Granular Dynamics in Chrono

Jonathan A. Fleischmann, Ph.D.
Assistant Professor of Mechanical Engineering, Marquette University
Formerly Assistant Scientist, Simulation-Based Engineering Laboratory (SBEL), University of Wisconsin-Madison
Chrono::Granular

Description

• Predefined and user-definable specimen geometries (box and cylinder)
  • STANDARD_TRIAXIAL and SMALL_TRIAXIAL
  • STANDARD_BOX and SMALL_BOX
  • STANDARD_JENIKE, HARTL_OOI, OSULLIVAN, etc.

• Predefined and user-definable granular material fabric:
  • MONO_SPHERES_5mm, MONO_SPHERES_6mm, etc.
  • TRI_SPHERES_4mm_5mm_6mm
  • OTTAWA_SAND (spheres with log-normal particle size distribution)
  • MONTEREY_SAND (spheres, cylinders, and boxes with log-normal particle size distribution)

• Predefined and user-definable particle materials:
  • GLASS, STEEL, QUARTZ, etc.

• Separate specimen generation from tests (so multiple tests can be performed on the same granular material specimen)

• Analyze discrete stress/strain based on inter-particle forces/displacements

• Easily Expandable!
**Chrono::Granular**

Shear Test Validation

- HARTL_OOI specimen geometry with MONO_SPHERES_6mm fabric and GLASS particle material, compared with physical experiments of Härtl and Ooi, *Granular Matter*, 2008:

<table>
<thead>
<tr>
<th>Uniform Glass Beads (Randomly Packed)</th>
<th>Physical Experiment</th>
<th>Chrono Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of spheres</td>
<td>~ 5,000</td>
<td>5,000</td>
</tr>
<tr>
<td>Sphere diameter (m)</td>
<td>0.006</td>
<td>0.006</td>
</tr>
<tr>
<td>Sphere density (kg/m³)</td>
<td>2,550</td>
<td>2,550</td>
</tr>
<tr>
<td>Shear displacement speed (m/s)</td>
<td>~ 0.00002</td>
<td>0.001</td>
</tr>
<tr>
<td>Coulomb friction coefficient for Glass-on-Glass</td>
<td>0.18</td>
<td>0.18</td>
</tr>
<tr>
<td>Coulomb friction coefficient for Glass-on-Boundary</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>Young’s Modulus for Glass (Pa)</td>
<td>$4\times10^{10}$</td>
<td>$4\times10^{7}$</td>
</tr>
<tr>
<td>Poisson’s Ratio for Glass</td>
<td>0.22</td>
<td>0.22</td>
</tr>
<tr>
<td>Void ratio (loose)</td>
<td>~ 0.7</td>
<td>0.7 – 0.6</td>
</tr>
</tbody>
</table>
• HARTL_OOI specimen geometry with MONO_SPHERES_6mm fabric and GLASS particle material, compared with physical experiments of Härtl and Ooi, *Granular Matter*, 2008:

Shear Test Validation
**Chrono::Granular**

**Triaxial Test Validation**

- OSULLIVAN specimen geometry with MONO_SPHERES_5mm fabric and STEEL particle material, compared with physical experiments of Cui, O’Sullivan, and O’Neill, *Géotechnique*, 2007:

<table>
<thead>
<tr>
<th>Uniform Steel Spheres (Randomly Packed)</th>
<th>Physical Experiment</th>
<th>Chrono Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of spheres</td>
<td>~ 15,000</td>
<td>~ 15,000</td>
</tr>
<tr>
<td>Sphere diameter (m)</td>
<td>0.005</td>
<td>0.005</td>
</tr>
<tr>
<td>Sphere density (kg/m$^3$)</td>
<td>7,800</td>
<td>7,800</td>
</tr>
<tr>
<td>Axial strain rate (% /s)</td>
<td>~ 0.008</td>
<td>1</td>
</tr>
<tr>
<td>Coulomb friction coefficient for Steel-on-Steel</td>
<td>0.096</td>
<td>0.096</td>
</tr>
<tr>
<td>Coulomb friction coefficient for Steel-on-Boundary</td>
<td>0.228</td>
<td>0.228</td>
</tr>
<tr>
<td>Young’s Modulus for Steel (Pa)</td>
<td>2($10^{11}$)</td>
<td>2($10^8$)</td>
</tr>
<tr>
<td>Poisson’s Ratio for Steel</td>
<td>0.28</td>
<td>0.28</td>
</tr>
<tr>
<td>Void ratio (loose)</td>
<td>~ 0.6</td>
<td>~ 0.6</td>
</tr>
</tbody>
</table>
Chrono::Granular Triaxial Test Validation

