Molecular Dynamics Simulations

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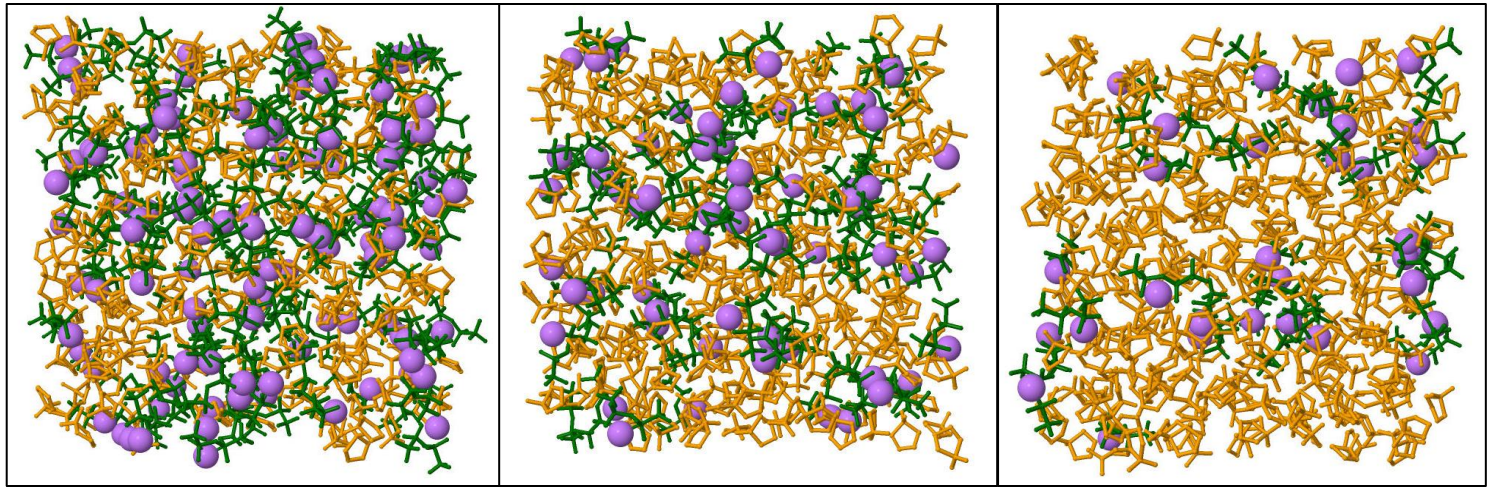
Outline

- **Part 1**

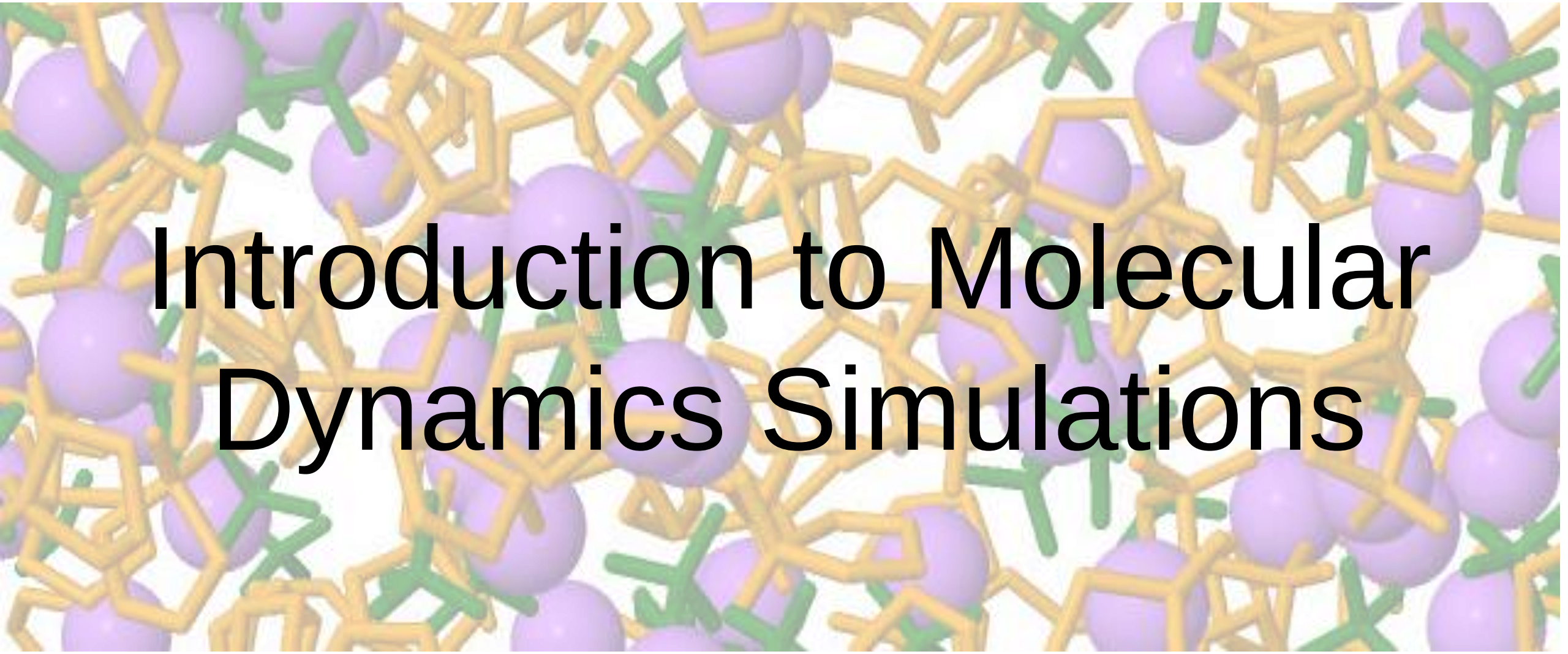
  1. Introduction to Molecular Dynamics Simulations
  2. Molecular Dynamics Simulation packages
  3. HPC LSU and LONI Software environment

