An open-source perspective at CFD-DEM for particle-laden flows

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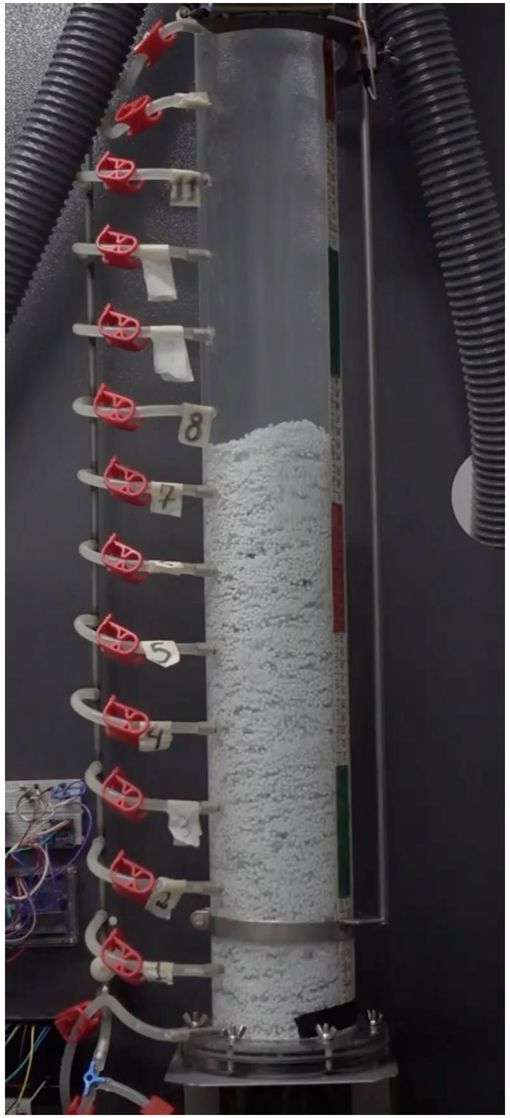
Particle-laden flow

Industrial applications of interest to us

Solid-fluid contactor: Fluidized-bed

Fluidized bed contactor

- Uniform fluid jet
- Strong particle-fluid mixing
- Many regimes
- Geldart B particles

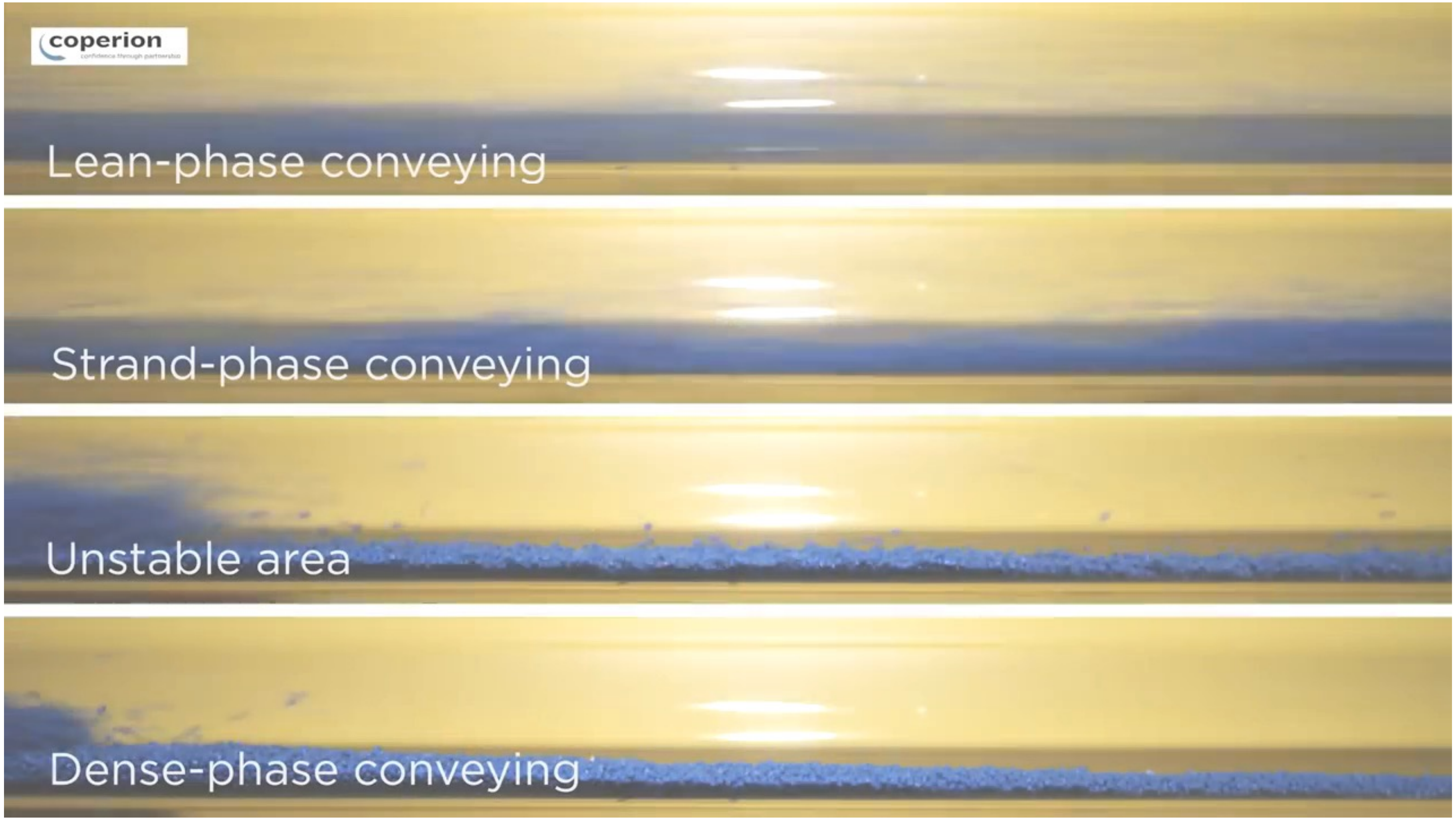


Solid-fluid contactor: Spouted-bed

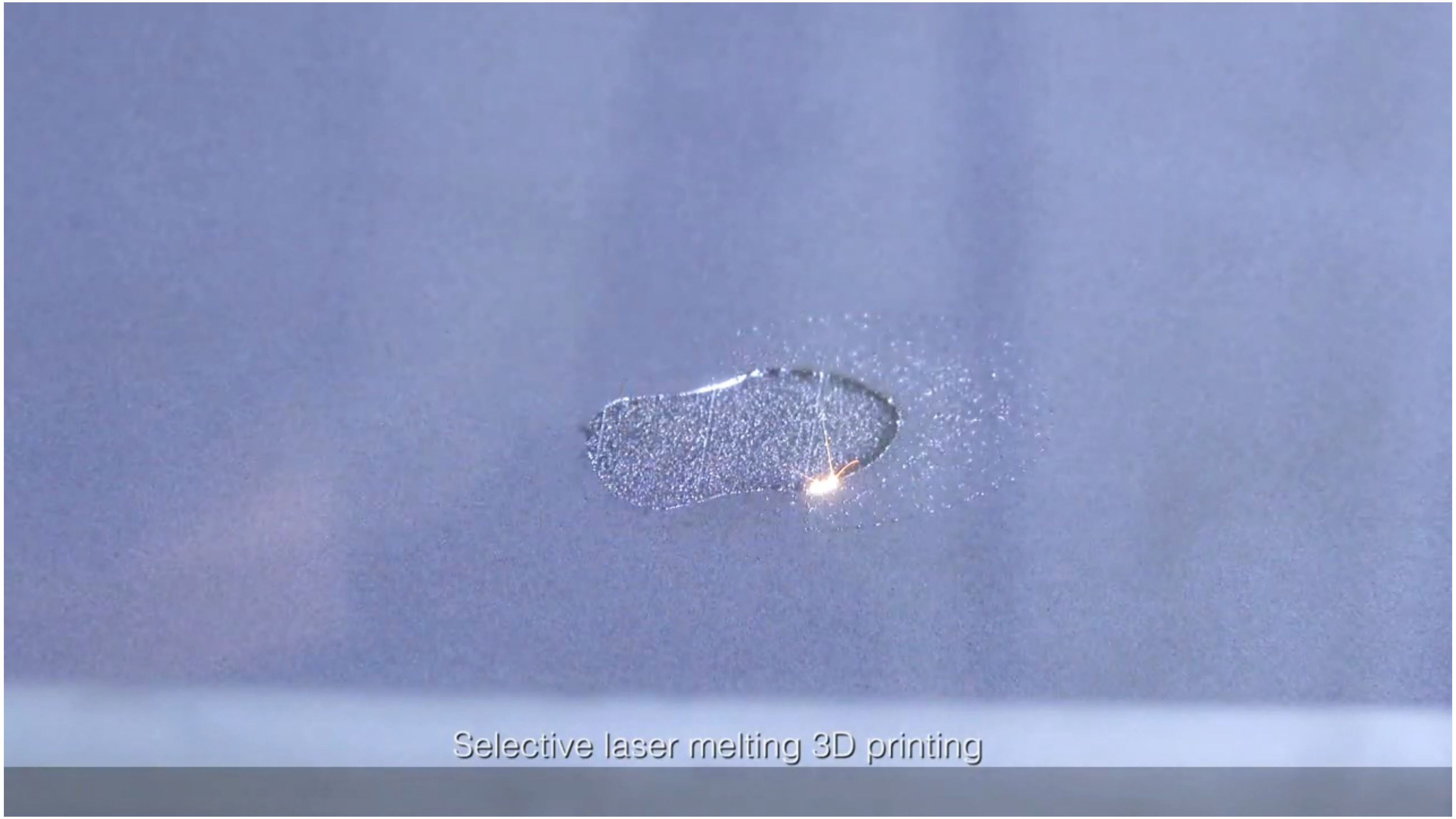
Spouted-bed contactor

- Air jet in a small slit
- Contact in upward movement of fluid
- Geldart D particles

Pneumatic conveying



Novel processes: LPBF 3D printing



Summary

Quick recap on high-order methods

Lethe: open-source high-order CFD/DEM/CFD-DEM

Illustration using two turbulent benchmarks

High-order Unresolved CFD-DEM

- VANS equation formulation
- Void fraction projection scheme
- Interesting validation cases

Conclusions and future work

High-order methods for CFD

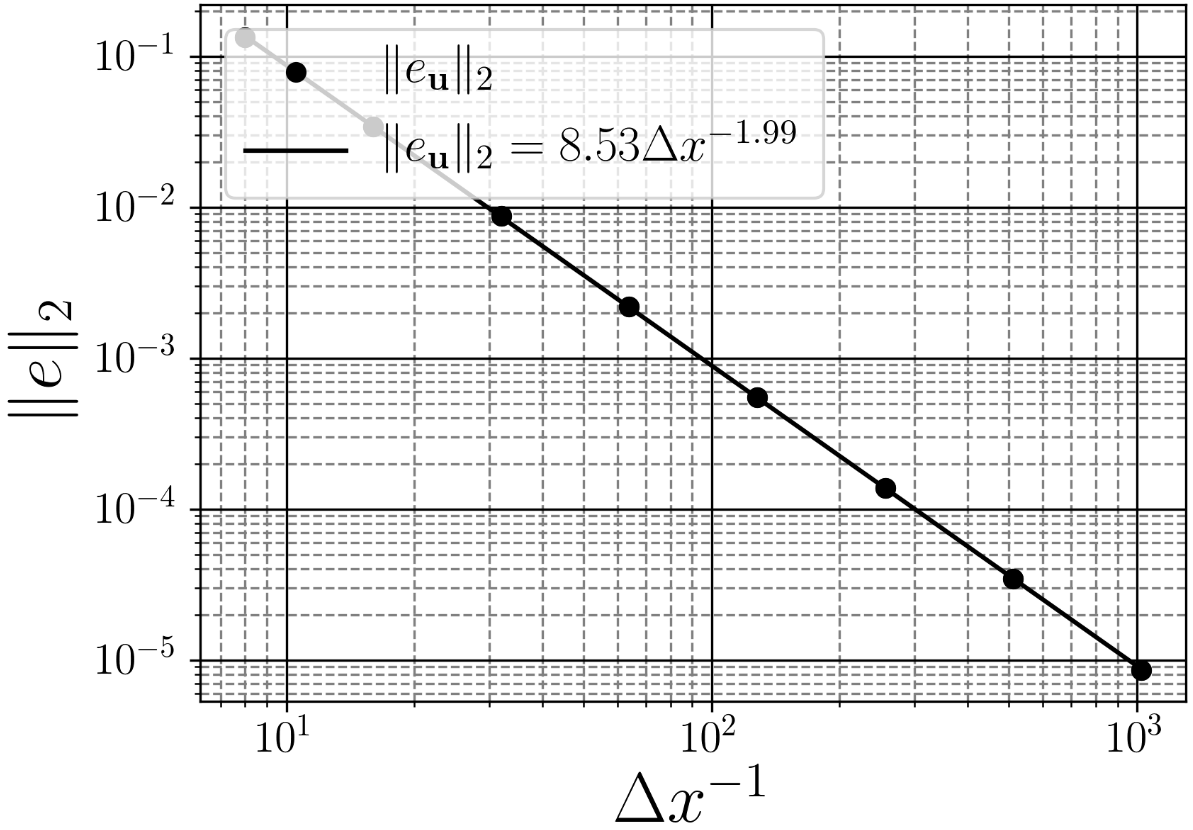
A quick introduction

Order of a scheme?

The order characterizes how the error will evolve as the mesh (or time step) is refined (or coarsened)

I.e. :

$$\frac{e(\Delta x_1)}{e(\Delta x_2)} = \left(\frac{\Delta x_1}{\Delta x_2}\right)^{p+1}$$



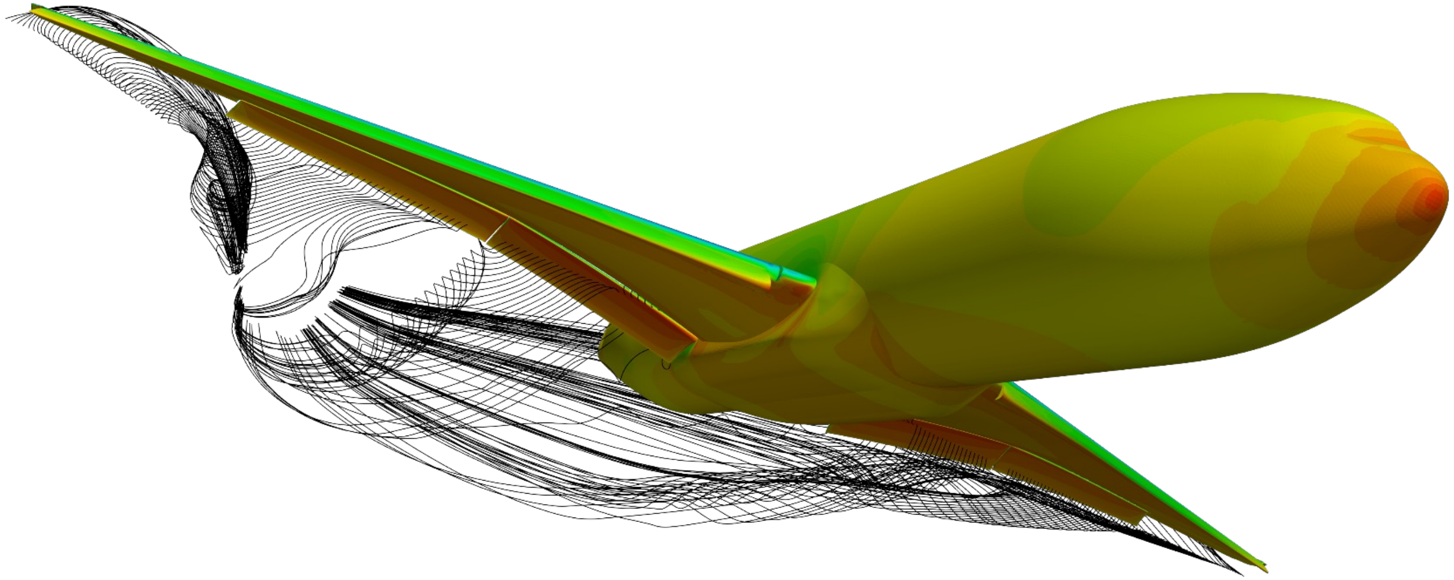
Traditional CFD

The traditional state of the art in commercial and open source software is mostly centered around 2nd order accurate scheme

Commercial:
- Fluent
- Star-CCM+

Open-source
- OpenFOAM
- SU2

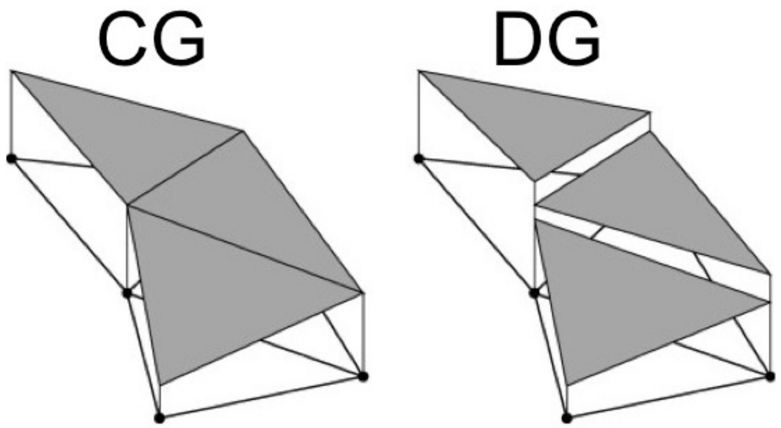
Why stop there?

