

HIGH PERFORMANCE RESEARCH COMPUTING

Running Molecular Dynamics Simulations Using LAMMPS

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November 14, 2025



High Performance
Research Computing
DIVISION OF RESEARCH



High Performance Research Computing | hprc.tamu.edu

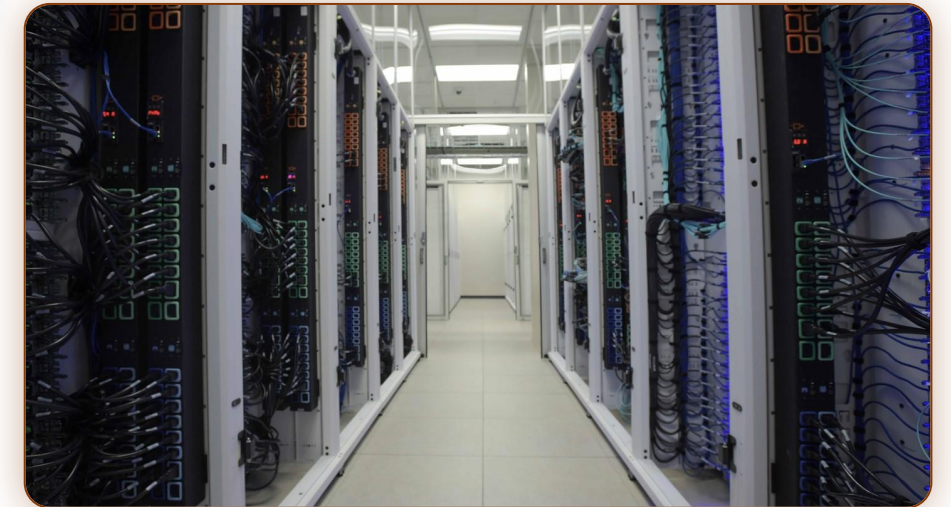
Grace Hardware

Grace is a 925-node Intel cluster from Dell with an InfiniBand HDR-100 interconnect, A100 GPUs, RTX 6000 GPUs, and T4 GPUs. The 925 nodes are based on the Intel Cascade Lake processor.

48 cores/node

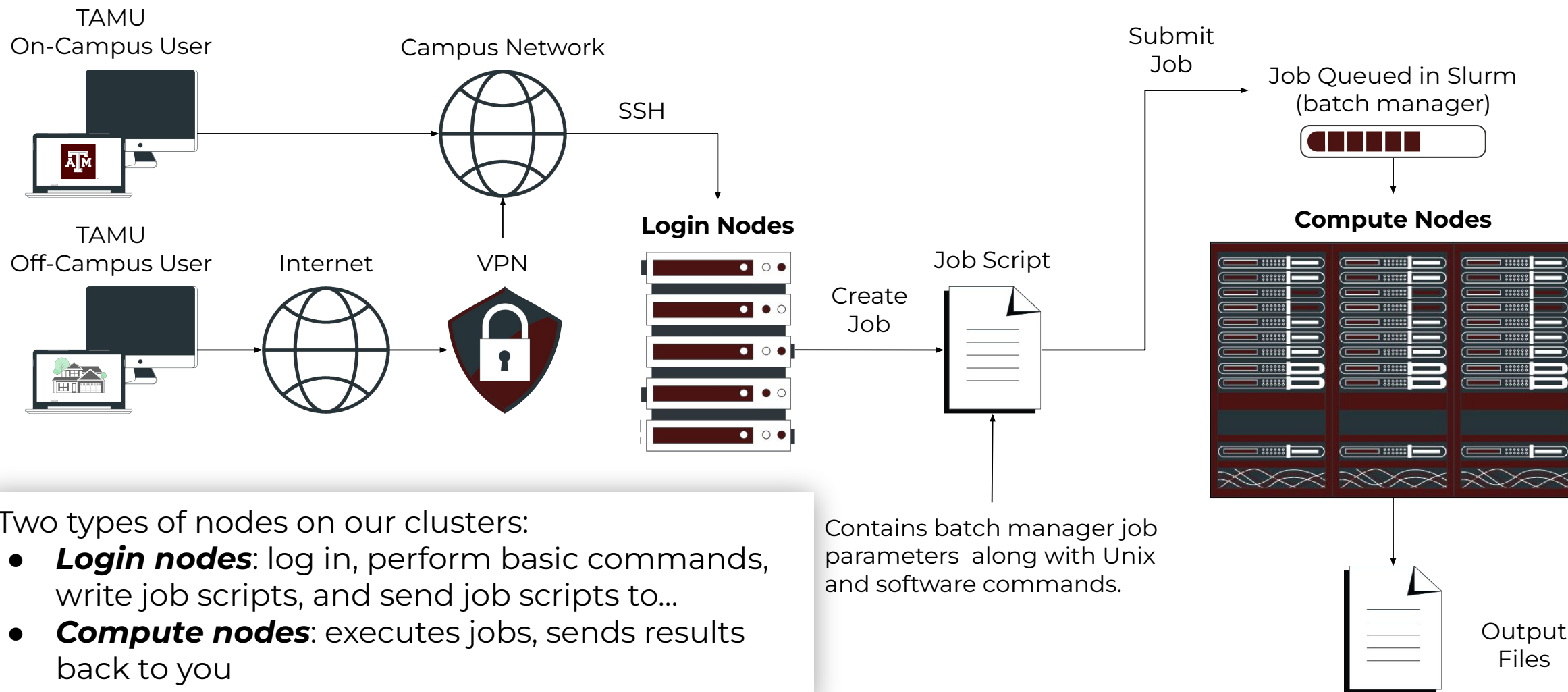
3TB Large Memory-80 cores/node
Login Nodes: 10 GbE TAMU network connection

Resource	Count
Login Nodes	5
384GB memory general compute nodes	800
GPU - A100 nodes with 384GB memory	100
GPU - RTX 6000 nodes with 384GB memory	9
GPU - T4 nodes with 384GB memory	8
3TB Large Memory	8

