

# Parallelization of Discrete Element method

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# Motivation and Objective

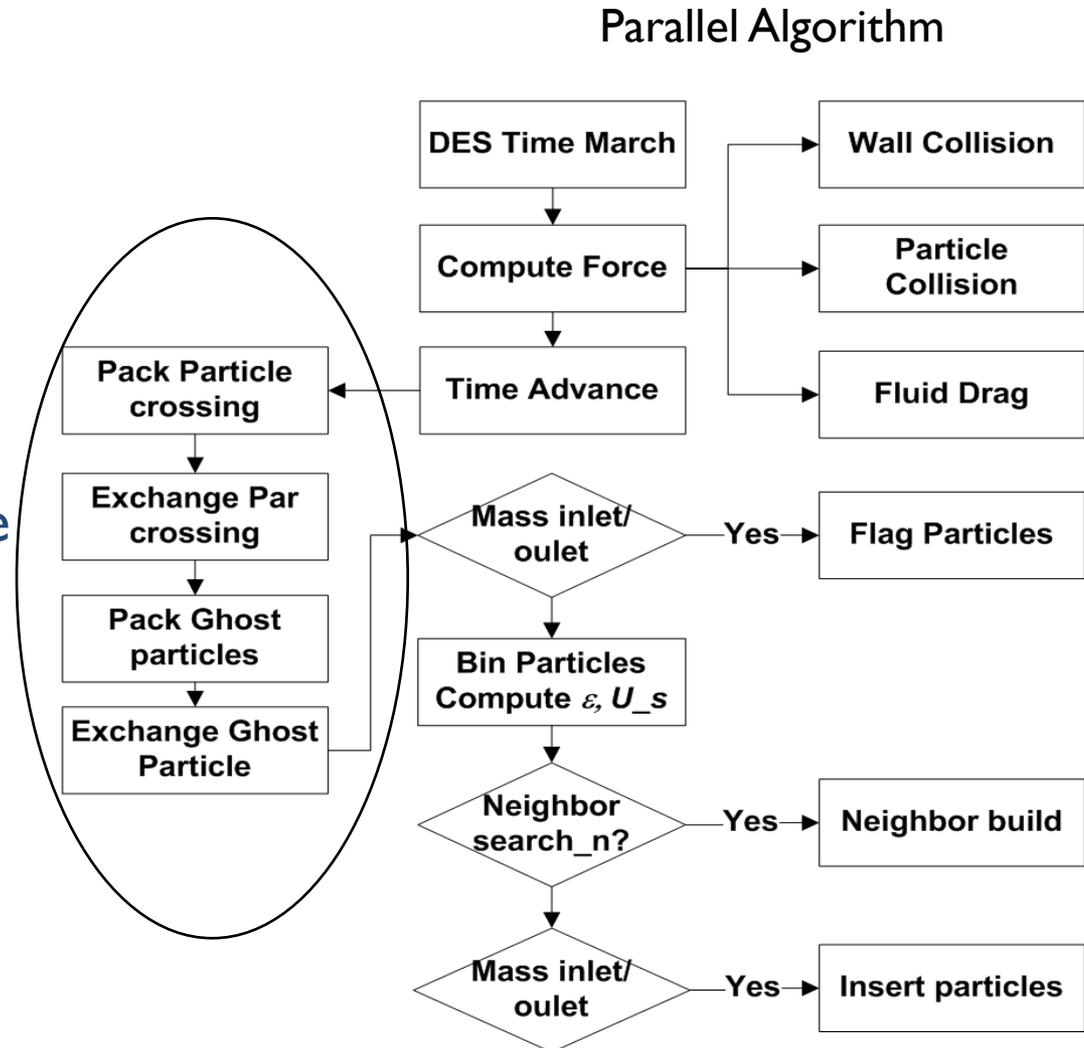
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- ▶ Discrete Element Method (DEM) offers accurate simulation of multiphase flows and could be used to obtain closure laws for reduced order models
- ▶ DEM is computationally expensive due to small time step, which is required to resolve particle-particle interaction
- ▶ Current MFIX release version supports only serial DEM, which limits number of particles that can be simulated within reasonable computational time.
- ▶ *Develop efficient parallel DEM which can simulate millions of particles within reasonable computational time*

# Design

## ▶ Considerations

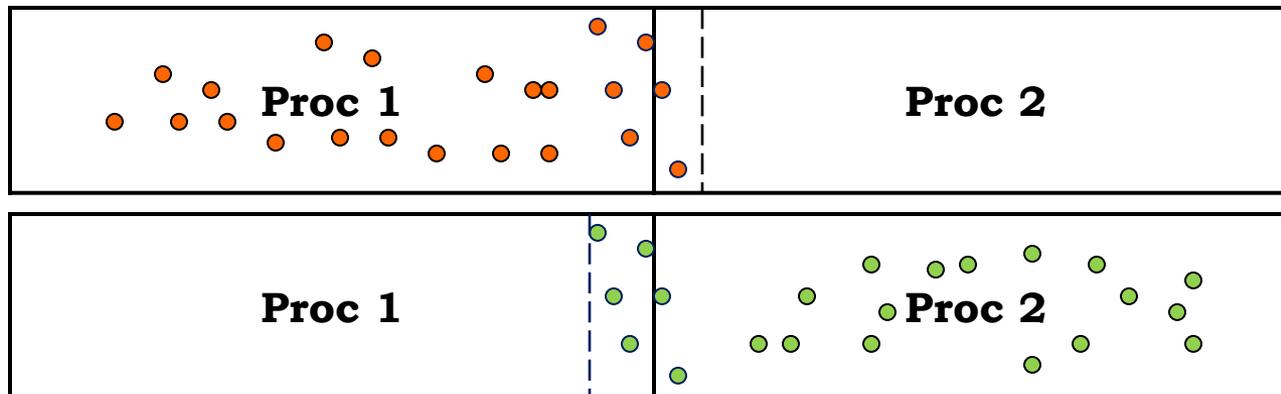
- ▶ Developing efficient parallel algorithm in compliance with existing MPI architecture of MFIX
- ▶ minimal changes to the code
- ▶ adherence to existing coding standards and naming convention



# Development

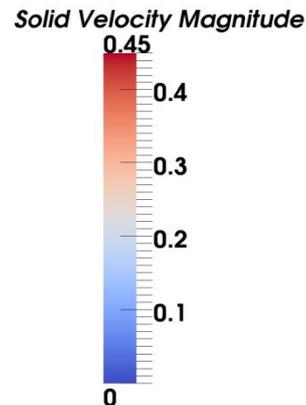
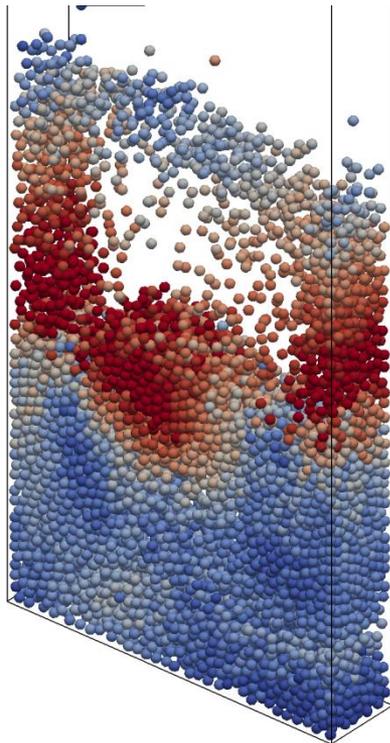
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- ▶ point to point communications
  - ▶ particles crossing processor boundary (entire particle information)
  - ▶ exchanging information for particles in ghost cell (position and velocity)
- ▶ collective communication for IO
- ▶ Supports
  - ▶ Periodic, mass inlet and outlet boundary conditions
  - ▶ output formats VTK and Tecplot; distributed and single IO



