2018 Review Meeting for Crosscutting Research

MFIX-DEM Enhancement for Industry-Relevant Flows

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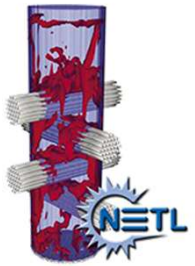
NREL
NATIONAL RENEWABLE ENERGY LABORATORY

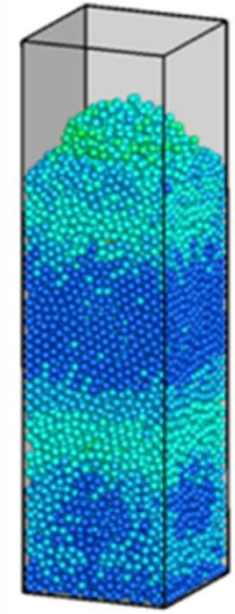
PSRI



Funded by the U.S. Department of Energy: FE0026298

Motivation

?



✘

Laboratory
$N_p \sim 10^{10}$

CFD-DEM
$N_p \sim 10^4$ - 10^7

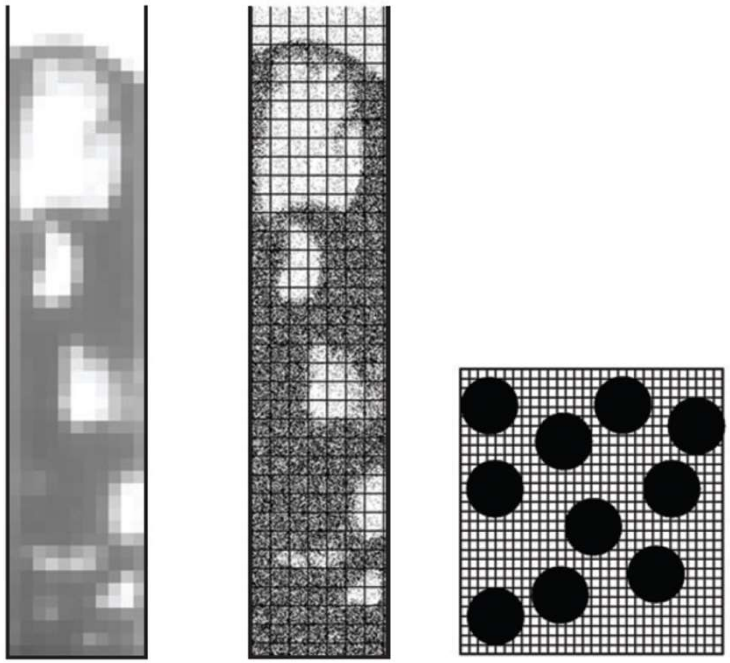
Industry
$N_p \sim 10^{14}$

Goal: DEM application toward industrially relevant flows

Challenges

- Speed ⇒ **Optimization & Algorithms (this talk)**
- Results reliability ⇒ Validation

Background:
Numerical Methods for Studying Gas-Solid Flows

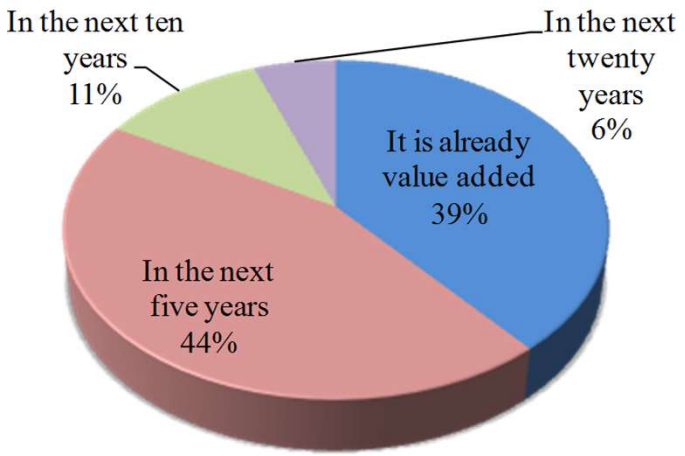


More detail, fewer closures

Less CPU time

van der Hoef et al. ARFM (2008)

