Running Molecular Dynamics Simulations Using LAMMPS

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High Performance
Research Computing
DIVISION OF RESEARCH

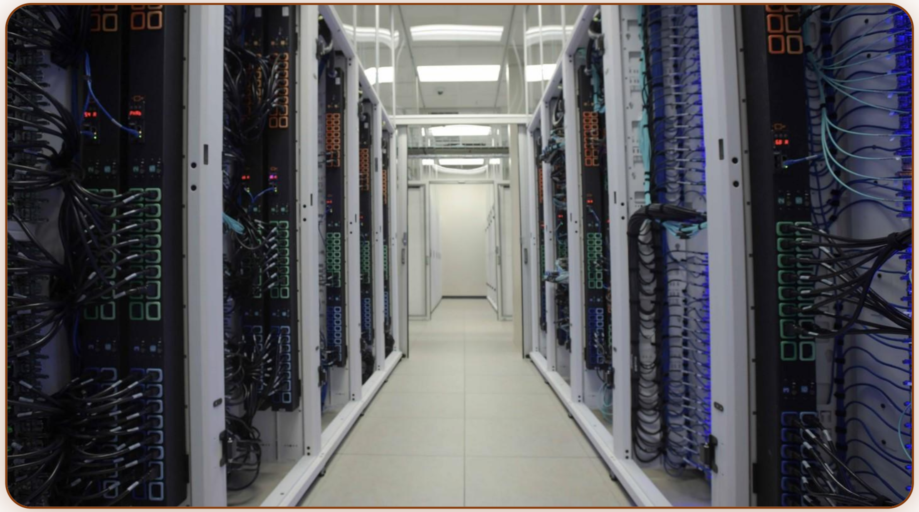
Grace Hardware

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

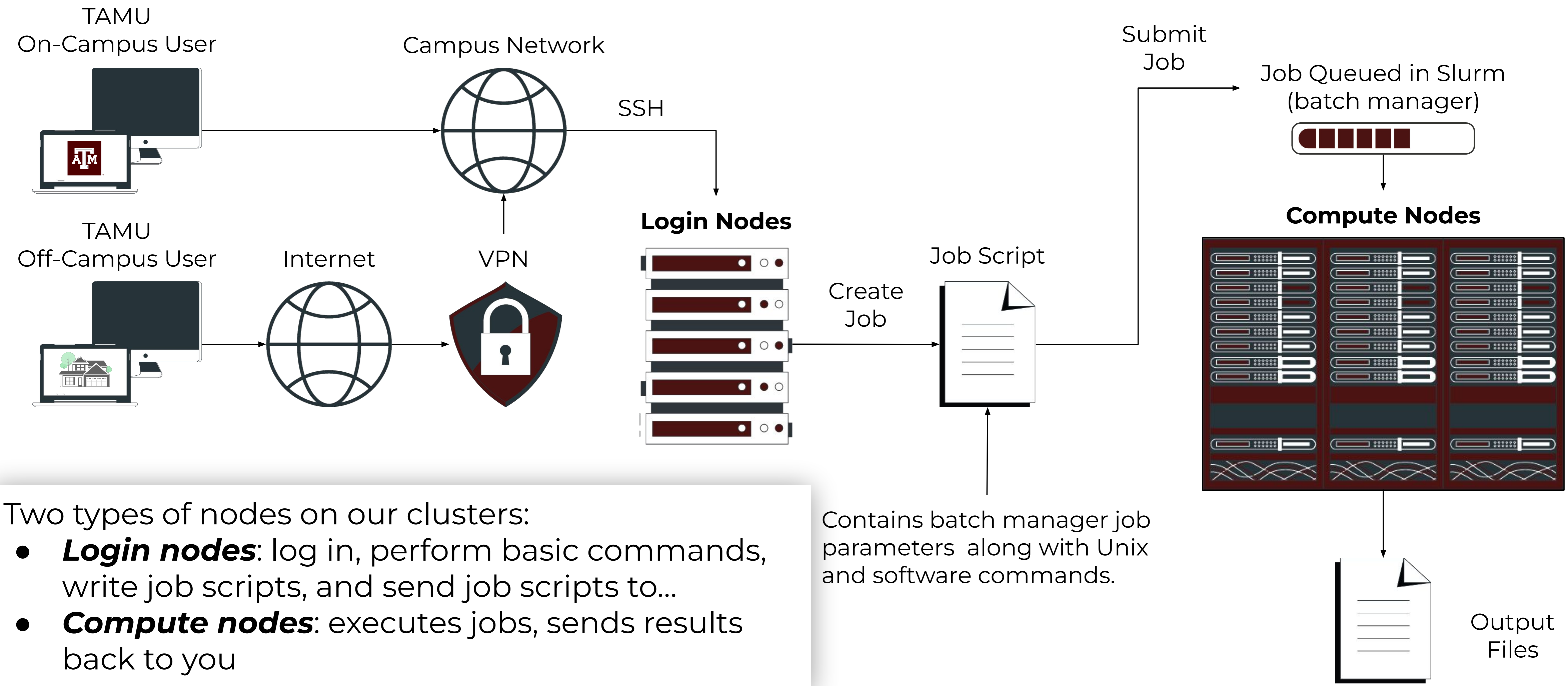
3TB Large Memory-80 cores/node
Login Nodes: 10 GbE TAMU network connection

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]