# Verification

Pseudo-2D Fluidized bed similar to Muller et al. 2008

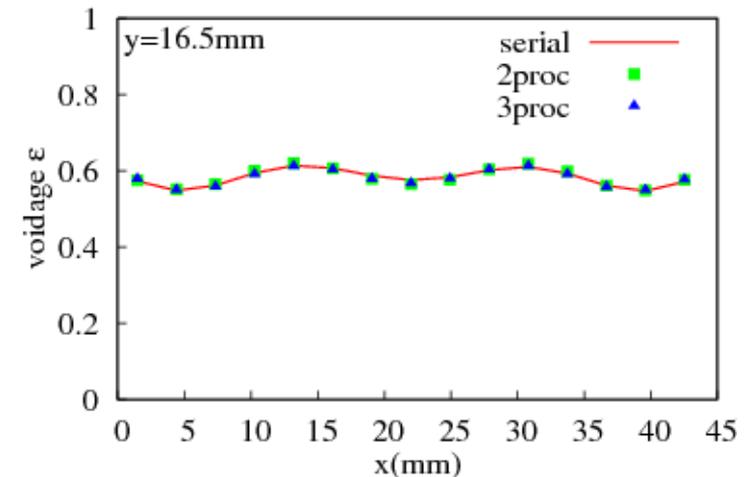
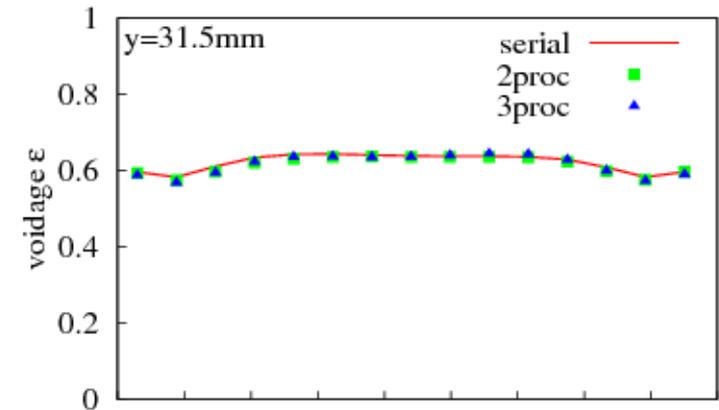


**U = 0.9 m/s**  
**Time = 19.50 s**

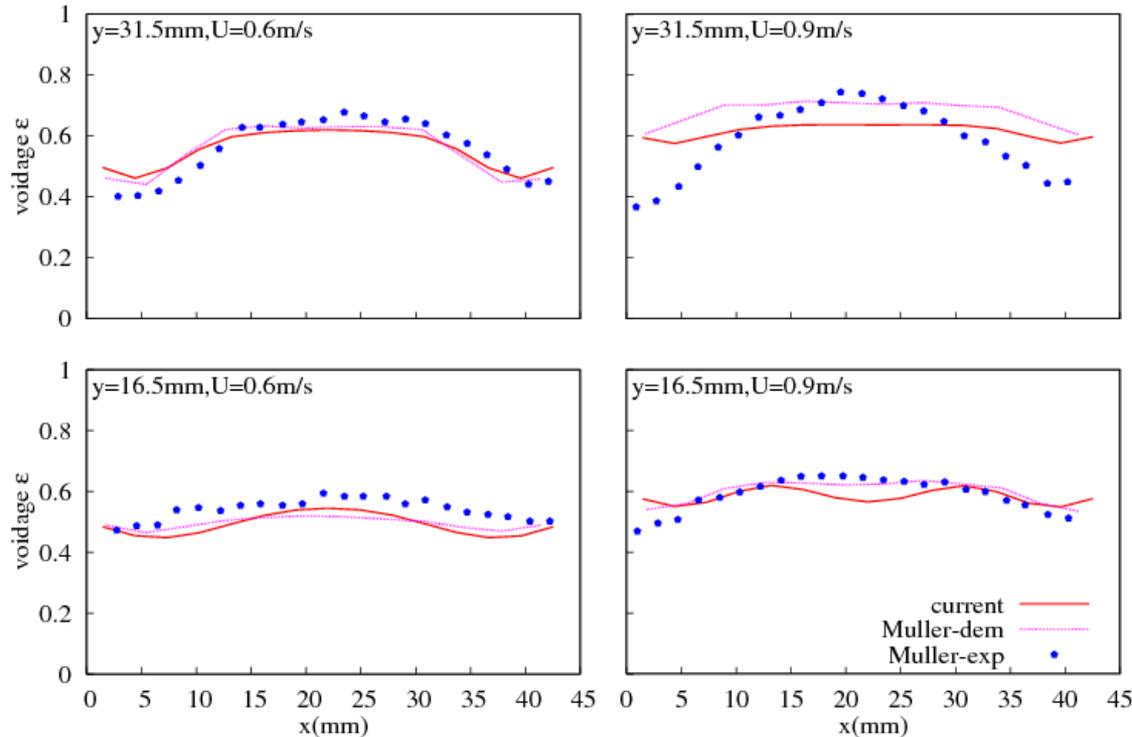
Parameter <sup>1</sup>	Value
Total Particles	9240
Diameter	1.2 mm
Density	1000 kg/m <sup>3</sup>
Coef. of restitution Particle, Wall	0.9, 0.9
Friction coefficient Particle, Wall	0.1, 0.1
Spring constant Particle, Wall	200, 200 N/m
Dimension Grid size	44x120x10 mm 15x40x3
Superficial Velocity	0.6, 0.9 m/s
Time Step (Fluid, Solid)	2e-4, 1.49e-5 (14 steps)

# Comparison Serial and Parallel

- ▶ In order to verify the parallel implementation, simulation is carried out with
  - ▶ Current released version
  - ▶ New Parallel version with 2 and 3 processors
- ▶ Compared average void fraction for a period of 20 secs at 100 Hz at two different axial heights
- ▶ No deviation between the results
- ▶ Comparison made for average lateral velocity also shows good agreement



# Comparison with experiments



- ▶ Reasonable agreement with experiments
- ▶ Current DEM and previous DEM by Muller et al. (2009) over predict the void fraction near the walls.
- ▶ Current DEM matches well with the previous DEM simulation.
- ▶ Similar comparisons were obtained for  $U=0.6$  m/s and for lateral velocity profiles.

# Strong Scaling Analysis

- ▶ A total of 2.56 million particles simulated
- ▶ Total grid cells ~ 800K
- ▶ Up to 256 processor is used (for 256 processors ~10,000 particles and 3200 cells/processor)
- ▶ Scaling analysis is carried out for 0.1 secs after initial 5 secs simulation of settling period.
- ▶ TAU profiling is used to identify the computational cost associated with each routines.