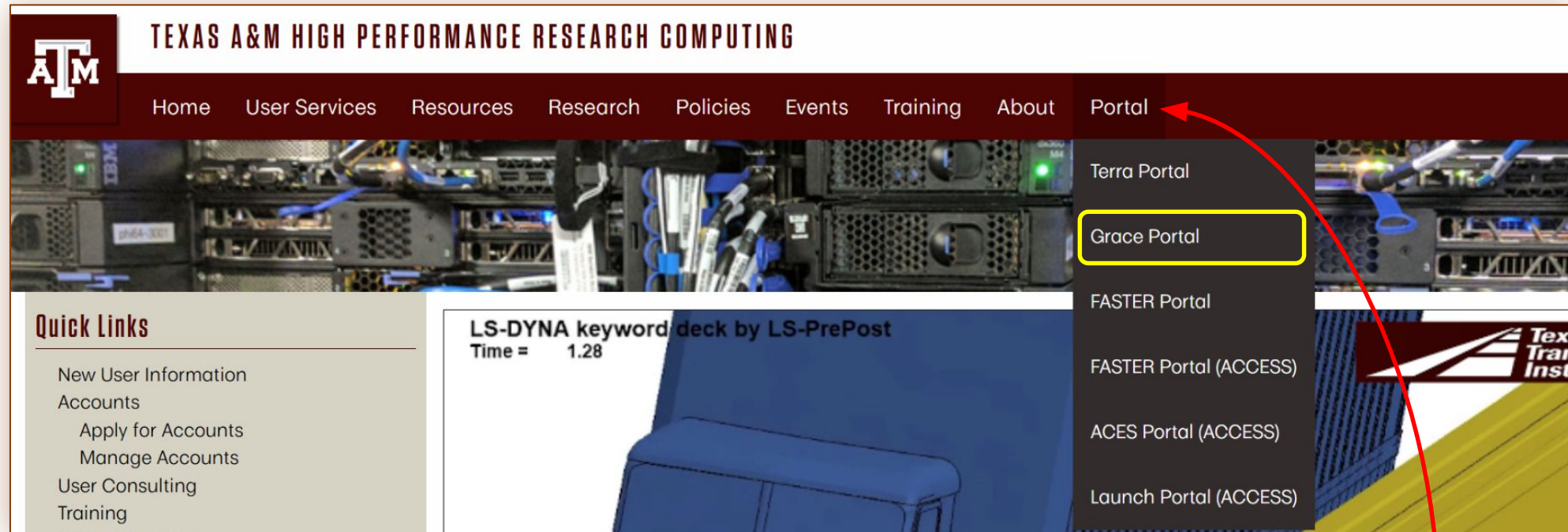


For more information: [Grace User Guide](#)

Computing on HPRC Clusters



Accessing Grace via the Portal



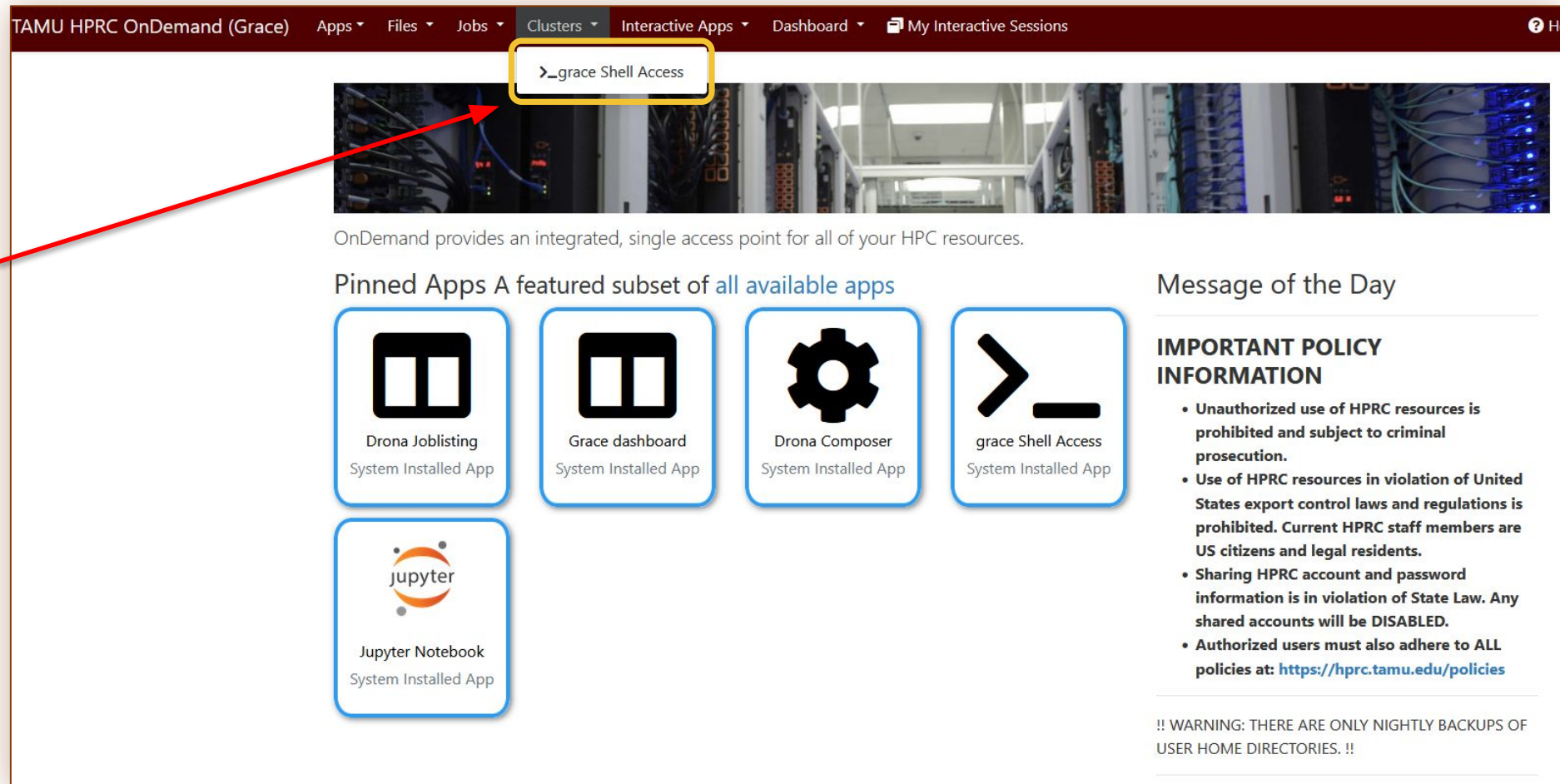
Access the HPRC portals through most web browsers:

1. Go to portal.hprc.tamu.edu or use the Portal dropdown menu on the HPRC homepage: [TAMU HPRC](https://hprc.tamu.edu)
2. Choose **Grace Portal**

<https://hprc.tamu.edu/kb/User-Guides/Grace/Access/>

Accessing Grace via the Portal

Select at the top:
“Clusters” → “_grace
Shell* Access”



TAMU HPRC OnDemand (Grace) Apps Files Jobs Clusters Interactive Apps Dashboard My Interactive Sessions

