Simulating Complex Flows with a Parallel Lattice Boltzmann Method

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Numerical Methods and Algorithms for
High Performance Computing
CIRM, Marseille
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Overview

- Motivation: How fast are computers today (and tomorrow)
  - and what we might want to do with them
- How fast should our Solvers be
  - Scalable Parallel Multigrid Algorithms for PDE
  - Matrix-Free Multigrid FE solver: Hierarchical Hybrid Grids (HHG)
- A Multi-Scale & Multi-Physics Simulation (with grain size resolution)
  - Rigid Body Dynamics for Granular Media
  - Flow Simulation with Lattice Boltzmann Methods
    - free surface flows
  - Fluid-Structure Interaction with Moving Rigid Objects
    - particle ladden flows
- Towards a Systematic Perfomance Engineering
  - GPU performance comparison
- Conclusions

Motivation

What can we do with Exa-Scale Computers (1)?

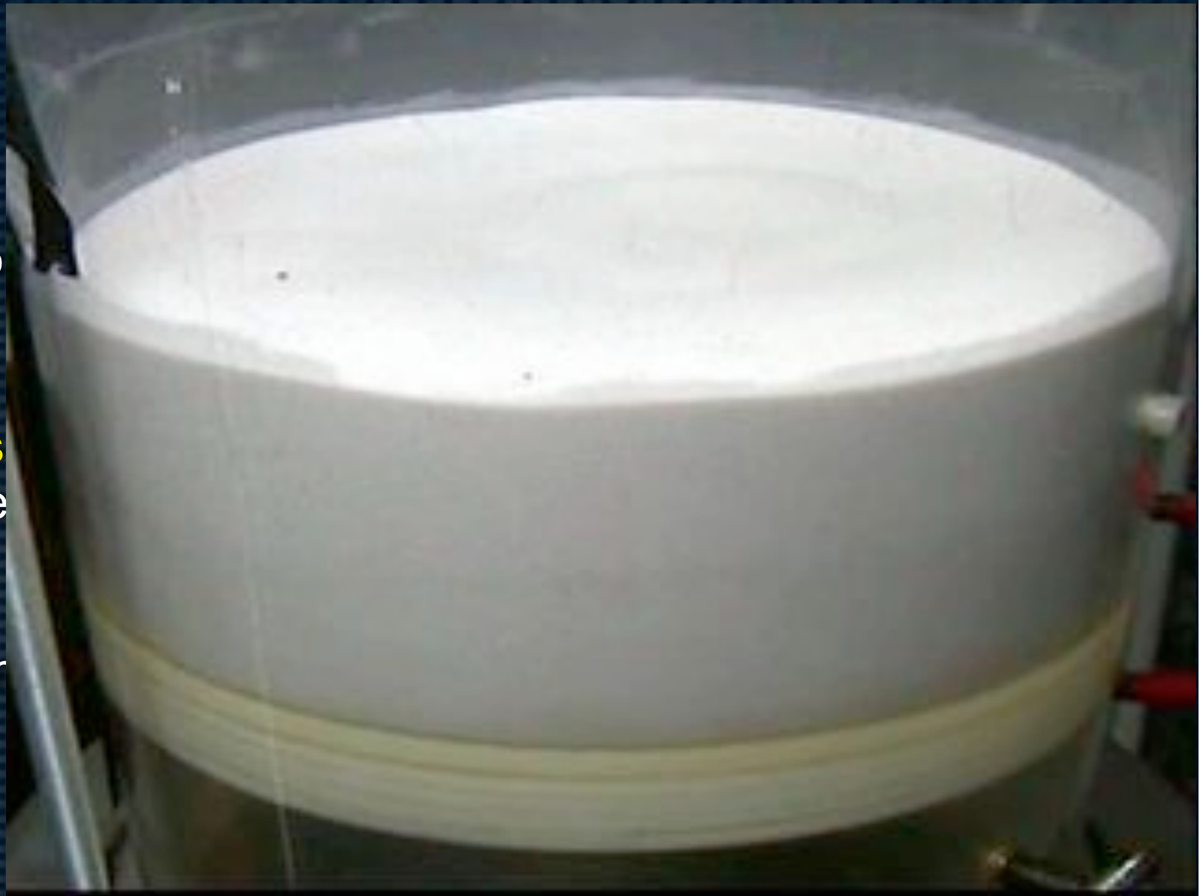
- The *recirculatory system* contains
  - ca. 0.006 m^3 volume
    - discretize with 10^{12} finite volumes
    - mesh size of 0.02 mm
    - 10^6 operations per second and per volume.
  - ca. 2.5×10^{13} red blood cells
    - 4×10^4 flops per second and blood cell
- The *brain* has
  - ca. 10^{11} Neurons
    - 10^7 flops per sec and neuron
  - ca. 0.0015 m^3 volume
    - discretize with 10^{14} finite elements
    - resolve the brain with a mesh size ~0.0025 mm
    - 10^4 operations per second and per element.

What can we do with Exa-Scale Computers(2)?

Fluidized Bed

Even if we want

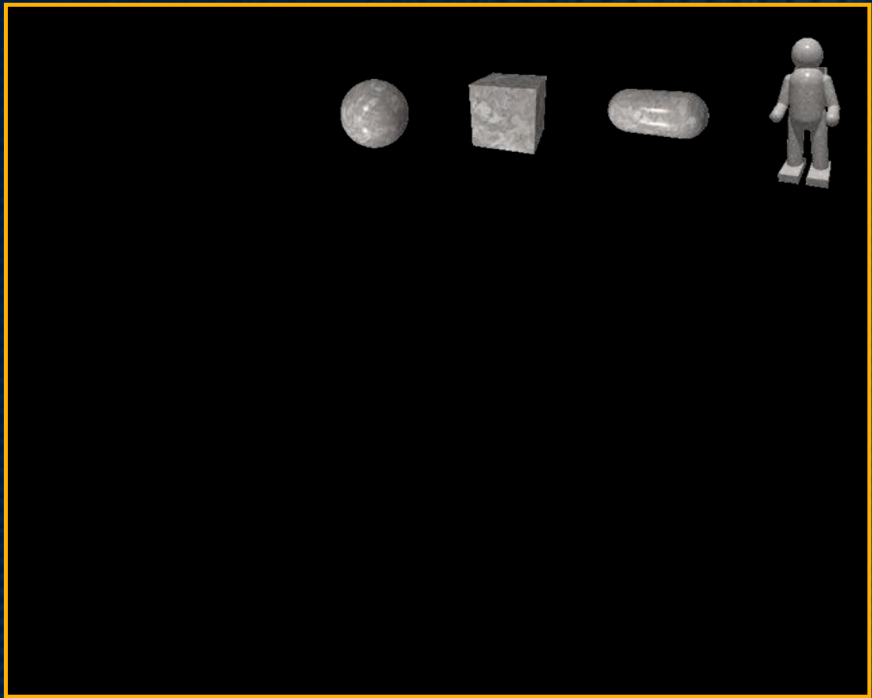
- to simulate a billion (10^9) objects (particles): we can do a billion (10^9) operations for each of them in each second
- a trillion (10^{12}) finite elements (finite volumes) to resolve the flow between particles: we can do a million (10^6) operations for each of them in each second



Fluidized Bed
(movie: thanks to K.E. Wirth, Erlangen)