- **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

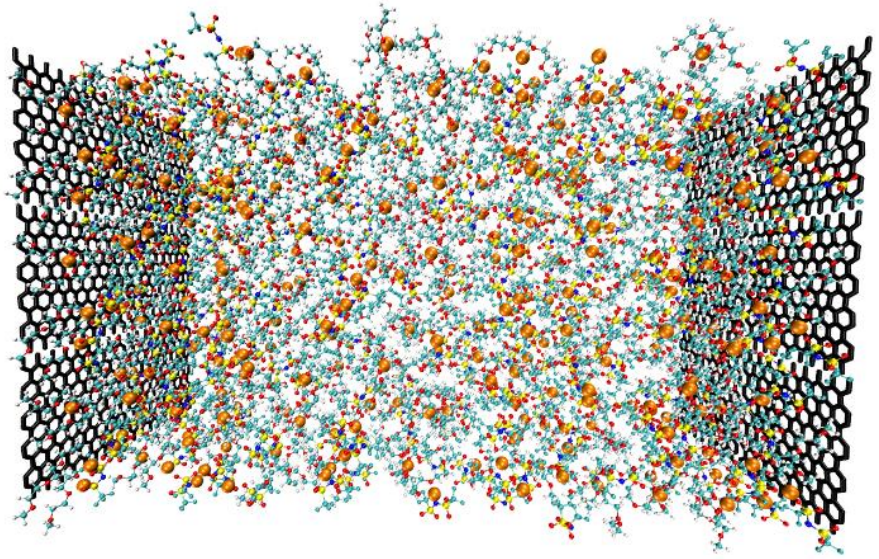


Introduction to Molecular Dynamics Simulations

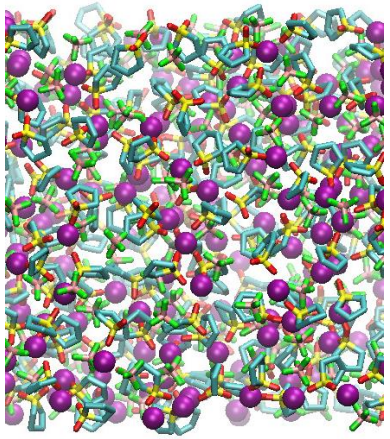
Introduction to Molecular Dynamics Simulations

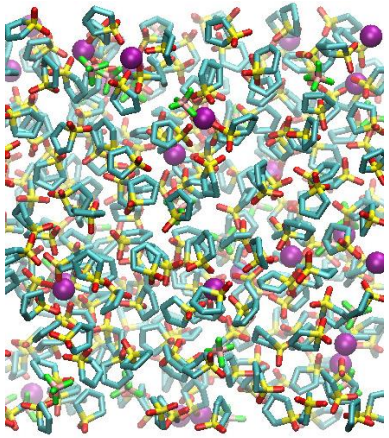
Molecular dynamics (MD) is a versatile tool for calculating structural and dynamics properties of molecular systems at equilibrium as a function of time. The molecular systems should obey the laws of classical physics.

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 force fields

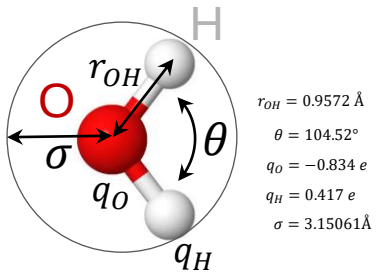
Molecular dynamics simulations

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

Thermodynamic properties

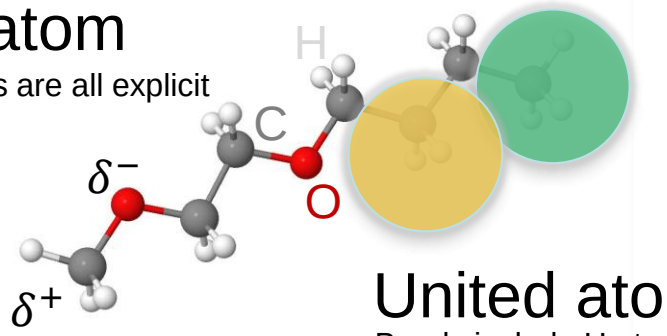
1. Calculate structural and dynamic properties as a time average of an ensemble of atoms.

