Introduction to QXMD

Subodh Tiwari
Lindsay Bassman, Aravind Krishnamoorthy
Collaboratory for advanced computing and Simulation
Department of Material Science & Department of Physics
University of Southern California

Materials Genome Software Courseware 2019

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QXMD

Capabilities

QXMD is scalable parallel quantum molecular dynamics engine.

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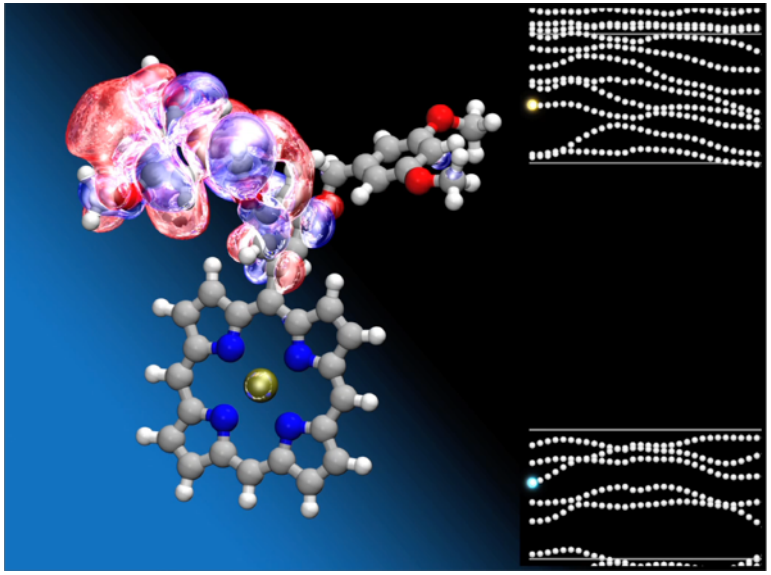
QXMD

Capabilities

QXMD is scalable parallel quantum molecular dynamics engine.

Non-adibatic Quantum Molecular Dynamics (NAQMD)



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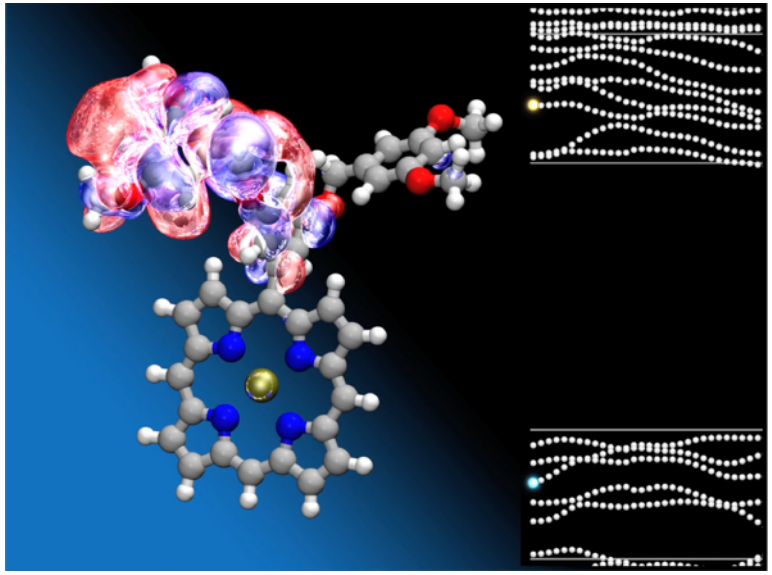
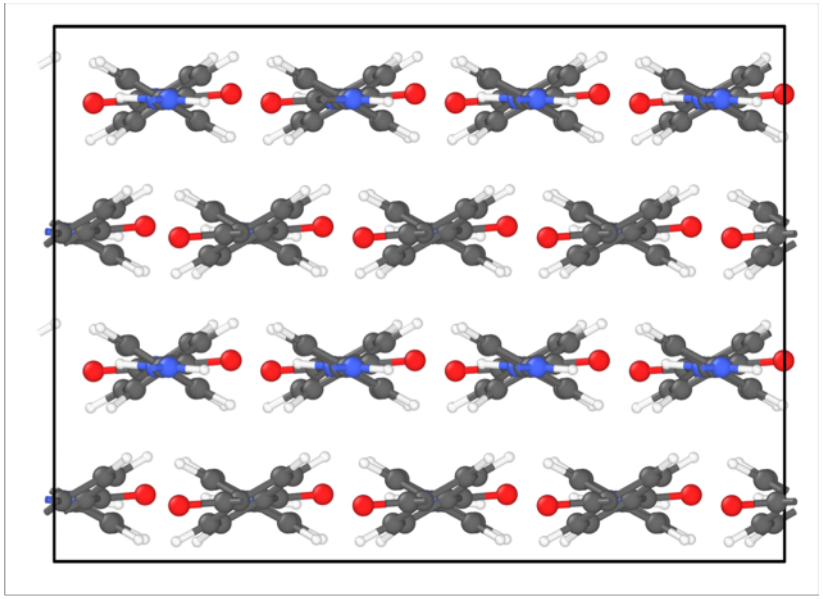
Capabilities

QXMD is scalable parallel quantum molecular dynamics engine.

Non-adibatic Quantum Molecular Dynamics (NAQMD)



Multiscale Shock theory (MSST)



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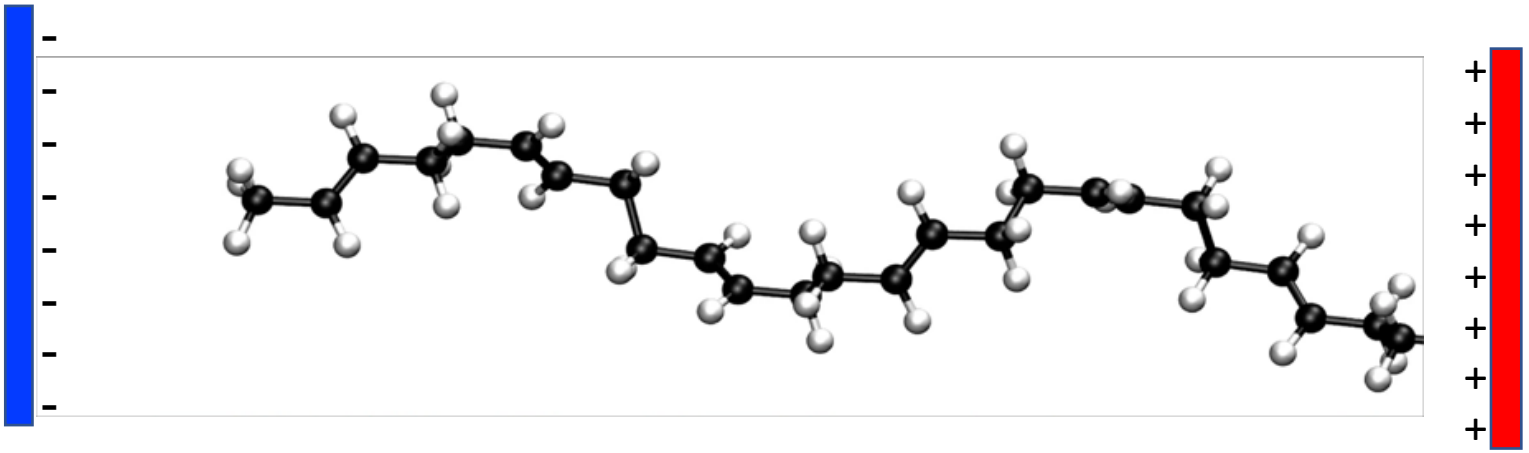
External Electric Field