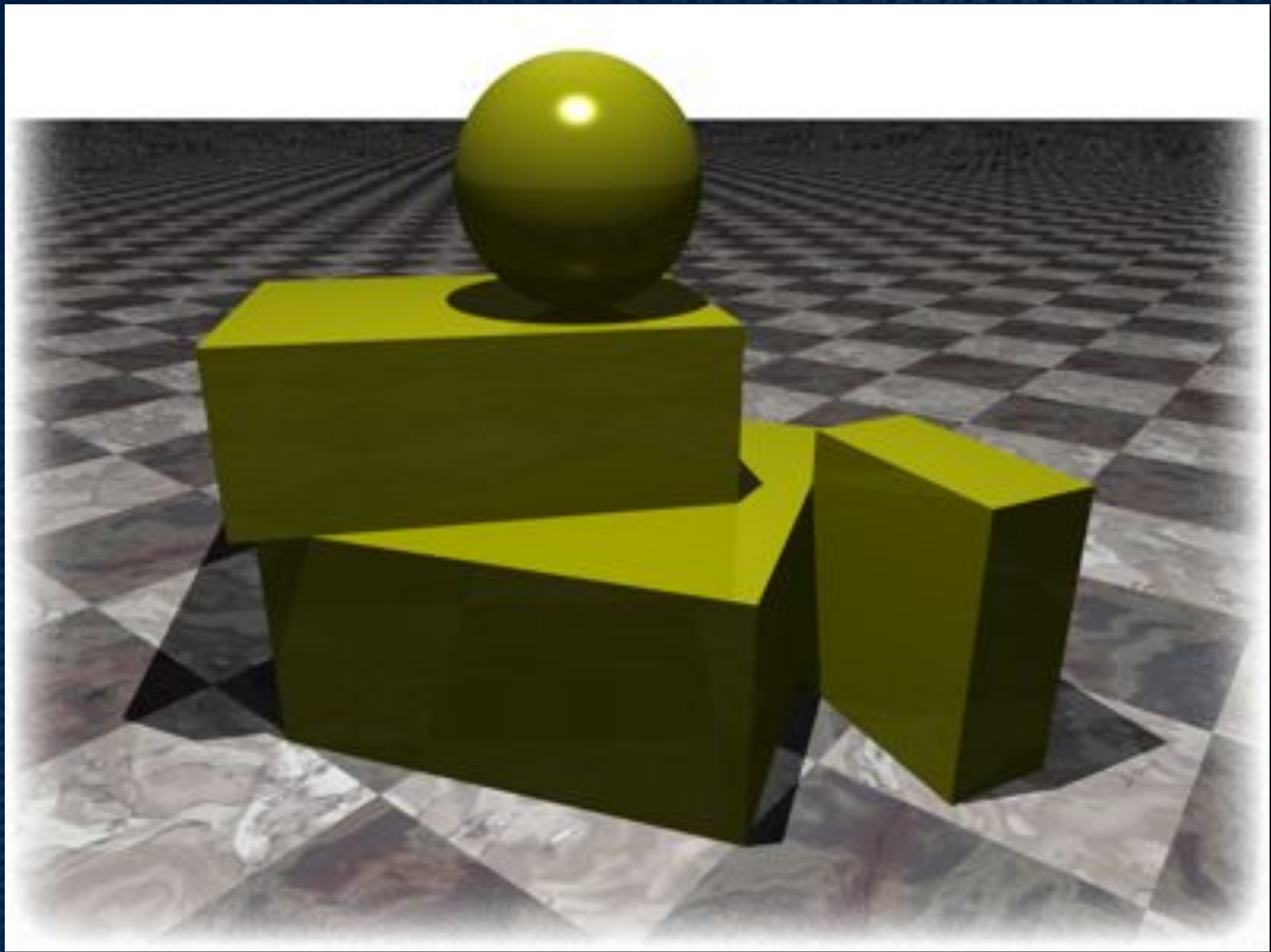
An Example of High Performance Multi-Scale and Multi-Physics Simulation

Rigid Body Dynamics (aka „physics engines“)

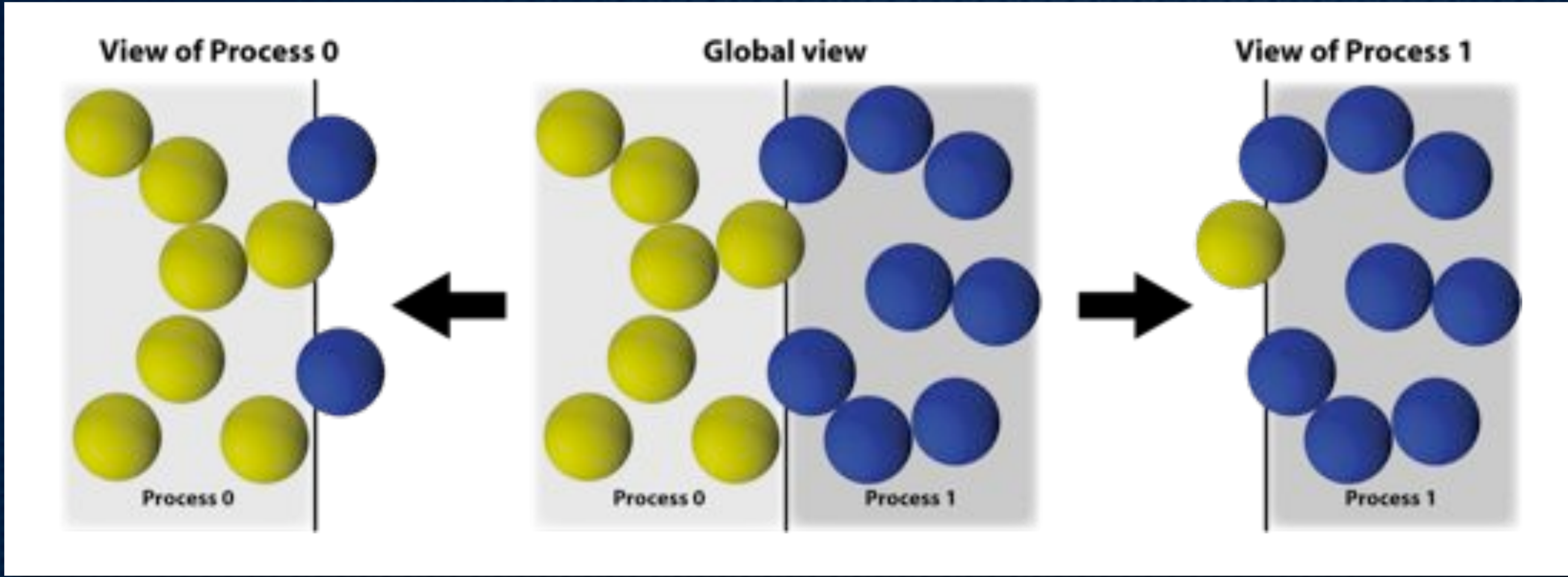


- Newton‘s Laws of Motion
  - including rotations
- Contact Detection
  - in each time step
- Collisions modelled by
  - cofficient of restitution: forces in normal direction
  - (Coulomb) friction laws: forces in tangential direction

Collisions & Contacts between Rigid Objects



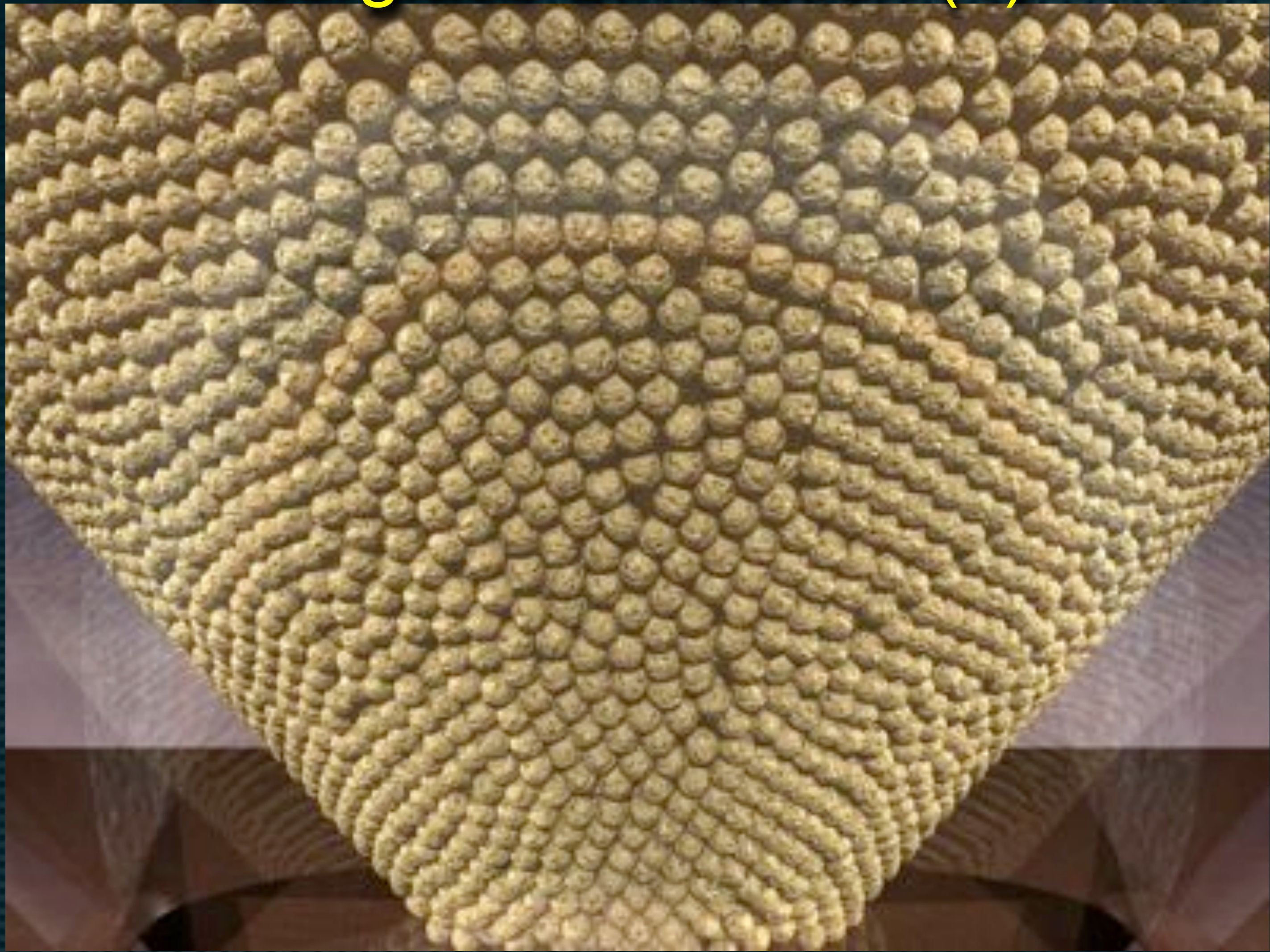
Parallel Rigid Body Dynamics



- 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 Media Simulations

Hourglass Simulation (1)



1 250 000 spherical particles, 256 CPUs, 300 300 time steps, runtime: 48 h (including data output)

How far can we go? Scaling Results!