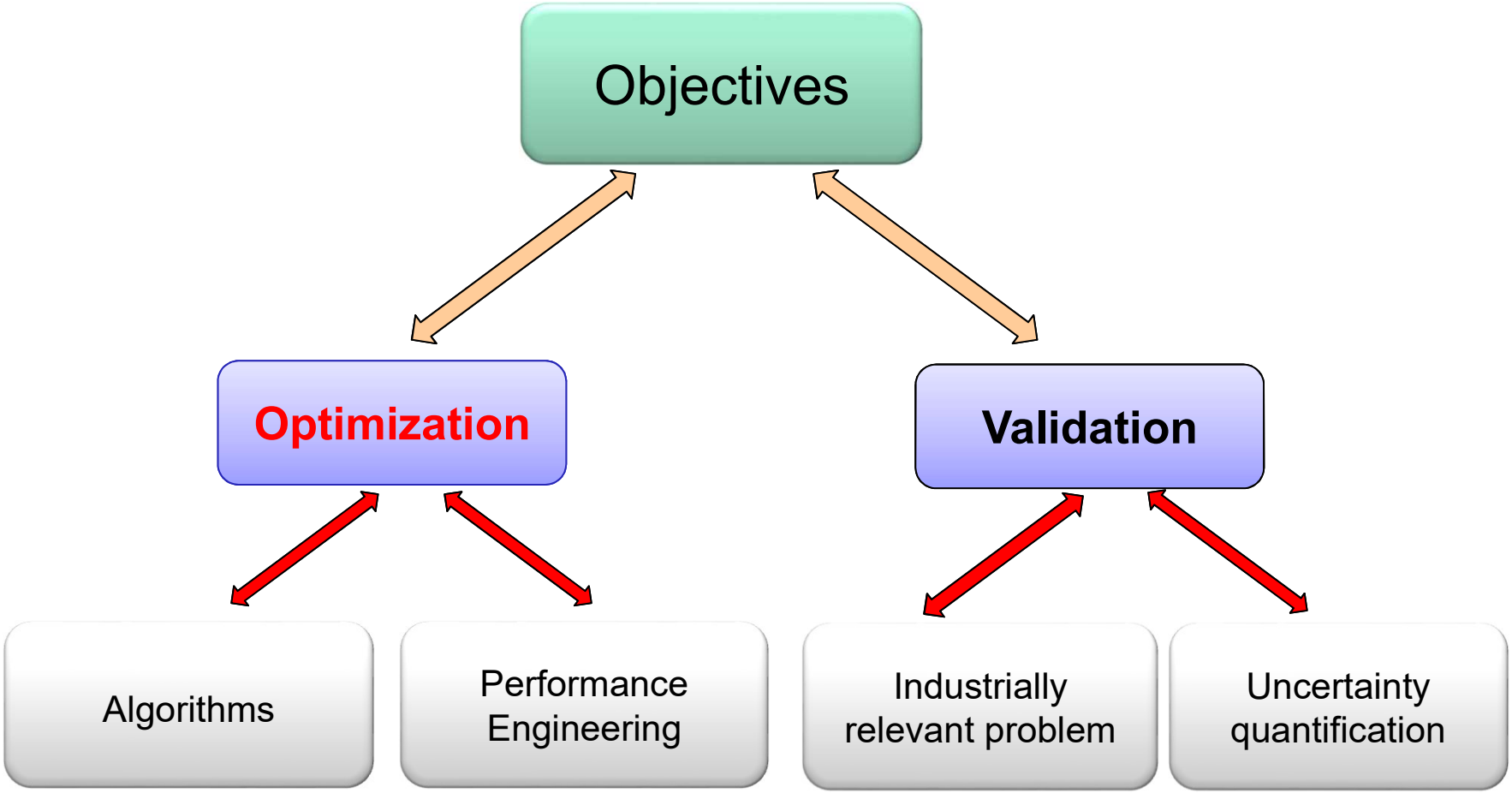
Expected value added through DEM



Expected value added through DEM:
PSRI Industrial Survey
(Cocco et al., *Chem. Eng. Prog.*, in press)

DEM: a balance between computational overhead and sources of uncertainty

Overall Project:
MFIX-DEM Enhancement towards Industrial Applications



Team

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DEM modeling of granular and gas-solid flows, MFIX


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PSRI
Industrial Application and Experiments of Particle Flows

Tasks

- Porting to MFiX 2017
  - Integrating Benchmarks and Simulations into GUI
- Tuning (Optimization & Algorithm)
- Expanding Benchmark Sets

Profiling and Optimization

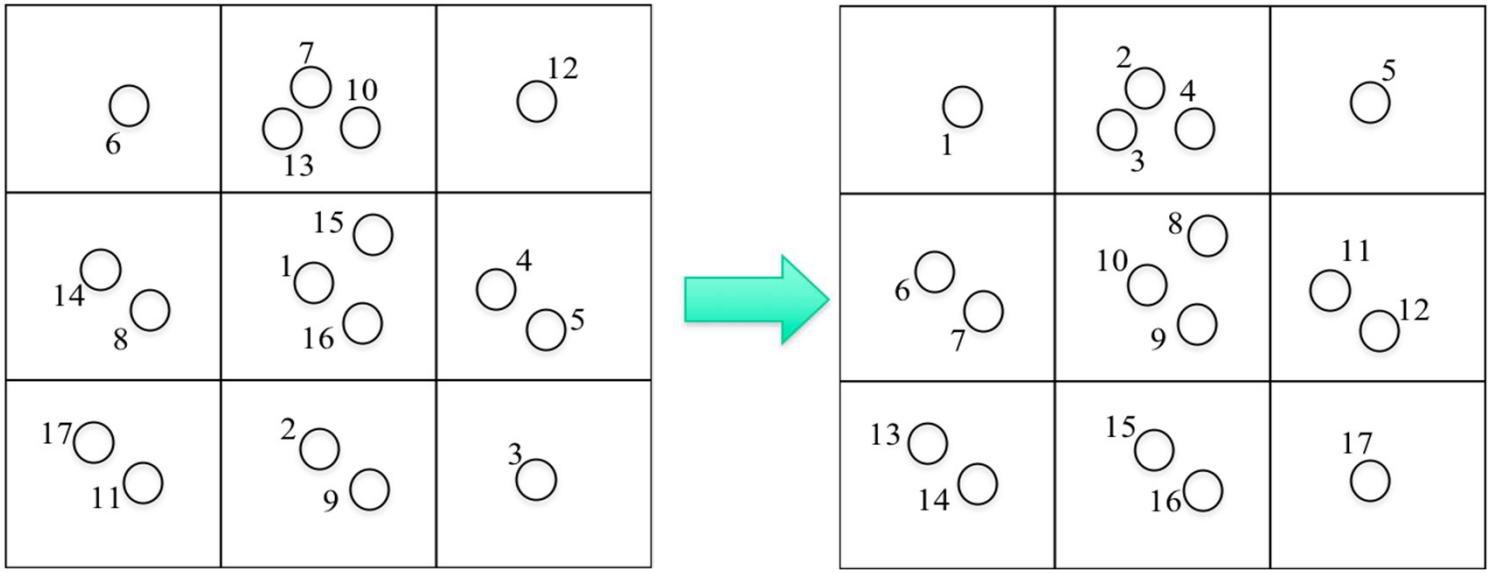
- **Hot Spots and Bottlenecks**
  - Multi-Levels
- **Computational Code**
  - Algorithms
  - Implementations
  - Compilations
- **I/O**
