Performance-Enhancement of Large-Scale DEM Simulations with a Novel Particle Contact Computation Disabling Technique

GPS Génie par la simulation
SBES Simulation - Based Engineering Science

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MOTIVATION FOR OPTIMIZATION

- DEM and unresolved CFD-DEM are useful for many engineering applications in which particle-particle collisions occur.
- Improve performance of large-scale DEM simulations.
- Dense system has a high computational cost for particle interactions.

GRANULAR MODELING THEORIES

Discrete Element Method (DEM)

Lagrangian approach where particles have translational and rotational motion obeying Newton's second law.

$$m_i \frac{d\mathbf{v_i}}{dt} = \sum_{j\in\mathcal{C}_i} (\mathbf{F}^n_{ij} + \mathbf{F}^t_{ij}) + m_i\mathbf{g} + \mathbf{F}^{ext}_i$$

$$I_i \frac{d\omega_\mathbf{i}}{dt} = \sum_{j\in\mathcal{C}_i} (\mathbf{M}^t_{ij} + \mathbf{M}^r_{ij}) + \mathbf{M}^{ext}_i$$

DEM Architecture in Lethe Software

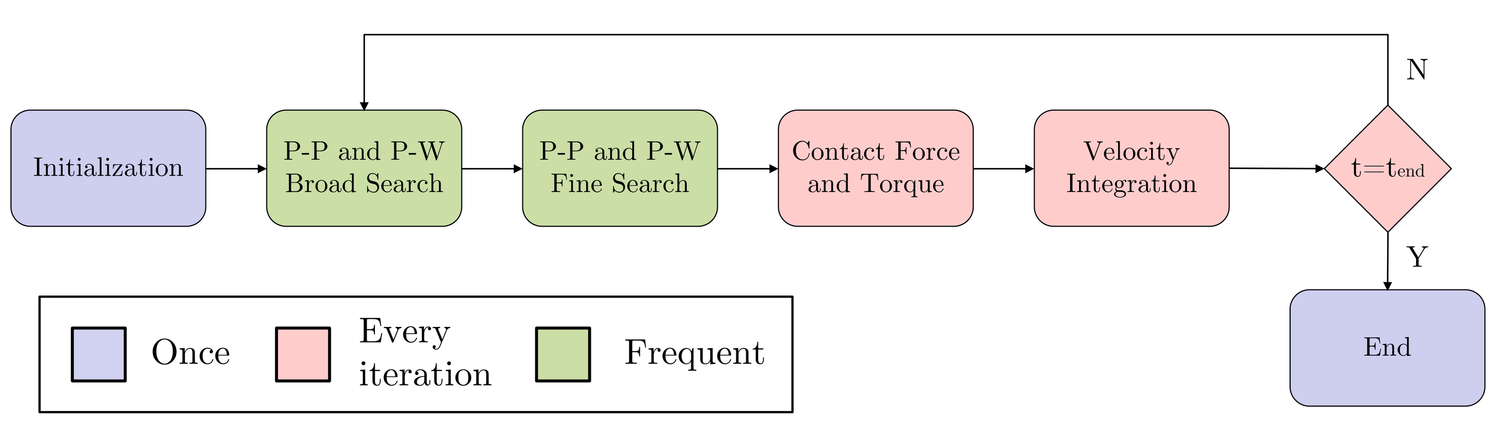

Figure 1. Simplified diagram of DEM architecture in Lethe-DEM. (Golshan *et al.*, 2022)

Granular Temperature Concept

Granular temperature is a concept in the kinetic theory of granular flow that measures the fluctuations of particles.

$$v_i = \frac{1}{n}\sum_{k=1}^{n} c_{ik}$$

$$\langle C_i C_i \rangle = \frac{1}{n}\sum_{k=1}^{n} (v_{ik} - v_i)^2$$

It is given by the average of particle normal stresses per unit bulk density. (*Jung et al.*, 2005)

$$\theta_p = \frac{1}{3}\sum_{i=1}^{3} \langle C_i C_i \rangle$$

OBJECTIVES

1. Build a benchmark to evaluate the potential of performance enhancement.
2. Define a metric to evaluate the mobility of particles.
3. Develop a dynamic algorithm to identify particles with negligible mobility.