# Cores	# Particles	Partitioning	Runtime [s]
128	2 000 000	8 x 4 x 4	727.096
256	4 000 000	8 x 8 x 4	726.991
512	8 000 000	8 x 8 x 8	727.150
1 024	16 000 000	16 x 8 x 8	727.756
2 048	32 000 000	16 x 16 x 8	727.893
4 096	64 000 000	16 x 16 x 16	728.593
8 192	128 000 000	32 x 16 x 16	728.666
16 384	256 000 000	32 x 32 x 16	728.921
32 768	512 000 000	32 x 32 x 32	729.094
65 536	1 024 000 000	64 x 32 x 32	728.674
131 072	2 048 000 000	64 x 64 x 32	728.320

* Jugene simulation results of 1000 time steps of a dense granular gas contained in an evacuated box without external forces.

Computational Fluid Dynamics with the Lattice Boltzmann Method

Falling Drop with Turbulence Model
(slow motion)

Computational Fluid Dynamics

- The flow modelling is based on the Navier-Stokes equations (here incompressible form)

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla p + \nu \Delta \mathbf{v} + \mathbf{f}.$$

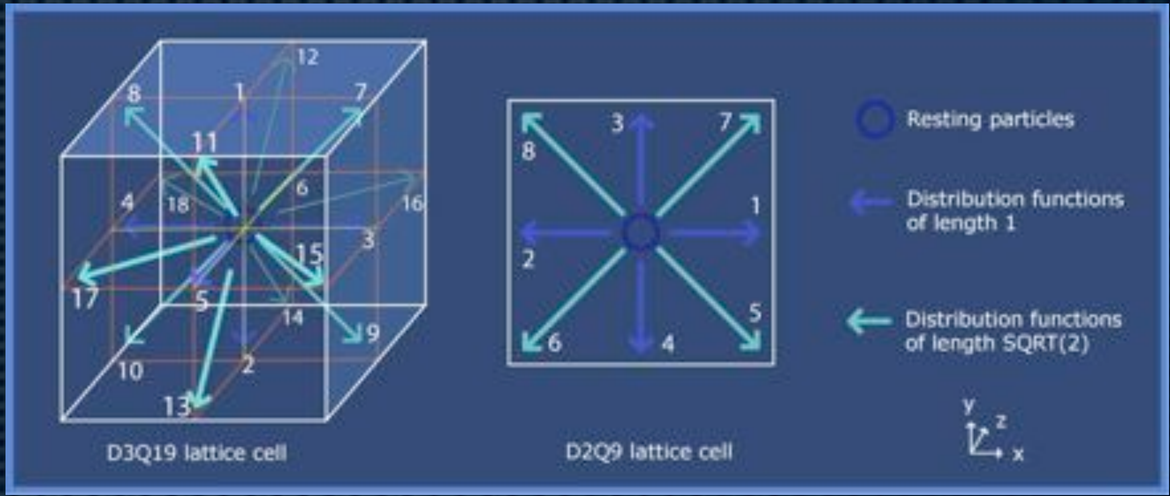
$$\nabla \cdot \mathbf{v} = 0,$$

- More recently, the Lattice Boltzmann method (LBM) has been developed as an alternative

$$\partial_t f(\vec{x}, \vec{v}, t) + \vec{v} \nabla_{\vec{x}} f(\vec{x}, \vec{v}, t) + \frac{\vec{F}}{m} \nabla_{\vec{v}} f(\vec{x}, \vec{v}, t) = \mathrm{I_c}(f),$$