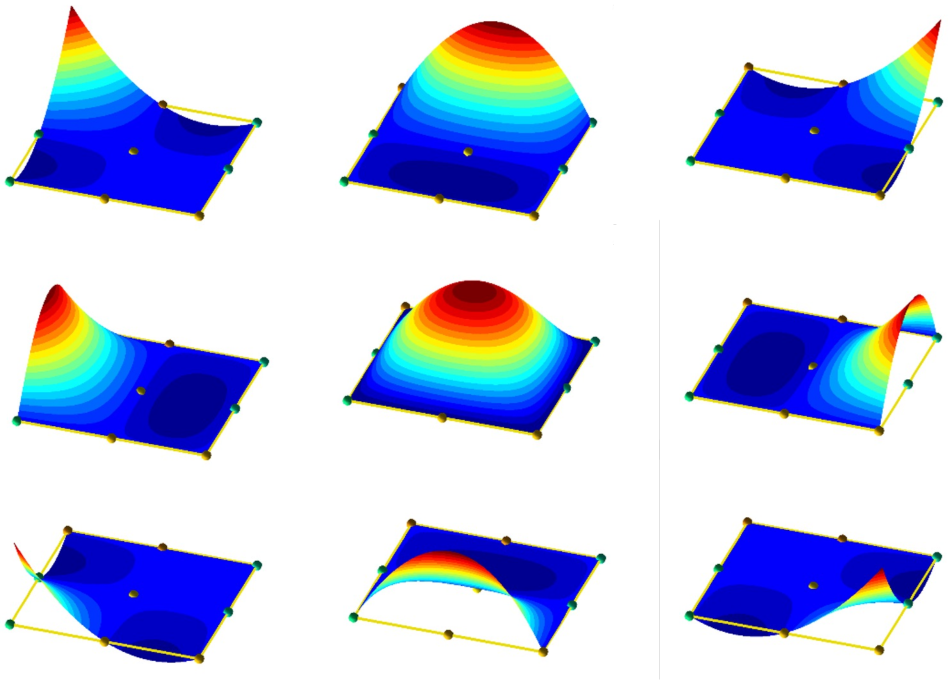


High-order and FEM

In the case of FEM using high-order methods entails using high order polynomial interpolations. This can be done using either:

- Continuous Galerkin - CG
- Discontinuous Galerkin - DG



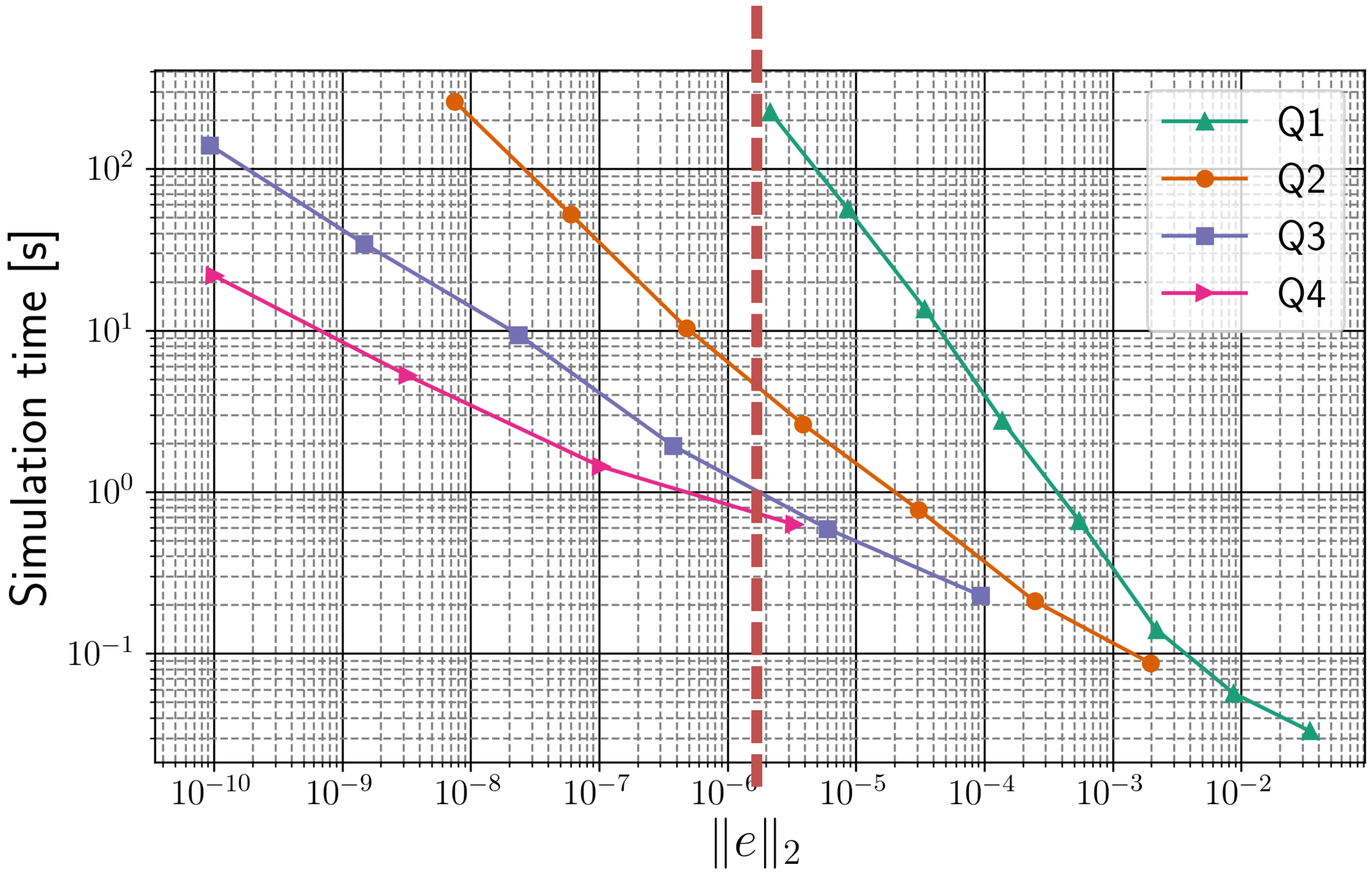


Efficiency of high-order methods

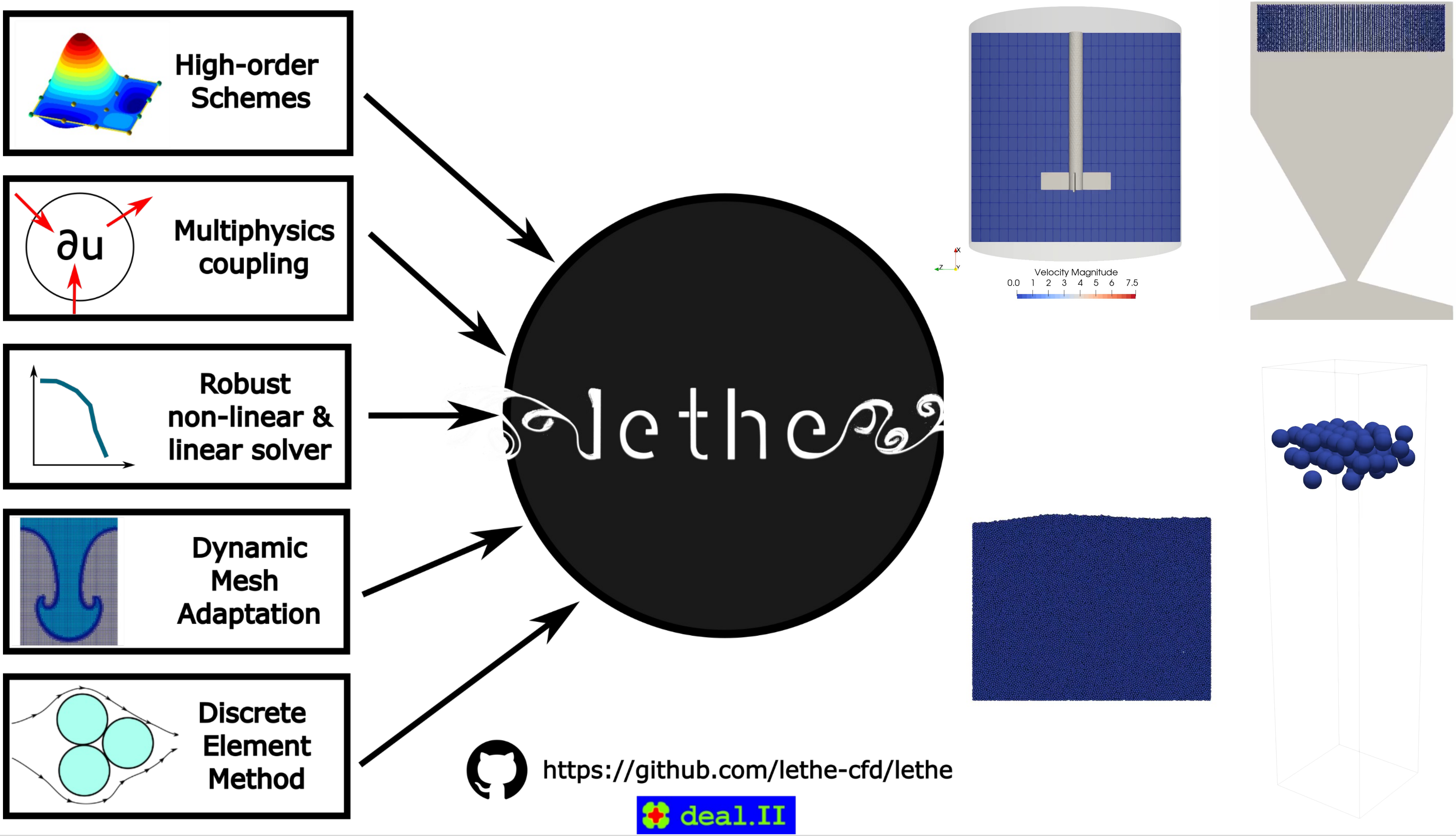
Same accuracy in shorter solution time

Depends on:

- Geometry
- Reynolds number



Lethe


High-order Schemes
∂u
Multiphysics coupling
Robust non-linear & linear solver
Dynamic Mesh Adaptation
Discrete Element Method
lethe
Velocity Magnitude
0.0 1 2 3 4 5 6 7.5
https://github.com/lethe-cfd/lethe
deal.II

Lethe

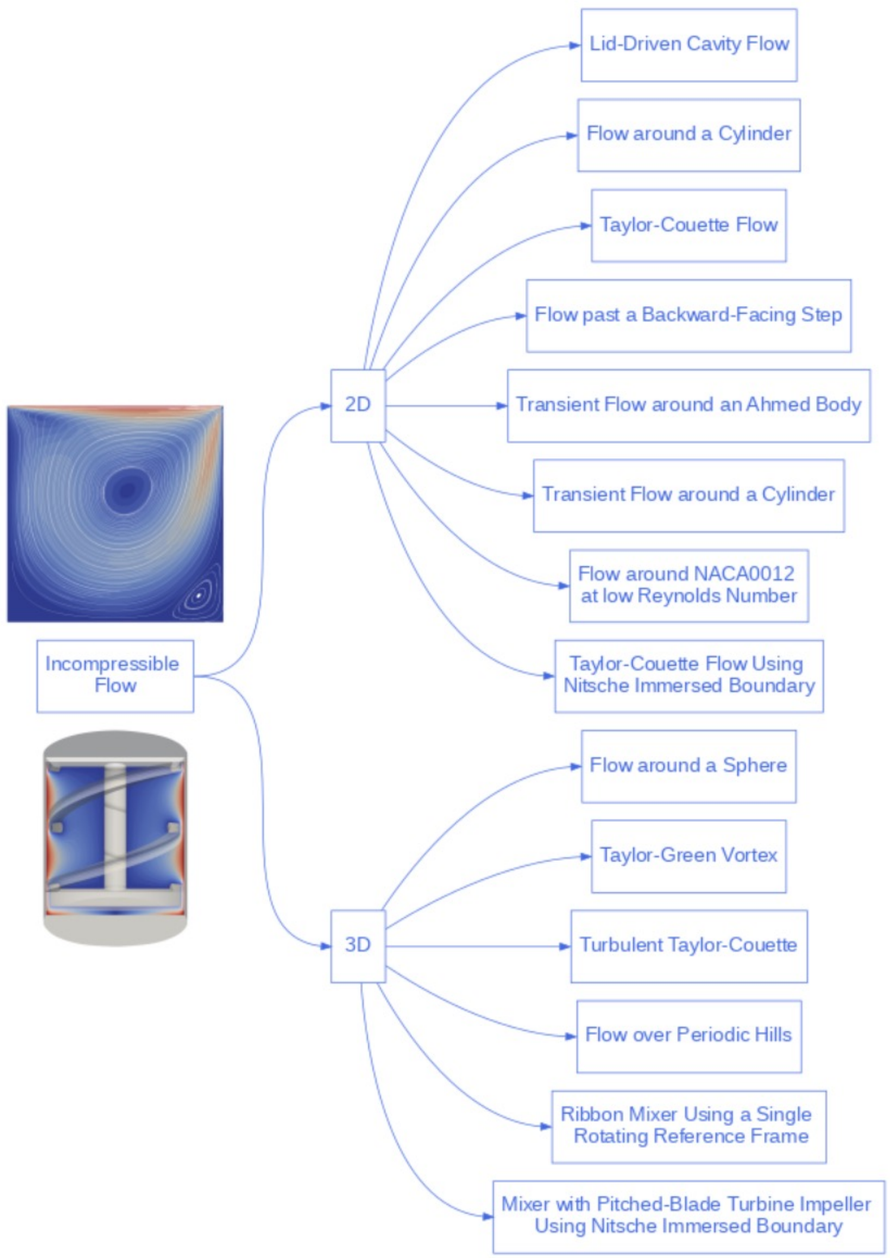
Solid open-source foundations

- Based on the deal.II framework
- Tested (>340 tests run daily)
- Documented (>50 examples)
- Used in 5 countries

 (Canada, Germany, UK, Australia, USA)

What is the FEM formulation used in Lethe for the Navier-Stokes equations?

Incompressible Flow



Continuity

$$\int_{\Omega} \nabla \cdot \boldsymbol{u} q \,\mathrm{d}\Omega + \underbrace{\sum_{K} \int_{\Omega_k} \mathcal{SR} \cdot (\tau_u \nabla q)\, \mathrm{d}\Omega_k}_{\text{PSPG}} = 0$$

Momentum

$$\int_{\Omega} \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) \cdot \boldsymbol{v} \,\mathrm{d}\Omega + \int_{\Omega} \nu \left(\nabla \boldsymbol{u} : \nabla \boldsymbol{v} \right) \mathrm{d}\Omega$$

$$- \int_{\Omega} \left(p \nabla \cdot \boldsymbol{v} \right) \mathrm{d}\Omega + \underbrace{\sum_{K} \int_{\Omega_k} \mathcal{SR} \cdot (\tau_u \boldsymbol{u} \cdot \nabla \boldsymbol{v})\, \mathrm{d}\Omega_k}_{\text{SUPG}} = 0$$

Comments

Stabilized formulation:

- Allows QnQn elements, circumvents LBB conditions
- Implicit LES

Non-linear problem solution strategy

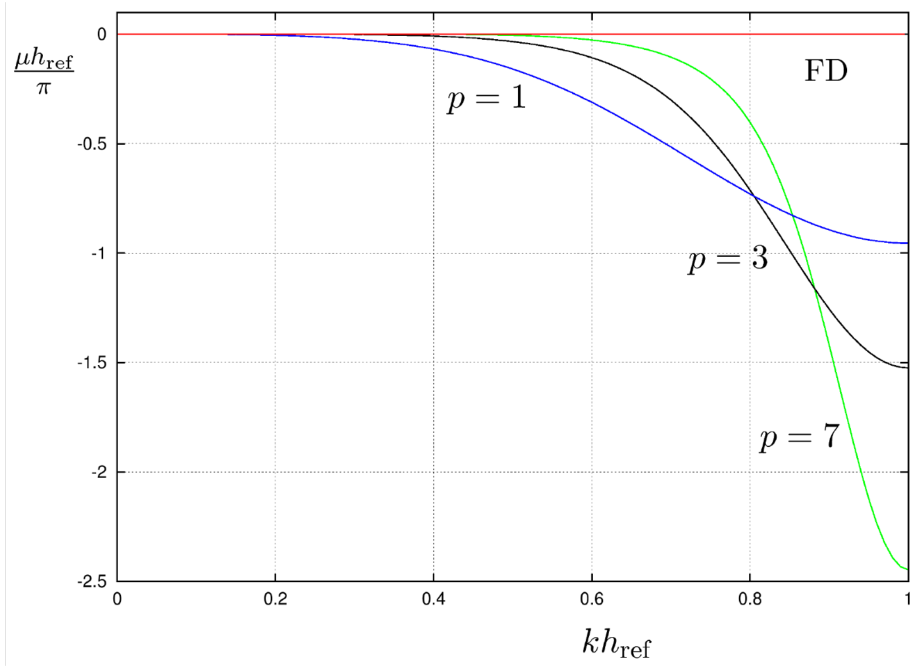
- Newton-Raphson method with dynamic recalculation of the Jacobian matrix

Linear solver strategy

- Monolithic solver using AMG, ILU or GMG preconditioning

High order

- High order methods move the numerical dissipation to higher wave number. Closer to where the real viscosity is acting



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A simple turbulent benchmark

Taylor-Green vortex at Re=1600

Wang, Zhijian J., et al. "High-order CFD methods: current status and perspective." International Journal for Numerical Methods in Fluids (2013) – Test 3.5

Blais et al. "Lethe: An open-source parallel high-order adaptative CFD solver for incompressible flows." *Software X* 12 (2020)

Taylor-Green test case

Unsteady flow of decaying vortices

In 2D:

- Exponential decay of the vortices

In 3D:

- Generation of a fully 3D flow patterns
- Turbulent cascade that generate smaller flow structures which then dissipate

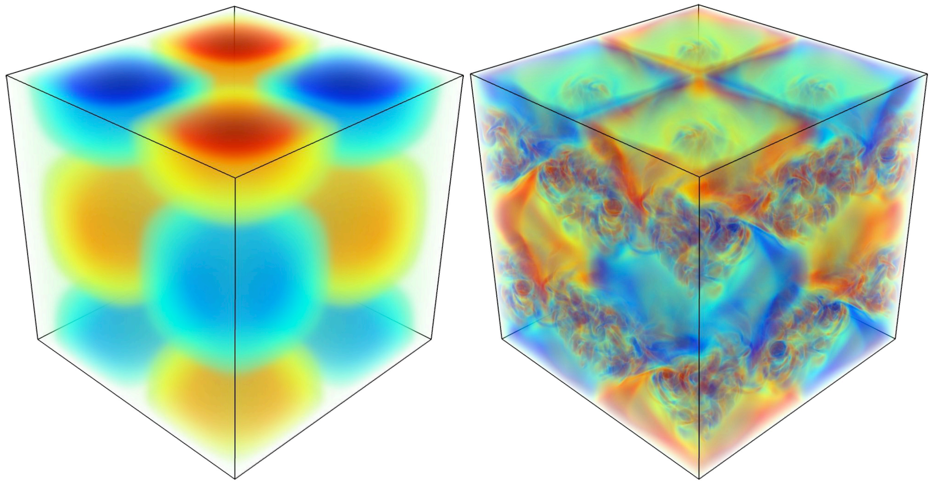
The TGV test case is a great benchmark for DNS and ILES

$$u = V_0 \sin\left(\frac{x}{L}\right)\cos\left(\frac{y}{L}\right)\cos\left(\frac{z}{L}\right)$$

$$v = -V_0 \cos\left(\frac{x}{L}\right)\sin\left(\frac{y}{L}\right)\cos\left(\frac{z}{L}\right)$$

$$w = 0$$

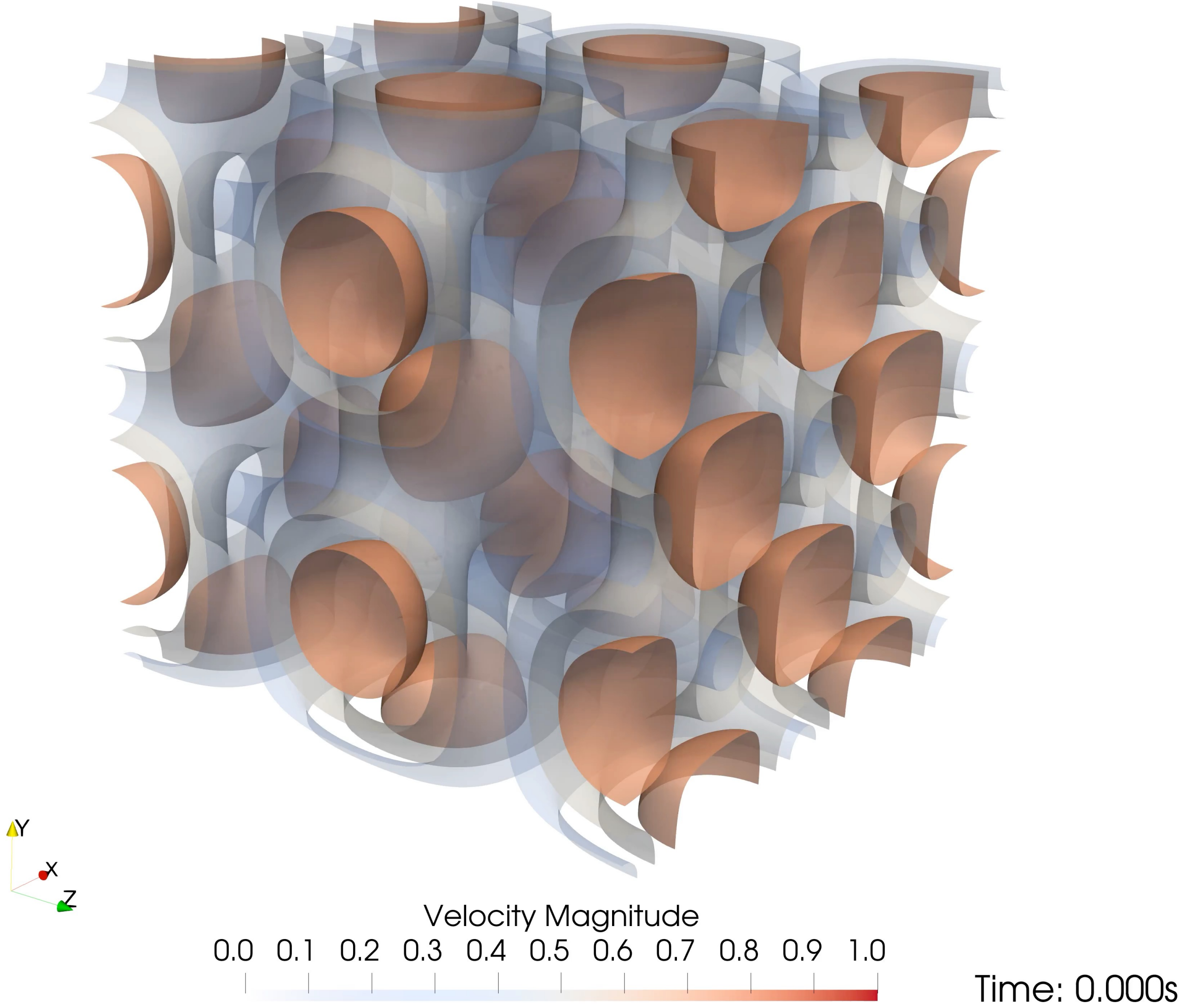
$$p = p_0 + \frac{\rho V_0^2}{16}\left(\cos\left(\frac{2x}{L} + \cos\left(\frac{2y}{L}\right)\right)\right)\left(\cos\left(\frac{2z}{L}\right)+2\right)$$



