Molecular Dynamics Simulations

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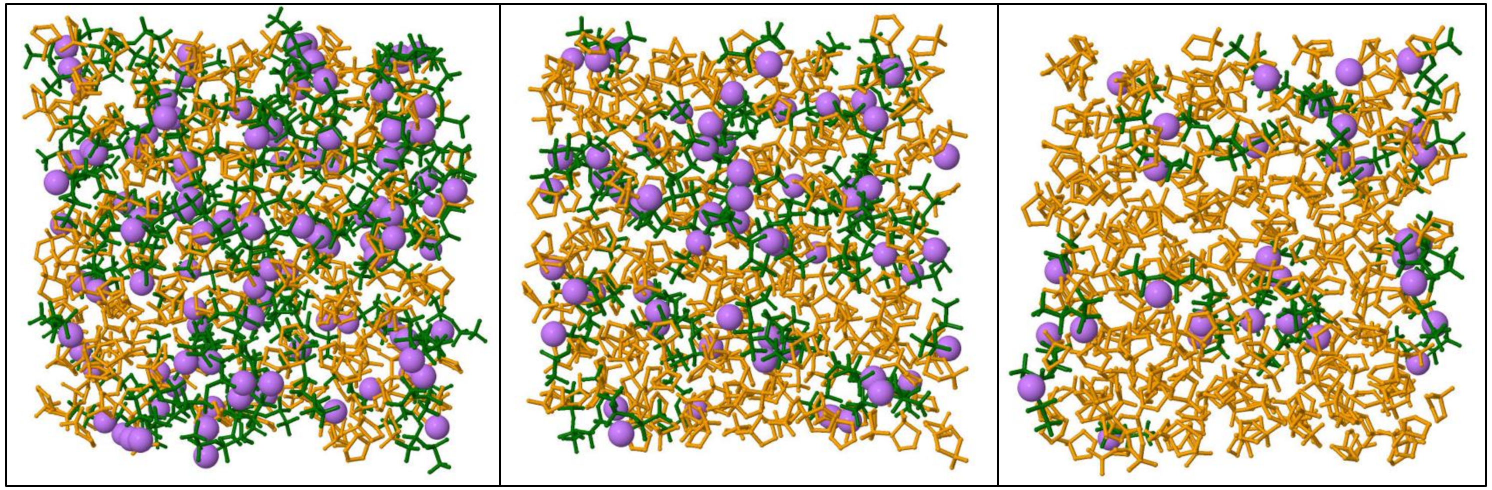
Outline

- **Part 1**

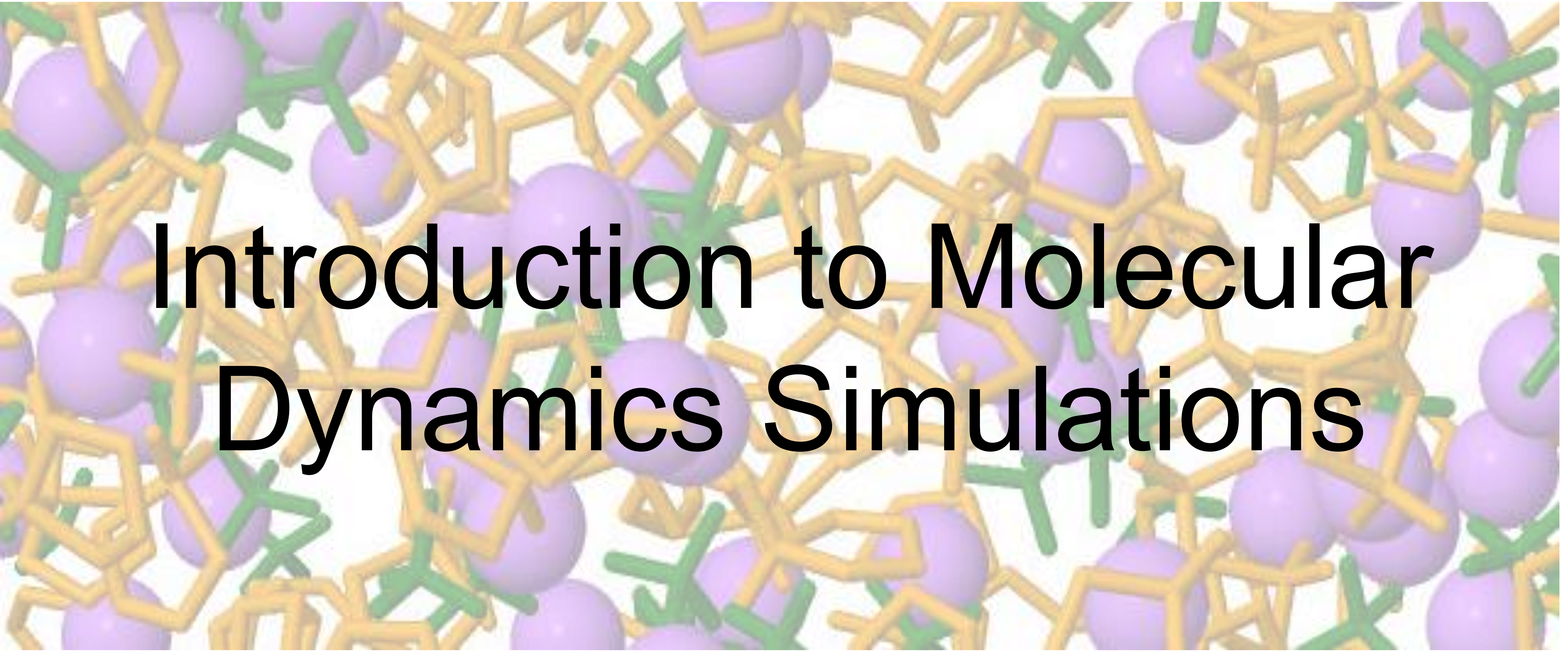
  1. Introduction to Molecular Dynamics Simulations
  2. Molecular Dynamics Simulation packages
  3. HPC LSU and LONI Software environment