TIP3P water model



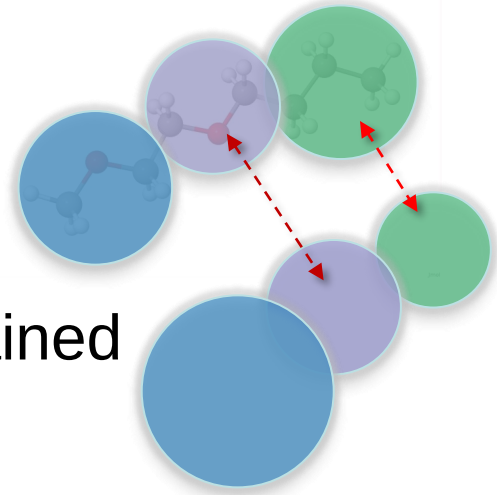
All atom

H atoms are all explicit



United atom

Beads include H atoms in CH2 CH3

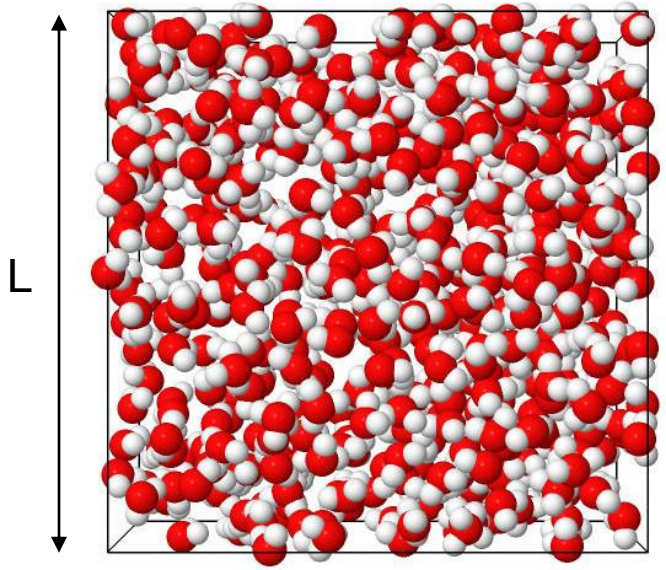


Coarse-Grained models

Beads include entire functional groups

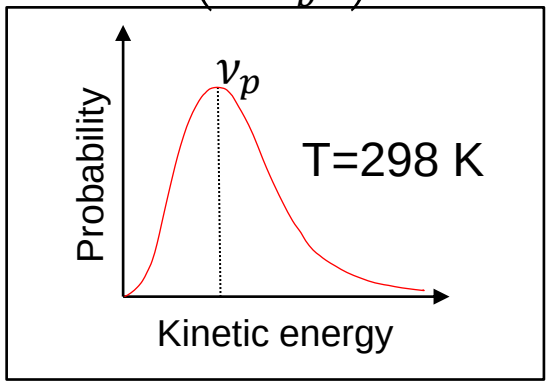
Introduction to Molecular Dynamics Simulations

Simulation box, L



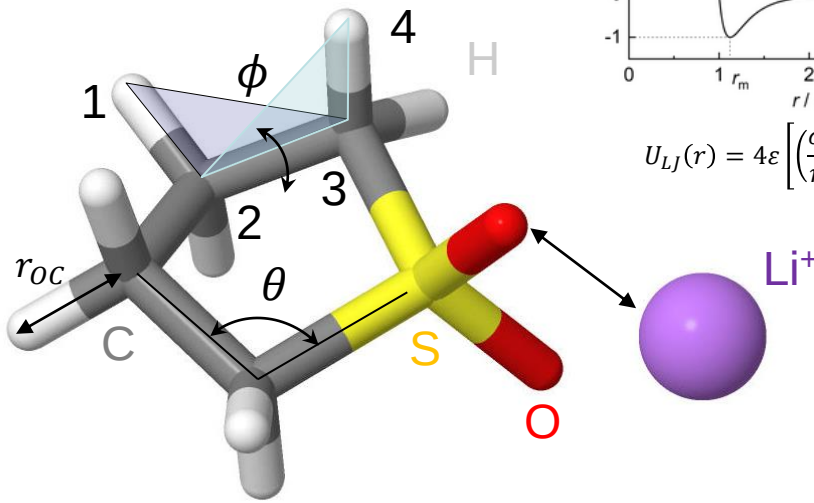
$N = 1536 \quad r_i = x, y, z$

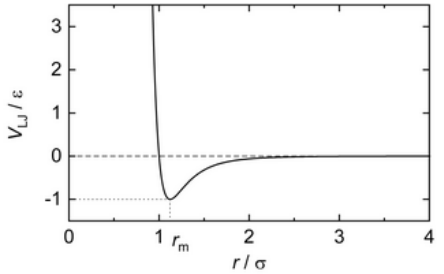
$$P(v_{i,r}) = \left(\frac{m}{2\pi k_b T}\right)^{\frac{1}{2}} e^{-\frac{mv_{i,r}^2}{2\pi k_b T}}$$



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





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

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

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

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

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

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

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

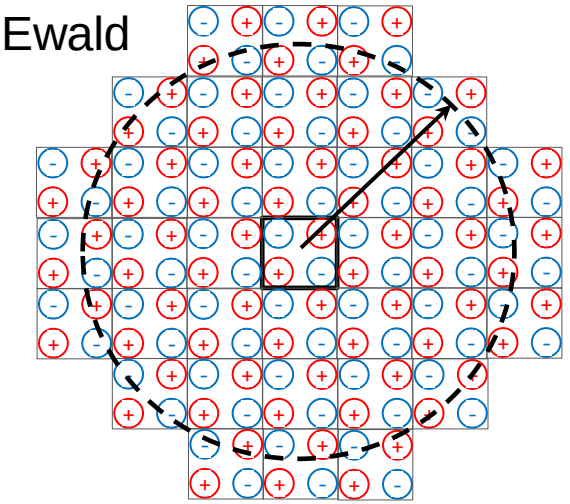
$$v(t+\Delta t) = v(t) + \frac{1}{2}\Delta t[a(t) + a(t+\Delta t)]$$

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

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

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

Ewald



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

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

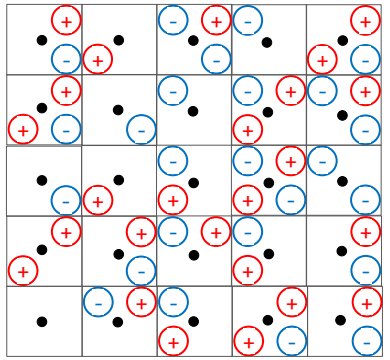
$$U^{real} = \frac{1}{2}\sum_{i,j}^{N}\sum_{n} q_i q_j \frac{\mathrm{erfc}(\alpha r_{ij,n})}{r_{ij}}$$

