Simulation of Particulate Solids Processing Using Discrete Element Method

Oleh Baran
Outline

- DEM overview
- DEM capabilities in STAR-CCM+
  - Particle types and injectors
  - Contact physics
  - Coupling to fluid flow
  - Coupling with passive scalar
- Performance and scalability
- Simulation assistant benefits
- Scaled particle approach
- Summary
DEM is applicable to solid flows

- When part or whole solid phase is in dense shear flow regime
- With particles of different shape and size distribution
DEM examples
DEM Governing Equations

⚠️ **Momentum conservation**

\[
m_i \frac{dv_i}{dt} = \sum_j F_{ij} + F_g + F_{\text{fluid}}
\]

- \( m_i \) and \( v_i \) are mass and velocity of particle \( i \), \( F_g = m_i g \) is gravity force, \( F_{ij} \) is contact force between particle \( i \) and element \( j \).
- DEM is a meshless method!
- DEM is computationally intensive method!

⚠️ **Conservation of angular momentum**

\[
\frac{d}{dt} I_i \omega_i = \sum_j T_{ij}
\]

- \( i, I_i \) and \( \omega_i \) are the momentum on inertia and rotational velocity of particle \( i \).
- \( T_{ij} = r_{ij}(F_{ij} + F_r) \) is the torque produced at the point of contact and it is the function of the rolling friction force \( F_r \).
DEM in STAR-CCM+ overview: Contact Forces

❖ Base model is non-linear Herz-Mindlin model
  – Other models available (next slide)

❖ The normal and tangential components, $F_n$ and $F_t$, of contact force depends on overlap, particle properties
  – Young’s modulus
  – Density
  – Size
  – Poisson ratio,
  – and interaction properties, for example friction, rolling friction, restitution, etc
## DEM Capabilities: Contact models

### Basic models

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hertz-Mindlin</td>
<td>Classical nonlinear contact force model for rigid bodies</td>
<td>Friction, restitution (normal and tangential)</td>
</tr>
<tr>
<td>Walton-Brawn</td>
<td>Linear model for deformable particles</td>
<td>Compression and tensile stiffnesses</td>
</tr>
</tbody>
</table>

### Optional models (for adding to basic model)

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rolling Resistance</td>
<td>Force proportional</td>
<td>Set of rolling friction parameters</td>
</tr>
<tr>
<td></td>
<td>Constant Torque</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Displacement Damping</td>
<td></td>
</tr>
<tr>
<td>Linear Cohesion</td>
<td>Constant attractive force matching either JKR force or DMT model for zero overlap</td>
<td>Work of cohesion, model blending factor</td>
</tr>
<tr>
<td>Artificial Viscosity</td>
<td>Additional velocity dependent damping model</td>
<td>Linear and Quadratic coefficients</td>
</tr>
<tr>
<td>Parallel Bonds</td>
<td>For modelling consolidated particles</td>
<td>Max tensile and shear stress, Bond radius</td>
</tr>
<tr>
<td>Conduction Heat transfer</td>
<td>For both particle-particle and particle-geometry contacts</td>
<td>Ranz-Marshall or user set heat transfer</td>
</tr>
</tbody>
</table>
## DEM- Capabilities: Particles

<table>
<thead>
<tr>
<th>Particle Type</th>
<th>Spherical</th>
<th>Composite</th>
<th>Rigid, unbreakable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clumps</td>
<td>Flexible, breakable</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Particle Initialization

<table>
<thead>
<tr>
<th>Volumetric injection</th>
<th>• Random Injector: on region <strong>or Part</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• Lattice injector:</td>
</tr>
<tr>
<td></td>
<td>• Part injector: on volume cells</td>
</tr>
</tbody>
</table>

| Surface injection | Surface or Part Injector: on boundary cells, or on planar grid |

All injectors: - ability to set particle size distributions: constant, normal, log-normal, other - ability to specify flow rate, initial velocities, orientation, etc
### DEM Coupling to Fluid Flow

