Parallelization of Discrete Element method

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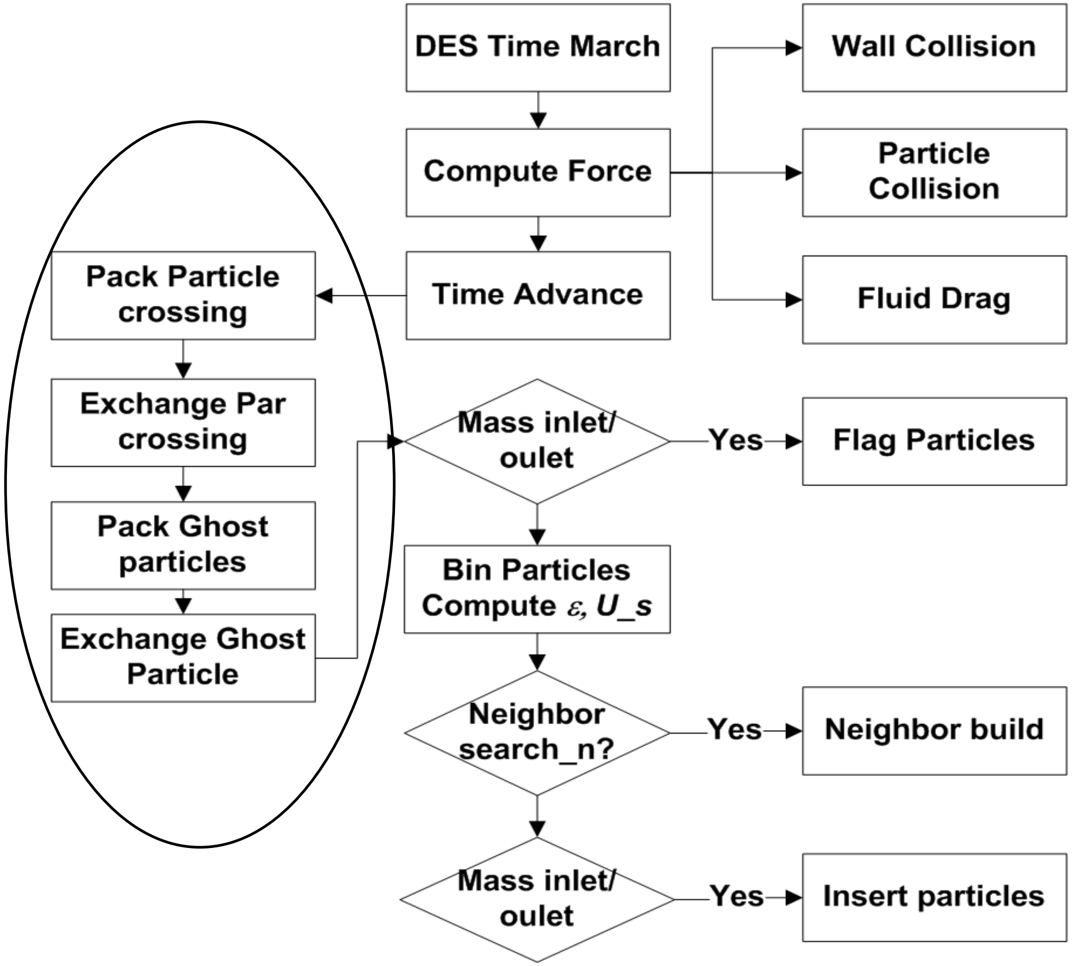
Motivation and Objective

- 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

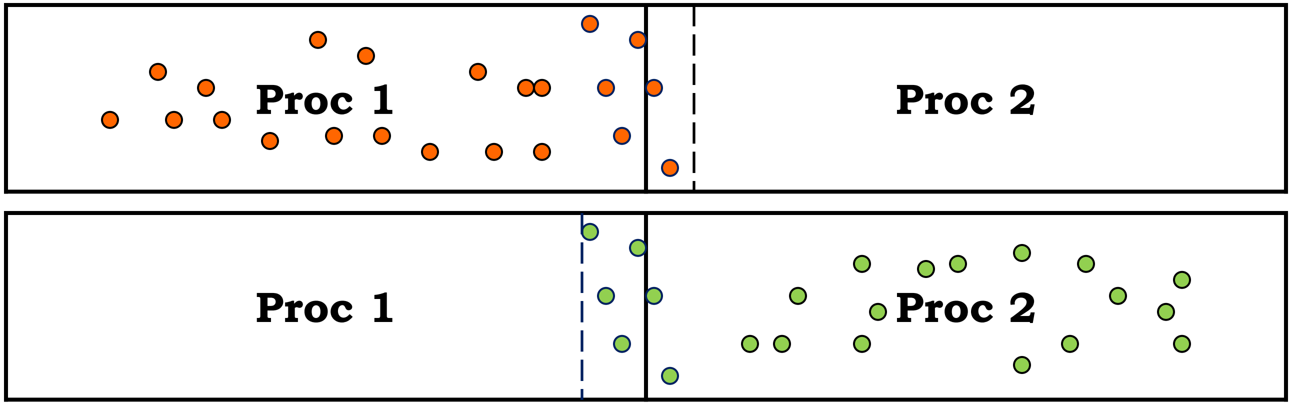
- Considerations
  - Developing efficient parallel algorithm in compliance with existing MPI architecture of MFIX
  - minimal changes to the code
  - adherence to existing coding standards and naming convention