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

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

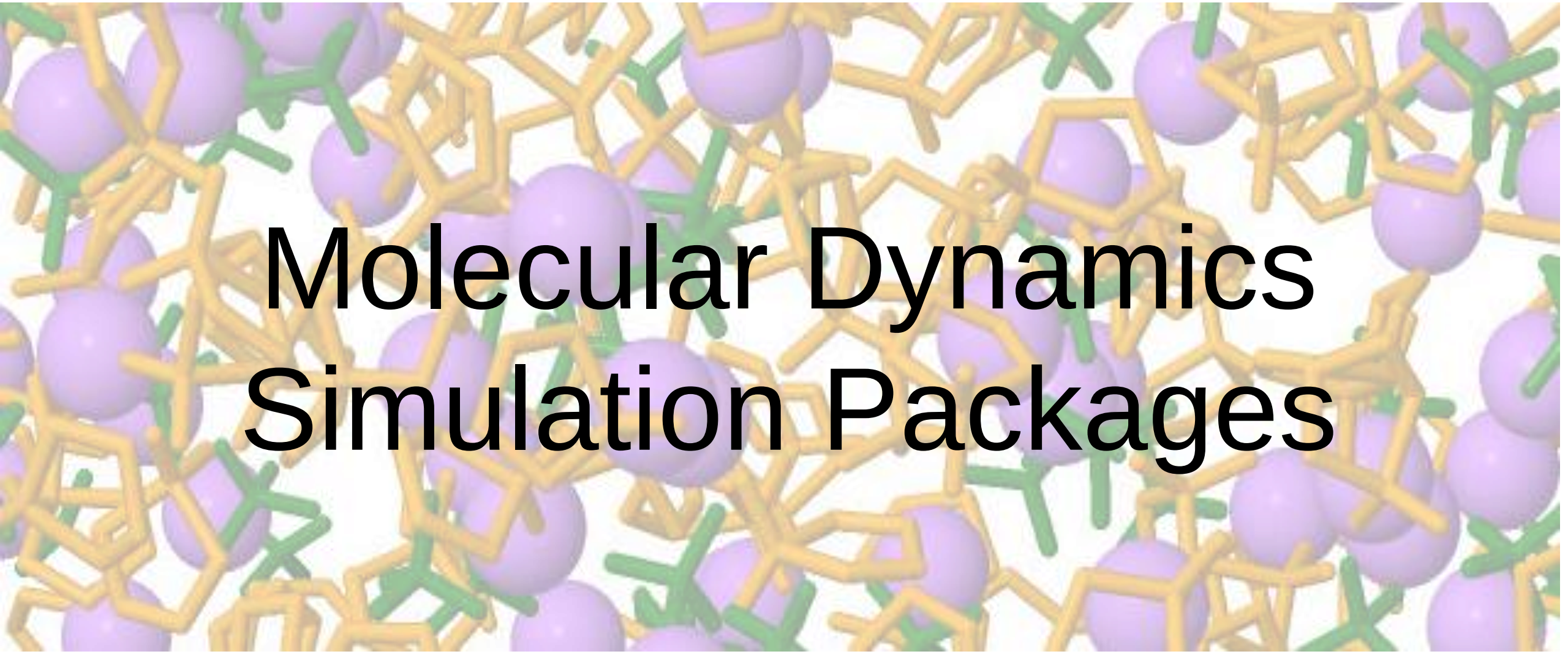
A three-dimensional grid is introduced to optimize the computation of long-range interactions and calculate the reciprocal space contribution.