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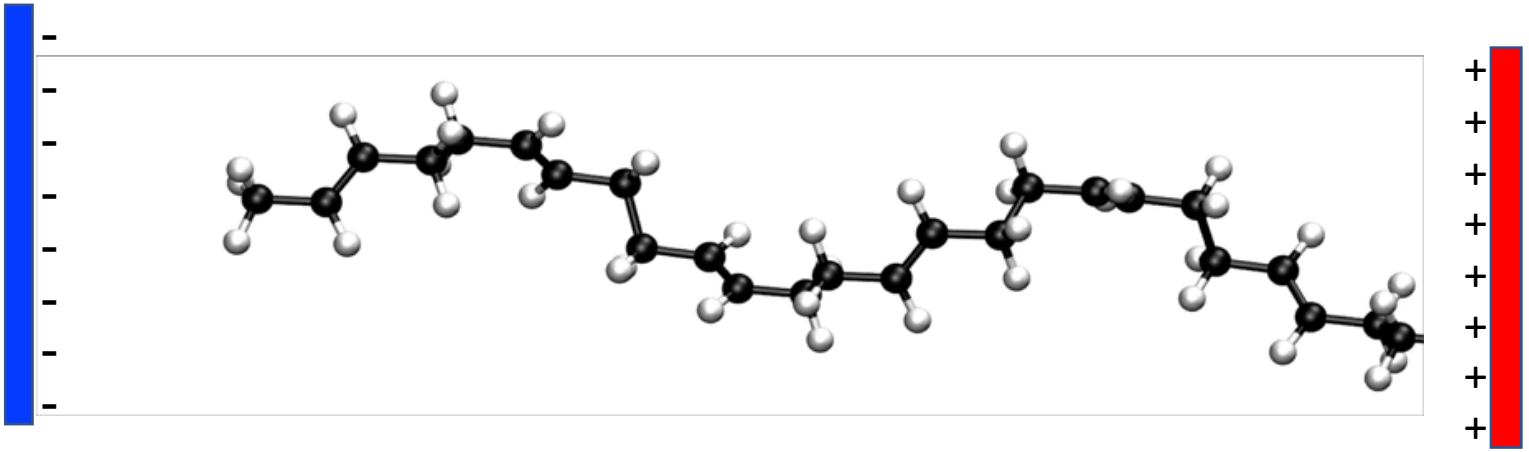
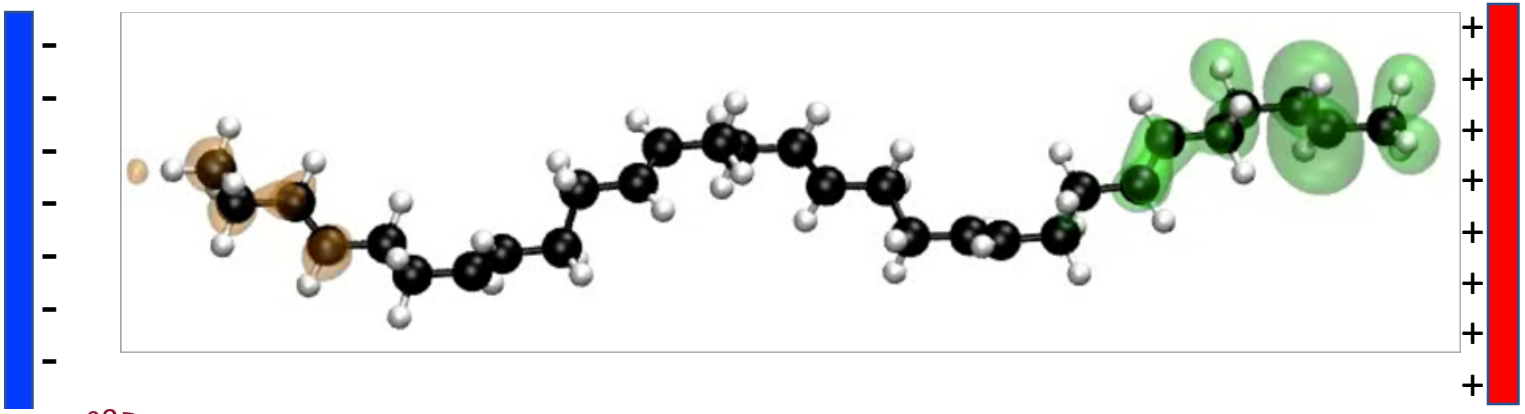
Capabilities

External Electric Field



NAQMD under External Electric Field



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Outline

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 $MoSe_2$**

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Download

Download from GitHub:
$ git clone https://github.com/USCCACS/QXMD.git
$ cd QXMD

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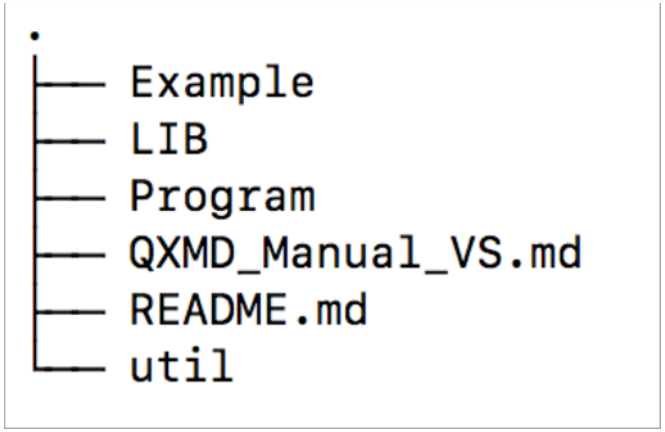
Software Package