- **Part 2**

  1. Running MD simulations using available packages on an HPC System



LiTFSI: 2.17 mol/dm^3 LiTFSI: 1.77 mol/dm^3 LiTFSI: 1.03 mol/dm^3

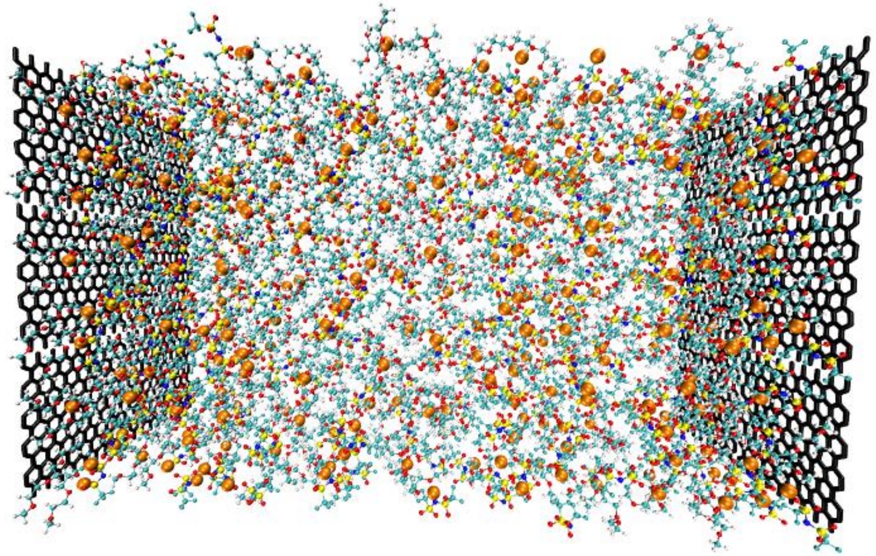


Introduction to Molecular Dynamics Simulations

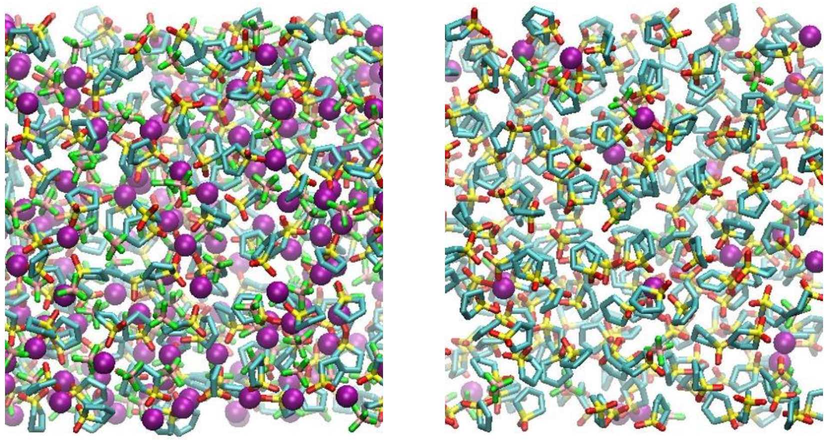
Introduction to Molecular Dynamics Simulations

Molecular dynamics (MD) is a versatile tool for calculating structural and dynamics properties of molecular systems at equilibrium as a function of time. The molecular systems should obey the laws of classical physics.

Molecular dynamics simulations are widely used in various fields like chemistry, physics, biology, and material science. The most popular research studies include the dynamics of proteins, DNA and RNA structures, ionic liquids (ILs), lipid bilayers and membranes, battery electrolytes, and …



Ion dynamics in battery electrolytes



Introduction to Molecular Dynamics Simulations

Molecular dynamics simulation models

1. Ensemble of atoms, each has a point mass m.
2. Group of atoms (OPLS-UA)
3. Coarse-grained models (MARTINI model)
4. Machine learning models

Force fields

1. Pair-wise classical force fields (AMBER, CHARMM, OPLS, GROMOS)
2. Many-body force fields include (EAM, Tersoff, REBO)
3. Reactive force fields (ReaxFF)
4. Machine learning models (potentials)

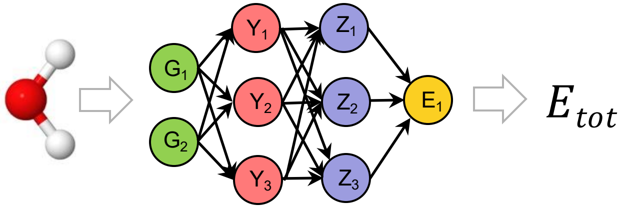
Molecular dynamics simulations

1. Integrate Newton's equation of motion, F = ma
2. Set 3N ODEs to propagate over time (Velocity Verlet Algorithm)

Thermodynamic properties

1. Calculate structural and dynamic properties as a time average of an ensemble of atoms.

Per-atom NN

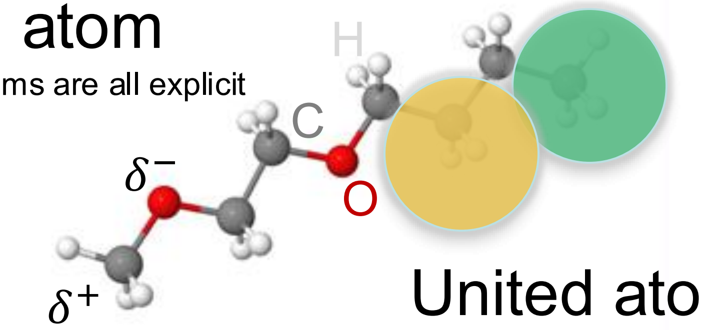


Democritus ~400 B.C.

The Greek word ατομοσ – invisible.

