Statistical Analysis on Large-scale Direct Numerical Simulation of Gas-solid Flow

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Outline

- Background
- Enabling Large-scale DNS
- Numerical Results
- Conclusions
Multi-scale Modelling for Gas-solid Flow

Two-fluid Model (TFM)  Discrete Particle Model (DPM or CFD-DEM)  Direct Numerical Simulation (DNS)

Fluid phase  Pseudo-fluid phase  Larger than particle size  Particle size  Smaller than particle size
Particle-resolved DNS

The mesh is reduced to below the size of particle, and the flow field around particle is fully resolved. The fluid-solid interaction force is directly obtained by integrating the viscous stress on the surface of the particles.

DNS can be regarded as the most accurate method, but it’s huge computational cost leads to small-scale simulation domain.
DNS VS Real Constitutive Laws

Real gas-solid flows
A computational grid
$N_p \sim O(10^5)$


Particle-resolved DNS
$N_p \sim O(10^2)$
Strategies for Enabling Large-scale DNS

- **Gas:**
  - Fluid Dynamics
  - Fast algorithm
- **Solid:**
  - Fluid-Solid Coupling
  - High density ratio
  - Particle Motion

**Large-scale Simulation**
- GPU-based parallelization

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Discrete Modeling of Particle-Fluid System

Newton's second law

\[ F = ma \]

Inter-particle collision

Boltzmann equation

\[ \frac{Df}{Dt} = \frac{\partial f(t, x, v)}{\partial t} + v \frac{\partial f(t, x, v)}{\partial x} = \Omega \]

Discrete form

\[ f(x + e_i \Delta t, t + \Delta t) - f(x, t) = \Omega \]

Issac Newton
(1643.1.4-1727.3.31)

Ludwig Edward Boltzmann
(1844.2.20-1906.9.5)
Improved Solution for Gas Flow

Navier-stokes equation

\[ \rho \frac{d\mathbf{u}}{dt} = -\nabla p + \mu \Delta \mathbf{u} + \rho \mathbf{g} \]

Implicit, Serial, Euler

parallelization

Lattice Boltzmann equation

\[ f (x + e_i \Delta t, t + \Delta t) - f (x, t) = \Omega_i \]

Explicit, Parallel, Lagrange
Lattice Boltzmann method

Simple rule: bounce-back boundary condition

Molecular Model

Continuous Model

Boltzmann eq.

Collisionless Boltzmann eq.

Euler eq.  Navier—Stokes eq.

Conservation eq. is not closed

Kn = \frac{\lambda}{L}

Inviscid flow

Free molecular flow
Collision and Streaming Steps

Histogram view of the distribution function, $f$.

D2Q9 model

D3Q19 model

Lattice Unit

Discrete velocities $e_i$

Directional densities $f_i$

Macroscopic velocity $u = \frac{1}{\rho} \sum_i e_i f_i$

Macroscopic density $\rho = \sum_i f_i$
Streaming step \( f_i(x + e_i\delta_i, t + \delta_i) = f_i^*(x, t) \)

(a) From the node to its neighboring nodes

(b) From the neighboring nodes to local node
Collision step

\[ f_i^* (x, t) = f_i (x, t) + \frac{1}{\tau} [f_{i eq} (x, t) - f_i (x, t)] \]
Computation’s Speedup 3000x

Traditional algorithm: 1024 particles, 1024CPU takes one month
New algorithm: 1400 particles, single CPU takes 7 days!
\[ f_i(x + \varepsilon_i \Delta t, t + \Delta t) = f_i(x, t) + \frac{1}{\tau} (1 - \beta(\varepsilon_s, \tau))(f_i^{eq}(\rho, \mathbf{v}) - f_i(x, t)) + \beta(\varepsilon_s, \tau) \Omega_i^s \]

Weighting function

\[ \beta(\varepsilon_s, \tau) = \frac{\varepsilon_s (\tau - 0.5)}{(1 - \varepsilon_s) + (\tau - 0.5)} \]

Additional collision term

\[ \Omega_i^s = f_{-i}(x, t) - f_i(x, t) + f_i^{eq}(\rho, \mathbf{V}_s) - f_{-i}^{eq}(\rho, \mathbf{v}) \]

Solid volume fraction

\[ \varepsilon_s = \frac{V_{solid}}{V_{cell}} \]

Fluid-structure Interactions

Force acting on particle:

\[ F_{f \rightarrow p} = \frac{h^2}{\Delta t} \sum_{j=1}^{n} \left( \beta_j \sum_{i=1}^{8} \Omega_i^s e_i \right) \]

Fluid-induced torque:

\[ T_{f \rightarrow p} = \frac{h^2}{\Delta t} \sum_{j=1}^{n} \left( (\mathbf{x}_j - \mathbf{x}_c) \times \beta_j \sum_{i=1}^{8} \Omega_i^s e_i \right) \]
Enhance Stability of Parallel Algorithm

Traditional link-based LBM method

Our proposed LBM-DEM method

Time step by 100 times

Large-scale GPU Parallel Computing

Mole-8.5 (born on April 24)

(19th, June 2010, Top500)  (9th, Nov 2011, Green500)
Node layout of Mole-8.5
GPU Parallel Implementation

**CPU**

Center Processing Unit

**GPU**

Graphic Processing Unit

Flow Chart of GPU implementation:
- Init
  - Allocate memory on CPU and GPU
  - Read data from CPU and copy to GPU
- Inter-phase coupling
- Solid phase computing
- Lattices computing
- GPU to CPU data copy
- In same node
- Y: Share memory within processors in same node
  - N: MPI with data-transfer for different nodes
- CPU to GPU data copy
- While t <= tmax
  - Y: Continue
  - N: Finalize