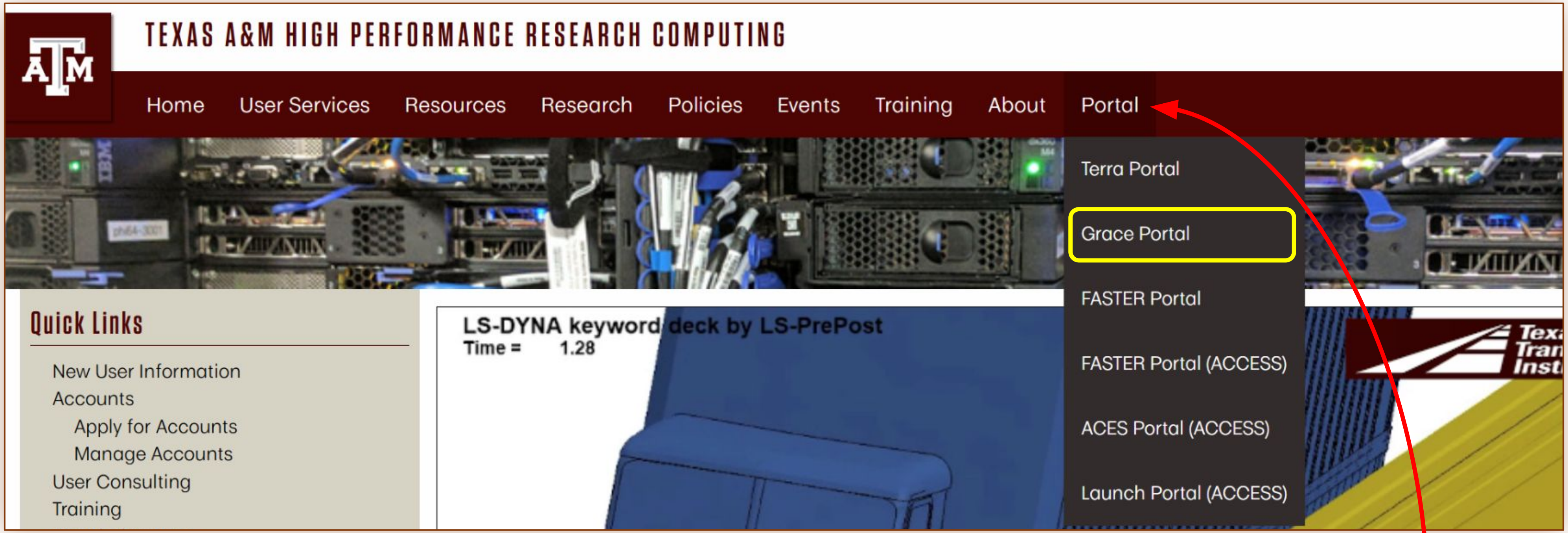
Computing on HPRC Clusters



Two types of nodes on our clusters:

- ***Login nodes***: log in, perform basic commands, write job scripts, and send job scripts to…
- ***Compute nodes***: executes jobs, sends results back to you

Accessing Grace via the Portal



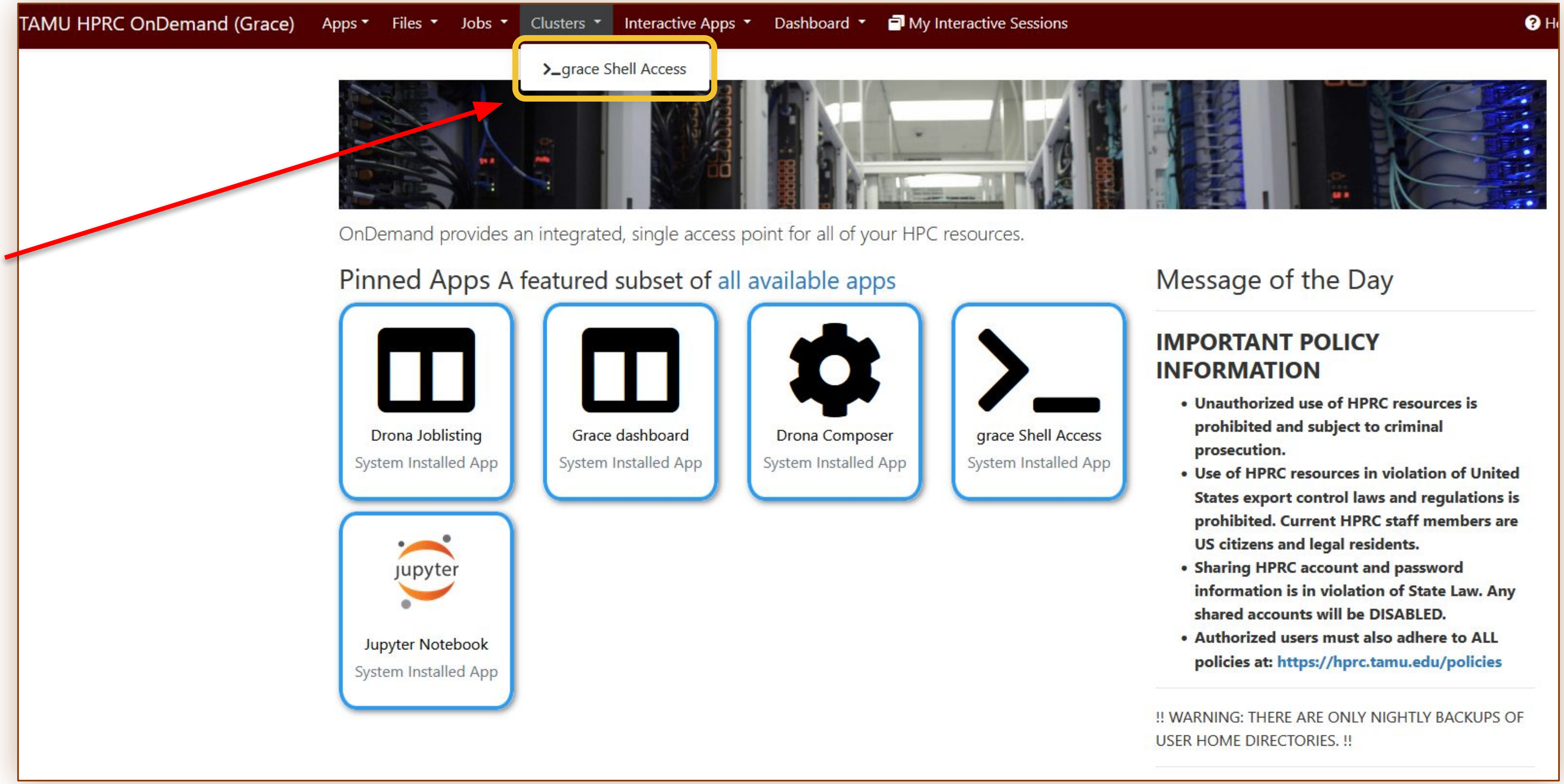
Access the HPRC portals through most web browsers:

