Ultrasound Simulations of Non-smooth Granular Dynamics

Ulrich Rüde (LSS Erlangen, ulrich.ruede@fau.de)
joint work with T. Preclik and D. Bartuschat
Lehrstuhl für Simulation
Erlangen-Nürnberg

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fully resolved geometry - hard particles - ultra-parallel

864 000 sharp-edged particles with a diameter between 0.25 mm and 2 mm.
Outline

- Motivation
- Supercomputers
- Towards the **direct simulation** of Particulate Flows
  1. Solid phase - **rigid body dynamics** (multi-body simulation)
  2. Fluid phase - lattice Boltzmann method (meso-sopic model)
  3. Electrostatics - finite volume multigrid (macro-sopic model)

Multi-physics applications
  - Coupling the models
  - Examples

Perspectives
Building Block I:

Current and Future High Performance Supercomputers
BIG Iron

JUQUEEN
- Blue Gene/Q architecture
- 458,752 PowerPC A2 cores
- 16 cores (1.6 GHz) per node
- 16 GiB RAM per node
- 5D torus interconnect
- 5.8 PFlops Peak
- TOP 500: #9

SuperMUC
- Intel Xeon architecture
- 147,456 cores
- 16 cores (2.7 GHz) per node
- 32 GiB RAM per node
- Pruned tree interconnect
- 3.2 PFlops Peak
- TOP 500: #20
Building block II:

Granular Media Simulations

with the physics engine


Particle Model

Single particle described by
  - **state variables**
    position $x$, orientation $\varphi$,
    translational and angular velocity $v$ and $\omega$
  - **parameterization of its shape** $S$
    e.g. geometric primitive, composite object, or mesh
  - **inertia properties**: mass $m$,
    principle moments of inertia $I_{xx}$, $I_{yy}$, and $I_{zz}$

The Newton-Euler equations for rigid objects

$$
\begin{align*}
\begin{pmatrix}
\dot{x}(t) \\
\dot{\varphi}(t)
\end{pmatrix}
&=egin{pmatrix}
v(t) \\
Q(\varphi(t))\omega(t)
\end{pmatrix} \\
M(\varphi(t))
\begin{pmatrix}
\dot{v}(t) \\
\dot{\omega}(t)
\end{pmatrix}
&=egin{pmatrix}
f(s(t),t) \\
\tau(s(t),t) - \omega(t) \times I(\varphi(t))\omega(t)
\end{pmatrix}
\end{align*}
$$
Contact Representation

A contact is described by
- the contact location \( \hat{x} \),
- the contact normal \( n \),
- and the signed contact distance \( \xi \).

For a pair of particles \((1, 2)\) with convex shapes \( S_1, S_2 \) and associated signed distance functions \( f_1, f_2 \) these can be defined to be

\[
\hat{x} = \arg \min_{f_2(y) \leq 0} f_1(y), \quad n = \nabla f_2(\hat{x}), \quad \xi = f_1(\hat{x}).
\]
Contact Models (2)

Hard contacts

- require impulses,
- exhibit non-differentiable but continuous trajectories,
- contact reactions are defined implicitly in general,
- have non-unique solutions,
- and can be solved numerically by methods from two classes.

⇒ measure differential inclusions

Time Stepping

• Discretization of the Newton-Euler differential equations:

\[
\begin{pmatrix}
    x'(\lambda) \\
    \varphi'(\lambda) \\
    v'(\lambda) \\
    \omega'(\lambda)
\end{pmatrix} = \begin{pmatrix}
    x \\
    \varphi \\
    v \\
    \omega
\end{pmatrix} + \delta t \begin{pmatrix}
    v'(\lambda) \\
    Q(\varphi)\omega'(\lambda)
\end{pmatrix},
\]

\[
\begin{pmatrix}
    v'(\lambda) \\
    \omega'(\lambda)
\end{pmatrix} = \begin{pmatrix}
    v \\
    \omega
\end{pmatrix} + \delta t M(\varphi)^{-1} \begin{pmatrix}
    f(\lambda) \\
    \tau(\lambda) - \omega \times I(\varphi)\omega
\end{pmatrix}.
\]

• Expression for the relative contact velocity:

\[
\delta v'(\lambda) = v'_1(\lambda) + \omega'_1(\lambda) \times (\hat{x} - x_1) - v'_2(\lambda) - \omega'_2(\lambda) \times (\hat{x} - x_2)
= A^T A \lambda - A^T b.
\]
Frictional contact models for rigid objects

<table>
<thead>
<tr>
<th>Non-penetration conditions</th>
<th>Coulomb friction conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \xi \geq 0 \perp \lambda_n \geq 0 )</td>
<td>( | \lambda_{to} |_2 \leq \mu \lambda_n )</td>
</tr>
<tr>
<td>( \dot{\xi} = 0 )</td>
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Signorini condition
impact law
friction cone condition
frictional reaction opposes slip

Coulomb solutions are not unique: new maximum dissipation friction model
Parallel Computation

Key features of the parallelization:

- domain partitioning
- distribution of data
- synchronization protocol
- subdomain NBGS
- accumulators and corrections
- aggressive message aggregation
- nearest-neighbor communication
Parallel solution

- Subdomain Non-linear Block Gauss-Seidel (NBGS).
- Subsystem solver
  - relaxes single contacts $F_j^{-1}$
- Data dependencies to other processes updated asynchronously (Jacobi)
- Parallel: two message exchanges per iteration
  - Send velocity corrections from shadow copies to owner.
  - Send velocity corrections to shadow copies

Matrix-free implementation avoids the explicit setup of $F$

Communication of velocity corrections instead of contact reactions avoids exchange of contact data
Dense granular channel flow with crystallization
Scaling and Efficiency Results

- Solver algorithmically not optimal for dense systems, hence cannot scale unconditionally, but highly efficient in many cases of practical importance
- Strong and weak scaling results for a constant number of iterations performed on SuperMUC and Juqueen
- Largest ensembles computed
  - $2.8 \times 10^{10}$ non-spherical particles
  - $1.1 \times 10^{10}$ contacts
- granular gas: scaling results

Breakup up of compute times on Erlangen RRZE Cluster Emmy

- "Scalability" alone would not mean that the method is fast!

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Granular Dynamics - Ulrich Rüde
Multi-Physics Simulations for Particulate Flows

Parallel Coupling with waLBerla and PE

sedimenting elongated particles with D. Bartuschat and K. Gustavsson (Stockholm)
Fluid-Structure Interaction
direct simulation of Particle Laden Flows (4-way coupling)


Heterogenous CPU-GPU Simulation

Fluidized Beds:

Direct numerical simulation
fully resolved particles

Fluid-structure-interaction

4-way-coupling

Particles: 31250, Domain: 400x400x200, Timesteps: 400 000
Devices: 2 x M2070 + 1 Intel „Westmere“, Runtime: 17.5 h


Conclusions and Perspectives

- Supercomputer power
- Versatile and efficient parallel tools
  - Lattice Boltzmann (for flow)
  - **Multibody Dynamics** (NCP based, for particles)
  - Multigrid (for electrostatics)
- Gain insight
  - Multi-Scale
  - Multi-Physics
- Challenges
  - validation
  - software
  - sustainability
Thank you for your attention!

Videos, preprints, slides at
https://www10.informatik.uni-erlangen.de