>_grace Shell Access

OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of [all available apps](#)

Drona Joblisting
System Installed App

Grace dashboard
System Installed App

Drona Composer
System Installed App

grace Shell Access
System Installed App

Jupyter Notebook
System Installed App

Message of the Day

IMPORTANT POLICY INFORMATION

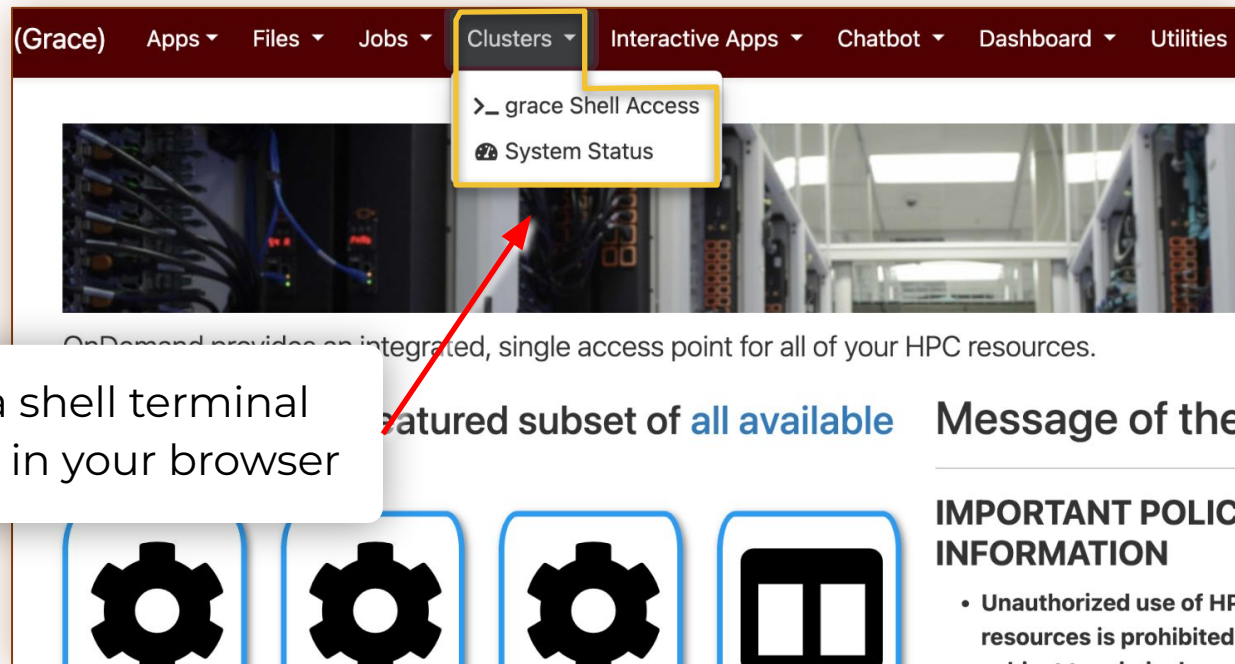
- Unauthorized use of HPRC resources is prohibited and subject to criminal prosecution.
- Use of HPRC resources in violation of United States export control laws and regulations is prohibited. Current HPRC staff members are US citizens and legal residents.
- Sharing HPRC account and password information is in violation of State Law. Any shared accounts will be DISABLED.
- Authorized users must also adhere to ALL policies at: <https://hprc.tamu.edu/policies>

!! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES. !!

*Shell is also called *terminal* or *command line*

<https://hprc.tamu.edu/kb/User-Guides/Grace/Access/>

Shell Access via the Portal



```
Host: login.gracelocal

*****
This computer system and the data herein are available only for authorized
purposes by authorized users. Use for any other purpose is prohibited and may
result in disciplinary actions or criminal prosecution against the user. Usage
may be subject to security testing and monitoring. There is no expectation of
privacy on this system except as otherwise provided by applicable privacy laws.
Refer to University SAP 29.01.03.M0.02 Acceptable Use for more information.
*****

Last login: Sat Nov 8 21:02:22 2025 from 172.31.6.22

=====
Texas A&M University High Performance Research Computing
=====
Consulting:      help@hprc.tamu.edu (preferred) or (979) 845-0219
Website:         https://hprc.tamu.edu
Knowledgebase:   https://hprc.tamu.edu/kb/
YouTube Channel: https://www.youtube.com/texasamhprc
=====

==== IMPORTANT POLICY INFORMATION ====
*
* - Unauthorized use of HPRC resources is prohibited and subject to
*   criminal prosecution.
* - Use of HPRC resources in violation of United States export control
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*   Texas State Law. Any shared accounts will be DISABLED.
* - Authorized users must also adhere to ALL policies at:
*   https://hprc.tamu.edu/policies/
*
=====

!! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES. !!
!! SCRATCH IS NOT BACKED UP AND IS NOT MEANT FOR LONG TERM STORAGE. !!

Please restrict usage to 8 CORES across ALL login nodes.
Users found in violation of this policy will be SUSPENDED.

**** Shared Storage Status for Grace and FASTER Clusters, September 12 ****

We are currently experiencing a significant performance issue with our
filesystem, which is impacting the Grace and FASTER clusters. You may be
observing long wait times, slow command execution, and unresponsive jobs.

Our systems administration team is actively working on a solution.
Unfortunately, running jobs may continue to experience slowness until
more free space is reclaimed as indicated by our email announcement at
2:03p September 12.

We apologize for this disruption to your work. As of now, we do not
have an estimated time of resolution but we will send another update
once the issue is resolved.

Thank you for your patience.

To see these messages again, run the motd command.

Your current disk quotas are:
Disk          Disk Usage  Limit  File Usage  Limit
/home/dineshd 1.3G       10.0G   9896       10000
/scratch/user/dineshd 820.1G    1.0T   244062    250000
/scratch/group/mittal-group 3.7T     5.0T   3935574   5000000
* Quota increase for /scratch/group/mittal-group will expire on Dec 8, 2025
Type 'showquota' to view these quotas again.
[dineshd@grace1 ~]$
```

Copying Training Materials to \$SCRATCH

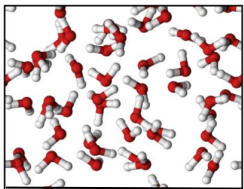
Login to Grace terminal and once you are there:

1. Copy “MD_LAMMPS” containing training materials from /scratch/training

```
cp -r /scratch/training/MD-LAMMPS/ $SCRATCH
```

2. Change now to training materials directory in your \$SCRATCH

```
cd $SCRATCH/MD-LAMMPS
```



What is Molecular Dynamics ?