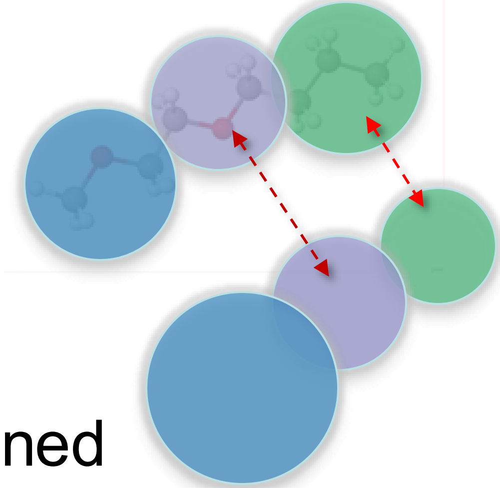
All atom

H atoms are all explicit



United atom

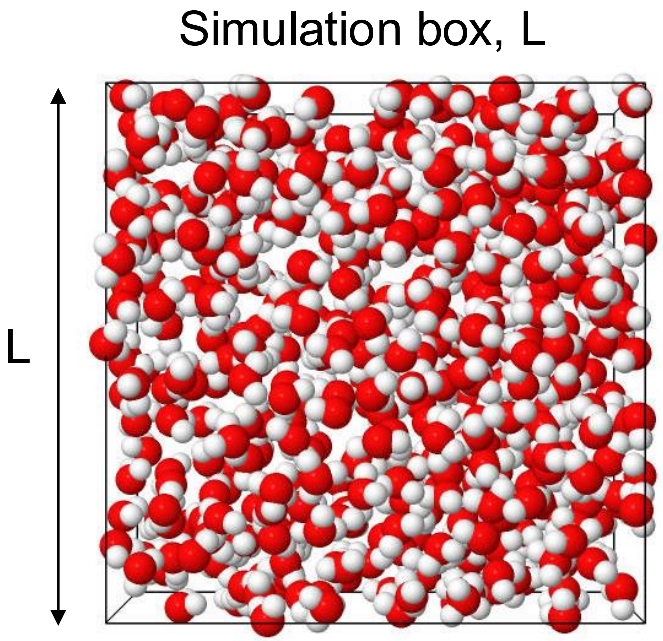
Beads include H atoms in CH2 CH3



Coarse-Grained models

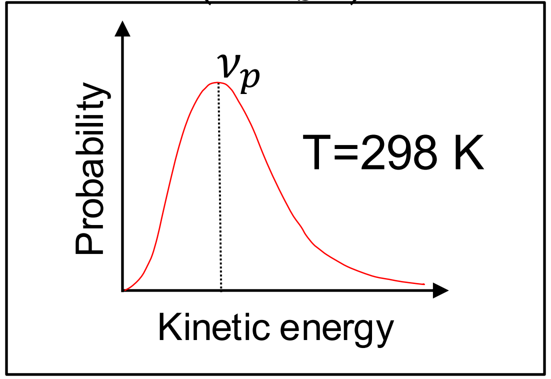
Beads include entire functional groups

Introduction to Molecular Dynamics Simulations



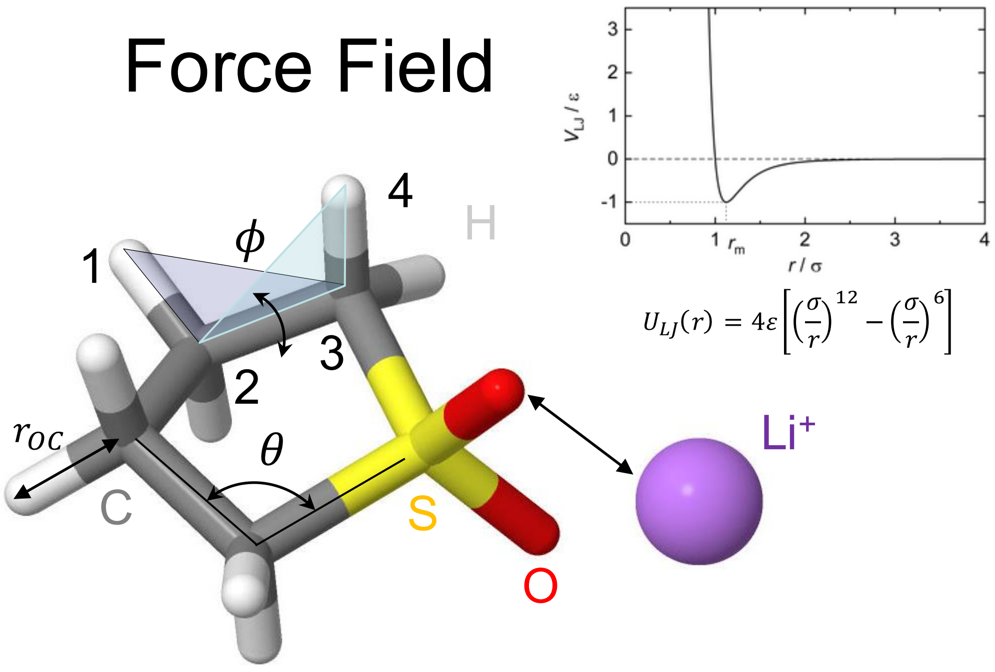
$N = 1536 \quad r_i = x, y, z$

$$P(v_{i,r}) = \left(\frac{m}{2\pi k_b T}\right)^{\frac{1}{2}} e^{-\frac{m v_{i,r}^2}{2\pi k_b T}}$$



1. Set up a system of N atoms.
2. Assign x, y, and z coordinates to each atom
3. Assign velocities using Maxwell-Boltzmann Distribution
4. Choose the right force field (Potential function)
5. Propagate atomic positions using integration algorithms (Velocity Verlet, Leap Frog, and …)

Force Field



$U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$

$$\boxed{U_{total} = U_{intra} + U_{inter}}$$

$$U_{intra} = U_{bond} + U_{bend} + U_{torsion} + U_{out\ of\ plane}$$

$$U_{inter} = U_{Coulomb} + U_{van\ der\ Waals}$$

Introduction to Molecular Dynamics Simulations

Time step: Δt

Intra-molecular interactions

Neighbor list

Inter-molecular Interactions:
van der Waals (LJ),
Electrostatic (Ewald)

Calculate forces, update positions, adjust temperature and pressure

$$r(t+\Delta t) = r(t) + \Delta t v(t) + \frac{\Delta t^2 a(t)}{2}$$

$$a(t+\Delta t) = \frac{f(t+\Delta t)}{m}$$

$$v(t+\Delta t) = v(t) + \frac{1}{2}\Delta t[a(t) + a(t+\Delta t)]$$

Introduction to Molecular Dynamics Simulations

1. Ewald summation (by Peter P. Ewald in 1921)
2. PPME (Particle-Particle mesh Ewald, Hockney 1981)
3. PME (Particle mesh Ewald, Darden 1993)

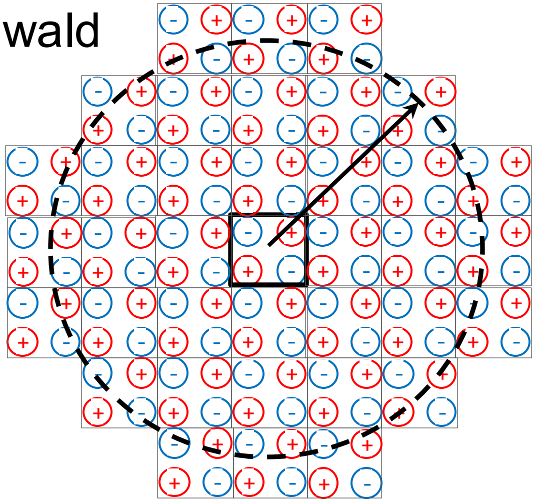
$$U^{Ewald} = U^{real} + U^{reciprocal} + U^{self}$$

$$\mathcal{O}(N^2) \longrightarrow \mathcal{O}(N \cdot log(N))$$

A three-dimensional grid is introduced to optimize the computation of long-range interactions and calculate the reciprocal space contribution.

A discrete set of points is introduced where charge densities and potentials are calculated significantly reducing the number of calculations needed for reciprocal space.

Ewald



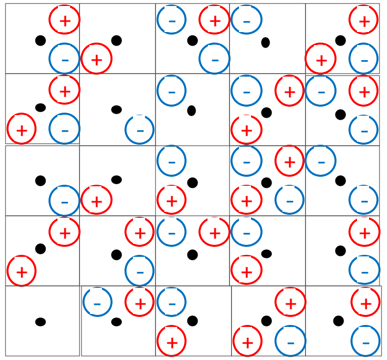
$$\sum_{i=1}^{N} q_i = 0$$

$$\mathcal{O}(N)$$

$$U^{real} = \frac{1}{2}\sum_{i,j}^{N}\sum_{n} q_i q_j \frac{\mathrm{erfc}(\alpha r_{ij,n})}{r_{ij}}$$

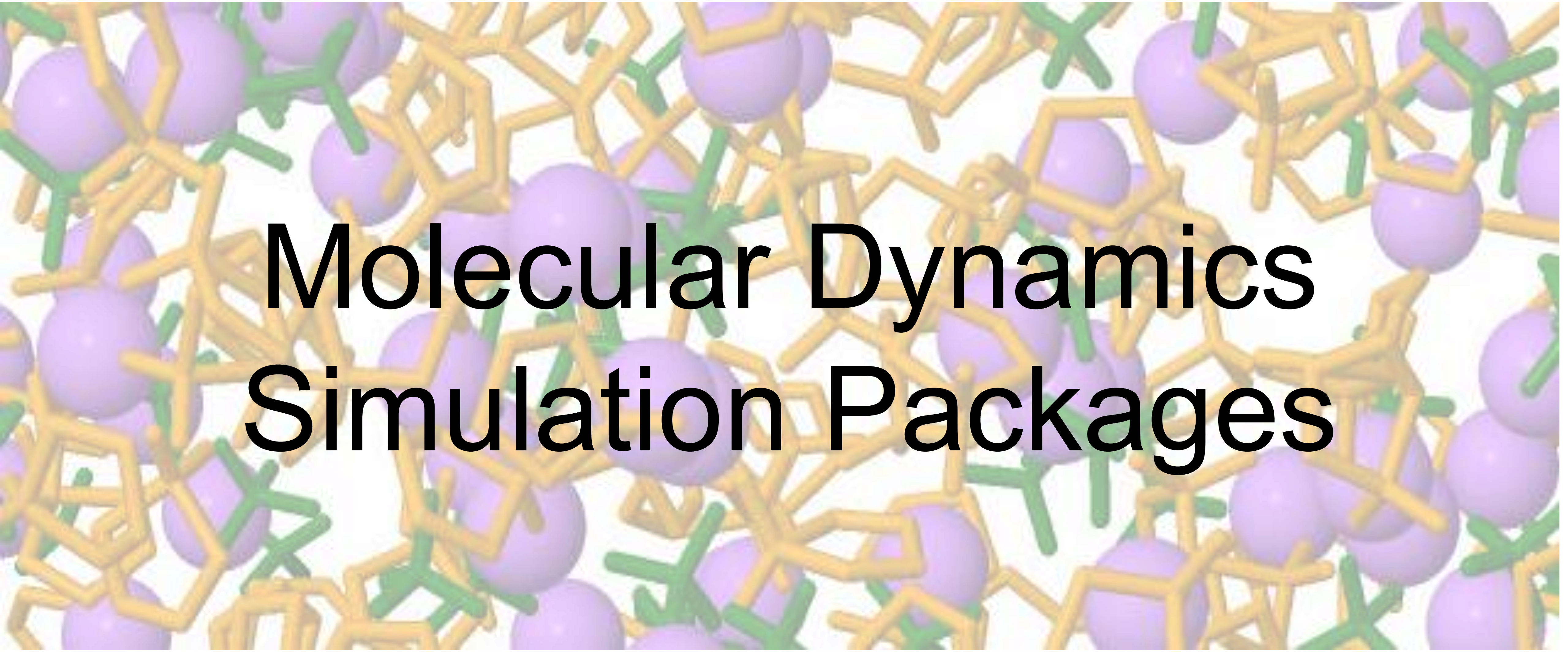
$$U^{self} = -\frac{\alpha}{\sqrt{\pi}}\sum_{i=1}^{N} q_i^2$$

$$U^{reciprocal} = \frac{1}{2\pi V}\sum_{i,j}^{N} q_i q_j \sum_{k\neq 0} \frac{exp\left(-\frac{\pi k^2}{\alpha}\right) + 2\pi i k \cdot (r_i - r_j)}{k^2}$$