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



PME

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



Molecular Dynamics Simulation Packages

MD Simulation Packages

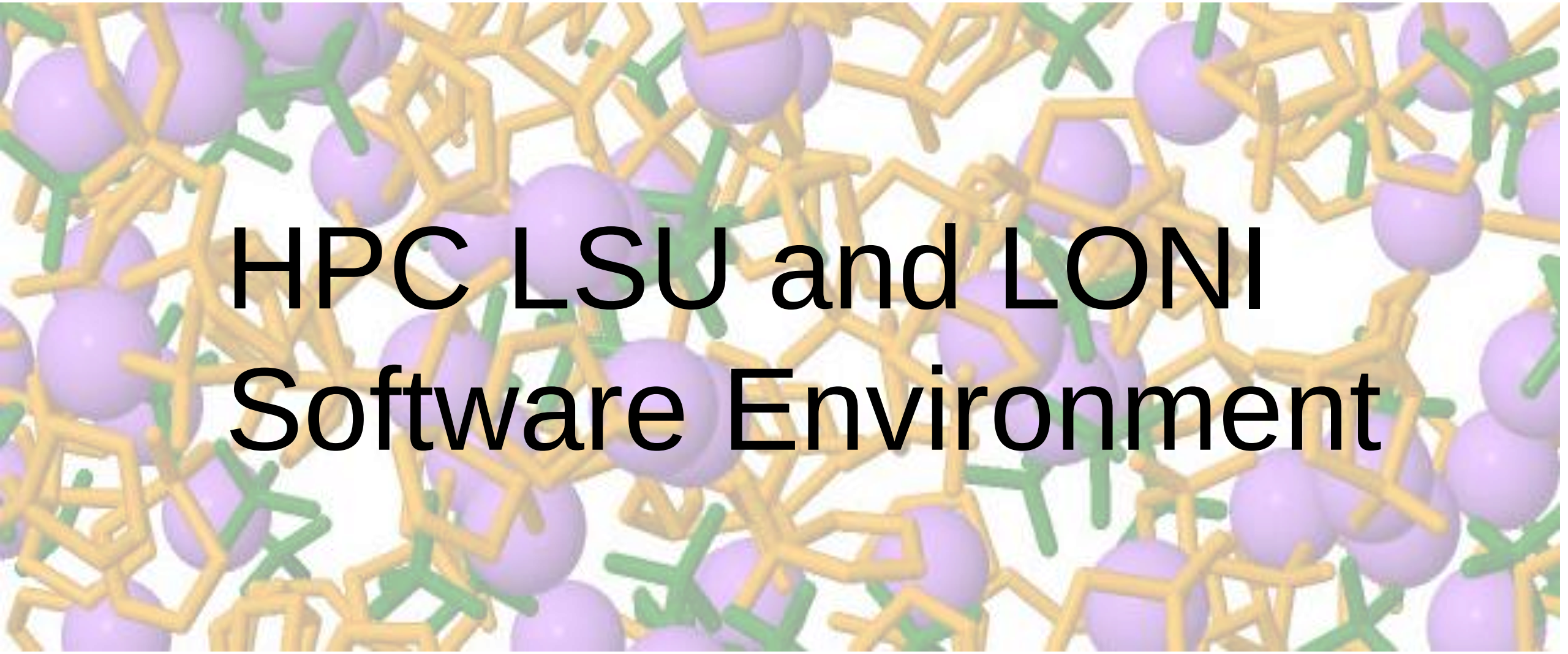
- LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator, Sandia National Lab, 1995) is a molecular dynamics simulation package, https://www.lammps.org
- GROMACS (GROningen Machine for Chemical Simulations, University of Groningen, 1991) is a molecular dynamics simulation package, https://www.gromacs.org
- 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

	LAMMPS	GROMACS	NAMD	AMBER	VMD
QB2	2020/10/29	2020.6	2.14	18	1.9.3
QBC	2020/03/03	2020.2	2.14	18	1.9.3
SMIC	2022/12/22	2022.0	2.14	18	1.9.3
MIKE	2022/06/23	2021.3	2.14	22	1.9.3



HPC LSU and LONI Software Environment

Software environment

[username@cluster ~]$ **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/23Jun2022/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1
lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1
.
namd/2.14/intel-2021.5.0
namd/2.14/intel-2021.5.0-cuda

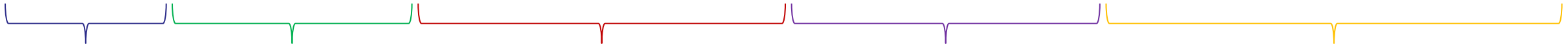
Software environment

No GPU

lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1

name package version compiler MPI library

lammps/23Jun2022/intel-2021.5.0-cuda-11.6.0-intel-mpi-2021.5.1



name package version compiler cuda version MPI library

GPU

Software environment

[username@mike2 ~]$ **module purge**

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

[username@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

[username@mike2 ~]$ **module display** lammps/23Jun2022/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

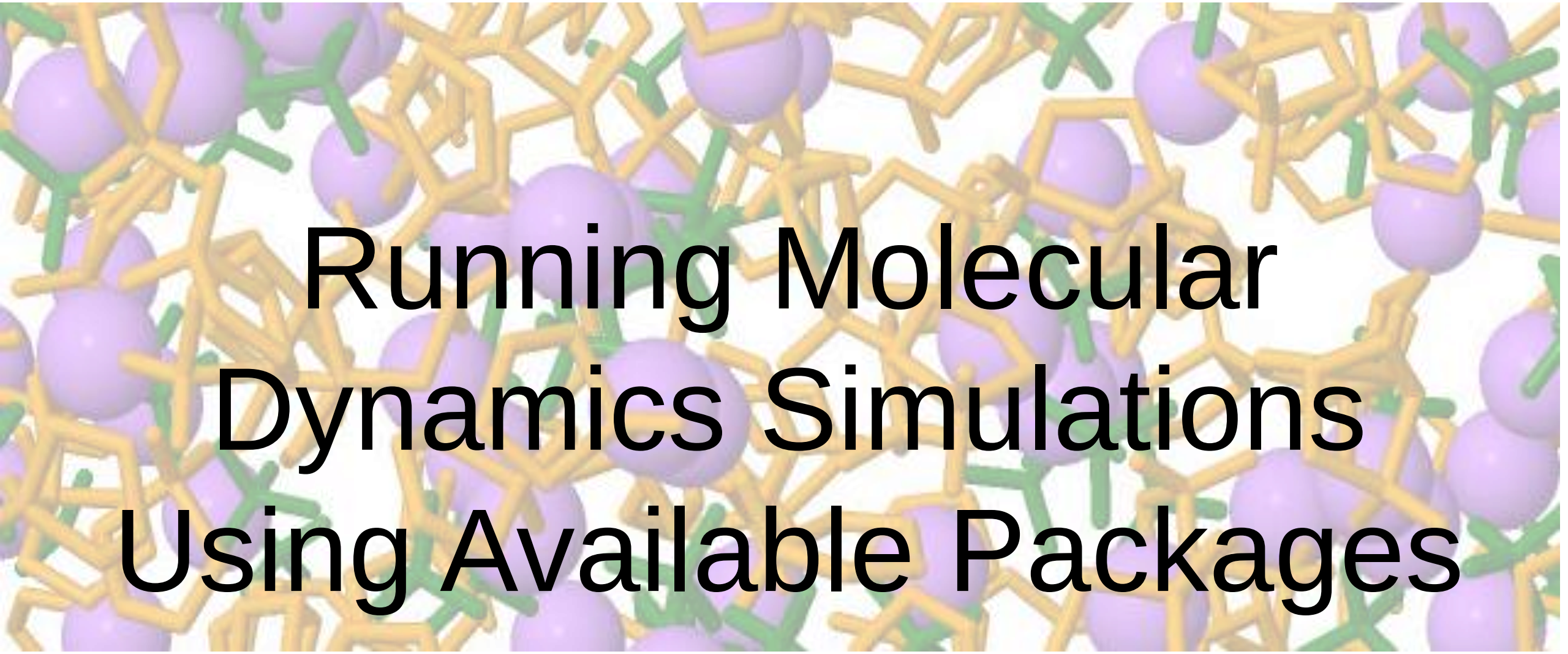
prepend-path PATH /usr/local/packages/lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1/bin