<table>
<thead>
<tr>
<th>Force Type</th>
<th>Methodology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drag Force</td>
<td>Di Felice</td>
</tr>
<tr>
<td></td>
<td>Schiller-Naumann</td>
</tr>
<tr>
<td></td>
<td>Gidaspow (for 2-way coupling only)</td>
</tr>
<tr>
<td></td>
<td>User defined field function</td>
</tr>
<tr>
<td>Drag Torque</td>
<td>With either Sommerfeld Rotational Drag or user defined rotational drag coefficient</td>
</tr>
<tr>
<td>Lift Force</td>
<td>Shear Lift: Choice of Saffman, Sommerfeld, user-set coefficients</td>
</tr>
<tr>
<td></td>
<td>Spin Lift: Choice of Sommerfeld or user-set coefficients</td>
</tr>
<tr>
<td>Pressure Gradient Force</td>
<td>Buoyancy force</td>
</tr>
<tr>
<td>Two-way coupling</td>
<td>Fluid is affected by particles: Momentum source is applied to continuous phase</td>
</tr>
<tr>
<td>Other interactions</td>
<td>Gravity force, User-Defined Body Force, Particle Radiation, Energy model, Passive Scalar</td>
</tr>
</tbody>
</table>
DEM Passive Scalar

arians in version 8.06
- Arbitrary number of new particle properties
  - Color
    - Tracing subset of particles
    - Analyzing mixing efficiency
  - Particle residence time or displacement
    - ‘dead zone’ or ‘risk zone’ analysis of granular flow
  - Coating amount
    - Residence time in user-defined ‘spray zone’
  - Wetness / dryness of particles
    - Contribution from several processes
  - Amount of chemically active component
- Can interact with Eulerian passive scalar
Passive scalar for binning and mixing

Source term:
${\text{ParcelCentroid}}[0] \times \text{ParticleDensity} \times \text{TimeStep} \times (\text{Time} > 0 ? 0 : 1)$

Source term:
(${\text{ParcelCentroid}}[0] < 0 ? 0 : 1)$
Passive scalar for coating applications

 отметить

 Positive: Improve inter-particle coating uniformity by using optimal spraying equipment settings
  – Solution: using DEM passive scalar capability

 Passive scalar source:
 (ParcelCentroid("Cyl")\[2\] > 0.0 && ParcelCentroid("Cyl")\[2\] < 0.22 && ParcelCentroid("Cyl")\[0\] < 0.05 + 1.12 \times ParcelCentroid("Cyl")\[2\]) ? 0.1 \times ParticleDensity : 0.0
  – Coating thickness is accumulated in ‘spray zone’
  – Single simulation provides solution for two different spray methods
Passive scalar: Lagrangian-Eulerian coupling

 Gors Example of particles in a pile ‘releasing gas’

- Left Inlet air flow 100 m/s, later 10 m/s
- Particles initialized with non-zero ‘Particle Gas’ value of passive scalar $\phi_1$
- Eulerian passive scalar $\phi_2$ has diffusion and convection on, initial value zero in all cells
- Volume weighted interaction model for flow rate between passive Lagrangian and Eulerian scalars:
  
  $J = k(\rho_1 \phi_1 - \rho_2 \phi_2)A_p$ here $k = 0.01$ is user controlled interaction coefficient, $\rho_1$ and $\rho_2$ are densities of Lagrangian and Eulerian phases, $A_p$ is the surface area of the particle
Performance and Scalability

<table>
<thead>
<tr>
<th>DEM timestep</th>
<th>Material density of least dense phase</th>
<th>$\rho$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sim d \sqrt{\frac{\rho}{E}}$</td>
<td>Diameter of smallest sphere</td>
<td>$d$</td>
</tr>
<tr>
<td></td>
<td>Young’s Modulus of hardest particle</td>
<td>$E$</td>
</tr>
<tr>
<td></td>
<td>DEM Solver Timescale</td>
<td></td>
</tr>
<tr>
<td><strong>Number of elements</strong></td>
<td>Total Number of spheres</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Number of CPU</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Number of faces in mesh</td>
<td></td>
</tr>
<tr>
<td><strong>Max Physical time</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**: Typical simulation time of Fluidized bed in version 8.02:**

