LAMMPS Molecular Dynamics

ACES Workshop 2025

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Outline

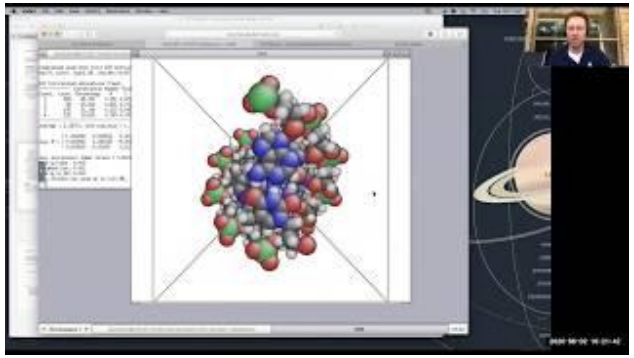
1. Learning Resources
2. LAMMPS Molecular Dynamics
3. Molecular Systems for Benchmarking
4. Using GPUs on ACES
    a. NVIDIA H100
    b. Intel GPU Max 1100 “PVC”
5. Discussion

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 = LJ (collisions) + EM (long range) + Bonding (neighbors)
- Benchmarks
  - LJ only
  - EAM = LJ + 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

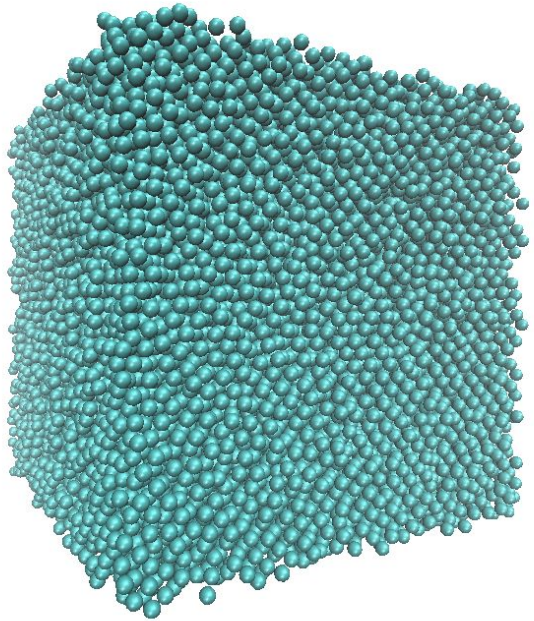
Files: `in.lj`

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

Interaction is collisions only

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

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



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

LAMMPS Benchmark System 2

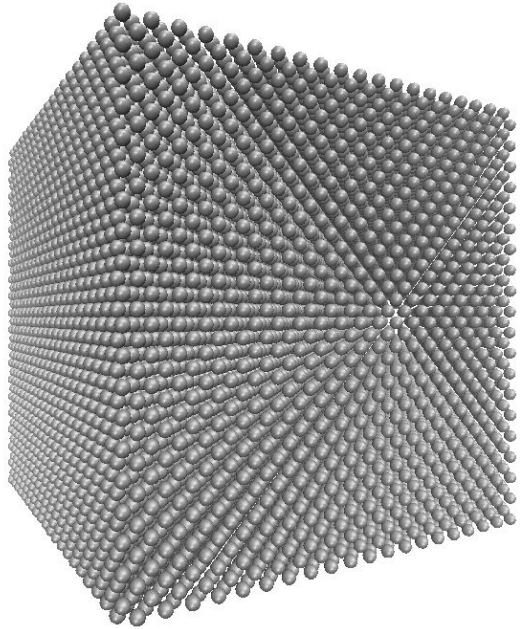
Files: `in.eam Cu_u3.eam`

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

Can be solid or liquid depending on temperature

Includes collisions and electrostatics

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



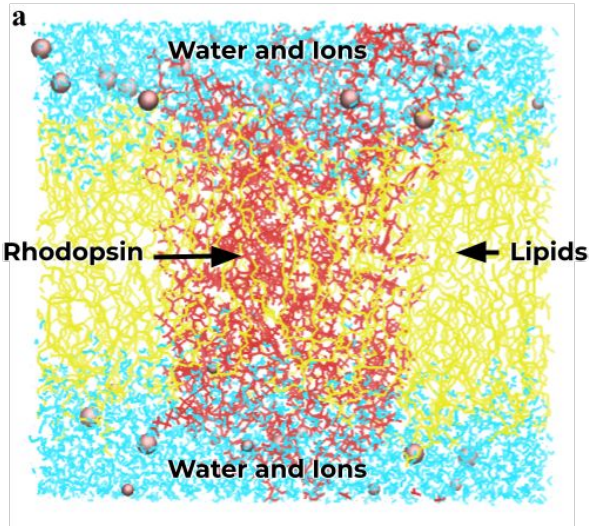
- https://docs.lammps.org/pair_eam.html
- Foiles et al, Phys Rev B, 33, 7983 (1986)