Velocity

Cascade from large turbulent structures to smaller ones

Small structures dissipate the energy



Energy dissipation - Enstrophy

$$\boxed{\frac{\partial}{\partial t}\left(\frac{u^2}{2}\right) = -\nabla\cdot\left[\left(\frac{u^2}{2}+\frac{p}{\rho}\right)\mathbf{u}+\nu\left(\nabla\times\mathbf{u}\right)\times\mathbf{u}\right]-\nu\left(\nabla\times\mathbf{u}\right)^2}$$

Integrating on a closed or periodic domain, we obtain:

$$\boxed{\frac{\partial}{\partial t}\int\left(\frac{u^2}{2}\right)dV = \int -\nu\left(\nabla\times\mathbf{u}\right)^2 dV}$$

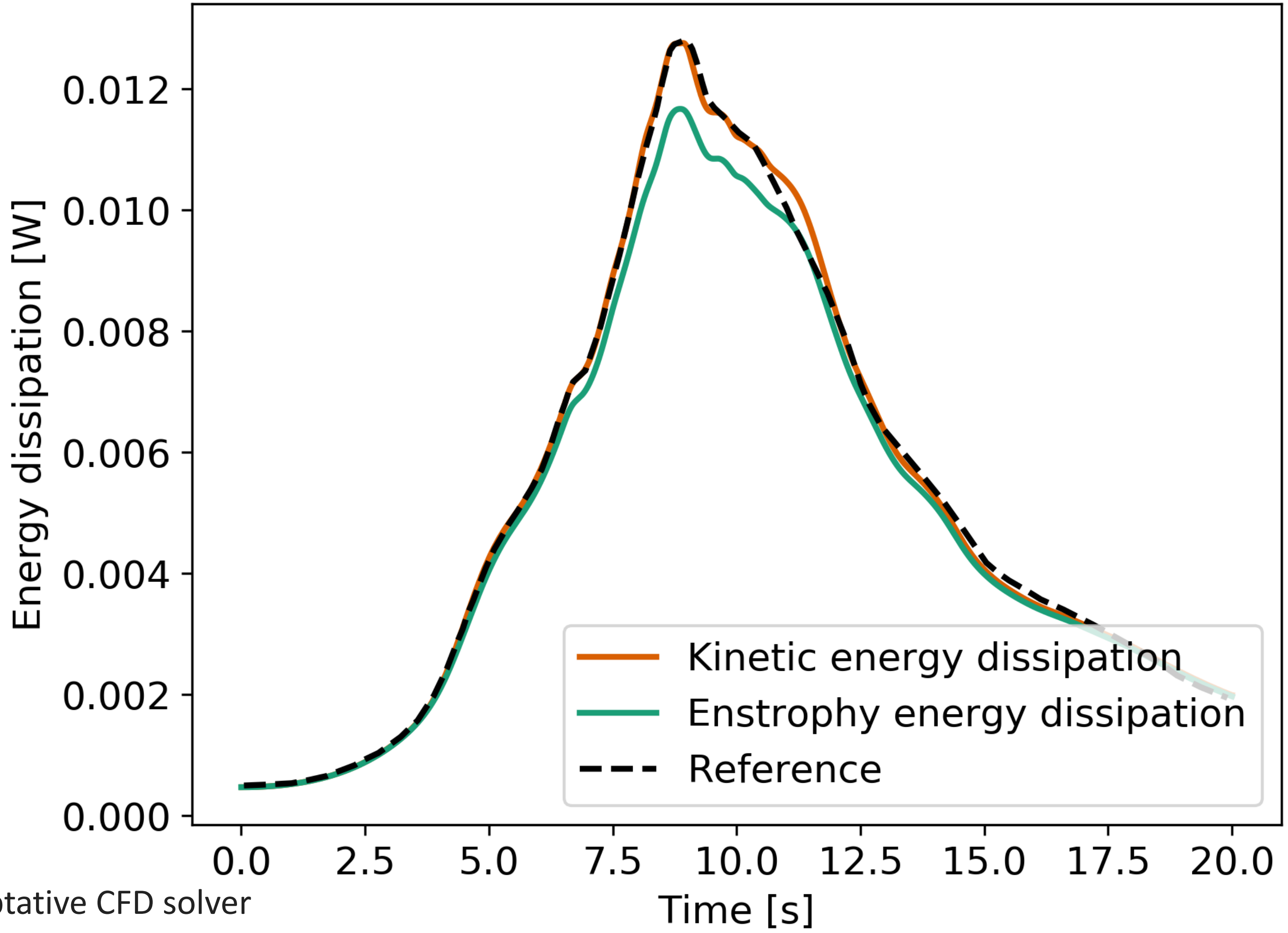
In absence of numerical dissipation, the integral of the enstrophy should be equal to the decay of kinetic energy

Q1-Q1 –$256x^3$

Kinetic energy dissipation makes sense

Enstrophy is off

<u>67.9M DOFs</u>



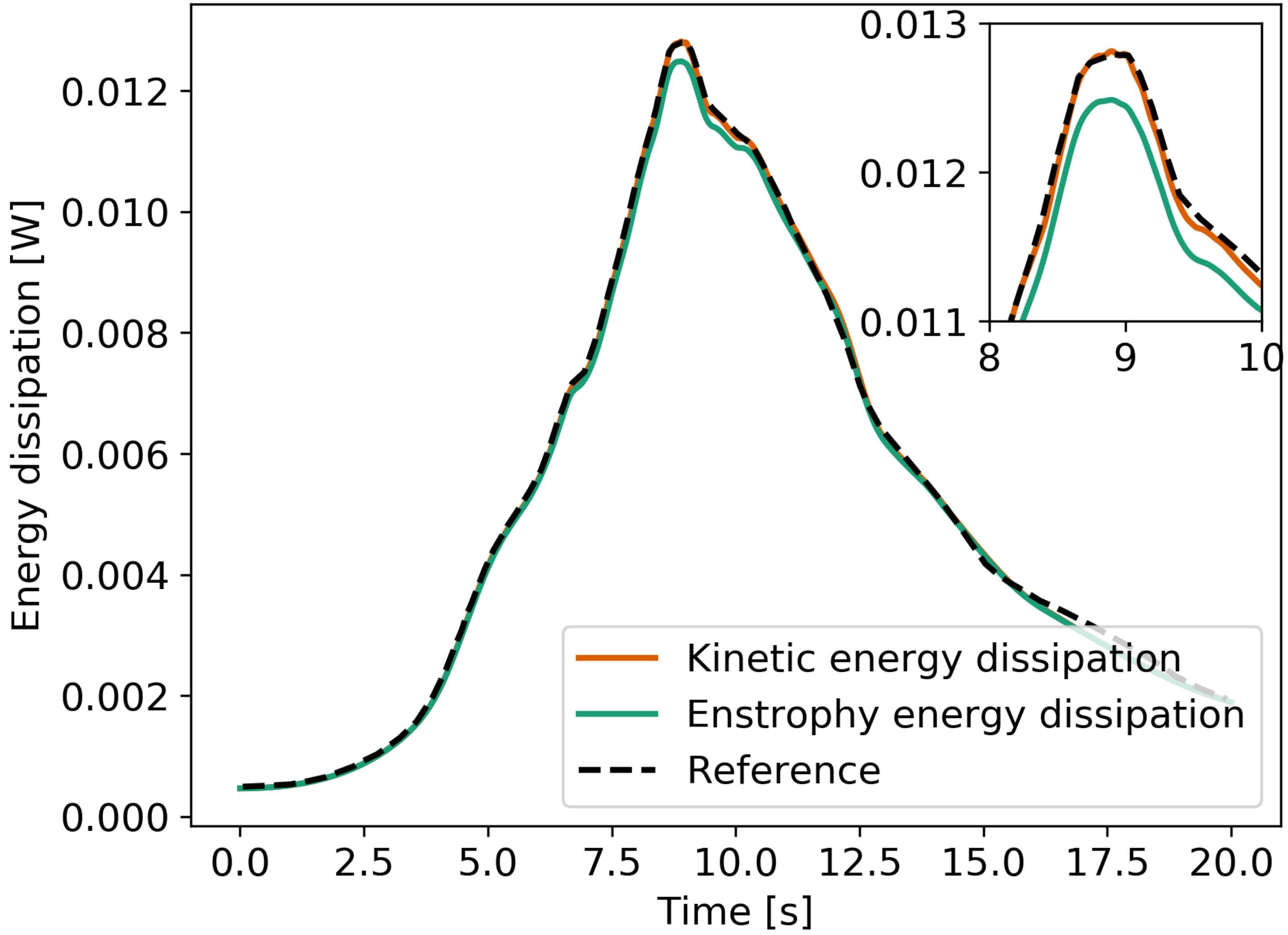
Blais et al. "Lethe: An open-source parallel high-order adaptative CFD solver for incompressible flows." *Software X* 12 (2020)

