

LAMMPS Molecular Dynamics

ACES Workshop 2025



Richard Lawrence
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Outline

1. Learning Resources
2. LAMMPS Molecular Dynamics
3. Molecular Systems for Benchmarking
4. Using GPUs on ACES
 - a. NVIDIA H100
 - b. Intel GPU Max 1100 “PVC”
5. Discussion



Learning Resources

These Slides

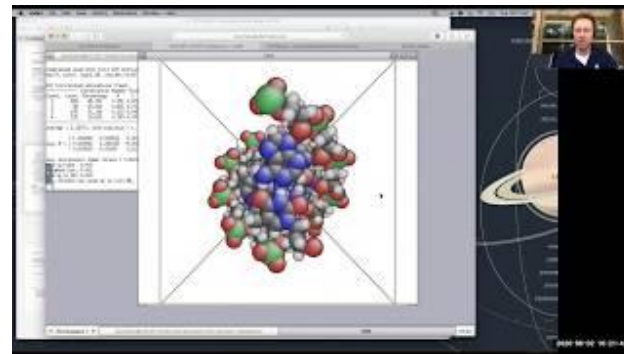
https://hprc.tamu.edu/aces/aces_workshop_2025.html

TAMU HPRC Knowledge Base

<https://hprc.tamu.edu/kb/Software/LAMMPS/>

TAMU HPRC on YouTube

<https://youtu.be/N2GMp3fHi-M>



LAMMPS Molecular Dynamics

- LAMMPS supports MPI, CUDA, OpenCL, and Kokkos
- General MD equation
 - $E = \text{LJ (collisions)} + \text{EM (long range)} + \text{Bonding (neighbors)}$
- Benchmarks
 - LJ only
 - $\text{EAM} = \text{LJ} + \text{EM}$
 - Rhodopsin = LJ + EM + Bonding



LAMMPS Syntax

- Command line use:

```
mpirun -np N lmp -in <filename> -var <extra var> -log <filename>
```

- Launcher `mpirun -np N` coordinates N processes
- Executable `lmp` may be named like `lmp_<platform>`
- Argument `-in` reads LAMMPS commands from file
- Argument `-var` sets extra variables defined by input file
- Argument `-log` sets a path to save a copy of stdout

- Important LAMMPS commands

- `pair_style` sets which forces will be applied
- `fix` sets constraints (such energy, temperature, pressure)
- `run` simulates a number of time steps



LAMMPS Benchmark System 1

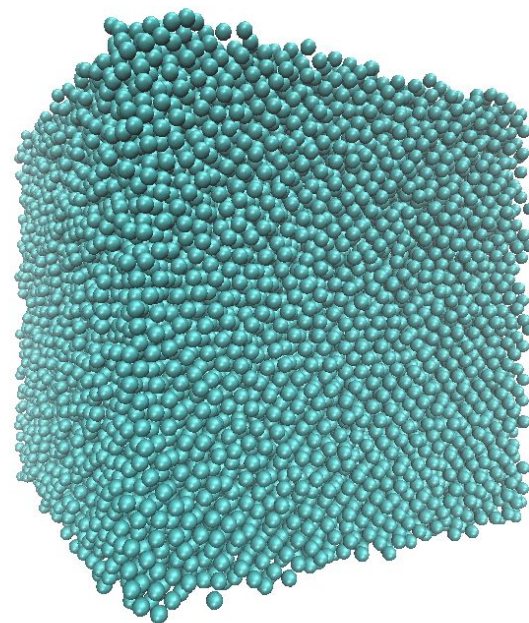
Files: in.lj

Lennard-Jones (LJ) system is an unordered liquid of atoms

Interaction is collisions only

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad r < r_c$$

- ϵ (energy units)
- σ (distance units)
- r_c cutoff (distance units)



- https://docs.lammps.org/pair_lj.html

LAMMPS Benchmark System 2

Files: `in.eam` `Cu_u3.eam`

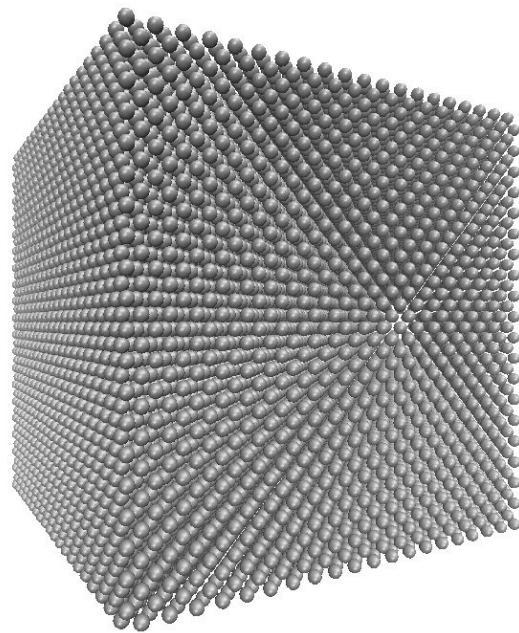
Embedded Atom Model (EAM) system is a lattice of metal atoms