Parameter <sup>1</sup>	Value
Total Particles	2.56 million
Diameter	4 mm
Density	2700 kg/m <sup>3</sup>
Coef. of restitution Particle, Wall	0.95, 0.95
Friction coefficient Particle, Wall	0.3 0.3
Spring constant Particle, Wall	2400, 2400 N/m
Dimension Grid size	640x640x2000 mm 160x160x500d <sub>p</sub> 64x64x200
Initial particle height	100d <sub>p</sub>
Superficial Velocity	2.0 m/sec
Time Step (Fluid, Solid)	5e-4, 4e-5 (12 sub steps)

# Strong Scaling Analysis

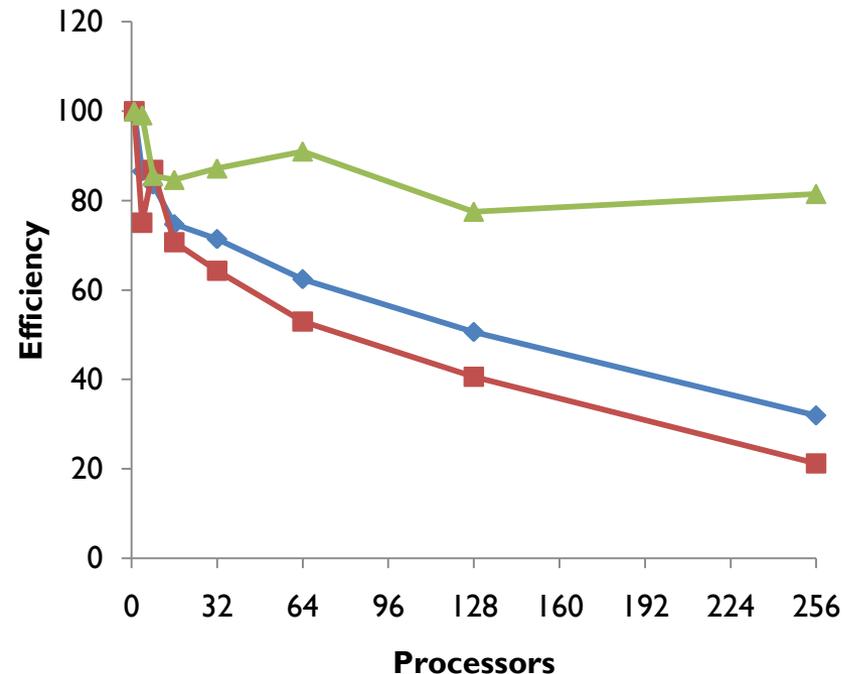
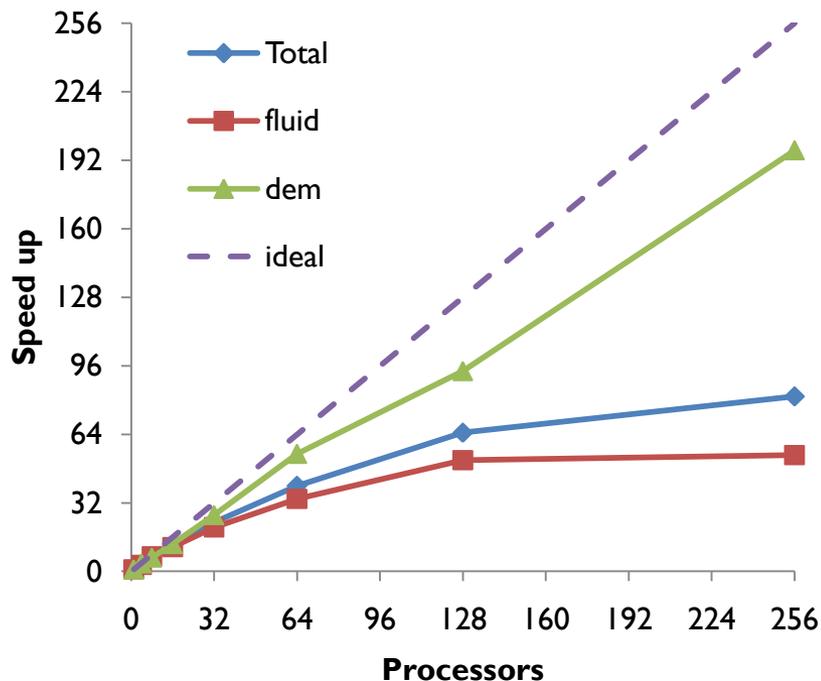
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## ▶ System configuration

- ▶ Athena cluster at VT
- ▶ Quad Socket AMD 2.3 GHZ Magny cour 8 core Processor
- ▶ 64 GB memory per node
- ▶ QDR Infiniband (40 Gb/sec)
- ▶ For simulation less than 32 processors, single node is blocked so that no other processes interfere with current study

Procs	Total time (hrs)	DEM time (hrs)
1	47.42	24.87
4	13.70	6.27
8	7.09	3.63
16	3.97	1.84
32	2.08	0.89
64	1.19	0.43
128	0.73	0.25
256	0.58	0.12