Input initial positions and velocities

*From random initialization,
PDB, or experiment*

Compute potential energies $U(r)$

*Using appropriate force
field parameters*

Calculate forces on atoms

$$F(r) = -\nabla U(r)$$

Compute acceleration → update atom
velocities → update positions

*Integrate Newton's
equations of motion $F = ma$*

$t \leq t_{\max}$

no

Output values of interest

yes

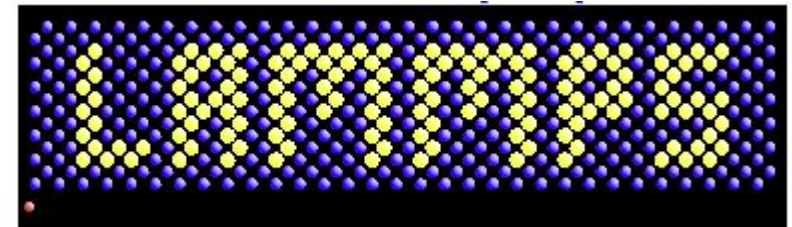
What is a Force Field?

- A mathematical model that describes how atoms interact with each other
- It provides equations and parameters needed to compute potential energies and forces.
- Force fields are usually fitted to material properties around a certain set of conditions.
 - They may not be accurate in regions outside where they were fitted!
- Some types of force fields usable in LAMMPS:
 - LJ, EAM, CHARMM, AMBER, COMPASS, AIREBO, and REAXFF

What is LAMMPS?

- Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
 - *“LAMMPS is a classical molecular dynamics (MD) code that models ensembles of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, solid-state (metals, ceramics, oxides), granular, coarse-grained, or macroscopic systems using a variety of interatomic potentials (force fields) and boundary conditions. It can model 2d or 3d systems with sizes ranging from only a few particles up to billions.”*
- Open source MD software
- Optimized to run parallelly on large numbers of CPUs and GPUs
- Documentation: [LAMMPS documentation](#)

[LAMMPS Molecular Dynamics Simulator](#)



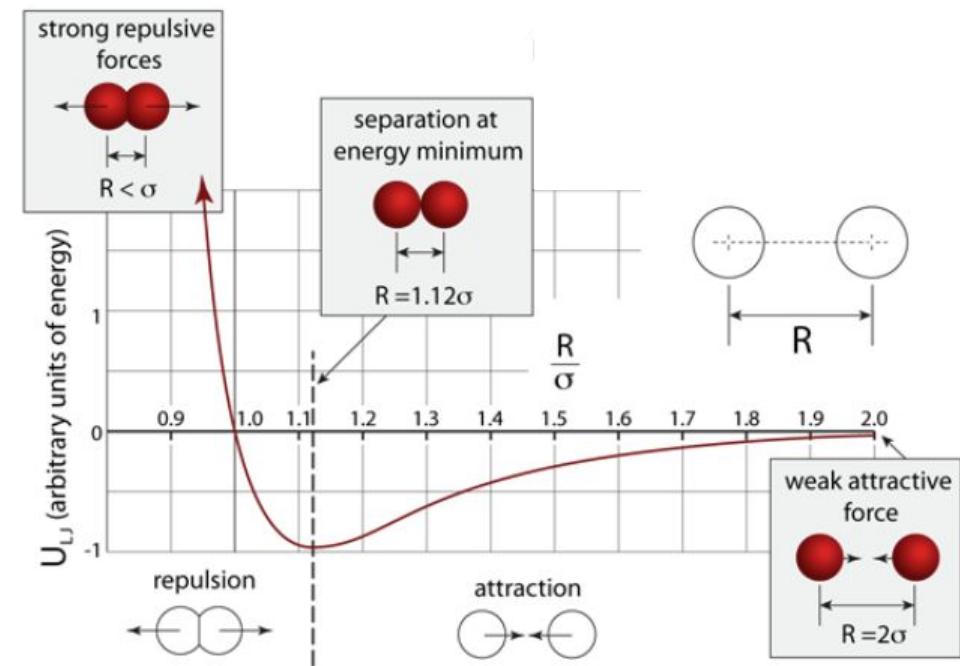
Lab 1: Lennard Jones (LJ) (Coarse-grained)

- To run a LAMMPS simulation, one needs three things:
 - *Topology file: describes number of atoms, describes initial positions, charges, masses, etc.*
 - *Input file: describes potential energy functional forms, simulation conditions, on-the-fly analysis computations*
 - *Job submission script: describes resources (number of cores, memory) required for the simulation to run*

LJ functional form

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

[pair_style lj/cut command — LAMMPS documentation](#)



<https://physicsatmcl.commons.msu.edu/lennard-jones-potential/>

Basics of LAMMPS Input & Data Files

- Change to the LJ directory.

```
cd LJ
```

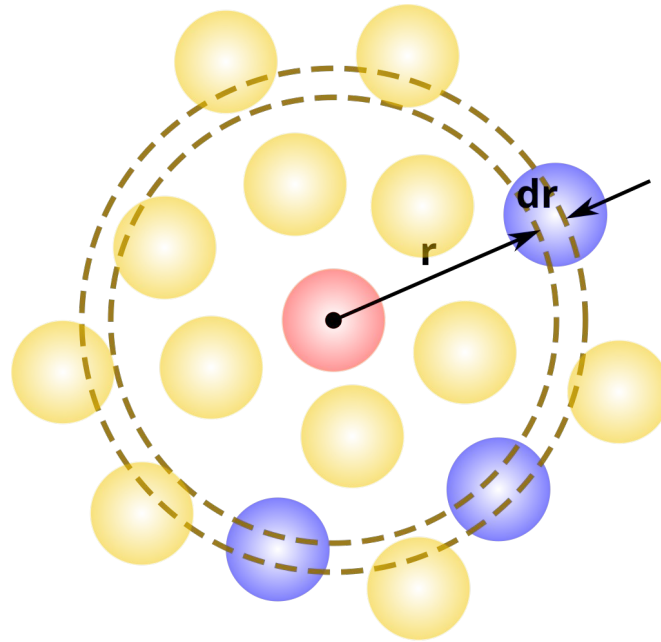
- Submit the job.

```
sbatch job.sh
```

- Let's inspect the LAMMPS input & data files before running the LJ simulation.
 - 'lj.in' → input file
 - 'initial_fcc.data' → data file or topology file

Radial Distribution Function (RDF)

- Normalized probability of finding an atom at a given separation distance from a reference atom
 - Normalized by the corresponding probability in the case of uniform probability distribution