Can be solid or liquid depending on temperature

Includes collisions and electrostatics

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

- https://docs.lammps.org/pair_eam.html
- Foiles et al, Phys Rev B, 33, 7983 (1986)

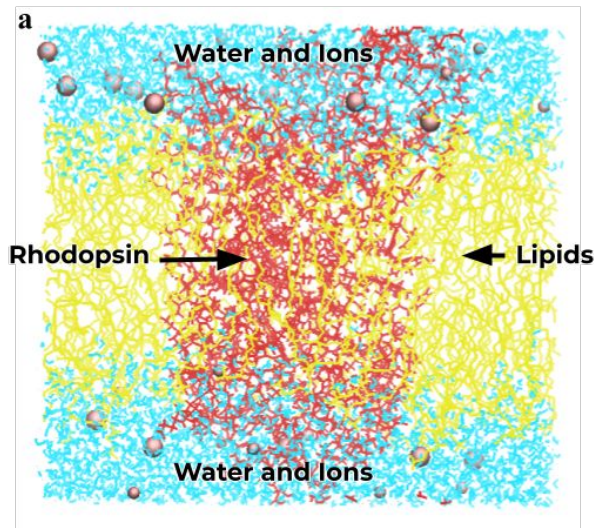


LAMMPS Benchmark System 3

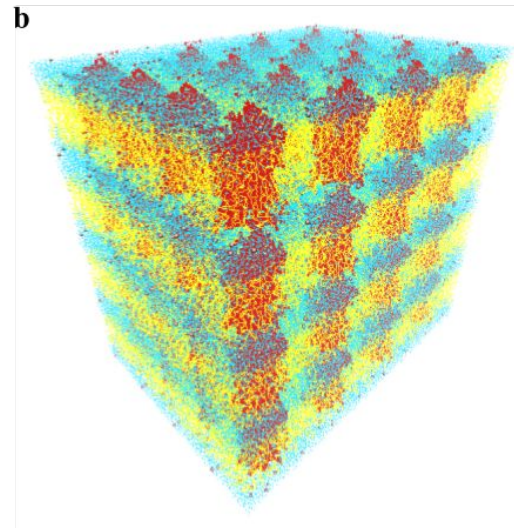
Files: data.rhodo
in.rhodo.extended

Rhodopsin system is a large protein molecule embedded in a solvated lipid bilayer

Includes collisions, electrostatics, and **bonding**



a. Single



b. Replicated 4x4x4

- <https://www.lammps.org/bench.html#rhodo>
- <https://doi.org/10.1145/3569951.3597556>

LAMMPS Software Modules on ACES

- How to choose a module

```
module spider LAMMPS
```

For Intel GPU

```
LAMMPS/patch_19Nov2024-intel-kokkos
```

```
...
```

universal interface

```
LAMMPS/29Aug2024_update2-kokkos-CUDA-12.4.1
```

```
...
```

LAMMPS version

For NVIDIA GPU

```
module spider LAMMPS/29Aug2024_update2-kokkos-CUDA-12.4.1
```

You will need to load all module(s) on any one of the lines below before the "LAMMPS/29Aug2024_update2-kokkos-CUDA-12.4.1" module is available to load.

