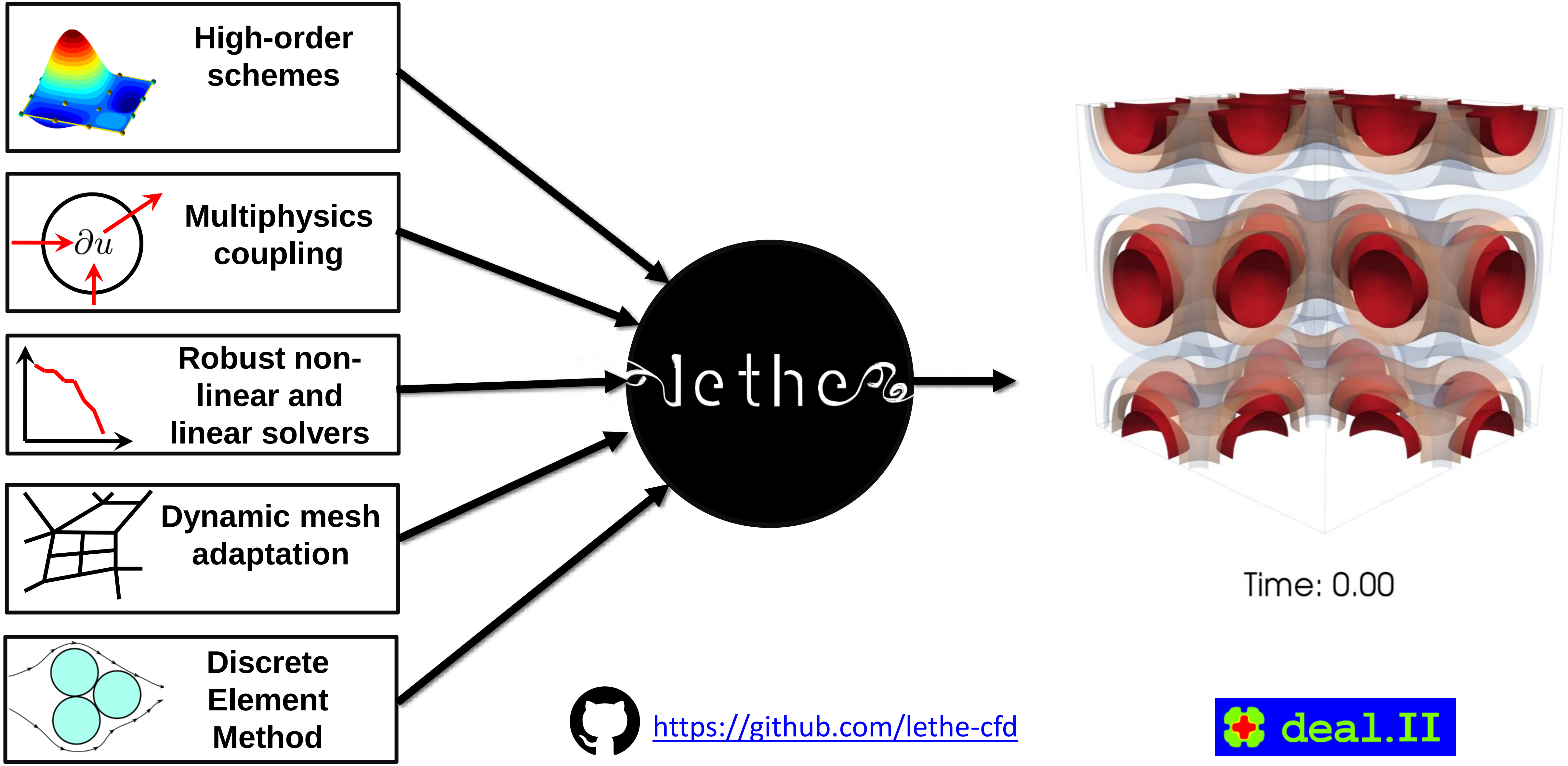
Lethe-DEM: A DEM Software Using Particle Class of deal.II

https://arxiv.org/abs/2106.09576

Lethe



https://github.com/lethe-cfd

deal.II

Introduction

Granular material is ubiquitous in nature and the second most used material in global industry after water.