Q2-Q2 –128^3

Dramatic change

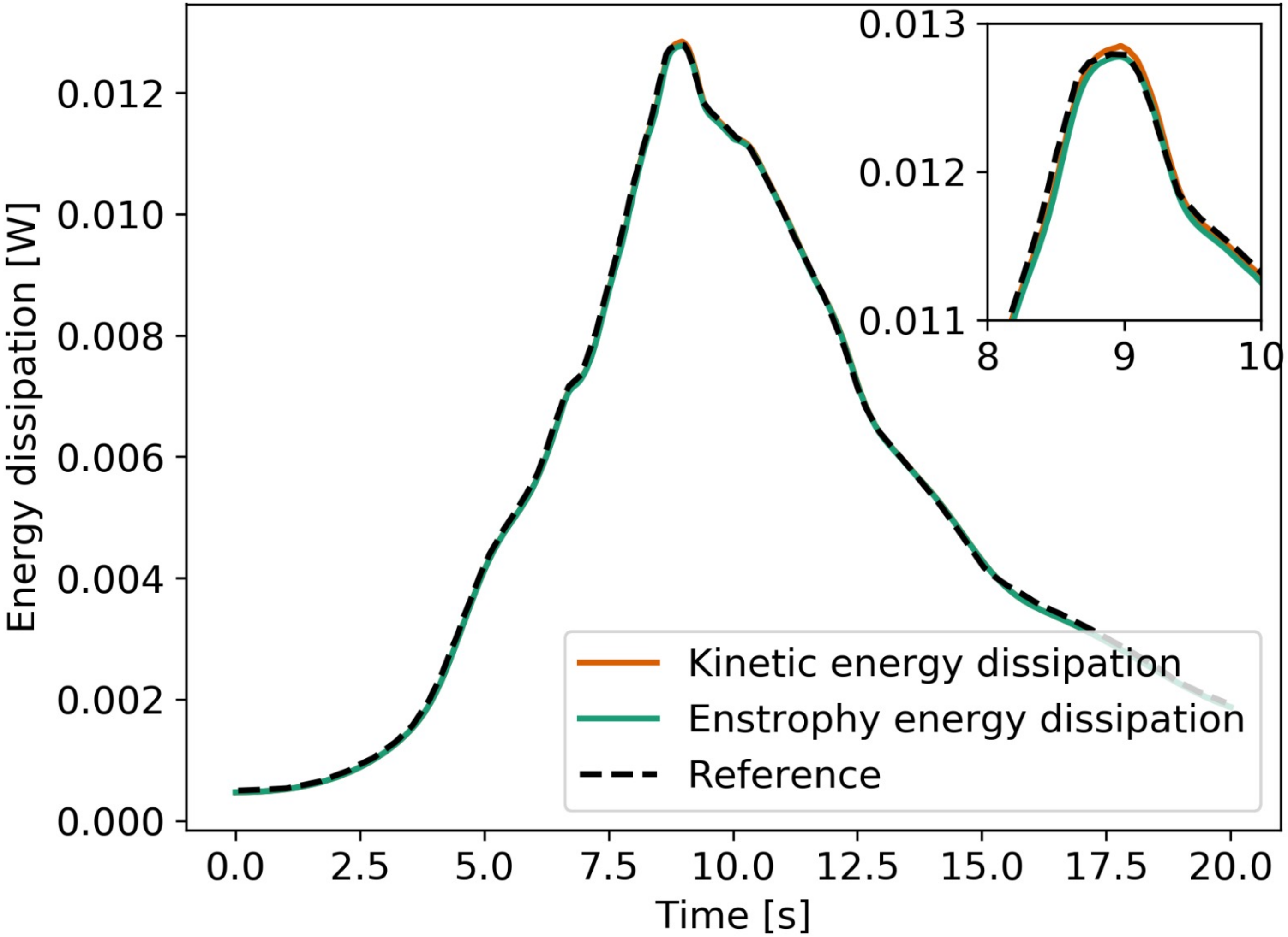
Good agreement for enstrophy

- 67.9M DOFs



Q3-Q3 –128^3

250M DOFs

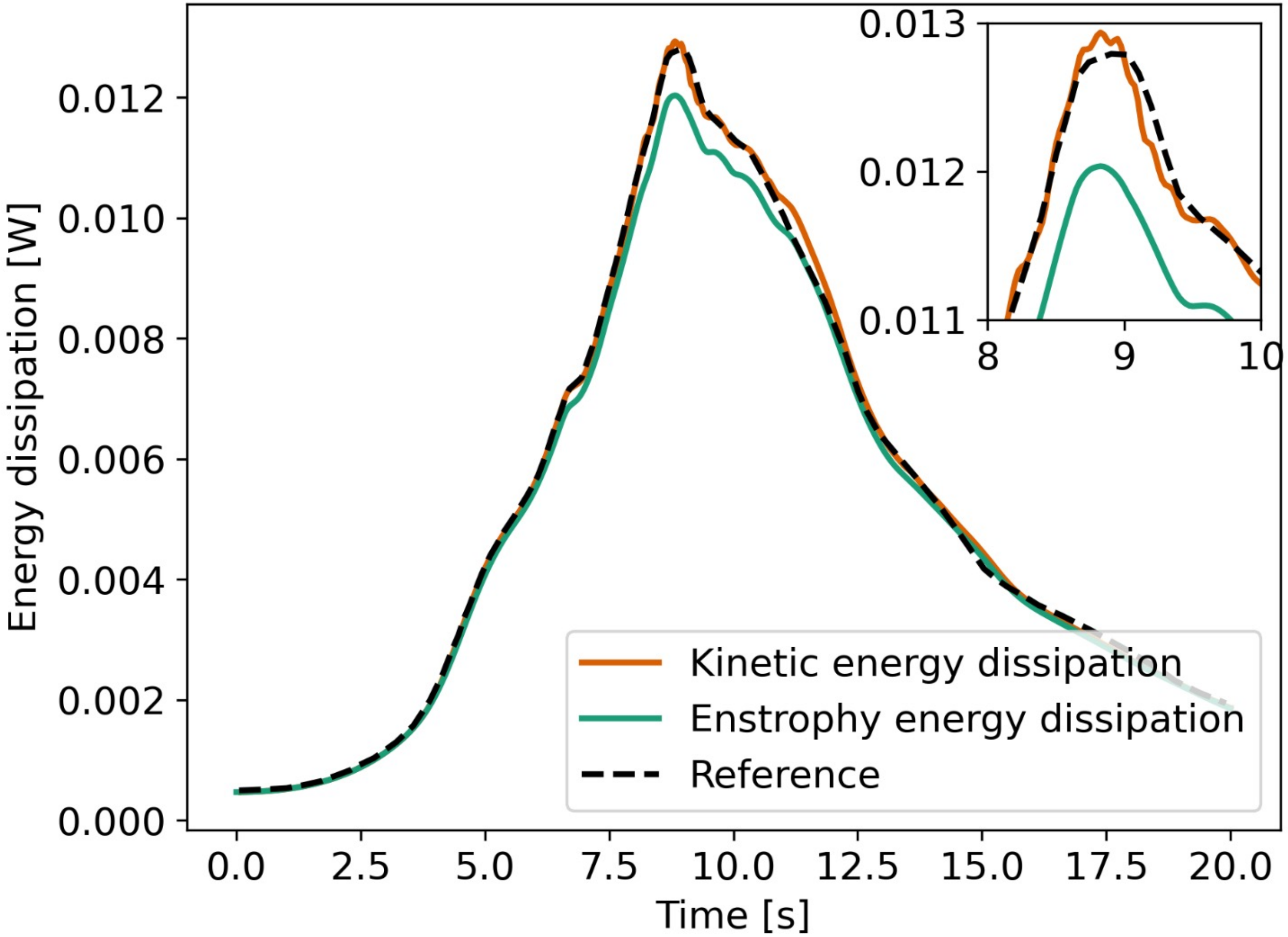


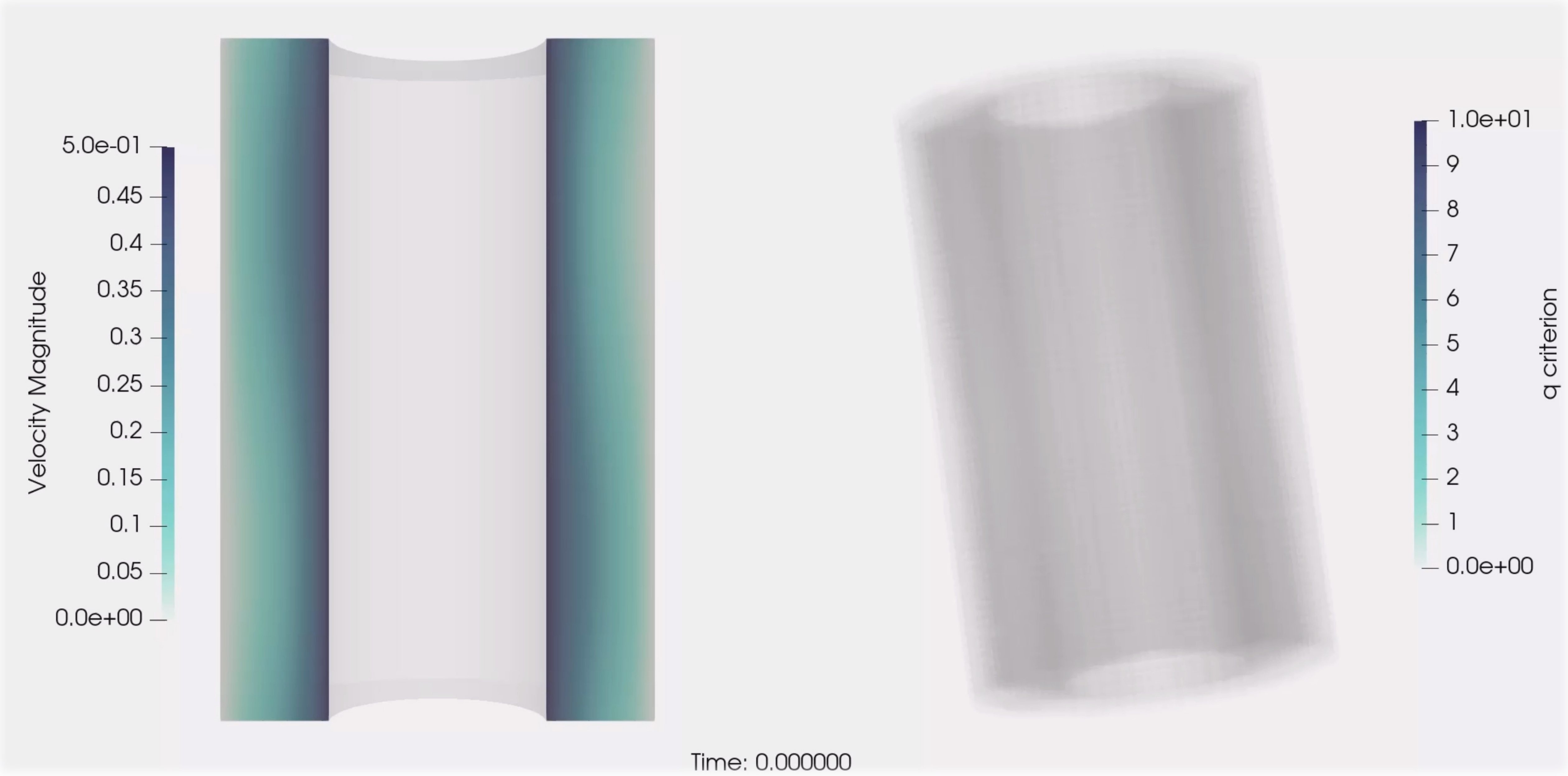
Q3-Q3 –64^3

Even coarser mesh give decent results

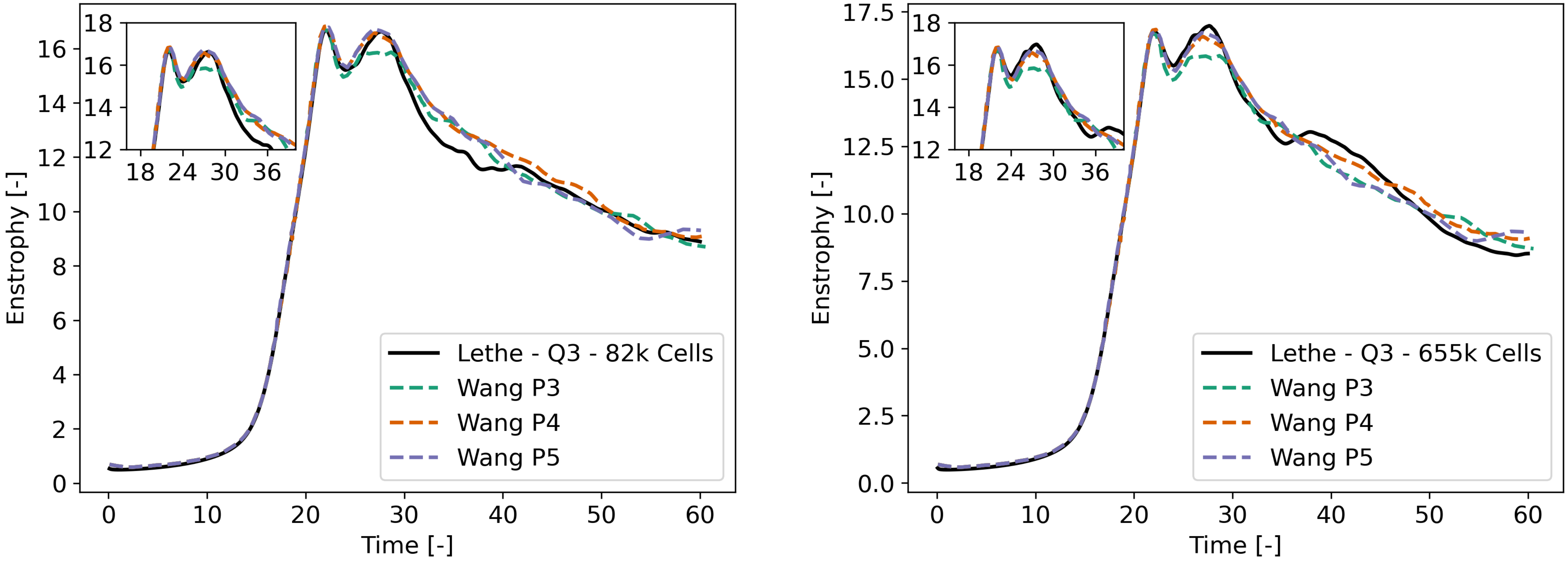
30M DOFs

- Runs in 2 hours on a desktop




5.0e-01
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0.0e+00
Velocity Magnitude
1.0e+01
9
8
7
6
5
4
3
2
1
0.0e+00
q criterion
Time: 0.000000

Enstrophy over time



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High-order Unresolved CFD-DEM

Model formulation

Volume-Averaged Navier-Stokes equations

$$\frac{\partial\left(\epsilon_f\right)}{\partial t} + \nabla \cdot \left(\epsilon_f \boldsymbol{u}_f\right) = 0$$

$$\frac{\partial\left(\epsilon_f \boldsymbol{u}_f\right)}{\partial t} + \nabla \cdot \left(\epsilon_f \boldsymbol{u}_f \otimes \boldsymbol{u}_f\right) = -\frac{\epsilon_f}{\rho_f}\nabla p + \epsilon_f \nabla \cdot \left(\boldsymbol{\tau}_f\right) + \frac{\boldsymbol{F_{pf}^{A}}}{\rho_f}$$

We discretize the VANS equations using stabilized FEM

Continuity

$$\int_\Omega \left(\frac{\partial \left(\epsilon_f\right)}{\partial t} + \epsilon_f \nabla \cdot \boldsymbol{u} + \boldsymbol{u} \nabla \epsilon_f \right) q d\Omega + \underbrace{\mathcal{SR} \cdot \left(\tau_u \nabla q\right) d\Omega_k}_{\text{PSPG}} = 0$$

Momentum

$$\int_\Omega \rho_f \left(\epsilon_f \frac{\partial \boldsymbol{u}}{\partial t} + \epsilon_f \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) \cdot \boldsymbol{v} d\Omega + \int_\Omega \Big(\epsilon_f \nu \left(\nabla \boldsymbol{u} : \nabla \boldsymbol{v} \right) \Big) + \Big(\nu \nabla \boldsymbol{u} \nabla \epsilon_f \cdot \boldsymbol{v} \Big) d\Omega$$

$$- \frac{1}{\rho_f} \int_\Omega \Big(\epsilon_f p \cdot \nabla \boldsymbol{v} + p \nabla \epsilon_f \cdot \boldsymbol{v} \Big) d\Omega + \frac{1}{\rho_f} \int_\Omega \frac{\boldsymbol{F_{pf}}}{V_\Omega} \cdot \boldsymbol{v} d\Omega d\Omega$$

$$+ \underbrace{\sum_K \int_{\Omega_k} \mathcal{SR} \cdot \left(\tau_u \boldsymbol{u} \cdot \nabla \boldsymbol{v}\right) d\Omega_k}_{\text{SUPG}} + \underbrace{\sum_K \int_{\Omega_k} \gamma \left(\frac{\partial \epsilon_f}{\partial t} + \nabla \cdot \left(\epsilon_f \boldsymbol{u}\right) \right) \left(\nabla \cdot \boldsymbol{v}\right) d\Omega_k}_{\text{grad}-\text{div}} = 0$$

Multiple stabilization term

$$\mathcal{SR} = \frac{\partial\left(\epsilon_f \boldsymbol{u}_f\right)}{\partial t} + \nabla \cdot \left(\epsilon_f \boldsymbol{u}_f \otimes \boldsymbol{u}_f\right) + \frac{\epsilon_f}{\rho_f}\nabla p - \epsilon_f \nu \nabla^2 \boldsymbol{u} - \frac{\boldsymbol{F}_{\boldsymbol{pf}}^{\boldsymbol{A}}}{\rho_f}$$

PSPG: Enables equal-order elements

$\sum_K \int_{\Omega_k} \mathcal{SR} \cdot \left(\tau_u \nabla q\right) d\Omega_k$

SUPG: Implicit LES model

$\sum_K \int_{\Omega_k} \mathcal{SR} \cdot \left(\tau_u \boldsymbol{u} \cdot \nabla \boldsymbol{v}\right) d\Omega_k$

Grad-div: Enhances mass conservation

$\sum_K \int_{\Omega_k} \gamma \left(\frac{\partial \epsilon_f}{\partial t} + \nabla \cdot \left(\epsilon_f \boldsymbol{u}\right)\right) \left(\nabla \cdot \boldsymbol{v}\right) d\Omega_k$

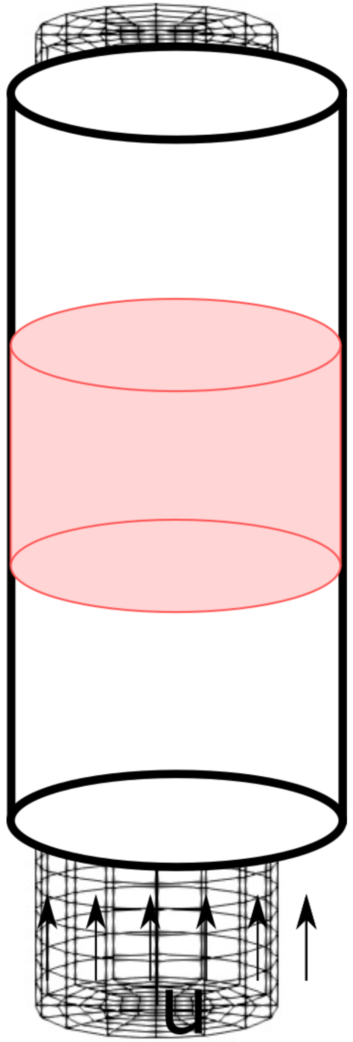
Simple example

Flow through a pipe

- Slip on the walls
- Constant velocity inlet
- Jump in the void fraction

$$\epsilon_f = \epsilon_f(\boldsymbol{x})$$

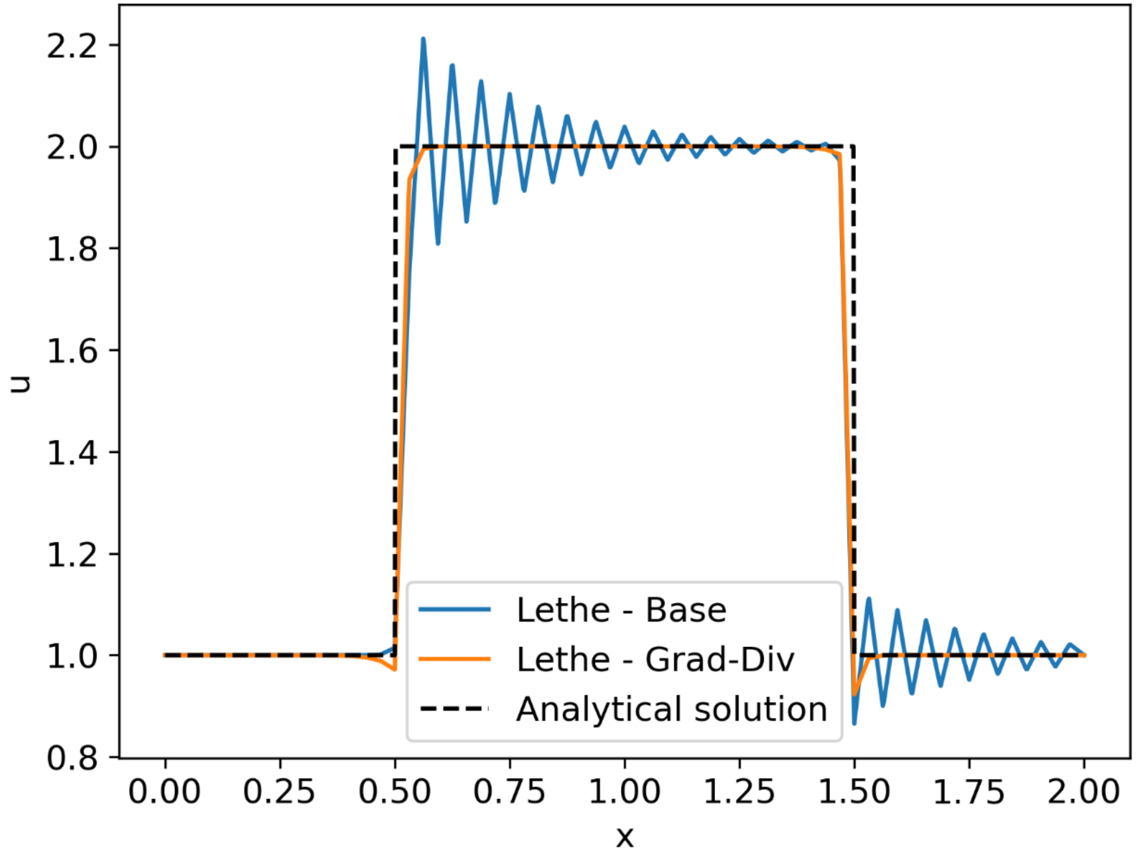
Mass must be conserved, so velocity must increase if the porosity decreases



Impact of stabilization

SUPG + PSPG leads to strong oscillation when the void fraction varies

Additional Grad-div stabilization in the momentum equation remedies this issue



Discrete Element Method

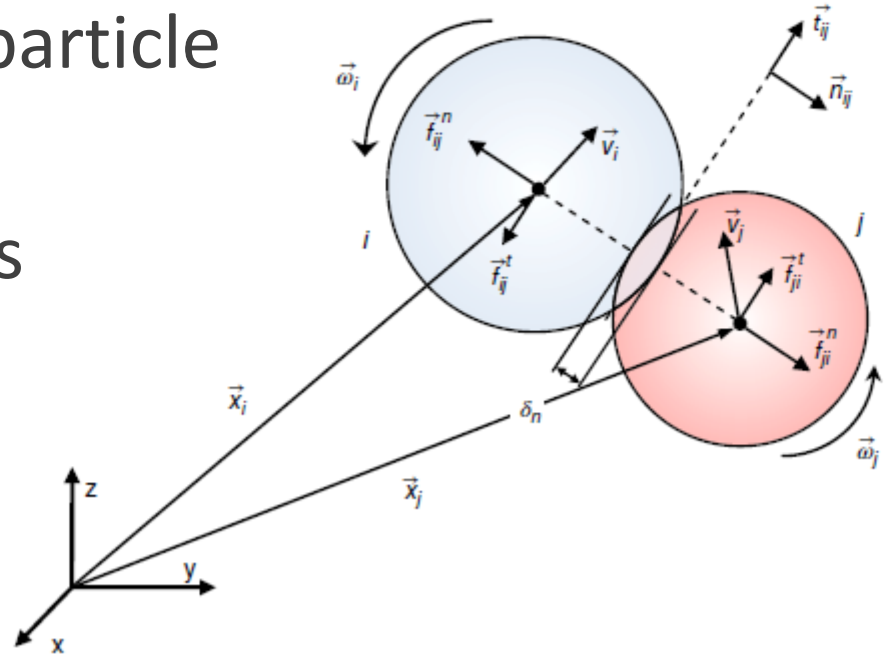
Newton second's law solved for each particle

$$m_i \frac{\partial \boldsymbol{u}_{p,i}}{\partial t} = \sum_{j \in C_i} \boldsymbol{f}_{c,ij} + \sum_{w} \boldsymbol{f}_{c,iw} + m_i \boldsymbol{g} + \boldsymbol{f}_{\boldsymbol{fp},\boldsymbol{i}}$$

Contact forces are calculated by allowing particle overlap

Overlap is decomposed into two directions

- Normal
- Tangential



Contact detection

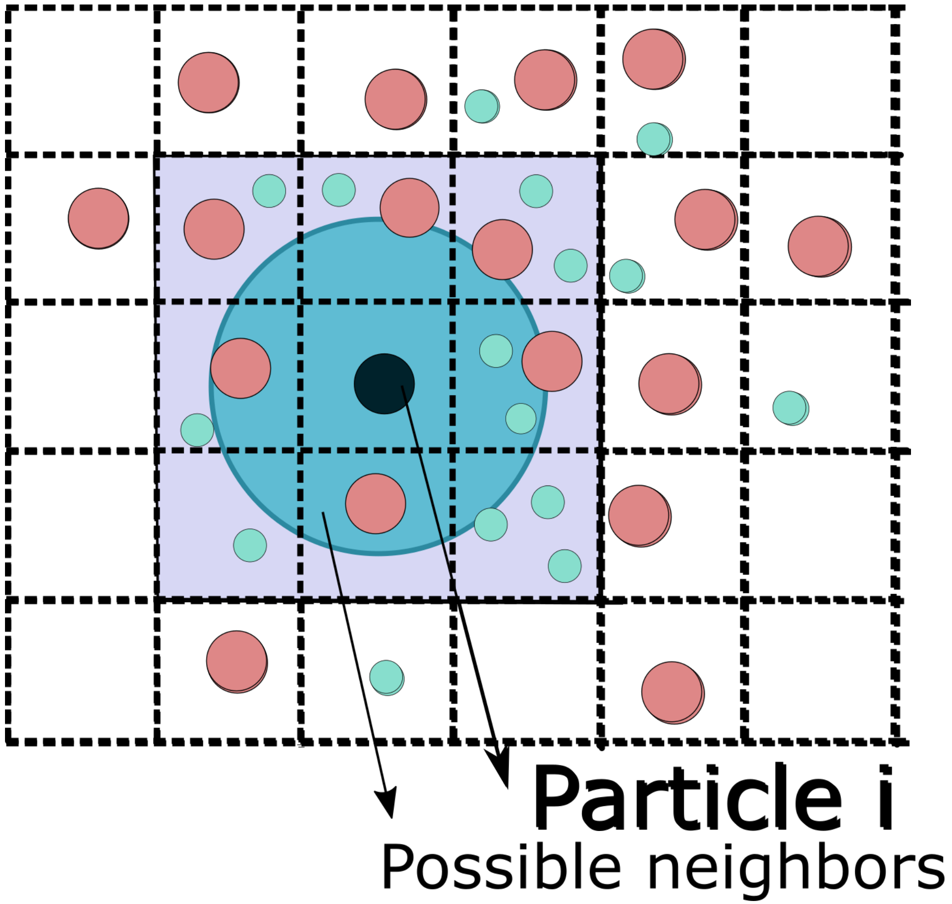
Binned list

- $O(n_p)$ scaling

Superposed by a Verlet list

Algorithmic decisions

- List is refreshed every n iterations dynamically
- CFD mesh is used as contact detection structure
- Domain decomposition is used to parallelize the calculations

