Lattice Boltzmann Methods on the way to exascale

Ulrich Rüde
(LSS Erlangen, ulrich.ruede@fau.de)

Lehrstuhl für Simulation
Universität Erlangen-Nürnberg
www10.informatik.uni-erlangen.de

HIGH PERFORMANCE COMPUTING
From Clouds and Big Data to Exascale and Beyond

An International Advanced Workshop
Cetraro – Italy, June 27 – July 1, 2016
Outline

Goals:
- drive algorithms towards their performance limits (scalability is necessary but not sufficient)
- sustainable software: reproducibility & flexibility
- coupled multi physics

Three software packages:
1. Many body problems: rigid body dynamics
   \(2.8 \times 10^{10}\) non-spherical particles
2. Kinetic methods: Lattice Boltzmann - fluid flow
   \(>10^{12}\) cells, adaptive, load balancing
3. Continuum methods: Finite element - multigrid
   fully implicit solves with \(>10^{13}\) DoF

Real life applications
The work horses

JUQUEEN
- Blue Gene/Q architecture
- 458,752 PowerPC A2 cores
- 16 cores (1.6 GHz) per node
- 16 GiB RAM per node
- 5D torus interconnect
- 5.8 PFlops Peak
- TOP 500: #13

SuperMUC
- Intel Xeon architecture
- 147,456 cores
- 16 cores (2.7 GHz) per node
- 32 GiB RAM per node
- Pruned tree interconnect
- 3.2 PFlops Peak
- TOP 500: #27
Building block I:

The Lagrangian View:

Granular media simulations

with the physics engine

### Nonlinear Complementarity and Time Stepping

#### Non-penetration conditions

- \( \xi \geq 0 \perp \lambda_n \geq 0 \)
- \( \dot{\xi}^+ \geq 0 \perp \lambda_n \geq 0 \)

#### Coulomb friction conditions

- \( ||\lambda_{to}||_2 \leq \mu \lambda_n \)
- \( ||\delta v_{to}^+||_2 \lambda_{to} = -\mu \lambda_n \delta v_{to}^+ \)

**Signorini condition**


Dense granular channel flow with crystallization
Scaling Results

- Solver algorithmically not optimal for dense systems, hence cannot scale unconditionally, but is highly efficient in many cases of practical importance
- Strong and weak scaling results for a constant number of iterations performed on SuperMUC and Juqueen
- Largest ensembles computed
  - $2.8 \times 10^{10}$ non-spherical particles
  - $1.1 \times 10^{10}$ contacts
- granular gas: scaling results

(b) Weak-scaling graph on the Juqueen supercomputer.

LBM on the way to ExaScale — Ulrich Rüde
Building Block III:

Scalable Flow Simulations with the Lattice Boltzmann Method


Partitioning and Parallelization

- Static block-level refinement ($\rightarrow$ forest of octrees)
- Allocation of block data ($\rightarrow$ grids)
- Static load balancing
- Separation of domain partitioning from simulation (optional)
- Compact (KiB/MiB) binary MPI I/O
Parallel AMR load balancing

forest of octrees: octrees are not explicitly stored, but implicitly defined via block IDs

distributed graph:
- nodes = blocks
- edges explicitly stored as $<\text{block ID, process rank}>$ pairs

different views on domain partitioning

2:1 balanced grid (used for the LBM)
AMR and Load Balancing with waLBerla


AMR Performance

• Benchmark Environments:
  • JUQUEEN (5.0 PFLOP/s)
    • Blue Gene/Q, 459K cores, 1 GB/core
    • compiler: IBM XL / IBM MPI
  • SuperMUC (2.9 PFLOP/s)
    • Intel Xeon, 147K cores, 2 GB/core
    • compiler: Intel XE / IBM MPI

• Benchmark (LBM D3Q19 TRT):

<table>
<thead>
<tr>
<th>level</th>
<th>initially</th>
<th>after refresh</th>
<th>after load balance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.383 (1)</td>
<td>0.328 (1)</td>
<td>0.328 (1)</td>
</tr>
<tr>
<td>1</td>
<td>0.656 (1)</td>
<td>0.875 (9)</td>
<td>0.875 (1)</td>
</tr>
<tr>
<td>2</td>
<td>1.313 (2)</td>
<td>3.063 (11)</td>
<td>3.063 (4)</td>
</tr>
<tr>
<td>3</td>
<td>3.500 (4)</td>
<td>3.500 (16)</td>
<td>3.500 (4)</td>
</tr>
</tbody>
</table>
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• Benchmark (LBM D3Q19 TRT):

  during this refresh process ...