Approximately half of the products and three quarters of the raw material in the chemical industry is in the form of granular materials.

Modeling approaches:

- Continuum models (Eulerian)
- Discrete models (Lagrangian)

https://en.wikipedia.org/wiki/Granular_material

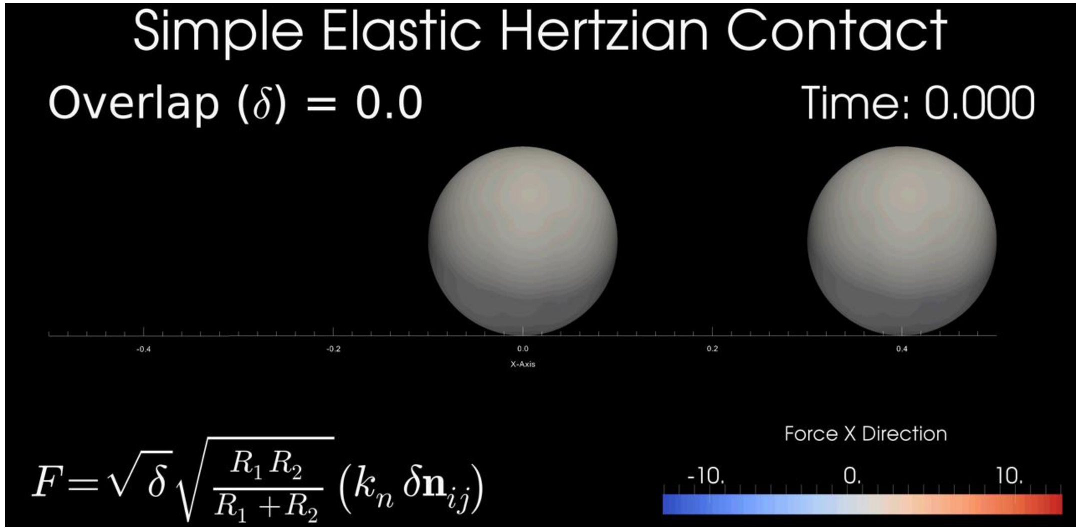
Discrete Element Method (DEM)

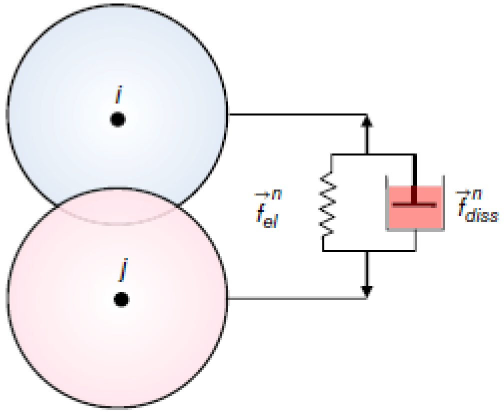
Lagrangian model for granular flows

Contact force derives from overlaps between particles (pair-wise contact)

DEM is very accurate, but with a cost of high computational cost

Computational cost: $O(n_p)$ < $\boldsymbol{O(n_p.\log n_p)}$ < $O(n_p^2)$





DEM Main Steps

Initialization

Initilize the simulation
Read input parameters

Broad Search

In broad search, list of all particle-particle and particle-wall contact candidates are obtained

Fine Search

The fine search finds the candidate contact pairs in a smaller domain

Contact Force

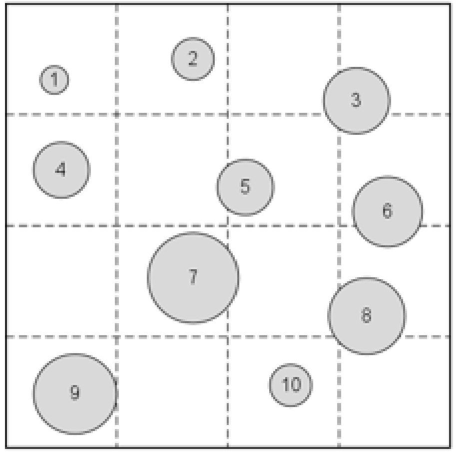
Calculation of the contact force according to fine search contact list output

