A STUDY ON THE DYNAMICS OF GRANULAR MATERIAL
WITH A COMPARISON OF DVI AND DEM APPROACHES

Master’s Thesis Defense
Martin Tupy
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Simulation-Based Engineering Lab
Department of Mechanical Engineering
University of Wisconsin-Madison
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Overview

- Motivation
- Discrete Element Method (DEM)
  - Formulation
  - Implementation and time comparison
- Differential Variational Inequality Approach (DVI)
  - Formulation
- Comparison between DVI and DEM
  - Sphere packing in a cylindrical container
  - Granular flow down an incline
  - Settling of spheres in a box
- Validation of DVI against Experimental Data
- Conclusion and Future Work
Motivation

- Industries:
  - Mining
  - Food & Pharmaceutics
  - Film & Game
  - etc.

- Problem examples:
  - Collapsing Silos
  - Mars Rover
  - etc.
Motivation

The Relevant Problem ⇒

Two Common Solutions ⇒

Solution Draws on ⇒

~ Large Scale Multibody Dynamics ~
Handling of the Frictional Contact Problem

Penalty Based Approach (DEM)

Differential Variational Inequality (DVI) Based Approach

Collision Detection.

Cone Complementarity Optimization Solution
Discrete Element Method

Loop
$t_{\text{start}}$ to $t_{\text{end}}$

Particle Initialization → Collision Detection → Contact Force Calculation → Newton’s 2nd Law → Velocity and Position Analysis → Output Data

Next time step
DEM

- **Spatial Subdivision**
- **2 particles**: $r_i, r_j$

$$r_{ij} = r_i - r_j$$

- If $r_{ij} \leq d$
  $$\delta_{ij} = d - r_{ij}$$
  $$n_{ij} = \frac{r_{ij}}{r_{ij}}$$

- Otherwise no collision
DEM

- Contact force components
  - normal
  - tangential

- Four different categories:
  - Continuous potential models
  - Linear viscoelastic models
  - Non-linear viscoelastic models
  - Hysteretic models
DEM

\[ v_{ij} = v_i - v_j \]
\[ v_{tij} = v_{ij} - v_{nij} - \frac{1}{2} (\omega_i - \omega_j) \times r_{ij} \]
\[ v_{nij} = (v_{ij} \cdot n_{ij}) n_{ij} \]
\[ u_{tij} = \int_{(coll)} v_{tij}(\tau) d\tau \]

- Normal Force \( F_{n_{ij}} \) computed as:
  \[ F_{n_{ij}} = f \left( \frac{\delta_{ij}}{d} \right) (k_n \delta_{ij} n_{ij} - \gamma_n m_{eff} v_{n_{ij}}) \]

- Tangential Force \( F_{t_{ij}} \) computed as:
  \[ F_{t_{ij}} = f \left( \frac{\delta_{ij}}{d} \right) (-k_t u_{t_{ij}} - \gamma_t m_{eff} v_{t_{ij}}) \]

\( k_n, k_t \) — spring stiffness
\( \gamma_n, \gamma_t \) — damping coefficient
DEM

- Coulomb-criterion

\[ |F_t| \leq |\mu F_n| \]

- decompose tangential force [1]:

\[ F_t = F_s + F_g \]

- each term needs to satisfy the criterion:

\[
F_s = -\min \gamma_t m_{eff} \left| v_{tij} \right|, \mu \left| F_{nij} \right| \frac{v_{tij}}{u_{tij}}
\]

\[
F_g = -\min k_t \left| u_{tij} \right|, \mu \left| F_{nij} \right| \frac{v_{tij}}{u_{tij}}
\]

DEM

- Force on one particle is the sum of its contact forces and gravity:
  \[ \mathbf{F}_{i\text{tot}} = m_i \mathbf{g} + \sum_j \mathbf{F}_{n ij} + \mathbf{F}_{t ij} \]

- Moment due to tangential force:
  \[ \mathbf{M}_{i\text{tot}} = -\frac{1}{2} \sum_j \mathbf{r}_{ij} \times \mathbf{F}_{t ij} \]

- Calculation of translational and rotational accelerations:
  \[ \mathbf{F}_{i\text{tot}} = m_i \mathbf{a}_i \rightarrow \mathbf{a}_i = \frac{\mathbf{F}_{i\text{tot}}}{m_i} \]
  \[ \mathbf{M}_{i\text{tot}} = I \alpha_i \rightarrow \alpha_i = \frac{\mathbf{M}_{i\text{tot}}}{I} \]
DEM

- Use explicit numerical integration methods like Explicit Euler or Velocity Verlet Integration