Parallel Algorithm



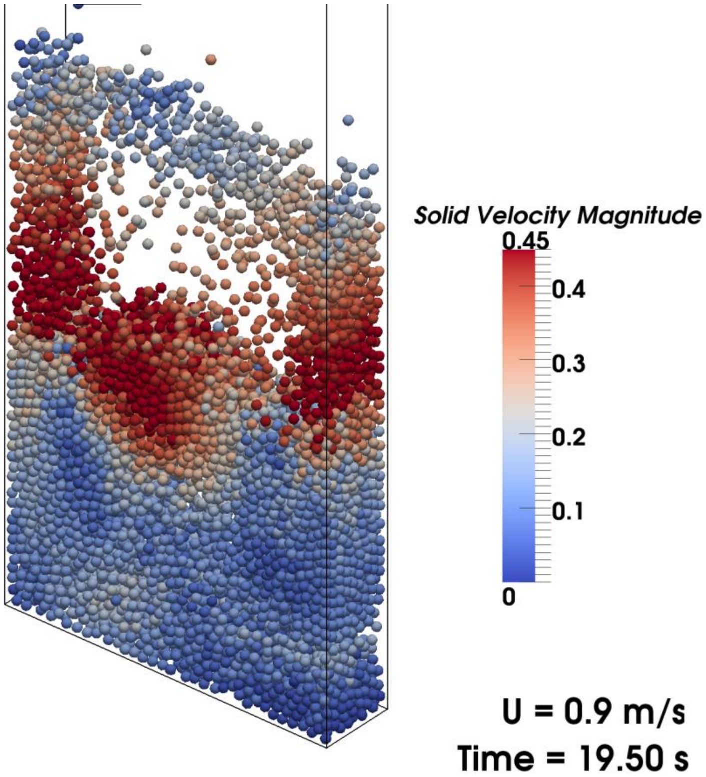
Development

- 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

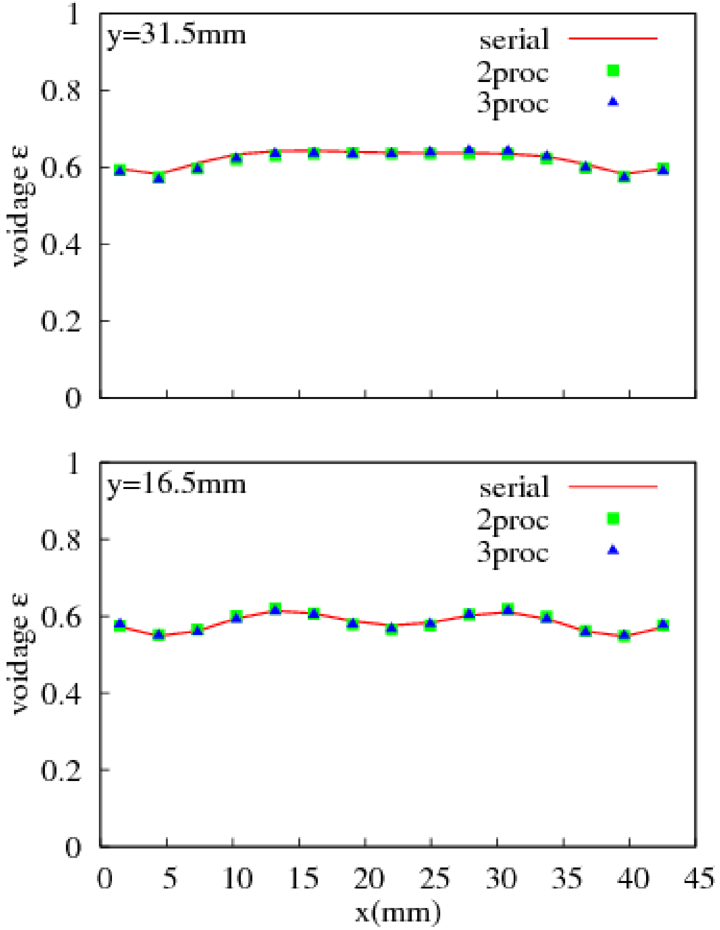
Psudo-2D Fluidized bed similar to Muller et al. 2008



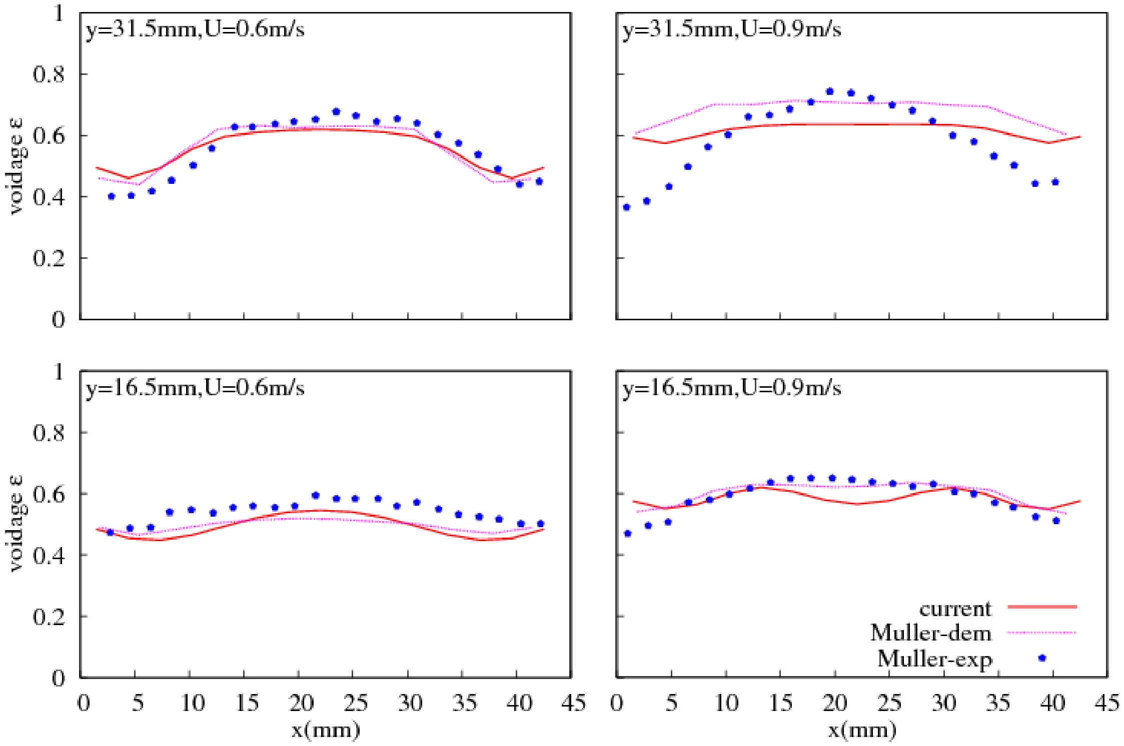
Parameter[1]	Value
Total Particles	9240
Diameter	1.2 mm
Density	1000 kg/m^3
Coef. of restitution Particle, Wall	0.9, 0.9
Friction coefficient Particle, Wall	0.1, 0.1
Spring constant Particle, Wall	200, 200 N/m
Dimension Grid size	44x120x10 mm 15x40x3
Superficial Velocity	0.6, 0.9 m/s
Time Step (Fluid, 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.

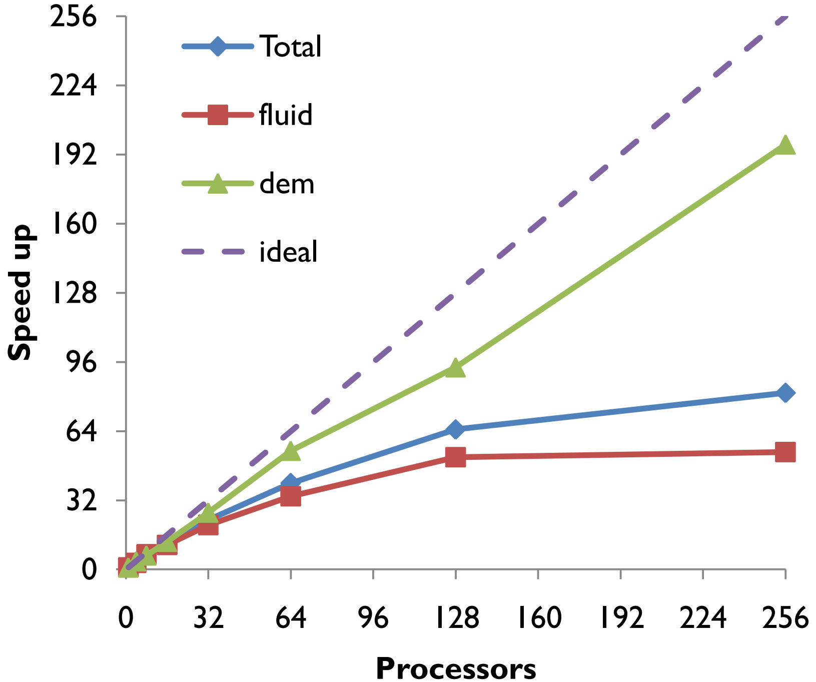
Parameter[1]	**Value**
Total Particles	2.56 million
Diameter	4 mm
Density	2700 kg/m^3
Coef. of restitution Particle, Wall	0.95, 0.95
Friction coefficient Particle, Wall	0.3 0.3
Spring constant Particle, Wall	2400, 2400 N/m
Dimension Grid size	640x640x2000 mm 160x160x500d_p 64x64x200
Initial particle height	100d_p
Superficial Velocity	2.0 m/sec
Time Step (Fluid, Solid)	5e-4, 4e-5 (12 sub steps)