Integration

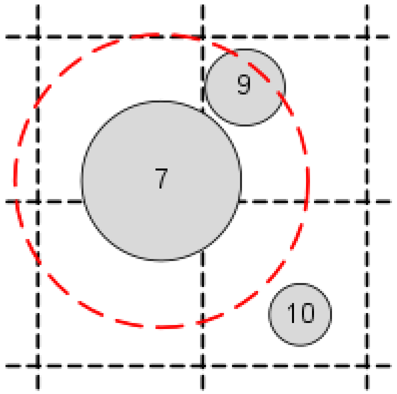
Integration of particles' velocities and positions using to the contact force

Mapping

Mapping the particles in the cells



Broad search



Fine search

Lethe-DEM & deal.II

Several features of deal.II are leveraged in Lethe-DEM.

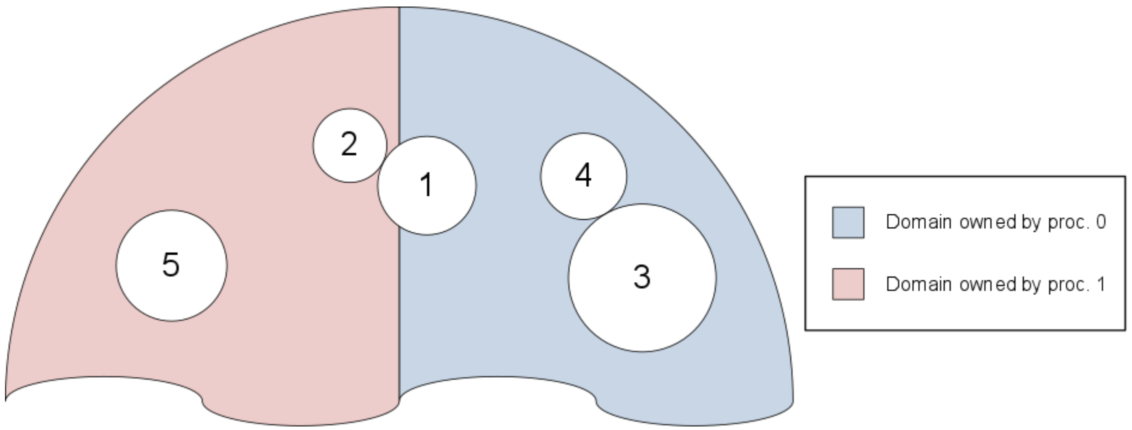
Lethe-DEM uses deal.II’s particle_handler.

Sort_particles_into_subdomains_and_cells is used for mapping of particles.