1 s Physical time for 28 h / 118 CPU for 1.3 millions of particles

d=2 mm, $\rho$=2440 kg/m3, $E$=10 MPa

**: Performance-improving features:**

- Load Balancing
- Per-continuum parallel solver
- Maximum Independent Set Algorithm in injectors
- Skinning
Skinning

 отметить

Contact detection optimized
  – New skin parameter in DEM solver
  – the larger the skin distance, the less often neighbor lists need to be re-built,
    • but more pairs must be checked for possible force interactions inside one neighborhood

![DEM Solver - Properties](image)
Simulation Assistant Benefits

1. Ensure presence of basic set in one click
2. Set Fluid Flow Scenes for DEM coupled to CFD cases
3. Synchronize View Settings for all Scenes

Fluidized Bed Analysis
- Set Fluidized Bed Analysis
- Check for Dangerous Cells
- Remove FB Analysis Functions

Particle Coarse-Graining
- Set Particle Coarse-Graining, if needed
  - Modify Primary Particle Diameter
  - Modify Coarse-Grained Particle Diameter
Can we use ‘larger particles’ to reduce particle count without significant change in accuracy of the model? In particular for fluidized bed application?

Scaled Particle Approach

Suggested correction to Gidaspow drag coefficient

\[ C_d \Rightarrow \left( \frac{d}{d_0} \right)^n C_d \]
Fluidized bed set up


- Size of particles – 0.503 mm
## Model parameters and studied configurations

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Particle size (mm)</th>
<th>Number of Particles</th>
<th>Values of drag scaling exponent n</th>
<th>Time to simulate 1 second</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>No coupling</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>1,271,020</td>
<td>1.576</td>
<td>18 h / 106 CPU</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>374,746</td>
<td>1.858</td>
<td>6.5 h / 46 CPU</td>
</tr>
<tr>
<td>3-9</td>
<td>4</td>
<td>156,506</td>
<td>1.889, 1.935, 1.977, 2.016, 2.052, 2.085, 2.116</td>
<td>5.1 h / 34 CPU</td>
</tr>
<tr>
<td>10-12</td>
<td>5</td>
<td>79,410</td>
<td>1.997, 2.077, 2.299</td>
<td>3.4 h / 10 CPU</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Material</th>
<th>E (MPa)</th>
<th>Poisson</th>
<th>$\rho$ (kg/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particles</td>
<td>polyester</td>
<td>10</td>
<td>0.34</td>
</tr>
<tr>
<td>Geometry</td>
<td>aluminum</td>
<td>68000</td>
<td>0.33</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Contacts</th>
<th>Friction</th>
<th>Restitution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle-Particle</td>
<td>0.8</td>
<td>0.01</td>
</tr>
<tr>
<td>Particle-Geometry</td>
<td>0</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Preparing initial configurations

1. Particles ‘poured down’

2. Bulk oscillation damped

3. User Body force applied to remove particles above 28 cm

Same process for each considered particle size
Pressure drop calculations

- **Two way-coupling activated**
  - All three inlets set to have same inlet velocity
  - Superficial velocity 0.0989 m/s

- **Simulated at least 0.5 s in steady state**

- **Pressure drop recorded**

Same process for all 12 configurations
Pressure Drop (d=4mm)
Pressure drop analysis

Compared to Ergun estimate for \( d_0 = 0.503 \, mm \) particles

Exponents \( > 2.1 \) correspond to fluidized state
Summary of fluidized bed study

Simple power-law correction to drag force was used for scaled particles

Results for pressure drop collapsed on single curve

- Perhaps limited for the particular choice of model parameters
  - Low coefficient of restitution
  - Further investigations are underway
- More accurate scaling can be set from force balance

Scaled particles can provide same pressure drop for less computation time
ありがとう