Supercomputing for Simulation in Science and Engineering


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

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Supercomputing Center of Chinese Academy of Sciences
Beijing, China
Overview

- Motivation (developments in computers)
- Towards Scalable Multilevel FE Solvers
  - Multigrid
  - HHG
  - Performance Results
- Flow Simulation with Lattice Boltzmann Methods
  - The LBM
  - Rigid Body Dynamics
  - Fluid-Structure Interaction with Moving Objects
  - Bubbly Flows and Foams
  - Animations
- Conclusions
Motivation
How much is a PetaFlops?

- $10^6 = 1$ MegaFlops: Intel 486
  33MHz PC (~1989)
- $10^9 = 1$ GigaFlops: Intel Pentium III
  1GHz (~2000)
  - If every person on earth computes one operation every 6 seconds, all humans together have ~1 GigaFlops performance (less than a current laptop)
- $10^{12} = 1$ TeraFlops: HLRB-I
  1344 Proc., ~2000
- $10^{15} = 1$ PetaFlops
  - 294,912 Cores (Jugene, 2009)
  - If every person on earth runs a 486 PC, we all together have an aggregate Performance of 6 PetaFlops.
- $10^{18} = 1$ ExaFlops (around 2020)?
Jugene @ Jülich

- IBM Blue Gene
- 0.825 petaflop/s performance speed running the Linpack benchmark.
- theoretical peak capability 1.0027 Petaflop/s
- 294 912 cores
- #4 on TOP 500 List
- Nov 2009

Björn Gmeiner (LSS) visiting Jülich Supercomputing Center
Picture taken March 2010
What’s the problem?

replacing 4 strong jet engines

Would you want to propel a Super Jumbo with 300,000 blow dryer fans?
Towards Scalable FE Software

Scalable Algorithms and Data Structures
How fast are our algorithms (multigrid) on current CPUs

Assumptions:
- Multigrid requires 27.5 Ops/unknown to solve an elliptic PDE (Griebel ’89 for Poisson)
- A modern laptop CPU delivers >10 GFlops peak

Consequence:
- We should solve one million unknowns in 0.00275 seconds
- ~ 3 ns per unknown

Revised Assumptions:
- Multigrid takes 500 Ops/unknown to solve your favorite PDE
- you can get 5% of 10 Gflops performance

Consequence: On your laptop you should
- solve one million unknowns in 1.0 second
- ~ 1 microsecond per unknown

Consider Banded Gaussian Elimination on the Play Station (Cell Processor), single Prec. 250 GFlops, for 1000 x 1000 grid unknowns
- ~2 Tera-Operations for factorization - will need about 10 seconds to factor the system
- requires 8 GB Mem.
- Forward-backward substitution should run in about 0.01 second, except for bandwidth limitations
Multigrid: V-Cycle

Goal: solve $A^h u^h = f^h$ using a hierarchy of grids

$A^h u^h = f^h$
$r^h = f^h - A^h u^h$
$r^H = I^H_h r^h$
$e^h = I^H_H e^H$
$A^H e^H = r^H$

Relax on Residual Restrict Correct Interpolate Solve by recursion...
Parallel High Performance FE Multigrid

- Parallelize "plain vanilla" multigrid
  - partition domain
  - parallelize all operations on all grids
  - use clever data structures

- Do not worry (so much) about Coarse Grids
  - idle processors?
  - short messages?
  - sequential dependency in grid hierarchy?

- Multigrid vs. Domain Decomposition
  - DD without coarse grid does not scale (algorithmically) and is inefficient for large problems/ many processors
  - DD with coarse grids is like multigrid and is as difficult to parallelize
  - We get good results for parallel multigrid ...

Bey's Tetrahedral Refinement
HHG refinement example

Input Grid
HHG Refinement example

Refinement Level one
HHG Refinement example

Refinement Level Two
HHG Refinement example

Structured Interior
HHG Refinement example

Structured Interior
HHG for Parallelization

Use regular HHG patches for partitioning the domain
HHG Parallel Update Algorithm

for each vertex do
    apply operation to vertex
end for
update vertex primary dependencies

for each edge do
    copy from vertex interior
    apply operation to edge
    copy to vertex halo
end for
update edge primary dependencies

for each element do
    copy from edge/vertex interiors
    apply operation to element
    copy to edge/vertex halos
end for
update secondary dependencies
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<th>#unkn. x 10^6</th>
<th>Ph.1: sec</th>
<th>Ph. 2: sec</th>
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<td>7.75*</td>
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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.