METHODOLOGY

1. Create a rectangular hopper case with periodic boundaries

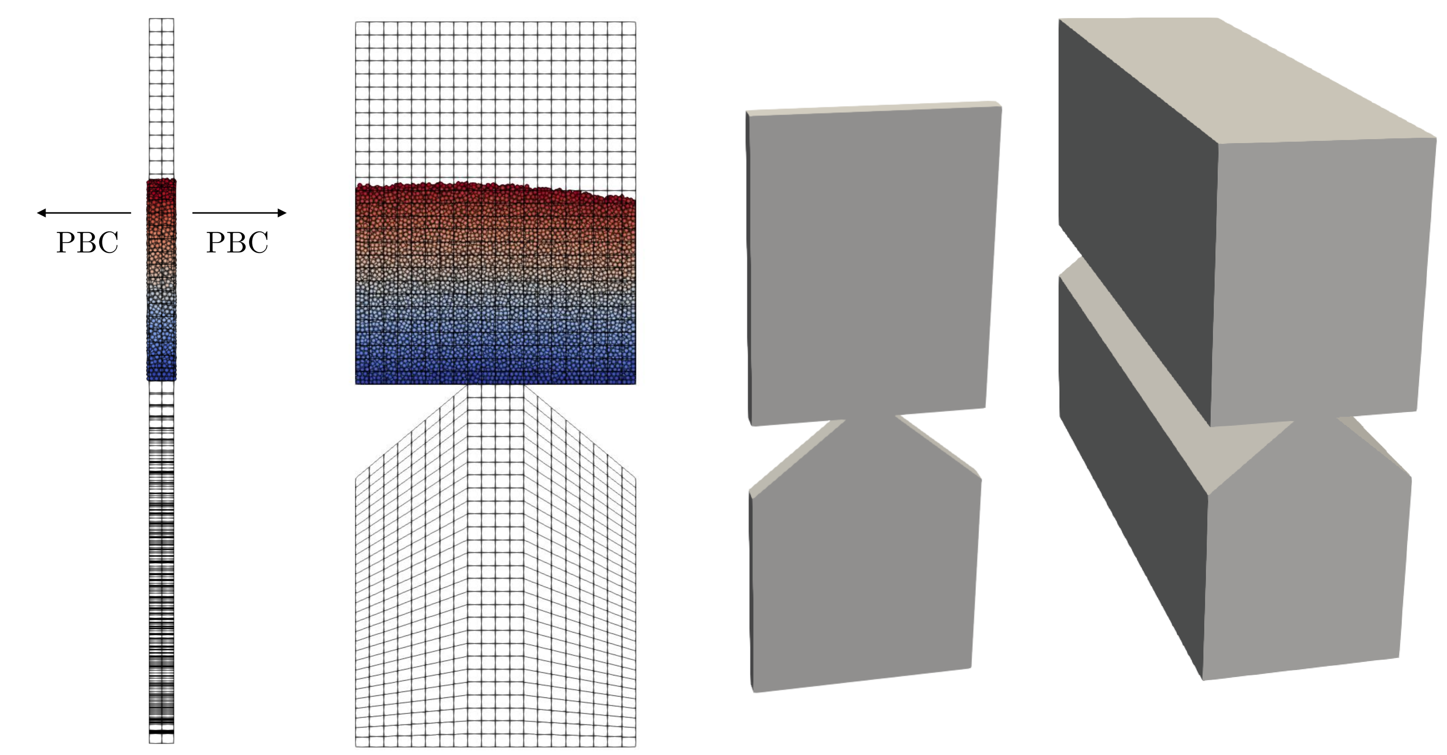

Figure 2. Hopper case mesh filled up with particles and width variations.