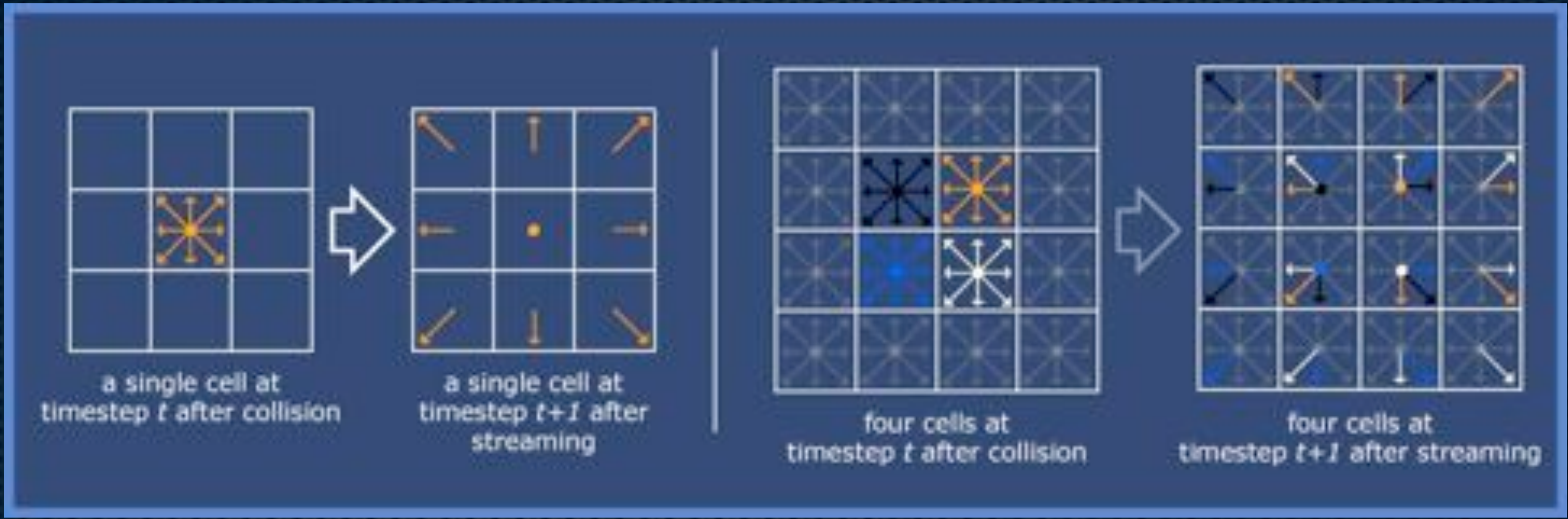
The Lattice-Boltzmann-Method

- 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



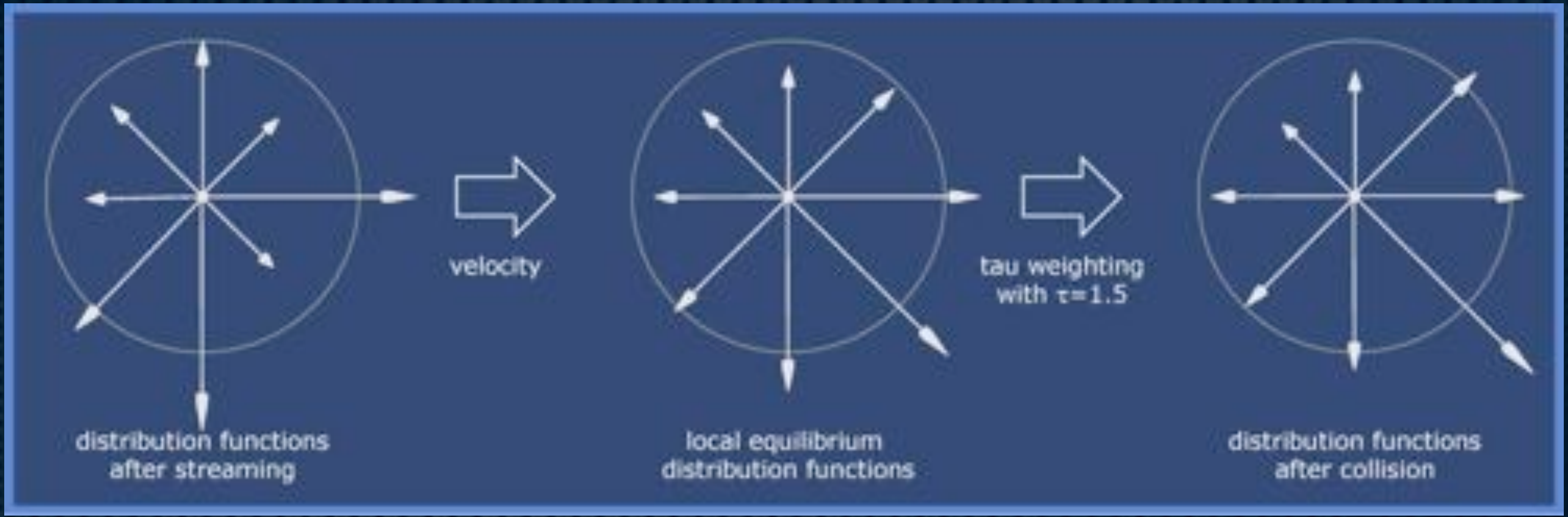
The stream step

Move particle (numbers)
into neighboring cells



The collide step

Compute new particle numbers according to the collisions



Boltzmann Equation

$$\frac{\partial f}{\partial t} + \langle u, \nabla f \rangle = Q$$

collision operator Q

$$Q = -\frac{1}{\tau}\left(f(x,t) - f^{(0)}(x,t)\right)$$

τ is the *relaxation time*

$f^{(0)}(x,t)$ *equilibrium distribution function*

Discretizing the Boltzmann Equation

$$\frac{\partial f}{\partial t} + \langle u, \nabla f \rangle = -\frac{1}{\tau}\left(f - f^{(0)}\right)$$

finite set $\{v_i\}, 0 \leq i \leq n$, of velocities

$$f_i(x,t) = f(x, v_i, t)$$

discrete Boltzmann equation

$$\frac{\partial f_i}{\partial t} + \langle v_i, \nabla f_i \rangle = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right)$$

$$F_i(x + c_i \Delta t, t + \Delta t) - F_i(x,t) = -\frac{1}{\tau}\left(F_i(x,t) - F_i^{(0)}(x,t)\right)$$

LBM in Equations (3D)

- 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:

$$F_i^{(0)}(x,t) = \frac{1}{3}\rho(x,t)\left(1 - \frac{3}{2}\frac{\langle u(x,t), u(x,t)\rangle}{c^2}\right)$$

for $i = \mathrm{C}$,

$$F_i^{(0)}(x,t) = \frac{1}{18}\rho(x,t)\left(1 + 3\frac{\langle c_i, u(x,t)\rangle}{c^2} + \frac{9}{2}\frac{\langle c_i, u(x,t)\rangle^2}{c^4} - \frac{3}{2}\frac{\langle u(x,t), u(x,t)\rangle}{c^2}\right)$$

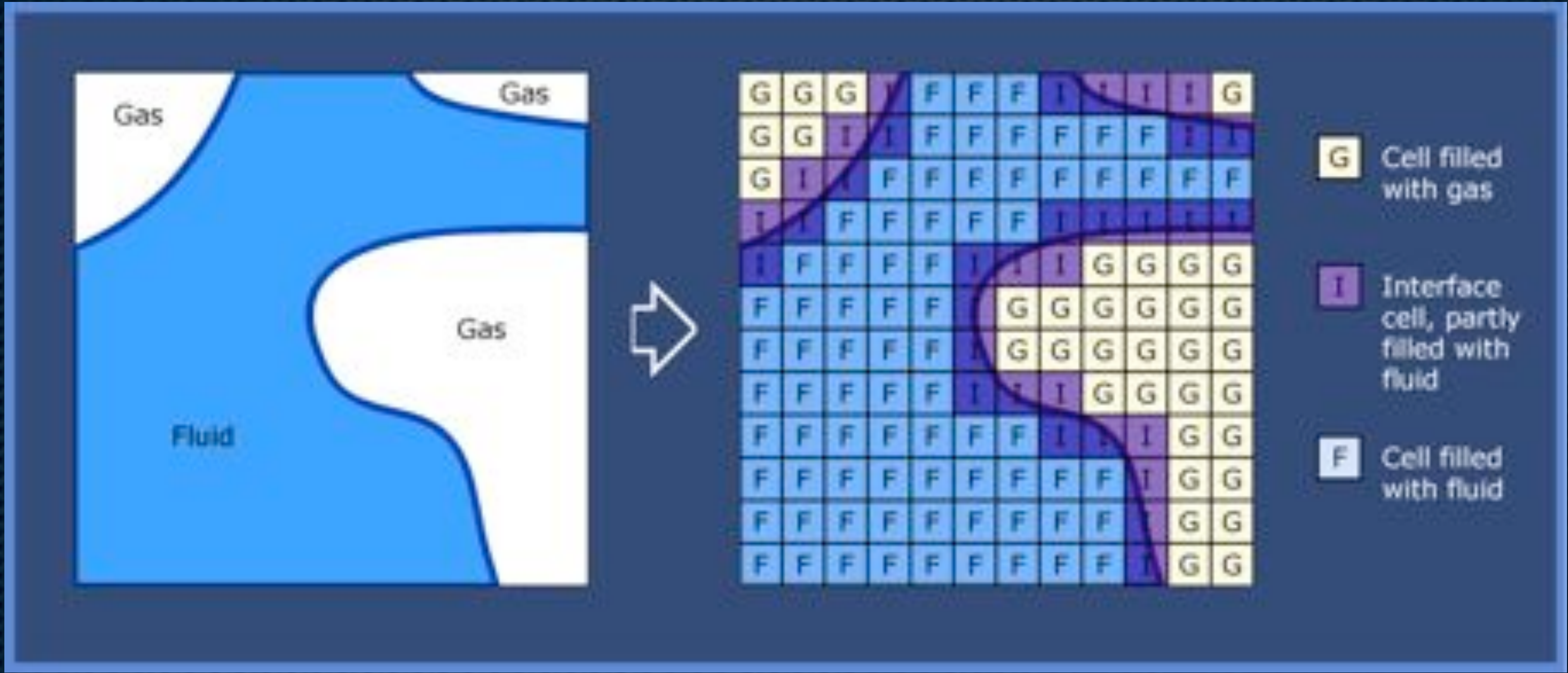
for $i \in \{\mathrm{N, E, S, W, T, B}\}$

$$F_i^{(0)}(x,t) = \frac{1}{36}\rho(x,t)\left(1 + 3\frac{\langle c_i, u(x,t)\rangle}{c^2} + \frac{9}{2}\frac{\langle c_i, u(x,t)\rangle^2}{c^4} - \frac{3}{2}\frac{\langle u(x,t), u(x,t)\rangle}{c^2}\right)$$

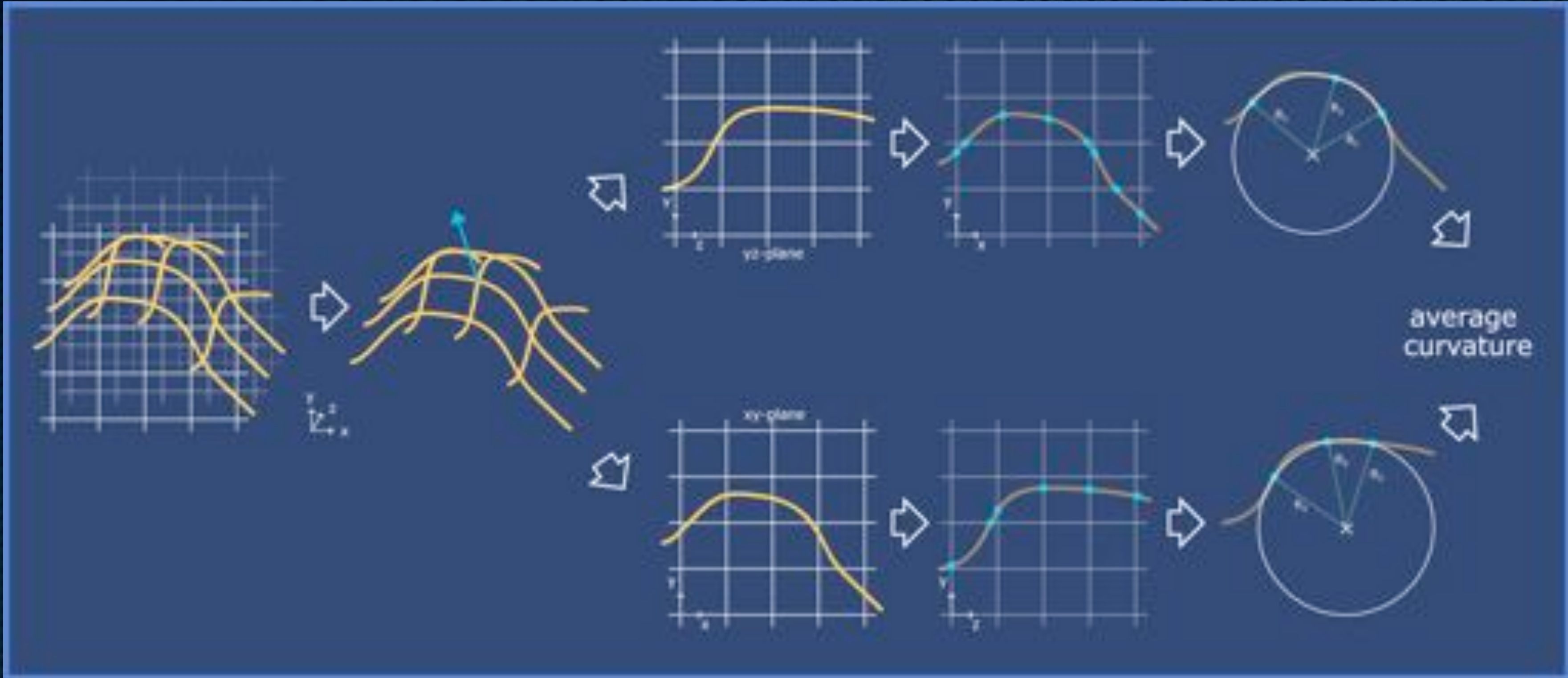
for $i \in \{\mathrm{TN, TS, BN, BS, TE, TW, BE, BW, NE, NW, SE, SW}\}$

