SPH IMPLEMENTATION LAMMPS

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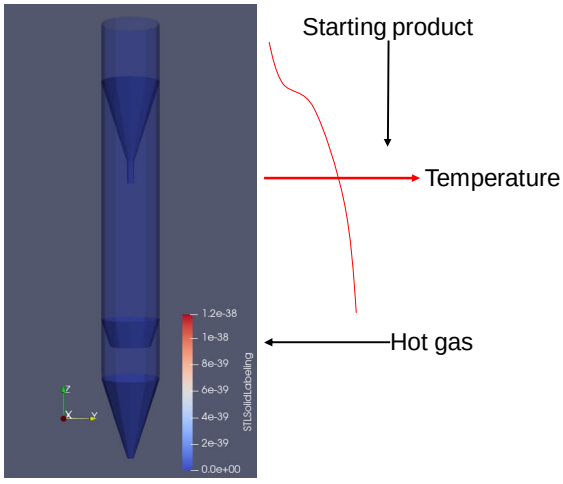
Industrial application of LAMMPS tools

Focus on production High Performance Engineering Materials

High Performance Engineering Materials
- Mechanical strength @ high temperatures
- High melt viscosity
- High conversion

Melt polymerization (often initial stages process)
- Free movement reactive groups
- Side reactions & branching

Solid state post condensation
- Limited movement reactive groups
- Limits side reactions & branching
- Requires extended residence time



Final product

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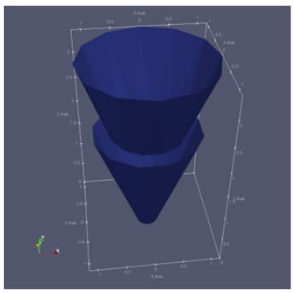
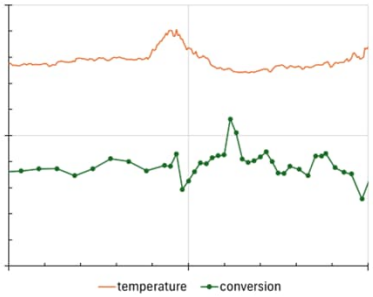
Typical challenges

Wrong placement internals
- Stagnant zones (workshop presentation)
- Gel formation

- Insufficient stress release between internals



Presence of fines in feed
- Segregation in reactor
- Maldistribution of gas flow
- Influencing flow profile
- Different reaction zones
  - Variability in end product conversion



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Goals of collaboration project

Short Description	General continuum solvers for particle flows, suitable for use in industry with adjustable boundary conditions and adjustable friction parameters, including a recipe for determining simulation (e.g., friction, restitution, continuum rheology) parameters from real powders.
Objectives	Obtain, test, and verify an open-source package for dense powder flows and apply in industry, including procedures to determine relevant parameters for real powders. Make package available to all IFPRI members, including standard flow simulations such as silo flow, chute flow and rotating drum flow.
Scope	Open-source, basic continuum solver for dense dry media, including an adjustable friction coefficient, wall friction coefficient, arbitrary geometries, and capability of forming new free surfaces, options for rapid flow effects on friction and the dependence of friction on evolving packing fraction. Make available to IFPRI members, documentation, and updates and examples.

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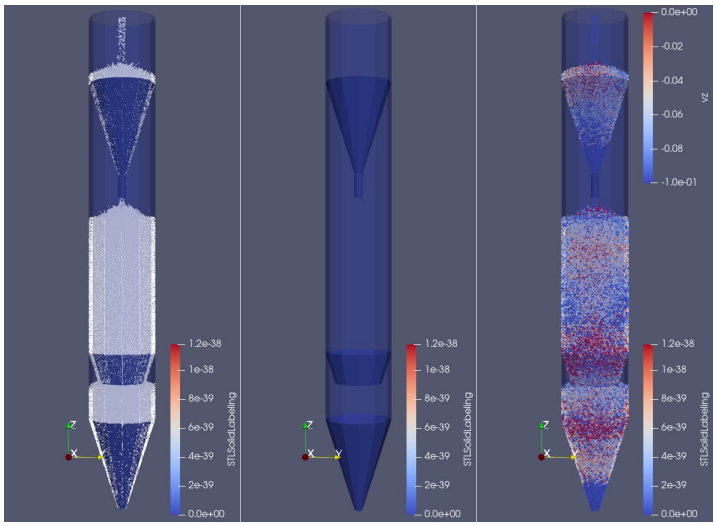
Test case

Standard processing silo with insert & feed cone

Geometry
- Feed cone + pipe
- Insert (e.g. gas inlet)
- Discharge cone

Powder characteristics
- 81900 packages of granules
- Fixed μ-rheology
  - $\mu_{granule}$ = 0.819 (Φ_E = 39°)
  - μ_{wall} = 0.135 (Φ_W = 7.7°)



