

LIGGGHTS

LIGGGHTS stands for “LAMMPS Improved for General Granular and Granular Heat Transfer Simulations”. It is an open-source Discrete Element Method (DEM) particle simulation software used for modeling granular material behaviors.

The software deployed on this cluster is compiled directly from the official baseline repository hosted at [GitHub - CFDEMproject/LIGGGHTS-PUBLIC](https://github.com/CFDEMproject/LIGGGHTS-PUBLIC).

Using LIGGGHTS on the cluster

To list all installed LIGGGHTS versions, run the command `module spider liggghts`.

For example, to access the version 3.8.0 and its dependencies, load the module using:

```
module load GCC/14.3.0 OpenMPI/5.0.8 LIGGGHTS/3.8.0
```

SLURM script

The following batch script is optimized for parallel execution on the newest cluster compute nodes available via the partition `mpp.share`. Resources are defined via `--ntasks-per-node`, and the parallel execution is performed via MPI using standard input redirection (`<`).

[liggghts_parallel_job.sh](#)

```
#!/bin/bash
#SBATCH --job-name=liggghts_job
#SBATCH --output=liggghts_%j.log
#SBATCH --error=liggghts_%j.err
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=128
#SBATCH --mem-per-cpu=3500
#SBATCH --time=12:00:00
#SBATCH --partition=mpp.share
#SBATCH --mail-type=BEGIN,END,FAIL

# Load the module
module load GCC/14.3.0 OpenMPI/5.0.8 LIGGGHTS/3.8.0

# Change to simulation workspace directory
cd $SLURM_SUBMIT_DIR

# Note: Replace "input.liggghts" with your actual input file name
mpirun -np $SLURM_NTASKS liggghts < input.liggghts
```

Visualization with ParaView

Simulation data is natively written directly into VTK files, eliminating the need for separate post-processing conversion scripts (such as the legacy LPP script).

To analyze and animate your particle simulation results, one convenient option is to use the interactive **ParaView App** available directly through the cluster's [Open OnDemand web interface](#). Alternatively, you can launch the **Remote Desktop App** via Open OnDemand or connect the cluster using the [X2Go client](#), and then activate **ParaView** by loading the appropriate module inside a terminal window. Once ParaView is open, the sequential VTK file series can be loaded directly to render and color the granular particle structures.

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