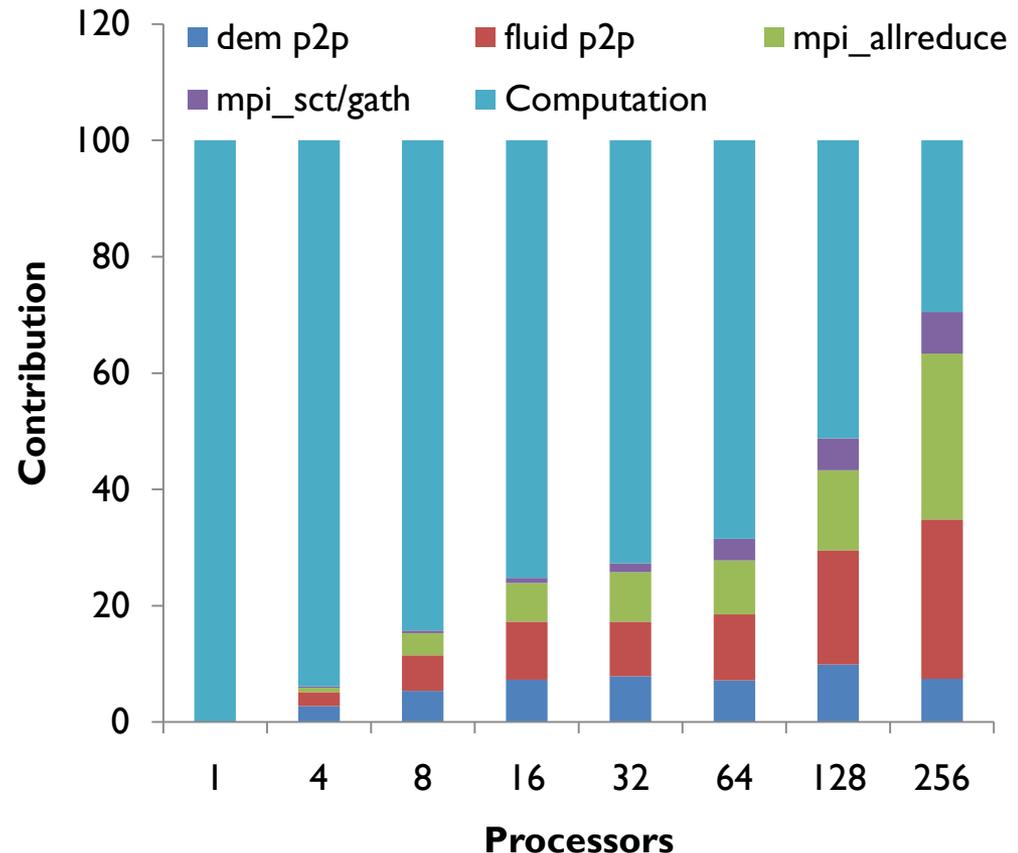
# Strong Scaling Analysis



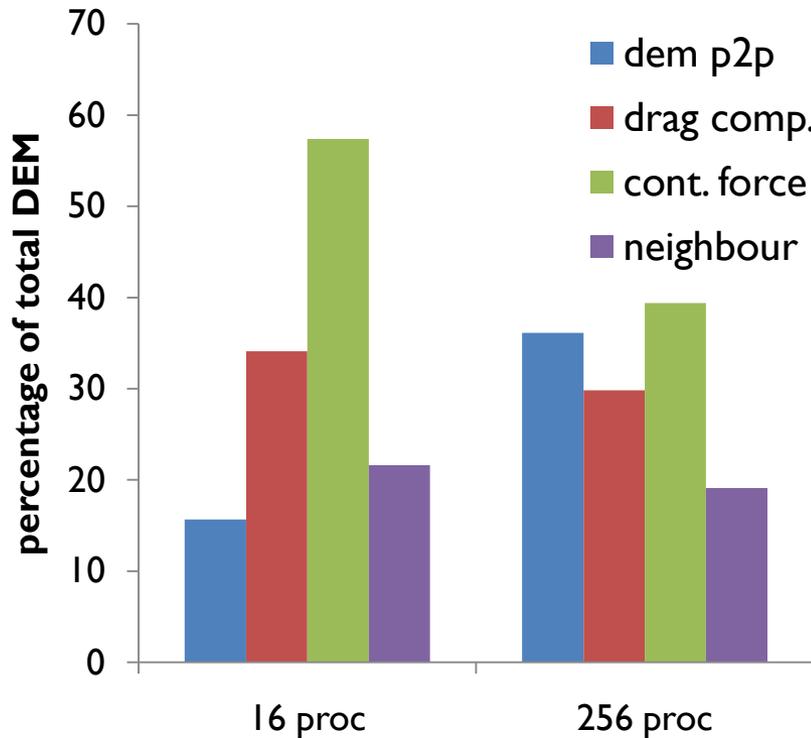
- ▶ For 256 processors (10,000 particles /proc,) a speed up of 208 for DEM and speed up of 81 for coupled solver are obtained.
- ▶ For fluid solver the scaling is poor due to low number of cells – only 3200 cells/processor for 256 processors
- ▶ Efficiency of DEM and Coupled solver are 81% and 31% , respectively.

# Communication overheads

- ▶ Graph shows communication overhead relative to total computation
- ▶ For fluid P2P communication % increases due to few number of cells.
- ▶ DEM P2P communication also increases.
- ▶ Global communications MPI\_allreduce, scatter and gather cost is high for 256 processors
- ▶ DEM shows good efficiency upto 10,000 particles/proc (80% efficiency), while flow solver has strong scaling up to 50,000 cells/proc (efficiency of 70%).



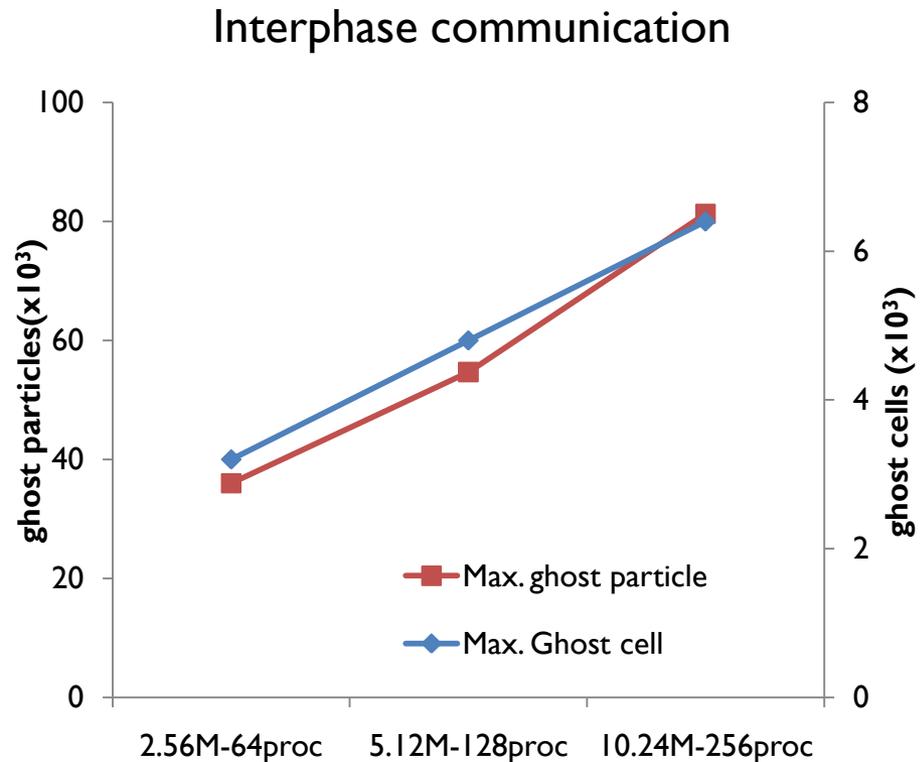
# DEM critical routines



- ▶ Relative % of DEM routines to total DEM time
- ▶ Contact force, drag force computation and neighbor list build are critical routines for DEM
- ▶ DEM P2P, which involves exchanging particles in ghost cell and particles crossing boundary contributes 15% for 16 proc and 30% for 256 proc simulation.

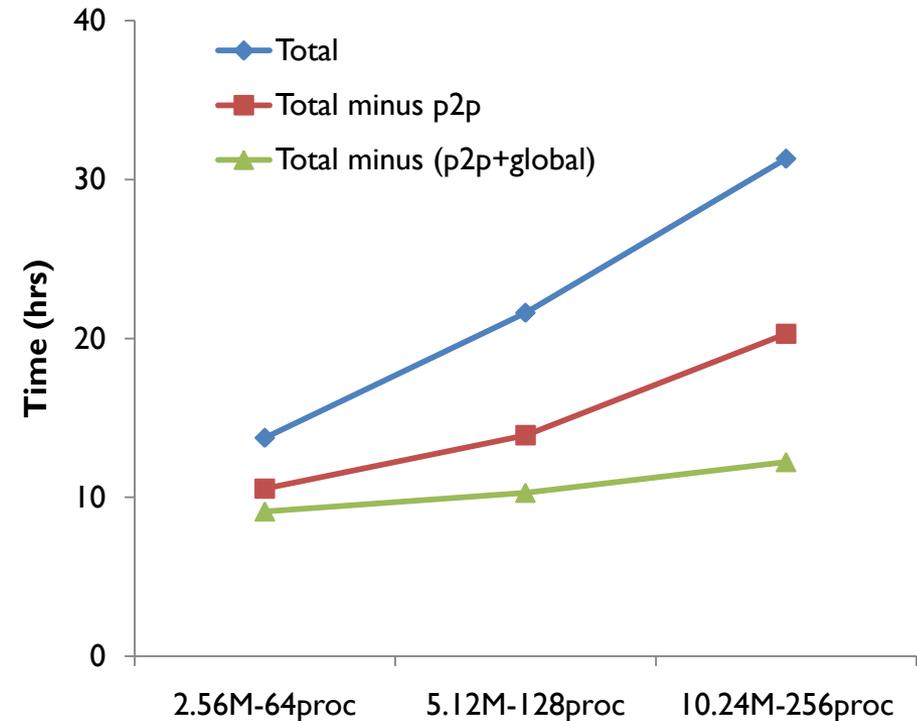
# Weak Scaling - Effect of bed height

- ▶ large scale system was analyzed by increasing the bed height
  - ▶  $H/W=0.625$  (64 proc-2.56 million)
  - ▶  $H/W=1.250$  (128 proc-5.12 million)
  - ▶  $H/W=2.500$  (256 proc-10.24 million)
- ▶ Width and depth are kept at 160dp
- ▶ Particles/proc and cells/proc are constant.
- ▶ interphase communication area increases with problem size, which will increase P2P cost.
- ▶ The study used to find relative contribution of global communication overheads