1. Go to portal.hprc.tamu.edu or use the Portal dropdown menu on the HPRC homepage: TAMU HPRC
2. Choose **Grace Portal**

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

Accessing Grace via the Portal

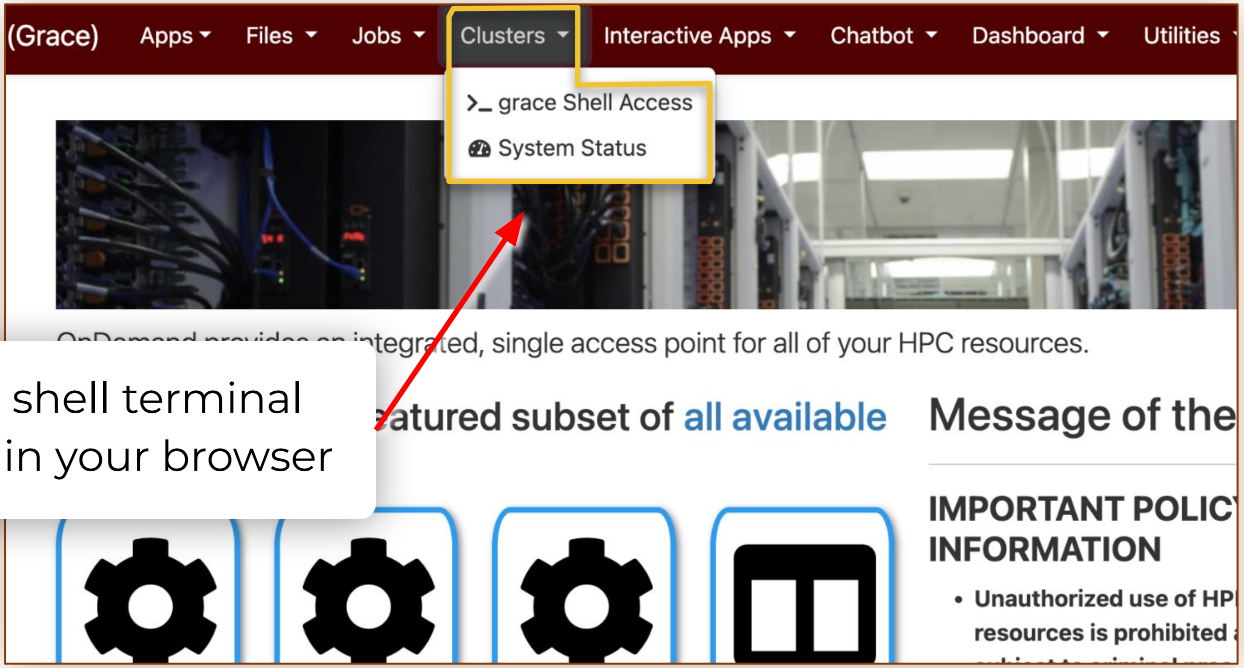
Select at the top: “Clusters” → “_grace Shell* Access”



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

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

Shell Access via the Portal



Get a shell terminal right in your browser

Copying Training Materials to $SCRATCH

Login to Grace terminal and once you are there:

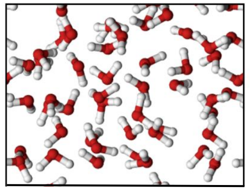
1. Copy “MD_LAMMPS” containing training materials from /scratch/training

```
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 $F = ma$

$t \leq t_{max}$

yes

no

Output values of interest

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?

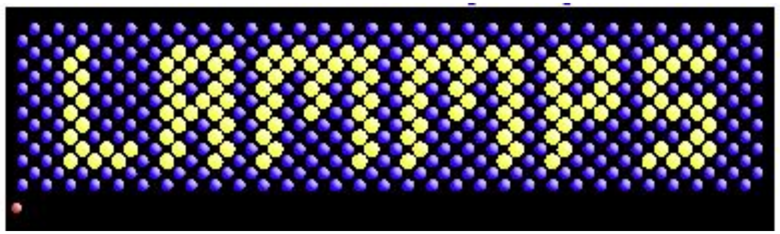
- Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
    - *"LAMMPS is a classical molecular dynamics (MD) code that models ensembles of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, solid-state (metals, ceramics, oxides), granular, coarse-grained, 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 parallely on large numbers of CPUs and GPUs

- Documentation: LAMMPS documentation

LAMMPS Molecular Dynamics Simulator



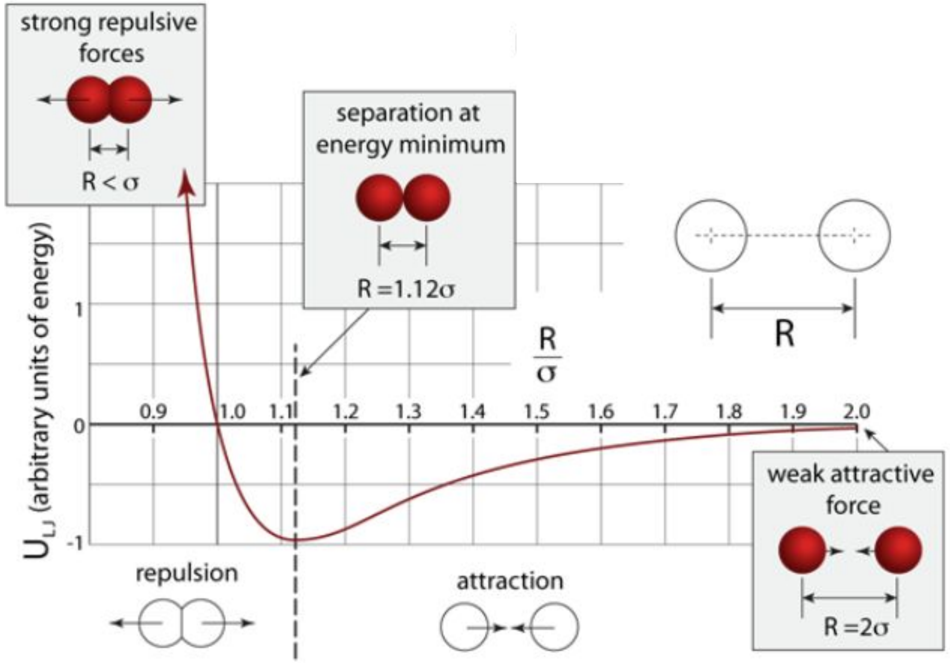
Lab 1: Lennard Jones (LJ) (Coarse-grained)

- 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

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

[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
```

