Peta-Scale Computing for the Direct Numerical Simulation of Particle Laden Flows


U. Rüde (LSS Erlangen, ruede@cs.fau.de)

Lehrstuhl für Informatik 10 (Systemsimulation)
Excellence Cluster Engineering of Advanced Materials
Universität Erlangen-Nürnberg

www10.informatik.uni-erlangen.de

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Overview

- Motivation: How fast are computers today (and next decade)
- Rigid Body Dynamics for Granular Media
- Flow Simulation with Lattice Boltzmann Methods
  - free surfaces
  - bubbly flows
- Fluid-Structure Interaction with Moving Rigid Objects
  - particle ladden flows
- preliminary GPU performance comparison
- Conclusions
Motivation
Example Peta-Scale System: Jugene @ Jülich

- PetaFlops = $10^{15}$ operations/second
- IBM Blue Gene
- 0.825 petaflop/s performance speed running the Linpack benchmark.
- theoretical peak capability 1.0027 Petaflop/s
- 294 912 cores
- #5 on TOP 500 List in June 2010

Exa-Scale: $10^{18}$ operations/second - expected around 2020
What can we do with Exa-Scale Computers?

- Even if we want
  - to simulate a billion objects (particles): we can do a billion operations for each of them in each second
  - a trillion finite elements (finite volumes) to resolve a PDE, we can do a million operations for each of them in each second
- Most existing software dramatically underperforms on contemporary HPC architectures
- This will get more dramatic on future exa-scale systems

Fluidized Bed
(movie: thanks to K.E. Wirth)
What's the problem?

replacing 4 strong jet engines

Would you want to propel a Super Jumbo with 300,000 blow dryer fans?
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
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
Granular Media Simulations
27270 randomly generated, non-spherical particles, 256 CPUs, 379300 time steps, runtime: 16.4 h (including data output), 0.154 s per time step
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Hourglass Simulation (1)

1250000 spherical particles, 256 CPUs, 300300 time steps, runtime: 48h (including data output)
### Scaling Results!

<table>
<thead>
<tr>
<th># Cores</th>
<th># Particles</th>
<th>Partitioning</th>
<th>Runtime [s]</th>
</tr>
</thead>
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<tr>
<td>128</td>
<td>2 000 000</td>
<td>8 x 4 x 4</td>
<td>727.096</td>
</tr>
<tr>
<td>256</td>
<td>4 000 000</td>
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<td>131072</td>
<td>2 048 000 000</td>
<td>64 x 64 x 32</td>
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</tr>
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</table>

*Jugene simulation results of 1000 time steps of a dense granular gas contained in an evacuated box without external forces.*
Flow Simulation with Lattice Boltzmann Methods
Computational Fluid Dynamics with the Lattice Boltzmann Method

Falling Drop with Turbulence Model (slow motion)
Simulation of Metal Foams

- Example application:
  - Engineering: metal foam simulations

- Based on LBM:
  - Free surfaces
  - Surface tension
  - Disjoining pressure to stabilize thin liquid films
  - Parallelization with MPI and load Balancing

- Collaboration with C. Körner (Dept. of Material Sciences, Erlangen)

- Other applications:
  - Food processing
  - Fuel cells
Larger-Scale Computation: 1000 Bubbles

Simulation
1000 Bubbles
510x510x530 = 1.4 \cdot 10^8 \text{ lattice cells}
70,000 \text{ time steps}
77 \text{ GB}
64 \text{ processes}
72 \text{ hours}
4,608 \text{ core hours}

Visualization
770 images
Approx. 12,000 \text{ core hours for rendering}

Best Paper Award for Stefan Donath (LSS Erlangen) at ParCFD, May 2009 (Moffett Field, USA)
Massively Parallel Particulate Flows
Mapping Moving Obstacles into the LBM Fluid Grid

(a) Initial setup: The velocities $u$ of the object cells $x_b$ are set to the velocity $u_w(x_b)$ of the object. In this example the object only has a translational velocity component. Fluid cells are marked with $x_f$.

(b) Updated setup: Two fluid cells have to be transformed to object cells and for two object cells the pdfs have to be reconstructed.

