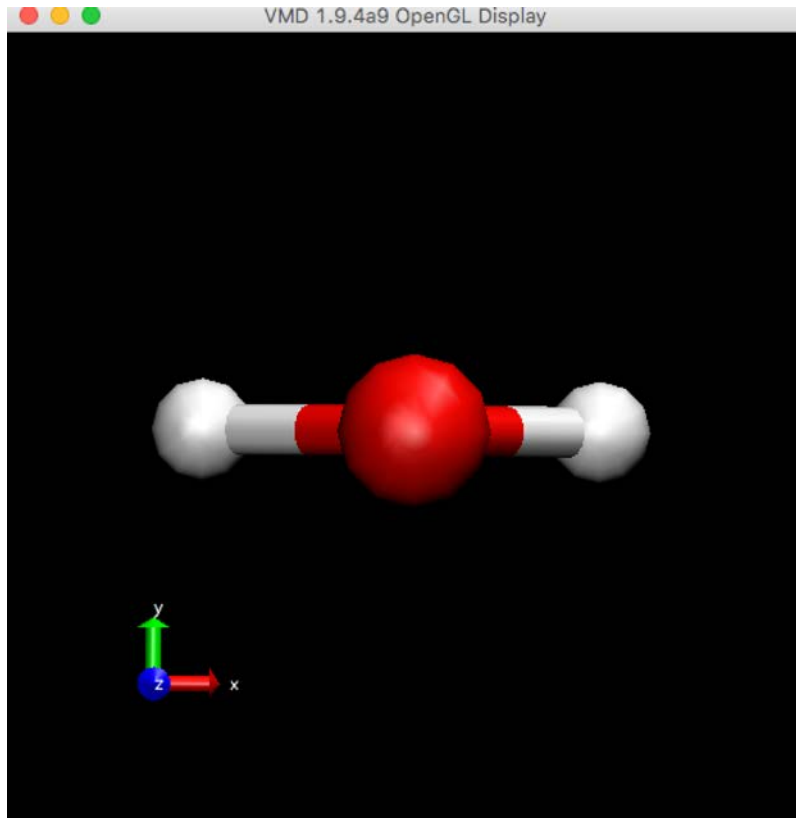
Display now looks like this

- In the Drawing Method menu, choose the DynamicBonds representation.

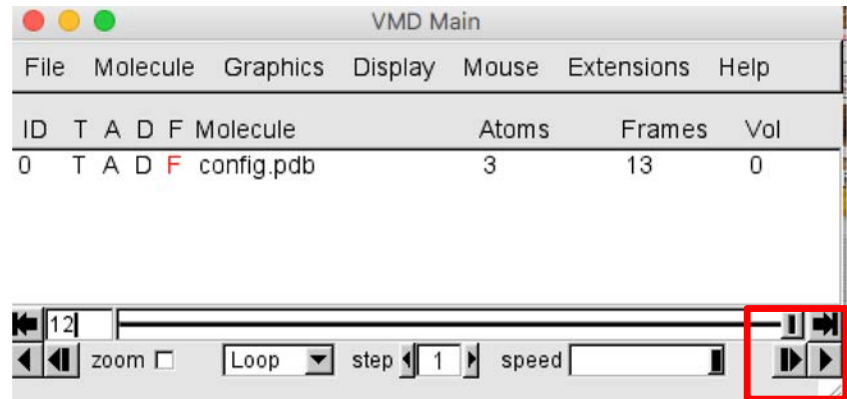


Play Movie

- In the Graphical Representations window; click on Create Rep



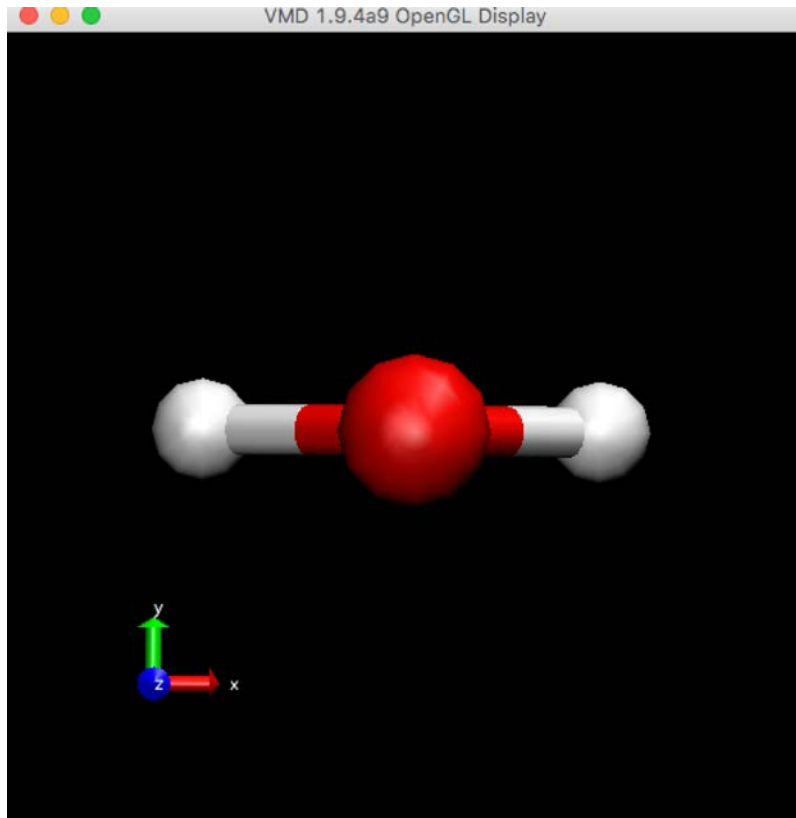
Display now looks like this



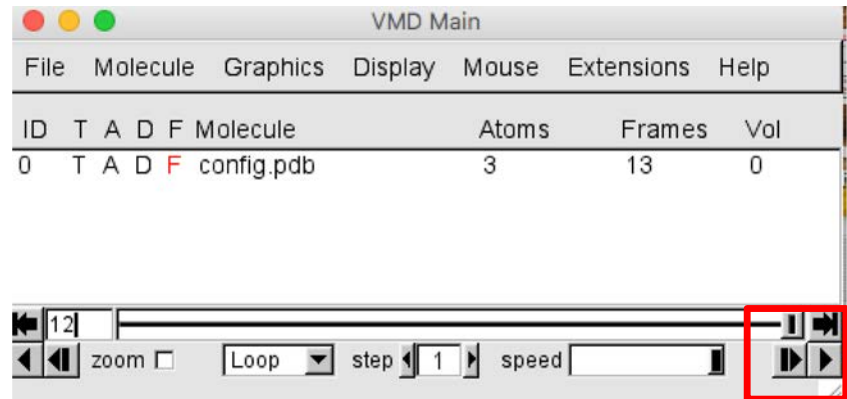
- Play movie by clicking on 
- Watch frame by frame 

Play movie

- In the Graphical Representations window; click on Create Rep



Display now looks like this



- Play movie by clicking on 
- Watch frame by frame movie 

Acknowledgement

[A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations](#)

F. Shimojo, R. K. Kalia, M. Kunaseth, A. Nakano, K. Nomura, S. Ohmura, K. Shimamura and P. Vashishta, Journal of Chemical Physics 140, 18A529 (2014).

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End of Section I

**Thank you for your
attention**