GCC/13.2.0 OpenMPI/4.1.6

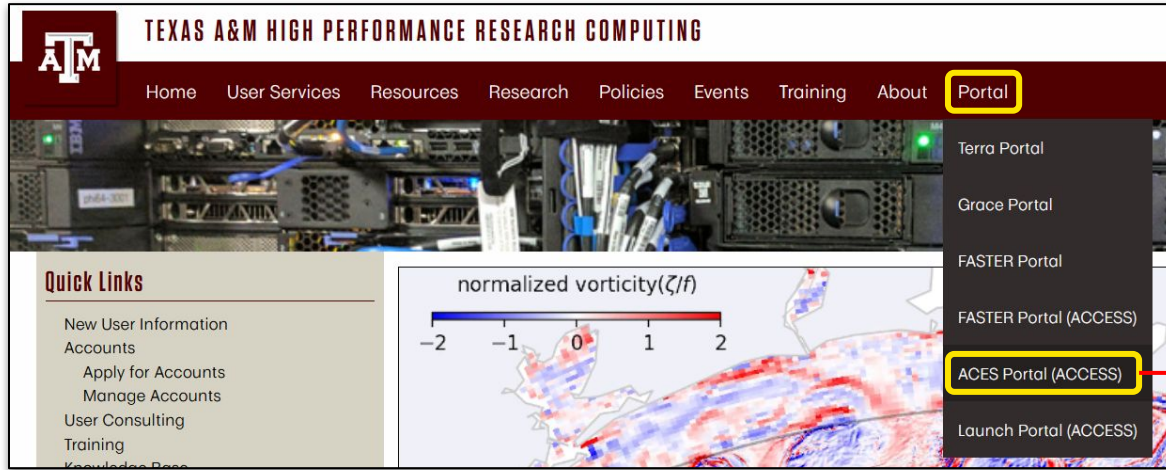
Prerequisites



Getting Started

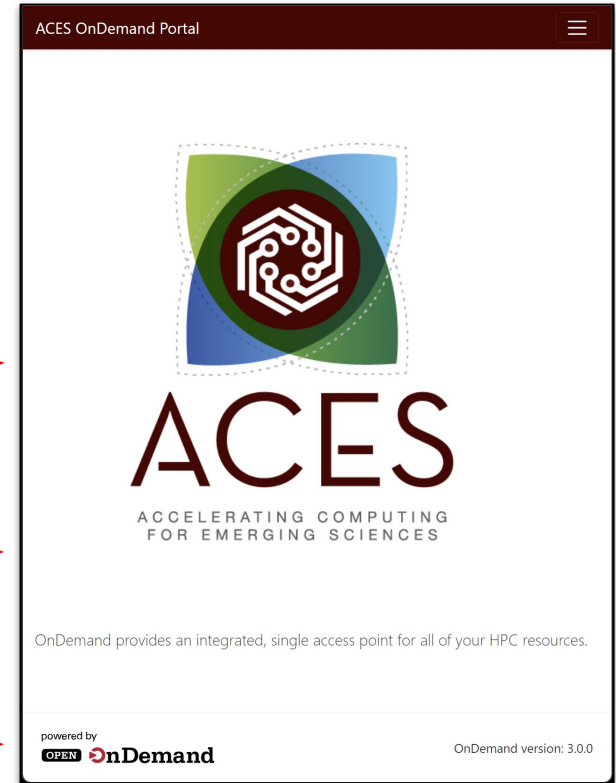


ACES Portal



ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

Open OnDemand (OOD) is an advanced web-based
graphical interface framework for HPC users



Get a Shell on ACES

Click on “Clusters” menu → _aces Shell Access



Success!

Welcome to the
ACES login node.

```
Last login: Wed Jul 10 16:37:19 2024 from 10.71.1.6
=====
|      Texas A&M University High Performance Research Computing      |
|-----|
| Website:           https://hprc.tamu.edu |
| Consulting:        help@hprc.tamu.edu (preferred) or (979) 845-0219 |
| ACES Documentation: https://hprc.tamu.edu/kb/User-Guides/ACES |
| FASTER Documentation: https://hprc.tamu.edu/kb/User-Guides/FASTER |
| Grace Documentation: https://hprc.tamu.edu/kb/User-Guides/Grace |
| Terra Documentation: https://hprc.tamu.edu/kb/User-Guides/Terra |
| 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 *
*   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 *
*   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. !!

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

To see these messages again, run the motd command.
Your current disk quotas are:
Disk                               Disk Usage    Limit    File Usage    Limit
/home/u.jw123527                   170M          10.0G      632          10000
/scratch/user/u.jw123527           36.5G         1.0T      124995       250000
/scratch/group/p.tra230003.000      4K            1.0T         1          500000
/scratch/group/p.tra220029.000      4K            1.0T         1          500000
/scratch/group/p.sta220004.000      4K            1.0T         1          500000
Type 'showquota' to view these quotas again.
[u.jw123527@aces-login3 ~]$
```