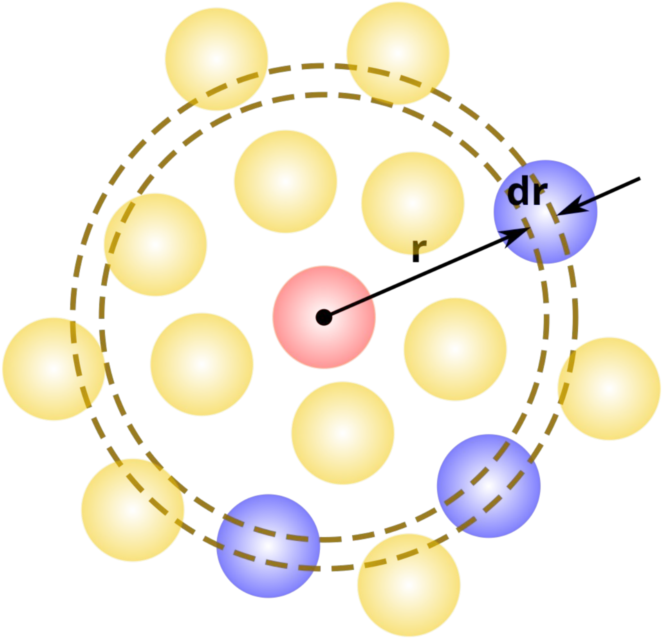
- Submit the job.

```
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

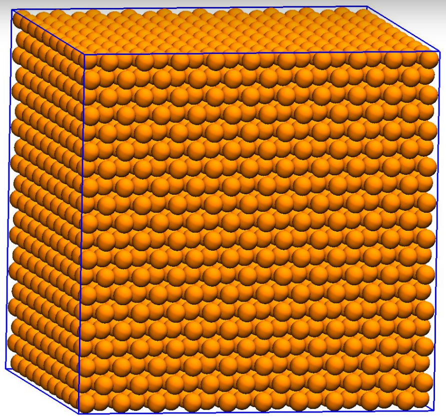
1. Compute system density ρ and confirm that the value is 0.85, which we defined in the input script → Hint: ρ = number of atoms/volume

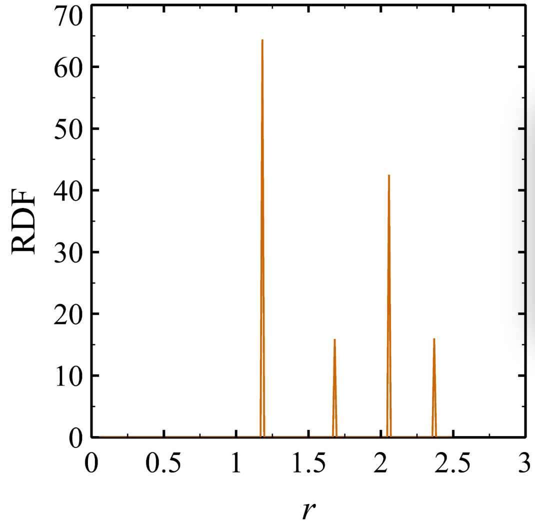
2. Visualize the output trajectory 'traj.lj.dump' using VMD (Visual Molecular Dynamics) → Hint: Load through Interactive Apps as shown in the morning session

3. Plot the RDF outputs 'rdf_initial.txt' and 'rdf_lastHalf.txt'. Based on the two RDF plots, <u>what would you call the structure of initial system configuration ('rdf_initial.txt') and final structure configuration ('rdf_lastHalf.txt')?</u>

Solution: Interpreting Structure Via RDF

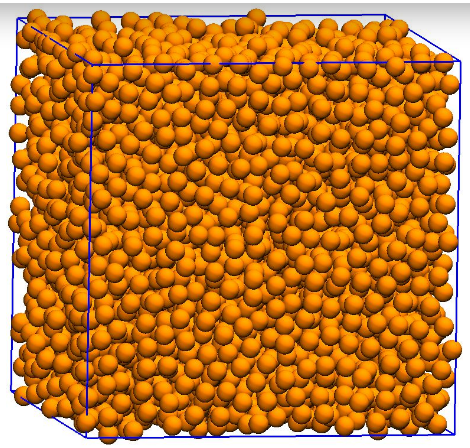
Initial configuration

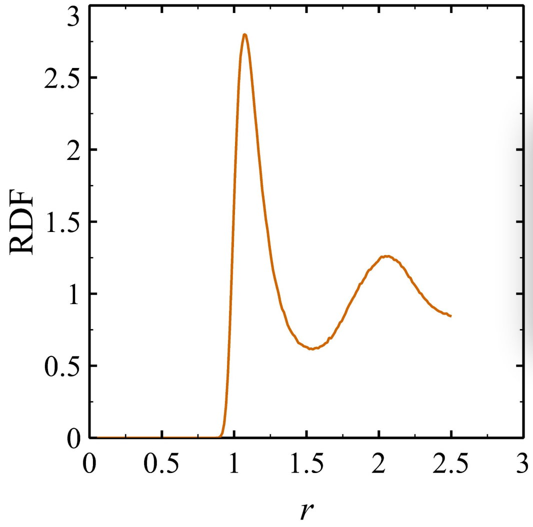




what does it represent: crystal?, liquid?

Final configuration

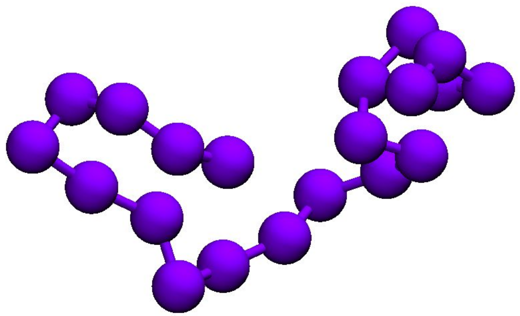