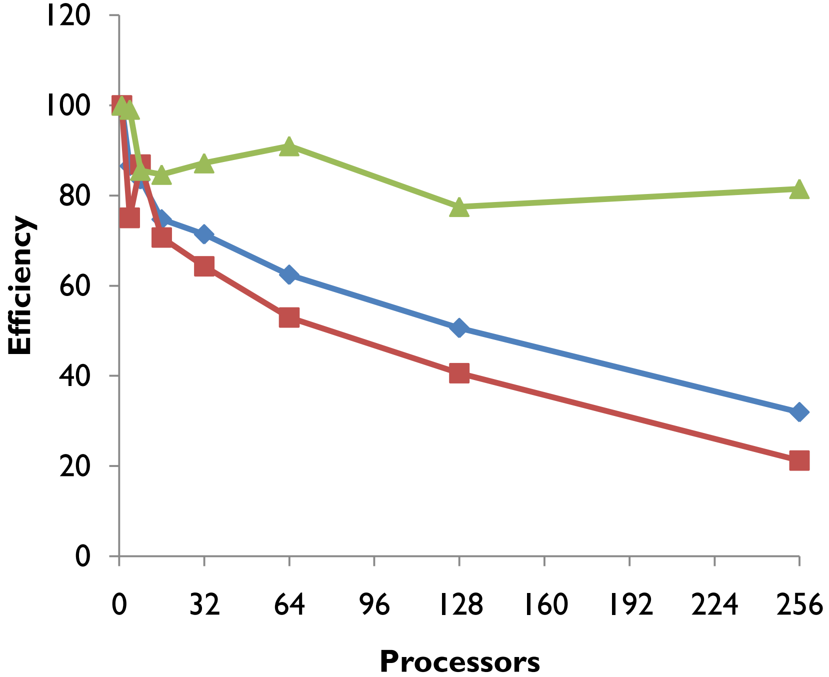
Strong Scaling Analysis

- 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

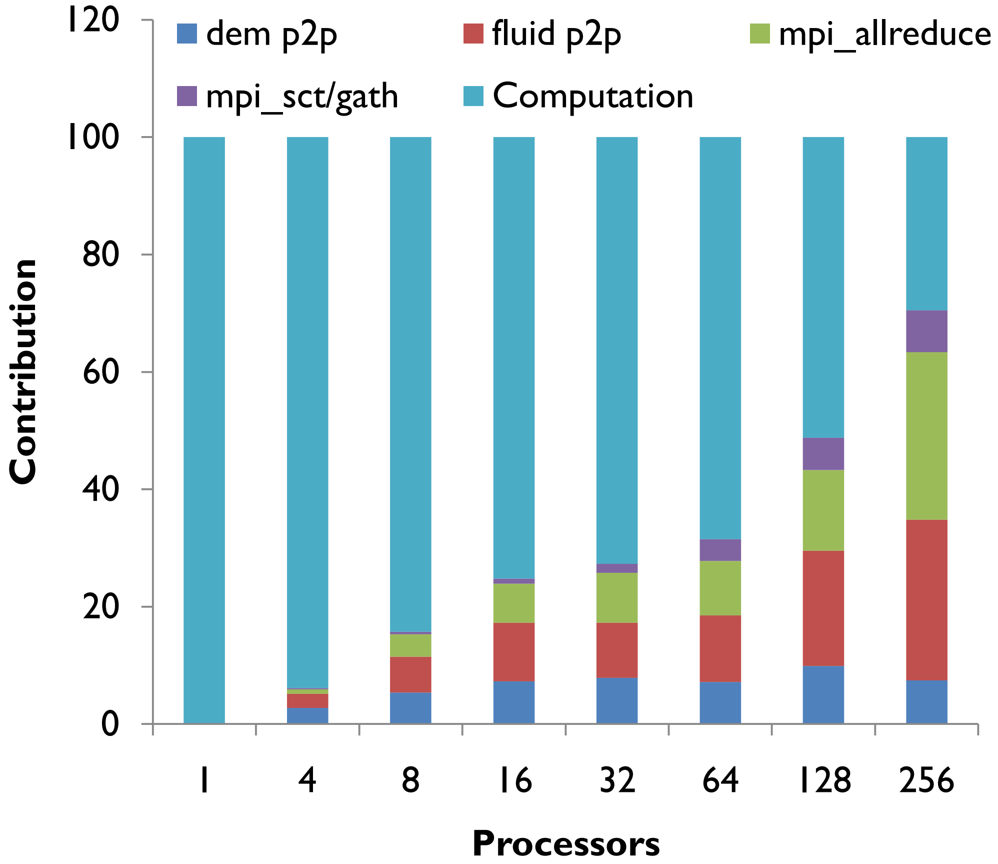




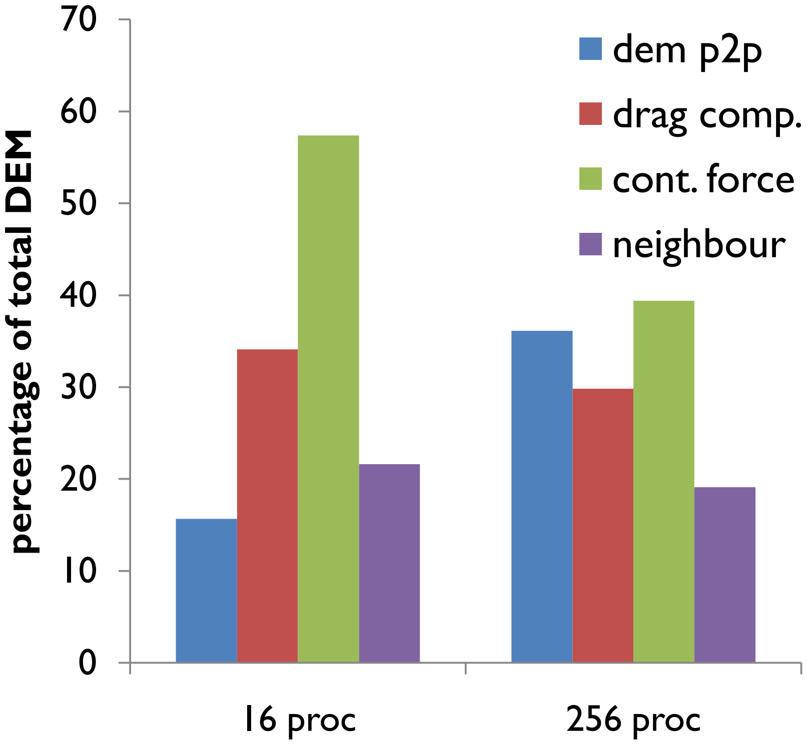
- For 256 processors (10,000 particles /proc,) a speed up of 208 for DEM and speed up of 81for coupled solver are obtained.
- For fluid solver the scaling is poor due to low number of cells – only 3200 cells/processor for 256 processors
- Efficiency of DEM and Coupled solver are 81% and 31% , respectively.