QXMD Manual in markdown

Examples: Example problem of QXMD

Lib: Psuedopotential

Program: Program executable and input template

Util: Utility files for QXMD codes

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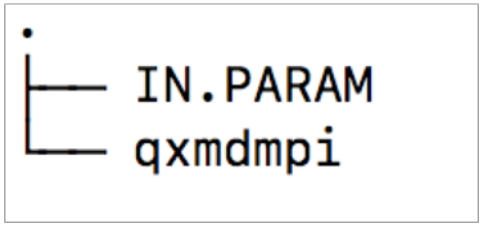
Directory Structure

```
$ cd Program
```

```
$ ls
```



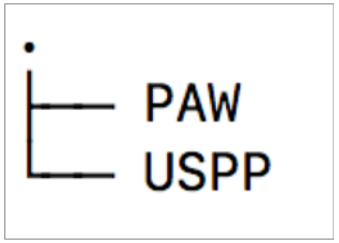
Input template

Executable

IN.PARAM: Template input file with complete input settings

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

LIB



Projector Augmented wave Pseudopotential

Ultra soft Pseudopotential

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Directory Structure

```
$ cd ../Examples
```

01_Optimization
02_Adiabatic
03_NAQMD
04_MSST

```
$ cd 01_Optimization
```

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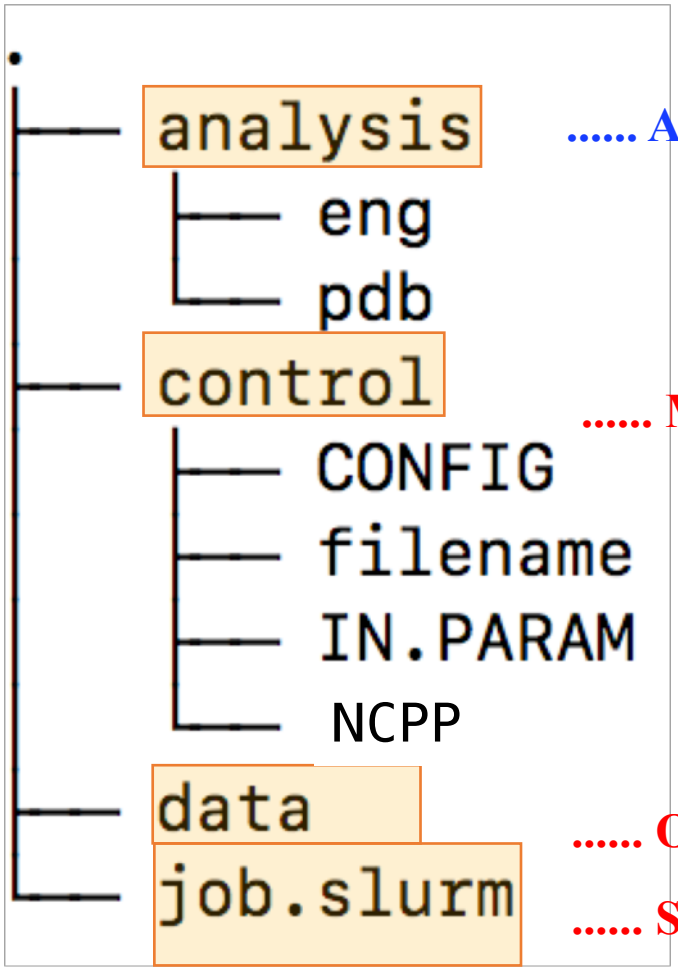
Directory Structure: 01_Optimization

```
$ cd 01_Optimization
```

```
$ cd 01_Water
```

Directory Structure



..... Analysis directory (optional)

..... Main control directory (mandatory)

..... Output data directory (mandatory)

..... Script to submit job (mandatory)

```
$ cd control
```

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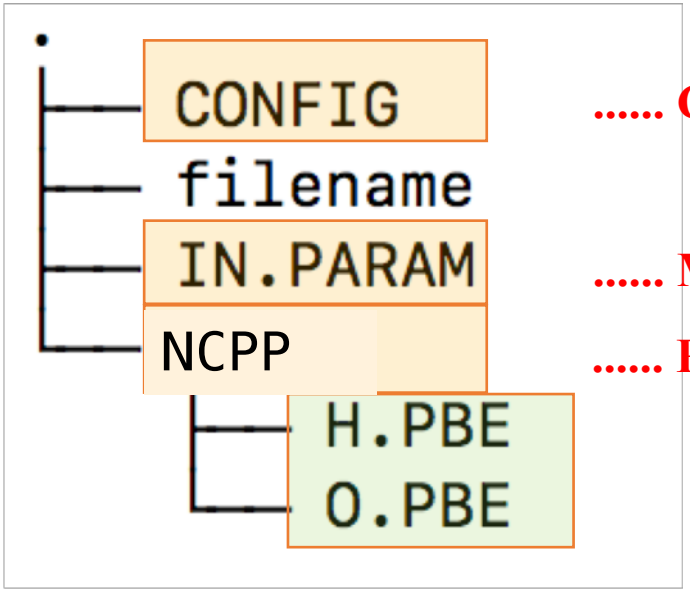
Directory Structure-Control



..... Configuration of structure (mandatory)

..... Main control file (mandatory)

..... Pseudopotential directory (mandatory)

PAW directory should be replaced with USPP for ultra soft Pseudopotential

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Control Directory

control/NCPP/

NCPP directory must contain potential file for each atom used in

Example: For H_2O, 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

```
75
1     0.853  0.625   0.321
1     0.836  0.670   0.415
……..
```