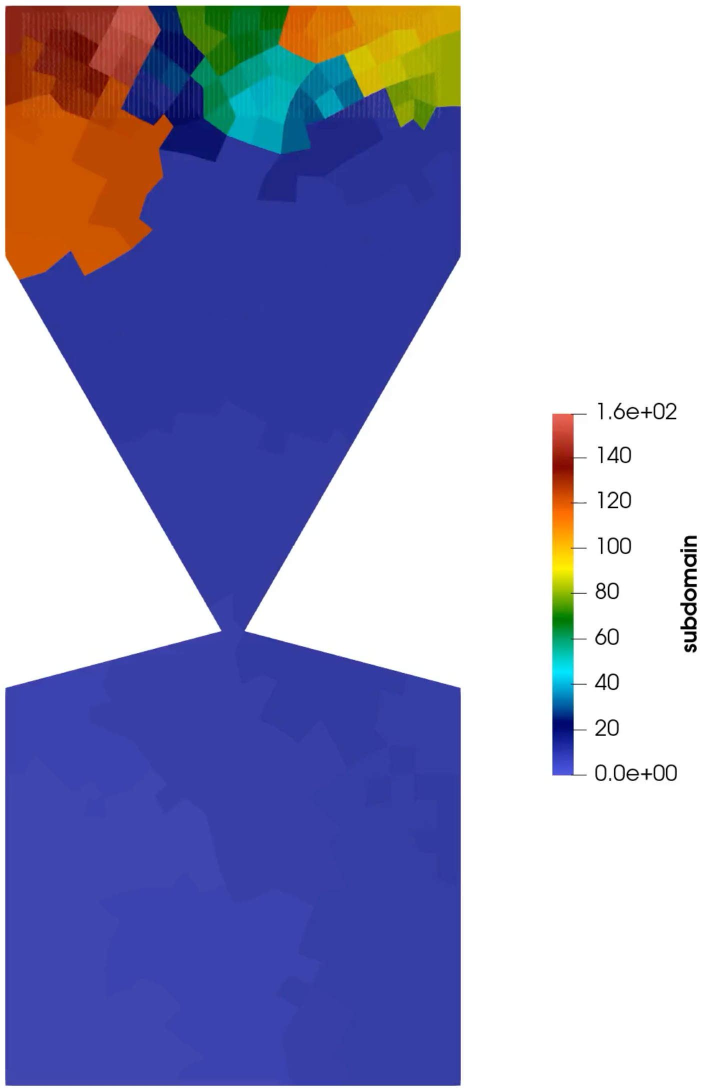


Parallelization and load-balancing

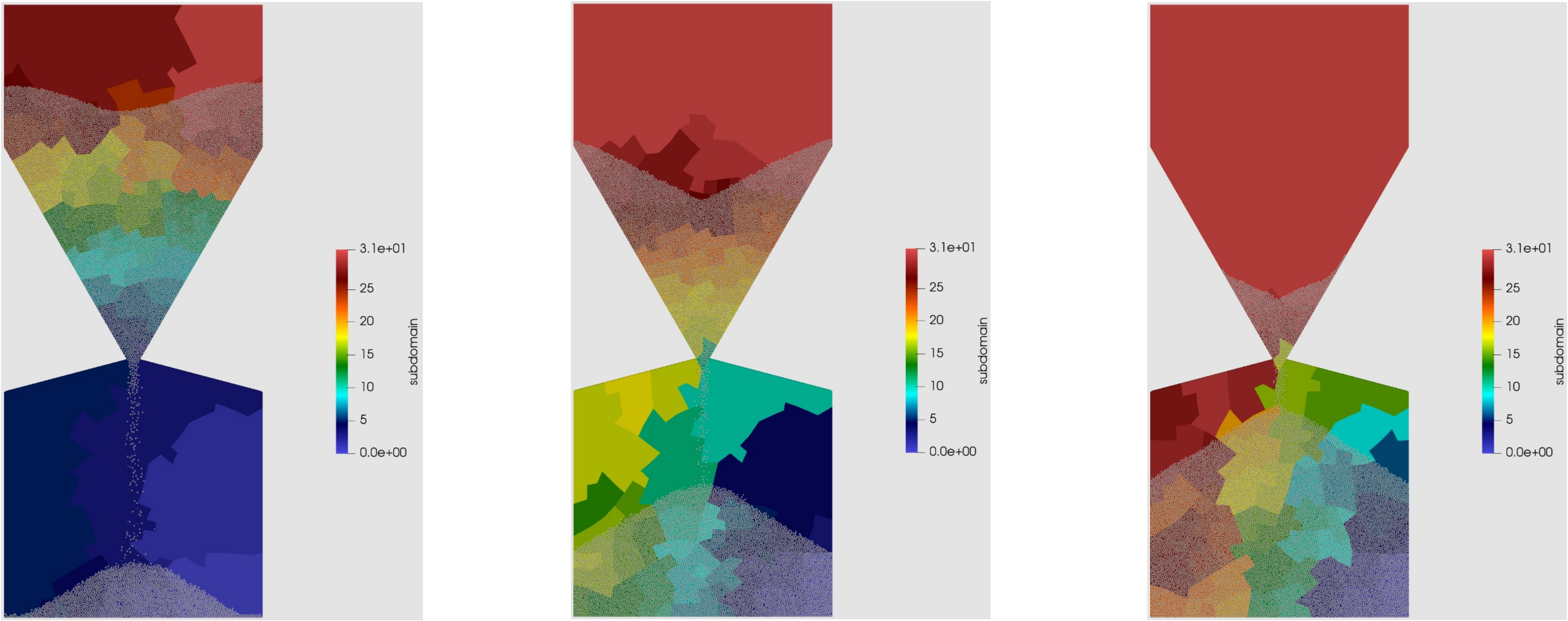
Underlying grid can be decomposed

As particle move, load dynamically evolve

Parallel decomposition must thus follow



Load-balancing



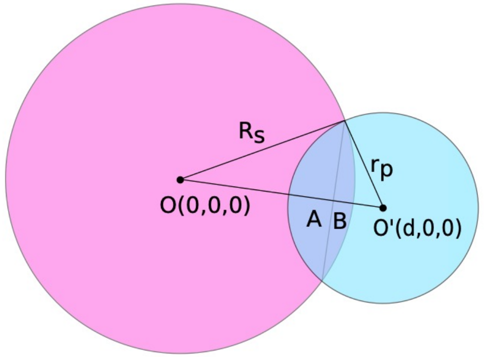
Time

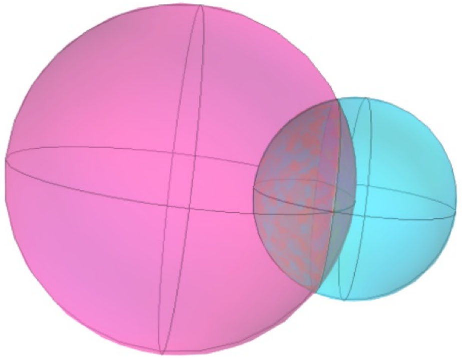
Void fraction calculation

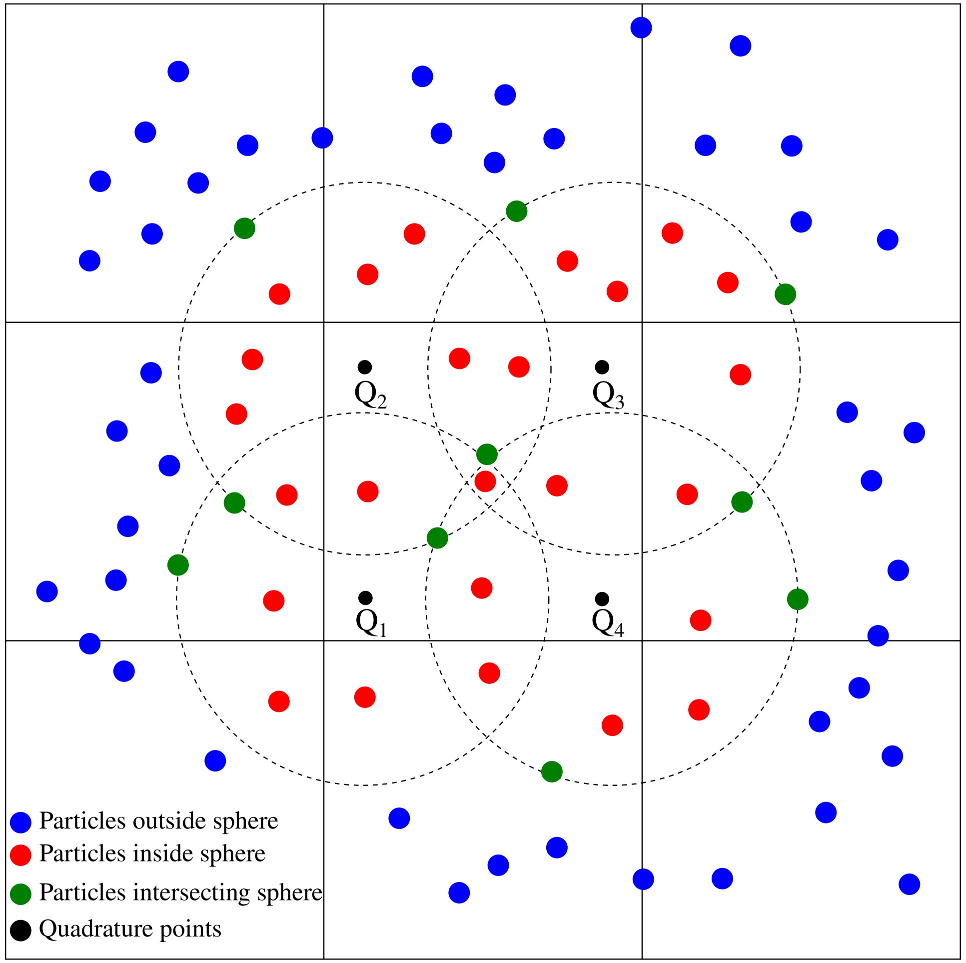
Challenges:

- Continuity in time
- Ideally as independent of the mesh as possible

Solution is a spherical quadrature centered void fraction calculation







Unresolved CFD-DEM model

Fluid

Volume-Averaged Navier-Stokes
(VANS form A)

$$\frac{\partial\left(\epsilon_f\right)}{\partial t}+\nabla\cdot\left(\epsilon_f\boldsymbol{u}_f\right)=0$$

$$\frac{\partial\left(\epsilon_f\boldsymbol{u}_f\right)}{\partial t}+\nabla\cdot\left(\epsilon_f\boldsymbol{u}_f\otimes\boldsymbol{u}_f\right)=-\frac{\epsilon_f}{\rho_f}\nabla p+\frac{\epsilon_f}{\rho_f}\nabla\cdot\left(\boldsymbol{\tau}_f\right)+\frac{\boldsymbol{F}_{\boldsymbol{pf}}^{\boldsymbol{A}}}{\rho_f}$$

Solid particles

Newton's second law

$$m_i\frac{\partial\boldsymbol{u}_{p,i}}{\partial t}=\sum_{j\in C_i}\boldsymbol{f}_{c,ij}+\sum_{w}\boldsymbol{f}_{c,iw}+m_i\boldsymbol{g}+\boldsymbol{f}_{\boldsymbol{fp,i}}$$

Hydrodynamic forces

$$\boldsymbol{F}_{pf}=\frac{1}{\Delta V}\sum_{i}^{n_p}\boldsymbol{f}_{pf,i}$$

$$\boldsymbol{f}_{pf,i}=\boldsymbol{f}_{d,i}+\boldsymbol{f}_{\nabla p,i}+\boldsymbol{f}_{\nabla\cdot\boldsymbol{\tau},i}+\boldsymbol{f}_{\mathrm{Saff},i}$$

- **Pressure gradient**
- **Viscous stress**
- **Drag**
- **Lift forces**

Case 1: Spouted bed

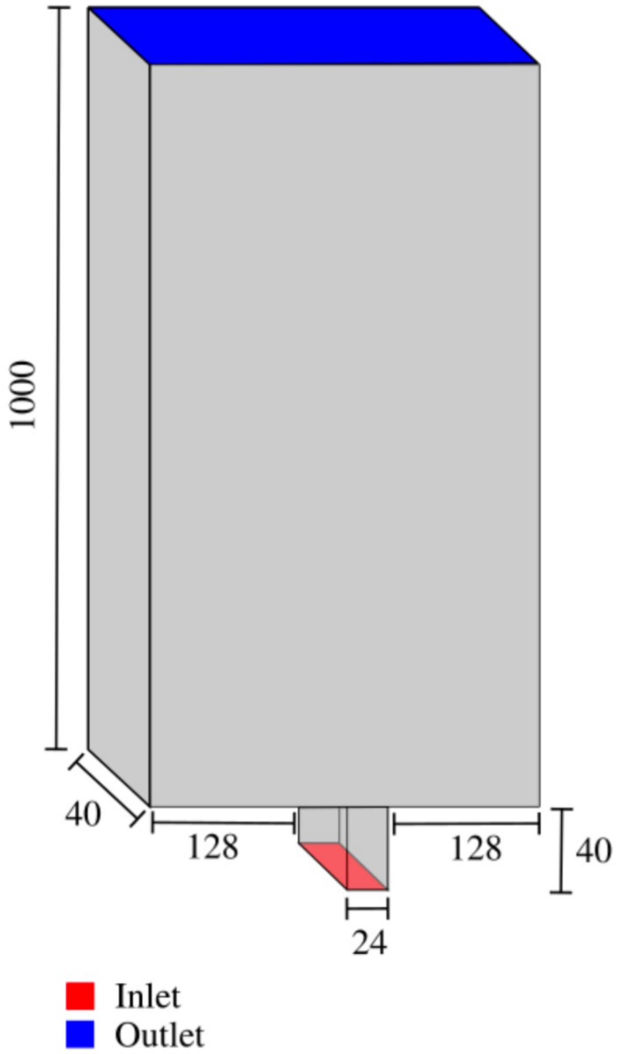
Unresolved CFD-DEM

El Geitani, T., Golshan, S., & Blais, B. (2023). Toward High-Order CFD-DEM: Development and Validation. *Industrial & Engineering Chemistry Research*, *62*(2), 1141-1159.

Spouted bed contactor

Physical parameters

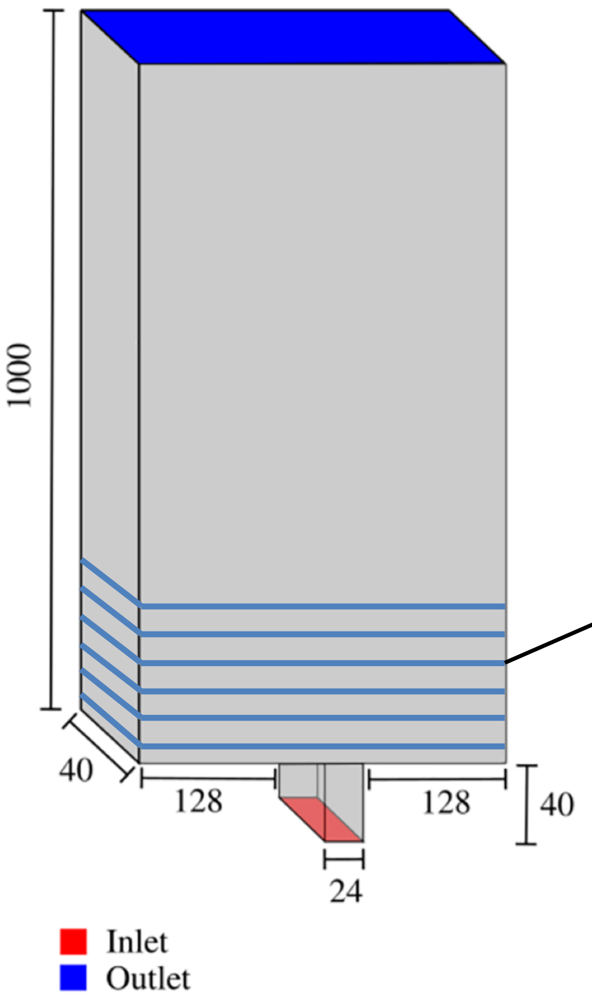
- Glass beads ($\rho_s = 2500 \frac{kg}{m^3}$ and $d_p = 2.5mm$)
- Approx 180k particles
- Air
- 30s of flow simulated

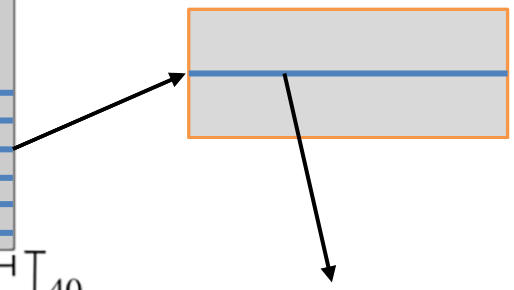


El Geitani, T., Golshan, S., & Blais, B. (2023). Toward High-Order CFD-DEM: Development and Validation. *Industrial & Engineering Chemistry Research*, *62*(2), 1141-1159.

Validation strategy

Simulation Setup

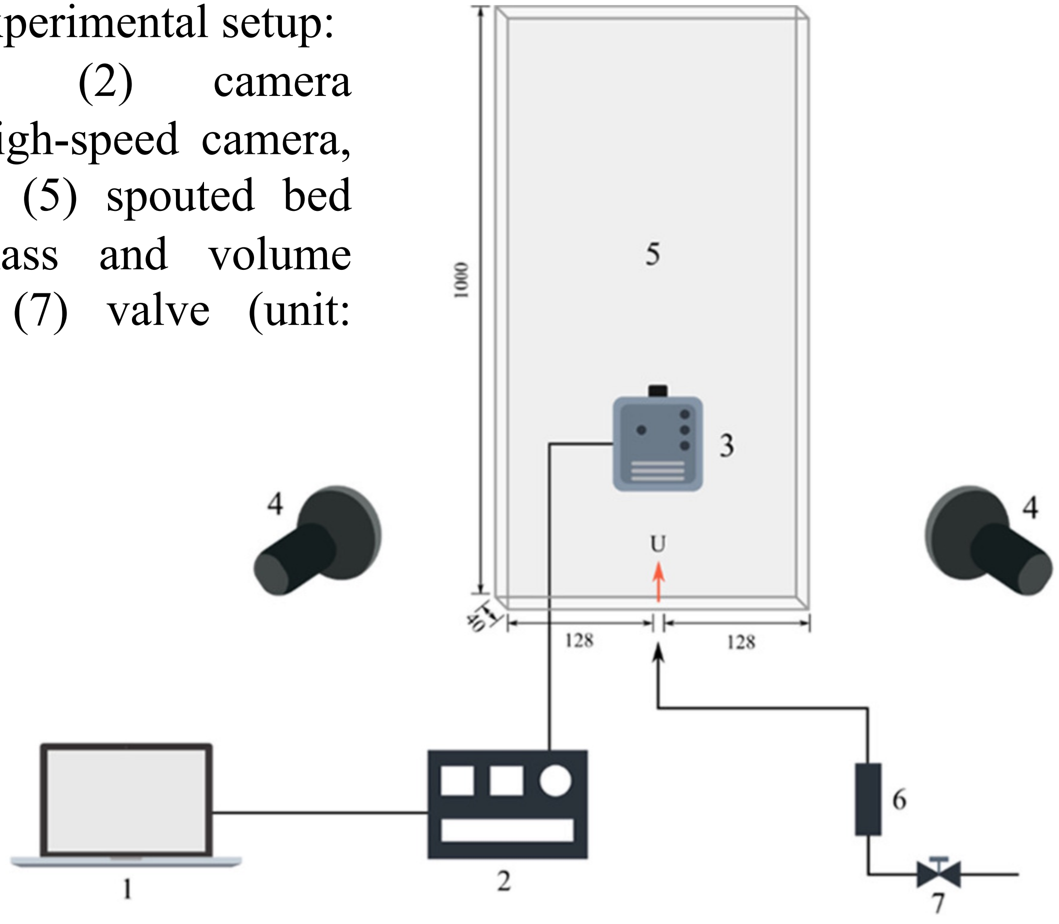




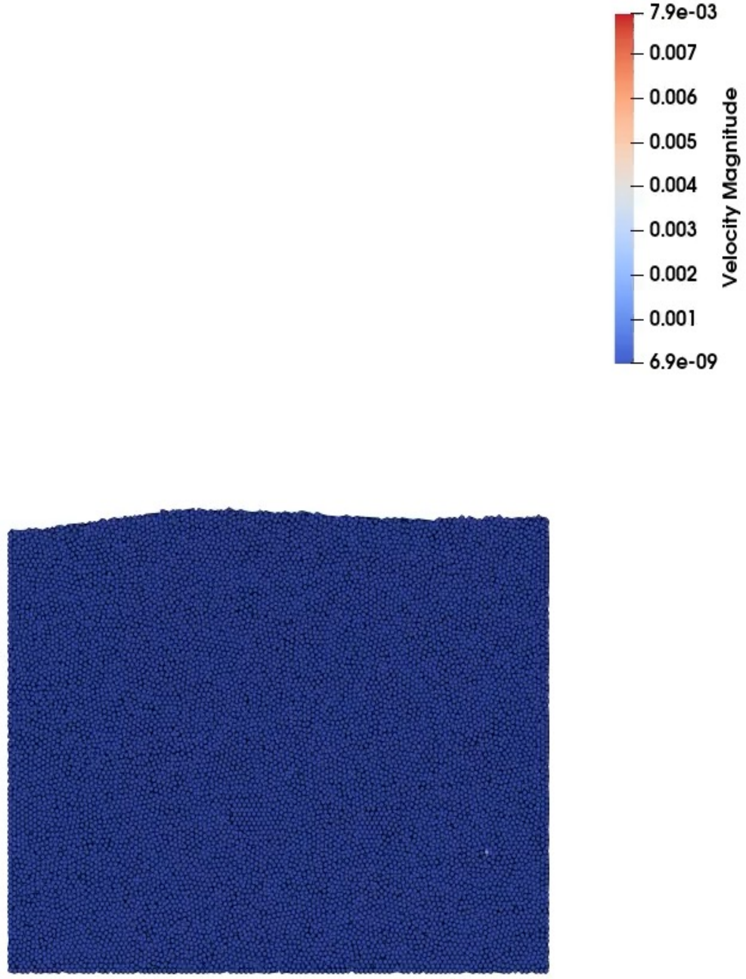
Calculate time-averaged particle velocity magnitude

Experimental Setup

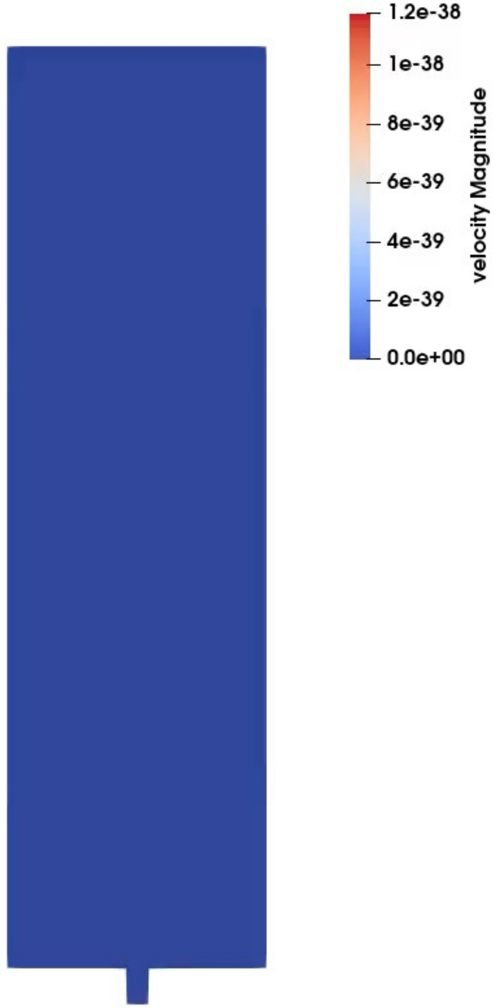
Scheme of the experimental setup: (1) computer, (2) camera controller, (3) high-speed camera, (4) LED lights, (5) spouted bed column, (6) mass and volume controller, and (7) valve (unit: mm) [9].