  ... all cells on the finest level are coarsened and
the same amount of fine cells is created by splitting coarser cells
→ 72% of all cells change their size
AMR Performance

- JUQUEEN – space filling curve: Morton

![Graph showing performance with increasing number of cores and cells.](image)

**hybrid MPI+OpenMP version with SMP**

- 1 process ↔ 2 cores ↔ 8 threads
- 14 billion cells
- 58 billion cells
- 197 billion cells

- **#cells per core**:
  - 31,062
  - 127,232
  - 429,408

Extreme Scale LBM Methods - Ulrich Rüde
• JUQUEEN – diffusion load balancing
Performance on Coronary Arteries Geometry

Color coded proc assignment


**Weak scaling**

458,752 cores of JUQUEEN over a trillion ($10^{12}$) fluid lattice cells
- cell sizes 1.27μm
- diameter of red blood cells: 7μm
- 2.1 $10^{12}$ cell updates per second
- 0.41 PFlops

**Strong scaling**

32,768 cores of SuperMUC
- cell sizes of 0.1 mm
- 2.1 million fluid cells
- 6000+ time steps per second

Flow through structure of thin crystals (filter)

work with Jose Pedro Galache and Antonio Gil
CMT-Motores Termicos, Universitat Politecnica de Valencia
Building Block IV (electrostatics)

Direct numerical simulation of charged particles in flow


6-way coupling

- Charge distribution
- Finite volumes
- MG
  - treat BCs
  - V-cycle
- Electrost. force
- Object motion
- LBM
  - treat BCs
  - stream-collide step
- Hydrodynam. force
- Object distance
- Lubrication correction

- Newtonian mechanics
- Collision response

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Separation experiment

240 time steps fully 6-way coupled simulation
400 sec on SuperMuc
weak scaling up to 32 768 cores
7.1 Mio particles
Volume of Fluids Method for Free Surface Flows

joint work with Regina Ammer, Simon Bogner, Martin Bauer, Daniela Anderl, Nils Thürey, Stefan Donath, Thomas Pohl, C Körner, A. Delgado


Free Surface Flows

- Volume-of-Fluids like approach
- Flag field: Compute only in fluid
- Special “free surface” conditions in interface cells
- Reconstruction of curvature for surface tension
Free Surface Bubble Model

- Data of a Bubble:
  - Initial Volume (Density=1)
  - Current Volume
  - Density/Pressure = initial volume / current volume

- Update Management
  - Each process logs change of volume due to cell conversions (Interface – Gas / Gas – Interface) and mass variations in Interface cells
  - All volume changes are added to the volume of the bubble at $p_G = \frac{V_b^*}{V_b(t)}$ the timestep (which also has to be communicated)
Simulation for hygiene products (for Procter&Gamble)

- Capillary pressure
- Inclination
- Surface tension
- Contact angle
Additive Manufacturing
Fast Electron Beam Melting


Electron Beam Melting Process
3D printing

- EU-Project Fast-EBM
- ARCAM (Gothenburg)
- TWI (Cambridge)
- FAU Erlangen

- Generation of powder bed
- Energy transfer by electron beam

- penetration depth
- heat transfer
- Flow dynamics
- melting
- melt flow
- surface tension
- wetting
- capillary forces
- contact angles
- solidification


Simulation of Electron Beam Melting

Simulating powder bed generation using the PE framework

WaLBerla Simulation

High speed camera shows melting step for manufacturing a hollow cylinder

Inter-node Strong Scaling SuperMUC: 16 - 4096 tasks

MLUPS vs. number of tasks

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Conclusions
CSE research is done by teams

Harald Köstler
Christian Godenschwager
Kristina Pickl
Regina Ammer
Simon Bogner
Florian Schornbaum
Sebastian Kuckuk
Christoph Rettinger
Dominik Bartuschat
Martin Bauer
Thank you for your attention!

Videos, preprints, slides at https://www10.informatik.uni-erlangen.de