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### Performance of GPU vs. CPU

(Single GPU)  

<table>
<thead>
<tr>
<th>Domain size (W×H×L)</th>
<th>Steps per second (Fermi GPU)</th>
<th>Steps per second (Intel E5520)</th>
<th>Speedup</th>
<th>Perf. (MLUPS) (double precision)</th>
</tr>
</thead>
<tbody>
<tr>
<td>32×64×32</td>
<td>1784.1</td>
<td>65.71</td>
<td>27.1</td>
<td>116.8</td>
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<tr>
<td>64×64×64</td>
<td>458.6</td>
<td>16.44</td>
<td>27.9</td>
<td>120.2</td>
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<tr>
<td>64×128×64</td>
<td>237.5</td>
<td>8.167</td>
<td>29.1</td>
<td>124.5</td>
</tr>
<tr>
<td>128×128×128</td>
<td>60.4</td>
<td>2.043</td>
<td>29.6</td>
<td>126.6</td>
</tr>
<tr>
<td>128×256×128</td>
<td>33.3</td>
<td>1.056</td>
<td>31.5</td>
<td>139.8</td>
</tr>
</tbody>
</table>

*MLUPS: mega-lattice-updates-per-second*
### Performance of Large-scale Simulation

<table>
<thead>
<tr>
<th>Case</th>
<th>Lattice</th>
<th>GPU</th>
<th>Steps</th>
<th>Time</th>
<th>Perf. (MLUPS)</th>
<th>Perf./GPU</th>
<th>Gflops</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1024 \times 1152 \times 1024$</td>
<td>$8 \times 8 \times 8$</td>
<td>2000</td>
<td>100.2</td>
<td>24111</td>
<td>47.1</td>
<td>10558</td>
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<tr>
<td>2</td>
<td>$1536 \times 1728 \times 1536$</td>
<td>$12 \times 12 \times 12$</td>
<td>2000</td>
<td>106.2</td>
<td>76741</td>
<td>44.4</td>
<td>33611</td>
</tr>
</tbody>
</table>

The number of float operations per step of case1: **529 Gflop**, case2: **1785.6 Gflop**

D3Q19 TDHS-LBM (Multi GPUs)

Strong scaling for large-scale gas-solid simulations on Mole-8.5
Largest Scale DNS of Gas-solid Suspensions

1M solid particles & 1G fluid lattices @ 576 GPUs

130K solid particles in 3D @ 224 GPUs

3D: 0.384cm x 1.536cm x 0.384cm, 130000 particles (512 X 2560 X 512)

Snapshots for 3D DNS and Drag Distribution

Force Magnitude

0.25
0.5
0.75
1
1.2

$t=2.5 \times 10^6$
$t=3 \times 10^6$
$t=3.5 \times 10^6$
$t=4 \times 10^6$
$t=4.5 \times 10^6$
$t=5 \times 10^6$
Effect of Mesoscale Structure on Drag

\[ F_{g \leftrightarrow s, i} = \beta \cdot (u_g - u_s) \]

\[ \beta \cdot (u_g - u_s) \approx \beta I \cdot (u_g - u_s) = \beta (u_g - u_s) \]


Scale-dependence of Domain Size

Granular Temperature

Fluctuating velocity distribution

<table>
<thead>
<tr>
<th>Sampling box</th>
<th>$\Theta_x$</th>
<th>$\Theta_y$</th>
<th>$\Theta_z$</th>
<th>$\Theta$</th>
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</thead>
<tbody>
<tr>
<td>$4 \times 4 \times 4$</td>
<td>$3.21 \times 10^{-6}$</td>
<td>$2.61 \times 10^{-6}$</td>
<td>$1.68 \times 10^{-6}$</td>
<td>$2.50 \times 10^{-6}$</td>
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<tr>
<td>$8 \times 8 \times 4$</td>
<td>$5.85 \times 10^{-6}$</td>
<td>$4.23 \times 10^{-6}$</td>
<td>$1.74 \times 10^{-6}$</td>
<td>$3.94 \times 10^{-6}$</td>
</tr>
<tr>
<td>$12 \times 12 \times 4$</td>
<td>$8.96 \times 10^{-6}$</td>
<td>$5.98 \times 10^{-6}$</td>
<td>$1.76 \times 10^{-6}$</td>
<td>$5.57 \times 10^{-6}$</td>
</tr>
<tr>
<td>$16 \times 16 \times 4$</td>
<td>$1.25 \times 10^{-5}$</td>
<td>$7.56 \times 10^{-6}$</td>
<td>$1.77 \times 10^{-6}$</td>
<td>$7.28 \times 10^{-6}$</td>
</tr>
</tbody>
</table>
Effect of Mesoscale Structure on Statistical Properties of Particles

Fluctuating velocity of particle $i$ at $j$ direction

$$u'_{i,j} = \begin{cases} u_{i,j} - u_{\text{dilute},j} \\ u_{i,j} - u_{\text{dense},j} \end{cases}$$

Voronoi tessellation

Simplified TFM with EMMS Drag

Prediction of STFM coupled with EMMS drag also agrees with experimental data.

Simplified TFM is 2.14 times faster than full TFM!

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Presented gas-solid statistical analysis of where we have used three strategies for enabling large-scale DNS including:

- A LBM-based DNS algorithm is proposed to simulate gas-solid flow
- LBM-DEM algorithm is feasible to be implemented on GPU
- Large-scale DNS of gas-solid flow has been efficiently run on GPU cluster
- The effects of mesoscale structure on both drag and statistical properties of particles were explored

Further investigations needed in constitutive laws (drag, solid stress, transfer of heat and mass, chemical reactions)
Better ways to link resolved models to coarse-grid simulation
Acknowledgements

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