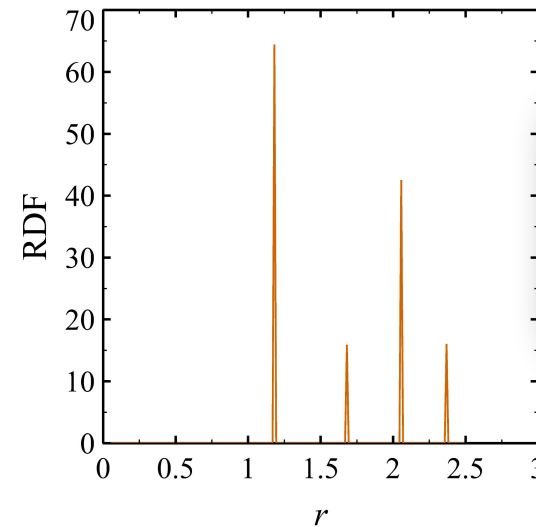
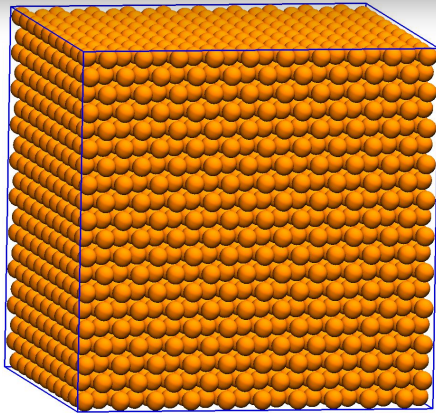
https://en.wikipedia.org/wiki/Radial_distribution_function

Post-Simulation Exercises

1. Compute system density ρ and confirm that the value is 0.85, which we defined in the input script → Hint: ρ = number of atoms/volume
2. Visualize the output trajectory 'traj.lj.dump' using VMD (Visual Molecular Dynamics) → Hint: Load through Interactive Apps as shown in the morning session
3. Plot the RDF outputs 'rdf_initial.txt' and 'rdf_lastHalf.txt'. Based on the two RDF plots, what would you call the structure of initial system configuration ('rdf_initial.txt') and final structure configuration ('rdf_lastHalf.txt')?

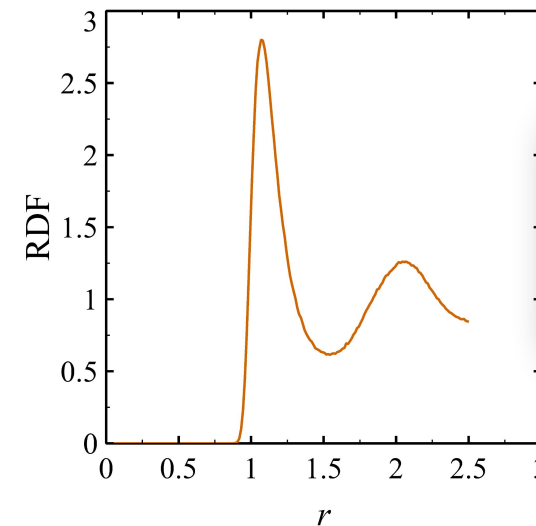
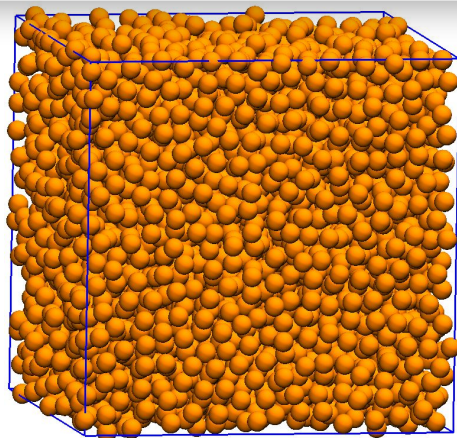
Solution: Interpreting Structure Via RDF

Initial configuration



what does it represent:
crystal?, liquid?

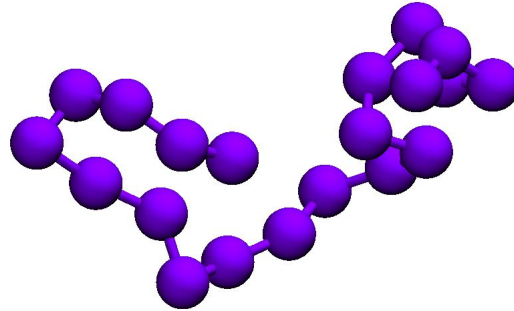
Final configuration



what does it represent:
crystal?, liquid?

Lab 2: LJ Polymer Melt (Coarse-grained)

- Next, we will simulate LJ polymer melt that introduces bonded interactions.



- Change into the LJ_polymer directory and submit the job.

```
cd ../LJ_polymer
```



```
python chains20.py & sbatch job.sh
```

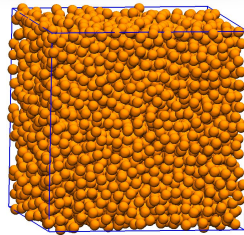
- Let's inspect the input & data files before running the LJ polymer simulation.
 - 'lj_polymer.in' → input file
 - 'chains20.data' → data file or topology file

Post-Simulation Exercises

1. Visualize the output trajectory 'traj.lj_polymer.dump' using VMD (Visual Molecular Dynamics) → Hint: Load through Interactive Apps as shown in the morning session.
2. Plot the RDF outputs 'rdf_lastHalf.txt' from pure LJ simulation and LJ polymer melt simulation on the same plot. What is the difference when you compare the RDFs from pure LJ system and LJ polymer melt?
3. Plot the MSD outputs 'msd_lastHalf.txt' from pure LJ simulation and LJ polymer melt simulation on the same plot. What do you infer from the two MSD curves?