  - Big Cases
- **Parallelization**
  - MPI (nodes)
  - OpenMP (processors/threads)
  - Hybrid
  - Instructions
  - Data

Profiling Examples

Top Three Most Time Consuming Functions (MFiX-exa)

Benchmark	Function	Run Time (%)
HCS (Serial)	solve_bicgstab	42.41
	FillBoundary	26.31
	calc_particle_collisions	3.47
HCS (MPI)	FillBoundary	46.71
	solve_bicgstab	29.99
	EvolveParticles	4.94
Fluidized Bed (Serial)	updateNeighbors	26.39
	calc_particle_collisions	22.06
	calc_wall_collisions	18.24
Fluidized Bed (MPI)	EvolveParticles	31.58
	fillNeighborsMPI	24.18
	updateNeighbors	10.75

Spatial Sorting of Particles

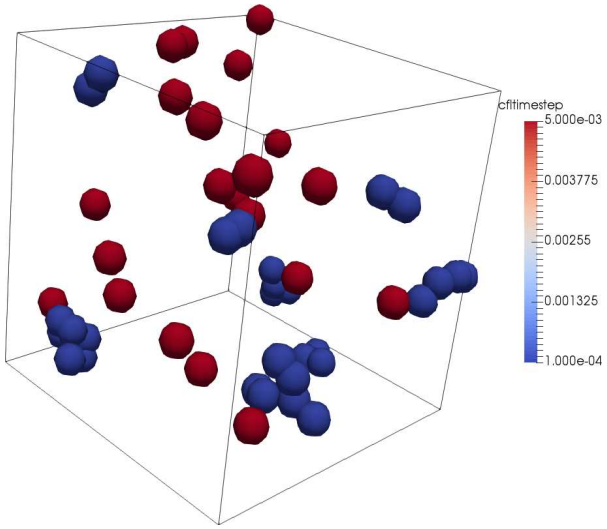


Spatial sorting (done at beginning of des time march)

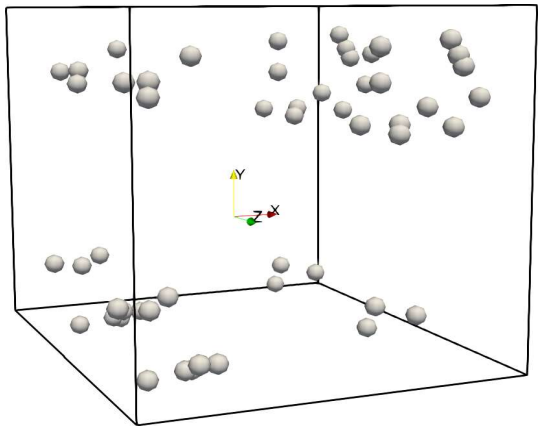
➡ **increase spatial data locality** in memory while

- Finding neighbors
- Calculating inter particle forces
- Drag calculations
- Interpolating mean fields.