- Velocity Verlet Integration:

\[ \mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t + \frac{1}{2} \mathbf{a}_i(t)\Delta t^2 \]

\[ \mathbf{v}_i(t + \Delta t / 2) = \mathbf{v}_i(t) + \frac{1}{2} \mathbf{a}_i(t)\Delta t \]

\[ \mathbf{v}_i(t + \Delta t) = \mathbf{v}_i(t + \Delta t / 2) + \frac{1}{2} \mathbf{a}_i(t + \Delta t)\Delta t \]

- Same for angular velocity respectively
DEM – Implementation Hierarchies

MATLAB
- Brute-force collision detection
- Serial Implementation

C++/CPU
- Bullet Physics collision detection (spatial subdivision)
- Serial Implementation

C++/GPU
- GPU collision detection (spatial subdivision)
- Parallel Implementation
DEM – Time Comparison

- Scenario used:
  - Cube of spheres
  - 500 μm diameter
  - Simulation time 0.5 sec
  - Step size 5*10^-5 seconds
DEM – Time Comparison

- 1 million spheres
- 0.5 sec long simulation
- ~12,000 sec computational time
- GPU
DEM – Time Comparison

- 3.375 million spheres
- 0.5 sec long simulation
- ~ 42,000 sec computational time
- GPU
GPU Computing

- Computational Model: SIMD (Single Instruction Multiple Data)
- Tesla C1060 simultaneously manages up to 30,720 threads on 240 scalar processors
- Ideal match for simulating granular dynamics

<table>
<thead>
<tr>
<th></th>
<th>Tesla C1060</th>
<th>Intel I7 975 Extreme</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cores</td>
<td>240</td>
<td>4</td>
</tr>
<tr>
<td>Memory</td>
<td>4 GB</td>
<td>32 KB L1 cache/core</td>
</tr>
<tr>
<td></td>
<td></td>
<td>256 KB L2 cache/core</td>
</tr>
<tr>
<td></td>
<td></td>
<td>8 MB L3 for all cores</td>
</tr>
<tr>
<td>Clock</td>
<td>1.33 GHz</td>
<td>3.20 GHz</td>
</tr>
<tr>
<td>Bandwidth</td>
<td>102 GB/s</td>
<td>32.0 GB/s</td>
</tr>
<tr>
<td>FLOPS</td>
<td>933 x 10⁹ (SP)</td>
<td>70 x 10⁹ (DP)</td>
</tr>
</tbody>
</table>
Differential Variational Inequality Approach

Equation of Motion:

\[ \dot{q} = T(q)v \]
\[ M(q)\dot{v} = f(t, q, v) - g_q^T(q, t)\lambda + \sum_{i=1}^{N_c} (\gamma_n^i D_n^T D_n^T + \gamma_u^i D_u^T D_u^T + \gamma_w^i D_w^T D_w^T) \]

- Generalized Positions
- Generalized Mass Matrix
- Kinematic Differential Equations
- Force Balance Equations
- Holonomic Kinematic Constraints
- Contact Complementarity Conditions
- Coulomb Friction Model
- Velocity Transformation Matrix
- Generalized Velocities
- Frictional Contact Force
- Reaction Force
- Applied Force
- Contact Impulse, for Contact “i”
- Total Number of Contacts
- Friction Impulse Components, for Contact “i”

\[ g(q, t) = 0 \]
\[ 0 \leq \Phi^i(q, t) \perp \gamma_n^i \geq 0 \]

\[ (\gamma_u^i, \gamma_w^i) = \arg\min_{\gamma_n^i \geq 0} \left( \gamma_n^i \sqrt{v^T D_n^T D_n^T v + v^T D_u^T D_u^T v + v^T D_w^T D_w^T v} \right) \]


Simulation-Based Engineering Laboratory
http://sbel.wisc.edu
Comparison between DVI and DEM

- **spherical packing in a cylindrical container**
  - comparison of packing fraction
  - force comparison

- **granular flow down an incline**
  - comparison of packing fraction
  - comparison of velocity profiles

- **settling of spheres in a box**
  - time comparison
Scenario 1: Sphere packing in a cylindrical container

- **Model:**
  - Spherical granular material: 1mm diameter
  - Cylinder: 20mm diameter
  - Number of particles: 1210 up to 6050 particles

- **Initialization:**

  ![Top view](top view)
  ![Lateral view](lateral view)
Scenario 1: Sphere packing in a cylindrical container