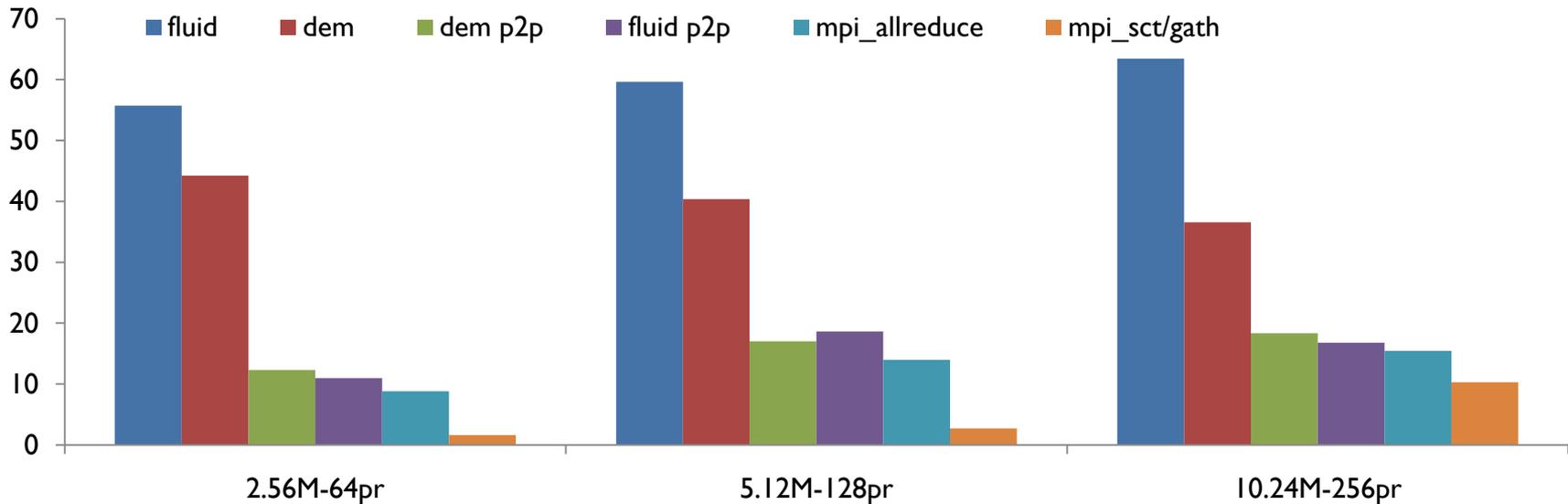


# Weak scaling

- ▶ Total time increases as problem size increases
- ▶ In the current study, P2P communication cost increases as interphase area also increases.
- ▶ Global communication cost (reduction operation and scatter/gather for IO) is major factor affecting the performance of large systems.
- ▶ Pure computational time (total time  $-(p2p+global\ comm.)$ ) is approximately constant for all three simulations



# Weak scaling



- ▶ Global communication is around 30% for 10 million case while it is around 10% for 2.56 million case.
- ▶ Scatter/gather communication increases from 1% to 10%.
- ▶ P2P communication also increases as the interphase area increases with the problem size.

# Void fraction at the center of the Bed

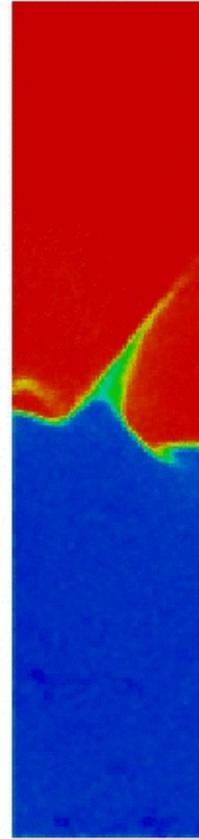
2.5 Million particles  
 $H/W = 0.625$



5 Million particles  
 $H/W = 1.25$



10 Million particles  
 $H/W = 2.5$

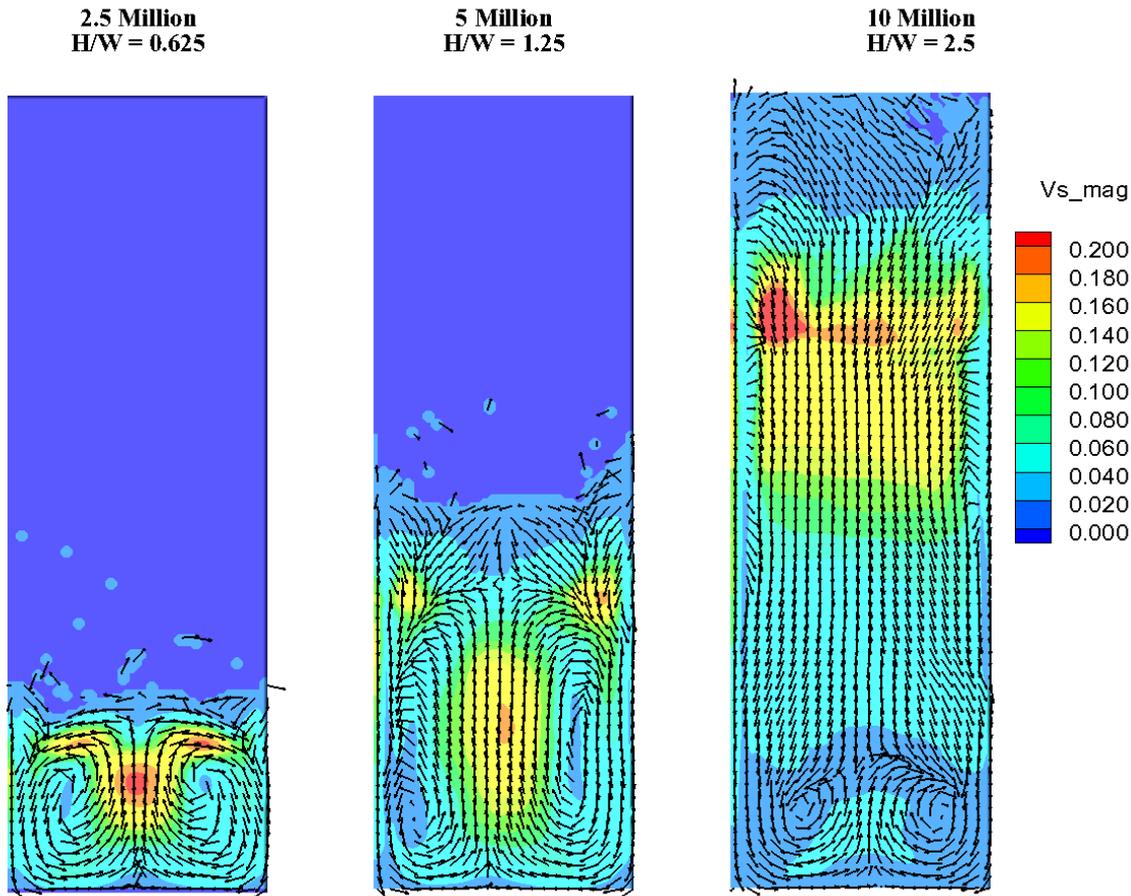


Time: 2.00

ep\_g  
1  
0.8  
0.6  
0.4  
0.35

- ▶ Bubble rise velocity and frequency identical for all bed heights
- ▶ As bed height increases, bubbles grows to entire width (slug flow) and collapses in the middle of the bed.