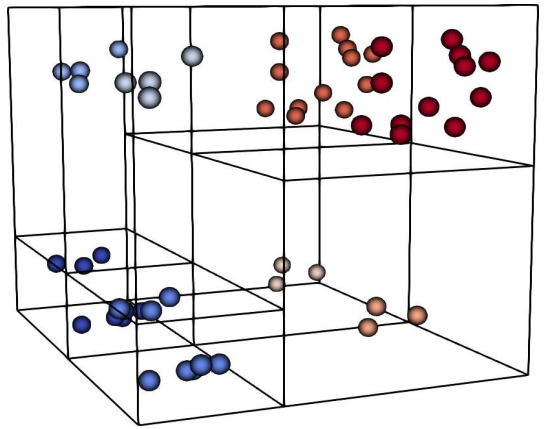
Explicit Scheme with Orthogonal Recursive Bisection



- Local Time Step for Particles
- Particles that are far apart can advance with large time steps (red)
- Particles that are going to collide need small time steps (blue)



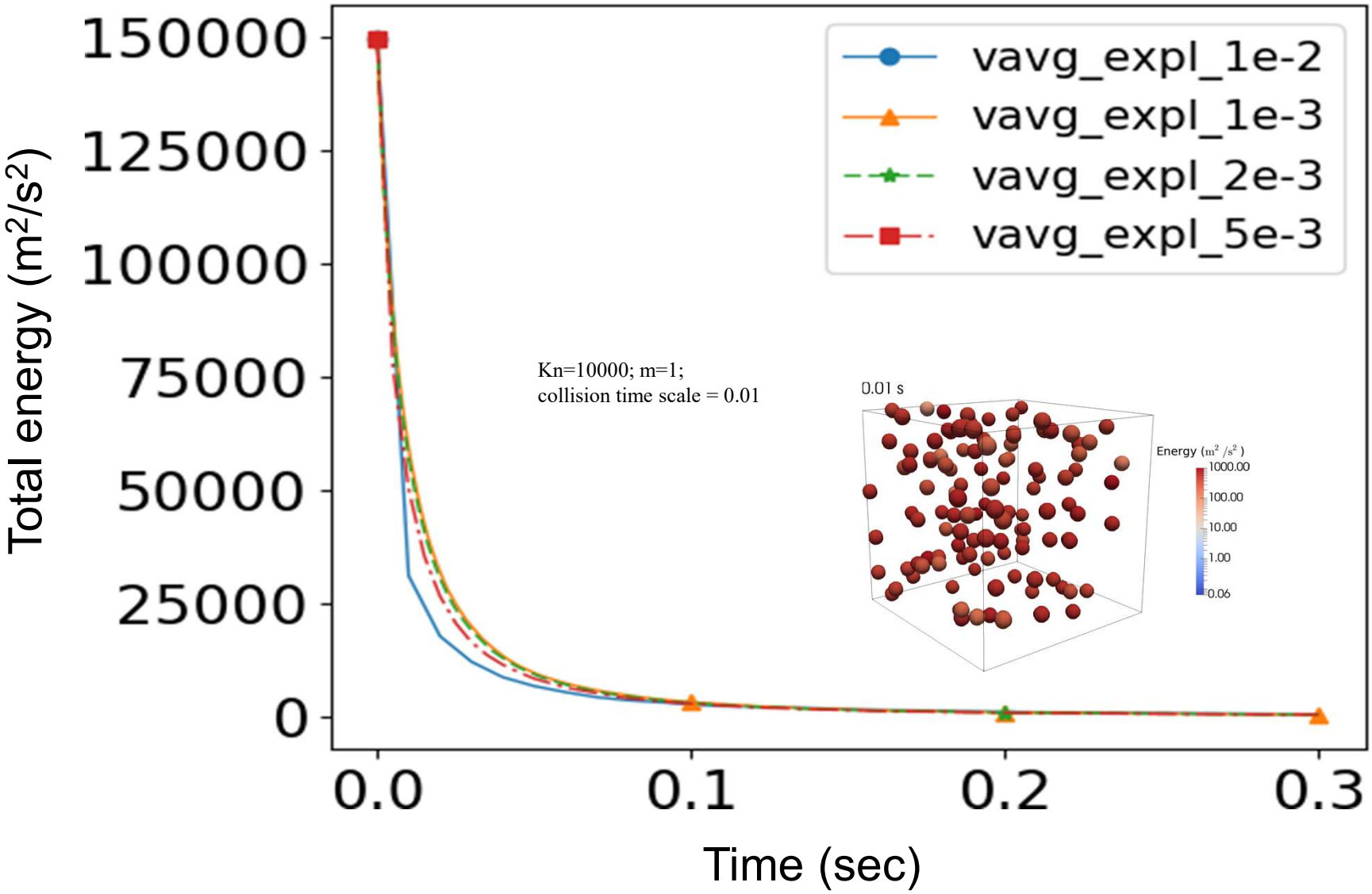
Classic Explicit Scheme



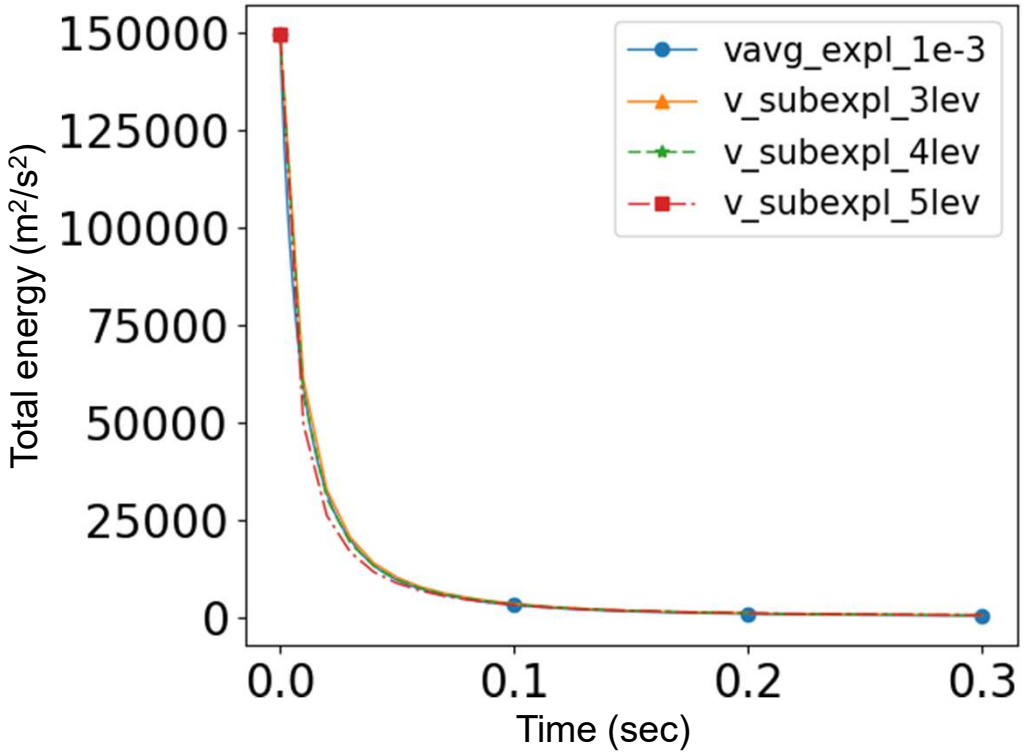
Explicit ORB Scheme

Baseline:

Time Step and Accuracy for Explicit Scheme (HCS)



Subset Explicit Solution and Exact Solution



Explicit time stepping

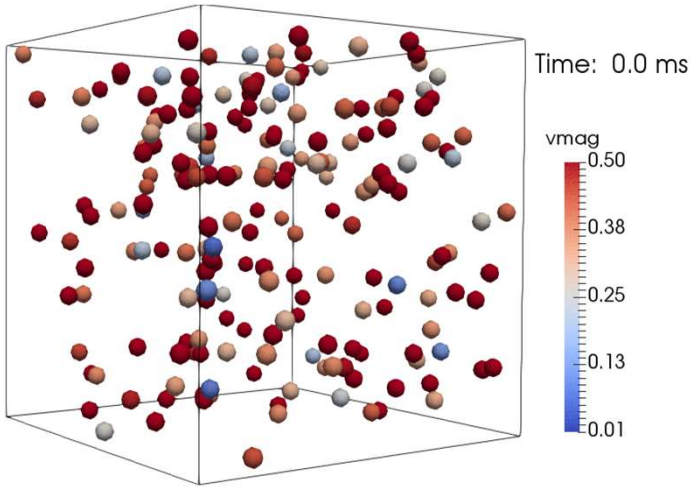
Time step	Wall time
1e-3	250 sec
2e-3	138 sec
5e-3	52 sec

Explicit ORB

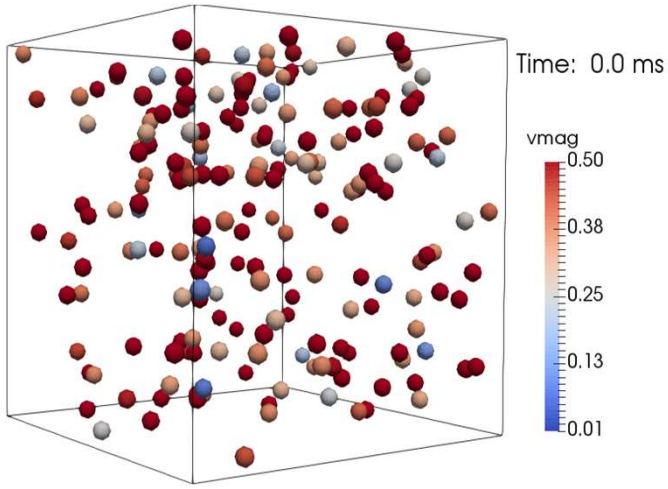
Time step	ORB levels	Wall time
1e-2	3	29 sec
1e-2	4	15 sec
1e-2	5	12 sec

Comparisons (Benchmark examples)