Packing Fraction Comparison

$$\phi_f = \frac{V_s}{V_c}$$

<table>
<thead>
<tr>
<th>Number of spheres</th>
<th>$\phi_f$ - DEM approach</th>
<th>$\phi_f$ - DVI approach</th>
<th>% - Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1210</td>
<td>0.4924</td>
<td>0.4850</td>
<td>1.50</td>
</tr>
<tr>
<td>2420</td>
<td>0.5544</td>
<td>0.5455</td>
<td>1.60</td>
</tr>
<tr>
<td>3630</td>
<td>0.5746</td>
<td>0.5645</td>
<td>1.75</td>
</tr>
<tr>
<td>4840</td>
<td>0.5872</td>
<td>0.5799</td>
<td>1.24</td>
</tr>
<tr>
<td>6050</td>
<td>0.5937</td>
<td>0.5904</td>
<td>0.55</td>
</tr>
</tbody>
</table>

Comparison of Packing Fraction
Scenario 1: Sphere packing in a cylindrical container

Force Comparison

<table>
<thead>
<tr>
<th>Number of spheres</th>
<th>Weight [mN]</th>
<th>Force – DVI [mN]</th>
<th>% - Error</th>
<th>Force – DEM [mN]</th>
<th>%-Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1210</td>
<td>12.430</td>
<td>12.431</td>
<td>+0.008</td>
<td>12.430</td>
<td>0</td>
</tr>
<tr>
<td>2420</td>
<td>24.861</td>
<td>24.863</td>
<td>+0.008</td>
<td>24.863</td>
<td>+0.008</td>
</tr>
<tr>
<td>3630</td>
<td>37.291</td>
<td>37.298</td>
<td>+0.019</td>
<td>37.290</td>
<td>-0.003</td>
</tr>
<tr>
<td>4840</td>
<td>49.721</td>
<td>49.715</td>
<td>-0.012</td>
<td>49.716</td>
<td>-0.010</td>
</tr>
<tr>
<td>6050</td>
<td>62.152</td>
<td>62.165</td>
<td>+0.021</td>
<td>62.152</td>
<td>0</td>
</tr>
</tbody>
</table>
Comparison between DVI and DEM

- **spherical packing in a cylindrical container**
  - comparison of packing fraction
  - force comparison

- **granular flow down an incline**
  - comparison of packing fraction
  - comparison of velocity profiles

- **settling of spheres in a box**
  - time comparison
Scenario 2: Granular flow down an incline

- Spherical granular material: 1mm diameter
- Tilt angle $\alpha$: 10°-30°
- Periodic boundary
Scenario 2: Granular flow down an incline

Packing Fraction

DEM - different Tilt Angles

DVI - different Tilt Angles

Tilt Angle $\alpha = 10^\circ$

Tilt Angle $\alpha = 20^\circ$

Tilt Angle $\alpha = 25^\circ$

Tilt Angle $\alpha = 30^\circ$
Scenario 2: Granular flow down an incline

Velocity Profile Comparison

DEM approach \( t = 0.4 \text{ sec} \) DVI approach
Comparison between DVI and DEM

- spherical packing in a cylindrical container
  - comparison of packing fraction
  - force comparison

- granular flow down an incline
  - comparison of packing fraction
  - comparison of velocity profiles

- settling of spheres in a box
  - time comparison
Scenario 3: Settling of Spheres in a box

- DEM step size highly sensitive to parameter values used in contact formulation
- Higher contact stiffness implies to smaller step size as a result of higher natural frequencies
- Simulation length: 0.5 seconds
DVI: Experimental Validation

<table>
<thead>
<tr>
<th>GRANULAR FLOW THROUGH DIFFERENT CHANNEL SIZES</th>
<th>GRANULAR FLOW WITH DIFFERENT WEIGHT LOADING</th>
</tr>
</thead>
<tbody>
<tr>
<td>• receptacle: trough shape</td>
<td>• receptacle: rectangular shape</td>
</tr>
<tr>
<td>• 39000 glass spheres</td>
<td>• 39000 glass spheres</td>
</tr>
<tr>
<td>• 0.5 mm diameter</td>
<td>• 0.5mm diameter</td>
</tr>
<tr>
<td>• gap sizes 1.5-3.0mm</td>
<td>• one steel sphere</td>
</tr>
<tr>
<td></td>
<td>• 6.35mm diameter</td>
</tr>
<tr>
<td></td>
<td>• gap size 3mm</td>
</tr>
</tbody>
</table>
DVI: Experimental Validation (Experiment 1)

- Experimental Setup
  - Newport LTA-HL Precision Linear Actuator
  - Newport UMR8.25 Linear Translational Stage
  - Cooper LFS 242 Tension/Compression Cell
DVI: Experimental Validation (Experiment 1)

- **Simulation Model:**
  - built in Chrono::Engine
  - 39,000 spheres
  - diameter 500µm
  - 45° slope angle

- **Selection of friction coefficient**
  - Multiple simulations with different friction coefficient values
  - Fitting of second order polynomials through data points
  - Chosen friction coefficient of 0.15