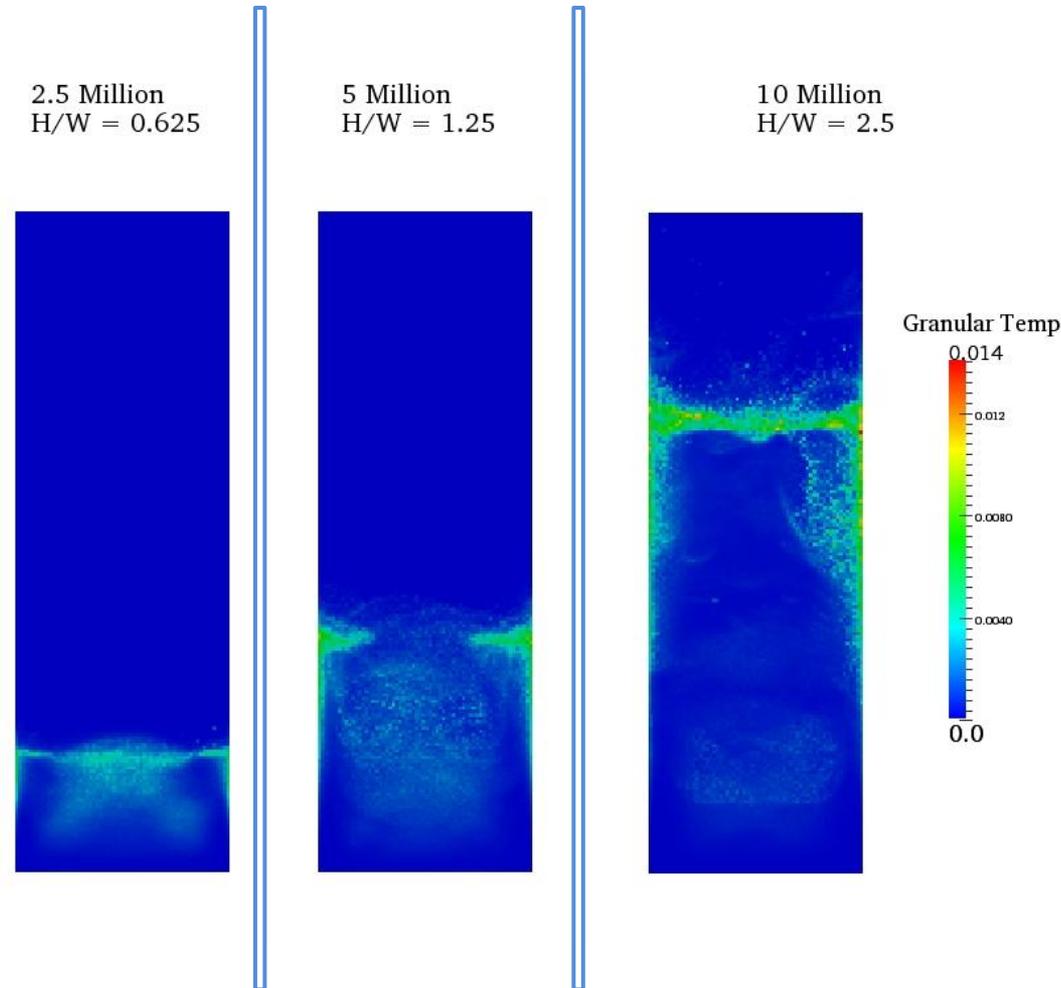
# Average solid velocity



Average solid velocity vectors  
(contour solid velocity magnitude)

- ▶ The average velocity contours show circulation of solids (spouting bed) for shallow bed.
- ▶ For large bed height, the recirculation region is small and does not extend up to top surface
- ▶ High gas velocity near the wall creates secondary solid circulation at the top surface. (this effect increases as bed height increases)

# Average Granular Temperature



- ▶ The profiles are identical for all three bed heights, with higher temperature near top surface close to wall.
- ▶ Granular temperature is high in regions where bubbles flow
- ▶ The value of granular temperature increases with increases in bed height

# Summary

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- ▶ Developed parallel DEM for MFIx, which is now capable of simulating millions of particles.
- ▶ Parallel DEM supports all existing features including mass inlet outlet for particles, periodic boundaries and interpolation routines for interphase momentum transfer and drag computation
- ▶ Distributed and parallel IO capability were added for restart and output files (supports Tecplot and VTK format)
- ▶ Strong Scaling: Speedup of 81 is obtained for combined CFD/DEM simulations for 256 processors, 2.56 million particles, 800K cells.
- ▶ Weak scaling shows that computational time remains constant for large system. Global communication increases with problem size.
- ▶ The scatter/gather used for single IO could be avoided using distributed IO
- ▶ *Future: Domain decomposition framework can lead to load imbalance. Hybrid MPI/OpenMP framework will provide better performance for complex systems with dilute and dense regions.*

# Acknowledgment

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- ▶ This technical effort was performed in support of the National Energy Technology Laboratory's ongoing research in advanced numerical simulation of multiphase flow under the RES contract DE-FE0004000.

# Design

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- ▶ **Distributed Memory Parallelization**
  - ▶ In accordance with existing MFIX domain decomposition
  - ▶ DES parallelization is based on separate grid (DESGRID)
    - ▶ Uniform – easy to bin the particles
    - ▶ Grid size selected based on the large diameter of the particles
  - ▶ One ghost cell enough for DES



# Development - Initialization

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- ▶ For new run
  - ▶ Read from `particle_input.dat` (either distributed IO or single IO) **or** Generate particle position based on input initial bed configuration
  - ▶ In case of single IO, particles will be scattered to respective processor based on its position
  - ▶ Each particle will be assigned with a unique global ID ; global ID is used to identify particles during ghost exchange and particle crossing exchange
- ▶ For restart run
  - ▶ Particles are read from restart file (either distributed IO or single IO)
  - ▶ In case of single IO, particles will be scattered; Further in case of single IO neighbor and contact particle details will have global ID; this will be modified to local particles number.

# Development – DES grid

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## ▶ DES grid

- ▶ A separate module contains all information related to desgrid
- ▶ Used for all DES MPI communication and neighbor build
- ▶ Uniform size  $\sim 3*$  largest solid diameter
- ▶ Easy to bin the particles
- ▶ Variables similar to existing MFIx fluid grid with “dg\_” prefix.  
Example dg\_istartI,dg\_iendI,dg\_imaxI,dg\_iminI
- ▶ Desgrid\_functions.inc contains IJK functions for desgrid

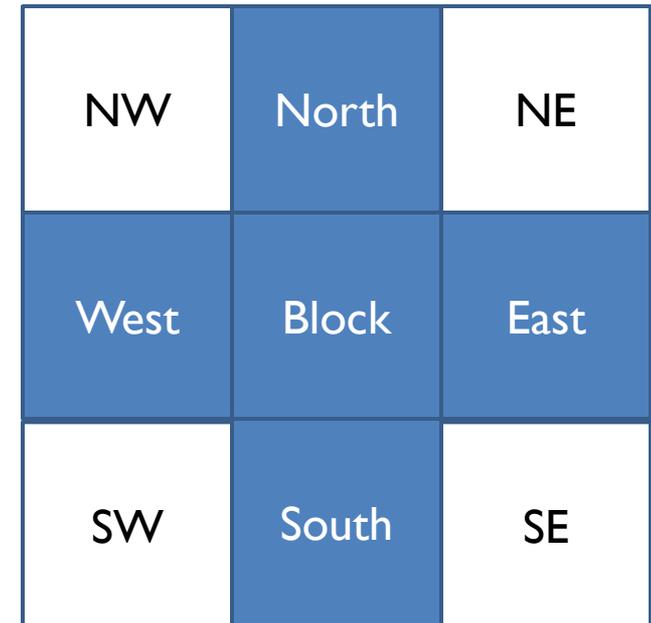
Note: Fluid grid is used to find the voidage, solid velocity and interphase momentum transfer terms