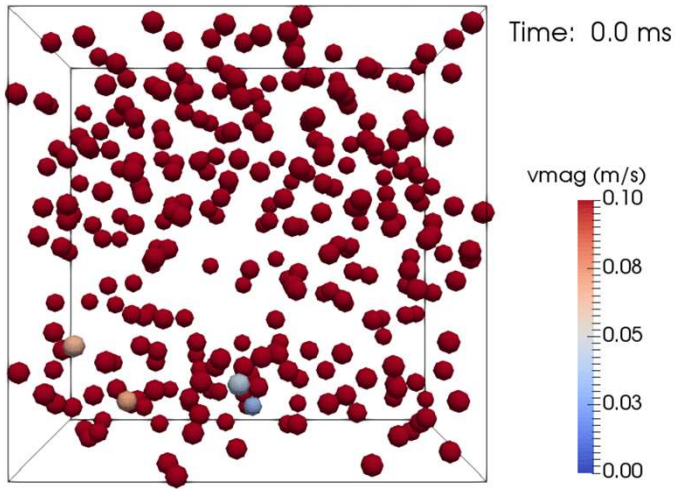
Mfix-exa – Traditional Explicit Scheme

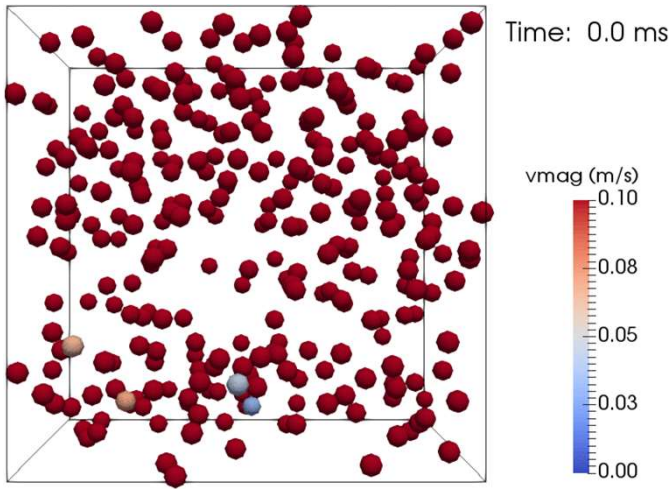


Mfix-exa – Explicit ORB Scheme



HCS: ~2X Faster for Evolve Particles





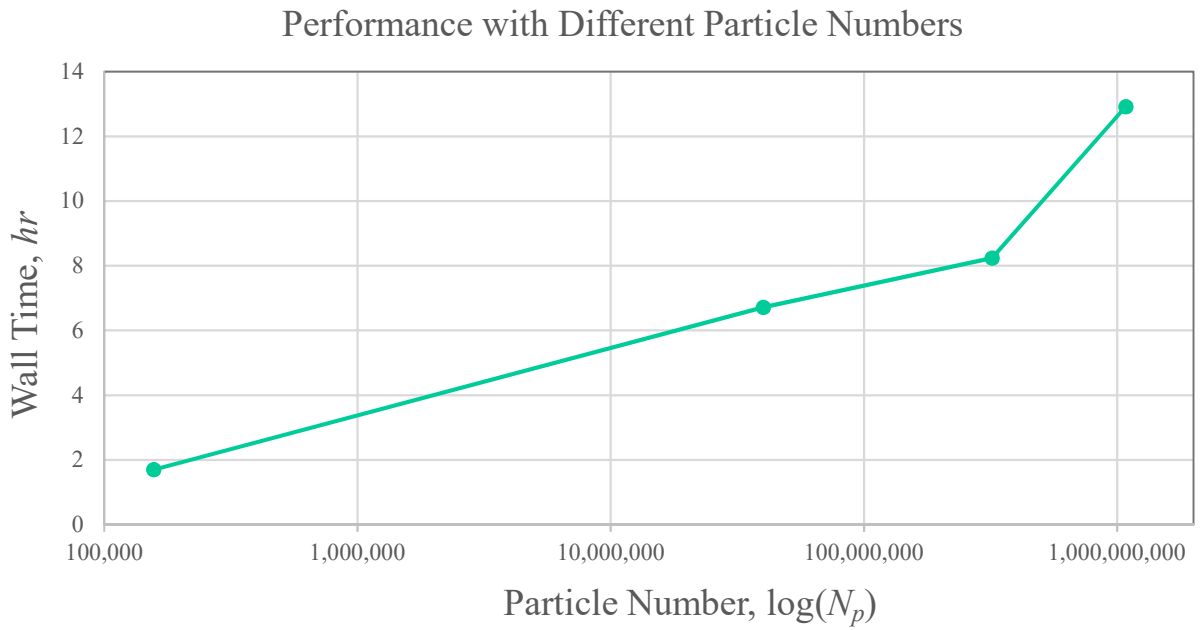
Settle: ~1.3X Faster for Evolve Particles

Big Case: Large Number of Particles

- **Challenges**
  - Particle Data (input file)
  - Space
  - Time
- **Solutions**
  - Generating the particles on the fly.
  - Distributing to Multiple CPUs

10^9 Particle Simulation (HCS Weak Scaling)

Cores (n_p)	Physical Domain (m)	Particle Tile Size	Particle Count (N_p)	Wall Time (hr)
1	0.020 x 0.020 x 0.020	101 x 101 x 101	156486	1.7
256	0.128 x 0.128 x 0.128	640 x 640 x 640	40052736	6.72
2048	0.256 x 0.256 x 0.256	1280 x 1280 x 1280	320421888	8.24
6912	0.384 x 0.384 x0.384	1920 x 1920 x 1920	1081423872	12.92



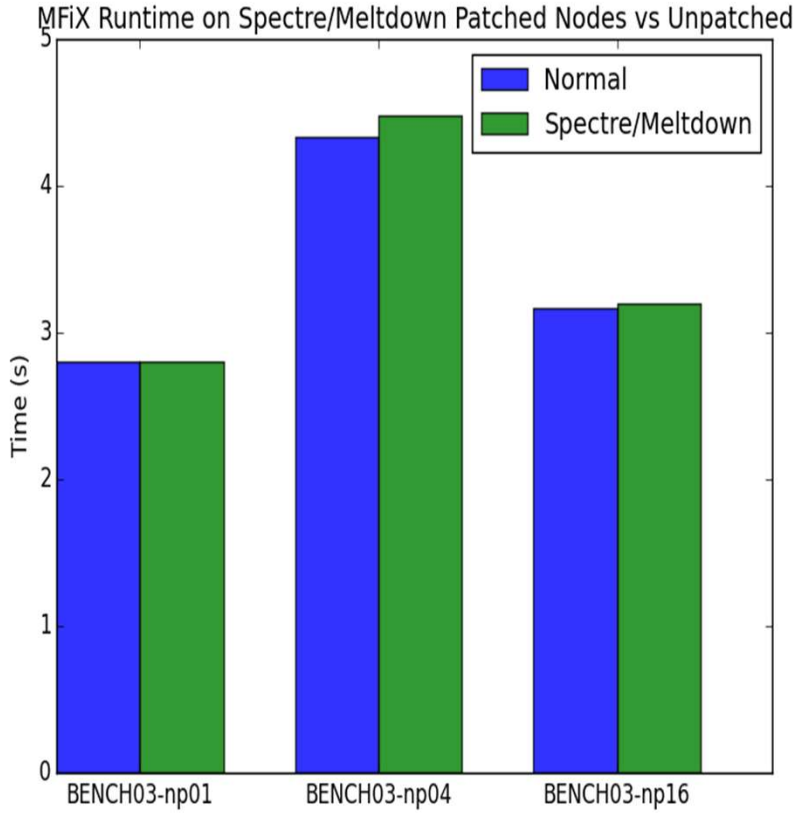
Effect of Spectre and Meltdown Patches

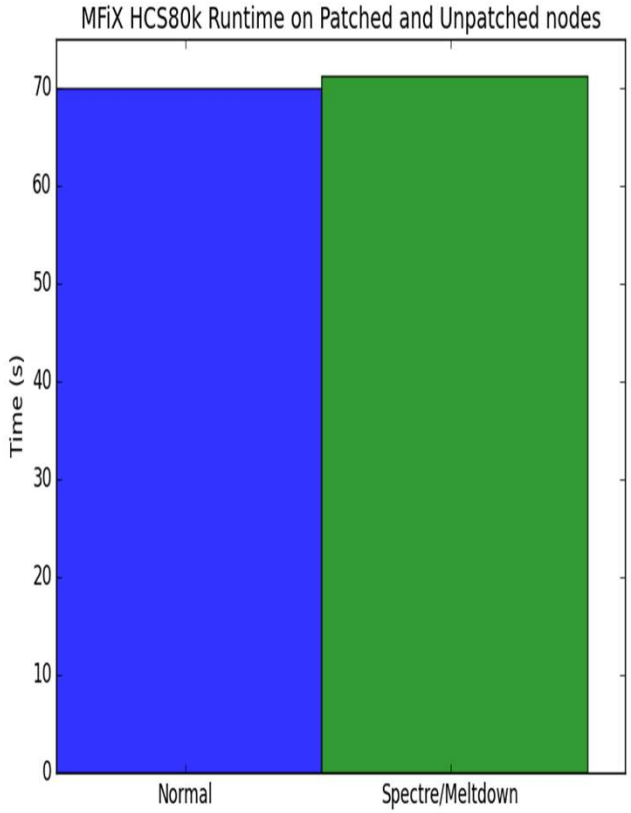
Fluidized Bed:

np01: 1 cpu, 2500 particles
np04: 4 cpus, 10000 particles
np16: 16 cpus, 40000 particles,