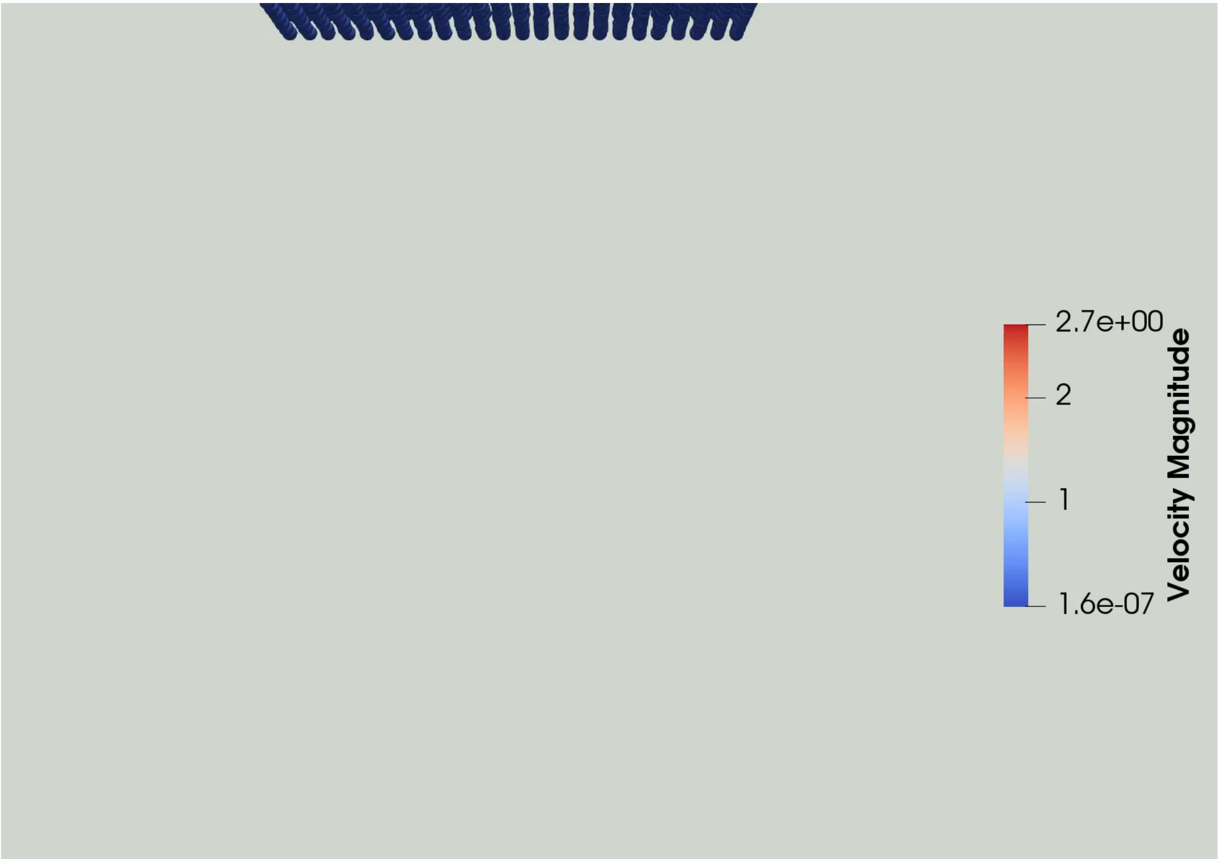
Update_ghost is used to update the information of ghost particles.