Unitless

Real

```
75
1     0.000   0.000   0.0
2     1.757   -0.586   0.0
……..
```

Units are Å or bohr

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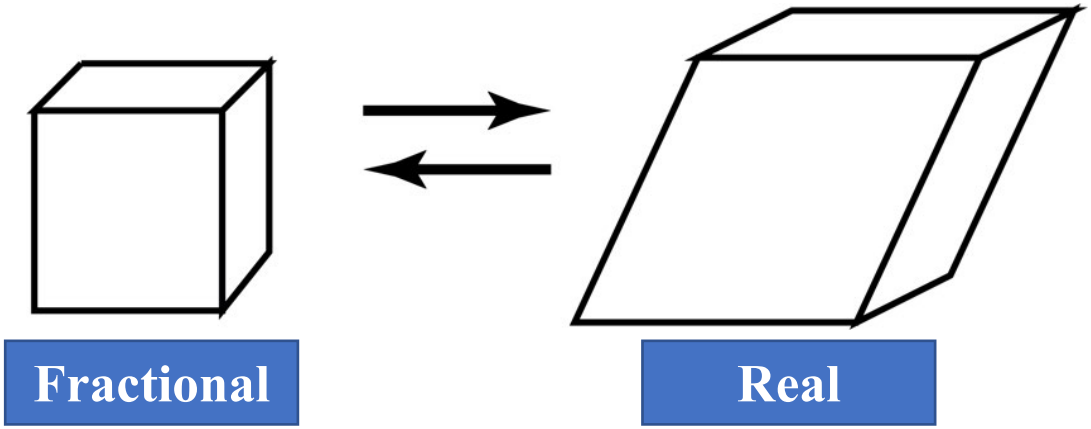
CONFIG

control/CONFIG

Both fractional or real can be given as input



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CONFIG (Water/$MoSe_2$)

control/CONFIG

Real

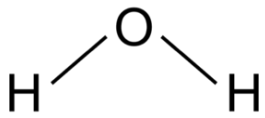
75

1 0.000 0.000 0.0

2 1.757 -0.586 0.0

……..

Units are Å or bohr



Water:

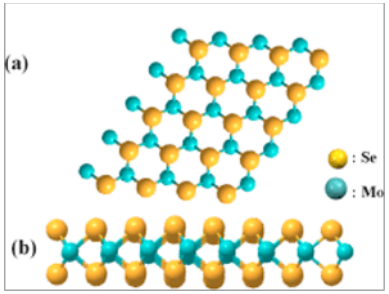
O- 1

H- 2

$MoSe_2$

Mo- 1

Se - 2



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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                   :
```

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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 divide-conquer-recombine algorithm for order N DFT code

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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

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Mandatory Input: Exchange Correlation

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

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

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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

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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.

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Mandatory Input: Molecular Dynamics

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

Method

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

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QXMD

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.

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Mandatory Input: Molecular Dynamics

(temperature)	: only for real dynamics (NVE-, NVT-, NPT-MD)
300.d0	: (treq) temperature in [K]
(check temperature)	:
.false.	: (liscale) .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

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QXMD

Mandatory Input: Molecular Dynamics

```
(temperature)              : only for real dynamics (NVE-, NVT-, NPT-MD )
  300.d0                   : (treq) temperature in [K]
(check temperature)        :
  .false.                  : (liscale) .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

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Mandatory Input: Molecular Dynamics

```
(stabilizer for quasi-Newton)  :
  0.1d0                        : (gammamin)
                               :
(clear Hessian)                :
  0                            : (ibfgsclear) clear Hessian every ibfgsclear step
```

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

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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
```

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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                          :
```

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Mandatory Input: Supercell/Cutoff Energy

```
*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                            :
```

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

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

Empty band= 1-20

Unit of smearing is Kelvin

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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
                                    :
```

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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

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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

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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                         :
```

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Example:01

```
$ pwd
../QXMD/Examples/01_Optimization/01_water/control
```

```
$ cd ..

Run qxmdmpi executable
```

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
```

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Output files

Output files: qm_ion.d

```
$ less qm_ion.d
```

Comment

```
#  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
```

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Output file: 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

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Output File: 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

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Output File: 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

```
$ press q to exit
```

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Output File: qm_box.d

```
$ less qm_box.d
```

```
#  supercell (FFT cell) vectors (lengths & angles)
#        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
```

Comment

Box length in bohr (a.u.)

```
$ press q to exit
```

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Output File: md_eng.d

Output files: md_eng.d

```
$ less md_eng.d
```

```
# step    P.E. [hartree]
      0 -2.1951549312E+01
      1 -2.1954246118E+01
      2 -2.1959473771E+01
      3 -2.1961990569E+01
      4 -2.1972379455E+01
      5 -2.1978050971E+01
      6 -2.1983590094E+01
      7 -2.2000540405E+01
      8 -2.2001983644E+01
      9 -2.2002236635E+01
     10 -2.2002297278E+01
     11 -2.2002316458E+01
```

Comment

Step and energy (hartree)