HCS:

1 cpu, 80000 particles





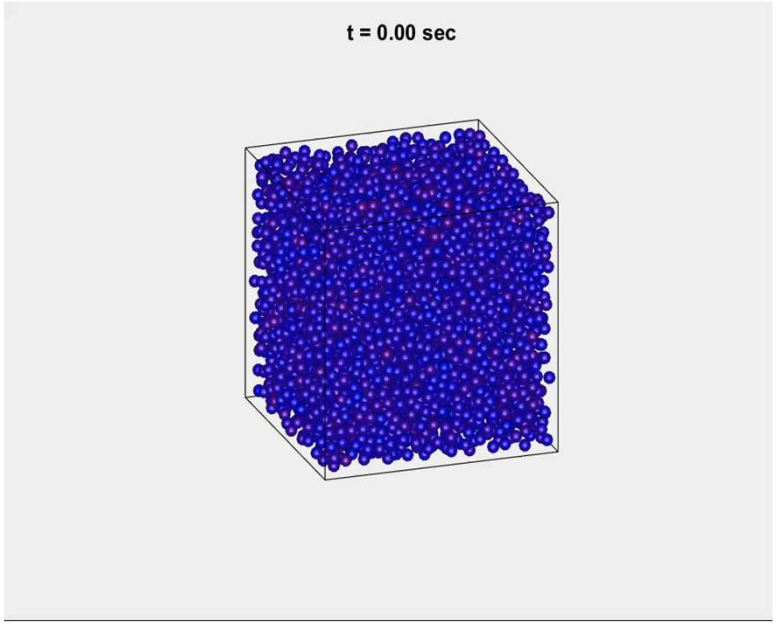
Expand Benchmark Sets

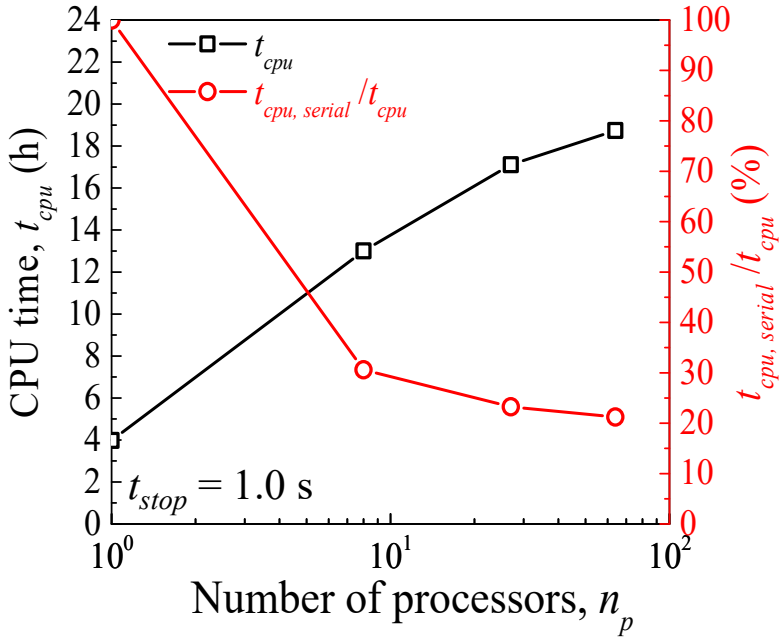
- Current Benchmarks (Rectangular, MFiX and MFiX-exa)
  - Homogeneous Cooling System (HCS)
  - Settling
  - Fluidized Bed
  - Riser Flow

- New Benchmarks (MFiX)
  - Tumbler (Square)
  - Non-Rectangular

Tumbler benchmarks (monodisperse)

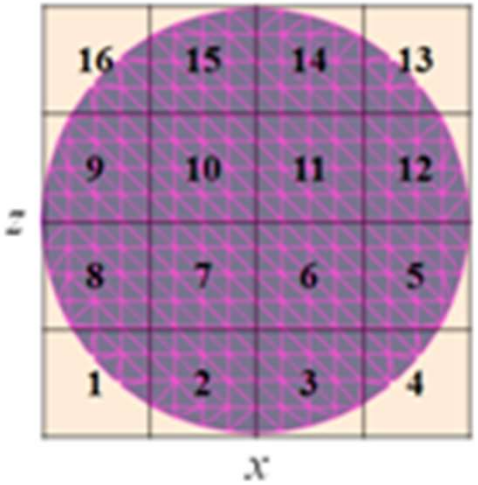
Cores (n_p)	Domain ($n_x \times n_y \times n_z$)	CFD Cell ($N_x \times N_y \times N_z$)	Particle count (N_p)
1	$1 \times 1 \times 1$	$10 \times 10 \times 10$	4,584
8	$2 \times 2 \times 2$	$20 \times 20 \times 20$	36,672
27	$3 \times 3 \times 3$	$30 \times 30 \times 30$	123,768
64	$4 \times 4 \times 4$	$40 \times 40 \times 40$	293,376