Local and ghost particles:

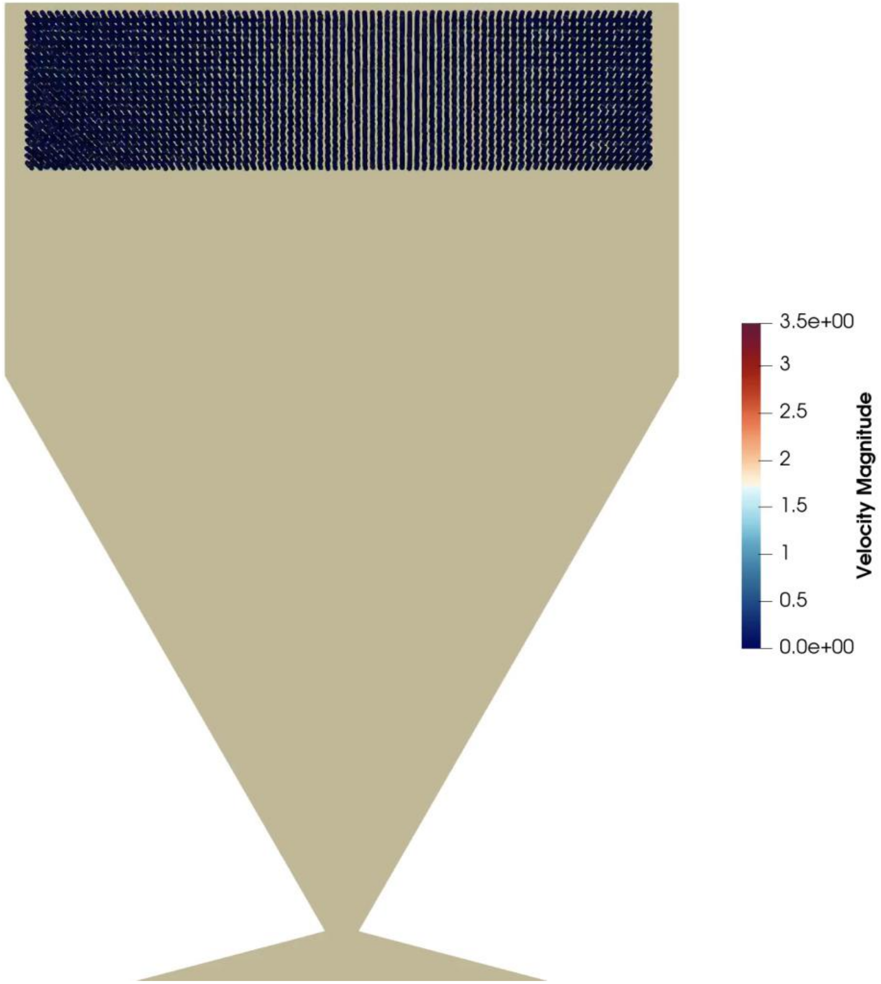
- Local-local and local-ghost collisions