```
$ press q to exit
```

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Analysis

Go to data directory

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

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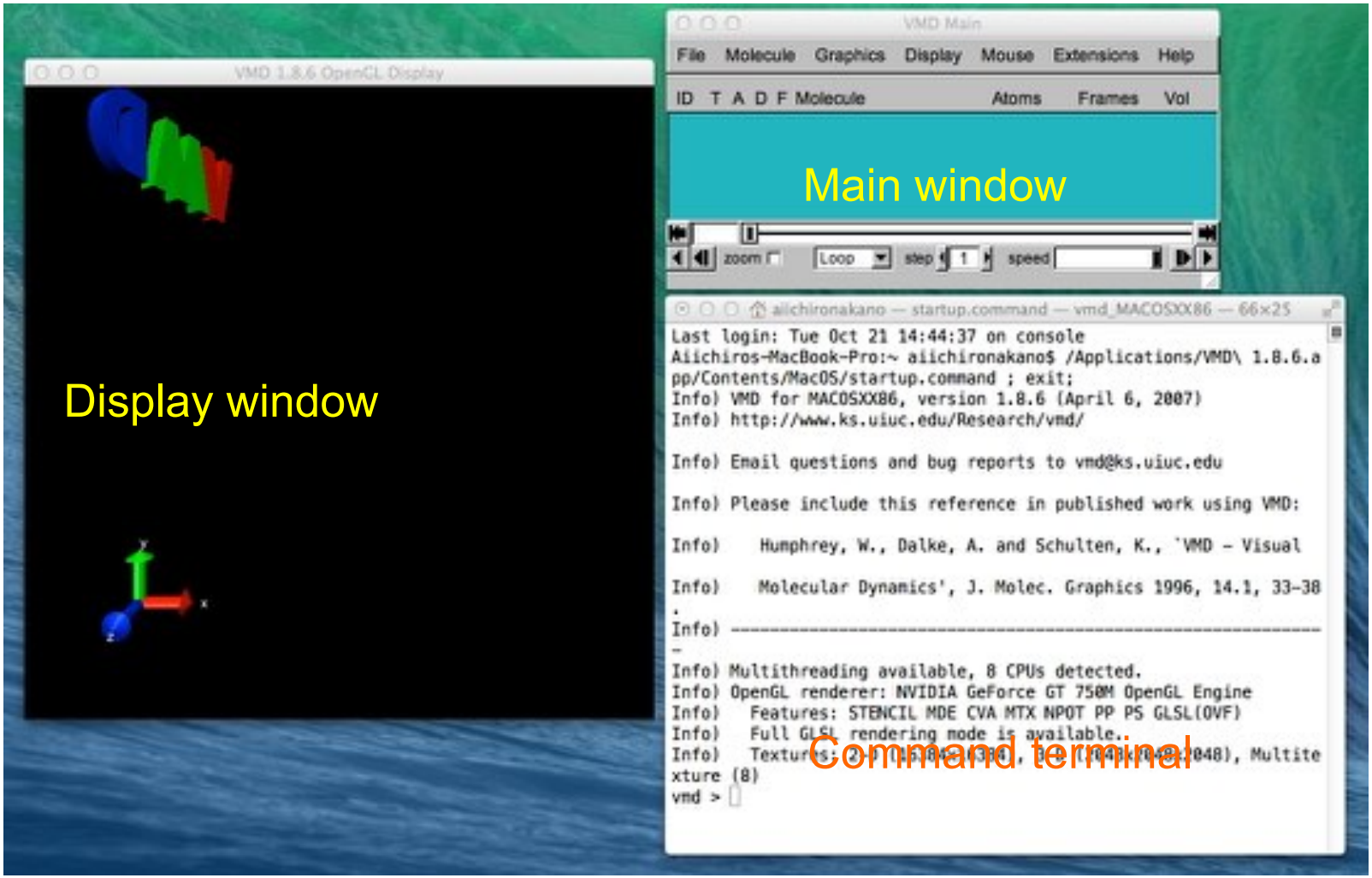
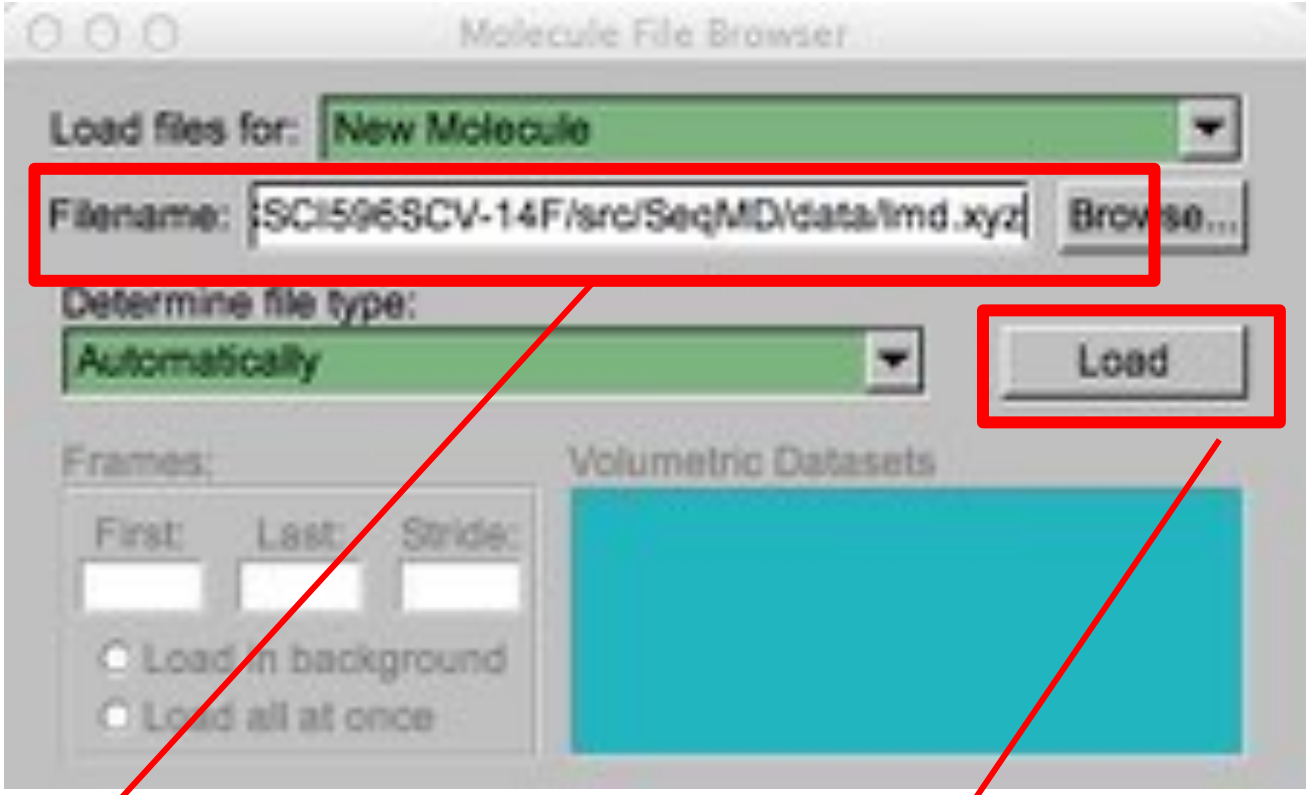
Start VMD

- 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 XYZ 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.

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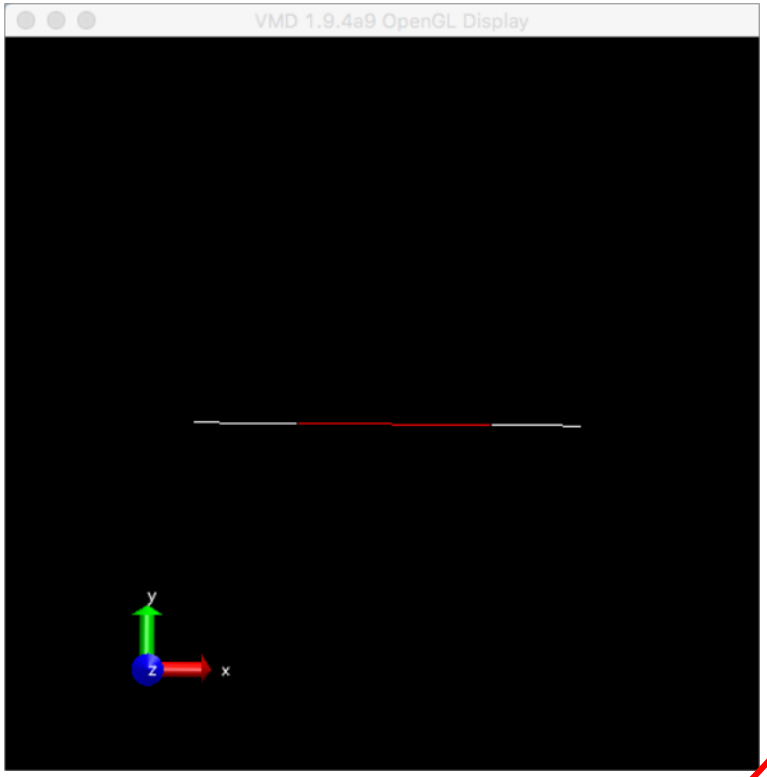
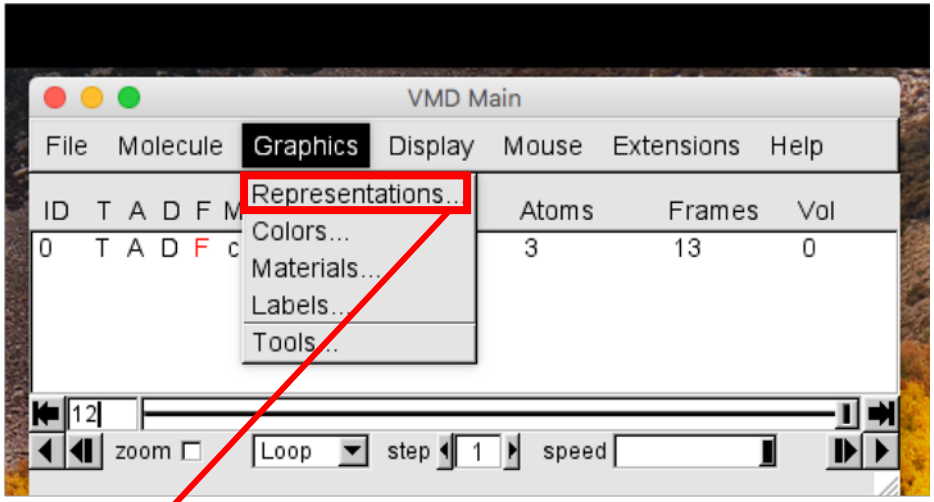
Load the MD-Trajectory PDB File