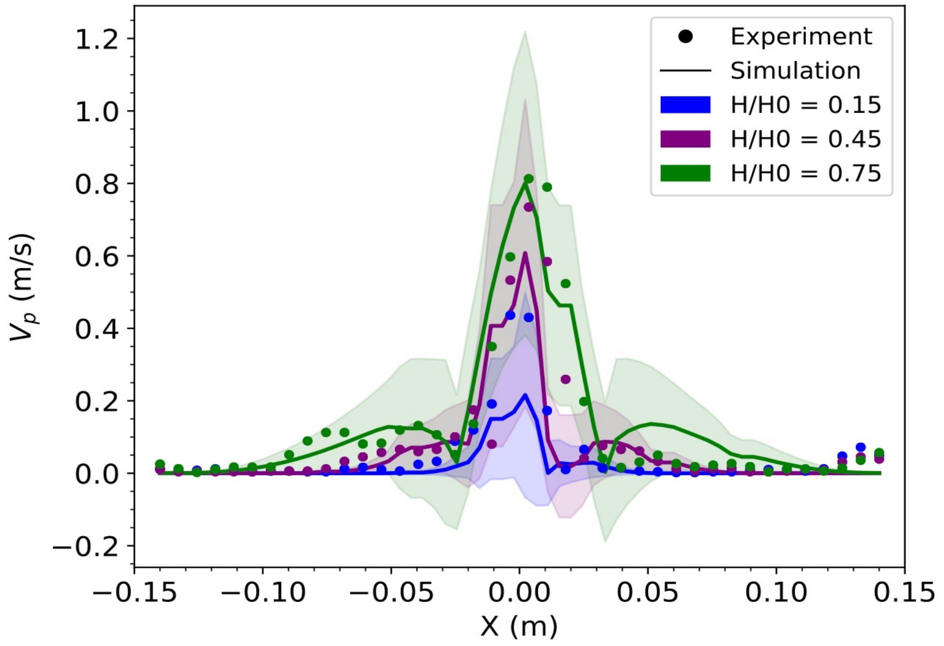
Q1 results

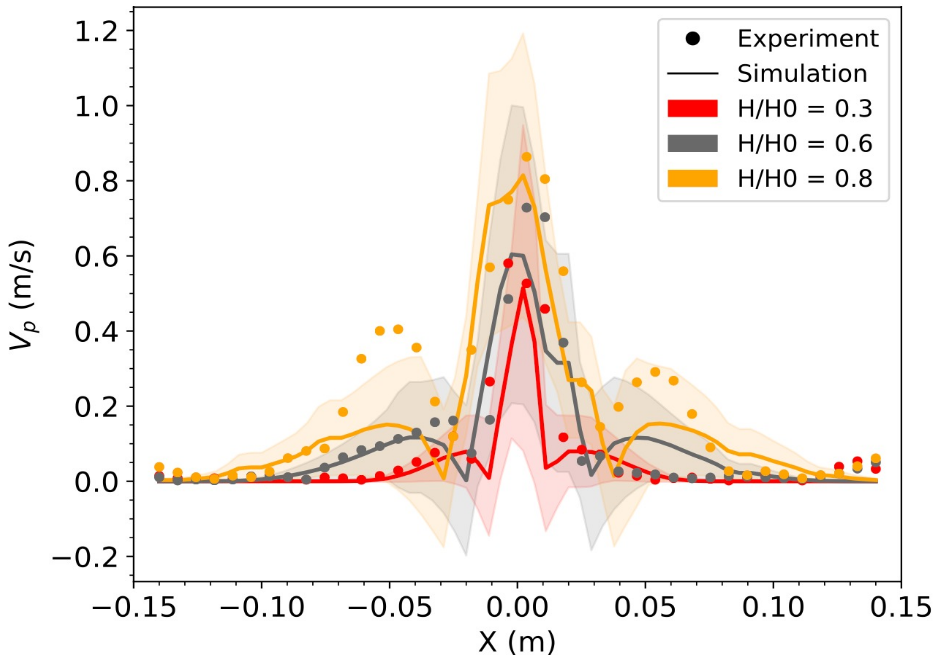


Particles velocity

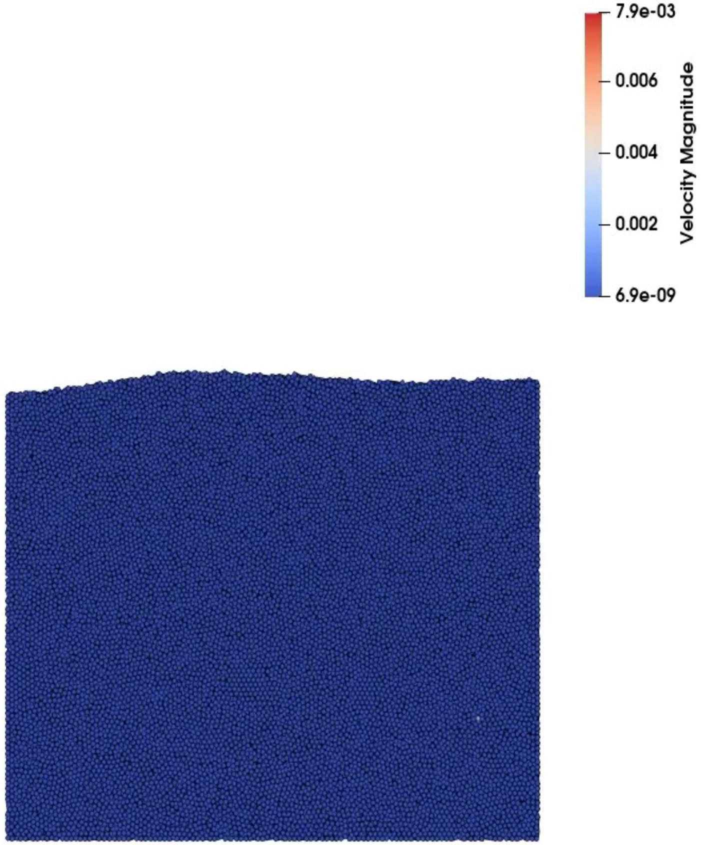


Fluid velocity

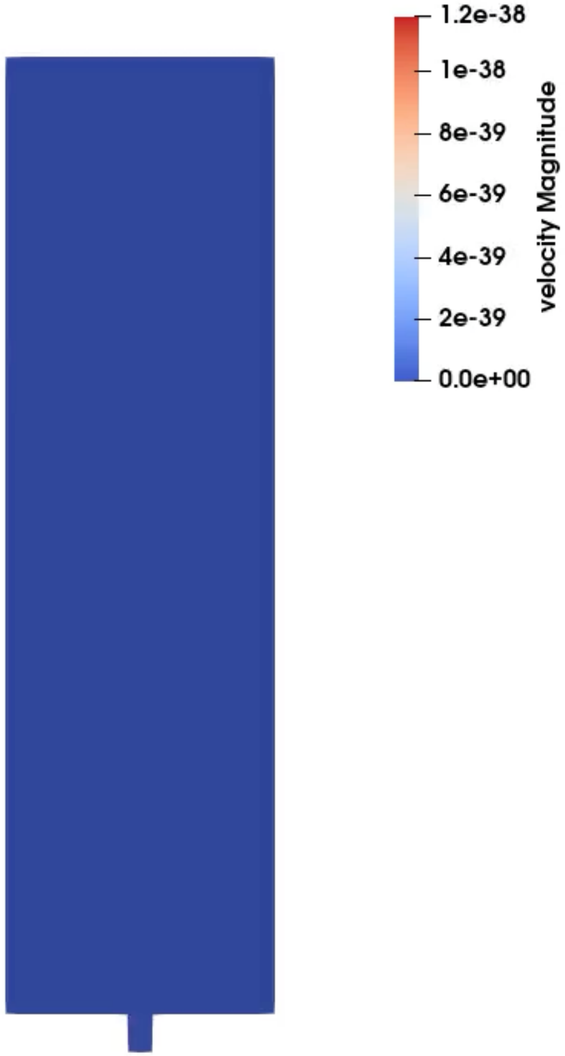




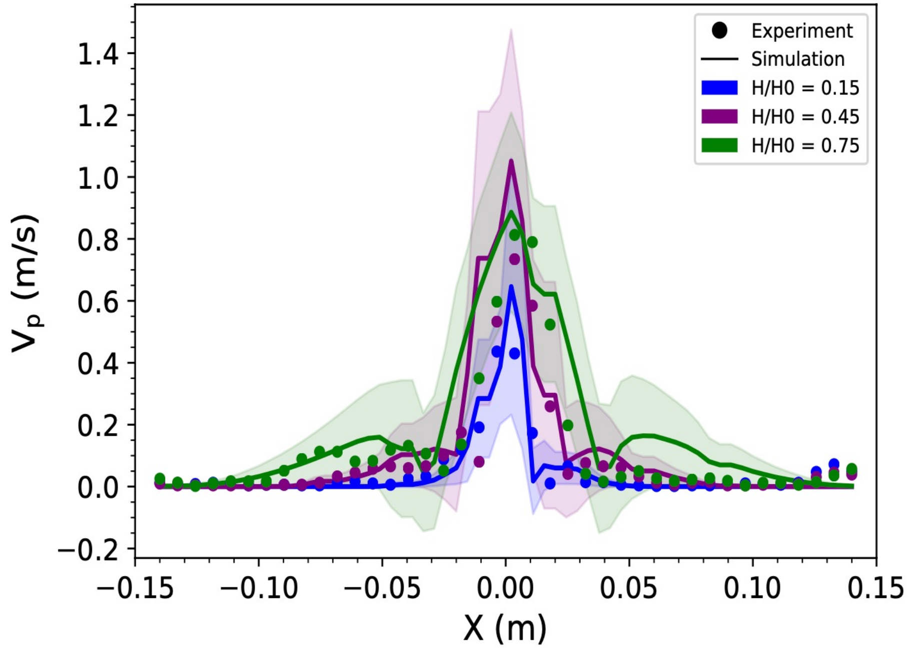
Q2 results

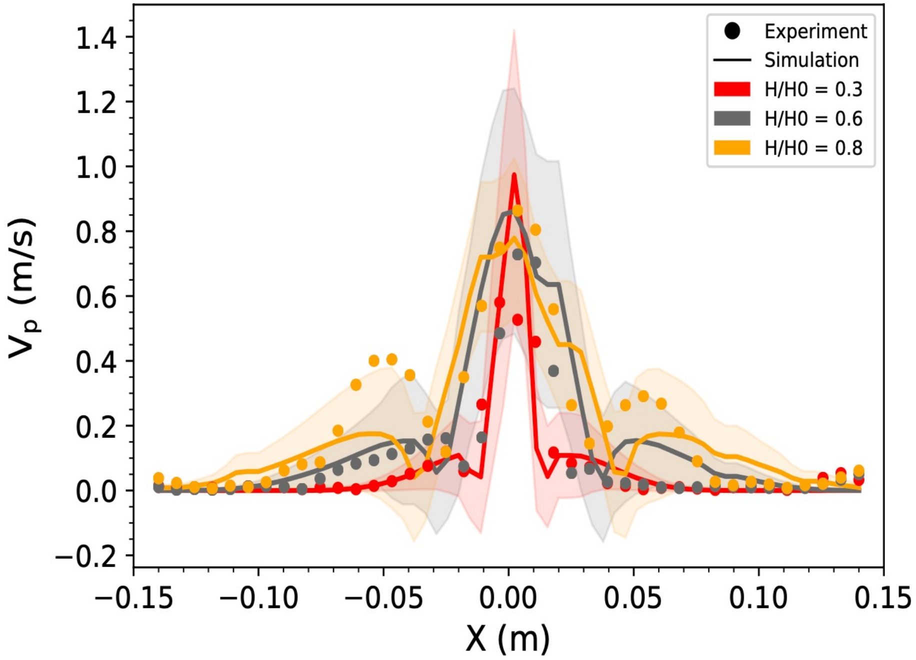


Particles velocity

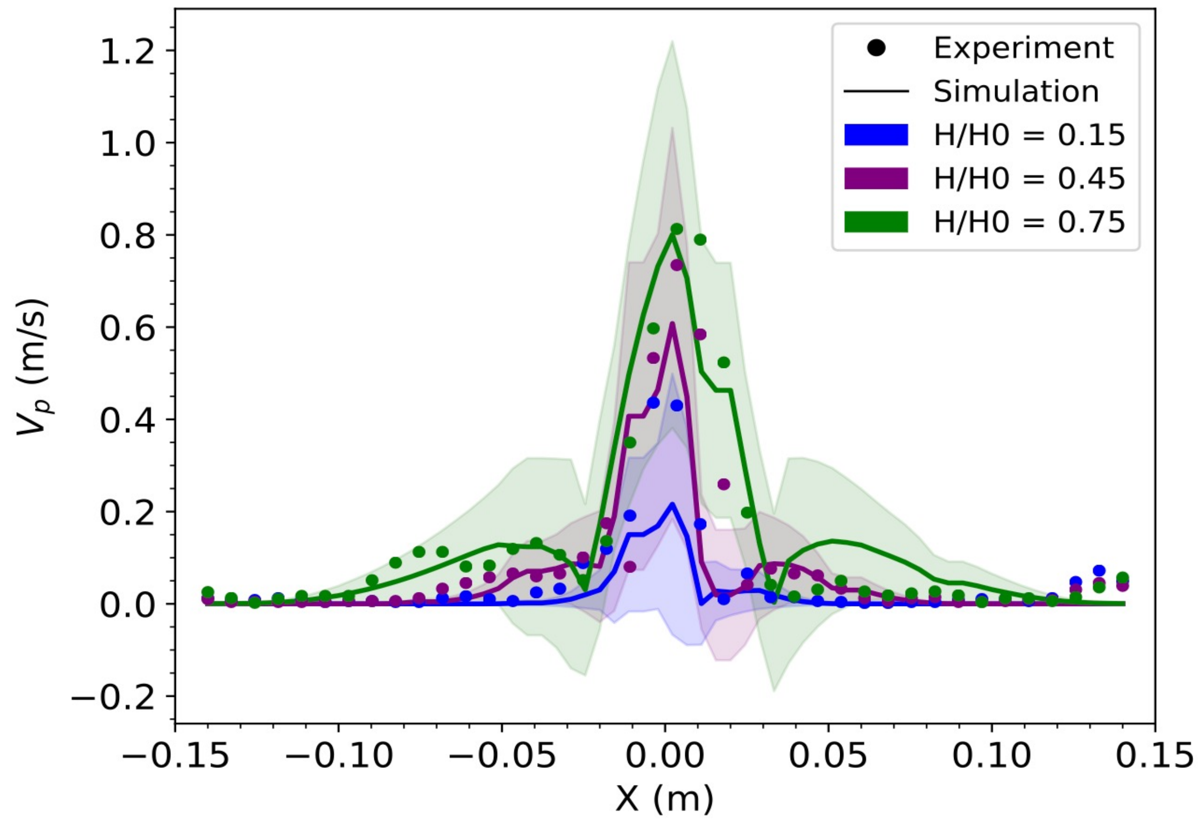


Fluid velocity

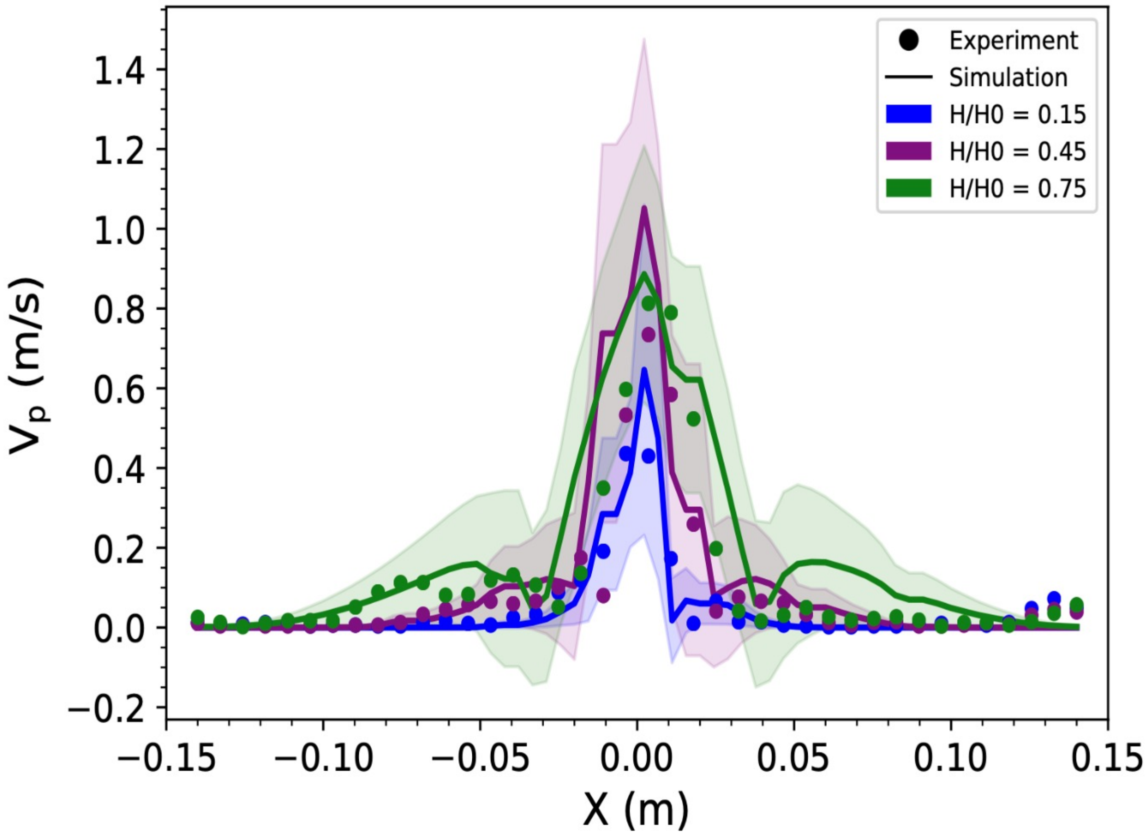




A more direct comparison



Q1 (2nd order)



