Parallel Simulation and Animation of Free Surface Flows with the Lattice Boltzmann Method

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Lehrstuhl für Informatik 10 (Systemsimulation)
Universität Erlangen-Nürnberg
www10.informatik.uni-erlangen.de
Georgia Tech, March 12, 2008
Overview

- Motivation
  - How fast are computers today?
- Towards Scalable Finite Element Solvers
  - Scalable Algorithms: Multigrid
  - Scalable Architecture: Hierarchical Hybrid Grids (HHG)
  - Parallel Performance Results
- Flow Simulation with Lattice Boltzmann Methods
  - The LBM
  - Free Surfaces
  - Metal Foams as an Example Application
  - Parallel Performance Results
  - Towards fluid-structure iteration with moving objects
  - Computational Haemodynamics using the PlayStation
  - Visualization and Animation
- Conclusions
Part III - a

The Lattice Boltzmann Method
Free surface flow: Breaking Dam
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
The stream step

Move particle (numbers) into neighboring cells

a single cell at timestep $t$ after collision

a single cell at timestep $t+1$ after streaming

four cells at timestep $t$ after collision

four cells at timestep $t+1$ after streaming
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:

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

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

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

Lattice Boltzmann Methods

*Free Surface Flow Simulation*  
*(for metal foams)*
The interface between liquid and gas

- Compute only fluid
- Special “free surface” conditions on interface
Falling Drop with Turbulence Model (slow)
Rising Bubbles
Numerical Experiment: Single Rising Bubble

![Graph showing bubble position and velocity over time]

**Y-axis:**
- Bubble position [m]

**X-axis:**
- Time [s]

**Legend:**
- 1 × σ
- Reference simulation

**Graph Details:**
- The graph plots bubble position and velocity against time.
- It compares the measured data (1 × σ) with the reference simulation.
Simulation of Metal Foams

- Free Surface Flows

- Applications:
  - Engineering: metal foam simulations
  - Computer graphics: special effects

- Based on LBM:
  - Mesoscopic approach to solving the NS equations
  - Good for complex boundary conditions
  - Details: D3Q19 model, BGK collision and grid compression
Part III - d

Lattice Boltzmann Methods

Parallel Performance
Parallelization

Standard LBM-Code: Scalability on SR 8000-F1

Largest Simulation:
1,08*10^9 cells
370 GByte memory

Communication Cost because of large data volume (64 MByte)

→ Efficiency ~ 75%

Dissertation T. Pohl
(2007/8)
Performance lousy on a single node!
Conditionals: 2,9 SLBM $\rightarrow$ 51 free surface LBM
Pentium 4: almost no degradation $\sim$ 10%
SR 8000: enormous degradation (pseudo-vector, predictable jumps)
OpenMP Parallelization

- OpenMP for shared memory architectures
- Partition along Y-axis, synchronize layers
OpenMP Performance

Performance results with 2/4-way Opterons:

Dual Core Node

Quad Core Node

Total Computation Time [s]

CPUs

1 2

1 2 4

Single Grid

Adaptive Grids (2 Coarser Levels)

CPUs

1 2 4

1 2 4

Single Grid

Adaptive Grids (2 Coarser Levels)
MPI Parallelization

- MPI for distributed memory architectures
- Partition along x-axis
- Transfer boundary layer over the network
MPI Performance

Measurements on up to $8 \times 4$-way Opteron with Infiniband interconnect:
MPI Performance with adaptive Grids:

- Same Opteron-cluster, with and without adaptive coarsening:

![Graphs showing performance comparison between single grid and adaptive coarsening with and without MPI]

Single Grid, Quad Nodes with MPI, Test Case Q

Adaptive Coarsening, Quad Nodes with MPI, Test Case Q

Single Grid, Quad Nodes with MPI, Test Case W

Adaptive Coarsening, Quad Nodes with MPI, Test Case W
waLBerla

- widely applicable Lattice Boltzmann framework erlangen
  - Complex geometries/porous media
  - Moving obstacles/fluid-structure interaction
  - Free surfaces
  - Ionized fluids/charged colloids

- Efficient implementation
  - High performance
  - Low memory consumption
  - Parallelization
  - Adaptivity

- Validation
Parallel Performance on the Woodcrest Cluster (RRZE)
Part III-e

Lattice Boltzmann Methods

Computational Haemodynamics on the Play Station
Aneurysms

- Aneurysm are local dilatations of the blood vessels
- Localized mostly at large arteries in soft tissue (e.g. aorta, brain vessels)
- Can be diagnosed by modern imaging techniques (e.g. MRT, DSA)
- Can be treated e.g. by clipping or coiling
Goal: demanding (flow) simulations at moderate cost but very fast, e.g. for simulation of blood-flow in an aneurysm for therapy and surgery planning

Available cell systems:
- Blades
- Playstation 3
A data structure for simulating flow in blood vessels

- In a brain geometry only about 3-10% of the nodes are filled with blood

- Domain partitioning in equally sized blocks, so-called patches
- only allocate patches containing fluid cells
- Memory requirements and the computational time reduced significantly
- For the Cell processor we use patches of size 8x8x8, fitting into the SPU local memory
Performance Results

LBM performance on a single core
(8x8x8 channel flow)

- Xeon 5160: 10.4 MFLUPS
- PPE: 4.8 MFLUPS
- SPE*: 49.0 MFLUPS

*on Local Store without DMA transfers

- Straight-forward C code
- SIMD-optimized assembly
Performance Results

Playstation 3 LBM performance (94x94x94 channel flow)

![Bar chart showing MFLUPS vs. Number of SPEs used](image-url)
Part III - e

Flow Simulation

Fluid Structure Interaction: Moving Objects
Particle Technology

Applications for the LBM:

- Simulate the behavior of particles and particle agglomerates in solutions (e.g. breaking up or further agglomeration)
- Properties of materials and products determined by the structure of nano-scale particles
Dynamics of many objects (rigid body dynamics)
Dynamics of many objects (now with friction)
Dynamics of many objects
(composed of more shape primitives)
Part III - f

Free Surface Flow Simulation

Visualization and Animation
Parallel “Tsunami”-Simulation

Resolution: 880*880*336; 260M cells, 6.5M active on average
Example Coupled Simulations
Simulations with Fluid Control
Part IV

Conclusions
Conclusions

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: disguise HitMe within “clever data structures” that introduce a lot of overhead

- 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 (such as multigrid)
  - the more primitive the algorithm the easier to maximize your MachoFlops.
Talk is Over
Please wake up!