PME

$$\mathcal{O}(N \cdot log(N))$$



Molecular Dynamics Simulation Packages

MD Simulation Packages

- LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator, Sandia National Lab, 1995) is a molecular dynamics simulation package, https://www.lammps.org
- GROMACS (GROningen Machine for Chemical Simulations, University of Groningen, 1991) is a molecular dynamics simulation package, https://www.gromacs.org
- NAMD (Not Another Molecular Dynamics Program, University of Illinois Urbana-Champaign, 1995) is a molecular dynamics simulation package (CHARMM force field), https://www.ks.uiuc.edu/Research/namd
- AMBER (Assisted Model Building with Energy Refinement, University of California, 2002) is a molecular dynamics simulation package (DNA force fields), https://ambermd.org

MD Simulation Packages

Name	Model builder	Min	MD	MC	GPU	License
LAMMPS	Yes	Yes	Yes	Yes	Yes	Free
GROMACS	No	Yes	Yes	No	Yes	Free
NAMD	Yes	Yes	Yes	No	Yes	Free
AMBER	Yes	Yes	Yes	Yes	Yes	Proprietary

MD Simulation Packages

- **<module available>**

	LAMMPS	**GROMACS**	**NAMD**	**AMBER**	**VMD**
QBC (QB3)	2020/03/03	2020.2	2.14	18/22	1.9.3
QBD (QB4)	2020/2023	2021.7	2.14/3.0bX	22	1.9.3
SMIC			2.14	22	1.9.3
MIKE	2022/2023	2021.3	2.14	18/22	1.9.3

MD Simulation Packages

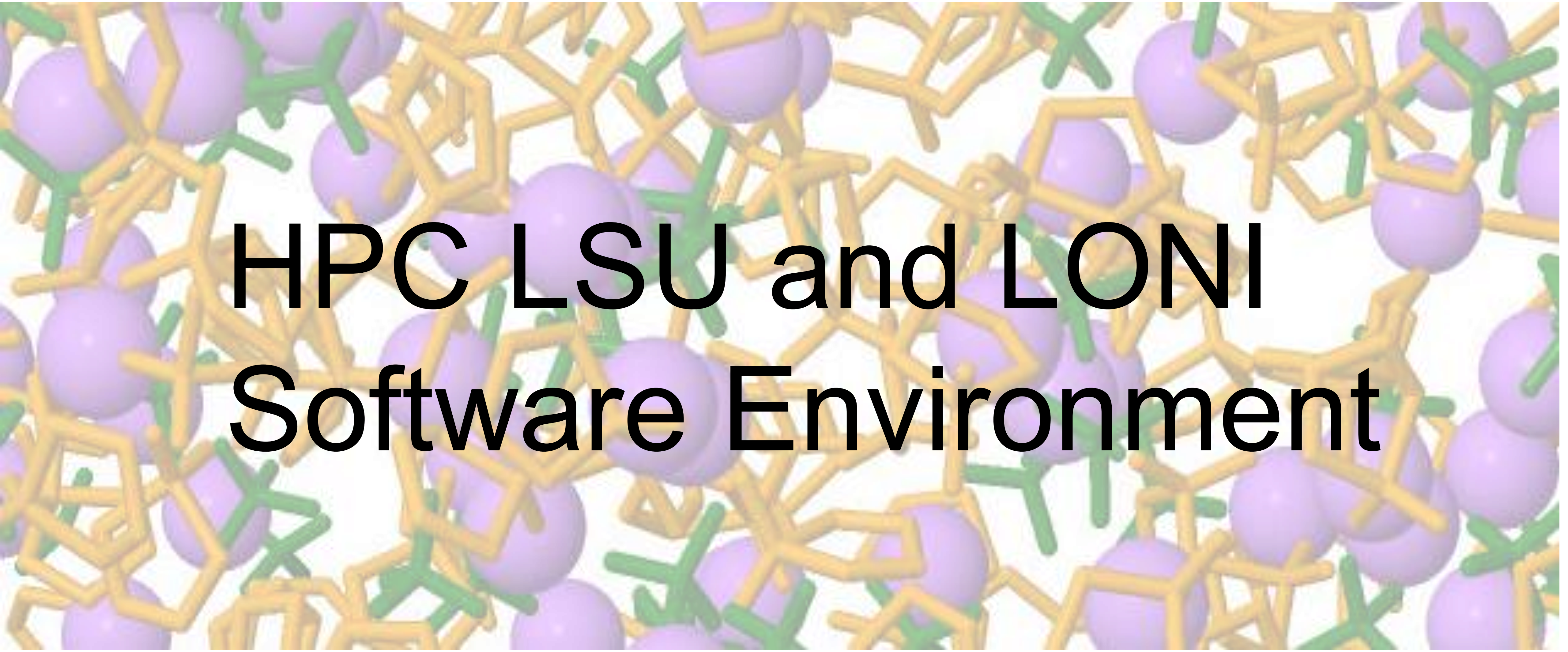
- **QBC (QB3)**

	LAMMPS	GROMACS	NAMD	AMBER	VMD
RHEL **8**	2023/08/02	2021.7	3.0b7		1.9.3
RHEL **7**	2019/2020/2022	2018/2020	2.14	18/22	1.9.3

This is valid only for QBC cluster.

To run packages installed on RHEL **7** version, you need to follow this link.

https://github.com/lsuhpchelp/singularity/tree/main/recipes/centos7



HPC LSU and LONI Software Environment

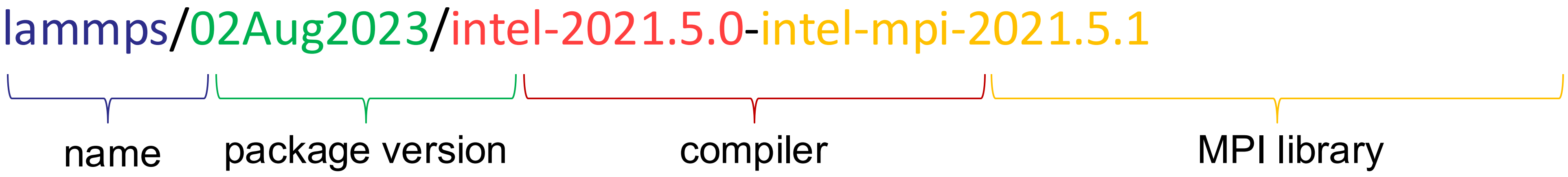
Software environment

```
[user@mike2 ~]$ module av

amber/18/intel-2021.5.0-intel-mpi-2021.5.1
amber/22/intel-2021.5.0-cuda-11.5.0-intel-mpi-2021.5.1
amber/22/intel-2021.5.0-intel-mpi-2021.5.1
.
gromacs/2021.3/intel-2021.5.0-intel-mpi-2021.5.1
.
lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1
lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1
.
namd/2.14/intel-2021.5.0
namd/2.14/intel-2021.5.0-cuda
```

Software environment

No GPU



lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1

name

package version

compiler

MPI library

lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

name

package version

compiler

cuda version

MPI library

GPU

Software environment

```
[user@mike2 ~]$ module purge

[user@mike2 ~]$ module load lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1

[user@mike2 ~]$ module list


Currently Loaded Module files:

 1) intel/2021.5.0
 2) intel-mpi/2021.5.1
 3) lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1
```

Software environment

```
[user@mike2 ~]$ module display lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1

module-whatis   {LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator. This package uses patch
releases, not stable release. See https://github.com/spack/spack/pull/5342 for a detailed discussion. }

conflict        lammps

prepend-path    PATH /usr/local/packages/lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1/bin

prepend-path    MANPATH /usr/local/packages/lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1/share/man
```

Software environment

```
[user@mike2 ~]$ ls /usr/local/packages/lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1/bin

binary2txt  chain.x  lmp_mpi  micelle2d.x  msi2lmp  phana  stl_bin2txt
```

Running jobs on HPC

There are two types of jobs in the High-Performance Computing (HPC) environment.

