LAMMPS Molecular Dynamics on ACES

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Outline

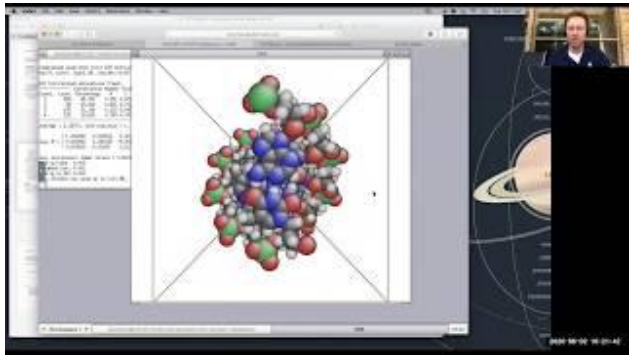
1. Learning Resources
2. LAMMPS Molecular Dynamics
3. Molecular Systems for Benchmarking
4. Using GPUs on ACES
    a. NVIDIA H100
    b. Intel GPU Max 1100 “PVC”
5. Discussion

Learning Resources

These Slides
https://hprc.tamu.edu/aces/aces_workshop_2024.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
  - LJ + EM
  - 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

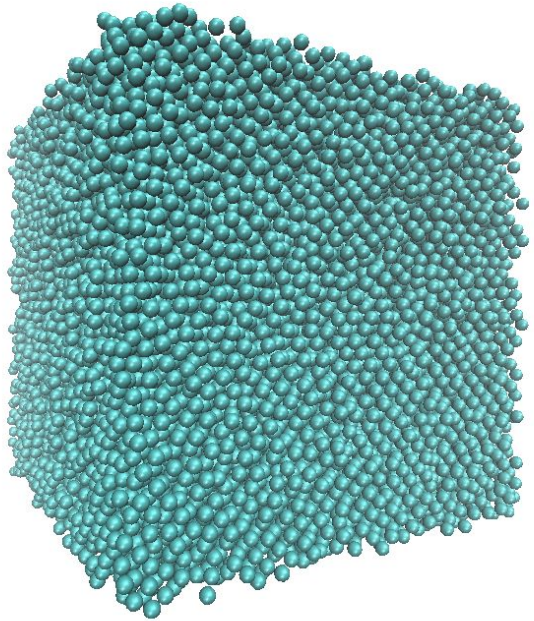
Files: `in.lj`

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

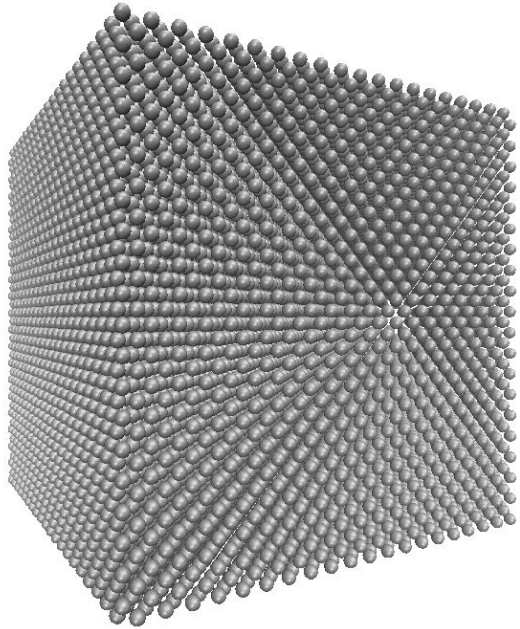
Files: `in.eam Cu_u3.eam`

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

Can be solid or liquid depending on temperature

Includes collisions and electrostatics

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



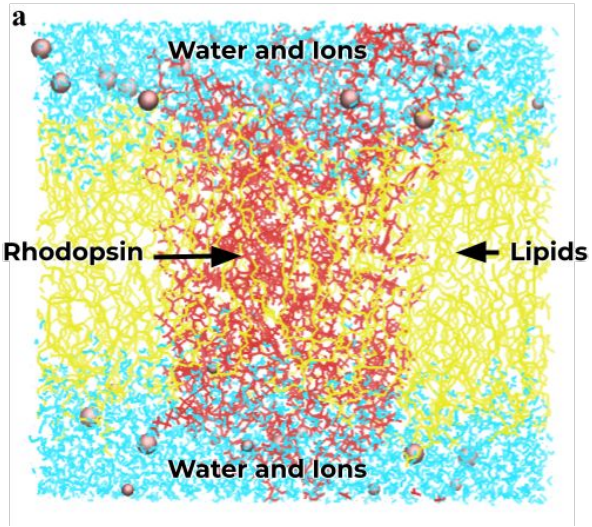
- https://docs.lammps.org/pair_eam.html
- Foiles et al, Phys Rev B, 33, 7983 (1986)