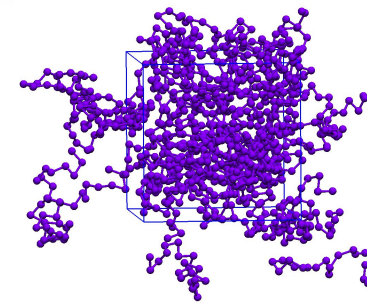
Solution: Interpreting RDFs & MSDs

Pure LJ

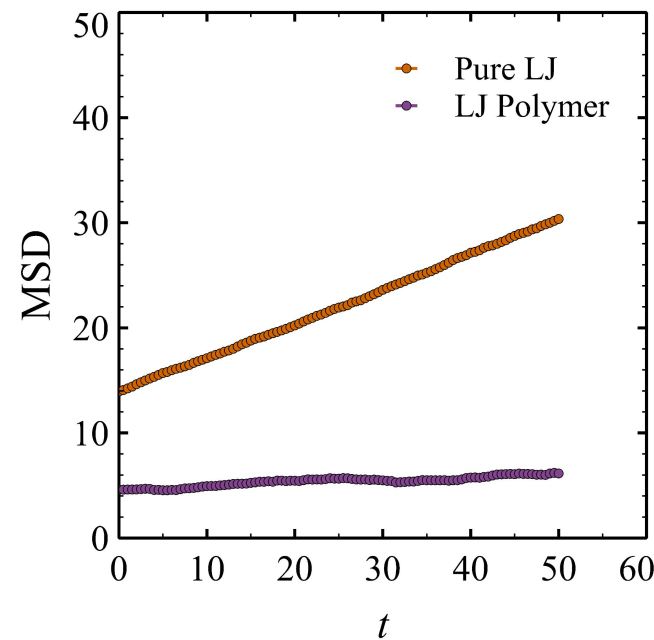
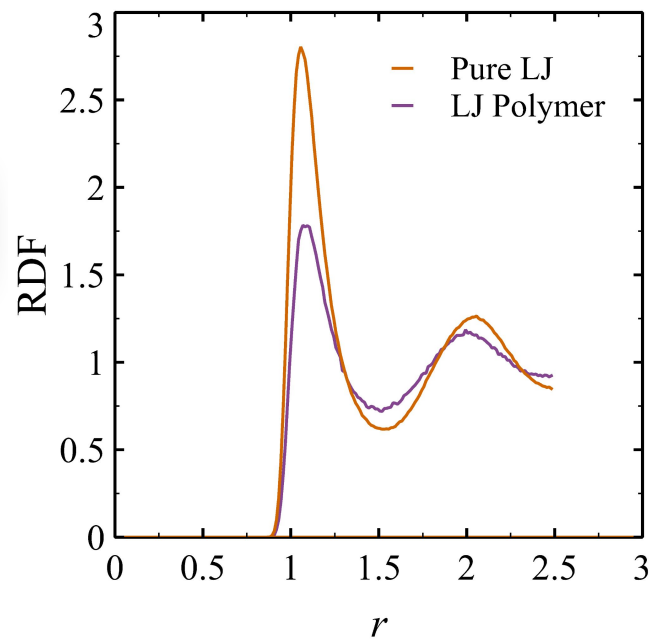


introducing bonded
interactions

LJ polymer



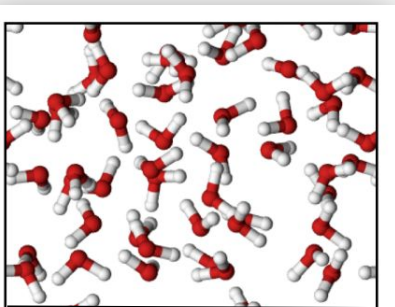
RDF



MSD

mean squared
displacement of atoms

Lab 3: Pure Water System (All-Atom)



- Building on previous 2 labs, now let us introduce angle constraints & electrostatics for accurate chemical interactions.
- We will use the TIP3P water model and perform constant pressure simulation to get to desired water density at room temperature.
- Let's inspect the input & data files before running the pure water simulation.
 - 'water_tip3p.in' → input file
 - 'water_tip3p.data' → data file or topology file

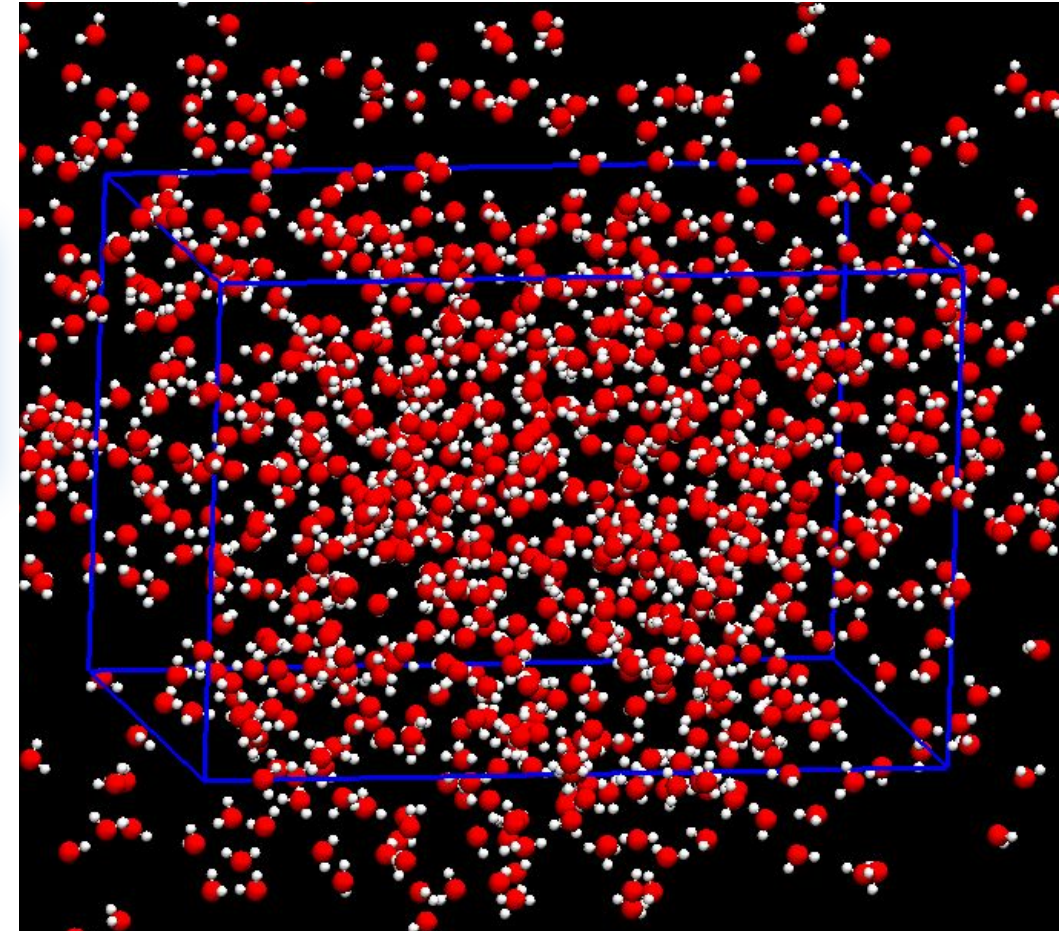
Post-Simulation Exercises

1. Before submitting the job, fix the input script 'water_tip3p.in' to compute average density of water after the run (Hint: Use fix ave/time).
 - a. Are you getting the correct density of water?
2. Visualize the output trajectory 'traj.water.dump' using VMD (Visual Molecular Dynamics) → Hint: Load through Interactive Apps as shown in the morning session.