The Interface Between Liquid and Gas

- Volume-of-Fluids like approach
- Flag field: Compute only in fluid
- Special “free surface” conditions in interface cells



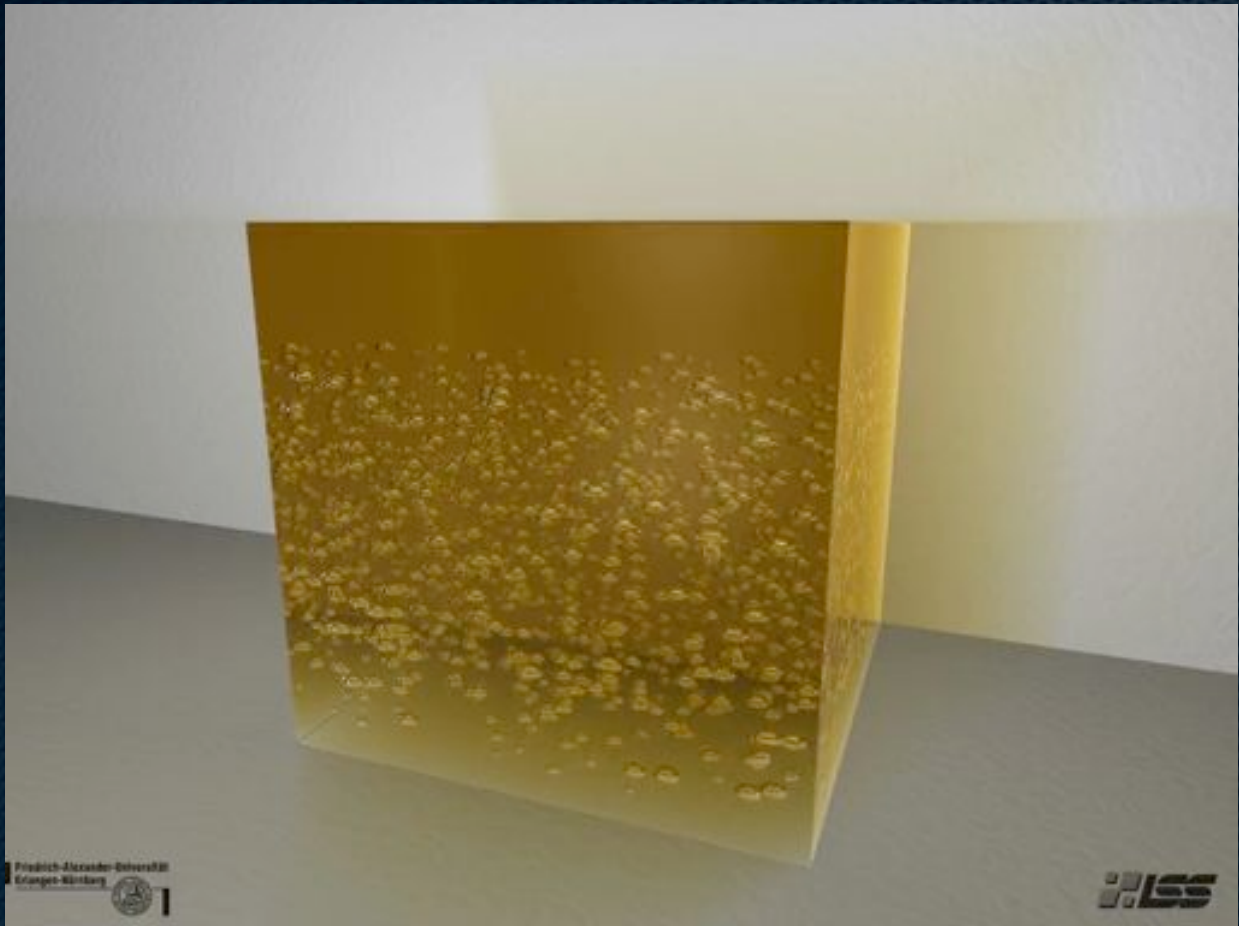
Curvature calculation (version I)



- Alternative approaches:
  - Integrate normals over surface (weighted triangles)
  - Level set methods (track surface as implicit function)

Walberla Software Framework

Computational Fluid Dynamics
Lattice Boltzmann Method



- 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

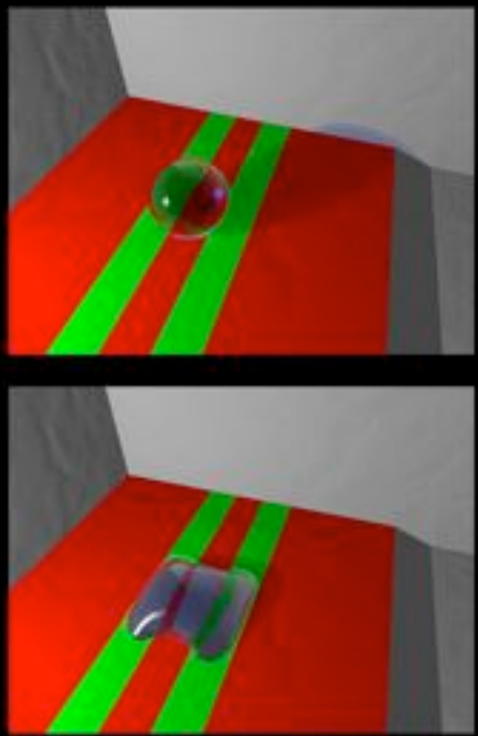
Best Paper Award for Stefan Donath (LSS Erlangen) at ParCFD, May 2009 (Moffett Field, USA)

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

Computational Fluid Dynamics
Wetting Effects/Contact Angles

Department of Computer Science
Chair for System Simulation
University of Erlangen-Nürnberg