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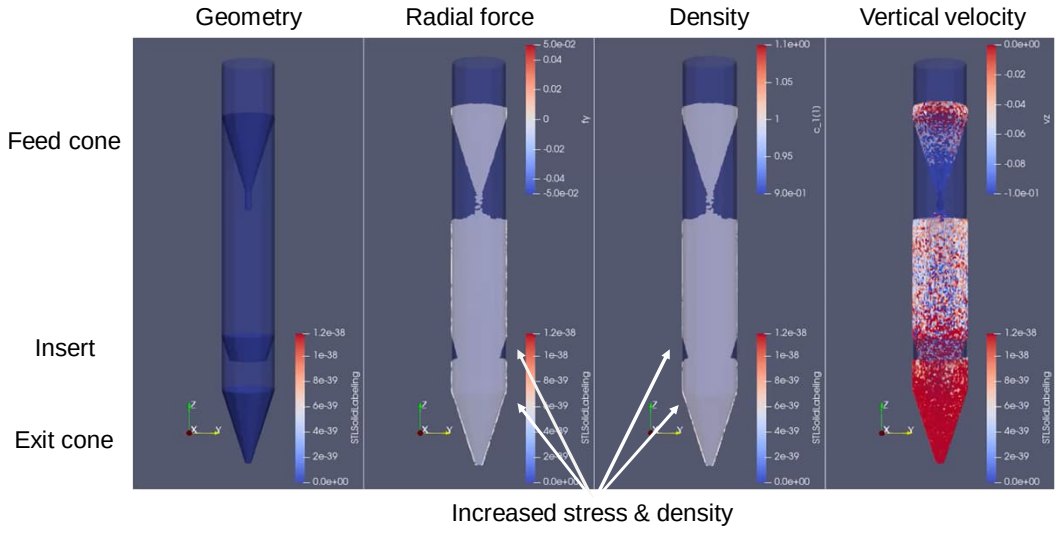
Visualization of test case



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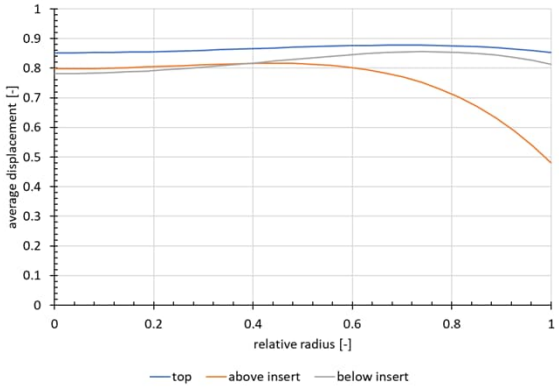
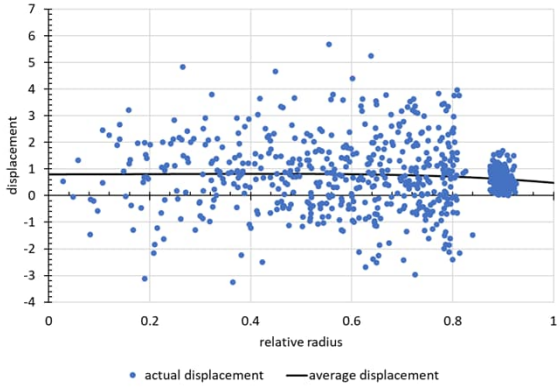
Results on velocity profile

Average displacement



Actual displacement



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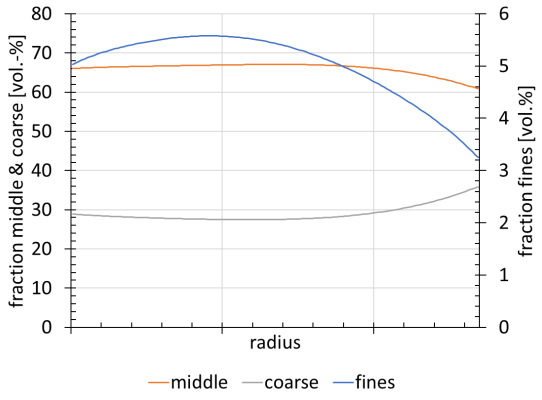
Conclusion test case

Application in industry

- Model applied on real world case
- Velocity profile extracted from results
  - Large dynamic variations
- Estimation made of segregation in column
  - Quantitative understanding

However

- Speed of calculation depends on complexity stl-grid



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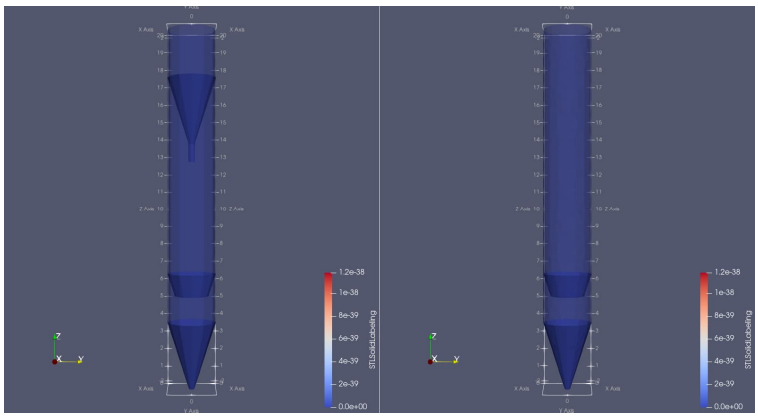
Testing complexity STL files

Low resolution

High resolution



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Variations in test cases

LAMMPS SPH-plasticity, Liggghts coarse grain model, details STL-grid

Test case	Lammps.Red	Lammps.Ext	Liggghts.Red	Liggghts.Ext
Platform	LAMMPS	LAMMPS	LIGGGHTS	LIGGGHTS
Interaction	SPH-Plasticity	SPH-Plasticity	Rolling friction	Rolling friction
STL-file	Low resolution	High resolution	Low resolution	High resolution
Particles/packages	68250	3588	50000	50000
Time step	1e-5	1e-5	2e-5	2e-5
Simulated time (s)	2 s	2 s	8 s	8 s
CPU/cores used	8	4	4	4
Run time (hrs)	36757	88629 s	5965 s	5733 s

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Conclusions

- Detailed STL files increase CPU load
  - Higher complexity wall interaction compared to DEM
    - Multiple layers of powder packages versus single particle interaction
- Possible improvements:
  - Application of single primitives for cones, walls…
    - Already applied in LAMMPS-DEM

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