2. Sum of forces and granular temperature evaluation

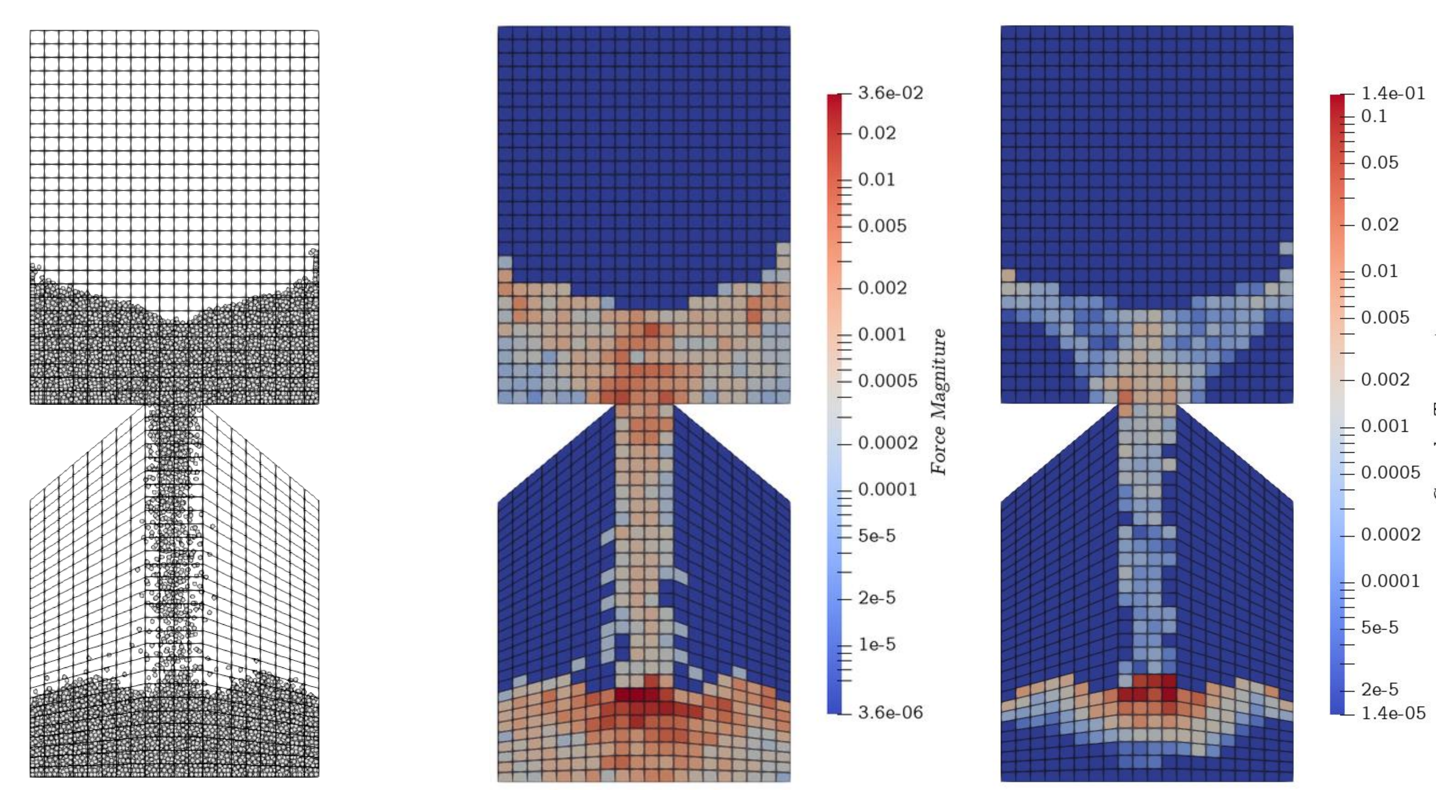

Figure 3. Computation of sum of forces and granular temperature per cell where granular temperature has a better delimitation of areas with negligible particle movement.