LAMMPS Benchmark System 3

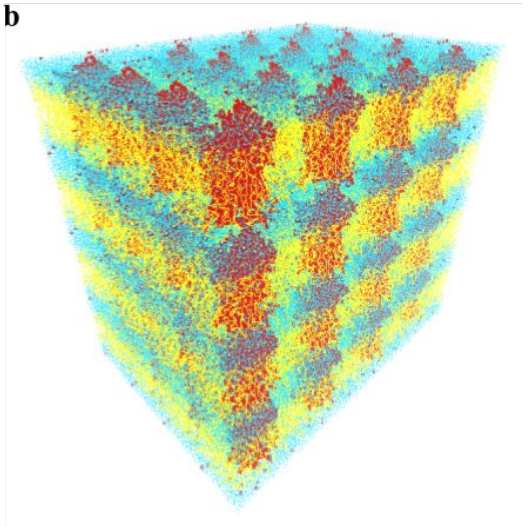
Files: `data.rhodo`
`in.rhodo.extended`

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

  LAMMPS/2Aug2023_update2-CUDA-11.8.0-sm90
  LAMMPS/2Aug2023_update2-intel-2023.07
  LAMMPS/2Aug2023_update2-kokkos-CUDA-12.1.1
  ...
```

For NVIDIA GPU

H100 specifically

LAMMPS version

For Intel GPU

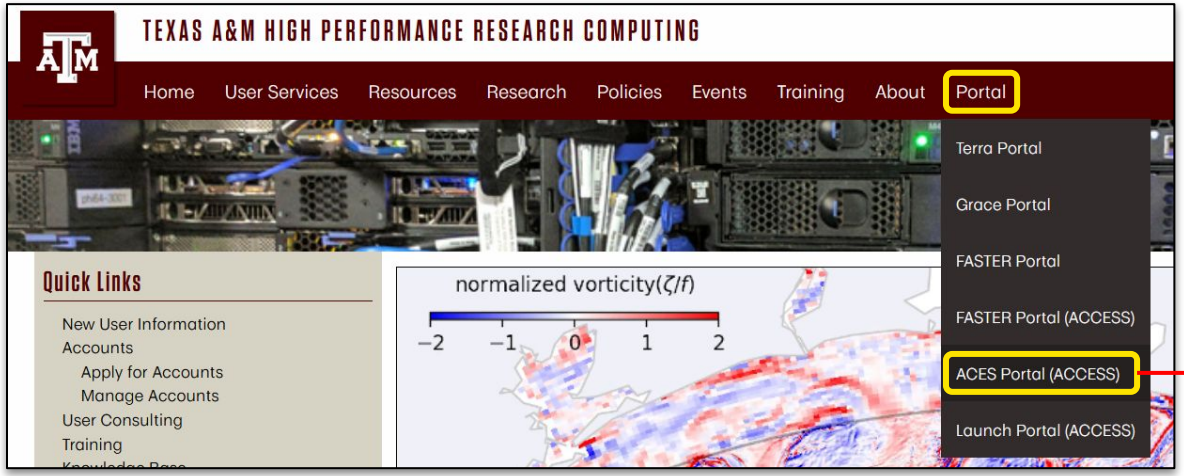
```
module spider LAMMPS/2Aug2023_update2-kokkos-CUDA-12.1.1
  You will need to load all module(s) on any one of the lines below before the
"LAMMPS/2Aug2023_update2-kokkos-CUDA-12.1.1" module is available to load.