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%).



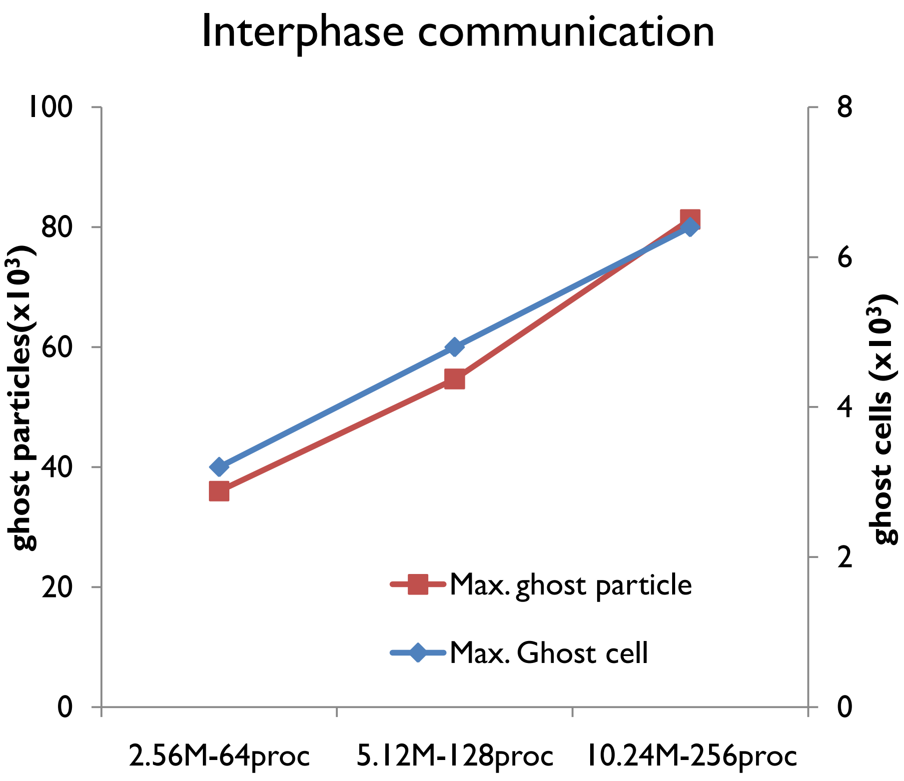
DEM critical routines



- 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.