prepend-path MANPATH /usr/local/packages/lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1/share/man

Software environment

[username@mike2 ~]$ ls /usr/local/packages/lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1/bin

combinefm_no_gro.x lmp lmp_omp lmp_serial newfm_no_gro.x rangefinder_no_gro.x



Running Molecular Dynamics Simulations Using Available Packages

Running LAMMPS jobs on HPC

Every LAMMPS simulation needs two essential files:

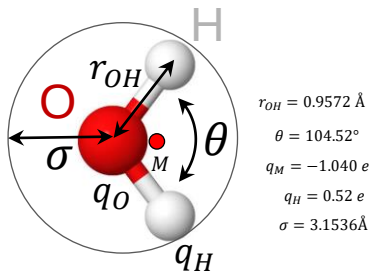
1. structure / topology (.lammps),
2. parameters (.in).

Structure/topology

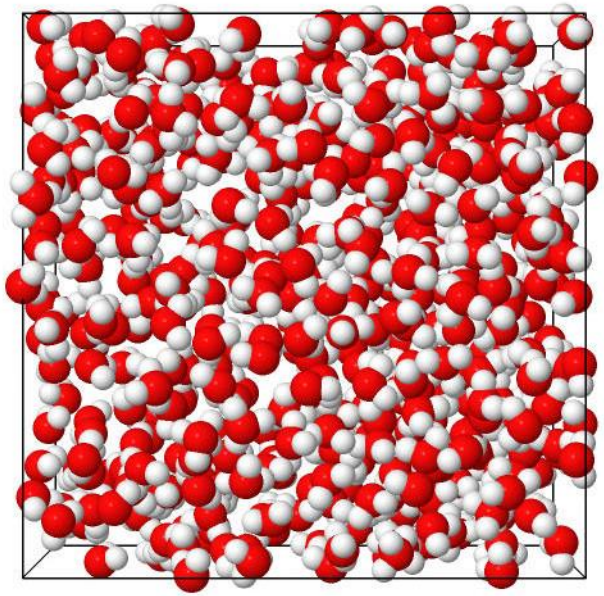
```
1536 atoms
Atoms
   1   1   1 -1.04840   23.067397   25.992172   12.516813
   2   1   2  0.52420   23.651513   25.756170   13.277936
   3   1   2  0.52420   23.106625   25.196754   11.981115
   ...
```

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
...
```



TIP4P water model



Running LAMMPS jobs on HPC

Running LAMMPS interactively

```
[user@cluster LAMMPS]$ srun -N1 -n64 -p workq --time=05:00:00 -A  hpc_allocation --pty bash
[user@cluster LAMMPS]$ module purge
[user@cluster LAMMPS]$ module load lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1
[user@cluster LAMMPS]$ module list

Currently Loaded Modulefiles:
 1) intel/2021.5.0   2) intel-mpi/2021.5.1   3) lammps/23Jun2022/intel-2021.5.0-intel-mpi-2021.5.1

[user@cluster LAMMPS]$ srun --overlap –n 1  lmp -in tip4p_512.in > tip4p_512.out
[user@cluster LAMMPS]$ top

[user@cluster LAMMPS]$ srun --overlap –n 64 lmp -in tip4p_512.in > tip4p_512.out
[user@cluster LAMMPS]$ ls

log.lammps  tip4p_512.in  tip4p_512.lammps  tip4p_512.out  tip4p_512.traj
```

Running LAMMPS jobs on HPC

Running LAMMPS jobs using PBS system

```
#!/bin/bash
#PBS -q workq
#PBS -N test
#PBS -l nodes=1:ppn=20
#PBS -l walltime=HH:MM:SS
#PBS -A loni_allocation
#PBS -o lammps.${PBS_JOBID}.out
#PBS -e lammps.${PBS_JOBID}.err
#PBS -m bea
#PBS -M your@email.address

module purge
module load lammps/20201029/intel-19.0.5-cuda-mvapich-2.3.3

echo "Date              = $(date)"
echo "Hostname          = $(hostname -s)"
echo "Working directory  = $(pwd)"

