Towards Direct Numerical Simulation of a Billion Fully Resolved Rigid Bodies Immersed in a Fluid

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Overview:

Contents

- Motivation
- waLBerla: A Software Framework for CFD
- pe: A Rigid Body Simulation Framework
- Coupling CFD and Rigid Bodies
- Results
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Motivation: Large-Scale Particulate Flow Simulations
Motivation: Fluidization Experiment
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- Transport of granular particles is crucial for
  - Understanding of physical phenomena
  - Industrial processes
- Current paradigm in the simulation of particulate flows: Simulation of the immersed particles as point masses
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- Current paradigm in the simulation of particulate flows:
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- Need for a paradigm change in order to make decisive progress in the modeling and simulation of particulate flows

  Simulation of particles as fully resolved entities
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  - Understanding of physical phenomena
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- Current paradigm in the simulation of particulate flows:
  Simulation of the immersed particles as point masses

- Need for a paradigm change in order to make decisive progress in the modeling and simulation of particulate flows
  Simulation of particles as fully resolved entities

- Demand on increased efforts to tackle the growing complexities (physics and software design)

- Requirement to develop software and tools for the next generation of supercomputers ($>10^6$ execution units)
Motivation: Large-Scale Particulate Flow Simulations
Motivation

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walBerla: A Software Framework for CFD

WALBErla

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**waLBerla: A Software Framework for CFD**

**Widely Applicable Lattice Boltzmann from Erlangen**

- Massively parallel CFD software framework based on Lattice Boltzmann Method
- Modular software concept
  - Supports various applications
    - Blood flow in aneurysms
    - Moving particles and agglomerates
    - Free surfaces to simulate foams, fuel cells, and m.m.
    - Charged colloids
    - Arbitrary combinations of above
- Integration of highly efficient and specialized kernels
waLBerla: A Software Framework for CFD

Best paper award ParCFD 2009: S. Donath, "A Parallel Free Surface Lattice Boltzmann Method for Large-Scale Applications"

Accepted for publication at SC’10: J. Götz, K. Iglberger, “Direct Numerical Simulation of Particulate Flows on 294912 Processor Cores”

Montag, 28. Juni 2010
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Montag, 28. Juni 2010
A Rigid Body Simulation Framework

- Software infrastructure for rigid body simulation algorithms (DEM, RBD, ...)
- Focus on massively parallel rigid body simulations
Example 1: The Silo Scenario

27270 randomly generated, non-spherical particles, 256 CPUs, 379300 time steps, runtime: 16.4h (including data output), 0.154s per time step

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27270 randomly generated, non-spherical particles, 256 CPUs, 379,300 time steps, runtime: 16.4h (including data output), 0.154s per time step.
Example 1: The Silo Scenario

Domain partitioning for 64 processes used in the silo scenario
Distributed Rigid Body Simulations

- No point masses, but volumetric and geometrically defined objects
- Objects may (geometrically) span several processes
- Objects overlapping processes boundaries must be synchronized
- Objects are assigned logically with exactly one process
The Parallel FFD Algorithm: Algorithm Formulation

1. Force synchronization
2. for each body \( B \) do
   3. first position half step
   4. first velocity half step
   5. end
3. Update of remote and notification of new rigid bodies
4. for each body \( B \) do
   5. find all contacts \( C(B) \)
   6. for each violated contact \( k \) in \( C(B) \) do
      7. add collision and friction constraints to \( B \)
   8. end
   9. end
10. Exchanging constraints on the rigid bodies
11. for each body \( B \) do
12.   if \( B \) has constraints then
13.     find post-collision velocity
14.     select friction response
15.   end
16.   else
17.     second velocity half-step
18.   end
19.   second position half-step
20. end
21. Update of remote and notification of new rigid bodies

## The Parallel FFD Algorithm: Scaling Results

<table>
<thead>
<tr>
<th># Cores</th>
<th># Particles</th>
<th>Partitioning</th>
<th>Runtime [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>128</td>
<td>20000000</td>
<td>8 x 4 x 4</td>
<td>727.096</td>
</tr>
<tr>
<td>256</td>
<td>40000000</td>
<td>8 x 8 x 4</td>
<td>726.991</td>
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<td>1024</td>
<td>160000000</td>
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<td>320000000</td>
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<td>2560000000</td>
<td>32 x 32 x 16</td>
<td>728.921</td>
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<td>5120000000</td>
<td>32 x 32 x 32</td>
<td>729.094</td>
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<td>10240000000</td>
<td>64 x 32 x 32</td>
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<tr>
<td>131072</td>
<td>20480000000</td>
<td>64 x 64 x 32</td>
<td>728.32</td>
</tr>
</tbody>
</table>