Silo Simulations

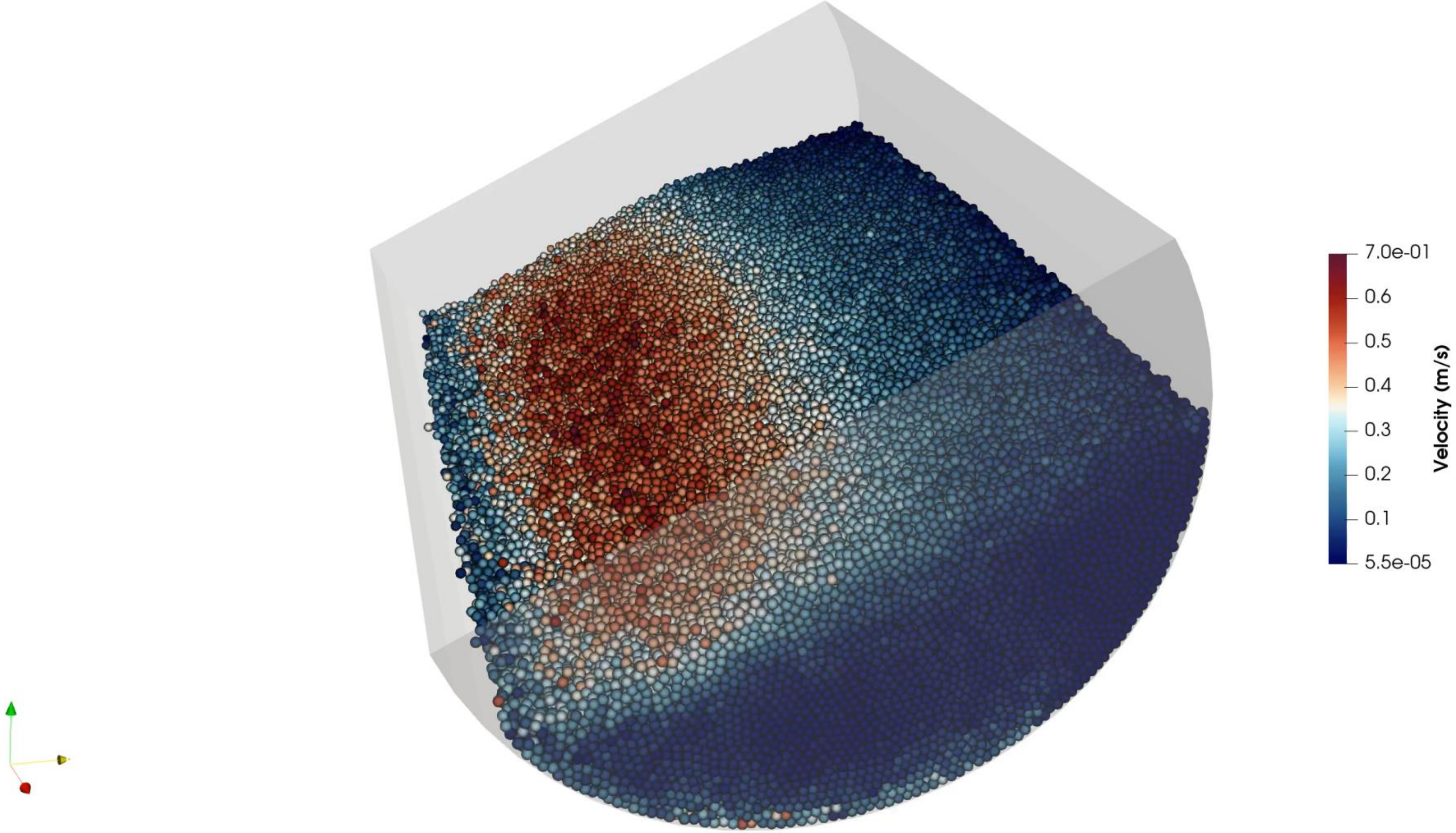


Flat-bottomed silo



Wedge-shaped silo

Rotating Drum Simulations



Scalability

Strong scaling is defined as how the solution time varies with the number of processors for a fixed total problem size.

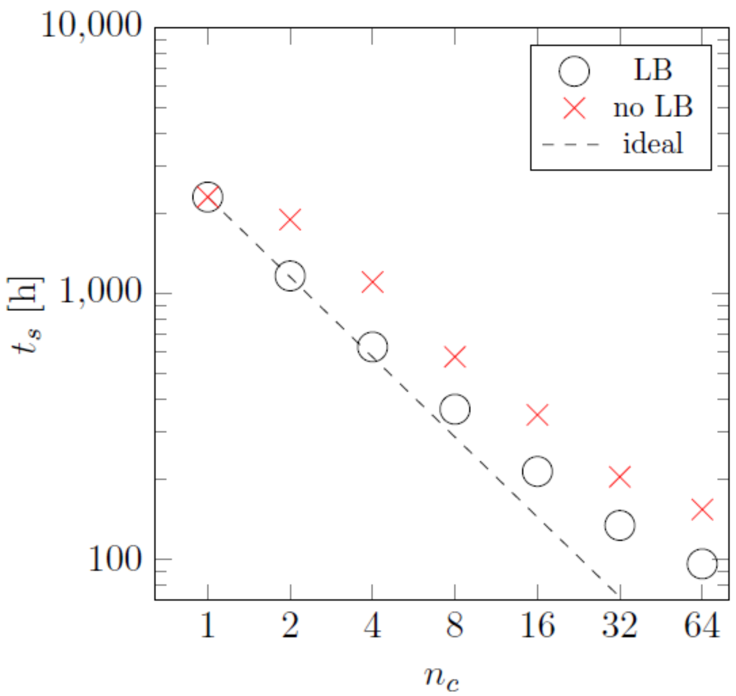
Weak scaling is defined as how the solution time varies with the number of processors for a fixed problem size per processor.