echo $PBS_O_WORKDIR
cd   $PBS_O_WORKDIR

time mpirun -np 20 lmp_mpi -in tip4p_512.in \
> tip4p_512.out
```

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.out
#SBATCH -e lammps.%j.err
#SBATCH --mail-user your@email.address

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

echo $SLURM_JOBID
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 -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

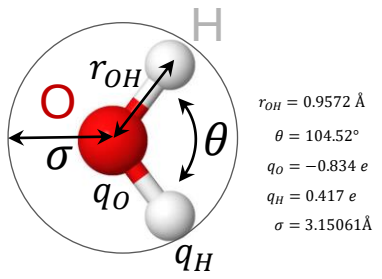
```
TIP3P water
 1536
   1SOL    OW    1   2.308   1.150   1.290  0.0374 -0.1946  0.1896
   1SOL   HW1    2   2.242   1.208   1.328 -0.7293 -1.1860  0.4498
   1SOL   HW2    3   2.376   1.143   1.357  1.6678  2.7051 -0.9958
   ...
```

Topology

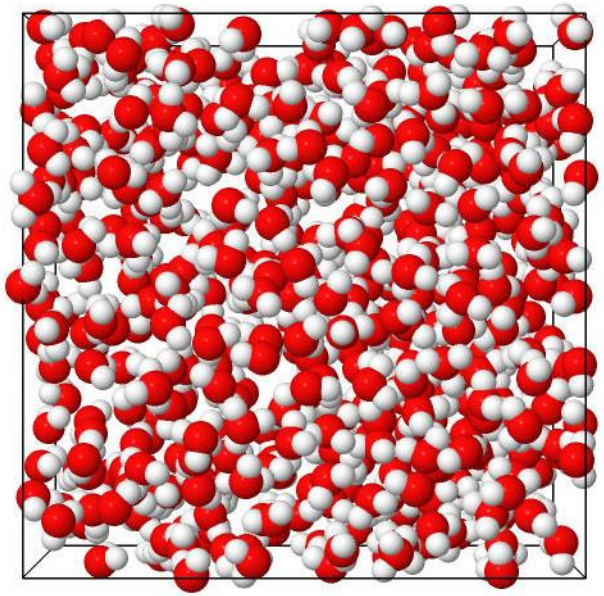
```
; Include forcefield parameters
#include "charmm27.ff/forcefield.itp"

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

Parameters

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



TIP3P water model



Running GROMACS jobs on HPC

Running GROMACS interactively

```
[user@cluster GROMACS]$ srun -N1 -n64 -p workq --time=05:00:00 -A  hpc_allocation0 --pty bash
[user@cluster GROMACS]$ module purge
[user@cluster GROMACS]$ module load gromacs/2021.3/intel-2021.5.0-intel-mpi-2021.5.1
[user@cluster 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@cluster GROMACS]$ srun --overlap gmx_mpi grompp  -f  min.mdp -c npt.gro -p topol.top -o min.tpr
[user@cluster GROMACS]$ srun --overlap gmx_mpi  mdrun --deffnm min –v
[user@cluster GROMACS]$ ls

min.edr  min.gro  min.log  min.mdp  min.tpr  min.trr

[user@cluster GROMACS]$ srun --overlap gmx_mpi grompp  -f  eql.mdp -c min.gro -p topol.top -o eql.tpr
[user@cluster GROMACS]$ srun --overlap gmx_mpi  mdrun --deffnm eql –v
[user@cluster GROMACS]$ ls

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 PBS system

```
#!/bin/bash
#PBS -q workq
#PBS –N test
#PBS -l nodes=1:ppn=20
#PBS -l walltime=HH:MM:SS
#PBS -A loni_allocation
#PBS -o gromacs.${PBS_JOBID}.out
#PBS -e gromacs.${PBS_JOBID}.err
#PBS -m bea
#PBS -M your@email.address

module purge
module load gromacs/2020.6/intel-19.0.5-mvapich-2.3.3


echo "Date              = $(date)"
echo "Hostname          = $(hostname -s)"
echo "Working Directory = $(pwd)"

echo $PBS_O_WORKDIR
cd  $PBS_O_WORKDIR

time mpirun -np 20 gmx_mpi mdrun –deffnm npt -v
```

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.out
#SBATCH -e gromacs.%j.err
#SBATCH --mail-user your@email.address

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

echo $SLURM_JOBID
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 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)

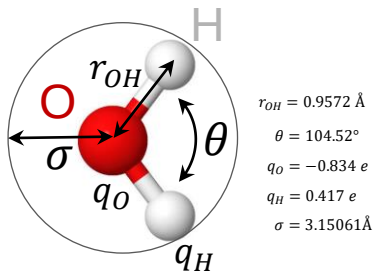
```
   1536 !NATOM
      1 WW1  5    TIP3 OH2  OT    -0.834000       15.9994           0
      2 WW1  5    TIP3 H1   HT     0.417000       1.0080            0
      3 WW1  5    TIP3 H2   HT     0.417000       1.0080            0
     ...
```

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
...
```

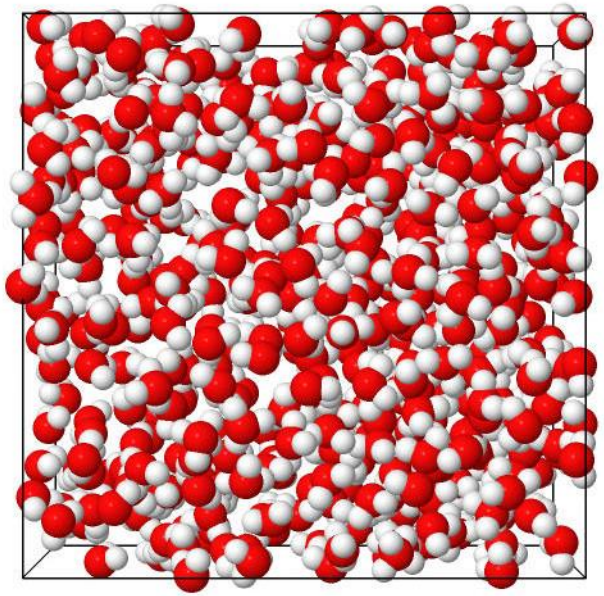
Parameters (.input)