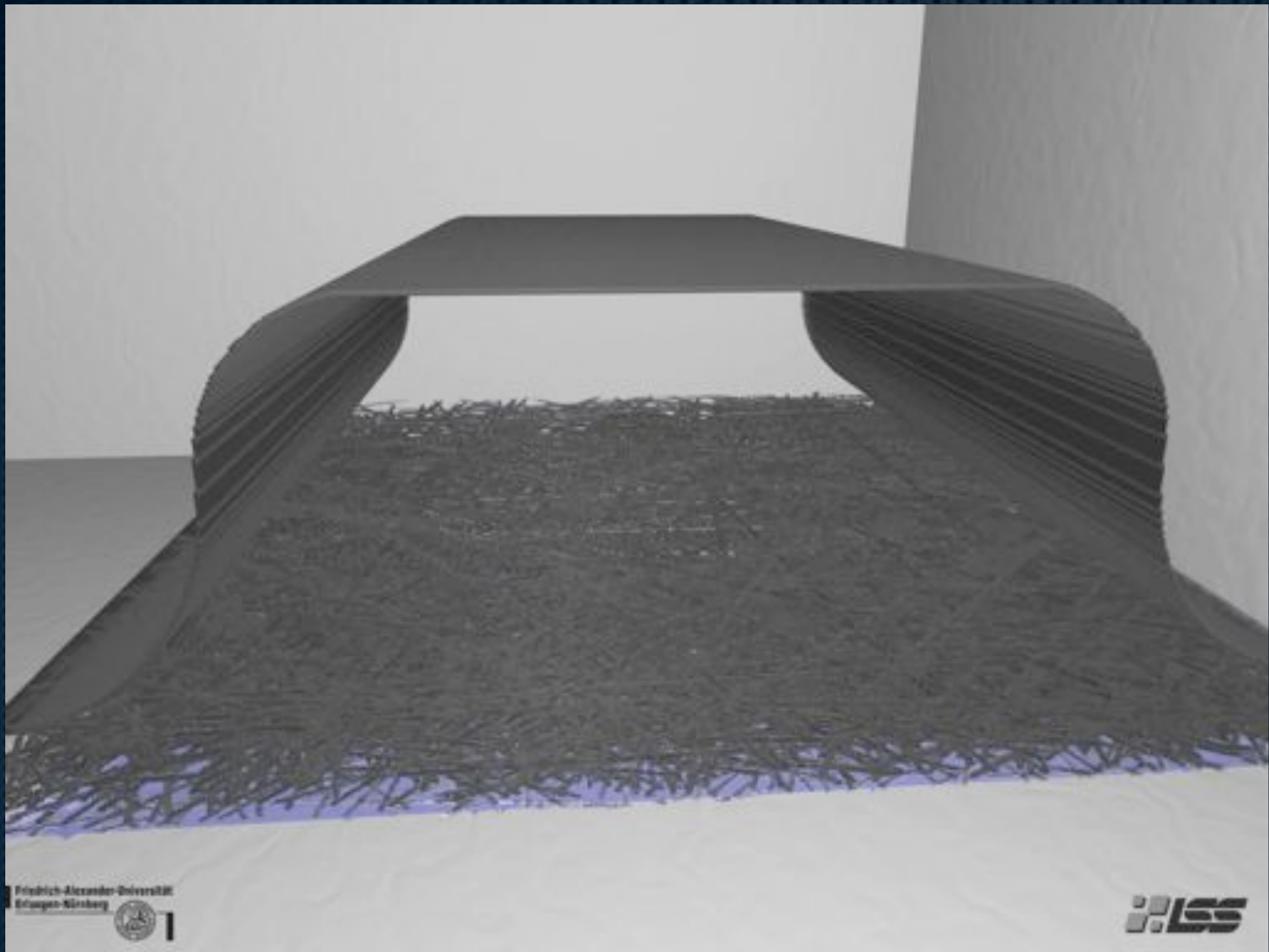


Stefan Donath and Ulrich Rüde

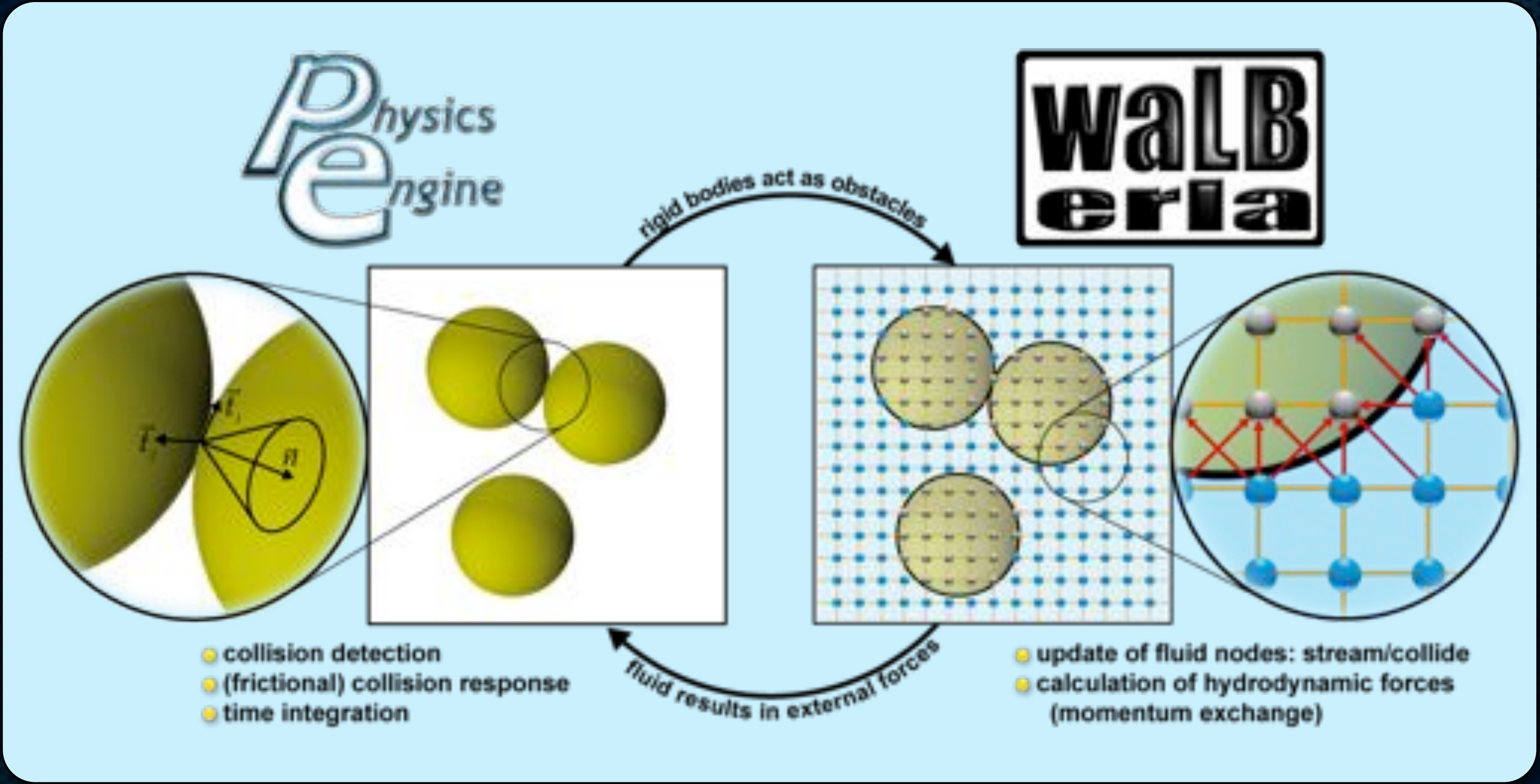
Microdrops on hydrophobic surface between two hydrophilic stripes

December 2010

Computational Fluid Dynamics for Fuel Cells
Water Transport through Hydrophobic Fibers