what does it represent: crystal?, liquid?

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

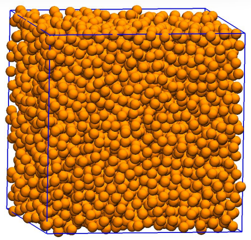
1. Visualize the output trajectory ‘traj.lj_polymer.dump’ using VMD (Visual Molecular Dynamics) → Hint: Load through Interactive Apps as shown in the morning session.

2. Plot the RDF outputs ‘rdf_lastHalf.txt’ from pure LJ simulation and LJ polymer melt simulation on the same plot. <u>What is the difference when you compare the RDFs from pure LJ system and LJ polymer melt?</u>

3. Plot the MSD outputs ‘msd_lastHalf.txt’ from pure LJ simulation and LJ polymer melt simulation on the same plot. <u>What do you infer from the two MSD curves?</u>

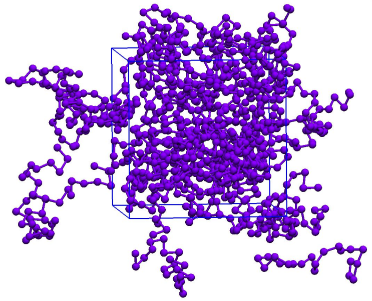
Solution: Interpreting RDFs & MSDs

Pure LJ

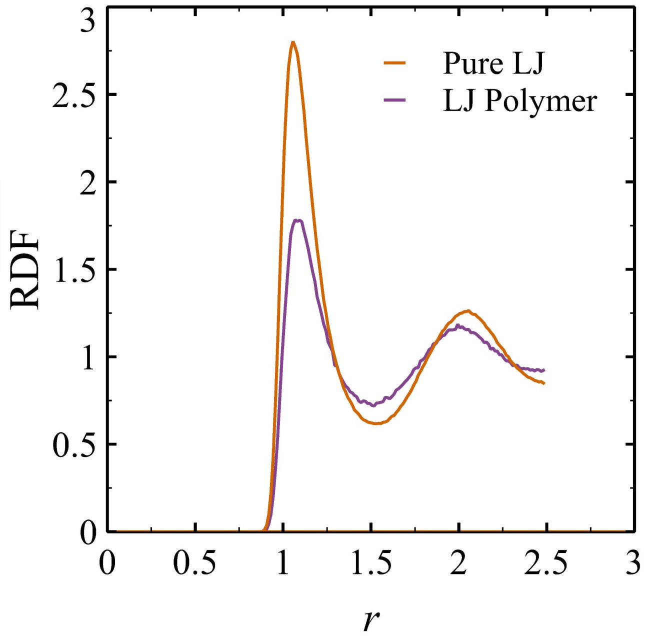


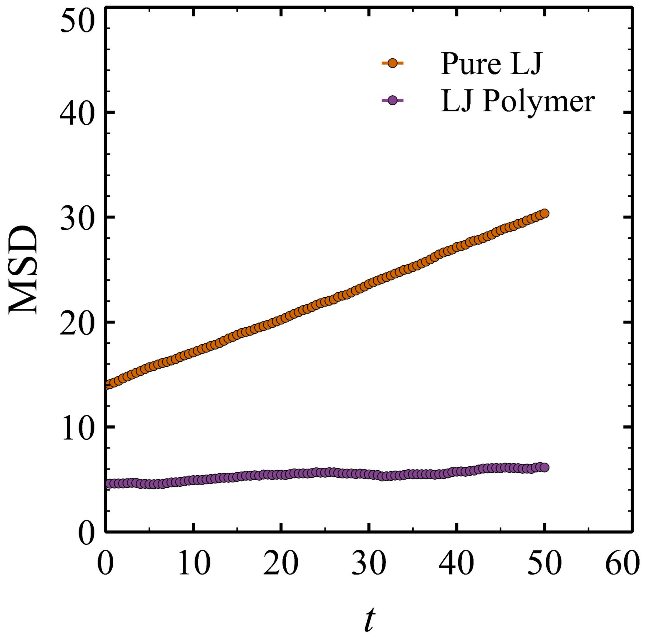
introducing bonded interactions

LJ polymer



RDF

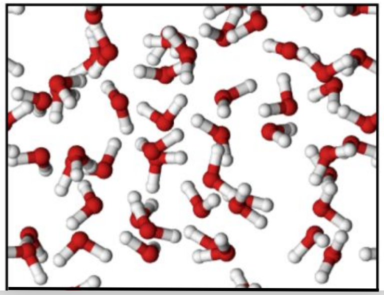




MSD

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