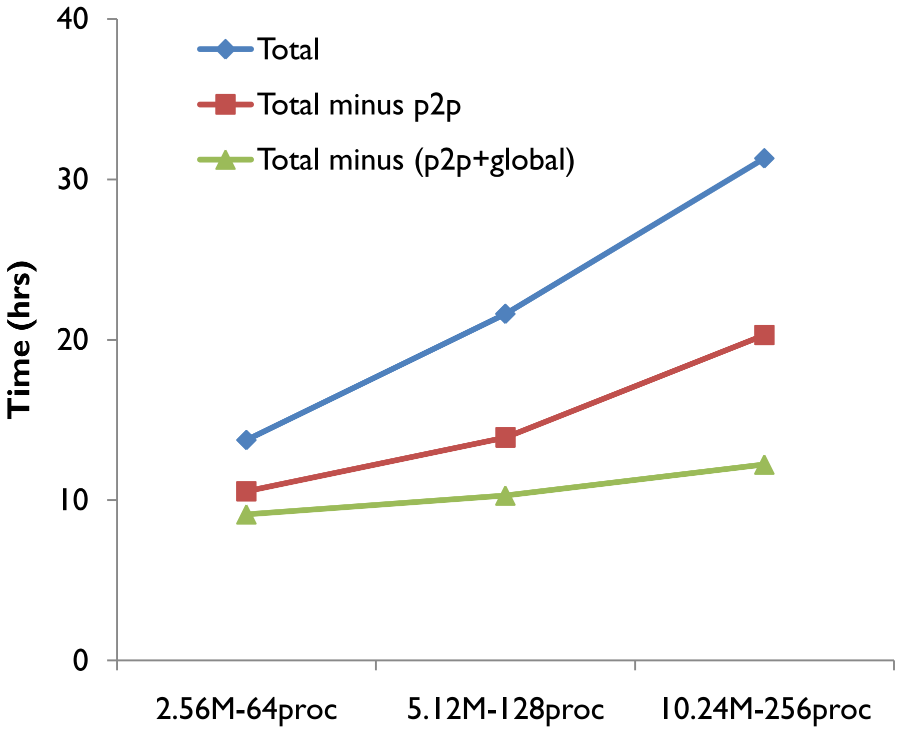
Weak Scaling - Effect of bed height

- 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

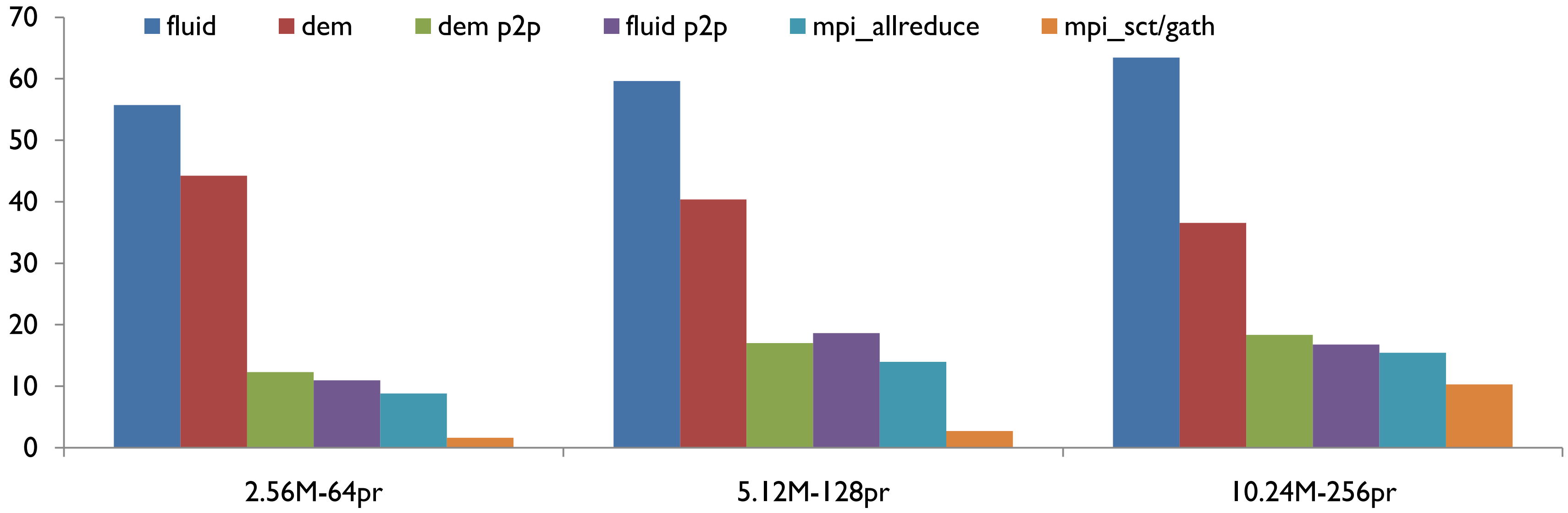


Weak scaling

- 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

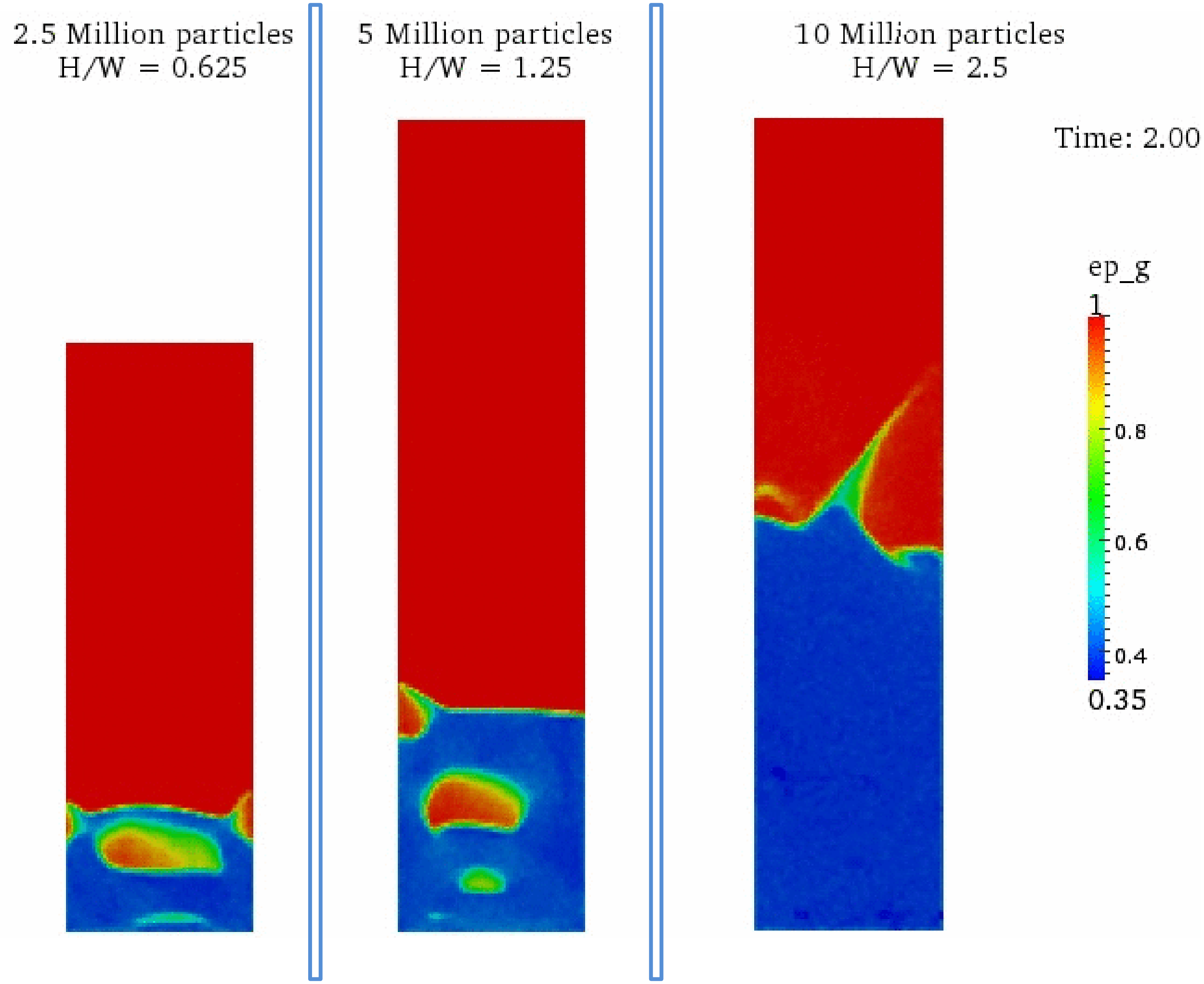


Weak scaling



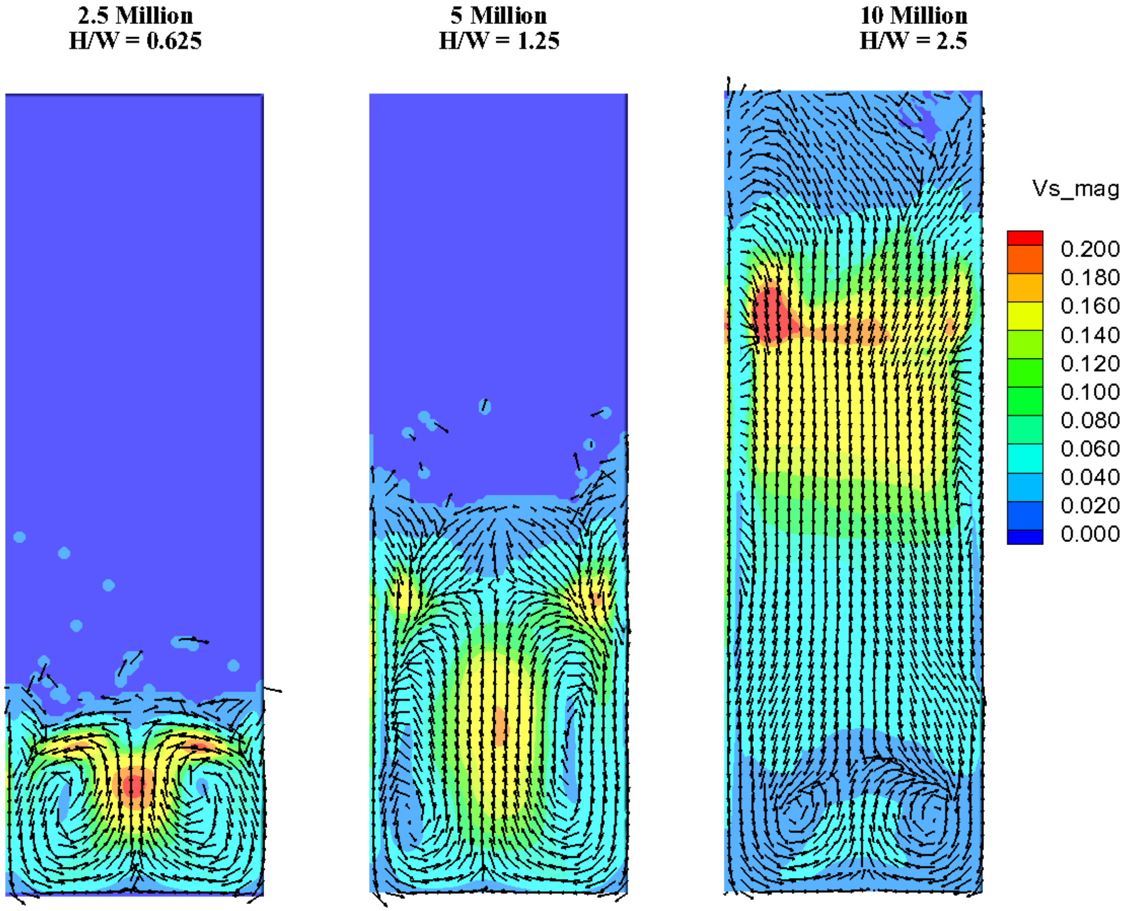
- Global communication is around 30% for 10 million case while it is around 10% for 2.56 million case.
- Scatter/gather communication increases from 1% to 10%.
- P2P communication also increases as the interphase area increases with the problem size.