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

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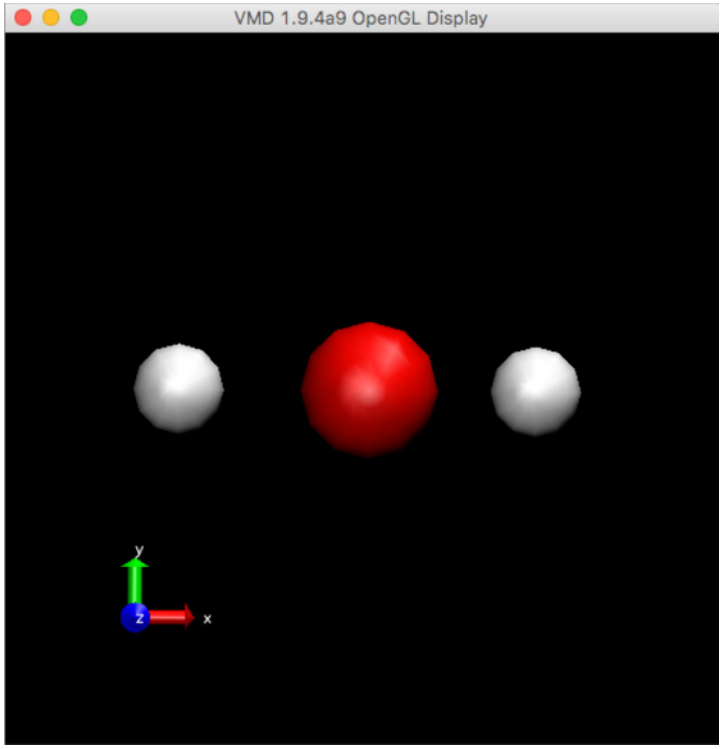
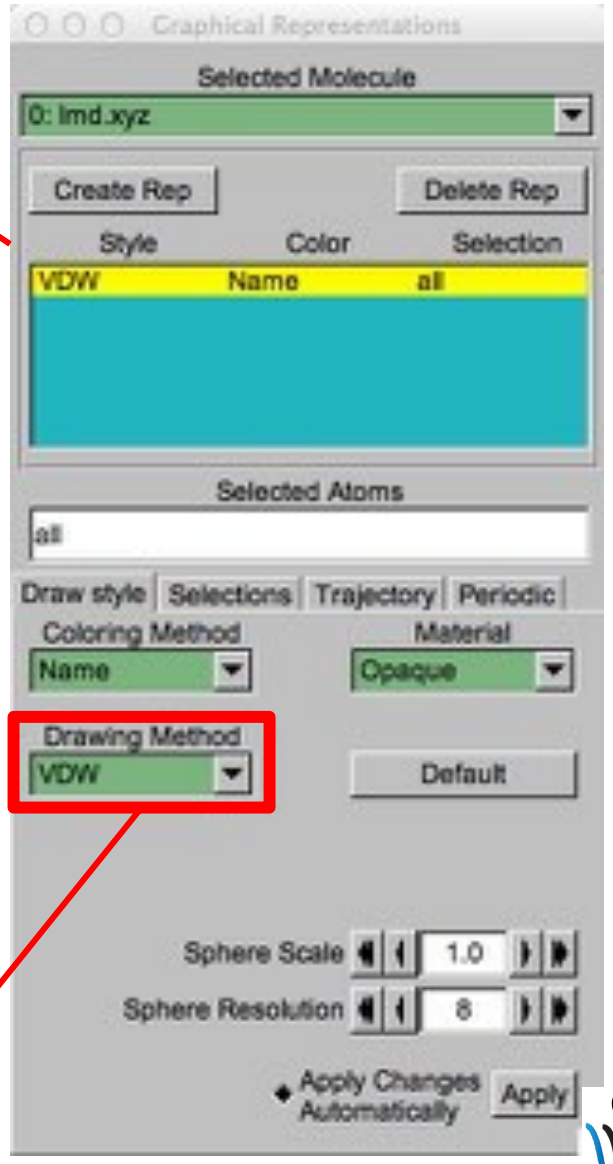
Choose the Graphic Representation

- 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.



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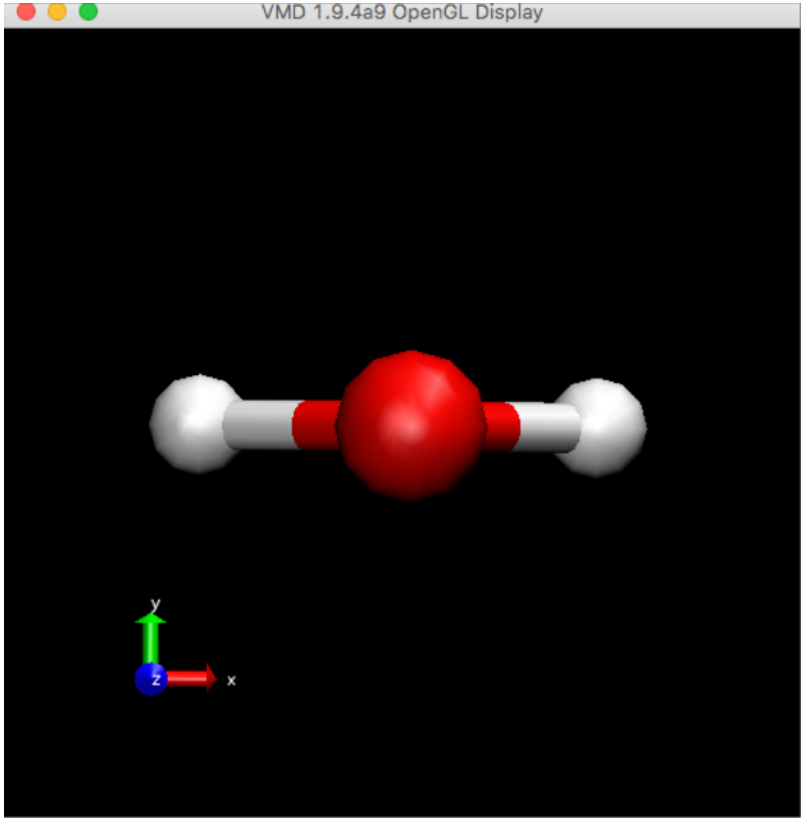
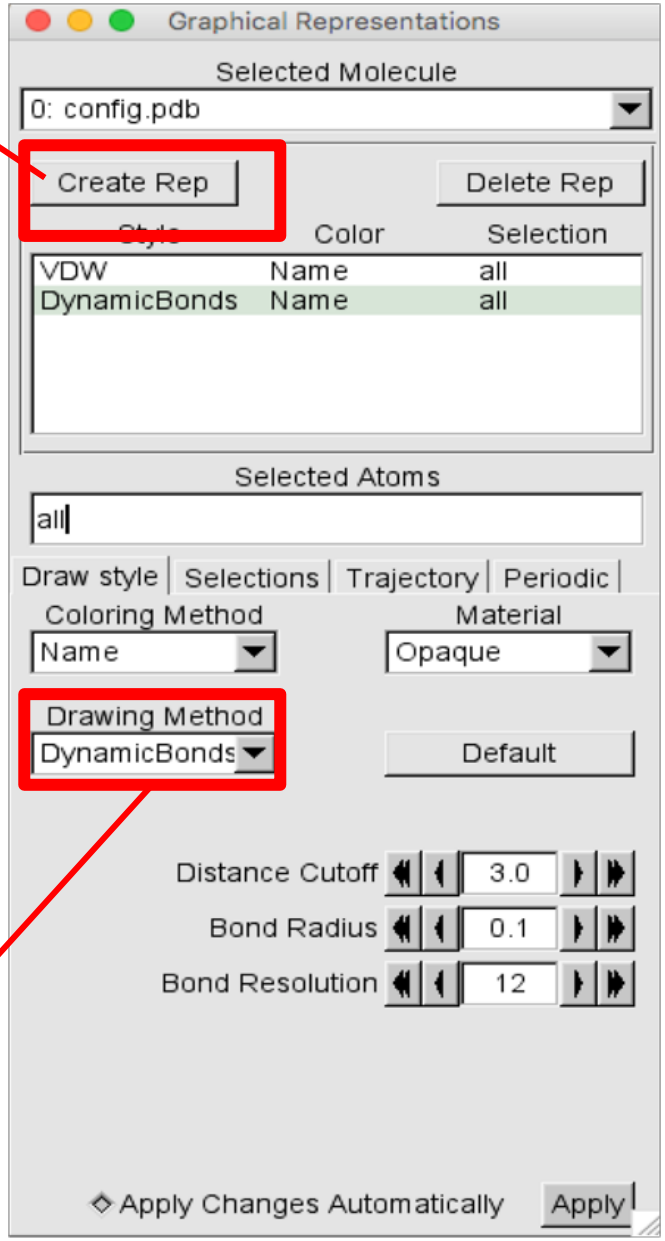
Choose the Graphic Representation

- In the Graphical Representations window; click on Create Rep



Display now looks like this

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