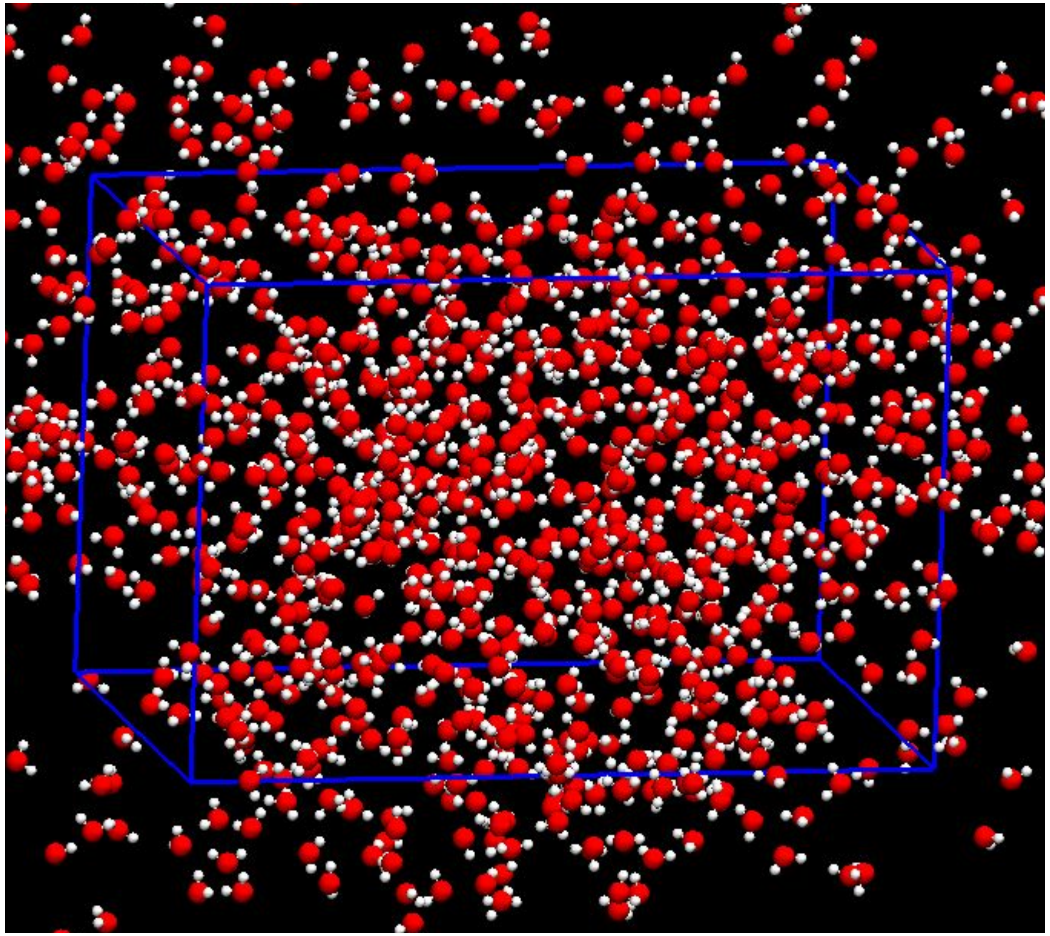
1. Before submitting the job, fix the input script ‘water_tip3p.in’ to compute average density of water after the run (Hint: Use fix ave/time).
    a. <u>Are you getting the correct density of water?</u>

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.

$$HO(CH2CH2O)_{n=20}H$$

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

CHARMM-GUI

CHARMM-GUI
Effective Simulation Input Generator and More

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: H- [PEO 20] 1 -OH Add monomer unit

Next Step:
Build Polymer Chains

CHARMM-GUI: System Size

System Size Determination Options

1. Box Type: Cubic

Length of XYZ: 50 (Å)

Solvation Options:

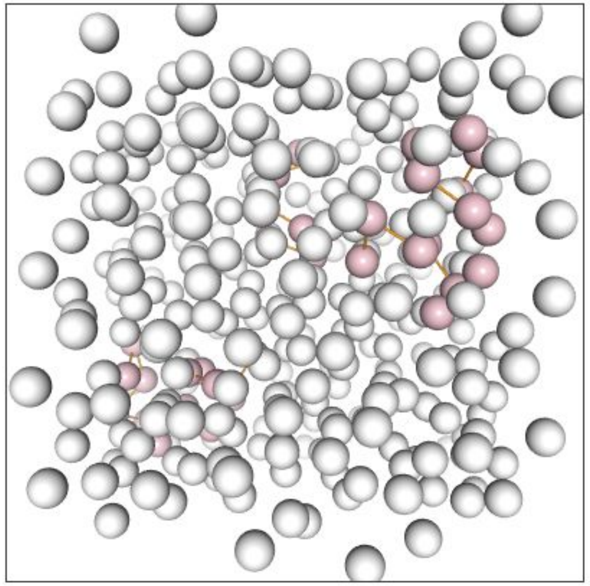
Select type of the solvent in PBC box.

Solvent water

show system size info 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:

PA

Bead	#Bead per Chain	Sequence	σ
PA	7/7	$ETHOX_{2.9}$	6 Å
SOLV	1	TIP3	6 Å

3. Interaction Matrix: Δδ ?

