Dynamic Simulation of Particle-Filled Hollow Spheres

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Motivation

Mathematical Modelling
  Molecular Dynamics
  Time Integration
  Potentials

Numerical Results

Current Cooperation: Fraunhofer Institute for Manufacturing Technology and Advanced Materials, Dresden (Ulrike Jehring)
vibration can cause many problems, e.g., noise and wear

development of light-weight material at Fraunhofer Institute for Manufacturing Technology and Advanced Materials (Ulrike Jehring)

research on hollow sphere structures
Motivation
Advantages of hollow sphere structures

- easily adaptable to different shapes
- solvent resistance, thermal resistance, noise reduction
Advantages of hollow sphere structures

- easily adaptable to different shapes
- solvent resistance, thermal resistance, noise reduction

Additionally
- hollow spheres with particles
Advantages of hollow sphere structures
Simulation of a sphere

Two basic possibilities

Collision Detection

- computation of the next collision following paths of particles
- 2D: diploma thesis (Denise Holfeld)
- high complexity
Simulation of a sphere

Two basic possibilities

<table>
<thead>
<tr>
<th>Collision Detection</th>
<th>Time Integration</th>
</tr>
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<tbody>
<tr>
<td>computation of the next collision</td>
<td>well established methods available for 3D case</td>
</tr>
<tr>
<td>following paths of particles</td>
<td></td>
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Molecular Dynamics

- discrete element method
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- discrete element method
- millions of molecules
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- millions of molecules
- equally distributed particles
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- periodic boundaries
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- potential-based
Molecular Dynamics

- discrete element method
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- cuboid simulation region
- potential-based
- basic program available Thermodynamics and Energy Technology (Jadran Vrabec)
Adaptations for filled spheres

- sphere with reflective boundary conditions
Adaptations for filled spheres

- sphere with reflective boundary conditions
- gravity
Adaptations for filled spheres

- sphere with reflective boundary conditions
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- friction
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- deformation and movement of the boundary
Adaptations for filled spheres

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- deformation and movement of the boundary
- different particle shapes
Adaptations for filled spheres

- sphere with reflective boundary conditions
- gravity
- friction
- deformation and movement of the boundary
- different particle shapes
- particles as aggregation of spheres
Translation

- problem is derived from the equation of motion
  \[ \ddot{x} = \dot{v} = \frac{F}{m} \]

- formulation as system of first order ODEs
  \[ \dot{v} = \frac{F}{m} \]
  \[ \dot{x} = v \]
The Leapfrog-Algorithm

- positions and velocities are calculated alternately

\[ v_{i}^{n+\frac{1}{2}} = v_{i}^{n-\frac{1}{2}} + \frac{dt}{m_{i}} F_{i}^{n} \]

\[ x_{i}^{n+1} = x_{i}^{n} + dtv_{i}^{n+\frac{1}{2}} \]

- \( F \) is based on a potential

\[ F_{ij} = \frac{\partial V_{ij}}{\partial r_{ij}} \]
Lennard-Jones Potential

- pairwise-potential
- potential has two parts, one attracting and one rejecting

\[ V(r) = -4\epsilon \left( \left( \frac{r}{\sigma} \right)^{12} - \left( \frac{r}{\sigma} \right)^6 \right) \]

- usually cut off at a distance \( r_c \)
- for reflections: hull potential
Lennard-Jones potential

\[ V(r) = 4 \varepsilon \left( \left( \frac{r_m}{r} \right)^{12} - \left( \frac{r_m}{r} \right)^6 \right) \]

\[ r_m = \sigma \left( \frac{2^{1/6}}{\sigma} \right) \]

standard

new
Reflections at the boundary
Reflections at the boundary

With the current implementation, there are two possibilities

<table>
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Reflections at the boundary

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<td>Elastic or inelastic collisions</td>
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<tr>
<td>Potential forces</td>
<td>(Coeff. of restitution from experiments)</td>
</tr>
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Initialization

- sphere shaped
- include experimental data
- pseudo friction on contact
Movement of the simulation volume

- pulsing surface
- hopping
- deformation
Examples
Conclusions and Outlook

- MD can be used for fast particle calculations
- adapted MD towards our application
Conclusions and Outlook

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- adapted MD towards our application
- fitting with experiments (falling sphere)
- adaptive linked cell algorithm
- coupling of spheres
- modeling of friction
Conclusions and Outlook

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Thank you for your attention!
Rotation

- rotation is derived from the equation of rigid body rotational motion, e.g. angular momentum
  \[
  j_i^{n+\frac{1}{2}} = j_i^{n-\frac{1}{2}} + t_i^n
  \]

- angular velocity is related to the angular momentum by the inertia tensor
  \[
  \omega = I^{-1}j
  \]

- quaternions useful for the orientation
  \[
  q_i^{n+1} = q_i^n + \frac{dt}{2} Q(q_i^{n+\frac{1}{2}}) \hat{\omega}_i^{n+\frac{1}{2}} \text{ where } \hat{\omega} = (0, \omega)^T
  \]

- Fincham’s rotational quaternion algorithm
Complexity

current status: up to 20000 particles
quadratic complexity

goal: 200000 particles
Linked Cell algorithm

- LCA linear in particle number
- LCA divides simulation volume into cells
- reduction in the number of possible contact particles