# Development – Particle crossing comm.

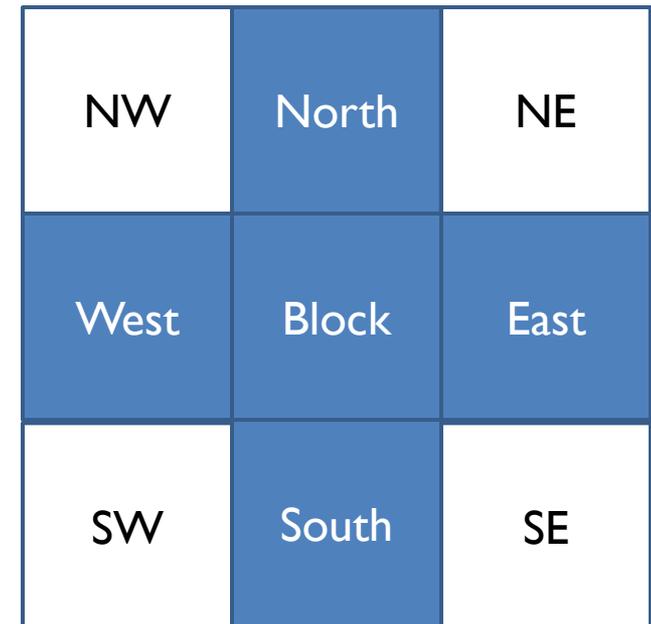
- ▶ When particle crosses boundary
  - ▶ Entire particle properties has to be transferred;
    - ▶ properties, position, velocity and forces
    - ▶ Neighbor and contact history –global id is sent along with their position
  - ▶ The communication takes place in the following order (grid-based network)
    - ▶ Top-Bottom Exchange
    - ▶ MPI\_barrier
    - ▶ North-South Exchange
    - ▶ MPI\_barrier
    - ▶ East-west Exchange
    - ▶ MPI\_barrier

This also takes care of particles moving from Center Block to NE,NW,SE,SW  
Adv: Less number of MPI calls.



# Development – Ghost comm.

- ▶ During each solid time step
  - ▶ Ghost particles are exchanged
    - ▶ properties, position, velocity
    - ▶ Ghost particles will be added/removed only before neighbor build
  - ▶ The communication takes place in the following order
    - ▶ East-west Exchange
    - ▶ MPI\_barrier
    - ▶ North-South Exchange
    - ▶ MPI\_barrier
    - ▶ Top-Bottom Exchange
    - ▶ MPI\_barrier



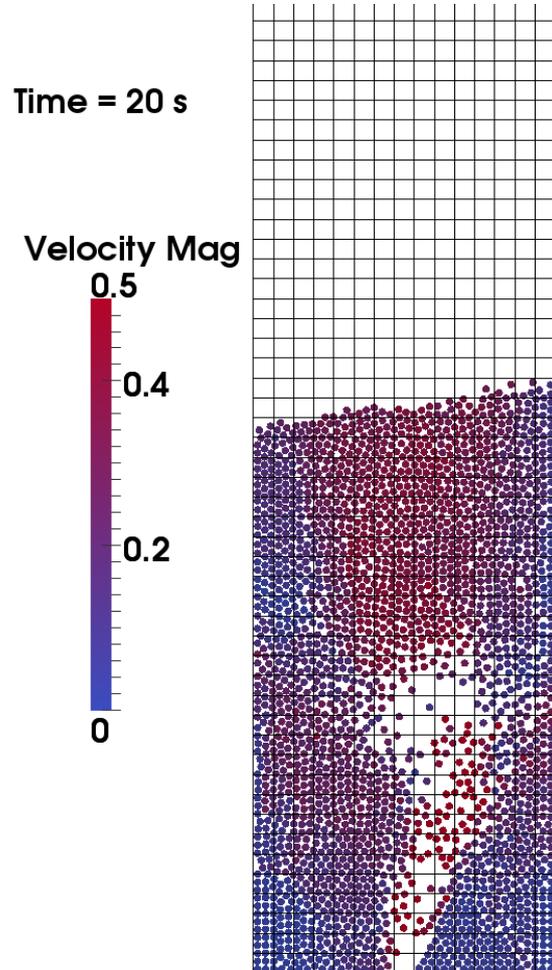
Particles in corner cells will be exchanged.  
Adv: Less number of MPI calls.

# Development – IO

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- ▶ Based on the option `bdist_io`
  - ▶ Single IO uses gather and scatter; restart files and VTK format, tecplot files
  - ▶ Distributed IO writes particle present in the processor (no ghost particles) to respective file

# Validation – 2D Bubbling bed



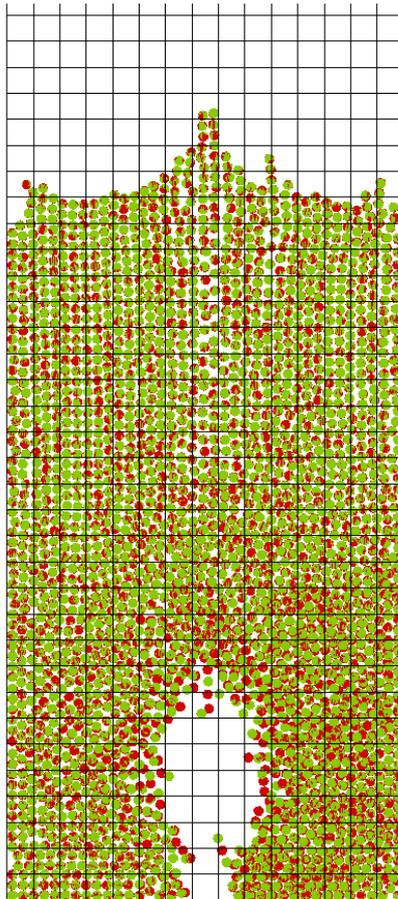
Parameter <sup>1</sup>	Value
Total Particles	2400
Diameter	4 mm
Density	2700 kg/m <sup>3</sup>
Coef. of restitution Particle, Wall	0.8, 0.8
Friction coefficient Particle, Wall	0.2, 0.2
Spring constant Particle, Wall	800, 1200 N/m
Dimension Grid size	150x900 mm 15x90
Superficial Velocity	2.8 m/s
Jet velocity	42 m/s
Time Step (Fluid, Solid)	5e-4, 7.5e-5 (7 steps)

# Validation – Instantaneous Particle

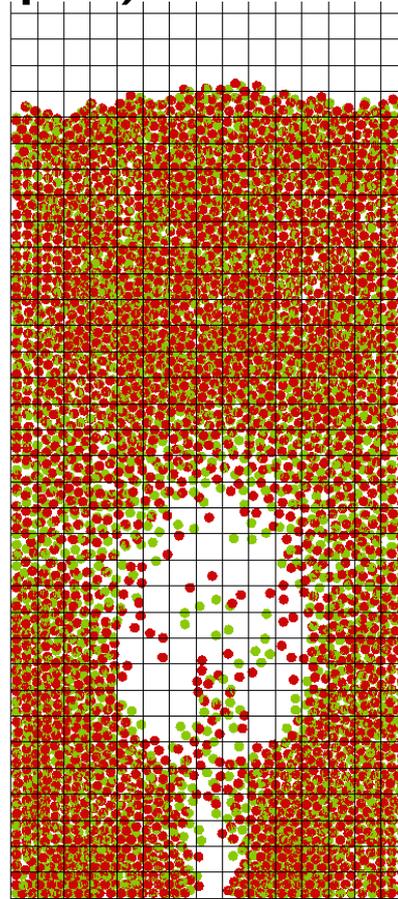
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**Green – Serial**