Void fraction at the center of the Bed



- 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.

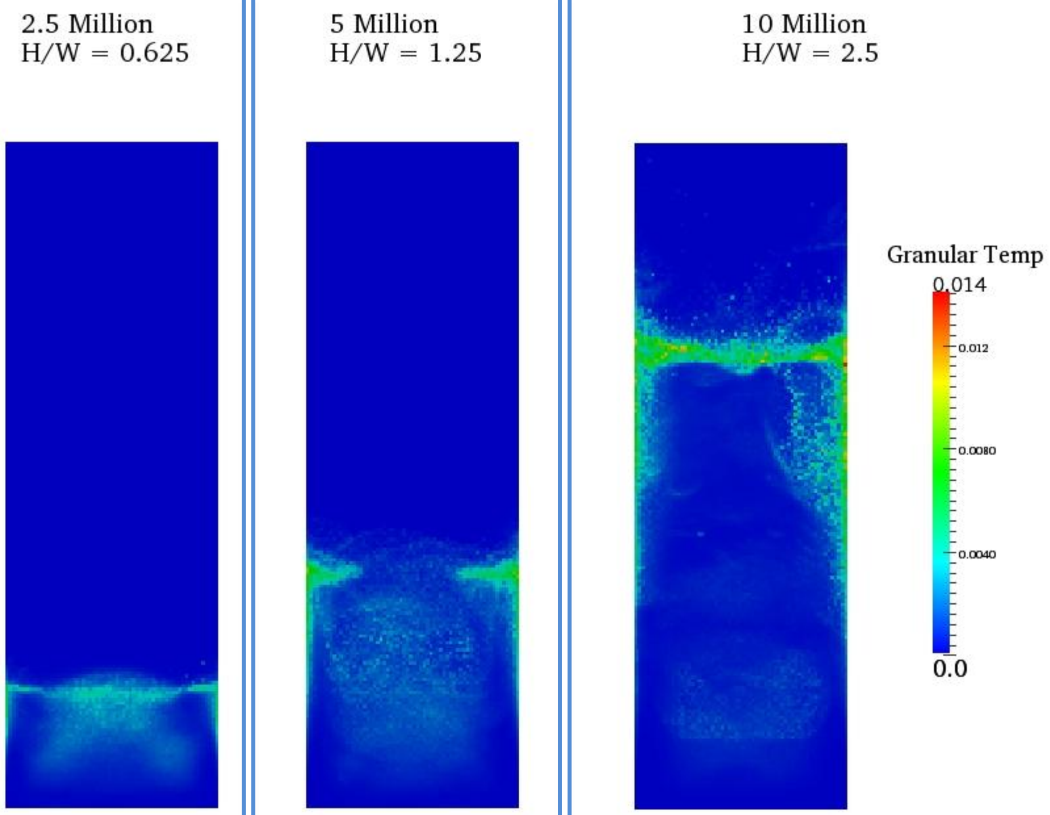
Average solid velocity



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 extent 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

- 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

- 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

- 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

Proc 1

istart4	Istart3	Istart2	istart1		iend1	Iend2	Iend3	Iend4
-1	0	1	2	3	4	5	6	7

Proc 2

istart4	Istart3	Istart2	istart1		iend1	Iend2	Iend3	Iend4
2	3	4	5	6	7	8	9	10

Development - Intialization

- 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

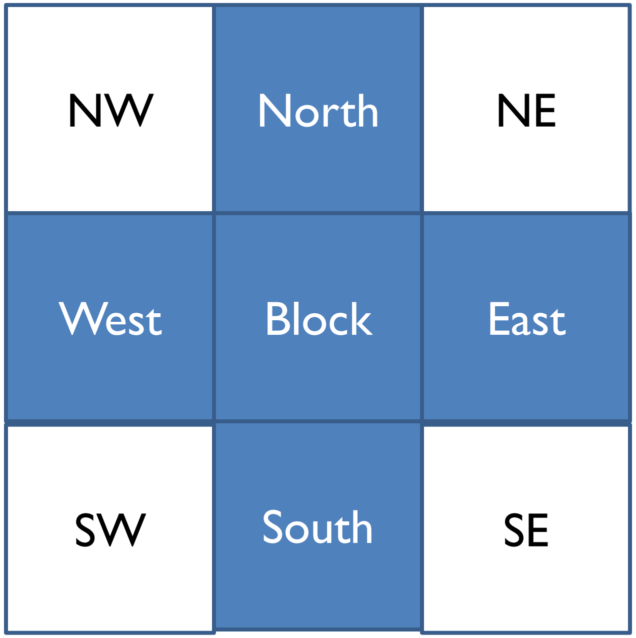
- DES grid
  - A separate module contains all information related to desgrid
  - Used for all DES MPI communication and neighbor build
  - Uniform size ~ 3* largest solid diameter
  - Easy to bin the particles
  - Variables similar to existing MFIX fluid grid with "dg_" prefix. Example dg_istart1,dg_iend1,dg_imax1,dg_imin1
  - 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.