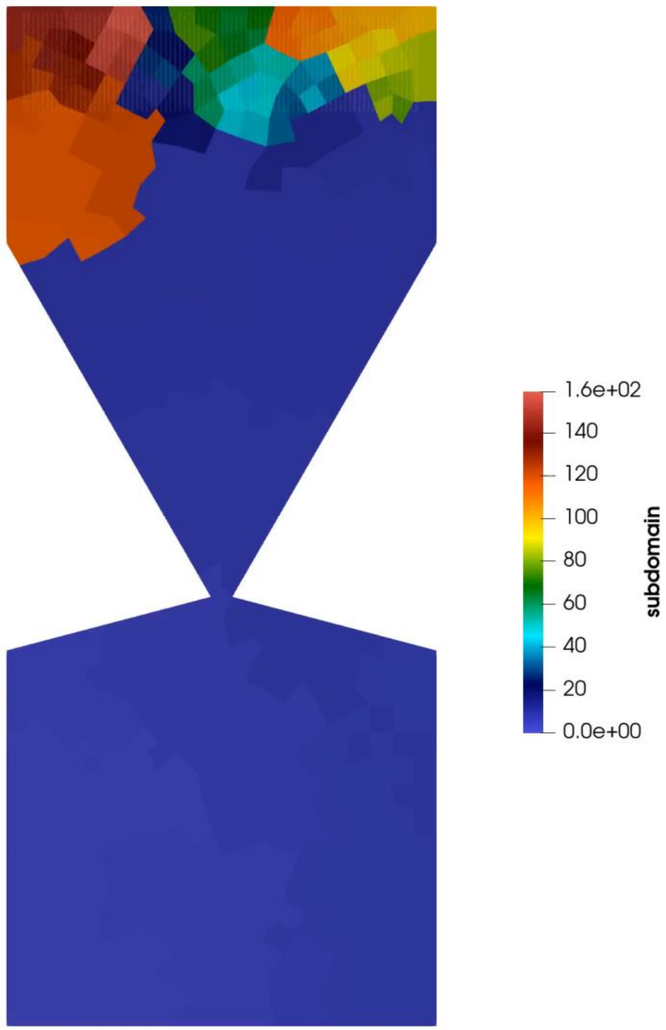
All the simulations are performed on ComputeCanada clusters on nodes with 32 cores (2 x Intel E5-2683 v4 Broadwell @ 2.1Ghz)

Strong Scaling (Silo)

As the particles move inside the simulation domain, the computational load changes on the processes. Consequently, we need to balance the computational load.

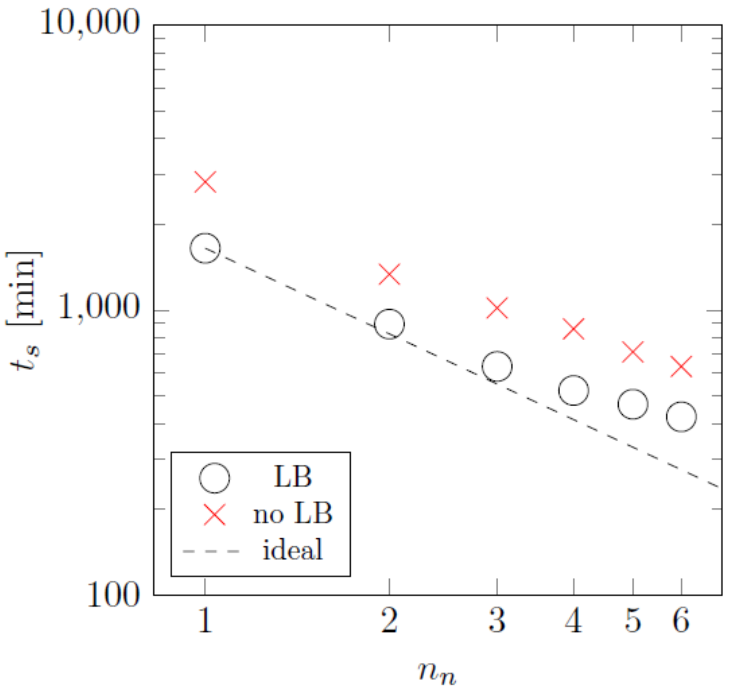
- f_{LB} = 1 Hz.
- For lower core counts, the strong scaling is quasi optimal.
- Load- balancing decreases the computational time by around 30%.