Set Up Your LAMMPS Workspace

- Activity:

```
cd $SCRATCH
cp -r /scratch/training/LAMMPS-tutorial .
cd LAMMPS-tutorial
ls
```

- Expected output:

Cu_u3.eam	lammps-h100-LJ.slurm
data.rhodo	lammps-h100-Rhodo.slurm
in.eam	lammps-pvc-EAM.slurm
in.lj	lammps-pvc-LJ.slurm
in.rhodo.extended	lammps-pvc-Rhodo.slurm
lammps-h100-EAM.slurm	



LAMMPS on NVIDIA H100 with Kokkos

Files: lammmps-h100-*.slurm

```
#SBATCH --gres=gpu:h100:1  
#SBATCH --partition=gpu
```

1 H100 from Slurm

```
module load GCC/13.2.0 OpenMPI/4.1.6
```

```
module load LAMMPS/29Aug2024_update2-kokkos-CUDA-12.4.1
```

```
lmp -k on g 1 -sf kk
```

CUDA with kokkos package



NVIDIA H100 Exercises

- Collect Data

```
sbatch lammops-h100-EAM.slurm  
sbatch lammops-h100-LJ.slurm  
sbatch lammops-h100-Rhodo.slurm
```

**Following along live? add
--reservation=workshop**

- Monitor

```
squeue --me  
watch ssh <node> nvidia-smi  
(ctrl+c when done)
```



LAMMPS on Intel PVC

Files: `lammops-pvc-*.slurm`

`#SBATCH --gres=gpu:pvc:1`

1 PVC from Slurm

`#SBATCH --partition=pvc`

`#SBATCH --exclusive`

These jobs don't get along

`module load patch_19Nov2024-intel-kokkos`

`lmp -k on g 1 -sf kk`

SYCL with kokkos package



Intel PVC Exercises

- Collect Data

```
sbatch lammops-pvc-EAM.slurm  
sbatch lammops-pvc-LJ.slurm  
sbatch lammops-pvc-Rhodo.slurm
```

**Following along live? add
--reservation=workshop**

- Monitor

```
squeue --me  
ssh <node> xpumcli dump -m 0  
(ctrl+c when done)
```



Discussion

- Compare Performance and Timing

```
sed -n '/lmp/p;/Performance:/p;/MPI task timing/,/^$/p' job.*
```



Texas A&M at PEARC25

Tutorials and Workshop	Date/Time	Room
Tutorial: ACES Tutorial for using Graphcore Intelligence Processing Units (IPUs) for AI/ML Workflows	Mon, July 21, 2025 1:30 PM-5:00 PM ET	Room A213
Tutorial: Open OnDemand Overview, Customization, and App Development	Mon, July 21, 2025 1:30 AM-5:00 PM ET	Room A226
Workshop: Collaborating with K12 Schools: Supporting Secondary Students and Teachers in Computing	Mon, July 21, 2025 1:30 PM-5:00 PM ET	Room B132



Texas A&M at PEARC25

Presentations and BoF	Date/Time	Room
WFT&E-2-3: ByteBoost: An advanced cybertraining program designed to enhance research on testbed systems	Tue, July 22, 2025 11:50 AM-12:05 PM ET	Room A216
A&SW-2-5: Generating Scientific Workflows With Drona Environments	Tue, July 22, 2025 12:00 PM-12:15 PM ET	Room A220-A221
WFT&E-3-2: Empowering NAIRR "Pilots" of all skill levels to become "ACES" with HPC	Tue, July 22, 2025 2:15 PM-2:30 PM ET	Room A114-A115
WFT&E-5-4: Exploring the Role of Academics, Research and Workforce Development in Establishing Research Computing Collaborations	Wed, July 23, 2025 11:55 AM-12:10 PM ET	Room A114-A115
A&SW-6-2: Comparison of GPU Performance Scaling for Molecular Dynamics <i>Don't miss my LAMMPS talk!</i>	Wed, July 23, 2025 2:15 PM-2:30 PM ET	Room A212-A213
BOF-18: Node to Joy: Finding the Right Compute Resources	Wed, July 23, 2025 4:15 PM-5:15 PM ET	Room A213-A215





High Performance
Research Computing
DIVISION OF RESEARCH

<https://u.tamu.edu/aces-survey>



Thank you

- We gratefully acknowledge support from National Science Foundation awards #2112356 (ACES), #2019129 (FASTER) and #19257614 (SWEETER)
- Please visit our talks and BoF at PEARC25
- Helpdesk: help@hprc.tamu.edu

