TEAM GENIE

LAMMPS… Not just for Moths!

HPC in the City Dallas ‘22

TEAM GENIE

‘Joba Adisa
Team Member

Hunter Marquette
Team Member

Diondre Deloatch
Team Member

Cole Mcknight
Mentor

LAMMPS…. - Not just for moths!

Goal:

To process and visualize grains flowing into a grain silo using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).

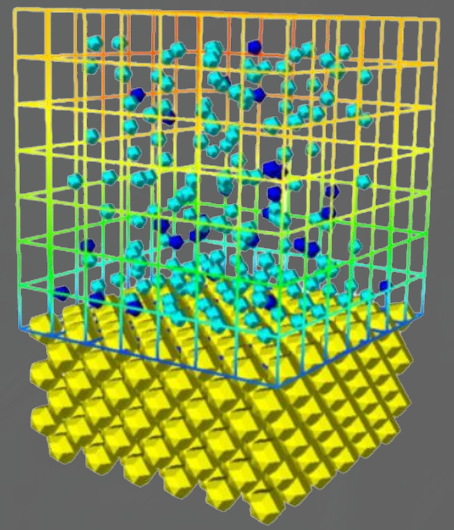


Figure 1: LAMMPS simulation showing Fluid electrolyte interacting dynamically with a solid electrode

Github:

https://github.com/hunter154321/2022HPC-Genie-LAMMPS

What is LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is an open-source molecular dynamics software that makes use of Message Passing Interface (MPI) for parallel particle simulation. LAMMPS can be used to model biomolecules, solid-state materials, and coarse grain matters. Source

For the purpose of this Hackathon, we decided to use LAMMPS to carry out a Granular Chute Flow simulation of grain particles flowing into a cylindrical silo.

Relevance to Texas

Challenge

Under certain conditions, flow of grain from the top and bottom of a silo can occur in such a way that heaps of grains are formed within the silo. With such heap, grains can rise to the top and eventually overflows through the surface.

This kind of event can lead to waste and infrastructure damage.

Source

Potential Solution

Granular modeling of grain flows in silos can help address this complicated behavior of grain particles by characterizing the approximate quantitative and qualitative conditions that allows for the rapid and smooth flow of grains in silos.

As a top ten producer of wheat crop in the US, commercial farmers and industries in Texas would find this kind of particle scale simulation useful.

Resources Utilized

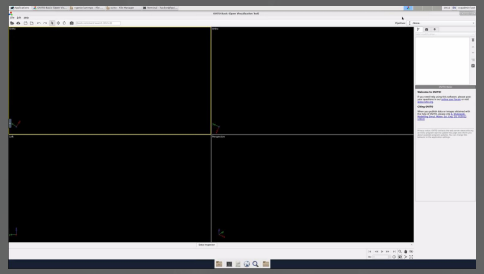
- Google Cloud (used to create custom VM)
- CloudyCluster HPC (used to submit batch HPC jobs)
- OpenOnDemand (used to create our desktop app)
- Github (used for version control of repo)
- SLURM (used to schedule batch HPC jobs)
- MPI (used to pass information between nodes)
- LAMMPS (for simulation of grain flows)
- OVITO (for visualization of LAMMPS outputs)
- Bash/CLI (used to write and run commands in the shell)

Project Timeline and Workflow

Day 1

TASKS COMPLETED

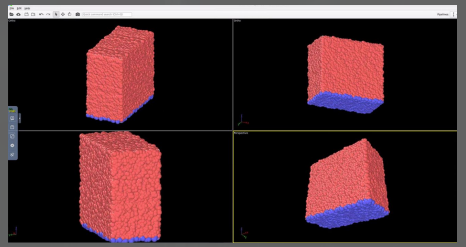
- ✓ Created VM on Google Cloud.
- ✓ Created Cloudy Cluster Image
- ✓ Installed & Run LAMMPS
- ✓ Installed OVITO



Day 2

TASKS COMPLETED

- ✓ Created a job script to run LAMMPS with MPI
- ✓ Visualization using OVITO

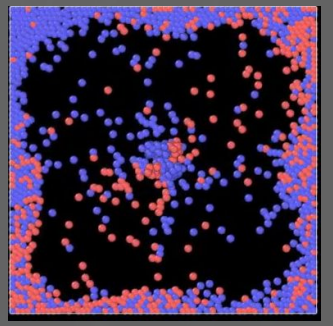


Project Timeline and Workflow

Day 3

TASKS COMPLETED

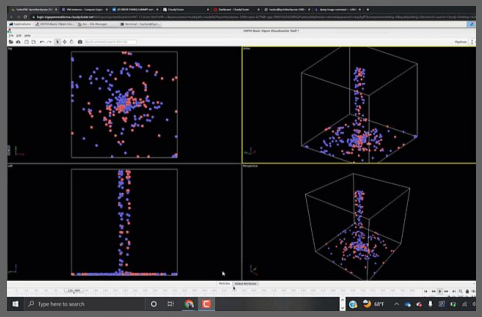
- ✓ Modify LAMMPS input file
- ✓ Switched simulations
- ✓ Visualize dumps using OVITO
- ✓ Rinse & Repeat



Day 4

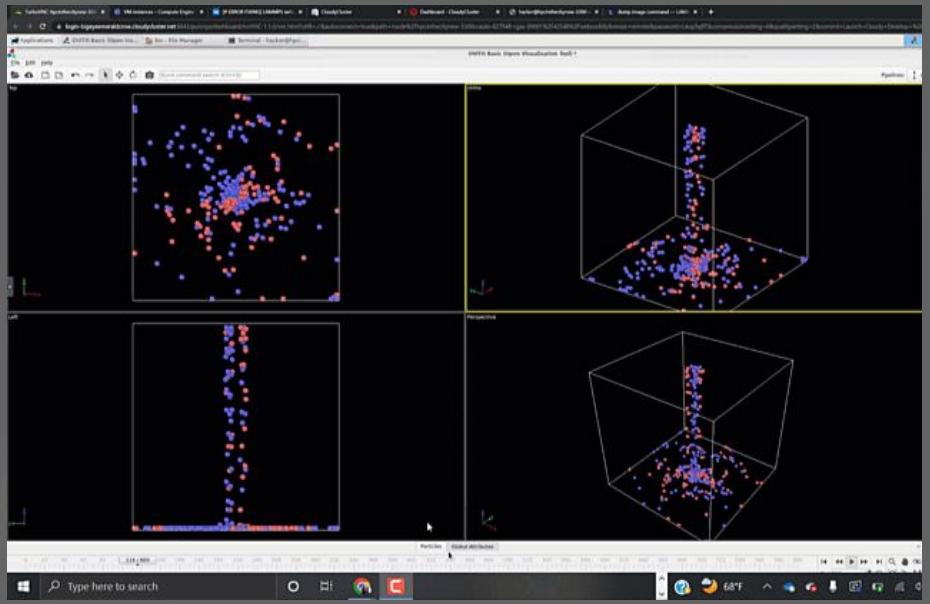
TASKS COMPLETED

- ❑ Modify model to fit cylindrical walls in a rectangular cuboid.
- ✓ Modify simulation to make spheres act look more like grain



Demo & Results

Link to Cloudy Cluster



Next Steps

Success:

We accomplished our tasks and produced something akin to grain falling into a square silo.

Challenges

We had wanted to use a cylindrical silo for our simulation but we have not been able to do that yet.

Next Steps:

- Modify model to fit cylindrical walls in a rectangular cuboid.
- Scale the simulation to more accurately model the physical properties of grains

Thank You

Sponsors and Supporters

MENTORS

Questions