Direct Numerical Simulation of Particulate Flows on 294.912 Compute Cores

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Cracking Hard Nuts - Simulating Complex Flows Beyond Hundred Thousand Cores
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CSE2011
Reno
Overview

- Motivation
  - Why another CFD Package?
  - Why Simulate Fluid-Structure Interaction?

- The Target System

- The Software
  - waLBerla: A Software Framework for CFD

- Fluid-Structure Interaction with Moving Rigid Objects
  - Rigid Body Dynamics
  - Fluid Flow Simulations with Lattice Boltzmann Methods
  - Coupling Rigid Body Dynamics and Fluid Flow Simulations

- Conclusions and Future Work
Motivation
Why we need another CFD program?

- In the last years many PhD students at our chair wrote nice programs for different CFD applications, but:
  - Programming and testing basic functionality takes a lot of time
  - Parallelizing takes even more time
  - When the PhD student leaves the chair, the program most times was not used any more, since nobody knows how to use it
Why Simulate Fluid-Structure Interaction?

- Transport of solid particles is crucial for:
  - Understanding of physical phenomena
  - Industrial processes

- But:
  - Fully resolved simulation of the obstacles is computational expensive
  - Up to now only moderate number of obstacles can be simulated

Montag, 11. April 2011
Target System: 
Jugene @ Jülich

- PetaFlops = $10^{15}$ operations/second
- IBM Blue Gene
- Theoretical peak capability 1.0027 Petaflop/s
- 294 912 cores
- #9 on TOP 500 List in November 2010

> 1 000 000 cores expected 2011

Extreme Scaling Workshop 2010 at Jülich Supercomputing Center
What's the Problem?
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Would you want to propel a Super Jumbo .....
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Would you want to propel a Super Jumbo ..... 

with four large turbines
What's the Problem?

Would you want to propel a Super Jumbo ..... with four large turbines or with 300,000 blow dryer fans?
What's the Problem?

Would you want to propel a Super Jumbo ..... with four large turbines (not from Rolls-Royce) or with 300,000 blow dryer fans?
The Software
waLBerla

- Created for desktop PCs and supercomputers
- Supporting multi-core PCs and GPUs
- Modular software concept
  - Supports various applications:
    - Blood flow in aneurysms
    - Moving particles and agglomerates
    - Free surfaces to simulate foams, fuel cells, a.m.m.
    - Charged colloids
waLBerla

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waLBerla

- Include restart mechanisms for field data, structures and unstructured data
- Input file is distributed in the parallel environment
- Global data is kept at a minimum
- Uses parallel visualization files for Paraview
- Include parallel algorithms to analyze simulation data
Fluid-Structure Interaction with Moving Rigid Objects
Fluid-Structure Interaction
Rigid Body Dynamics (without fluid)
Newton's laws of motion
- including rotations
- Contact detection
  - in each time step

Collisions modelled by
- coefficient of restitution: forces in normal direction
- friction laws: forces in tangential direction
Newton's laws of motion
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Collisions & Contacts between Rigid Objects
Collisions & Contacts between Rigid Objects
Parallel Rigid Body Dynamics

- No point masses, but volumetric, geometrically defined objects
- Objects may (geometrically) extend across several processors
- Objects overlapping with process boundaries must be synchronized
- Objects are assigned logically to exactly one process
- Unique identifier from rank of the process and local counter
1250000 spherical particles, 256 CPUs, 300300 time steps, runtime: 48h (including data output)
1,250,000 spherical particles, 256 CPUs, 300,300 time steps, runtime: 48h (including data output)
Fluid Flow Simulations with Lattice Boltzmann Methods
The Lattice Boltzmann Method

- Alternative to classical Navier-Stokes
- Discretization in cubes (cells)
- 9 (or 19) numbers per cell
- Repeat (many times)
  - stream
  - collide
The Stream Step

Move particle (numbers) into neighboring cells
The Collide Step

Compute new particle numbers according to the collisions

- distribution functions after streaming
- local equilibrium distribution functions
- distribution functions after collision

velocity

τ = 1.5
Coupling of Rigid Body Dynamics and Fluid Flow Solver
Mapping Moving Obstacles into the LBM Fluid Grid