3. Implement the node-based mobility status algorithm

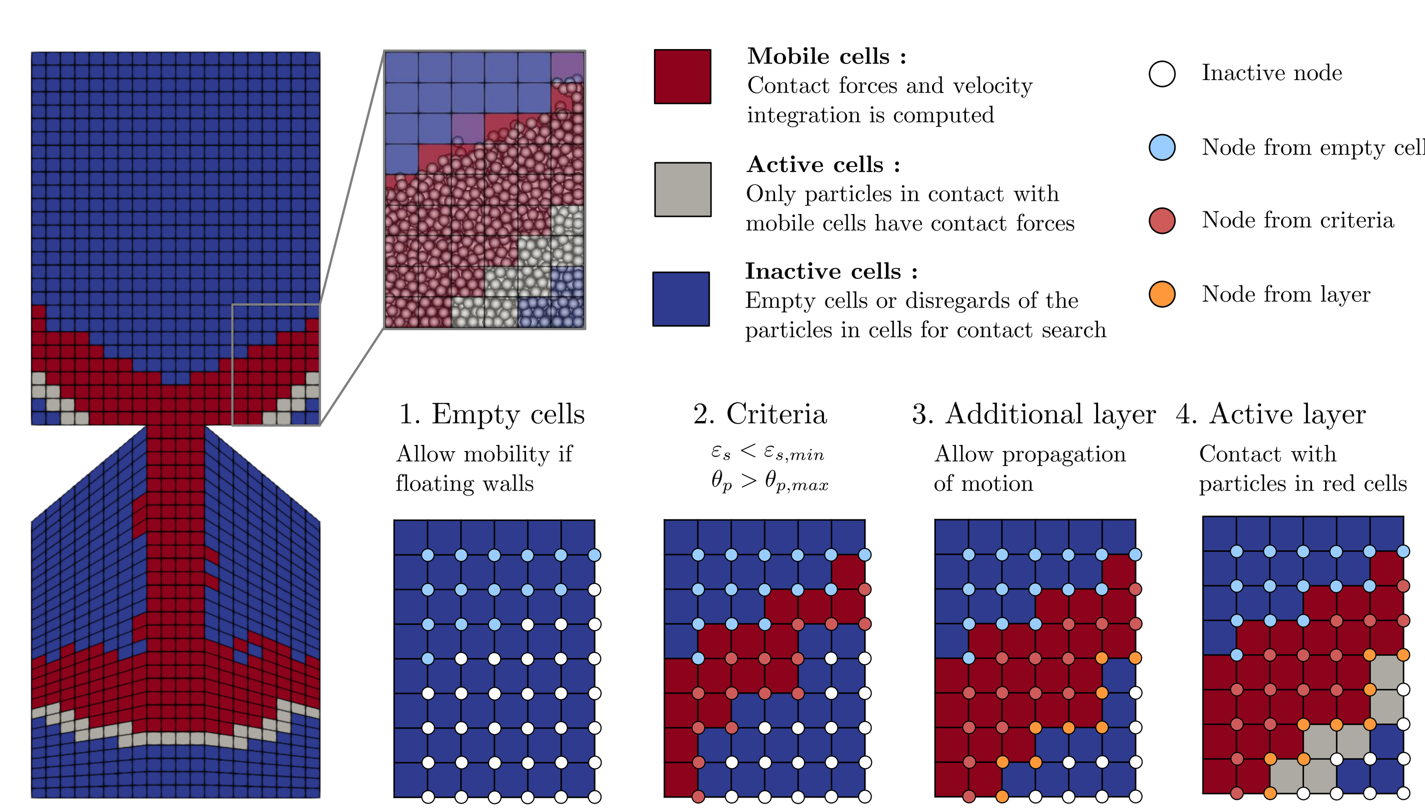

Figure 4. Schematic of the node assignment and cell mobility status per step.

PRELIMINARY RESULTS

Weak-scaling Analysis

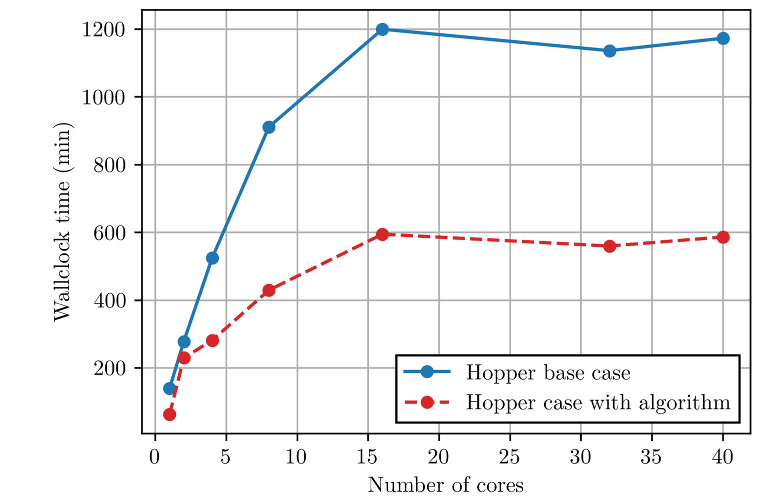

Figure 5. Weak-scaling analysis with simulation wall time for 1, 2, 4, 8, 16, 32, 40 cores with 13 580 particles/core.