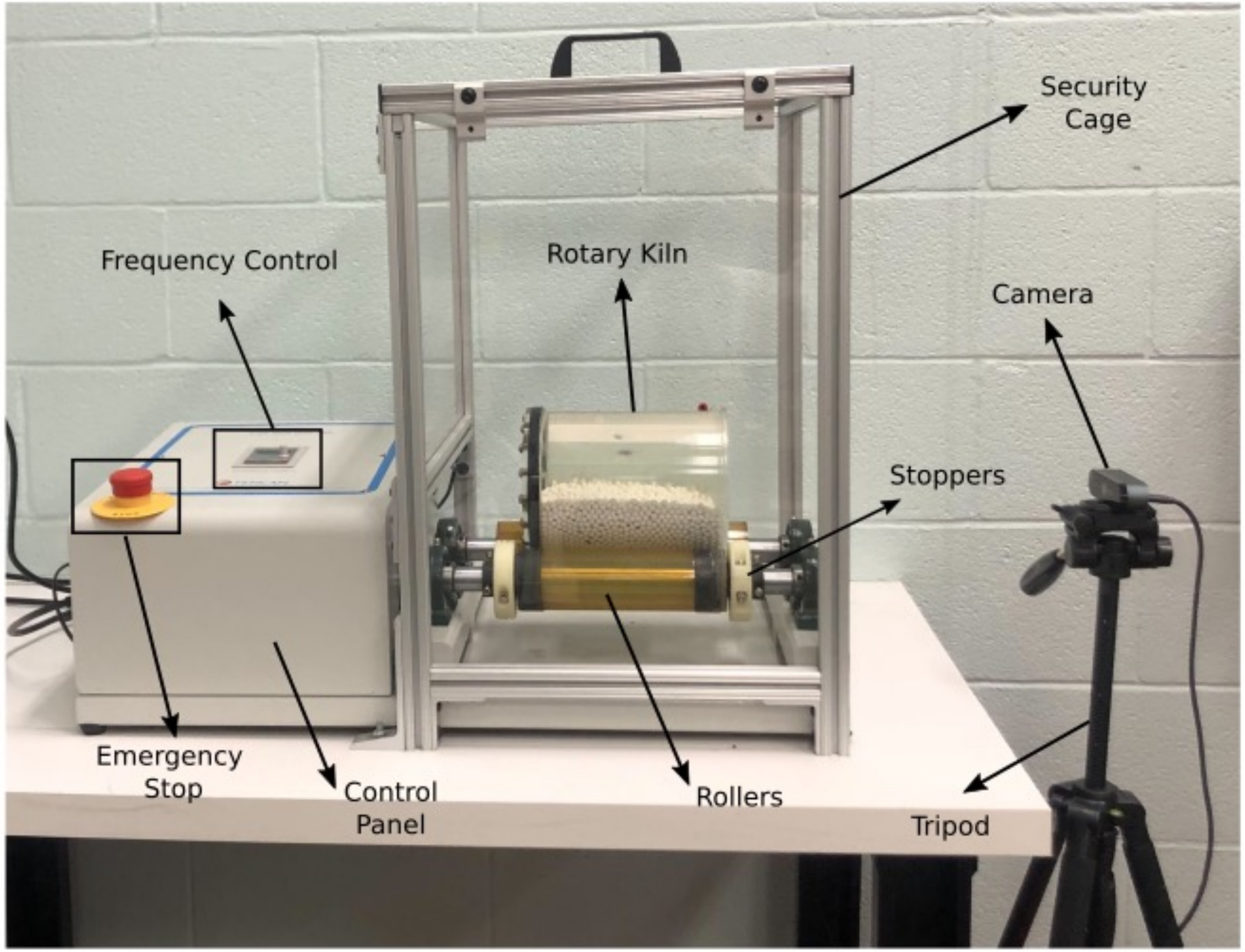
Q2 (3rd order)

Case 2: Solid-liquid mixing drum

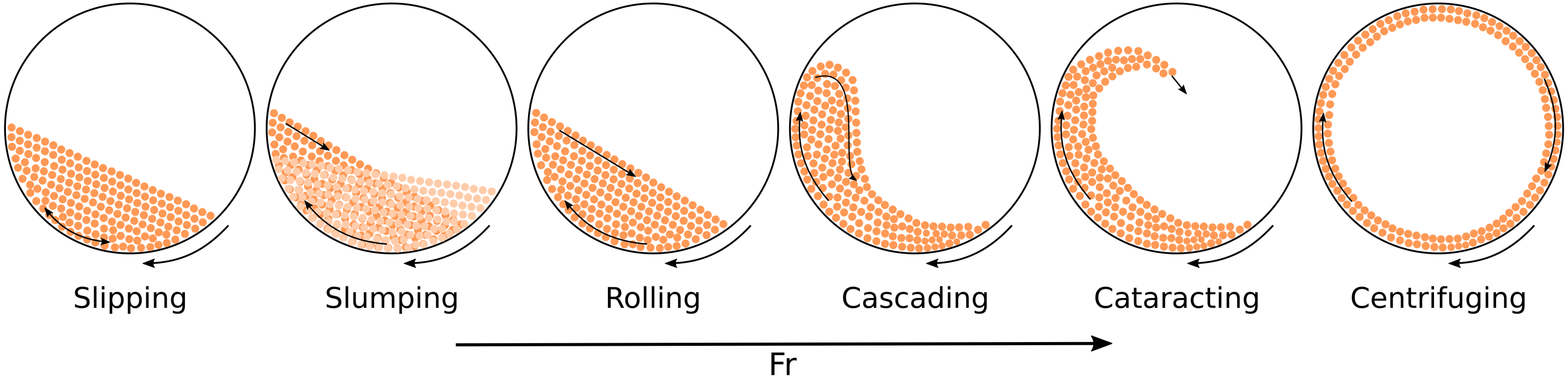
A simple benchmark for unresolved CFD-DEM

El Geitani, Toni, and Bruno Blais. "Solid-liquid rotary kilns: An experimental and CFD-DEM study." Powder Technology 430 (2023): 119008.

Solid-liquid mixing drum

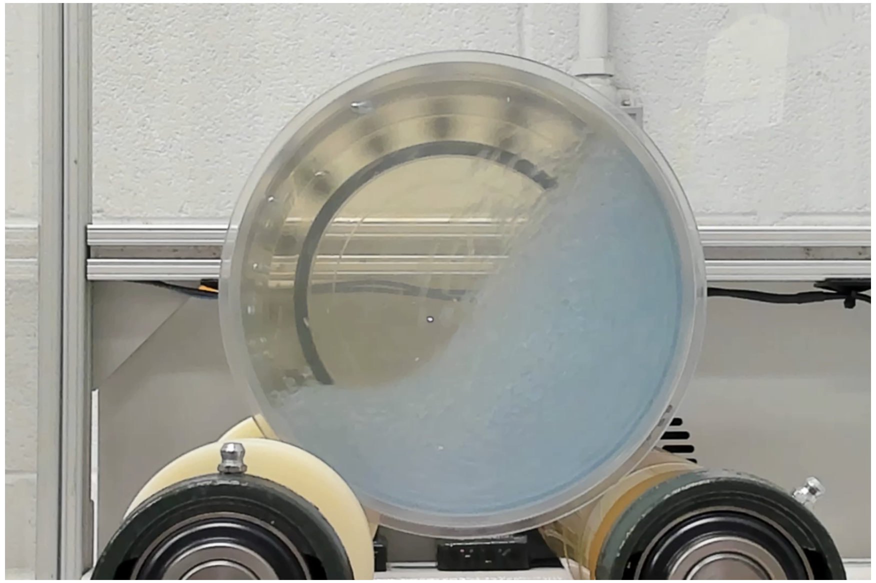


Experimental setup



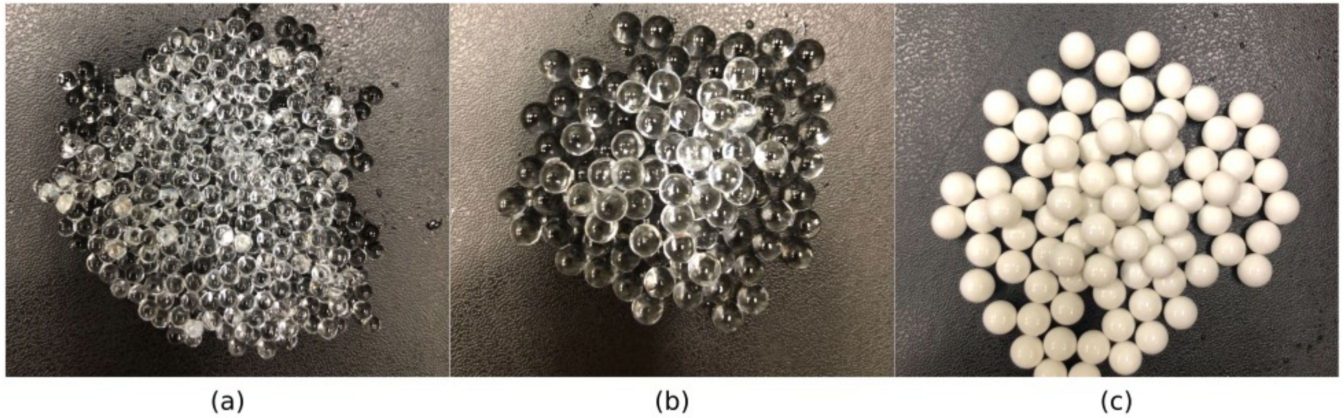
Besides, Froude number (Fr), the fill level as well as the particles' friction coefficient affect the regime change.

$$\boxed{Fr = \frac{\omega^2 R}{g}}$$



Materials used

Particles' Types

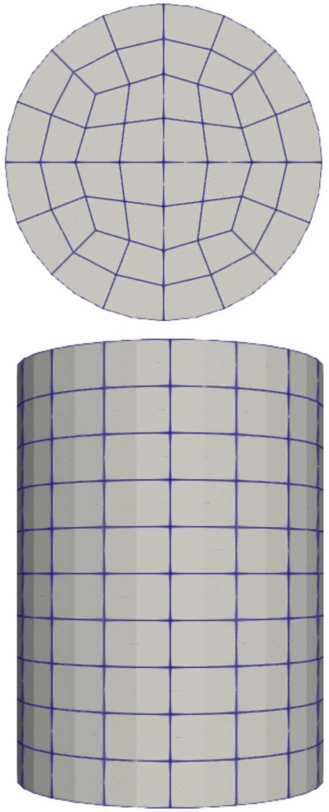


(a) 3 mm glass beads, (b) 5 mm glass beads and (c) 5.95 mm Acrylonitrile butadiene styrene (ABS) particles

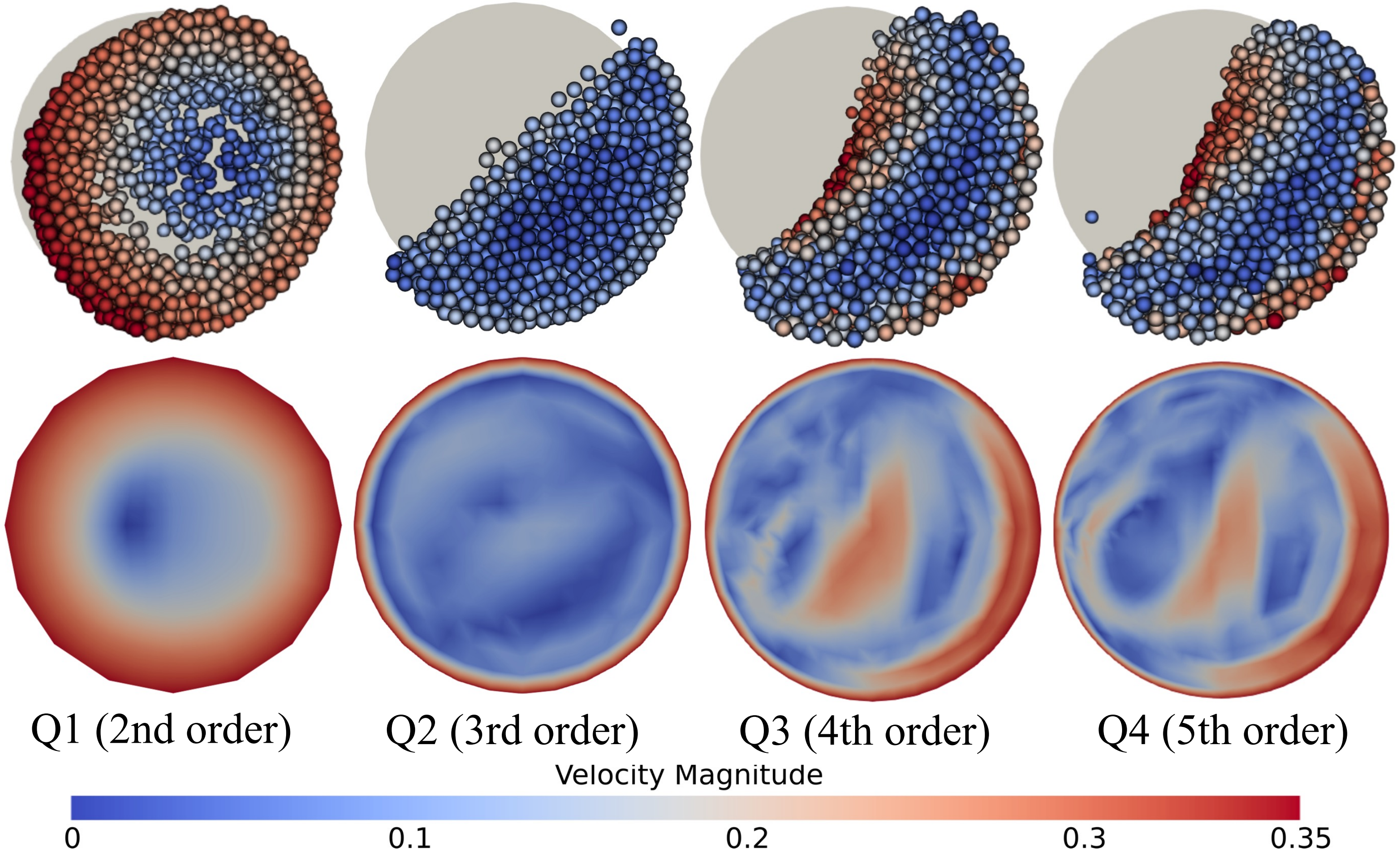
Fluids' Composition

	Air	Water	Sucrose Solution		
Sucrose Fraction (w_s/w_w)	0 %	0 %	50 %	66.66 %	100 %
Sugar Mass (kg)	0	0	1495.5	1993.8	2991
Fluid Mass (kg)	0	0	2991	2991	2991
Density $(\mathrm{kg\,m^{-3}})$	1.225	997	1138.5	1175.62	1224.25
Viscosity $(\mathrm{mPa \cdot s})$	0.016	1	3.49	5.17	11.5

Impact of simulation order



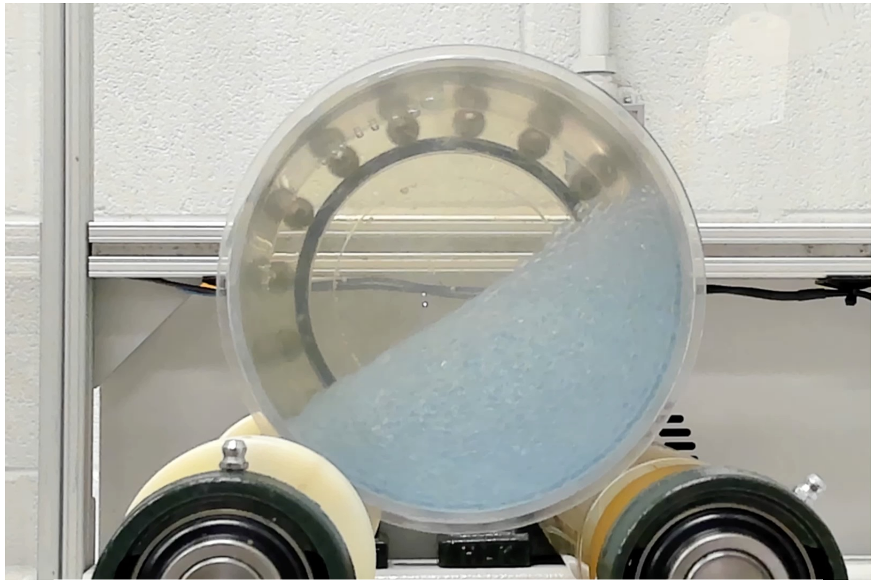
(b)

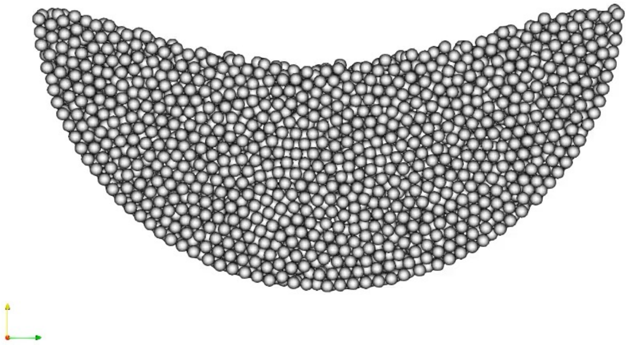


(e)