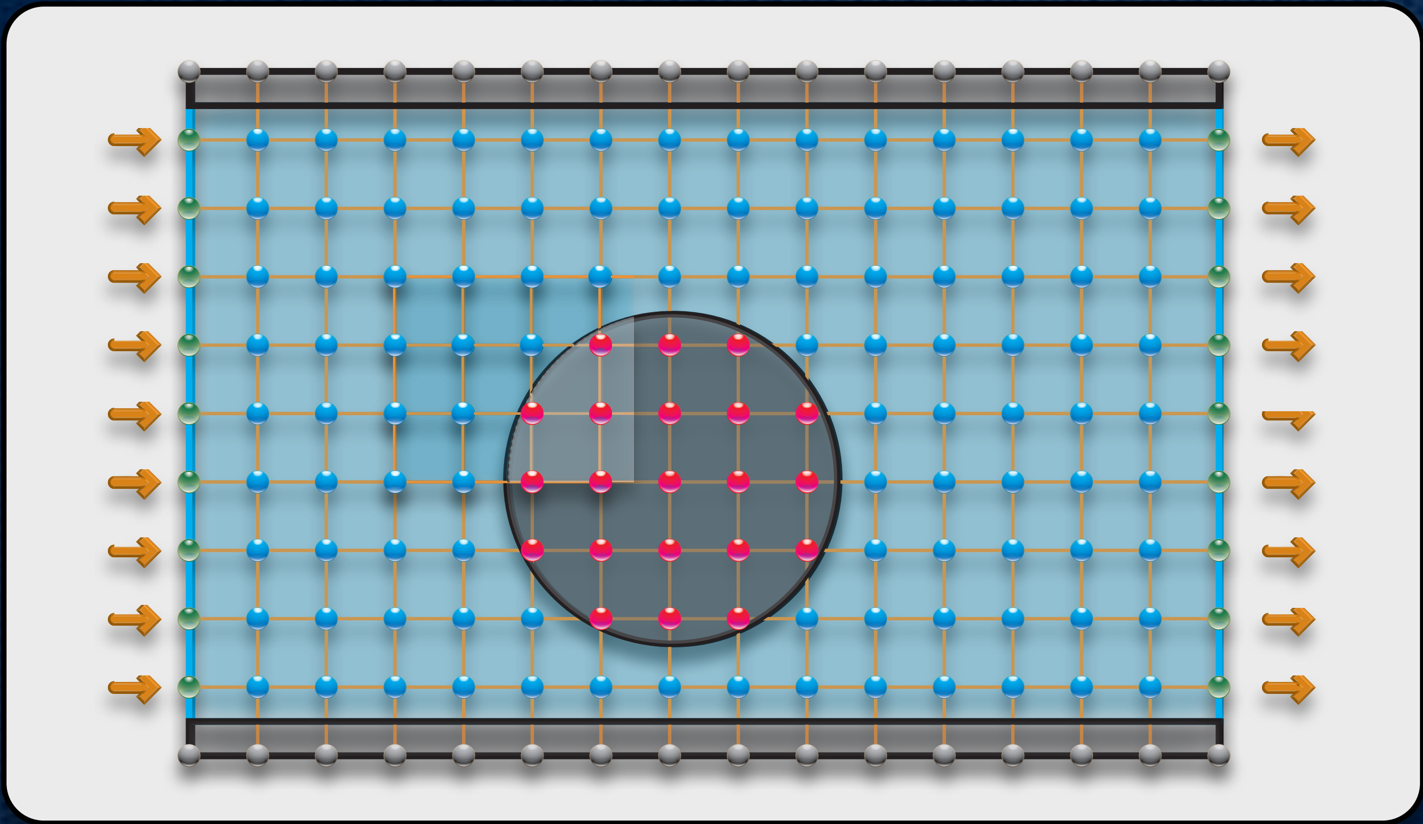


Fluid-Structure Interaction for particle ladden flows



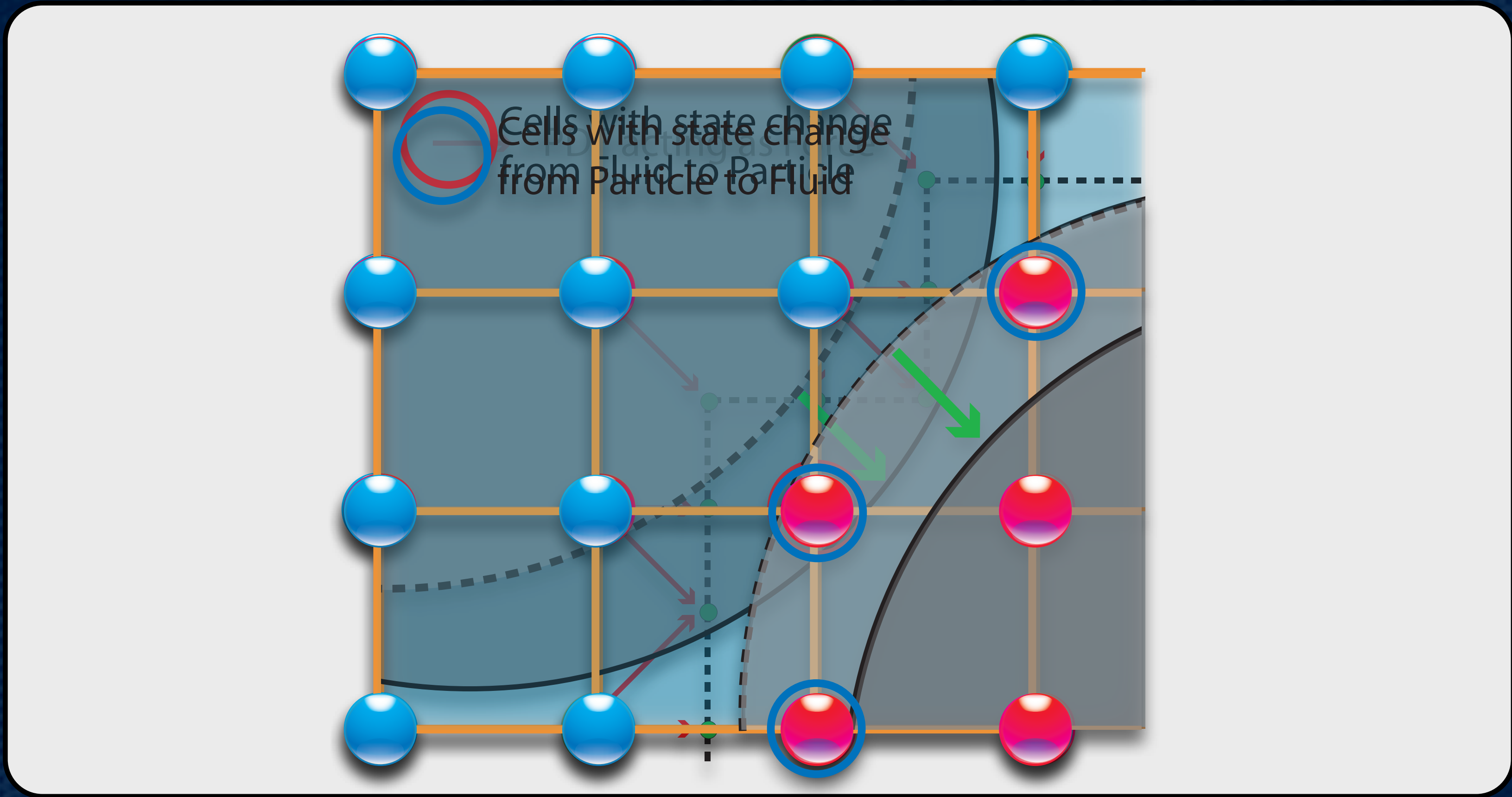
Mapping Moving Obstacles into the LBM Fluid Grid

An Example



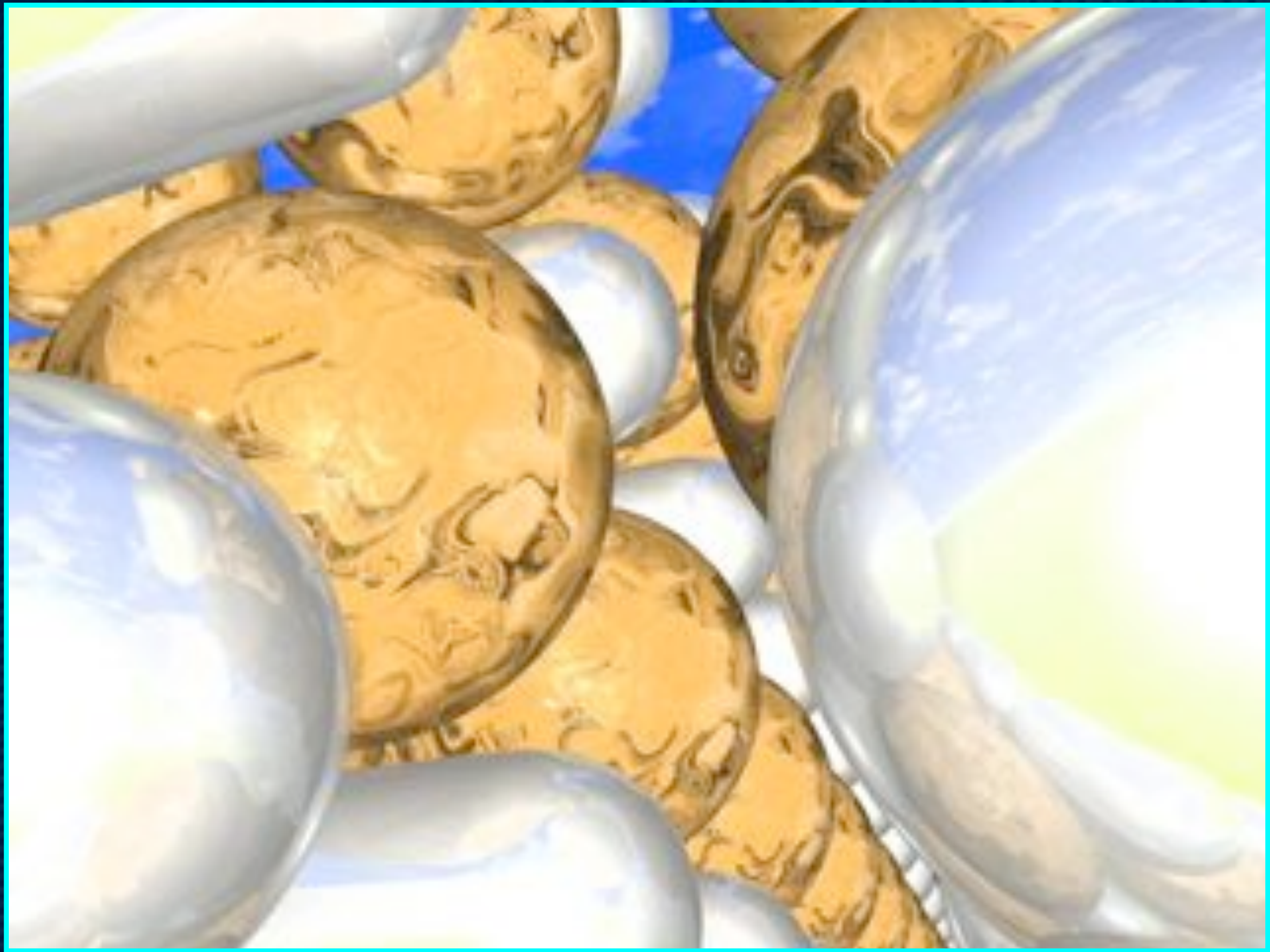
Mapping Moving Obstacles into the LBM Fluid Grid