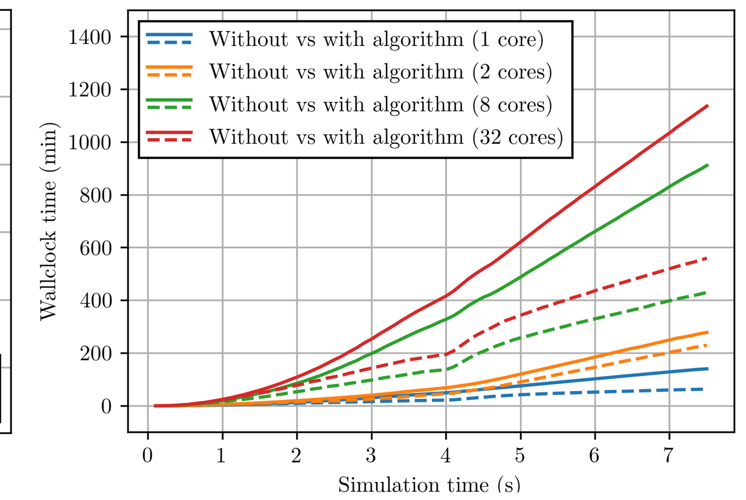

Figure 6. Wall time through simulations for 1, 2, 8, 16 and 32 cores with discharge at 4 s.

Mass Flow Rate

Table 1. Normalized mass flow rate results.

Cores	Flow rate without algorithm (g/s)	Flow rate with algorithm (g/s)	Relative difference
1	92.34	92.36	0.0%
2	92.27	92.52	0.3%
4	92.93	93.00	0.1%
8	92.53	91.88	0.7%
16	92.21	92.38	0.2%
32	92.26	92.35	0.1%
40	92.28	92.39	0.1%

Table 2. Average and standard deviation.

	Without algorithm (g/s)	With algorithm (g/s)
Average	92.40	92.41
S.D.	0.25	0.33

FUTURE WORK

Application on Pneumatic Conveying with CFD-DEM

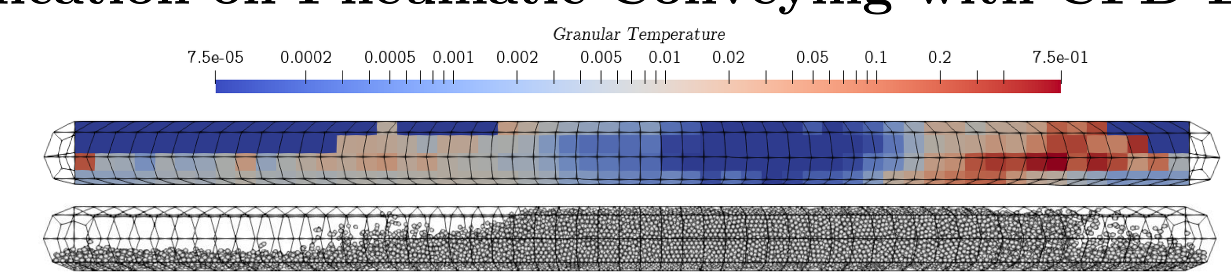

Figure 7. Small dense pneumatic conveying simulation forming plugs with its granular temperature.

DEM Simulation of Metal Additive Manufacturing

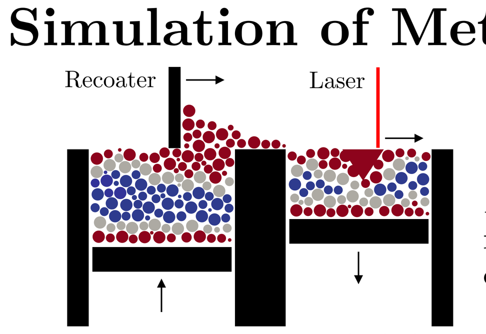

Figure 8. Diagram of a laser additive manufacturing process setup showing potential of disabling of particle contacts in some areas.

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ACKNOWLEDGMENTS

CRSNG NSERC
FONCER
Digital Research Alliance of Canada
Calcul Québec