*Jugene simulation results of 1000 time steps of a dense granular gas contained in an evacuated box without external forces.*
Example 2: The Hourglass Scenario

1,250,000 spherical particles, 256 CPUs, 300,300 time steps, runtime: 48h (including data output)
Example 2: The Hourglass Scenario

1250 000 spherical particles, 256 CPUs, 300 300 time steps, runtime: 48h (including data output)
Example 2: The Hourglass Scenario

1,250,000 spherical particles, 256 CPUs, 300,300 time steps, runtime: 48h (including data output)
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Example 3: Fluidization of Spherical Particles

23,985 spherical particles, $7.68 \cdot 10^6$ Cells (400x400x480), 512 CPUs, 252,000 time steps, runtime: 30 h, 0.43 s per time step
Example 3: Fluidization of Spherical Particles

- 23985 spherical particles, \(7.68 \times 10^6\) Cells (400x400x480), 512 CPUs, 252,000 time steps,
  
  runtime: 30h, 0.43s per time step
Example 4: Fluidization of Non-spherical Particles

1008 spheres and 900 capsules, $12.8 \cdot 10^6$ Cells (180x198x360), 512 CPUs, 210,000 time steps, runtime: 7.5 h, 0.128 s per time step
Example 4: **Fluidization of Non-spherical Particles**

1008 spheres and 900 capsules, \(12.8 \cdot 10^6\) Cells (180x198x360), 512 CPUs, 210,000 time steps, runtime: 7.5 h, 0.128 s per time step
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Segregation simulation of $242 \, 200$ spherical particles on $32 \, 768$ cores.
Largest simulation within the weak scaling experiment: $150 \cdot 10^9$ fluid cells and $264 \cdot 10^6$ spherical particles on $294 \, 912$ cores.

Two test scenarios:
- Test case A: 6.3% fraction of particle volume
- Test case B: 19.8% fraction of particle volume
Results: Weak Scaling Results on Jugene

Weak Scaling Testcase A

Efficiency

Number of Cores

40x40x40 lattice cells per core
80x80x80 lattice cells per core

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Results: Weak Scaling Results on Jugene

Weak Scaling Testcase B

Efficiency vs Number of Cores

- 40x40x40 lattice cells per core
- 80x80x80 lattice cells per core

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Results: Weak Scaling Results on Jugene

Weak Scaling Testcase B

Fraction of compute time

LBM Communication
Stream Collide
Object Mapping
Force Evaluation
Physics Engine

Number of cores
## Strong Scaling Results on Jugene

<table>
<thead>
<tr>
<th># Cores</th>
<th>Simulation time test case A</th>
<th>Simulation time test case B</th>
<th>Domain size per core</th>
</tr>
</thead>
<tbody>
<tr>
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<td>669.8</td>
<td>80 x 80 x 80</td>
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<tr>
<td>128</td>
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<td>40 x 80 x 80</td>
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<td>20 x 40 x 40</td>
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<tr>
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</tr>
<tr>
<td>4096</td>
<td>12.1</td>
<td>20.0</td>
<td>20 x 20 x 20</td>
</tr>
<tr>
<td>8192</td>
<td>7.6</td>
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<td>10 x 20 x 20</td>
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<td>16384</td>
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</tr>
<tr>
<td>32768</td>
<td>4.7</td>
<td>6.9</td>
<td>10 x 10 x 10</td>
</tr>
</tbody>
</table>

Simulation time and domain sizes for 500 time steps of strong scaling of coupled fluid-structure interaction simulations from 64 to 32768 compute cores with scenarios A and B.
Results: Strong Scaling Results on Jugene

Strong Scaling Testcase A

- LBM Communication
- Stream Collide
- Object Mapping
- Force Evaluation
- Physics Engine

Fraction of compute time vs Number of cores
Strong Scaling Results on Jugene

Strong Scaling Testcase B

Fraction of compute time

Number of cores

- LBM Communication
- Stream Collide
- Object Mapping
- Force Evaluation
- Physics Engine
Thank you very much for your attention!