1. Interactive jobs

Interactive jobs allow the user to run tasks interactively, usually directly connected to the system through a terminal or GUI.

These jobs are intended for tasks that require interaction from the user.

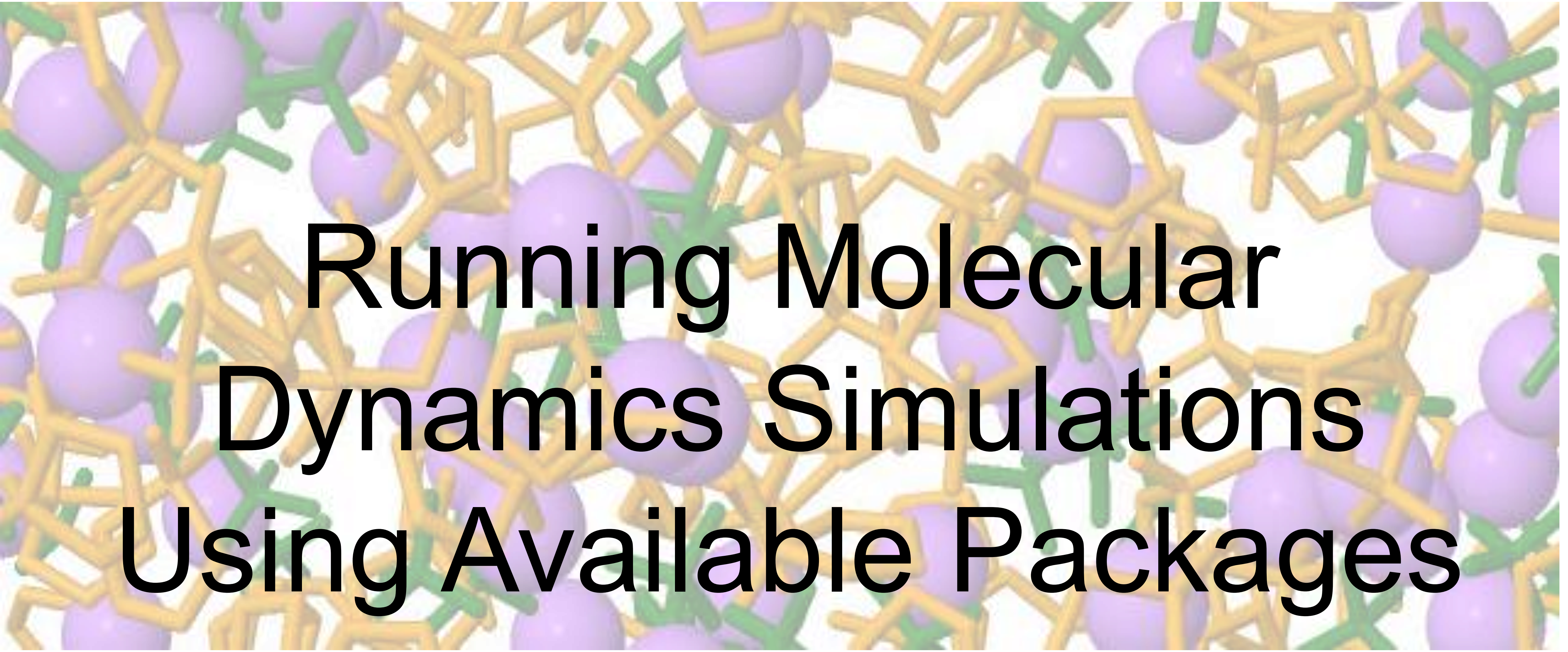
salloc and/or srun commands

2. Batch jobs

Batch jobs are computational tasks that are submitted to the HPC cluster without the need for interaction from the user.

These jobs are queued and executed by the Slurm resource manager.

sbatch <script.sh>



Running Molecular Dynamics Simulations Using Available Packages

Running LAMMPS jobs on HPC

Every LAMMPS simulation needs two essential files:

1. structure / topology (.lammps),
2. parameters (.in).

Structure/topology

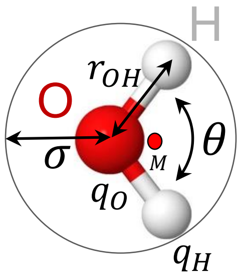
```
 1536 atoms
 Atoms
   1  1  1 -1.04840  23.067397  25.992172  12.516813
   2  1  2  0.52420  23.651513  25.756170  13.277936
   3  1  2  0.52420  23.106625  25.196754  11.981115
   ...
```

Parameters

```
units         real
atom_style     full
boundary       p p p

# Force Field
pair_style     lj/cut/tip4p/cut 1 2 1 1 0.125 8.0
bond_style     harmonic
angle_style    harmonic
kspace_style   none

#Read data
read_data      tip4p_512.lammps
...
```



$r_{OH} = 0.9572\,\text{Å}$

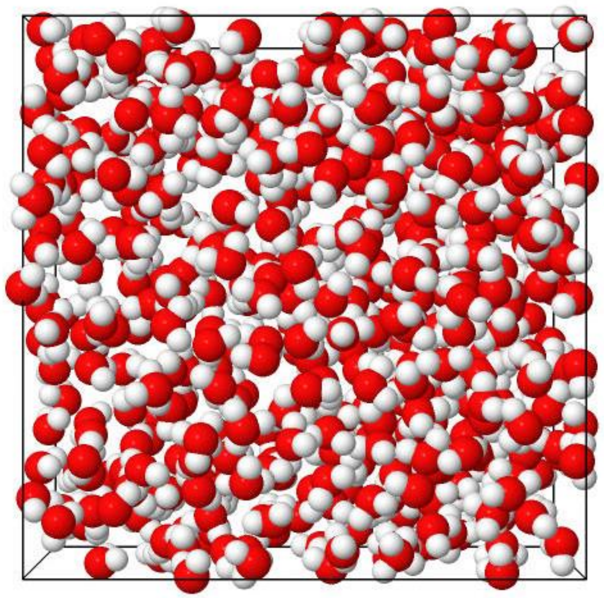
$\theta = 104.52°$

$q_M = -1.040\,e$

$q_H = 0.52\,e$

$\sigma = 3.1536\text{Å}$

TIP4P water model



Running LAMMPS jobs on HPC

Running LAMMPS interactively

```
[user@mike2 LAMMPS]$ salloc -A hpc_hpcadmin10 -p workq -t 01:00:00 -J Traning
[user@mike2 LAMMPS]$ module purge
[user@mike2 LAMMPS]$ module load lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1
[user@mike2 LAMMPS]$ module list

Currently Loaded Modulefiles:
 1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) lammps/02Aug2023/intel-2021.5.0-intel-mpi-2021.5.1

[user@mike171 LAMMPS]$ srun –n 1  lmp_mpi -in tip4p_512.in > tip4p_512.out &
[user@mike171 LAMMPS]$ top

[user@mike171 LAMMPS]$ srun -n64  lmp_mpi -in tip4p_512.in > tip4p_512.out &
[user@mike171 LAMMPS]$ ls
[user@mike171 LAMMPS]$ log.lammps  tip4p_512.in  tip4p_512.lammps  tip4p_512.out  tip4p_512.traj

[user@mike171 LAMMPS]$ tail –f log.lammps
[user@mike171 LAMMPS]$ ^C
```