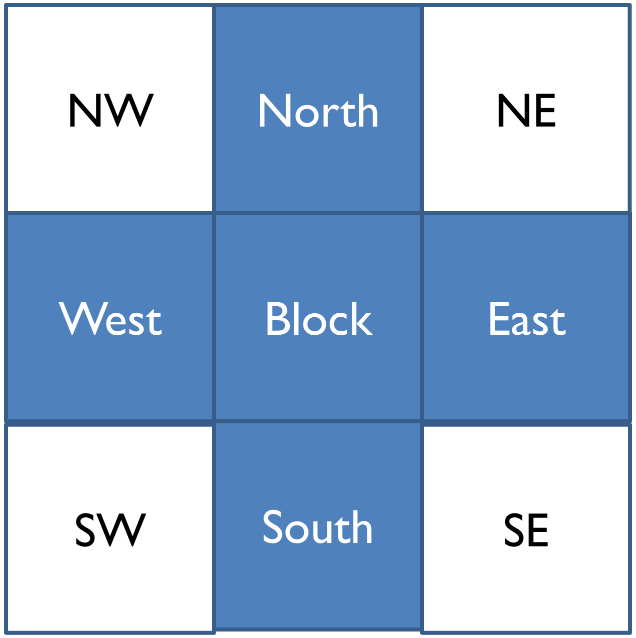
NW	North	NE
West	Block	East
SW	South	SE

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.

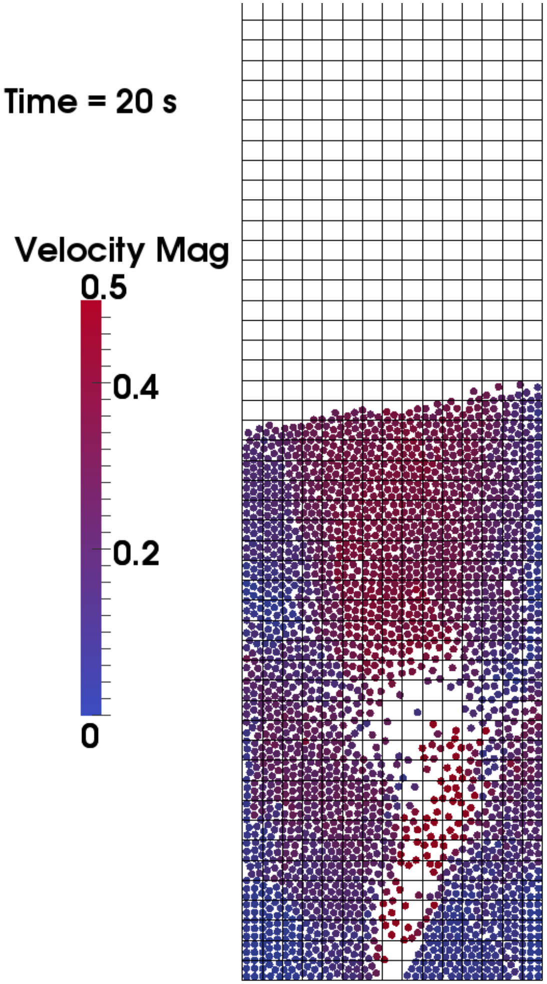


NW	North	NE
West	Block	East
SW	South	SE

Development – IO

- 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

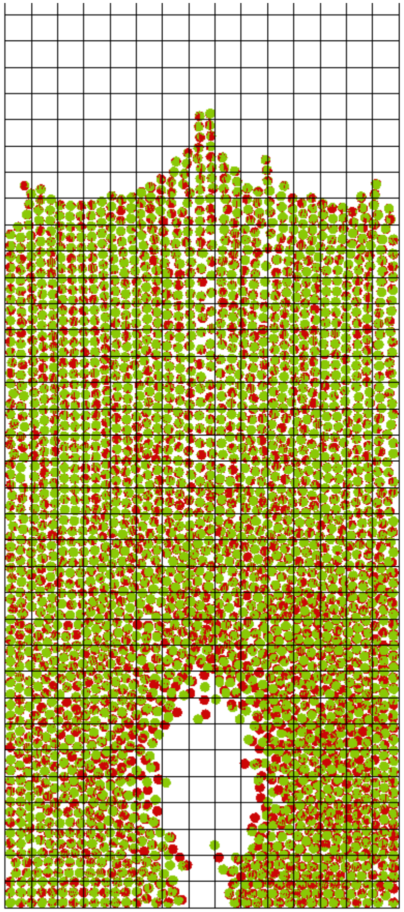


Parameter[1]	Value
Total Particles	2400
Diameter	4 mm
Density	2700 kg/m^3
Coef. of restitution Particle, Wall	0.8, 0.8
Friction coefficient Particle, Wall	0.2, 0.2
Spring constant Particle, Wall	800, 1200 N/m
Dimension Grid size	150x900 mm 15x90
Superficial Velocity	2.8 m/s
Jet velocity	42 m/s
Time Step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

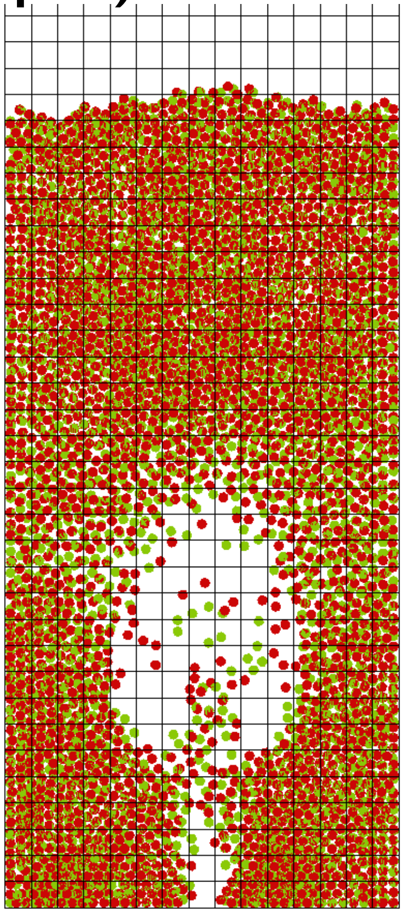
[1] Tsuij et al. (1993)

Validation – Instantaneous Particle

Green – Serial
Red – Parallel (2 proc)



