Simulation and Animation of Complex Flows on 294 912 Processor Cores


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Overview

- Motivation: How fast are computers today
- Rigid Body Dynamics for Granular Media
- Flow Simulation with Lattice Boltzmann Methods
  - free surfaces
  - bubbly flows
- Fluid-Structure Interaction with Moving Rigid Objects
  - particle laden flows
- preliminary GPU performance comparison
- Conclusions
Motivation
Example Peta-Scale System: Jugene @ Jülich

- PetaFlops = $10^{15}$ operations/second
- IBM Blue Gene
- 0.825 petaflop/s performance speed running the Linpack benchmark.
- theoretical peak capability 1.0027 Petaflop/s
- 294,912 cores
- #5 on TOP 500 List in June 2010

Exa-Scale: $10^{18}$ operations/second - expected around 2018?
What can we do with Exa-Scale Computers?

- Even if we want
  - to simulate a billion objects (particles): we can do a billion operations for each of them in each second
  - a trillion finite elements (finite volumes) to resolve a PDE, we can do a million operations for each of them in each second
- Most existing software dramatically underperforms on contemporary HPC architectures
- This will get more dramatic on future exa-scale systems

Fluidized Bed
(movie: thanks to K.E. Wirth)
Rigid Multibody Dynamics
(for simulating granular systems)
Rigid Body Dynamics

- Newton’s Laws of Motion
  - including rotations
- Contact Detection
  - in each time step
- Collisions modelled by
  - coefficient of restitution: forces in normal direction
  - friction laws: forces in tangential direction
Collisions & Contacts between Rigid Objects
Granular Media Simulations
Hour Glass Simulation

1250000 spherical particles, 256 CPUs, 300300 time steps, runtime: 48h (including data output)
27,270 randomly generated, non-spherical particles, 256 CPUs, 379,300 time steps, runtime: 16.4h (including data output), 0.154s per time step
### How far can we go? Scaling Results!

<table>
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<tr>
<th># Cores</th>
<th># Particles</th>
<th>Partitioning</th>
<th>Runtime [s]</th>
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*Jugene simulation results of 1000 time steps of a dense granular gas contained in an evacuated box without external forces.*
Flow Simulation with Lattice Boltzmann Methods
Computational Fluid Dynamics with the Lattice Boltzmann Method

Falling Drop with Turbulence Model (slow motion)
Larger-Scale Computation: 1000 Bubbles

Simulation
1000 Bubbles
510x510x530 = 1.4 \cdot 10^8 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)
Massively Parallel Particulate Flows
Fluid-Structure Interaction

Physics Engine

Walberla

- collision detection
- (frictional) collision response
- time integration

- fluid results in external forces

- update of fluid nodes: stream/collide
- calculation of hydrodynamic forces (momentum exchange)
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:
07h 12 min
**How Far Can We Go?**

**Scaling Results!**

![Graph showing efficiency of core number scaling](image)

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

- **Scaling 64 to 294 912 cores**

- **sparsely packed particles**

- **150 994 944 000 lattice cells**

- **83 804 982 rigid spherical objects**

Largest simulation to date:
- 8 Trillion ($10^{12}$) variables per time step (LBM alone)
- 50 TByte

Friedrich-Alexander-Universität Erlangen-Nürnberg

Lehrstuhl für Informatik 10 (Systemsimulation)
LBM on Clusters with GPUs
GPU Performance Results and Comparison

- Up to 500 MLup/s on a single GPU for plain LBM kernel (SP)
- 250 MLups/s for GPU in cluster
- Compares to 75 MLup/s for Nehalem Node (8 cores)
- A GPU node (2 GPUs) delivers performance like
  - 6 Nehalem Nodes (48 cores)
  - 75 IBM Blue Gene/P Nodes
- 30 GPU nodes (60 GPUs) are equivalent to
  - 137 Nehalem nodes (1096 cores)
  - 1275 Jugene/P nodes (5100 cores)

How far is it to do „Real Time CFD“?

25 GLups would compute
- 25 Frames per second for a LBM grid with
- resolution 1000 x 1000 x 1000
Conclusions
CS&E Applications in
disciplinary areas such as
physics, chemistry, biology, etc.
multi-disciplinary and
emerging areas
industry

Modeling and Simulation
multi-physics and multi-scale problems
kinetic methods
meshless methods
molecular and particle based methods
discrete and event driven models
hybrid models
validation and verification
uncertainty quantification

Chairs:
Padma Raghavan, Pennsylvania State University
Ulrich Ruede, Erlangen
Conclusions :-)  

**Exa-Scale will be 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 “Hash-Brown Lookaside Table for the Multi-Threatened Cash-Filling Grid-Cloud” data structure
  - ... 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, Applied Mathematics, Theoretical Physics, etc.
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- International: Utah, Technion, Constanta, Ghent, Boulder, München, CAS, 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 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
- Prof. J. Oppelstrup, KTH Stockholm (DAAD), Conservation Laws

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

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Thank you for your attention!

Questions?

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