(unit of ε: Kcal/mol, unit of Δδ:$MPa^{1/2}$)

	PA	SOLV
PA	0	4.46
SOLV	4.46	0

4. ☑ **Equilibration by OpenMM:** ?

Nonbonded interaction:

◉ Weeks-Chandler-Andersen (WCA) Potential [set default]

poor good (solvent)

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

Running steps are ...

1) ☐ Equilibration with WCA potential

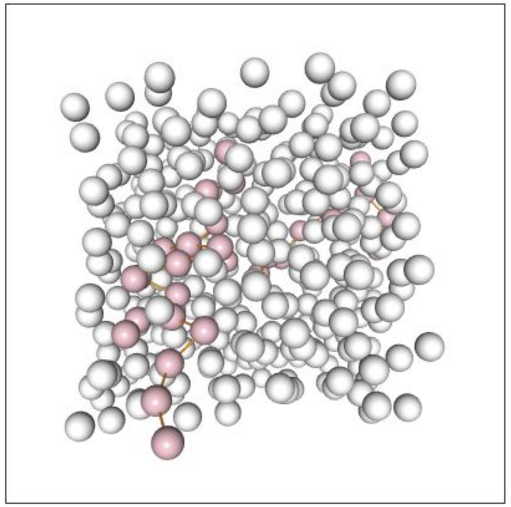
2) ☑ Equilibration with LJ potential

[show estimation] click this once you change below.

Temperature: 300.0 K (Reduced Temperature:0.61)

Simulation time: 10 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:

PA

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    IMPRopers
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
- [x] LAMMPS

Equilibration Input Generation Options:

(●) NVT ensemble

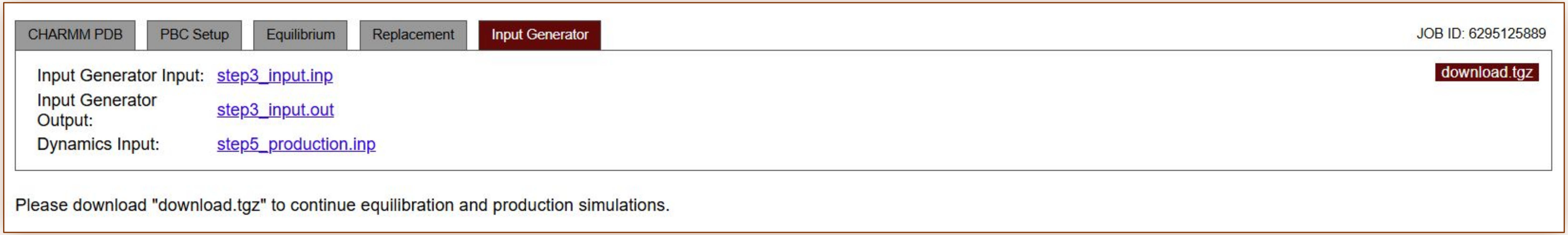
Temperature: 300.0 K

Dynamics Input Generation Options:

( ) NVT ensemble

(●) NPT ensemble

CHARMM-GUI: Download Files for Simulation



- To unzip .tgz file on the terminal:

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

- Then,

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

Minimization, Equilibration, and Production

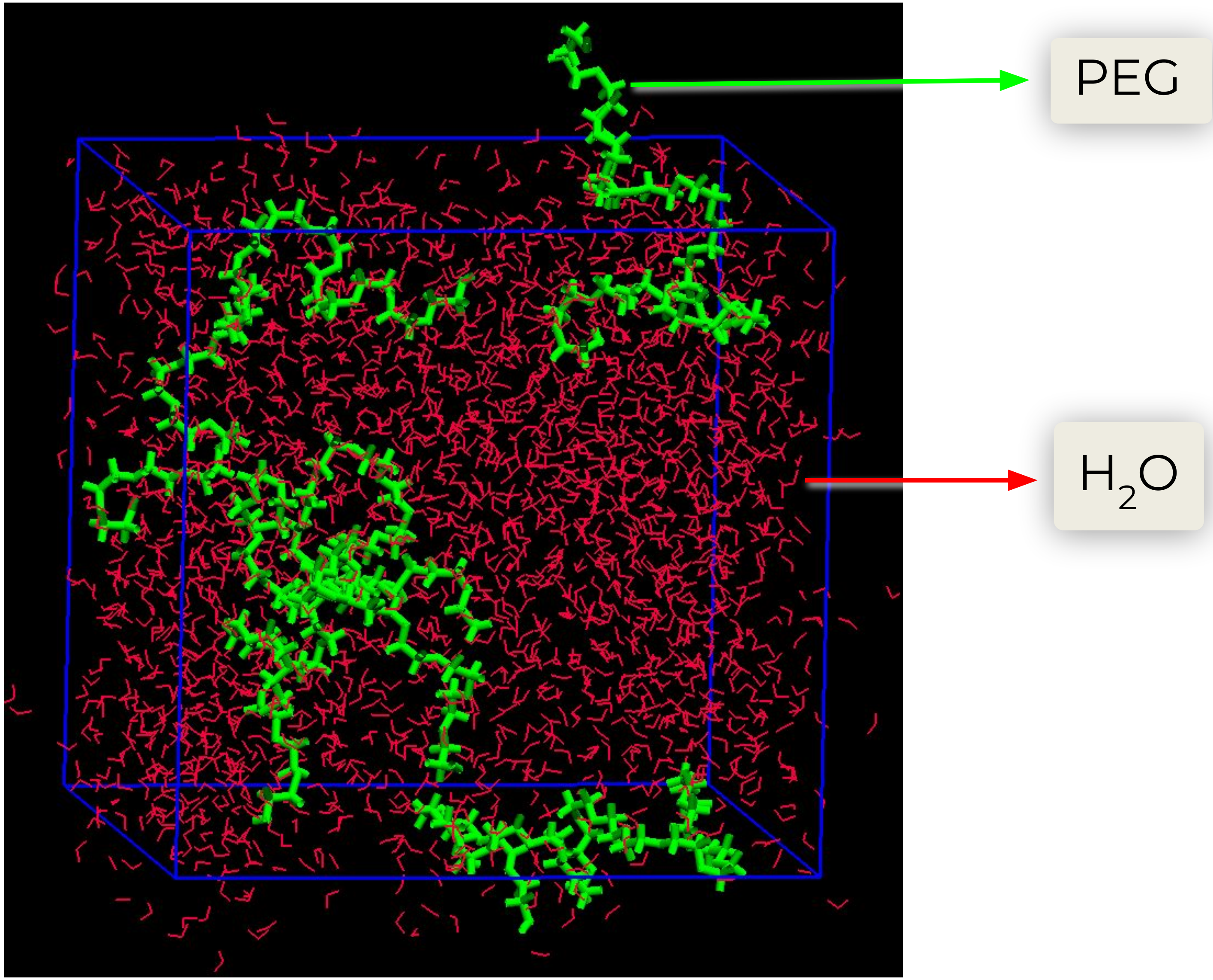
- Let’s inspect the input & data files before running the PEG in water simulation.
  - ‘step4.0_minimization.inp’ → input file for structure minimization
  - ‘step4.1_equilibration.inp’ → input file for structure equilibration
  - ‘step5_production.inp’ → input file for structure production
  - ‘step3_input.data’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

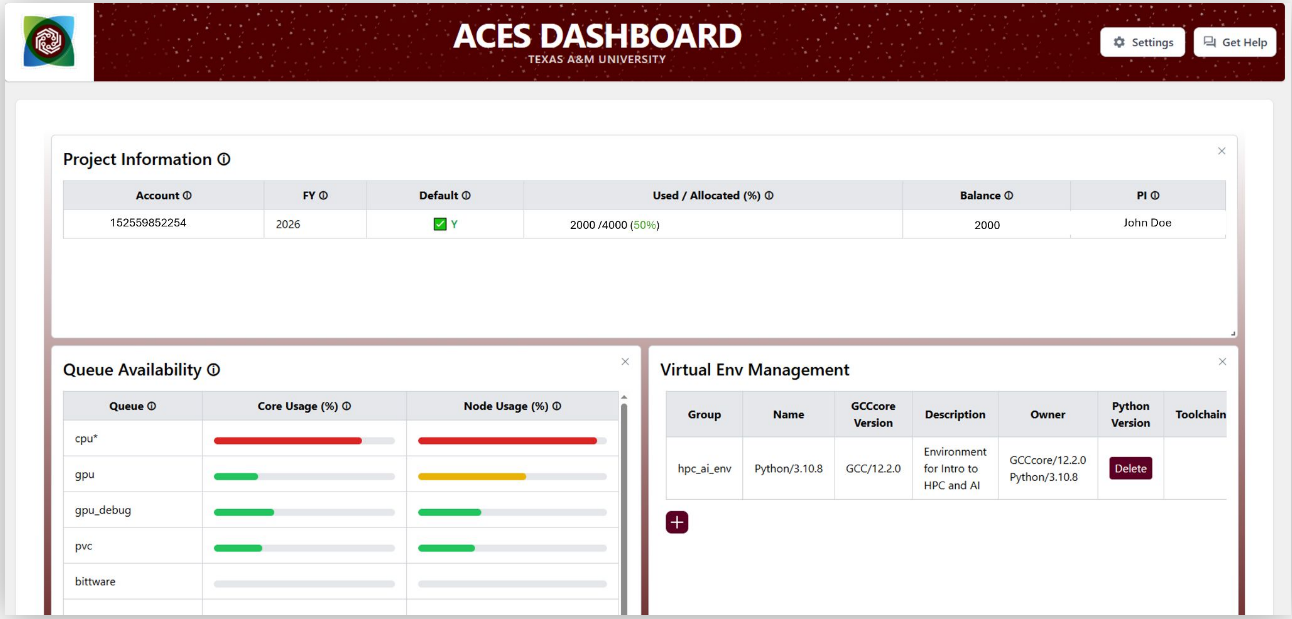
Solution: Visualizing Polymer in Water

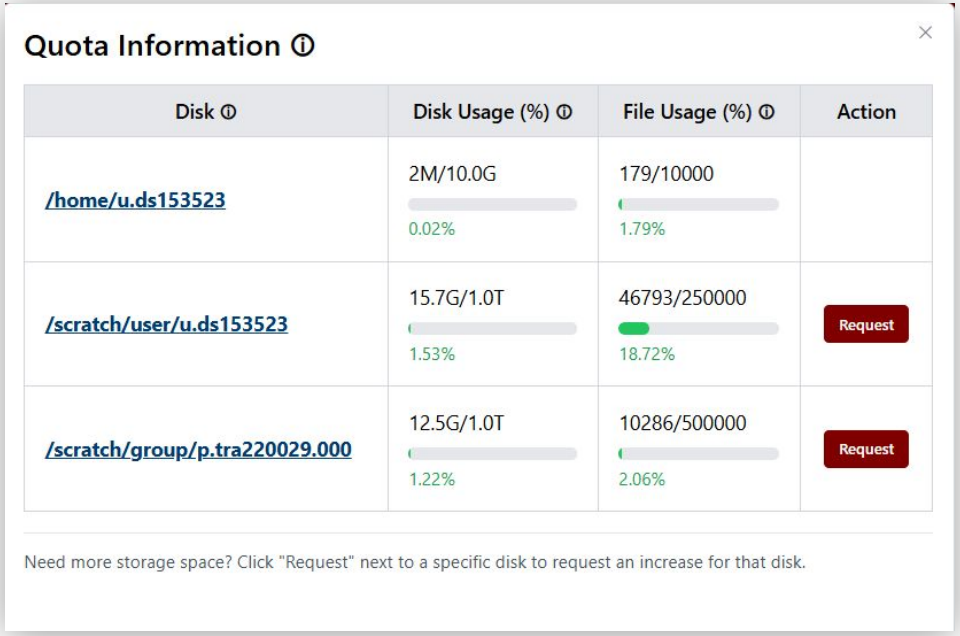


Need Help?

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





Remember the Dashboard!

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Thank you

Questions?

Give us feedback on the class with this survey:
https://u.tamu.edu/hprc_shortcourse_survey

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HPRC Survey