Running LAMMPS jobs on HPC

Running LAMMPS jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 1
#SBATCH -n 64
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o lammps_%j_%N.out
#SBATCH -e lammps_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load lammps/23Jun2022/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

echo $SLURM_NNODES
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun -N1 -n64 lmp_mpi -in water_tip4p.in > water_tip4p.out
```

Running LAMMPS jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 2
#SBATCH -n 128
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o lammps_%j_%N.out
#SBATCH -e lammps_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load lammps/23Jun2022/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

echo $SLURM_NNODES
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun –N2 –n128 lmp_mpi -in water_tip4p.in > water_tip4p.out
```

Running GROMACS jobs on HPC

Every GROMACS simulation needs three essential files:

1. structure (.gro/.pdb),
2. topology (.top), and
3. parameters (.mdp).

Structure

```
TIP3P water
 1536
   1SOL    OW    1   2.308   1.150   1.290  0.0374 -0.1946  0.1896
   1SOL   HW1    2   2.242   1.208   1.328 -0.7293 -1.1860  0.4498
   1SOL   HW2    3   2.376   1.143   1.357  1.6678  2.7051 -0.9958
   ...
```

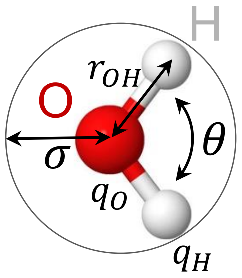
Topology

```
; Include forcefield parameters
#include "charmm27.ff/forcefield.itp"

; Include water topology
#include "charmm27.ff/tip3p.itp"
...
```

Parameters

```
; Run parameters
integrator       = md    ;leap-frog integrator
nsteps           = 5000 ;
dt               = 0.002 ;
...
```



$r_{OH} = 0.9572\,\text{Å}$

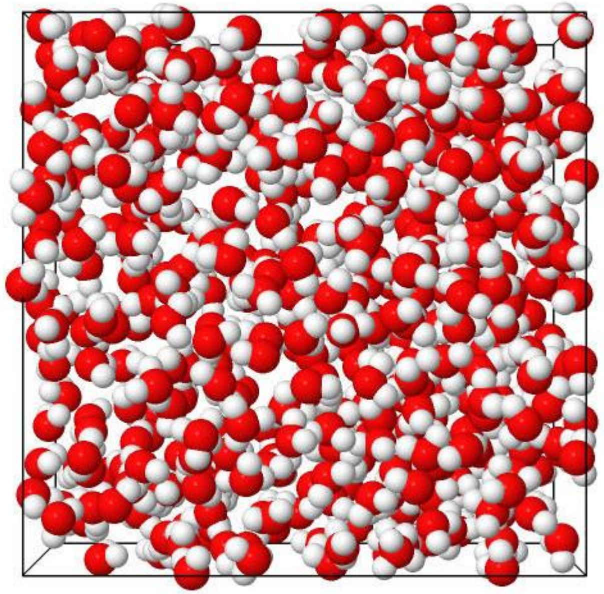
$\theta = 104.52°$

$q_O = -0.834\ e$

$q_H = 0.417\ e$

$\sigma = 3.15061\text{Å}$

TIP3P water model



Running GROMACS jobs on HPC

Running GROMACS interactively

```
[user@mike2 GROMACS]$ salloc -A hpc_hpcadmin10 -p workq -t 01:00:00 -J Traning
[user@mike2 GROMACS]$ module purge
[user@mike2 GROMACS]$ module load gromacs/2021.3/intel-2021.5.0-intel-mpi-2021.5.1
[user@mike2 GROMACS]$ module list

Currently Loaded Modulefiles:
 1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) gromacs/2021.3/intel-2021.5.0-intel-mpi-2021.5.1

[user@mike2 GROMACS]$ srun gmx_mpi grompp  -f  min.mdp -c npt.gro -p topol.top -o min.tpr
[user@mike2 GROMACS]$ srun gmx_mpi  mdrun --deffnm min
[user@mike2 GROMACS]$ ls
[user@mike2 GROMACS]$ min.edr  min.gro  min.log  min.mdp  min.tpr  min.trr


[user@mike2 GROMACS]$ srun gmx_mpi grompp  -f  eql.mdp -c min.gro -p topol.top -o eql.tpr
[user@mike2 GROMACS]$ srun –N1 –n64 gmx_mpi  mdrun --deffnm eql
[user@mike2 GROMACS]$ ls
[user@mike2 GROMACS]$ eql.cpt  eql.edr  eql.gro  eql.log  eql.mdp  eql.tpr  eql.trr  eql.xtc
```

Running GROMACS jobs on HPC

Running GROMACS jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 1
#SBATCH -n 64
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o gromacs_%j_%N.out
#SBATCH -e gromacs_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load gromacs/2021.3/intel-2021.5.0-intel-mpi-2021.5.1

echo $SLURM_NNODES
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun -N1 -n64 gmx_mpi mdrun –deffnm npt -v
```

Running GROMACS jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 2
#SBATCH -n 128
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o gromacs_%j_%N.out
#SBATCH -e gromacs_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load gromacs/2021.3/intel-2021.5.0-intel-mpi-2021.5.1

echo $SLURM_NNODES
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun –N2 –n128 gmx_mpi mdrun –deffnm npt -v
```

Running NAMD jobs on HPC

Every NAMD simulation needs three essential files:
Input files are identical to the input files used by **X-PLOR** and **CHARMM**.

1. coordinates (.pdb),
2. structure (.psf),
3. topology (.xplor),
4. parameters (.namd).

Coordinates (.pdb)

```
 REMARK original generated coordinate pdb file
ATOM      1  OH2 TIP3W   5      3.668  10.082  15.904  1.00  0.00      WW1  O
ATOM      2  H1  TIP3W   5      3.224  10.451  15.101  1.00  0.00      WW1  H
ATOM      3  H2  TIP3W   5      3.092  10.379  16.627  1.00  0.00      WW1  H
...
```

Structure (.psf)

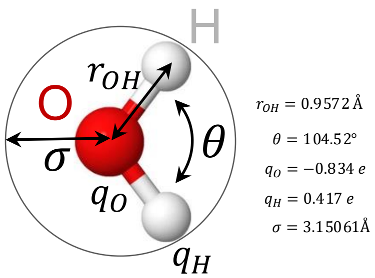
```
   1536 !NATOM
      1 WW1  5    TIP3 OH2  OT    -0.834000       15.9994        0
      2 WW1  5    TIP3 H1   HT     0.417000        1.0080        0
      3 WW1  5    TIP3 H2   HT     0.417000        1.0080        0
   ...
```

Topology (.xplor)

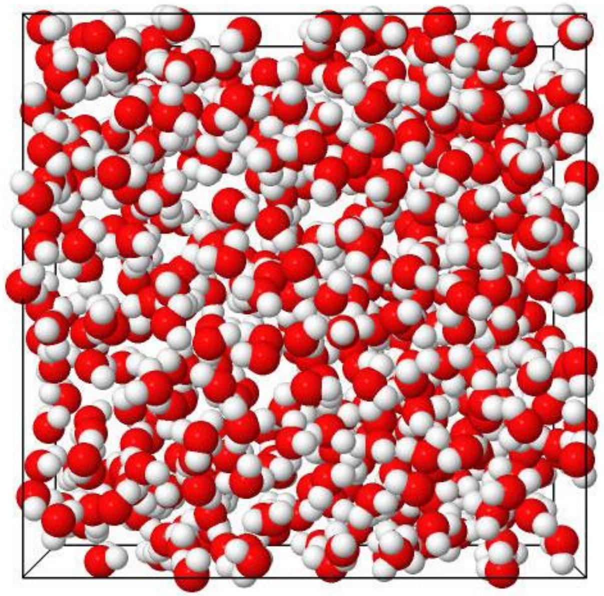
```
 BOND  OT   HT    450.000     0.9572 ! ALLOW   WAT
 BOND  HT   HT      0.000     1.5139 ! ALLOW WAT
ANGLE  HT    OT    HT      55.000 104.5200  ! ALLOW WAT
...
```

