Direct Numerical Simulation of Particulate Flows on 300,000 Compute Cores

K. Iglberger, S. Donath, C. Feichtinger, U. Rüde,

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Lehrstuhl für Informatik 10 (Systemsimulation)

www10.informatik.uni-erlangen.de

International Workshop on Multiscale Modelling, Simulation and Optimization
10-13 October, 2010

Excellence Cluster Engineering of Advanced Materials
Universität Erlangen-Nürnberg
Erlangen
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Overview

- Motivation
  - Why Simulate Particulate Flows?
  - Why Parallel Programming?

- The Software
  - waLBerla: A Software Framework for CFD
    - Fluid-Structure Interaction

- Rigid Body Dynamics for Granular Media

- Flow Simulation with Lattice Boltzmann Methods

- Fluid-Structure Interaction with Moving Rigid Objects
  - Particulate Flows

- Conclusions
Motivation
Why Simulate Particulate Flows?

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
Why Parallel Programming?
Why Parallel Programming?
Why Parallel Programming? (2)

- Latest standard processors are multicore processors
  - “The free lunch is over”
  - To exploit multicore performance, parallel algorithms are essential
  - CPUs will have 2, 4, 8, 16, …, 128, …, ??? cores

- Want to simulate problems which are not possible on „standard“ computers
Example Peta-Scale System: Jugene @ Jülich

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

For comparison: Current fast desktop PC is $\sim 20,000$ times slower

$> 1,000,000$ cores expected 2011
Think BIG!
What's the Problem?
What’s the Problem?

Would you want to propel a Super Jumbo .....
What's the Problem?

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 with 300,000 blow dryer fans?
The Software
waLBerla

- Created for Desktop PCs and Supercomputers
- Supporting Multi-Core PCs
- 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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Fluid-Structure Interaction
Rigid Multibody Dynamics
(for simulating granular systems)
Rigid Body Dynamics

- 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
Rigid Body Dynamics

- **Newton’s Laws of Motion**
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Collisions & Contacts between Rigid Objects
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27,270 randomly generated, non-spherical particles, 256 CPUs, 379,300 time steps, runtime: 16.4h (including data output), 0.154s per time step
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Flow Simulation with Lattice Boltzmann Methods
Computational Fluid Dynamics with the Lattice Boltzmann Method
Computational Fluid Dynamics with the Lattice Boltzmann Method

Falling Drop with Turbulence Model (slow motion)
The Lattice Boltzmann Method

- Discretization in cubes (cells)
- 9 (or 19) numbers per cell
  - = number of particles traveling towards neighboring cells
- Repeat (many times)
  - stream
  - collide
Stream/Collide:

\[ F_i(x + c_i \Delta t, t + \Delta t) - F_i(x, t) = -\frac{1}{\tau} \left( F_i(x, t) - F_i^{(0)}(x, t) \right) \]

Equilibrium DF:

For \( i = C \),

\[ F_i^{(0)}(x, t) = \frac{1}{3} \rho(x, t) \left( 1 - \frac{3}{2} \frac{\langle u(x, t), u(x, t) \rangle}{c^2} \right) \]

For \( i \in \{ N, E, S, W, T, B \} \),

\[ F_i^{(0)}(x, t) = \frac{1}{18} \rho(x, t) \left( 1 + 3 \frac{\langle c_i, u(x, t) \rangle}{c^2} + \frac{9}{2} \frac{\langle c_i, u(x, t) \rangle^2}{c^4} - \frac{3}{2} \frac{\langle u(x, t), u(x, t) \rangle}{c^2} \right) \]

For \( i \in \{ TN, TS, BN, BS, TE, TW, BE, BW, NE, NW, SE, SW \} \),

\[ F_i^{(0)}(x, t) = \frac{1}{36} \rho(x, t) \left( 1 + 3 \frac{\langle c_i, u(x, t) \rangle}{c^2} + \frac{9}{2} \frac{\langle c_i, u(x, t) \rangle^2}{c^4} - \frac{3}{2} \frac{\langle u(x, t), u(x, t) \rangle}{c^2} \right) \]
The Stream Step

Move particle (numbers) into neighboring cells
The Collide Step

Compute new particle numbers according to the collisions
Fluid-Structure Interaction with Moving Rigid Bodies
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
Mapping Moving Obstacles into the LBM Fluid Grid

An Example
Mapping Moving Obstacles into the LBM Fluid Grid

An Example

![Diagram of LBM fluid grid with moving obstacles](image-url)
Mapping Moving Obstacles into the LBM Fluid Grid

An Example
Mapping Moving Obstacles into the LBM Fluid Grid

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

Cells with state change from Fluid to Particle
Mapping Moving Obstacles into the LBM Fluid Grid

An Example (2)

Momentum calculation

PDF acting as Force
Simulation of a Segregation Process

Segregation simulation of 12,013 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

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

Number of Cores

Efficiency
Weak Scaling

Jugene
Blue Gene/P

Efficiency

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

![Graph showing weak scaling results for different number of cores and lattice cells per core](image)

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

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

Jugene
Blue Gene/P
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Supercomputer Center

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

![Diagram showing weak scaling for Blue Gene/P at Jugene, Jülich Supercomputer Center. The graph plots efficiency against the number of cores, with two lines representing different lattice cell counts per core: 40x40x40 and 80x80x80.](image-url)
Weak Scaling

Scaling 64 to 294,912 cores
Densely packed particles

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

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

Scaling 64 to 294,912 cores
Densely packed particles

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

Jugene Blue Gene/P
Jülich Supercomputer Center

150,994,944,000 lattice cells
264,331,905 rigid spherical objects
Conclusions
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- Parallel programming is necessary for multicore usage
- Lattice Boltzmann can handle complex fluid-structure simulations efficiently
- Supercomputers can be used
  - to do simulations in less time
  - to do larger simulations
  - for real world applications
  - to spend a lot of time, searching for programming mistakes
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- C. Feichtinger (LBM, waLBerla)


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