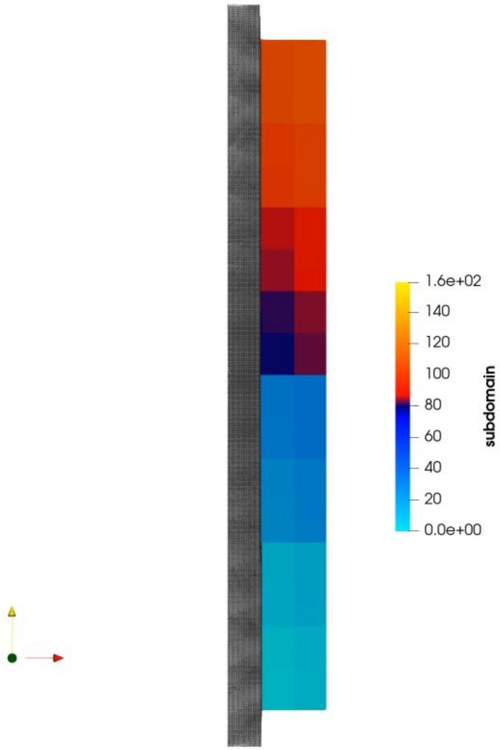


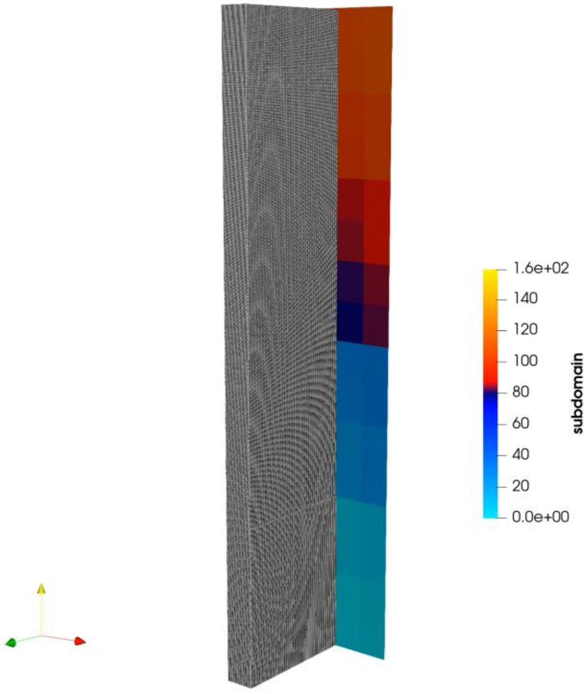
Strong Scaling (Drum)

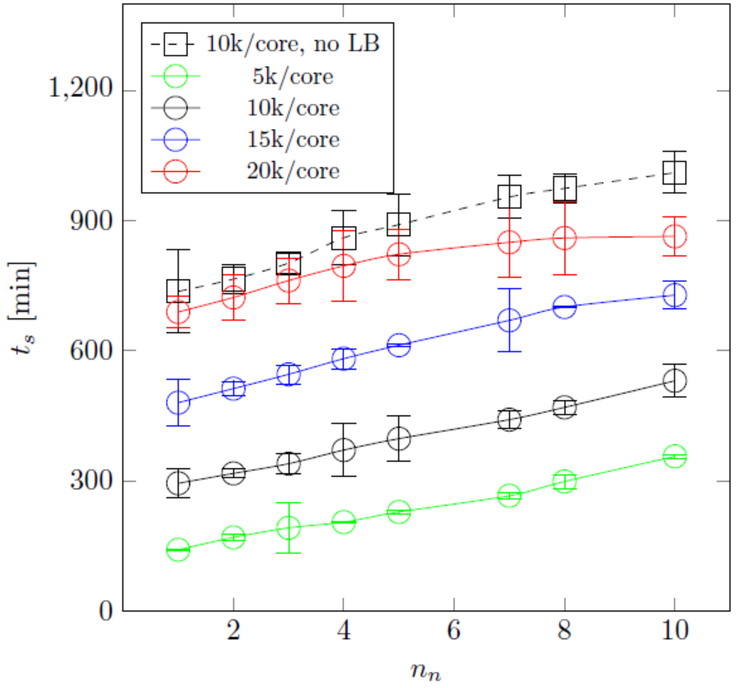
- t_{LB} = 1.5 s.
- Silo simulations are performed on 1 to 6 compute nodes, each with 32 cores.
- The deviation from the ideal speed-up increases with the number of cores.
- Using load-balancing decreases the computational time by around 35%.
- The simulation time per iteration decreases from 0.099 s to 0.025 s for this simulation on 1 to 6 nodes with load-balancing.



Weak Scaling







- The simulation times increase slightly with the number of processes at all the n_p/n_c values.
- For n_p/n_c = 20k on more than 6 nodes the simulation time does not further increase, which represents near ideal weak scalability.

Thanks!

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