An Example
Mapping Moving Obstacles into the LBM Fluid Grid

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An Example (2)

Cells with state change from Particle to Fluid

Cell change from particle to fluid
Mapping Moving Obstacles into the LBM Fluid Grid

An Example (2)

Cell change from fluid to particle
Mapping Moving Obstacles into the LBM Fluid Grid

An Example (2)

PDF acting as Force

Momentum calculation

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Algorithm 1 Coupled LBM-PE solver

1: for each body $B$ do
2: Map $B$ to lattice grid and reconstruct missing PDFs in case of cell changes
3: end for
4: for each lattice cell do
5: Apply boundary conditions and stream and collide PDFs
6: end for
7: for each surface cell do
8: Add forces from fluid to rigid objects
9: end for
10: Time step in the rigid body simulation
Virtual Fluidized Bed

512 processors

Simulation Domain
Size: 180x198x360
cells of LBM

900 capsules and
1008 spheres
= 1908 objects

Number of time steps:
252,000

Run Time:
07h 12 min
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512 processors

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Simulation of a Segregation Process

Segregation simulation of 242200 objects. Density values of 0.8 kg/dm$^3$ and 1.2 kg/dm$^3$ are used for the objects in water.
Weak Scaling

- **Jugene**
- **Blue Gene/P**
- **Jülich Supercomputer Center**

Graph showing efficiency vs. number of cores.

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

Jugene
Blue Gene/P

0.5
0.6
0.7
0.8
0.9
1

Efficiency

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

28

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Weak Scaling

Jugene
Blue Gene/P
Jülich Supercomputer Center

Efficiency

Number of Cores

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

![Graph showing weak scaling of Jugene Blue Gene/P supercomputer.](image)

- **Efficiency**
- **Number of Cores**
- **Jugene Blue Gene/P, Jülich Supercomputer Center**

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

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Weak Scaling

![Graph showing weak scaling results for Jugene Blue Gene/P Jülich Supercomputer Center. The graph compares efficiency for 40x40x40 and 80x80x80 lattice cells per core across different numbers of cores.]

- **Jugene** Blue Gene/P
- Jülich Supercomputer Center

- Red dots represent 40x40x40 lattice cells per core.
- Green squares represent 80x80x80 lattice cells per core.

**Legend:**
- Red dots: 40x40x40 lattice cells per core.
- Green squares: 80x80x80 lattice cells per core.
Weak Scaling

Scaling 64 to 294 912 cores
Densely packed particles

150 994 944 000 lattice cells
264 331 905 rigid spherical objects

Jugene
Blue Gene/P
Jülich Supercomputer Center

40x40x40 lattice cells per core
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Weak Scaling

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Largest simulation to date:
8 Trillion (10^{12}) variables per time step (LBM alone)
50 TByte

Jugene
Blue Gene/P
Jülich Supercomputer Center

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Simulations of particulate flows are of high interest in industrial applications and can help to understand physical phenomena in more detail.
Conclusions

- Simulations of particulate flows are of high interest in industrial applications and can help to understand physical phenomena in more detail.

- A coupled algorithm of Lattice Boltzmann and a rigid body dynamics solver can simulate fully resolved particulate flows.
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A coupled algorithm of Lattice Boltzmann and a rigid body dynamics solver can simulate fully resolved particulate flows.

`waLBerla` supports particulate flows on supercomputers.
Conclusions

- Simulations of particulate flows are of high interest in industrial applications and can help to understand physical phenomena in more detail.

- A coupled algorithm of Lattice Boltzmann and a rigid body dynamics solver can simulate fully resolved particulate flows.

- *waLBerla* supports particulate flows on supercomputers.

- Debugging a highly parallel implementation can be tedious.
Future Work

OK, the framework is working fine for many applications
Future Work

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Future Work

OK, the framework is working fine for many applications, but:

- How about test cases for validation of particulate flows and free surfaces
  - Suggestions for simulations including many particles are welcome ;-) 
- How about grid refinement + load balancing
- How to deal with massive parallelization:
  - Node crashes
  - Postprocessing
  - Restart mechanisms
Acknowledgements

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Thank you for your attention!
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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