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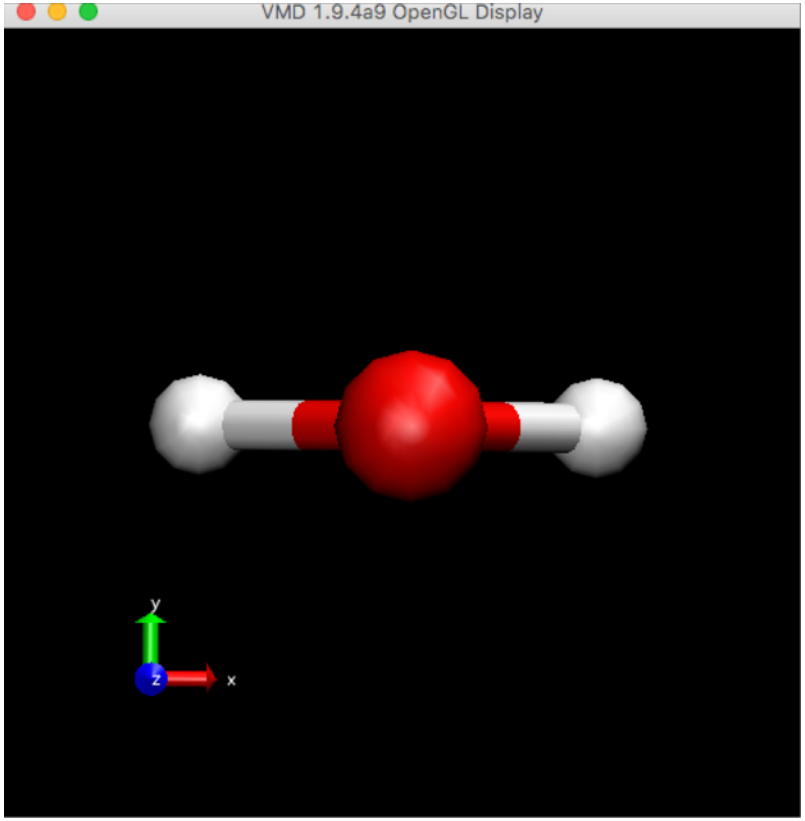
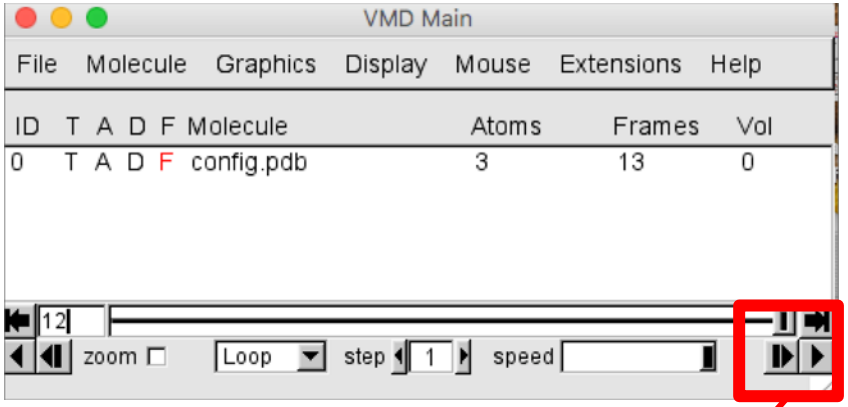
Play Movie



Display now looks like this

- In the Graphical Representations window; click on Create Rep



- Play movie by clicking on 
- Watch frame by frame 

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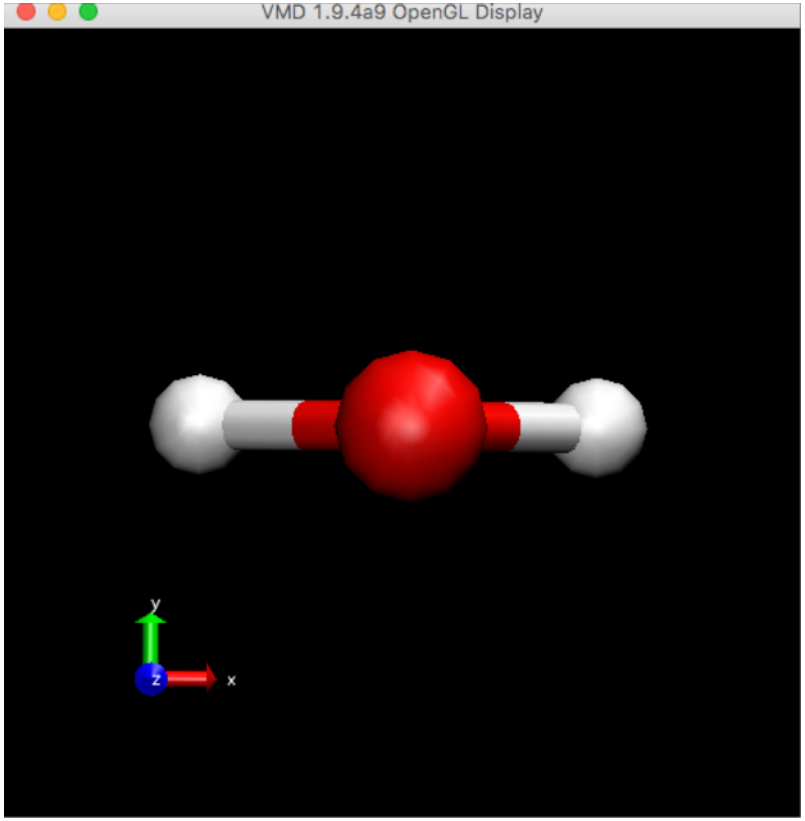
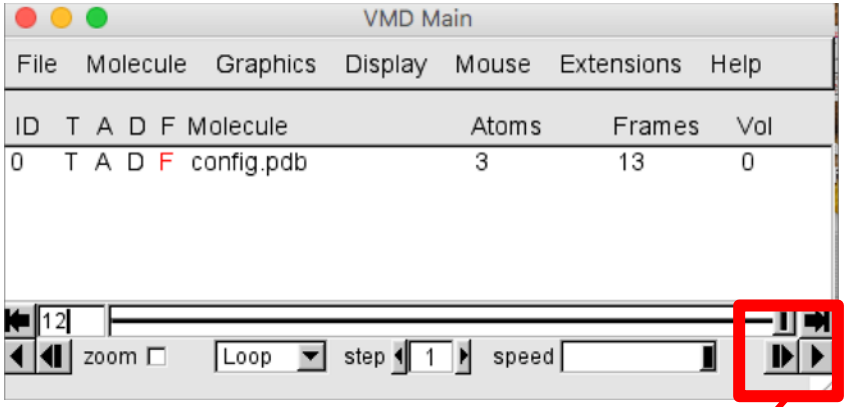
Play movie



Display now looks like this

- In the Graphical Representations window; click on Create Rep



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

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Visualizing Energy convergence

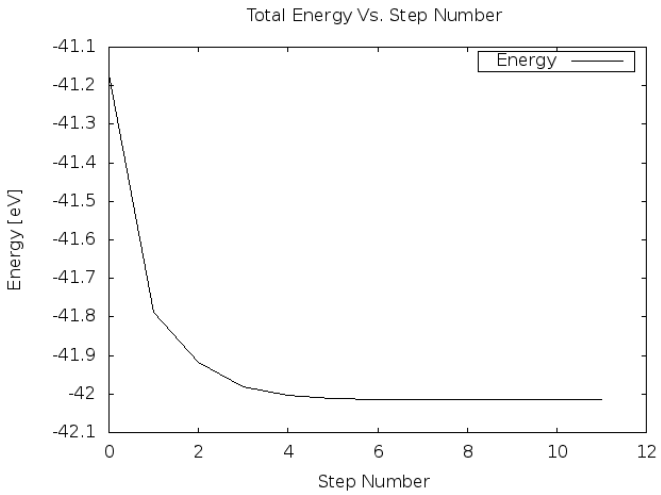
Go to “eng” analysis directory

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

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

```
$ gnuplot plot_eng.p
```

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



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End of Section I

Thank you for your attention

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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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