  GCC/12.3.0  OpenMPI/4.1.5
```

Prerequisites

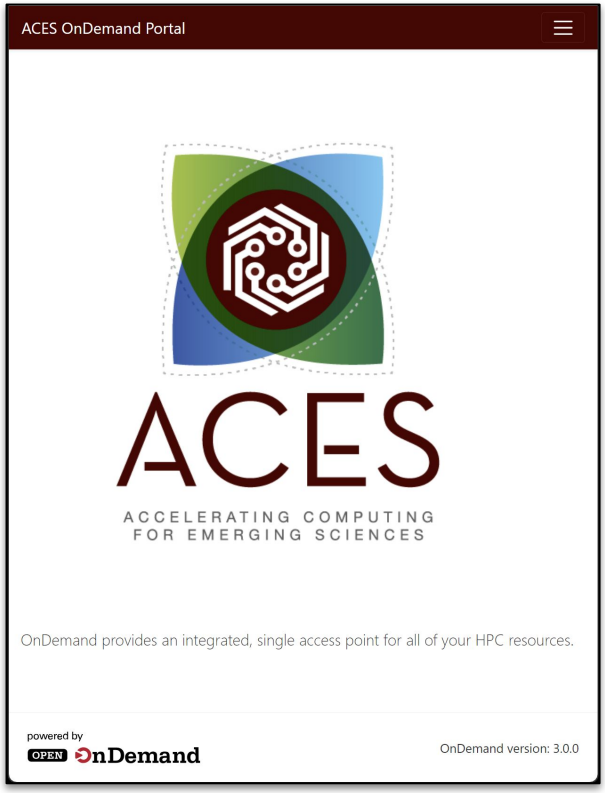
Getting Started

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/12.3.0  OpenMPI/4.1.5
module load LAMMPS/2Aug2023_update2-kokkos-CUDA-12.1.1

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

CUDA with kokkos package

NVIDIA H100 Exercises

- Collect Data

Following along live? add `--reservation=workshop_h100`

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

- 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 intel-compilers/2023.2.1  impi/2021.10.0
module load LAMMPS/3Aug2023-intel-2023.07
```

```
mpirun -np 24 lmp_oneapi -pk gpu 1 -sf gpu
```

GPU package requires cores, too

watch that executable name

OpenCL with GPU package

Intel PVC Exercises

- Collect Data

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

Following along live? add
`--reservation=workshop_pvc`

- 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 PEARC24

Talk/Event	Date/Time	Room
Tutorial: Hands-on exercises on the Intel Data Center GPU Max 1100 (PVC-GPU) for AI/ML and Molecular Dynamics Workflows on the ACES Testbed	Mon, July 22, 2024 9:00 AM-12:30 PM ET	Room 553B
Seventh Workshop on Strategies for Enhancing HPC Education and Training (SEHET24)	Mon, July 22, 2024 9:00 AM-12:30 PM ET	Room 557
Workshop: Providing cutting-edge computing testbeds to the science and engineering community	Mon, July 22, 2024 1:30 PM-5:00 PM ET	Room 554A
Workshop: Engaging Secondary Students in Computing: K12 Outreach	Mon, July 22, 2024 1:30 PM-5:00 PM ET	Room 553A
Cultivating Cyberinfrastructure Careers through Student Engagement at Texas A&M University High Performance Research Computing	Tue, July 23, 2024 11:00 AM-11:25 AM ET	Junior Ballroom
Insight Gained from Migrating a Machine Learning Model to Intelligence Processing Units	Tue, July 23, 2024 11:00 AM-11:25 AM ET	Room 551 A&B
BOF 4: What's in it for me? How can we truly democratize the research computing and data community?	Tue, July 23, 2024 1:30 PM-2:30 PM ET	Room 551 A&B

Texas A&M at PEARC24

Talk/Event	Date/Time	Room
BRICCs: Building Pathways to Research Cyberinfrastructure at Under Resourced Institutions	Tue, July 23, 2024 3:25 PM-3:50 PM ET	Junior Ballroom
Memory Bandwidth Performance across Accelerators	Tue, July 23, 2024 3:25 PM-3:50 PM ET	Ballroom B
Container Adoption in Campus High Performance Computing	Wed, July 24, 2024 11:00 AM-11:25 AM ET	Ballroom B
Engaging Secondary Students in Computing and Cybersecurity	Wed, July 24, 2024 3:15 PM-3:30 PM ET	Room 557
Exploring the Viability of Composable Architectures to Overcome Memory Limitations in High Performance Computing Workflows	Wed, July 24, 2024 3:45 PM-4:00 PM ET	Room 553 A&B
Performance of Molecular Dynamics Acceleration Strategies on Composable Cyberinfrastructure *Don't miss my LAMMPs talk!*	Wed, July 24, 2024 4:15 PM-4:30 PM ET	Room 551 A&B
BOF 17: Fantastic ACCESS Cyberinfrastructure Resources and Where to Find Them	Wed, July 24, 2024 4:45 PM-5:45 PM ET	Room 553 A&B
BOF 18: Recipes to build successful cross-institutional collaborative computing	Wed, July 24, 2024 4:45 PM-5:45 PM ET	Junior Ballroom

High Performance
Research Computing
DIVISION OF RESEARCH

Thank you

- We gratefully acknowledge support from National Science Foundation awards #2112356 (ACES)

- Please visit our talks and BoFs at PEARC24
- Helpdesk: help@hprc.tamu.edu