---

Finding $\mu$

- $\mu = 0.05$
- $\mu = 0.2$
- $\mu = 0.3$
- $\mu = 0.4$

- experiment
DVI: Experimental Validation (Experiment 1)

- **Simulation Model:**
  - built in Chrono::Engine
  - 39,000 spheres
  - diameter 500µm
  - 45° slope angle
DVI: Experimental Validation (Experiment 1)

Results

![Graph showing force vs. time for different gap sizes and friction coefficients.](image-url)
DVI: Experimental Validation (Experiment 1)

Results

![Graph showing force vs time for different trials with gap size 2.5mm. The graph includes lines for trials 1 to 8 and a dashed line for mu=0.15.](http://sbel.wisc.edu)
DVI: Experimental Validation (Experiment 1)

Results

![Graph showing force over time with legend indicating different runs and one marked with a mu value of 0.15.](image)
DVI: Experimental Validation
(Experiment 1)

Results

![Graph showing force in N against time in s with gap size 1.5mm. The graph includes multiple lines representing different data sets, with one line marked as 
\( \mu = 0.15 \).]
DVI: Experimental Validation (Experiment 1)

Results

Uncertainty by Student’s T distribution with 95% confidence

<table>
<thead>
<tr>
<th>Gap Size [mm]</th>
<th>Experimental [N/s]</th>
<th>Simulation [N/s]</th>
<th>% Error</th>
<th>Upper Bound [N/s]</th>
<th>Lower Bound [N/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>1.41E-02</td>
<td>1.40E-02</td>
<td>0.66</td>
<td>1.43E-02</td>
<td>1.38E-02</td>
</tr>
<tr>
<td>2</td>
<td>2.59E-02</td>
<td>2.62E-02</td>
<td>1.03</td>
<td>2.73E-02</td>
<td>2.45E-02</td>
</tr>
<tr>
<td>2.5</td>
<td>4.00E-02</td>
<td>4.05E-02</td>
<td>1.48</td>
<td>4.43E-02</td>
<td>3.56E-02</td>
</tr>
<tr>
<td>3</td>
<td>4.44E-02</td>
<td>4.48E-02</td>
<td>0.75</td>
<td>5.02E-02</td>
<td>3.87E-02</td>
</tr>
</tbody>
</table>

Simulation results match experimental data within 1.5 % error
DVI: Experimental Validation
(Experiment 1)

Repose Angle Validation
Granular material poured on a flat surface forms a pile
Angle formed is called angle of repose
  - Depends on shape, cohesion and friction
Angle of repose is approximately equal to friction angle

\[ \varphi = 19.5^\circ \]

\[ \mu_{\text{static}} = \tan(\varphi) \]

\[ \varphi = 19.5^\circ \]

\[ \mu = 0.35 \]
DVI: Experimental Validation (Experiment 2)

- Experimental Setup
  - Same as for previous one

- Simulation Model
  - built in Chrono::Engine
  - 39000 spheres
    - diameter 500µm
  - Additional load (sphere)
    - diameter 6.35mm
DVI: Experimental Validation (Experiment 2)

Results

Uncertainty: Student’s T distribution with 95% confidence
DVI: Experimental Validation (Experiment 2)

Results

Uncertainty: Student’s T distribution with 95% confidence

![Graph of Square Flow Mid Position 3mm Gap](image)
Results

Uncertainty: Student’s T distribution with 95% confidence
DVI: Experimental Validation (Experiment 2)

Results
Granular flow without additional loading

Gapsize 1.5mm

Gapsize 2.0mm
DVI: Experimental Validation (Summary)

● 1\textsuperscript{st} experiment
  ● Successful selection of friction coefficient \( \mu \) to be 0.15
  ● Simulation flow rates are within 1.5\% error

● 2\textsuperscript{nd} experiment
  ● Simulation results did not align with and without extra weight
  ● Discrepancy between experiment and simulation is in the neighborhood of 20\%

● Major difference:
  ● 1\textsuperscript{st} experiment – all particles are in motion
  ● 2\textsuperscript{nd} experiment – parts of the particle are in motion while others remain static
Conclusion

- Design and Implementation of DEM in MATLAB, C++/CPU, C++/GPU
- Development of two experiments
- First attempt at time-comparison between DVI and DEM in terms of accuracy and efficiency
- Development of an experimental setup for investigations of granular flow
- First micro-scale validation of DVI against experimental data
Reference

Future Work

- Further experiments for investigating the impact of different force parameters (DEM)

- Comprehensive calibration and validation of numerical simulations (DVI) using experimental data

- DEM and DVI on multiple GPUs to increase size of problems investigated
  - Leverage lab GPU-Cluster capable of 21 Teraflops in SP
Thank you.