Parameters (.input)

```
timestep             1.0
fullElectFrequency   4
numsteps             50000
outputtiming         20
...
```



TIP3P water model



Running NAMD jobs on HPC

Running NAMD interactively

```
[user@mike2 NAMD]$ salloc -A hpc_hpcadmin10 -p workq -t 01:00:00 -J Traning
[user@mike2 NAMD]$ module purge
[user@mike2 NAMD]$ module load namd/2.14/intel-2021.5.0
[user@mike2 NAMD]$ module list

Currently Loaded Modulefiles:
 1) intel/2021.5.0   2) namd/2.14/intel-2021.5.0

[user@mike2 NAMD]$ srun –N1 –n64 namd2 tip3p_512.namd > tip3p_512.out &
[user@mike2 NAMD]$ ls
[user@mike2 NAMD]$ par_all22_prot_lipid.xplor  tip3p_512.out  tip3p_512.out.coor.BAK
tip3p_512.out.vel.BAK  tip3p_512.out.xsc.BAK  tip3p_512.psf   tip3p_512.nam p3p_512.out.coor
tip3p_512.out.vel tip3p_512.out.xsc      tip3p_512.pdb
```

Running NAMD jobs on HPC

Running NAMD jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 1
#SBATCH -n 64
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o NAMD_%j_%N.out
#SBATCH -e NAMD_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load namd/2.14/intel-2021.5.0

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR


time srun -N1 -n64 namd2 tip3p_512.namd > tip3p_512.out
```

Running NAMD jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 2
#SBATCH -n 128
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o NAMD_%j_%N.out
#SBATCH -e NAMD_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load namd/2.14/intel-2021.5.0

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR


time srun –N2 –n128 namd2 tip3p_512.namd > tip3p_512.out
```

Running AMBER jobs on HPC

Every AMBER simulation needs three essential files:
Initial coordinate, topology, and parameter files.

1. coordinates (.inpcrd),
2. topology (.prmtop),
3. parameter (.inp).

Structure (.inpcrd)

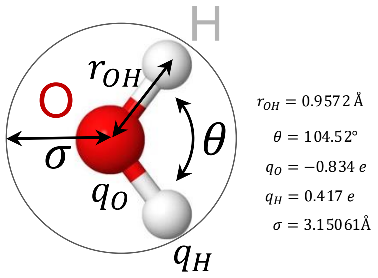
```
default_name
 1536
  16.5307255  19.4975686  18.1539268  13.3987255  16.6285686  12.9069268
  15.2747255  15.8905686  11.7989268  17.0747255  16.7645686  10.4629268
...
```

Topology (.prmtop)

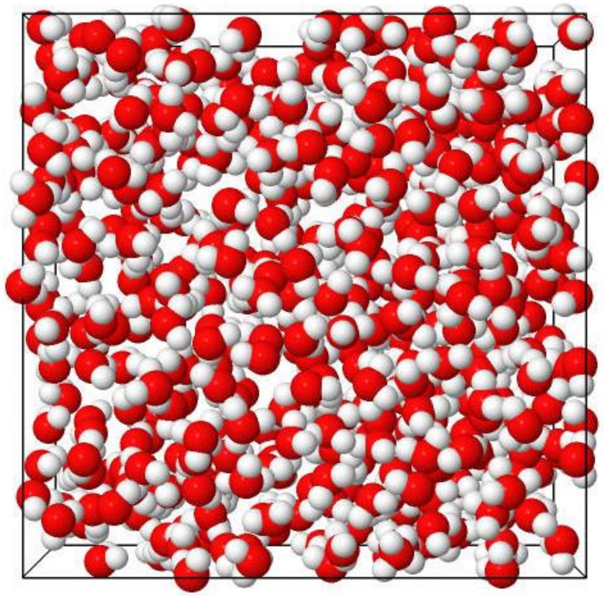
```
  %FORMAT(10I8)
    1536       2    1024       0     512       0  ...
    2048     512       0       0       0       2  ...
       0       0       0       0       0       0  ...
  ...
```

Parameters (.inp)

```
Production
 &cntrl
  imin=0,
  ntx=1,
  ntwv = 1
...
```



TIP3P water model



Running AMBER jobs on HPC

Running AMBER interactively

```
[user@mike2 AMBER]$ salloc -A hpc_hpcadmin10 -p workq -t 01:00:00 -J Traning
[user@mike2 AMBER]$ module purge
[user@mike2 AMBER]$ module load amber/22/intel-2021.5.0-intel-mpi-2021.5.1
[user@mike2 AMBER]$ module list

Currently Loaded Modulefiles:
  1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) amber/22/intel-2021.5.0-intel-mpi-2021.5.1

[user@mike2 AMBER]$ srun sander -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd &
[user@mike2 AMBER]$ ls

[user@mike2 AMBER]$ srun –n1 –N64 sander.MPI -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd &
[user@mike2 AMBER]$ ls


[user@mike2 AMBER]$ srun –n1 –N64  pmemd.MPI -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd &

[user@mike2 AMBER]$ ls
```

Running AMBER jobs on HPC

Running AMBER jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 1
#SBATCH -n 64
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A loni_allocation
#SBATCH -J test
#SBATCH -o amber_%j_%N.out
#SBATCH -e amber_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load amber/22/intel-2021.5.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun -N1 –n64 sander.MPI -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd
-r tip3p_512.rst
```

Running AMBER jobs using SLURM system

```
#!/bin/bash
#SBATCH -p workq
#SBATCH -N 2
#SBATCH -n 128
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A loni_allocation
#SBATCH -J test
#SBATCH -o amber_%j_%N.out
#SBATCH -e amber_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load amber/22/intel-2021.5.0-intel-mpi-2021.5.1

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun –N2 –n128 sander.MPI -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c
tip3p_512.inpcrd -r tip3p_512.rst
```

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- **Van der Waals, Johannes Diderik (1837 - 1923). *Over de Continuiteit van den Gas- en Vloeistoftoestand.* Leiden, 1873, (Nobel Prize 1910, van der Waal's equation of state) http://rbx-exhibit2000.scs.illinois.edu//vanderwaals.htm**
- **Fabbrizzi, L. "Beyond the Molecule: Intermolecular Forces from Gas Liquefaction to X−H···π Hydrogen Bonds" ChemPlusChem, Volume 87, Issue 1, 2022, Pages 1-23, ISSN 2192-6506, https://doi.org/10.1002/cplu.202100243**
- **Darden, T. York, D. and Pederson, L. "Particle mesh Ewald: An *N*·log(*N*) method for Ewald sums in large systems" J. Chem. Phys. 1993, 98, 10089-10092**
- **Plimpton, S. "Fast Parallel Algorithms for Short-Range Molecular Dynamics", Journal of Computational Physics, Volume 117, Issue 1, 1995, Pages 1-19, ISSN 0021-9991, https://doi.org/10.1006/jcph.1995.1039.**
- **Behler, J. and Parrinello, M. "Generalized Neural-Network Representation of High-Dimensional Potential Energy Surfaces" Physical Review Letters, 2007, 98, 146401 https://doi.org/10.1103/PhysRevLett.98.146401**

Thank You

Environment

Environment	Slurm
Job ID	$SLURM_JOBID
Submit directory	$SLURM_SUBMIT_DIR
Submit host	$SLURM_SUBMIT_HOST
Node list	$SLURM_JOB_NODELIST
Total number of nodes	$SLURM_NNODES
Total number of tasks	$SLURM_NTASKS

SLURM stands for Simple Linux Utility for Resource Management, which also provides a workload management system. It enables users to submit, monitor, and manage jobs on a supercomputer. It provides a framework for distributing computational tasks and a job scheduling system.

Running LAMMPS jobs on HPC with 1 GPU

Running LAMMPS interactively