**Red – Parallel (2 proc)**



Time = 0.1 s

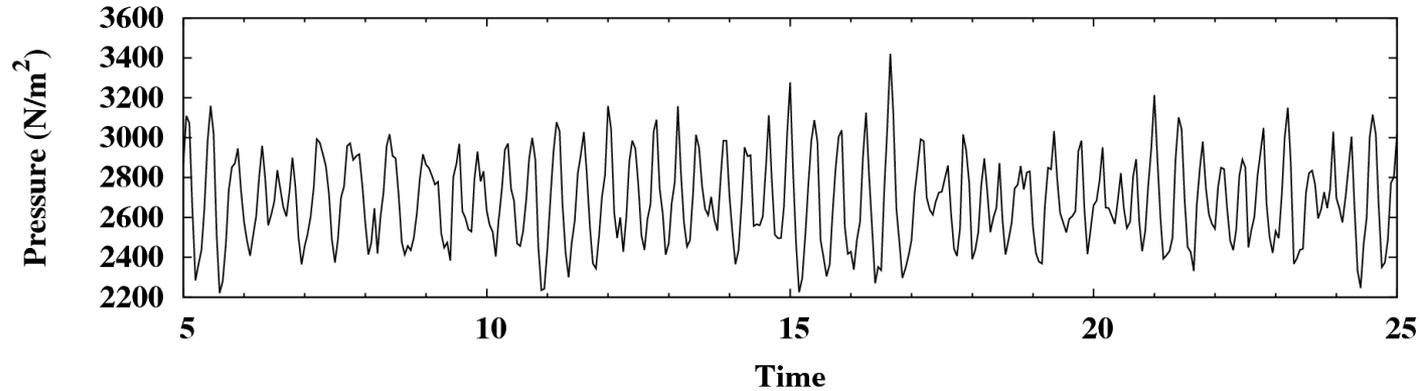


Time = 0.2 s

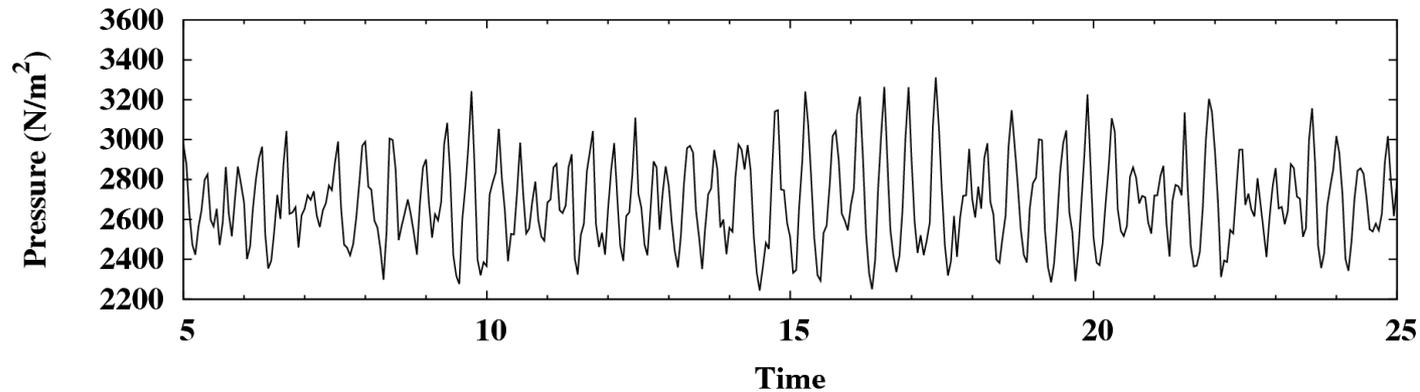
- **Instantaneous Particle position matches well up to 0.1 secs**
  - **It deviates as time progress due to numerical round of errors**
-

# Validation – Pressure drop

Serial Simulation

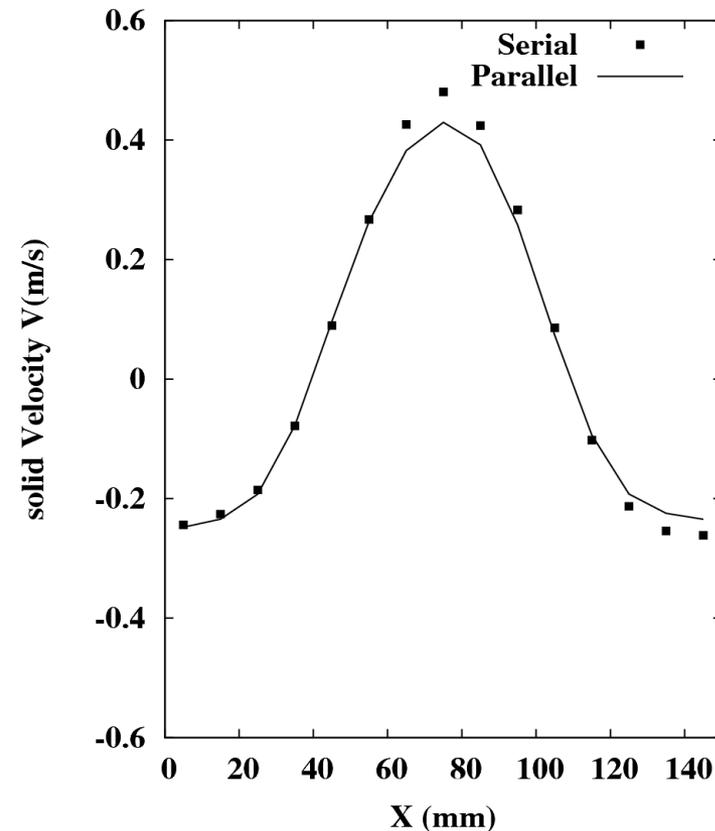
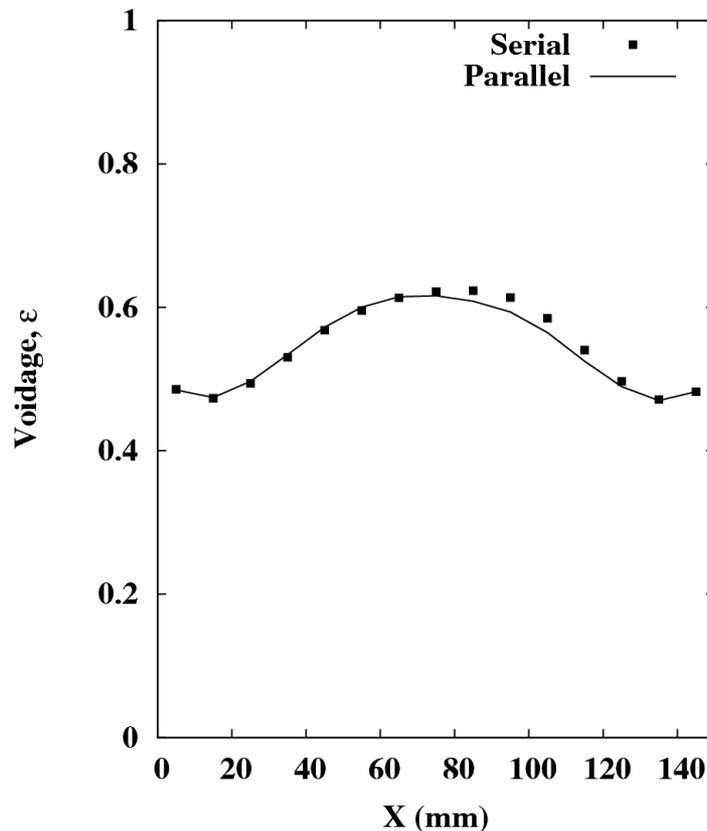


Parallel Simulation with 2procs



Pressure drop varies between 2200 and 3200 N/m<sup>2</sup> for both simulations

# Validation – Average profiles



Average profiles obtained for 20 secs at a frequency of 20 Hz.

Some asymmetry in the serial case.

