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 the 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

- 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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Particles</td>
<td>9240</td>
</tr>
<tr>
<td>Diameter</td>
<td>1.2 mm</td>
</tr>
<tr>
<td>Density</td>
<td>1000 kg/m³</td>
</tr>
<tr>
<td>Coef. of restitution</td>
<td>0.9, 0.9</td>
</tr>
<tr>
<td>Friction coefficient</td>
<td>0.1, 0.1</td>
</tr>
<tr>
<td>Spring constant</td>
<td>200, 200 N/m</td>
</tr>
<tr>
<td>Dimension</td>
<td>44x120x10 mm, 15x40x3 mm</td>
</tr>
<tr>
<td>Superficial Velocity</td>
<td>0.6, 0.9 m/s</td>
</tr>
<tr>
<td>Time Step (Fluid, Solid)</td>
<td>2e-4, 1.49e-5 (14 steps)</td>
</tr>
</tbody>
</table>

\[ U = 0.9 \text{ m/s} \]
\[ \text{Time} = 19.50 \text{ s} \]
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.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Total Particles</td>
<td>2.56 million</td>
</tr>
<tr>
<td>Diameter</td>
<td>4 mm</td>
</tr>
<tr>
<td>Density</td>
<td>2700 kg/m³</td>
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<tr>
<td>Coef. of restitution Particle, Wall</td>
<td>0.95, 0.95</td>
</tr>
<tr>
<td>Friction coefficient Particle, Wall</td>
<td>0.3 0.3</td>
</tr>
<tr>
<td>Spring constant Particle, Wall</td>
<td>2400, 2400 N/m</td>
</tr>
<tr>
<td>Dimension Grid size</td>
<td>640x640x2000 mm 160x160x500dₚ 64x64x200</td>
</tr>
<tr>
<td>Initial particle height</td>
<td>100dₚ</td>
</tr>
<tr>
<td>Superficial Velocity</td>
<td>2.0 m/sec</td>
</tr>
<tr>
<td>Time Step (Fluid, Solid)</td>
<td>5e-4, 4e-5 (12 sub steps)</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Procs</th>
<th>Total time (hrs)</th>
<th>DEM time (hrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>47.42</td>
<td>24.87</td>
</tr>
<tr>
<td>4</td>
<td>13.70</td>
<td>6.27</td>
</tr>
<tr>
<td>8</td>
<td>7.09</td>
<td>3.63</td>
</tr>
<tr>
<td>16</td>
<td>3.97</td>
<td>1.84</td>
</tr>
<tr>
<td>32</td>
<td>2.08</td>
<td>0.89</td>
</tr>
<tr>
<td>64</td>
<td>1.19</td>
<td>0.43</td>
</tr>
<tr>
<td>128</td>
<td>0.73</td>
<td>0.25</td>
</tr>
<tr>
<td>256</td>
<td>0.58</td>
<td>0.12</td>
</tr>
</tbody>
</table>
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

- 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.
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)
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

<table>
<thead>
<tr>
<th>istart4</th>
<th>Istart3</th>
<th>Istart2</th>
<th>istart1</th>
<th>iend1</th>
<th>lend2</th>
<th>lend3</th>
<th>lend4</th>
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<tbody>
<tr>
<td>-1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
</tr>
</tbody>
</table>

Proc 1

<table>
<thead>
<tr>
<th>istart4</th>
<th>Istart3</th>
<th>Istart2</th>
<th>istart1</th>
<th>iend1</th>
<th>lend2</th>
<th>lend3</th>
<th>lend4</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
<td>9</td>
</tr>
</tbody>
</table>

Proc 2
Development - Initialization

- **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.
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

- 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

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</tr>
<tr>
<td>Diameter</td>
<td>4 mm</td>
</tr>
<tr>
<td>Density</td>
<td>2700 kg/m$^3$</td>
</tr>
<tr>
<td>Coef. of restitution</td>
<td>0.8, 0.8</td>
</tr>
<tr>
<td>Friction coefficient</td>
<td>0.2, 0.2</td>
</tr>
<tr>
<td>Spring constant</td>
<td>800, 1200 N/m</td>
</tr>
<tr>
<td>Dimension Grid size</td>
<td>150x900 mm 15x90</td>
</tr>
<tr>
<td>Superficial Velocity</td>
<td>2.8 m/s</td>
</tr>
<tr>
<td>Jet velocity</td>
<td>42 m/s</td>
</tr>
<tr>
<td>Time Step (Fluid, Solid)</td>
<td>5e-4, 7.5e-5 (7 steps)</td>
</tr>
</tbody>
</table>

$^1$Tsuij et al. (1993)
Validation – Instantaneous Particle

Green – Serial
Red – Parallel (2 proc)

- 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/m² for both simulations.
Validation – Average profiles

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