B. Bergen, F. Hülsemann, U. Rüde, G. Wellein: ISC Award 2006, also: „Is \(1.7 \times 10^{10}\) unknowns the largest finite element system that can be solved today?“, SuperComputing, Nov’ 2005.
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
LBM in Equations

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:

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

\[ F_i^{(0)}(x, t) = \frac{1}{18} \rho(x, t) \left( 1 + \frac{3}{2} \frac{\langle c_i, u(x, t) \rangle}{c^2} + \frac{9}{2} \frac{\langle c_i, u(x, t) \rangle^2}{c^4} - \frac{3}{2} \frac{\langle u(x, t), u(x, t) \rangle}{c^2} \right) \quad \text{for } i \in \{N, E, S, W, T, B\} \]

\[ F_i^{(0)}(x, t) = \frac{1}{36} \rho(x, t) \left( 1 + \frac{3}{2} \frac{\langle c_i, u(x, t) \rangle}{c^2} + \frac{9}{2} \frac{\langle c_i, u(x, t) \rangle^2}{c^4} - \frac{3}{2} \frac{\langle u(x, t), u(x, t) \rangle}{c^2} \right) \quad \text{for } i \in \{TN, TS, BN, BS, TE, TW, BE, BW, NE, NW, SE, SW\} \]
walBerla

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
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 Flows with Non-Spherical Particles and Frictional Elastic Collisions

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

### 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

K. Iglberger (LSS)
PRACE Award 2010

<table>
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<tr>
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<th># Spheres</th>
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<td>1613.73</td>
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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.
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)
Algorithm for Coupling LBM and Multibody Dynamics

Algorithm 2 Coupled LBM-PE solver

1: MPI communicate ghost layer of velocity and density
2: for each body B do
3: Map B to lattice grid
4: end for
5: MPI communicate ghost layer of PDFs
6: for each lattice cell do
7: Stream and collide
8: end for
9: for each surface cell do
10: Add forces from fluid to rigid objects
11: end for
12: Time step in the rigid body simulation
Parallelization of Particle-laden Flows

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<th>Module</th>
<th>% of compute time</th>
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<td>Object mapping</td>
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<tr>
<td>PE communication</td>
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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 Processes

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
Simulation of a Segregation Process

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/dm\(^3\) and 1.2 kg/dm\(^3\) are used for the objects in water with density 1 kg/dm\(^3\) and a gravitation field. Lighter particles are rising to the top of the box, while heavier particle sink to the bottom.
Weak Scaling

![Graph showing weak scaling efficiency with respect to the number of cores.]

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

- **Scaling**: 64 to 294,912 cores
- **Largest simulation to date**: 8 Trillion ($10^{12}$) variables per time step (LBM alone)
- **50 TByte**

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

- **150,994,944,000 lattice cells**
- **83,804,982 rigid spherical objects**
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 \times 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)
Numerical Experiment: Single Rising Bubble

Comparison to (rotationally symmetric) 2D level-set volume-of-fluid method and experimental results (T. Pohl, D. Gerlach, F. Durst (Erlangen), G. Biswas (IIT Kanpur), more in the future jointly with V. Buwa, IIT Delhi)

Modified parameter: surface tension
Flow Simulation

Visualization and Animation
Simulations with Fluid Control
Part IV

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, Applied Mathematics, Theoretical Physics, 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. IgIberger, T. Preclik, K. Pickel (rigid body dynamics)
- J. Götz, C. Feichtinger (Massively parallel LBM software, suspensions)
- C. Mihoubi, D. Bartusch (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

Funding by KONWIHR, DFG, BMBF, EU, Elitenetzwerk Bayern
Thank you for your attention!

Questions?

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