```
[user@mike2 LAMMPS]$ salloc -N1 -n16 -p gpu --gres=gpu:1 --time=12:00:00 -A hpc_hpcadmin8
[user@mike2 LAMMPS]$ module purge
[user@mike2 LAMMPS]$ module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1
[user@mike2 LAMMPS]$ module list

Currently Loaded Modulefiles:
 1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1



[user@mike179 LAMMPS]$ time srun -N1 –n16 lmp_mpi -sf gpu -pk gpu 1 neigh yes newton off -in lj.in > lj.out &

[user@mike179 LAMMPS]$ nvidia-smi –l
```

Running NAMD jobs on RHEL7

1

mvapich2.modules

```
#!/bin/bash
export MODULEPATH=/usr/local/packages/Modules/modulefiles/apps:$MODULEPATH
module purge
module load namd/2.14b2/intel-19.0.5
module load fftw/3.3.8/intel-19.0.5-mvapich-2.3.3
```

https://github.com/lsuhpchelp/singularity/tree/main/recipes/centos7

Running NAMD jobs on RHEL 7

run_RHEL7.sh

2

```
#!/bin/bash
#SBATCH -p checkpt
#SBATCH -N 1
#SBATCH -n 64
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o namd_%j_%N.out
#SBATCH -e namd_%j_%N.err

module purge
module load centos7-runner/1.0

# use mvapich2.modules to load necessary modules from rhel7 software stack
export SINGULARITYENV_MODULE_FILE="$PWD/mvapich2.modules”

# Disables CMA (Cross Memory Attach) based intra-node communication at run time.
export MV2_SMP_USE_CMA=0

# Disables process affinity, which prevents MPI processes from being pinned to specific CPUs.
export MV2_ENABLE_AFFINITY=0

# this uses 1 thread per MPI process
export SINGULARITYENV_OMP_NUM_THREADS=1
time srun –n64 centos7run namd2 tip3p_512.namd > tip3p_512.out
```

Running LAMMPS jobs on HPC with 2 GPUs

Running LAMMPS interactively

```
[user@mike2 LAMMPS]$ salloc -N1 –n32 -p gpu --gres=gpu:2 --time=12:00:00 -A hpc_hpcadmin8
[user@mike2 LAMMPS]$ module purge
[user@mike2 LAMMPS]$ module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1
[user@mike2 LAMMPS]$ module list

Currently Loaded Modulefiles:
 1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1



[user@mike179 LAMMPS]$ time srun -N1 –n32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out &

[user@mike179 LAMMPS]$ nvidia-smi –l
```

Running LAMMPS jobs on HPC with GPU

Running LAMMPS jobs using 1 GPU

```
#!/bin/bash
#SBATCH -p gpu
#SBATCH –gres=gpu:1
#SBATCH -N 1
#SBATCH -n 16
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o lammps_%j_%N.out
#SBATCH -e lammps_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

echo $SLURM_NNODES
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun -N1 -n16 lmp_mpi -sf gpu -pk gpu 1 neigh yes newton off -in lj.in > lj.out
```

Running LAMMPS jobs using 2 GPUs

```
#!/bin/bash
#SBATCH -p gpu
#SBATCH –gres=gpu:2
#SBATCH -N 1
#SBATCH -n 32
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A hpc_allocation
#SBATCH –J test
#SBATCH -o lammps_%j_%N.out
#SBATCH -e lammps_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load lammps/02Aug2023/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1

echo $SLURM_NNODES
echo $SLURM_NTASKS
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun -N1 –n32 lmp_mpi -sf gpu -pk gpu 2 neigh yes newton off -in lj.in > lj.out
```

Running AMBER jobs on HPC with 1 GPU

Running AMBER interactively

```
[user@mike2 AMBER]$ salloc -N1 -n16 -p gpu --gres=gpu:1 --time=12:00:00 -A hpc_hpcadmin8
[user@mike2 AMBER]$ module purge
[user@mike2 AMBER]$ module load amber/22/intel-2021.5.0-cuda-11.5.0-intel-mpi-2021.5.1
[user@mike2 AMBER]$ module list

Currently Loaded Modulefiles:
  1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) amber/22/intel-2021.5.0-cuda-11.5.0-intel-mpi-2021.5.1

[user@mike2 AMBER]$ export CUDA_VISIBLE_DEVICES=“0”

[user@mike2 AMBER]$ time srun pmemd.cuda_DPFP.MPI –AllowSmallBox -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd -r tip3p_512.rst &

[user@mike2 AMBER]$ nvidia-smi –l
```

DPFP – stands for Double Precision Floating point (64 bits)

SPFP – stands for Single Precision Floating point (32 bits)

Running AMBER jobs on HPC with 2 GPUs

Running AMBER interactively

```
[user@mike2 AMBER]$ salloc -N1 –n32 -p gpu --gres=gpu:2 --time=12:00:00 -A hpc_hpcadmin8
[user@mike2 AMBER]$ module purge
[user@mike2 AMBER]$ module load amber/22/intel-2021.5.0-cuda-11.5.0-intel-mpi-2021.5.1
[user@mike2 AMBER]$ module list

Currently Loaded Modulefiles:
  1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) amber/22/intel-2021.5.0-cuda-11.5.0-intel-mpi-2021.5.1

[user@mike2 AMBER]$ export CUDA_VISIBLE_DEVICES=“0,1”

[user@mike2 AMBER]$ time srun pmemd.cuda_DPFP.MPI –AllowSmallBox -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd -r tip3p_512.rst &

[user@mike2 AMBER]$ nvidia-smi –l
```

DPFP – stands for Double Precision Floating point (64 bits)

SPFP – stands for Single Precision Floating point (32 bits)

Running AMBER jobs on HPC with GPU

Running AMBER jobs using 1 GPU

```
#!/bin/bash
#SBATCH –p gpu
#SBATCH –gres=gpu:1
#SBATCH -N 1
#SBATCH –n 16
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A loni_allocation
#SBATCH -J test
#SBATCH -o lammps_%j_%N.out
#SBATCH -e lammps_%j_%N.err
#SBATCH --mail-user=your@email.address
#SBATCH --mail-type=ALL

module purge
module load amber/22/intel-2021.5.0-cuda-11.5.0-intel-mpi-2021.1

export CUDA_VISIBLE_DEVICES="0"
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun pmemd.cuda_DPFP.MPI –AllowSmallBox -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c
tip3p_512.inpcrd -r tip3p_512.rst
```

Running AMBER jobs using 2 GPUs

```
#!/bin/bash
#SBATCH –p gpu
#SBATCH –gres=gpu:2
#SBATCH -N 1
#SBATCH –n 32
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A loni_allocation
#SBATCH -J test
#SBATCH -o lammps_%j_%N.out
#SBATCH -e lammps_%j_%N.err
#SBATCH --mail-user your@email.address
#SBATCH --mail-type=ALL

module purge
module load amber/22/intel-2021.5.0-cuda-11.5.0-intel-mpi-2021.1

export CUDA_VISIBLE_DEVICES="0,1"
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR

time srun pmemd.cuda_DPFP.MPI –AllowSmallBox -O -i eql.inp -o eql.out -p tip3p_512.prmtop -
tip3p_512.inpcrd -r tip3p_512.rst
```