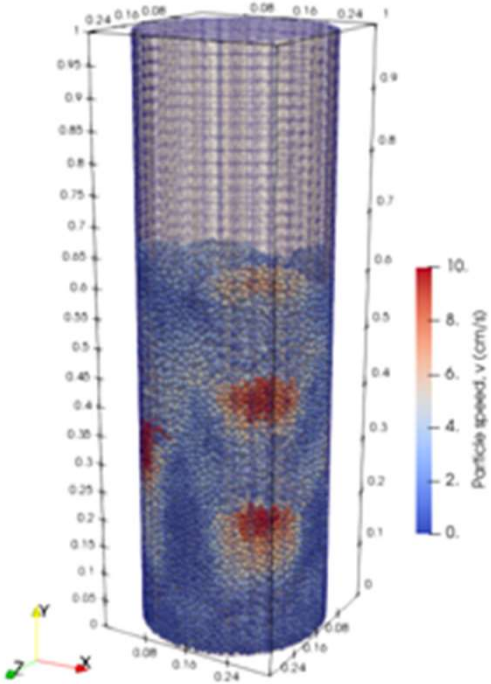


Non-Rectangular

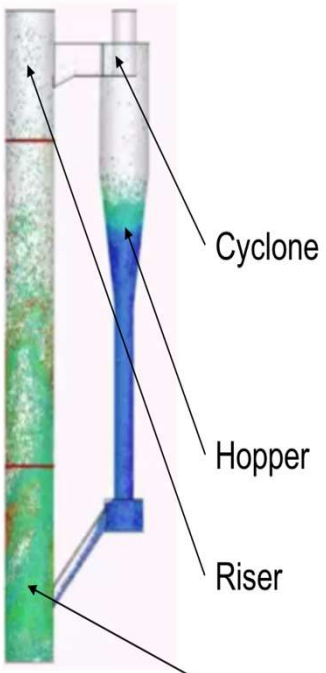
Cartesian cut-cells



Cylindrical Geometries

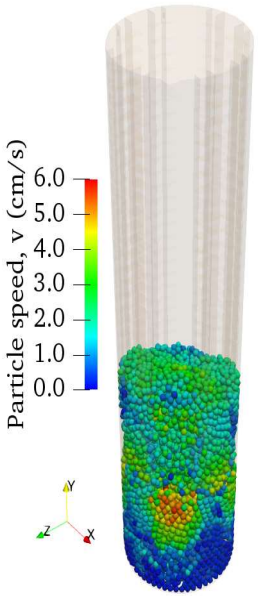


Non-Rectangular Benchmarks

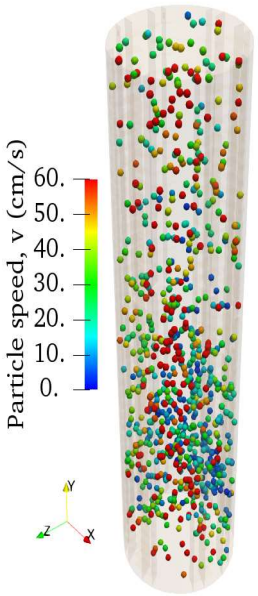


CFB

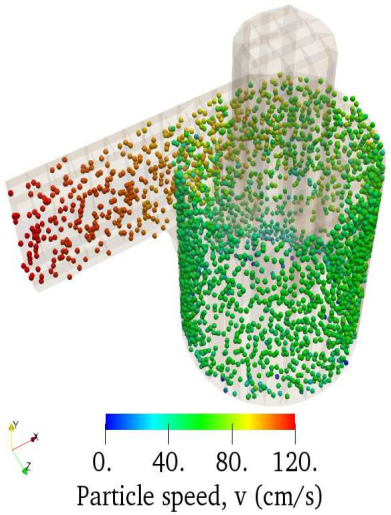
Hadi Wahyudi, et al
(https://www.youtube.com/watch?v=XYfiMO9o0yU)



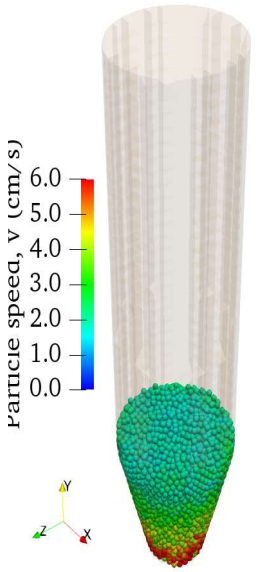
Fluidized bed
($N_p = 8{,}000$)



Riser
($N_p = 800$)

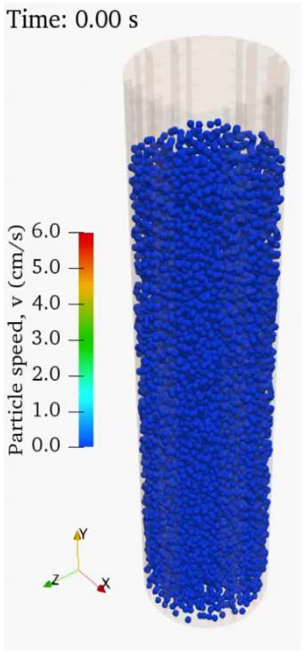


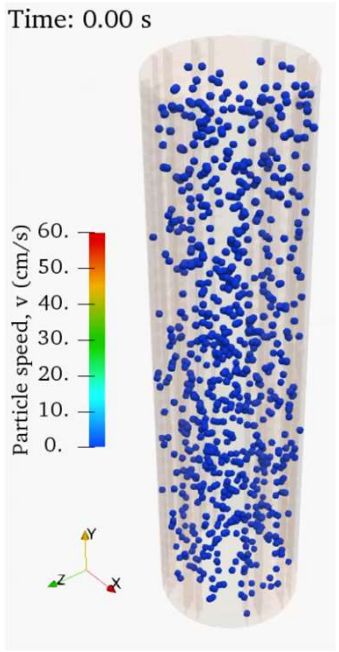
Cyclone
($N_p\ (t \to \infty) \approx 2{,}800$)

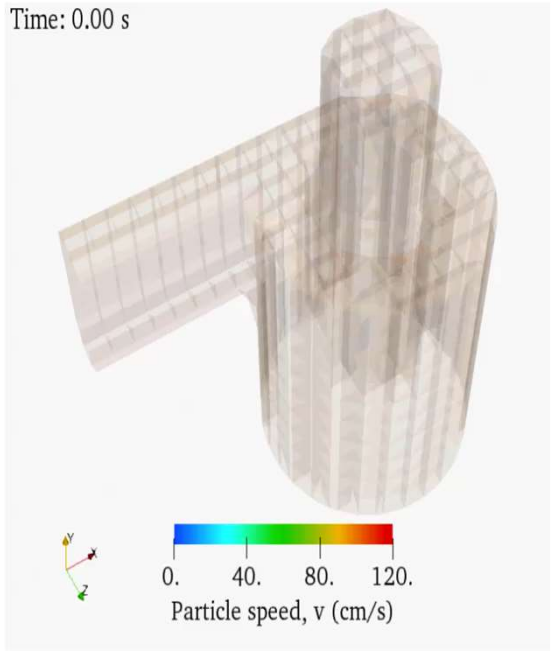


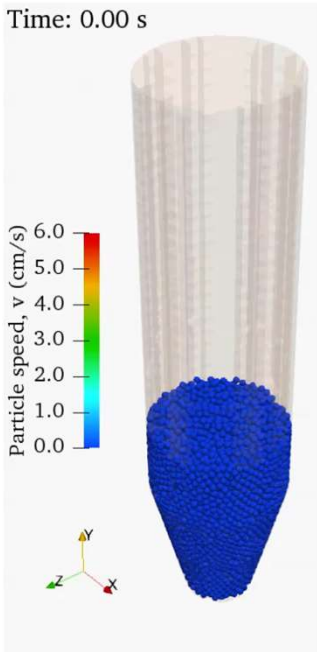
Hopper
($N_p\ (t = 0) = 8{,}000$)