Solution: Water Density & Visualization

```
# ---- computing average density ----  
fix AVG_RHO all ave/time 1 5000 35000 v_rho  
file avg_density.txt
```

Water density at 298 K = ~ 1 g/cc



Lab 4: Polymer in Water (All-Atom)

- Let us prepare and run a simulation of 5 polyethylene glycol (PEG) chains, each made up of 20 monomer units, in water.
 - Building on previous 3 labs, we are now going to simulate two-component systems and introduce dihedral potentials for polymer chains in addition to bond and angle potentials.
 - PEG is a synthetic hydrophilic polymer used widely across medical, industrial, and commercial sectors because of its non-toxicity, water solubility, and versatility.



- We will use CHARMM-GUI Polymer Builder to prepare the system.

[CHARMM-GUI](#)



CHARMM-GUI: System Type & Polymer Building Block

System Type: ?

- ☐ Single Polymer Chain
- ☒ Solution
- ☐ Melt

Building Block(s) of Polymer: ?

Select the polymer chain you want below. [Add polymer chain](#)

Polymer chain 1: [Add monomer unit](#)

Next Step: 
Build Polymer Chains

CHARMM-GUI: System Size

System Size Determination Options

1. Box Type: ▾

Length of XYZ: (Å)

Solvation Options:

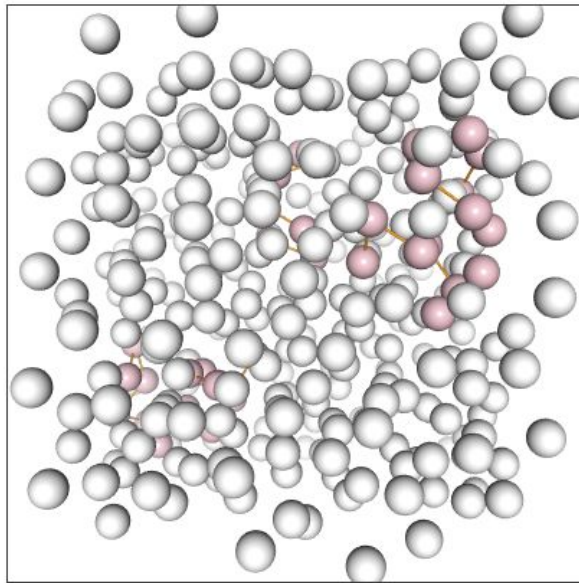
Select type of the solvent in PBC box.

☒ Solvent ▾

click this once you set the system size above.

Chain ID	Composition	Volume(Å ³)	#Chain	% v/v (approximated)
P1	ETHOX ₂₀	1276.7	5	

CHARMM-GUI: CG Equilibration



1. Determined System: (X:50 Å, Y:50 Å, Z:50 Å)

Chain ID	Composition	#Chain	Bead Composition
P1	ETHOX ₂₀	5	PA ₇
SOLV	TIP3	308	

2. Size & Constituent of Kuhn Bead:



Bead	#Bead per Chain	Sequence	σ
PA	7/7	ETHOX _{2,9}	6 Å
SOLV	1	TIP3	6 Å

3. Interaction Matrix: $\Delta\delta$
(unit of ϵ : Kcal/mol, unit of $\Delta\delta$: MPa^{1/2})

	PA	SOLV
PA	0	4.46
SOLV	4.46	0

4. ☒ Equilibration by OpenMM:

Nonbonded interaction:

☒ Weeks-Chandler-Andersen (WCA) Potential
poor good (solvent)

$\lambda_{\text{Solvent-PA}}$ 0.06

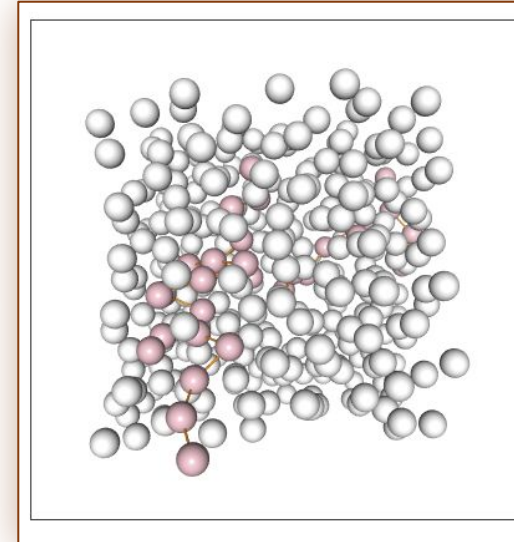
Running steps are ...

- ☐ Equilibration with WCA potential
- ☒ Equilibration with LJ potential

click this once you change below.

Temperature: K (Reduced Temperature: 0.61)

Simulation time: ns (recommended time: 10 ns)



1. Determined System: (X:44.6 Å, Y:44.6 Å, Z:44.6 Å)

Chain ID	Composition	#Chain	Bead Composition
P1	ETHOX ₂₀	5	PA ₇
SOLV	TIP3	308	

2. Size & Constituent of Kuhn Bead:



Bead	#Bead per Chain	Sequence	σ
PA	7/7	ETHOX _{2,9}	6 Å
SOLV	1	TIP3	6 Å

CHARMM-GUI: All-Atom Input Generation

Computed Energy:

Please beware of that the computed energy is CHARMM single-point energy and is displayed to make sure all the coordinates are defined.

ENER ENR:	Eval#	ENERGY	Delta-E	GRMS		
ENER INTERN:		BONDS	ANGLES	UREY-b	DIHedrals	IMProper
ENER EXTERN:		VDwaals	ELEC	HBONds	ASP	USER

ENER>	0	11368.43888	0.00000	19.69743		
ENER INTERN>		1377.09757	341.17613	177.24010	389.20067	0.00000
ENER EXTERN>		9348.58659	-264.86218	0.00000	0.00000	0.00000

Input Generation Options:

It may take some time to generate selected inputs.

- ☐ NAMD
- ☐ GROMACS
- ☐ AMBER
- ☐ OpenMM
- ☐ CHARMM/OpenMM
- ☐ GENESIS
- ☐ Desmond
- ☒ LAMMPS

Equilibration Input Generation Options:

- ☒ NVT ensemble

Temperature: K

Dynamics Input Generation Options:

- ☐ NVT ensemble
- ☒ NPT ensemble

CHARMM-GUI: Download Files for Simulation

CHARMM PDB

PBC Setup

Equilibrium

Replacement

Input Generator

JOB ID: 6295125889

Input Generator Input: [step3_input.inp](#)

Input Generator Output: [step3_input.out](#)

Dynamics Input: [step5_production.inp](#)

download.tgz

Please download "download.tgz" to continue equilibration and production simulations.