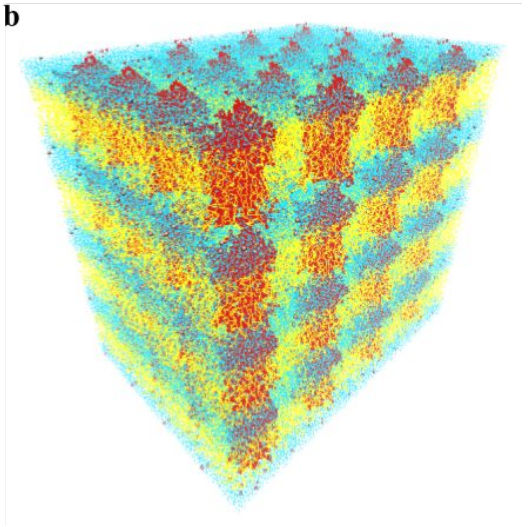
LAMMPS Benchmark System 3

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
  ...
```

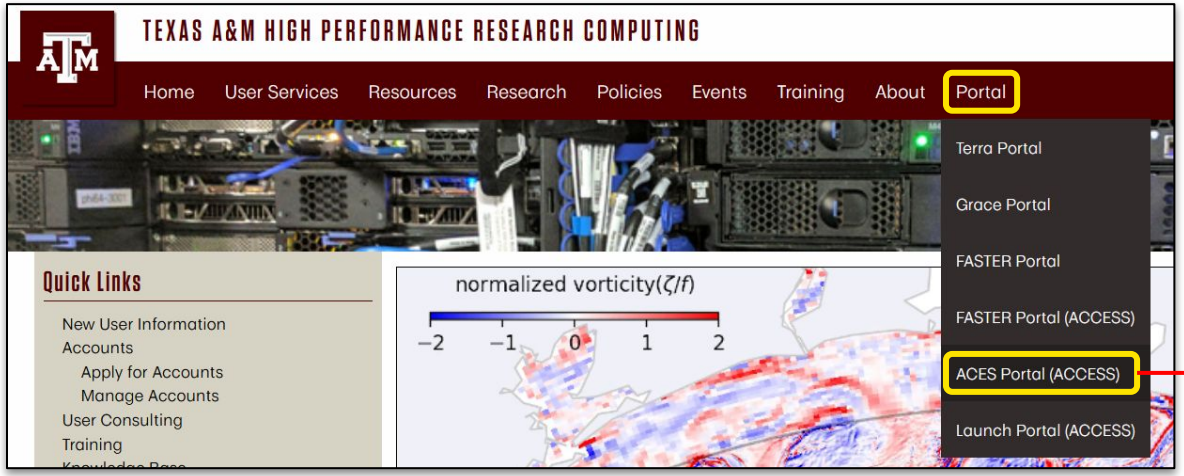
LAMMPS version For NVIDIA GPU

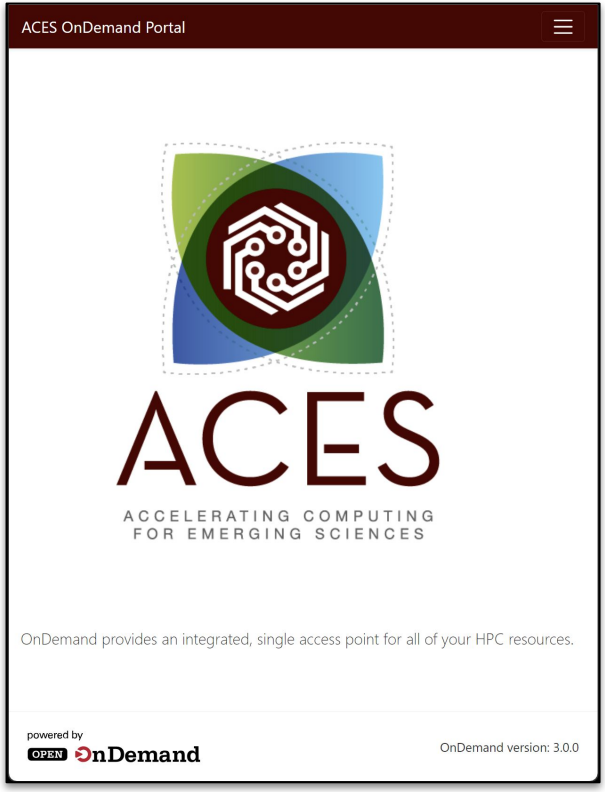
```
module spider LAMMPS/29Aug2024_update2-kokkos-CUDA-12.4.1

  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.

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: `lammps-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 lammps-h100-EAM.slurm
sbatch lammps-h100-LJ.slurm
sbatch lammps-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: `lammps-pvc-*.slurm`

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

1 PVC from Slurm

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

- Monitor

```
squeue --me
ssh <node> xpumcli dump -m 0
```

(ctrl+c when done)

Following along live? add

```
--reservation=workshop
```

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 *Don't miss my LAMMPs talk!*	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

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

High Performance
Research Computing
DIVISION OF RESEARCH

Thank you

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- Please visit our talks and BoF at PEARC25
- Helpdesk: help@hprc.tamu.edu