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



$r_{OH} = 0.9572$ Å
$\theta = 104.52°$
$q_O = -0.834\ e$
$q_H = 0.417\ e$
$\sigma = 3.15061$Å

TIP3P water model



Running NAMD jobs on HPC

Running NAMD interactively

```
[user@cluster NAMD]$ srun -N1 -n64 -p workq --time=05:00:00 -A  hpc_allocation0 --pty bash
[user@cluster NAMD]$ module purge
[user@cluster NAMD]$ module load namd/2.14/intel-2021.5.0
[user@cluster NAMD]$ module list

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

[user@cluster NAMD]$ srun --overlap namd2 tip3p_512.namd > tip3p_512.out &
[user@cluster NAMD]$ ls

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 PBS system

```
#!/bin/bash
#PBS -q workq
#PBS -N test
#PBS -l nodes=1:ppn=20
#PBS -l walltime=HH:MM:SS
#PBS -A loni_allocation
#PBS -e NAMD.${PBS_JOBID}.err
#PBS -o NAMD.${PBS_JOBID}.out
#PBS -m bea
#PBS -M your@email.address

module purge
module load namd/2.14/intel-19.0.5

echo "Date              = $(date)"
echo "Hostname          = $(hostname -s)"
echo "Working Directory = $(pwd)"

echo $PBS_O_WORKDIR
cd   $PBS_O_WORKDIR

time mpirun -np 20 namd2 tip3p_512.namd > tip3p_512.out
```

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.out
#SBATCH -e NAMD.%j.err
#SBATCH --mail-user your@email.address

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 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)

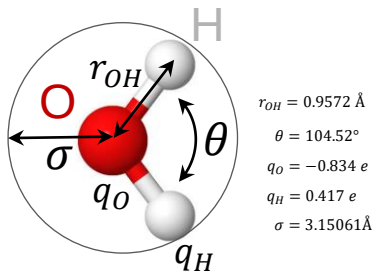
```
default_name
 1536
  16.5307255  19.4975686  18.1539268  13.3987255  16.6285686  12.9069268
  15.2747255  15.8905686  11.7989268  17.0747255  16.7645686  10.4629268
...
```

Topology (.prmtop)

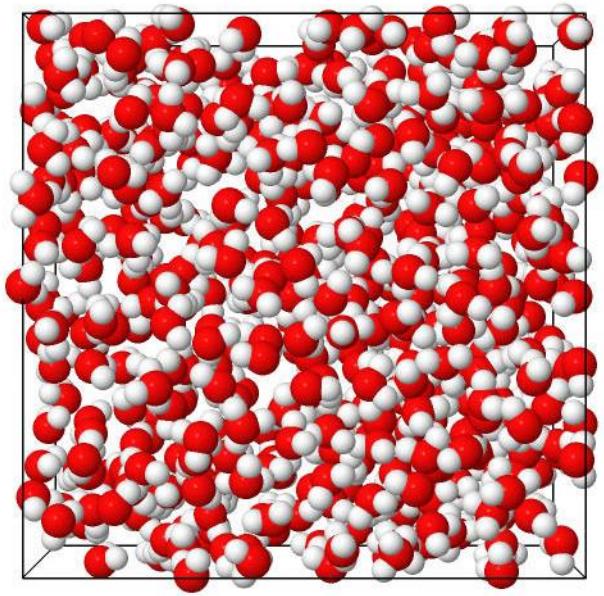
```
 %FORMAT(10I8)
   1536      2   1024      0    512      0 ...
   2048    512      0      0      0      2 ...
      0      0      0      0      0      0 ...
 ...
```

Parameters (.inp)

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



TIP3P water model



Running AMBER jobs on HPC

Running AMBER interactively

```
[user@cluster AMBER]$ srun -N1 -n64 -p workq --time=05:00:00 -A  hpc_allocation0 --pty bash
[user@cluster AMBER]$ module purge
[user@cluster AMBER]$ module load amber/22/intel-2021.5.0-intel-mpi-2021.5.1
[user@cluster 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@cluster AMBER]$ srun --overlap sander -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd
[user@cluster AMBER]$ ls
```

Running AMBER jobs on HPC

Running AMBER jobs using PBS system

```
#!/bin/bash
#PBS -q workq
#PBS -N test
#PBS -l nodes=1:ppn=20
#PBS -l walltime= HH:MM:SS
#PBS -A loni_allocation
#PBS -o lammps.${PBS_JOBID}.out
#PBS -e lammps.${PBS_JOBID}.err
#PBS -m bea
#PBS -M your@email.address

module purge
module load amber/18/intel-19.0.5-mvapich-2.3.3

echo "Date              = $(date)"
echo "Hostname          = $(hostname -s)"
echo "Working directory  = $(pwd)"

echo $PBS_O_WORKDIR
cd   $PBS_O_WORKDIR

time mpirun -np 20 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 1
#SBATCH -n 48
#SBATCH -c 1
#SBATCH -t HH:MM:SS
#SBATCH -A loni_allocation
#SBATCH -J test
#SBATCH -o amber.%j.out
#SBATCH -e amber.%j.err
#SBATCH --mail-user your@email.address

module purge
module load amber/18/intel-19.0.5-mvapich-2.3.3

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo $SLURM_SUBMIT_DIR
cd   $SLURM_SUBMIT_DIR


time srun -N1 -n48 sander.MPI -O -i eql.inp -o eql.out -p tip3p_512.prmtop -c tip3p_512.inpcrd
-r tip3p_512.rst
```

- Marrink, S. J. *et al*, "The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations" J. Phys. Chem. B 2007, 111, 27, 7812-7824, https://doi.org/10.1021/jp071097f
- 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.

Thank You