- OSULLIVAN specimen geometry with MONO_SPHERES_5mm fabric and STEEL particle material, compared with physical experiments of Cui, O’Sullivan, and O’Neill, Géotechnique, 2007:
Chrono::Granular

- Once generated, the same specimen (geometry and granular material) can be subjected to a variety of test scenarios:

**Versatility**
Chrono::Granular

Model Accuracy

• The geometry of the Jenike direct shear test (with cylindrical specimen shape), can be accurately modeled:

![Graph showing shear stress/normal stress vs shear displacement (m)]
Macro-scale (continuum) stress/strain distributions in bulk granular materials can be computed from micro-scale (discrete) inter-particle forces and displacements:

\[
\sigma_{ij} = \frac{1}{V_\sigma} \sum_c f^c_i l^c_j \quad [\text{e.g., Nemat-Nasser, } \textit{Plasticity}, \text{ 2004}]
\]

\[
\varepsilon_{ij} = \frac{1}{V_\varepsilon} \sum_e u^e_i d^e_j \quad [\text{Bagi, } \textit{Mechanics of Materials}, \text{ 1996}]
\]

\[
\varepsilon_{ij} \approx \sum_c u^c_i l^c_k \Lambda^{-1}_{jk} \quad \text{where} \quad \Lambda_{jk} = \sum_c l^c_j l^c_k \quad \text{is the fabric tensor}
\]
Chrono::Granular

- Macro-scale (continuum) stress/strain distributions in bulk granular materials can be computed from micro-scale (discrete) inter-particle forces and displacements:

\[ I_1 = \text{tr}(\sigma_{ij}) \]

\[ I_3 = \text{det}(\sigma_{ij}) \]
Macro-scale (continuum-based) yield surfaces for bulk granular materials can be generated from a series of templated cubical (true) triaxial tests, for validation or micro-scale parameter selection, and/or for coupling with FEM material models:

\[ \Delta U_f = \frac{1}{2} \sum_c |F_f^c| |v_t^c| \Delta t \]

Yield energy per particle:

\[ U_f = \sum_{sliding} \Delta U_f \]
Macro-scale (continuum-based) yield surfaces for bulk granular materials can be generated from a series of templated cubical (true) triaxial tests, for validation or micro-scale parameter selection, and/or for coupling with FEM material models:

\[ \mu = 0.5 \]

\[ \phi = 33^\circ \]

\[ (\mu_{macro} = \tan \phi \approx 0.65) \]

\( \pi \)-plane

\( \sigma_i \) positive in compression
Contact Models

\[ F_n = f(r_{\text{eff}}, \delta_n)(k_n \delta_n n - \gamma_n m_{\text{eff}} v_n) \]

**Coulomb friction:** If \( k_t |\delta_t| > \mu |F_n| \) then \( \delta_t \leftarrow \delta_t \frac{\mu |F_n|}{k_t |\delta_t|} \)

DEMT-Penalty

\[ F_t = f(r_{\text{eff}}, \delta_n)(-k_t \delta_t - \gamma_t m_{\text{eff}} v_t) \]

Tangential displacement history vector \( \delta_t \) must be stored and projected onto contact plane at each time step.
Contact Models

DEM-Penalty

Hertz/Deresiewicz contact model
(other models available)

\[ r_c = \left( \frac{3(1 - \nu^2)}{4E} F_n r_{\text{eff}} \right)^{1/3} \]

\[ k_n = \frac{2Gr_c}{1 - \nu} \]

\[ k_t = \frac{4Gr_c}{2 - \nu} \]

\[ \left( \frac{k_t}{k_n} = \frac{2(1 - \nu)}{2 - \nu} \right) \]

Conditional stability criterion: \( \Delta t < 0.2 \sqrt{\frac{m_{\text{min}}}{k_{\text{max}}}} \)
Contact Models

**DEM-Complementarity**

- **Generalized Positions**
- **Velocity Transformation Matrix**
- **Generalized Velocities**
- **Reaction Force**
- **Frictional Contact Force**

**Kinematic Differential Equations**

\[ \dot{q} = T(q)v \]

**Force Balance Equations**

\[ M(q)\ddot{v} = f(t, q, v) - g^T_q(q, t)\lambda + \sum_{i=1}^{N_c}(\dot{\gamma}^i_u D^i_u + \dot{\gamma}^i_u D^i_u + \dot{\gamma}^i_w D^i_w) \]

**Holonomic Kinematic Constraints**

\[ g(q, t) = 0 \]

**Contact Complementarity Conditions**

\[ 0 \leq \Phi^i(q, t) \perp \dot{\gamma}^i_n \geq 0 \quad i = 1, 2, \ldots, N_c \]

\[ (\dot{\gamma}^i_u, \dot{\gamma}^i_w) = \operatorname{arg\ min}_{\dot{\gamma}^i_u \geq \sqrt{(\overline{\gamma}^i_u)^2 + (\overline{\gamma}^i_w)^2}} \left( \gamma^i_u v^T D^i_u + \gamma^i_w v^T D^i_w \right) \]