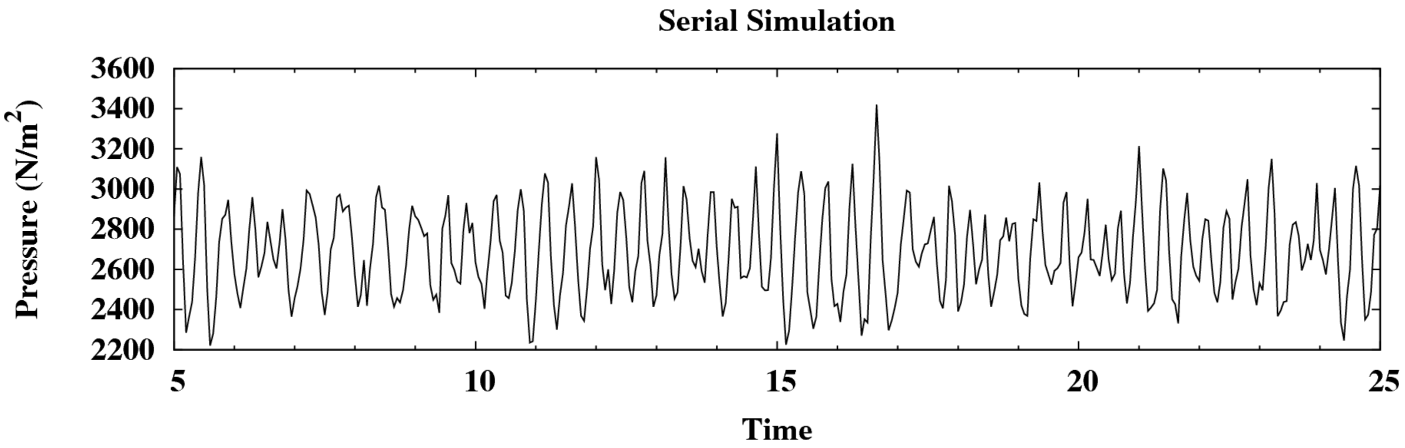
Time = 0.1 s

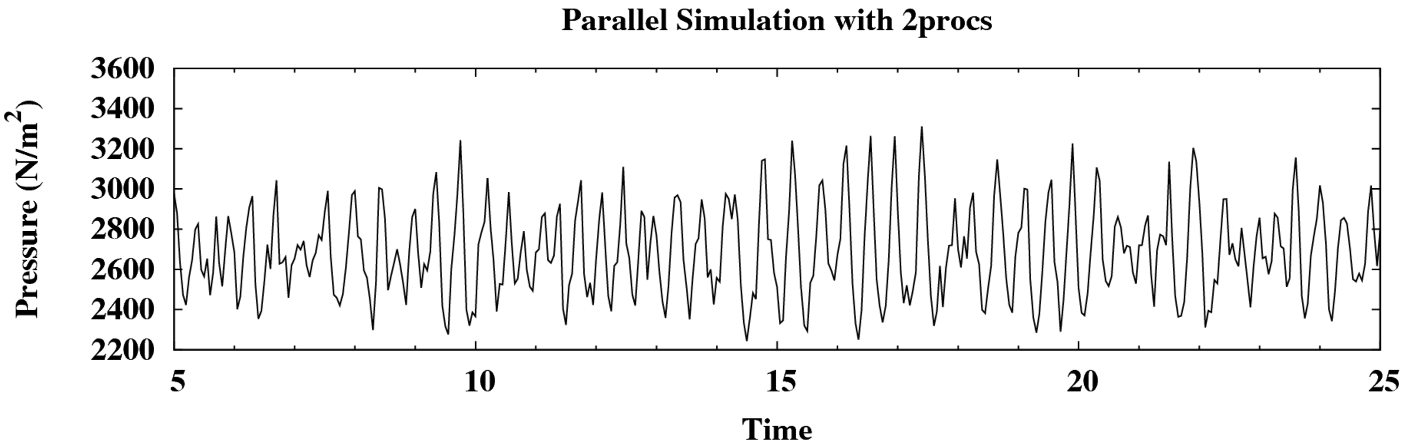


Time = 0.2 s

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

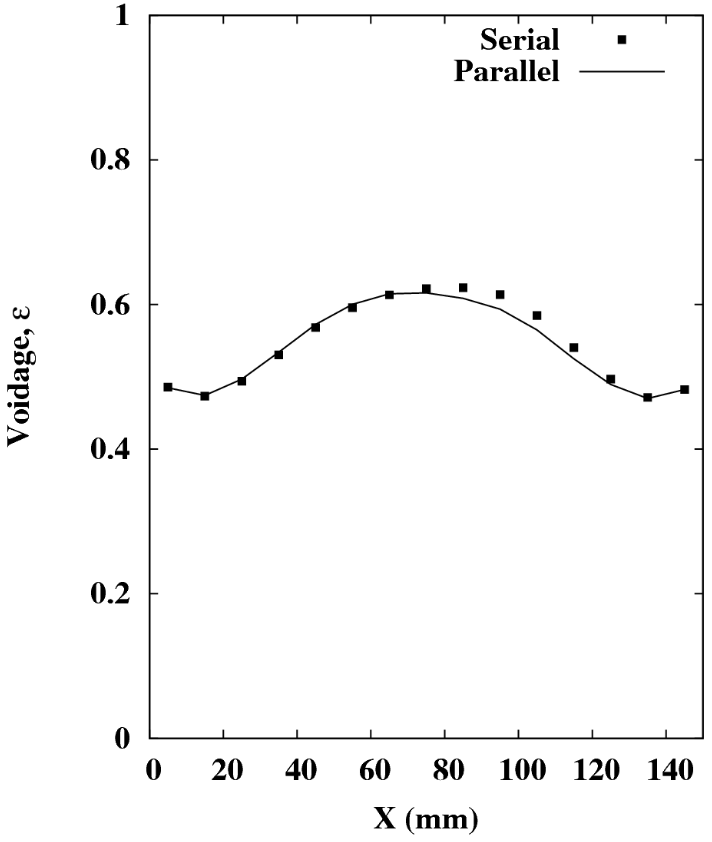
Validation – Pressure drop

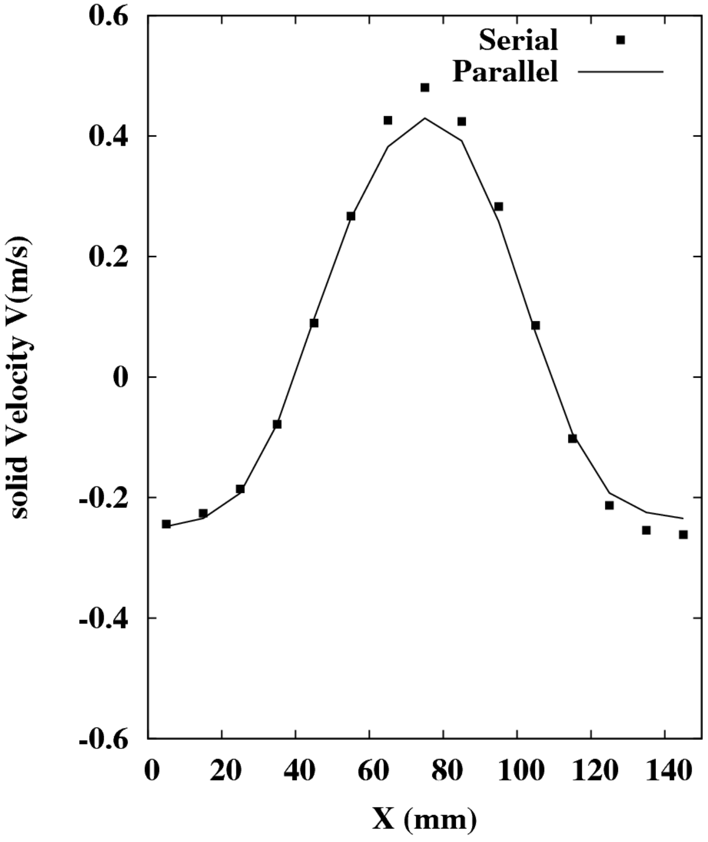




Pressure drop varies between 2200 and 3200 N/m^2 for both simulations

Validation –Average profiles





Average profiles obtained for 20 secs at a frequency of 20 Hz.
Some asymmetry in the serial case.