Supercomputing for Simulation in Science and Engineering

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in collaboration with many colleagues and students

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

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Presentation at
ABB Västerås
Friedrich-Alexander University
Erlangen-Nürnberg

- Founded 1743
- 5 Schools, 22 Departments, 24 Clinics
- 26,000 students in 132 programs
- ~ 500 tenured faculty (full and associate profs)
- ~ 900 PhD and Dr. habil. degrees in 2007
- ~ 92 Mio Euro external funding/ year
- School of Engineering founded in 1966
  - Currently about 4500 students
  - 5 departments, covering all engineering fields, including computer science
The **LSS Mission**

Development and Analysis of Simulation Technology for Applications in Science and Engineering

Applications from Physical and Engineering Sciences

Computer Science

**LSS**

Mathematics
Overview

- Motivation
  - How fast are computers today?

- Scalable Finite Element Solvers
  - Scalable Solver Algorithms
  - Scalable Architecture: Hierarchical Hybrid Grids (HHG)

- Complex Flow Simulation with Lattice Boltzmann Methods
  - The LBM
  - Bubbly Flows and Foams
  - Non-Newtonian models for blood flow and clotting
  - Multibody Dynamics
  - Fluid-Structure Interaction with Moving Objects
  - Fluctuating LBM for FSI with nano particles

- Conclusions
Towards Scalable FE Software

Scalable Algorithms and Data Structures
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Parallel scalability of scalar elliptic problem in 3D discretized by tetrahedral finite elements.

Times to solution on SGI Altix: Itanium-2 1.6 GHz.

Largest problem solved to date: $3.07 \times 10^{11}$ DOFS (1.8 trillion tetrahedra) on 9170 Procs in roughly 90 secs.

Computational Fluid Dynamics

Lattice Boltzmann Method
The Lattice-Boltzmann-Method

- Discretization in 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
Lattice Boltzmann Methods

Free Surface Flow Simulation
(for foams)
Large-Scale Application: 1000 Bubbles

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

Visualization
360 images
8 processes for 4 hours per image
11,520 core hours

Best Paper Award for Stefan Donath at ParCFD, May 2009 (Moffett Field, USA)
Simulation of Metal Foams

Applications:
- 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 (Material Sciences)
Rigid Multi Body Dynamics
Collisions & Contacts between Rigid Objects
Massively Parallel Particulate Flows
Fluidized Beds
(collaboration with K.E. Wirth, Chemical Engineering)
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.
Coupling the physics engine to the Lattice Boltzmann solver

- Example

**Timeloop**

1. Set boundary conditions
2. LBM stream collide
3. Add forces from fluid to obstacles
4. Move and collide obstacles
   - send to instance
   - move and collide locally
5. Move and collide obstacles on instance
6. Send values back
7. Receive and update values from instance
8. If obstacle getting near border, then send to neighbor
Parallel Performance of Fluid-Structure Interaction with Multibody Dynamics

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

Figure 4: Performance of simulations with rigid bodies incorporated in the fluid. The number of lattice cells per processor core is 4 million, spheres are used with a diameter of 6 lattice cells and a average spacing of 12 lattice cells between the spheres. For 8192 cores more than 37 million objects are simulated. Due to the architecture of the h1rb-2, 4 cores per memory channel are used instead of 2 when running on more than 7900 cores, which reduces the performance.
Free Surface Flow Simulation

Visualization and Animation
Conclusions
The Two Principles of Science

Theory
Mathematical Models, Differential Equations, Newton

Experiments
Observation and prototypes empirical Sciences

Computational Science
Simulation, Optimization (quantitative) virtual Reality
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 (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
- 3 Indian student interns

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

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