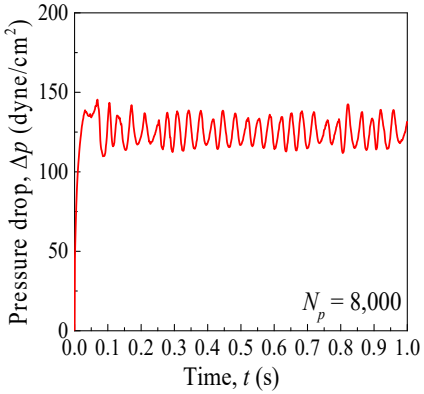
Non-Rectangular Benchmarks

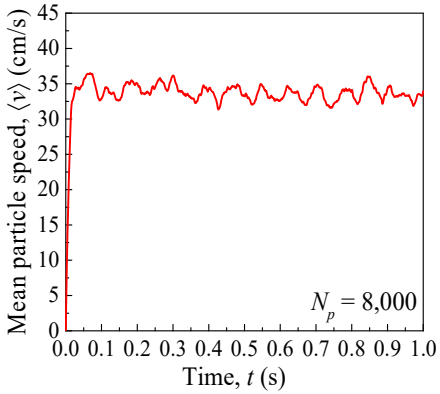


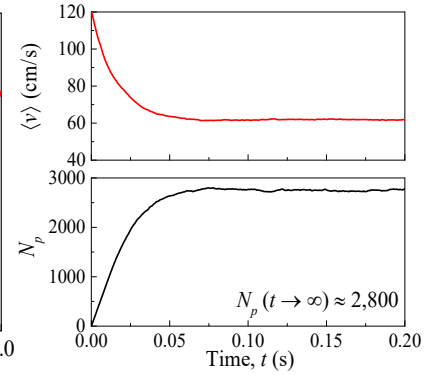


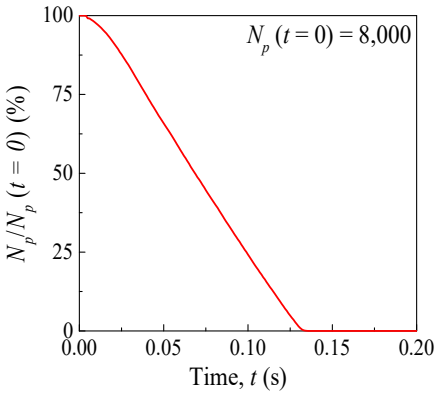




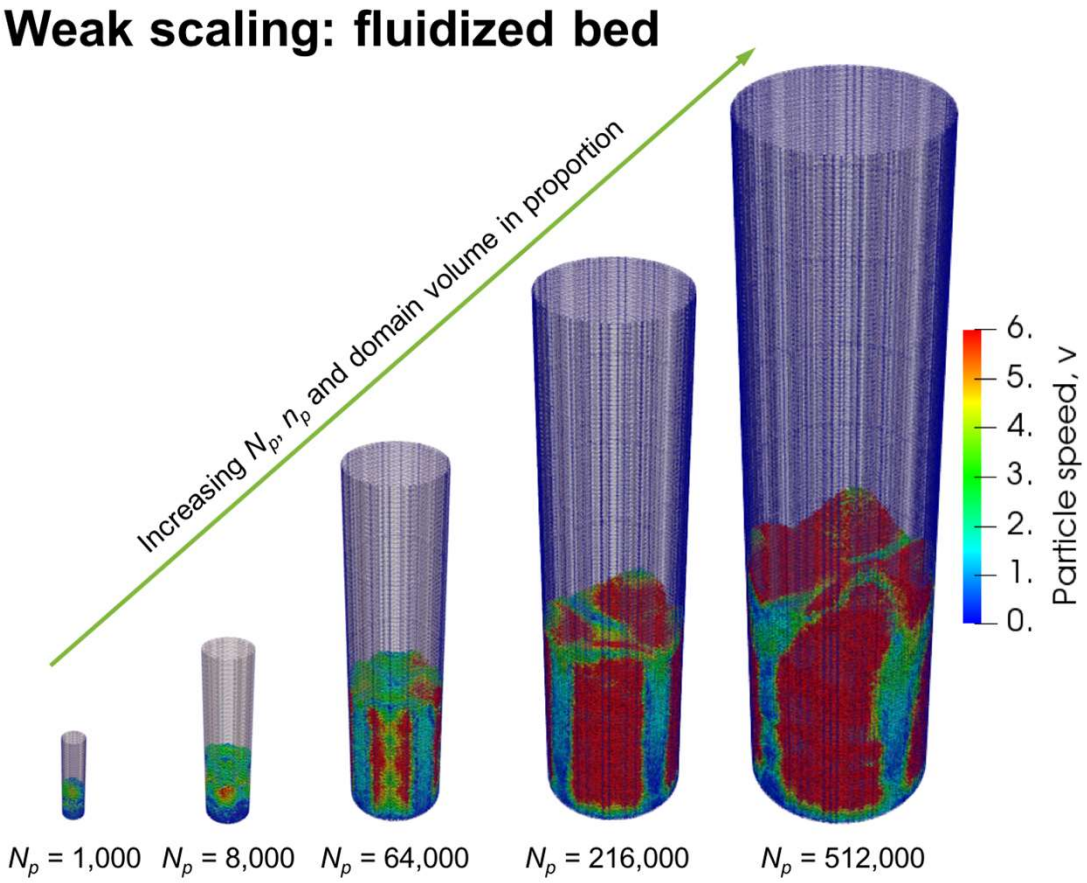


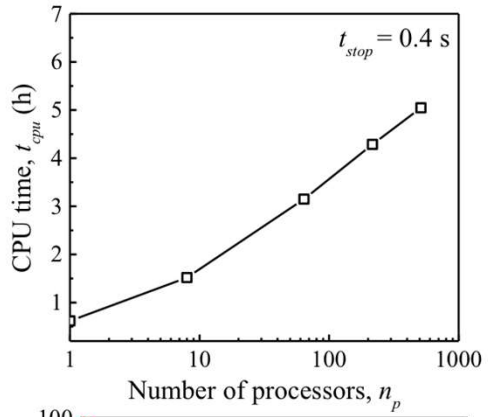


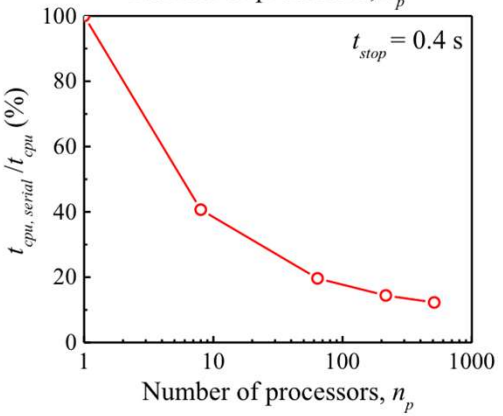




Non-Rectangular Benchmarks







Acknowledgements