Figure 1: 2D mapping example.
Fluid-Structure Interaction

- collision detection
- (frictional) collision response
- time integration

rigid bodies act as obstacles

fluid results in external forces

update of fluid nodes: stream/collide
- calculation of hydrodynamic forces
  (momentum exchange)
Virtual Fluidized Bed

512 Processors
HLRB-II

Simulation Domain Size: 180x198x360 cells of LBM

900 capsules and 1008 spheres = 1908 objects

Number time steps: 252,000

Run Time: 07h 12 min
Segregation simulation of 12,013 objects with two different shapes in different time steps simulated on 2,048 cores in a box. Density values of 0.8 kg/dm³ and 1.2 kg/dm³ are used for the objects in water with density 1 kg/dm³ and a gravitation field. Lighter particles are rising to the top of the box, while heavier particle sink to the bottom.
Weak Scaling

Jugene
Blue Gene/P
Jülich Supercomputer Center

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

Scaling 64 to 294,912 cores
sparsely packed particles

150,994,944,000 lattice cells
83,804,982 rigid spherical objects
LBM on Clusters with GPUs
waLBerla Software Architecture for GPU Usage

- **CPU**
  - CPU Buffers
  - Apply BC
  - Local Boundary Condition
  - PCI Express Transfer

- **GPU**
  - GPU Buffers
  - Local Communication
  - Swap
  - GPU - GPU Copy Operations

- **CPU**
  - MPI Buffers
  - MPI_Isend
  - MPI_Irecv
  - InfiniBand Transfer
  - MPI Communication

**Patch Architecture**
- Only LBM on GPU
  - no free surfaces
  - no FSI

**NEC Nehalem**
- Xeon E5560
- 2.8 GHz
- 12 GB per Node
- 2 GPUs per Node

**nVIDIA TESLA S1070**
- 30 Nodes
- up to 60 GPUs
GPU Performance Results and Comparison

- Up to 500 MLup/s on a single GPU for plain LBM kernel (SP)
- 250 MLups/s for GPU in cluster
- Compares to 75 MLup/s for Nehalem Node (8 cores)
- A GPU node (2 GPUs) delivers performance like:
  - 6 Nehalem Nodes (48 cores)
  - 75 IBM Blue Gene/P Nodes
- 30 GPU nodes (60 GPUs) are equivalent to:
  - 137 Nehalem nodes (1096 cores)
  - 1275 Jugene/P nodes (5100 cores)

How far is it to do „Real Time CFD“?

25 GLups would compute
- 25 Frames per second for a LBM grid with resolution 1000 x 1000 x 1000
Conclusions
The Two Principles of Science

Three

Theory
Mathematical Models, Differential Equations, Newton

Experiments
Observation and prototypes, empirical Sciences

Computational Science
Simulation, Optimization, (quantitative) virtual Reality
CS&E Applications in
disciplinary areas such as
physics, chemistry, biology, etc.
multi-disciplinary and
emerging areas
industry

Modeling and Simulation
multi-physics and multi-scale problems
kinetic methods
meshless methods
molecular and particle based methods
discrete and event driven models
hybrid models
validation and verification
uncertainty quantification

Chairs:
Padma Raghavan, Pennsylvania State University
Ulrich Ruede, Erlangen
Acknowledgements

Collaborators

- In Erlangen: WTM, LSE, LSTM, LGDV, RRZE, LME, Neurozentrum, Radiologie, Applied Mathematics, Theoretical Physics, etc.
- Especially for foams: C. Körner (WTM)
- International: Utah, Technion, Constanta, Ghent, Boulder, München, CAS, Zürich, Delhi, ...

Dissertationen Projects

- N. Thürey, T. Pohl, S. Donath, S. Bogner (LBM, free surfaces, 2-phase flows)
- M. Kowarschik, J. Treibig, M. Stürmer, J. Habich (architecture aware algorithms)
- K. Igilberger, T. Preclik, K. Pickel (rigid body dynamics)
- J. Götz, C. Feichtinger (Massively parallel LBM software, suspensions)
- C. Mihoubi, D. Bartuschat (Complex geometries, parallel LBM)

(Long Term) Guests in summer/fall 2009/10:

- Dr. S. Ganguly, IIT Kharagpur (Humboldt) - Electroosmotic Flows
- Prof. V. Buwa, IIT Delhi (Humboldt) - Gas-Fluid-Solid flows
- Felipe Aristizabal, McGill Univ., Canada (LBM with Brownian Motion)
- Prof. Popa, Constanta, Romania (DAAD) Numerical Linear Algebra
- Prof. N. Zakaria, Universiti Petronas, Malaysia
- Prof. Hanke, KTH Stockholm (DAAD), Mathematical Modelling

~25 Diplom- /Master- Thesis, ~30 Bachelor Thesis

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Thank you for your attention!

Questions?

Slides, reports, thesis, animations available for download at:
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