**Coulomb Friction Model**

Friction Components, for Contact “i”

Friction Dissipation Energy

Total Number of Contacts

Gap Function, for Contact “i”
Contact Models

DEM-Complementarity

1. Kinematic Differential Equations
   \[ \mathbf{q}^{(t+1)} = \mathbf{q}^{(t)} + h \mathbf{T}(\mathbf{q}^{(t)}) \mathbf{v}^{(t+1)} \]
2. Force Balance Equations
   \[ \mathbf{M}(\mathbf{v}^{(t+1)} - \mathbf{v}^{(t)}) = h \mathbf{f}(\mathbf{q}^{(t)}, \mathbf{q}^{(l)}, \mathbf{v}^{(l)}) - \mathbf{g}_a(\mathbf{q}^{(l)}, t)\lambda + \sum_{i=1}^{N_c} (\gamma_u^i \mathbf{D}_n + \gamma_u^i \mathbf{D}_u + \gamma_w^i \mathbf{D}_w) \]
3. Holonomic Kinematic Constraints
   \[ \frac{1}{h} g(\mathbf{q}^{(l)}, t) + \mathbf{g}(\mathbf{v}^{(l+1)}) + \mathbf{g}_i = 0 \]
4. Contact Complementarity Conditions
   \[ 0 \leq \frac{1}{h} \Phi_i(\mathbf{q}^{(l)}, t) + \mathbf{D}_n^T \mathbf{v}^{(l+1)} \perp \gamma_i^\pm \geq 0 \]
5. Coulomb Friction Model
   \[ (\gamma_u^i, \gamma_w^i) = \arg \min_{\mu} \frac{\mu' \gamma_u^i \mathbf{v}^T \mathbf{D}_u + \gamma_w^i \mathbf{v}^T \mathbf{D}_w}{\mu' \gamma_u^i + \gamma_w^i} \] for \( i = 1, 2, \ldots, N_c \), total number of contacts.
Contact Models

• Mass flow rate experiment
  • 500 µm spheres
  • Total mass of granular material: 6.38 g
  • Width of opening: 9.398 mm
  • Opening speed: 1 mm/s
  • Maximum opening gap: 2 mm

DEM-C vs. DEM-P

![Graph showing comparison between Experiment and Simulation (DEM-C) and Simulation (DEM-P)]
Contact Models

- **DEM-P**
  - Step-size: $10^{-5}$ s
  - Cost per step: 0.054 s
    - Collision detection: 0.026 s
    - Update: 0.010 s
    - Solver: 0.016 s
  - Average number contacts: 118,400

- **DEM-C**
  - Step-size: $10^{-4}$ s
  - Cost per step: 0.423 s
    - Collision detection: 0.054 s
    - Update: 0.010 s
    - Solver: 0.359 s
  - Average number contacts: 140,000

**Mass flow rate experiment**

- 39,000 particles
- $r = 0.25 \cdot 10^{-3}$ m
- $\mu = 0.3$
- 2 mm gap size
- 40 threads

Contact Models vs. DEM-P

- **DEM-C**
  - Step-size: $10^{-4}$ s
  - Cost per step: 0.423 s
    - Collision detection: 0.054 s
    - Update: 0.010 s
    - Solver: 0.359 s
  - Average number contacts: 140,000

- **DEM-P**
  - Step-size: $10^{-5}$ s
  - Cost per step: 0.054 s
    - Collision detection: 0.026 s
    - Update: 0.010 s
    - Solver: 0.016 s
  - Average number contacts: 118,400
Contact Models

- Direct shear test
  - 1,000 uniform glass spheres (randomly packed)
  - Particle diameter: $D = 6 \text{ mm}$
  - Shear Speed: 1 mm/s
  - Inter-Particle Coulomb Friction Coefficient (Glass-on-Glass): $\mu = 0.18$
  - Void Ratio (loose): $e = 0.7$
## Contact Models

### DEM-P
- **Direct shear test**
- 1,000 particles
- $r = 3 \text{ mm}$
- $\mu = 0.18$
- 1 mm/s shear speed
- 10 threads

#### DEM-C
- **Step-size:** $10^{-3}$ s
- **Cost per step:** 0.1615 s
  - Collision detection: 0.0036 s
  - Update: 0.0007 s
  - Solver: 0.1571 s
- **Average number contacts:** 4800

#### DEM-P
- **Step-size:** $10^{-5}$ s
- **Cost per step:** 0.0025 s
  - Collision detection: 0.0008 s
  - Update: 0.0007 s
  - Solver: 0.001 s
- **Average number contacts:** 4200