- To unzip .tgz file on the terminal:

```
tar -xvzf charmm-gui.tgz
```

- Then,

```
cd charmm-gui-6294776824/lammps
```

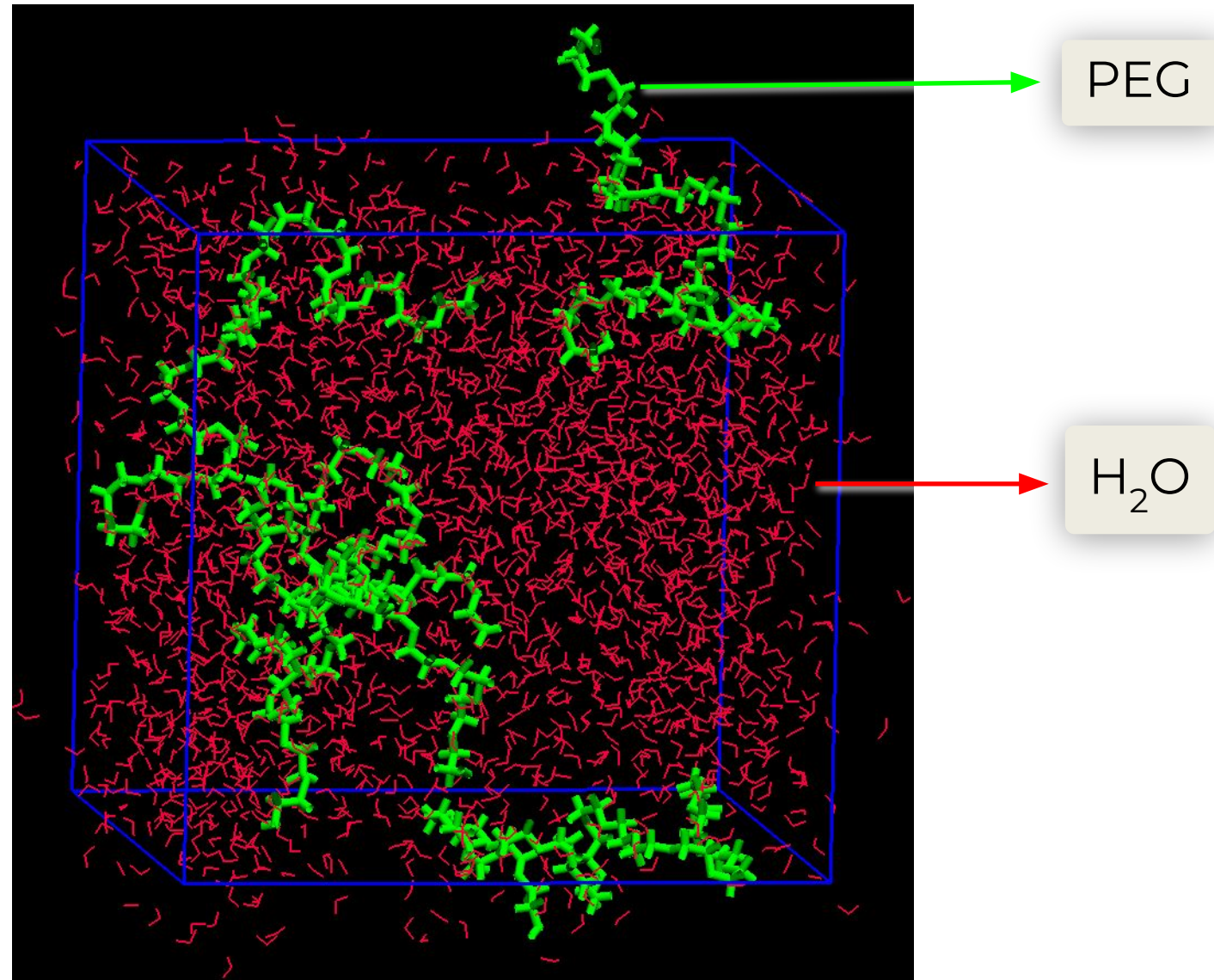
Minimization, Equilibration, and Production

- Let's inspect the input & data files before running the PEG in water simulation.
 - 'step4.0_minimization.inp' → input file for structure minimization
 - 'step4.1_equilibration.inp' → input file for structure equilibration
 - 'step5_production.inp' → input file for structure production
 - 'step3_input.data' → data file or topology file

Simulation Exercises

1. Change the information regarding input files in the job submission script to first run the minimizations step, then the equilibrations step, and finally the production simulation.
2. Visualize the output trajectory 'traj.water.dump' using VMD (Visual Molecular Dynamics). → Hint: Load through Interactive Apps as shown in the morning session.

Solution: Visualizing Polymer in Water



Need Help?

First check the FAQ: <https://hprc.tamu.edu/kb/FAQ/Accounts>

- Grace User guide: <https://hprc.tamu.edu/kb/User-Guides/Grace/>
- Email your questions to help@hprc.tamu.edu
- See our training sessions: hprc.tamu.edu/training

ACES DASHBOARD
TEXAS A&M UNIVERSITY

Settings Get Help

Project Information

Account	FY	Default	Used / Allocated (%)	Balance	PI
152559852254	2026	Y	2000 / 4000 (50%)	2000	John Doe

Queue Availability

Queue	Core Usage (%)	Node Usage (%)
cpu*	100%	100%
gpu	20%	80%
gpu_debug	10%	10%
pvc	10%	10%
bitware	10%	10%

Virtual Env Management

Group	Name	GCCL Version	Description	Owner	Python Version	Toolchain
hpc_ai_env	Python/3.10.8	GCCL/12.2.0	Environment for Intro to HPC and AI	GCCL/12.2.0 Python/3.10.8	Delete	

Quota Information

Disk	Disk Usage (%)	File Usage (%)	Action
/home/u.ds153523	2M/10.0G 0.02%	179/10000 1.79%	
/scratch/user/u.ds153523	15.7G/1.0T 1.53%	46793/250000 18.72%	Request
/scratch/group/p.tra220029.000	12.5G/1.0T 1.22%	10286/500000 2.06%	Request

Need more storage space? Click "Request" next to a specific disk to request an increase for that disk.

Remember the Dashboard!



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*Give us feedback on the class with this
survey:*

https://u.tamu.edu/hprc_shortcourse_survey

Thank you
Questions?