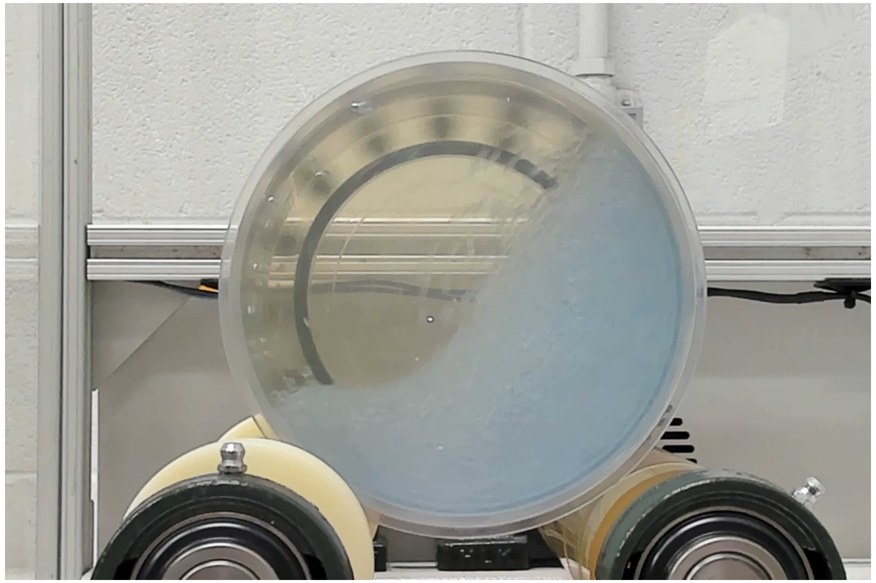
Observed regimes

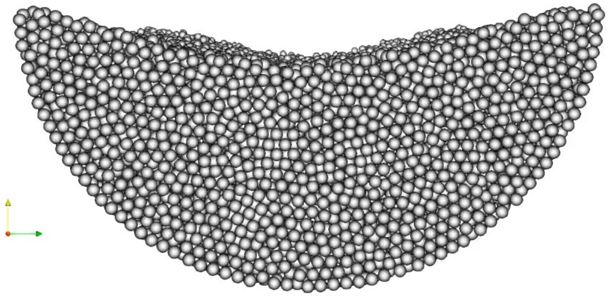
Rolling Regime





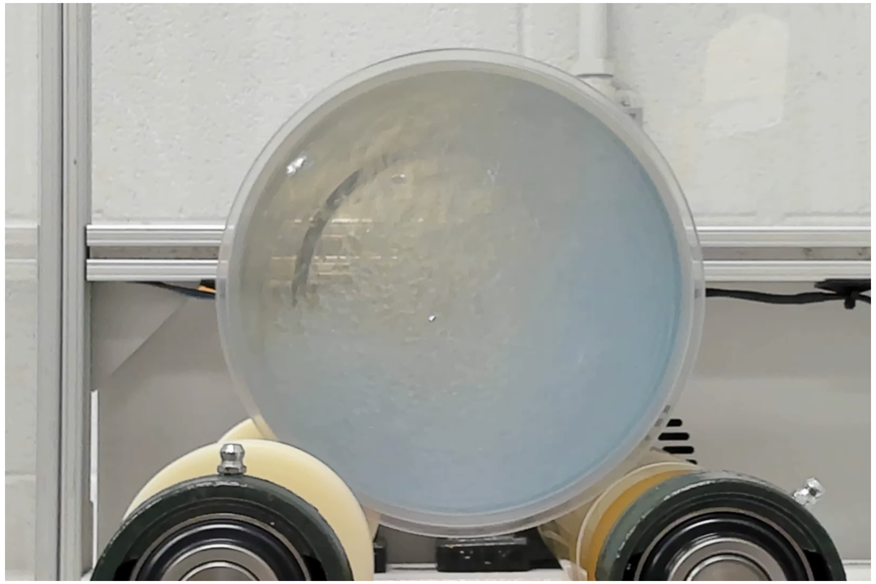
Cascading Regime

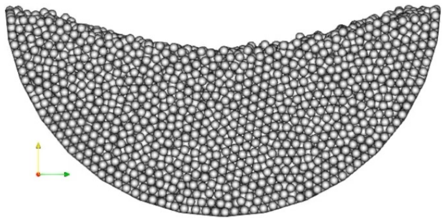




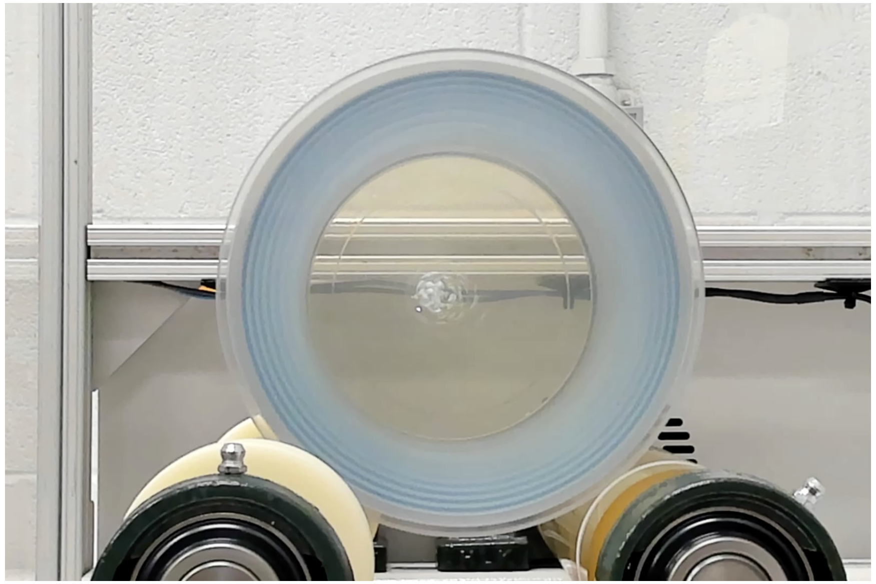
Observed regimes

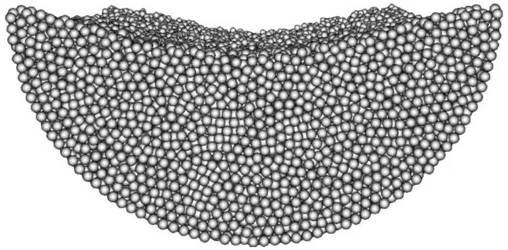
Cataracting Regime





Centrifuging Regime





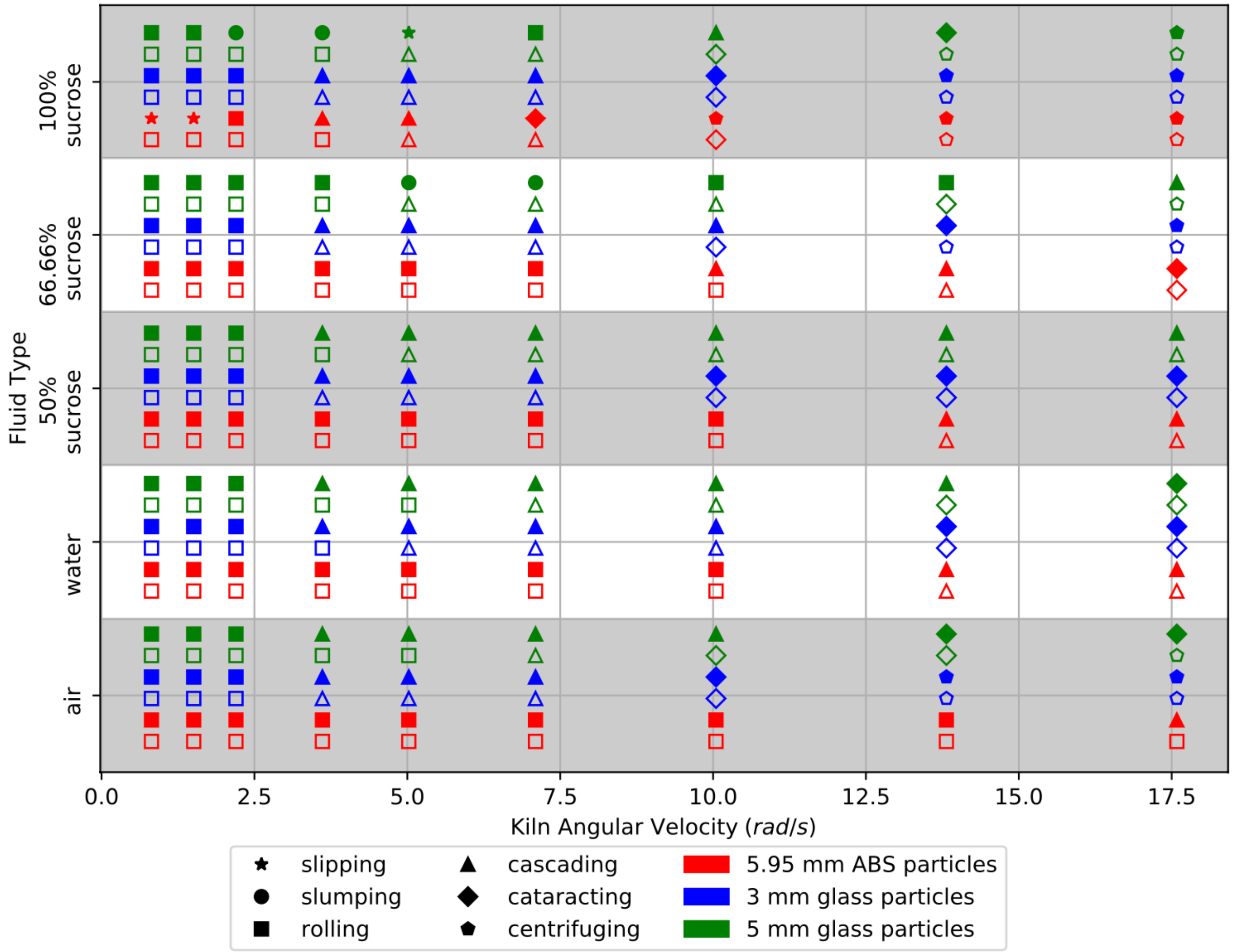
Regime capture efficiency

Methodology:

- Calibrate friction coefficients in rolling regime for a given fluid
- Simulate all velocity range and compare the regime obtained in the simulation with reality

Result for accuracy:

- 96% 3mm glass, 84% for 6mm ABS, 54% for 5mm glass



Interesting particle rotation

Challenge and future direction

Onwards to Matrix-free Methods

What are the challenges?

Time consuming part matrix-based algorithm

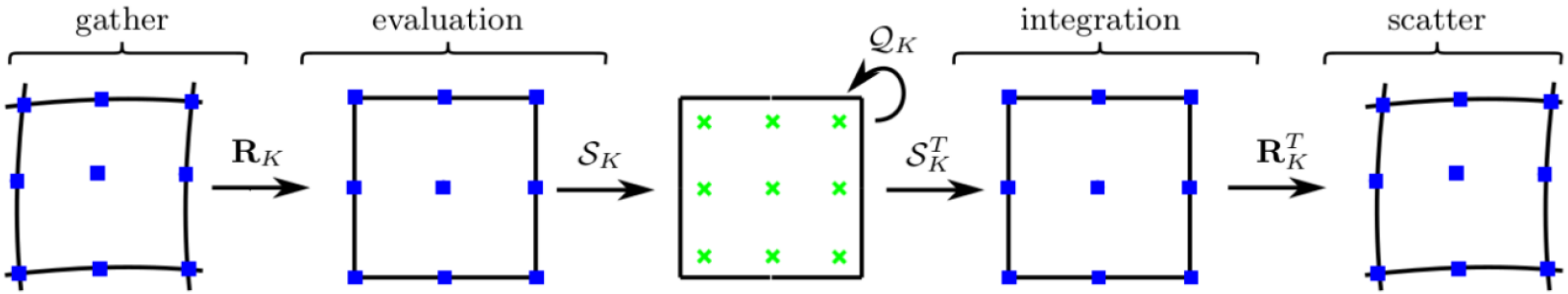
- Assembly of the system matrix
- Assembling the preconditioner (e.g. AMG)
- Solving the linear system

Motivation for a matrix-free approach

- On modern CPUs access to main memory is the bottleneck
- Krylov methods (e.g. GMRES) use matrix-vector multiplications
- For large problems, it is faster to compute matrix entries than to load them

Matrix-free: Main idea

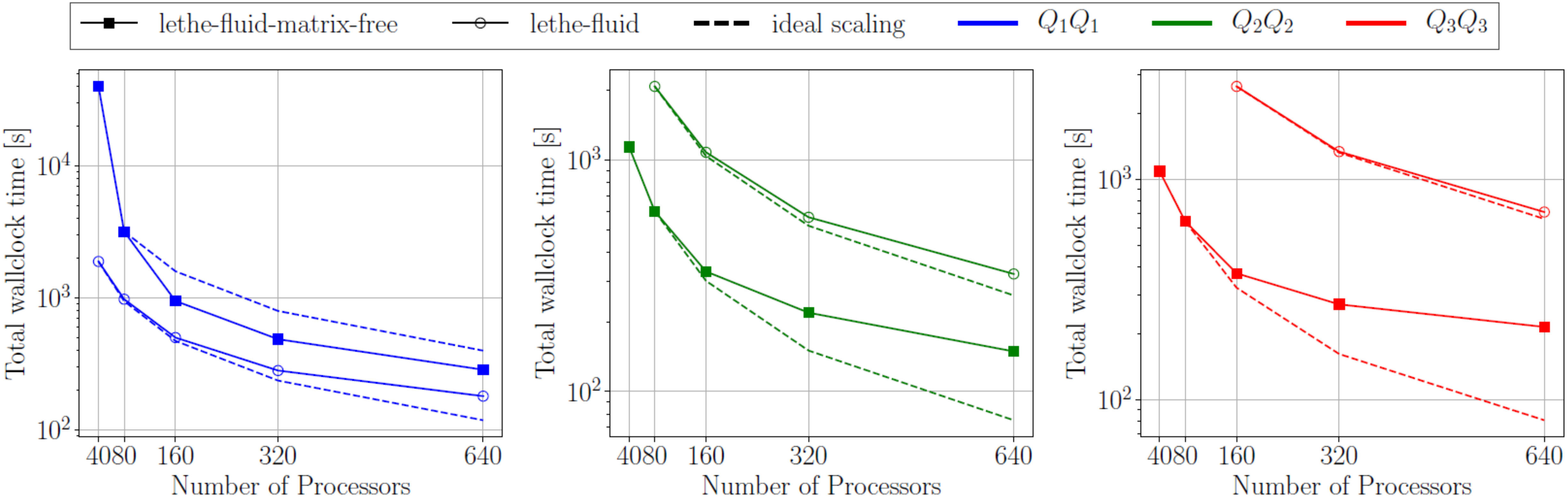
Calculate the matrix-vector multiplication defining an operator



Other elements

- Geometric multigrid preconditioning with global coarsening
- Other optimization (vectorization and sum-factorization)

Result for Taylor-Green vortex



As soon as go to Q2, matrix-free outperforms matrix-based

Conclusions

Challenges and conclusion

Modeling granular flow remains highly challenging

- Lagrangian strategies are computationally intensive
- Turbulent particle-fluid interaction and turbulence modeling in the presence of particles is difficult

High-order CFD-DEM are part of the solution

- Combined order and mesh resolution give lots of freedom
- Matrix-free is the way to go to reduce computational cost

Open-source computational model are a part of the solution

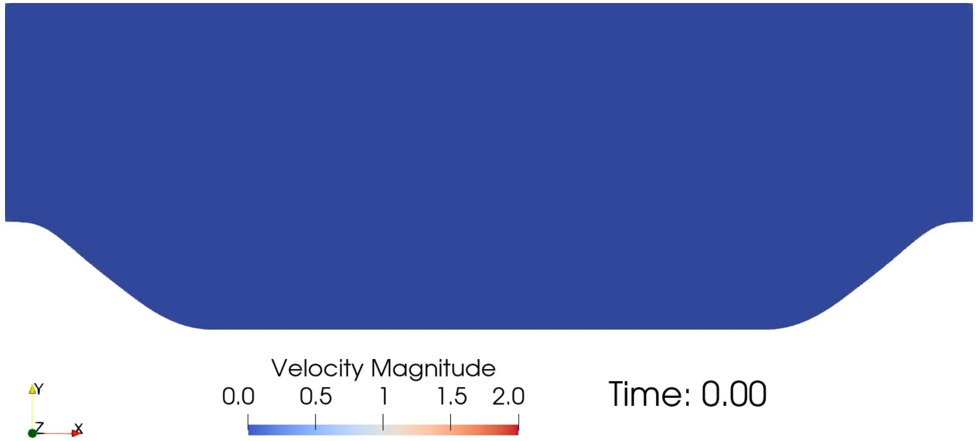
- Reproducibility
- Capacity to be launched at large scale
- Imperfect, but that's all right

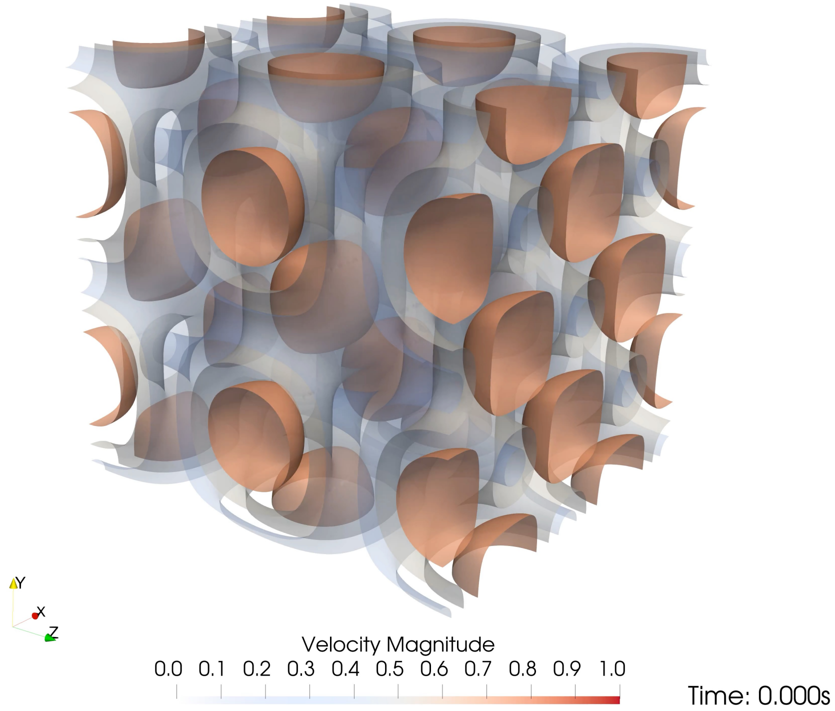
Thanks!

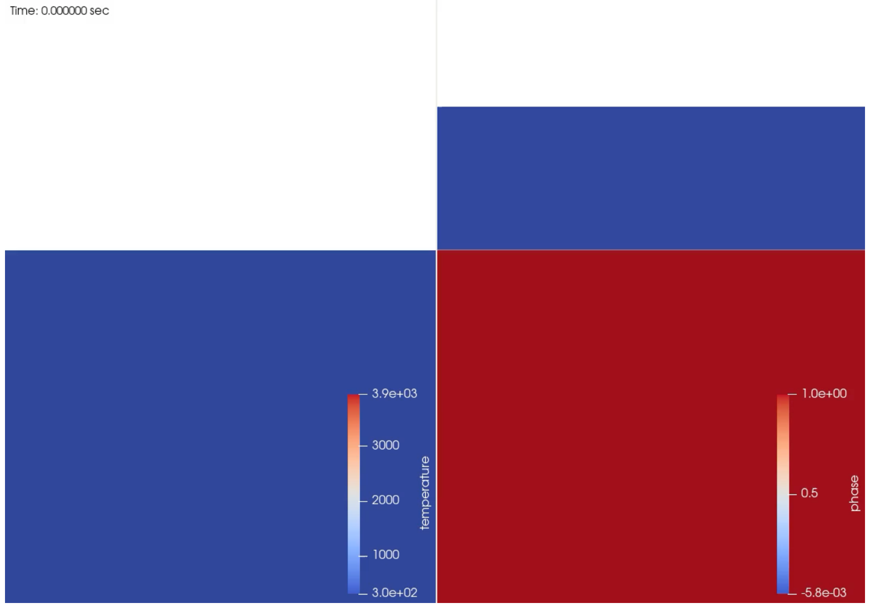
Bruno Blais

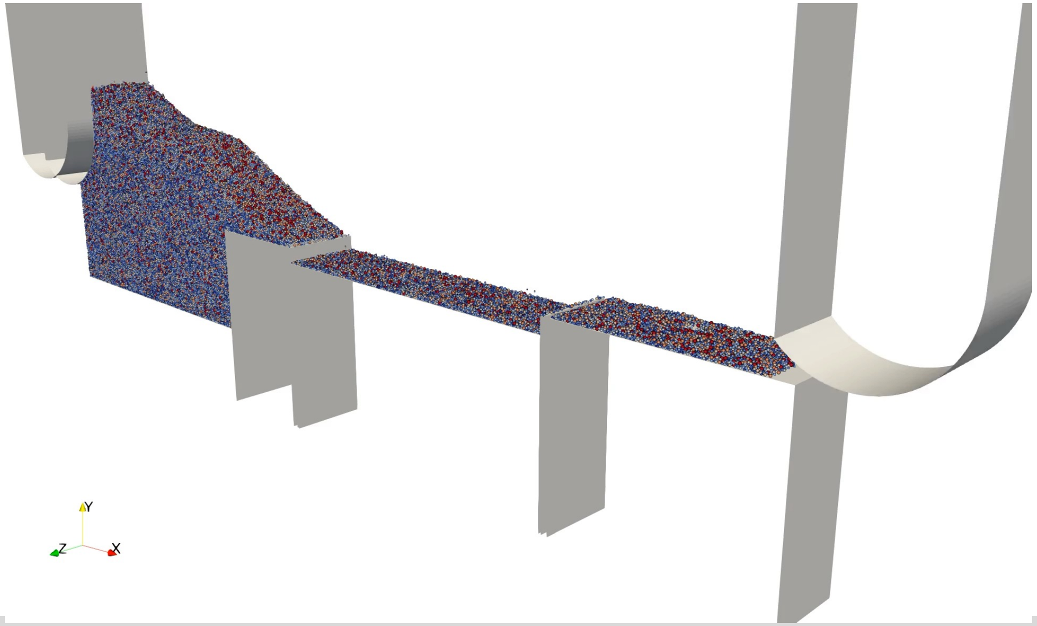
Bruno.Blais @polymtl.ca

https://github.com/lethe-cfd


Y
Z
X
Velocity Magnitude
0.0
0.5
1
1.5
2.0
Time: 0.00


Y
X
Z
Velocity Magnitude
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
Time: 0.000s


Time: 0.000000 sec
3.9e+03
3000
2000
1000
3.0e+02
temperature
1.0e+00
0.5
-5.8e-03
phase


Y
Z
X

Wish to learn more?

- El Geitani, T., Golshan, S., & Blais, B. (2023). Toward High-Order CFD-DEM: Development and Validation. *Industrial & Engineering Chemistry Research*, *62*(2), 1141-1159.
- El Geitani, T., & Blais, B. (2023). Quadrature-Centered Averaging Scheme for Accurate and Continuous Void Fraction Calculation in Computational Fluid Dynamics–Discrete Element Method Simulations. *Industrial & Engineering Chemistry Research*, *62*(12), 5394-5407.
- Ferreira, V. O., El Geitani, T., Junior, D. S., Blais, B., & Lopes, G. C. (2023). In-depth validation of unresolved CFD-DEM simulations of liquid fluidized beds. *Powder Technology*, 118652.
- Geitani, TE, Golshan, S, Blais, B. A high-order stabilized solver for the volume averaged Navier-Stokes equations. *Int J Numer Meth Fluids*. 2023; 95(6): 1011– 1033.
- Golshan, S., Munch, P., Gassmöller, R., Kronbichler, M., & Blais, B. (2023). Lethe-DEM: An open-source parallel discrete element solver with load balancing. *Computational Particle Mechanics*, *10*(1), 77-96.

Barbeau, Lucka, et al. "High-order moving immersed boundary and its application to a resolved CFD-DEM model." Computers & Fluids 268 (2024): 106094.

Barbeau, Lucka et al. In preparation (2024)