Simulation and Animation of Complex Flows on 10,000 Processor Cores


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in collaboration with many more

Lehrstuhl für Informatik 10 (Systemsimulation)
Universität Erlangen-Nürnberg
www10.informatik.uni-erlangen.de

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Supercomputing Masterworks 2009
Where is Erlangen?
Overview

- Flow Simulation with Lattice Boltzmann Methods
- The LBM
- Rigid Body Dynamics
- Fluid-Structure Interaction with Moving Objects
- Fluctuating LBM for FSI with nano particles
- Bubbly Flows and Foams
- Animations
- Conclusions
Computational Fluid Dynamics with the Lattice Boltzmann Method

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

- Discretization in squares or cubes (cells)
- 9 numbers per cell (or 19 in 3D)
  - number of particles traveling towards neighboring cells
- 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
Widely applicable lattice Boltzmann from Erlangen

- CFD SW 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, a.m.m.
    - Charged colloids
    - Arbitrary combinations of above
- Integration in efficient massively-parallel environment

- Patch concept enables
  - Extendability: new functionality
  - Parallelization
  - Load Balancing
  - Accelerators!
Rigid Multibody Dynamics
What is rigid body dynamics?
Rigid body dynamics with friction and objects of more general shape
(T. Preclik, K. Iglberger)

Solve linear complimentarity problem in each time step
Collisions & Contacts between Rigid Objects
Dynamics of many objects (composed objects)
Granular Flows with Non-Spherical Particles and Frictional Elastic Collisions

64 Processes, 62658 particles, each composed of 2-5 overlapping spheres, approx. 13 hours runtime

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
Weak Scaling

up to 9120 processor cores

more than one billion geometric objects

HLRB-II: SGI Altix
Leibniz Computing Center Garching

Itanium based
63 TFlop Peak
40 TByte memory

<table>
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<th>Partitioning</th>
<th>Runtime [s]</th>
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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.
Parallelization of Particle-laden Flows

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<th>% of compute time</th>
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<tr>
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xsize: 540, ysize: 500, zsize: 500

135 x 10^6 lattice cells

129 processes/cores

2,500 objects

27,000 time steps

12:54h
Fluidized Beds
Virtual Fluidized Bed

- 512 processors of HLRB2:
- Size of Simulation Domain
  400x400x480 cells of LBM
- number of rigid objects: 25,000
- number of time steps: 252,000
- Run time:
  30h 4min
- corresponds to 15,000 core hours.
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:
Parallel Performance of Fluid-Structure Interaction
with Multibody Dynamics

Largest simulation to date:
622 Billion unknowns per time step (LBM alone)
12 TByte

- 4 million fluid lattice cells per core
- 32 billion cells max in total
- spherical moving objects of diameter 6 lattice cells
- 37 million moving objects max in total
"Fluctuating" Lattice Boltzmann for Microfluidics: Brownian Motion

- cell size 1nm
- Domain size 100 nm x 100 nm
- 100 x 100 cells
- time step $10^{-13}$ sec
- > 100 000 time steps $\approx$ 1 ns
Lattice Boltzmann Methods

Free Surface Flow Simulation

for foams, fuel cells, food processing, etc.
The interface between liquid and gas

- Volume-of-Fluids like approach
- Flag field: Compute only in fluid
- Special “free surface” conditions in interface cells
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 time steps
77 GB
64 processes
72 hours
4,608 core hours

Visualization
770 images
Approx. 12,000 core hours for rendering

Best Paper Award for Stefan Donath (LSS Erlangen) at ParCFD, May 2009 (Moffett Field, USA)
Parallel Efficiency

Woodcrest cluster
moderate domain size per core
(strong: 6.5 GB, weak: 1 GB/core)

HLRB2, SGI Altix 4700
Full domain size (3.5 GB/core)
Largest domain size:
$6.1 \times 10^{10}$ cells ≈ 31 TB Mem
Flow Simulation

Visualization and Animation
Massively parallel simulations with many particles (LSS cluster)

- xsize: 540
- ysize: 240
- zsize: 400
- 52 x 10^6 lattice cells
- 31 processes/cores on LSS cluster
- 750 objects
- 10,000 timesteps
- 9:45h
Simulations with Fluid Control
Part IV

Conclusions
Conclusions :-) 

Parallel Supercomputer Performance is Easy!

- If parallel efficiency is bad, choose a slower serial algorithm
  - it is probably easier to parallelize
  - and will make your speedups look much more impressive
- Introduce the “CrunchMe” variable for getting high Flops rates
  - advanced method: disguise CrunchMe by using an inefficient (but compute-intensive!) algorithm from the start
- Introduce the “HitMe” variable to get good cache hit rates
  - advanced version: Implement HitMe in the “Transgalactic Hash-Brown Lookaside Table of the Multi-Threatened Cash-Filling Spock-Tree“ Class
  - ... impressing yourself and others
- Never cite “time-to-solution”
  - who cares whether you solve a real-life problem anyway
  - it is the MachoFlops that interest the people who pay for your research
- Never waste your time by trying to use a complicated algorithm in parallel
  - Use Primitive Algorithm => Easy to Maximize your MachoFlops
  - A few million CPU hours can easily save you days of reading in boring math books
Acknowledgements

Collaborators

- In Erlangen: WTM, LSE, LSTM, LGDV, RRZE, LME, Neurozentrum, Radiologie, etc.
- Especially for foams: C. Körner (WTM)
- International: Utah, Technion, Constanta, Ghent, Boulder, München, 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. Iglberger, 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:

- 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
- several Indian student interns

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

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Thanks for your attention!

Questions?

Slides, reports, thesis, animations available for download at:
www10.informatik.uni-erlangen.de