An Example (2)



Cell change from fluid to particle

Virtual Fluidized Bed



512 processors

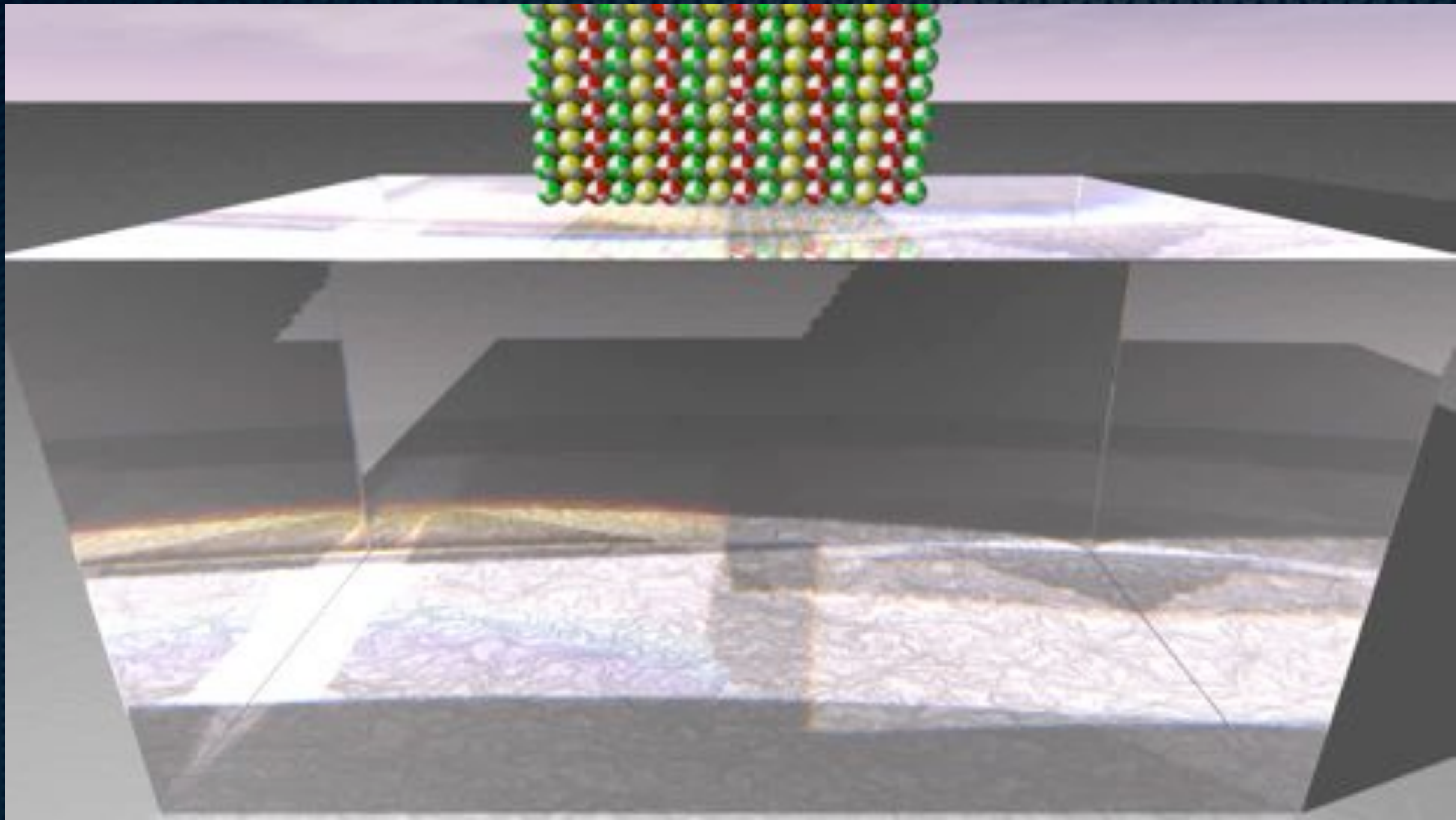
Simulation Domain Size: 180x198x360 cells of LBM

900 capsules and 1008 spheres
= 1908 objects

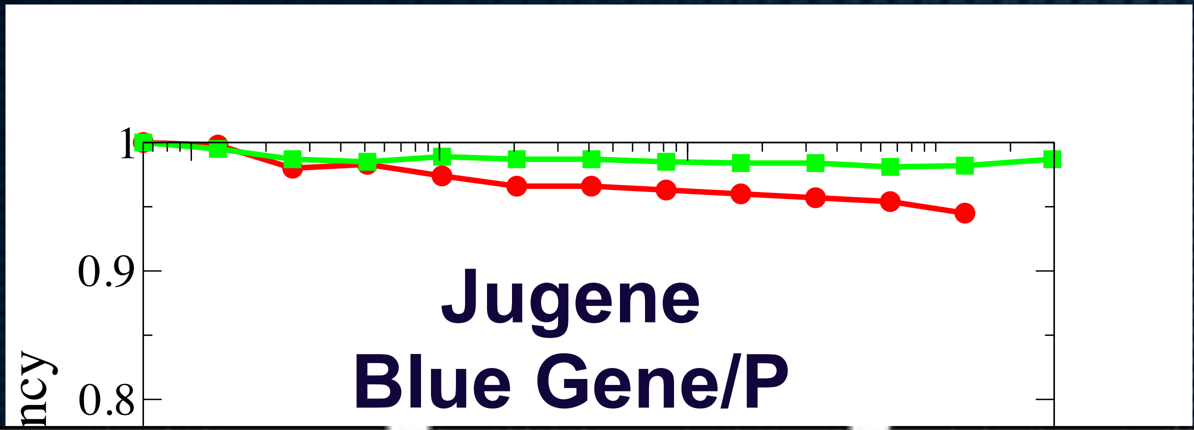
Number time steps:
252,000

Run Time:
07h 12 min

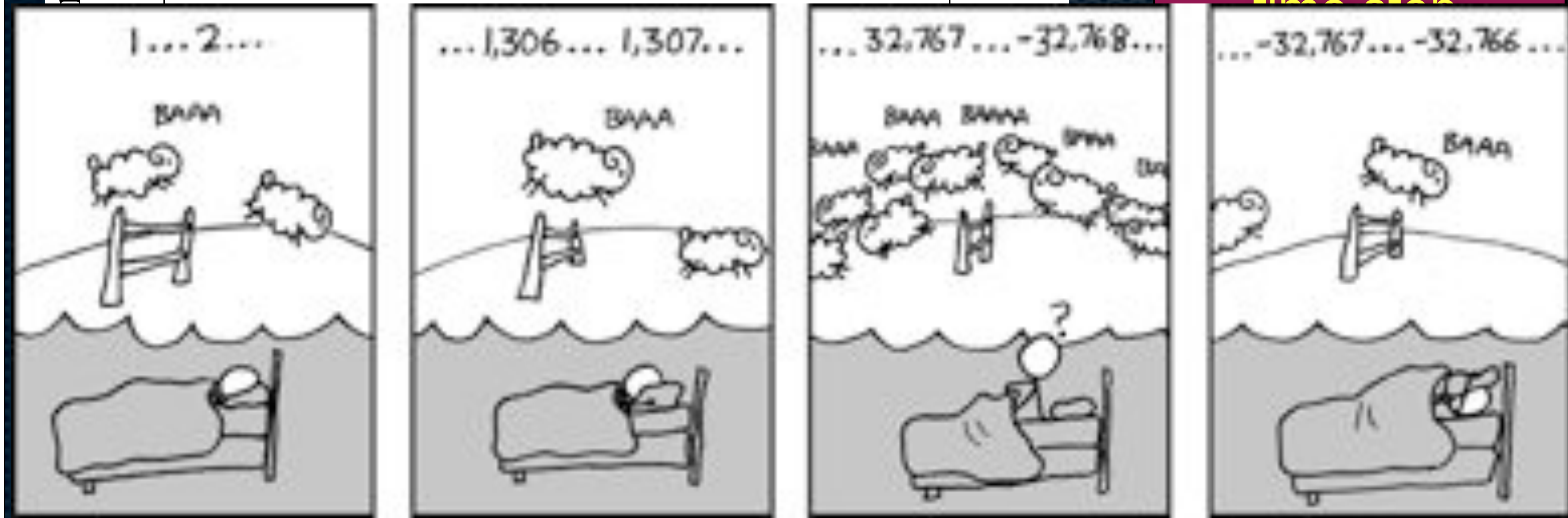
Fluid-Structure Interaction with Free Surface and Moving Objects



Weak Scaling



Largest simulation to date :
8 Trillion (10^{12}) variables per time step

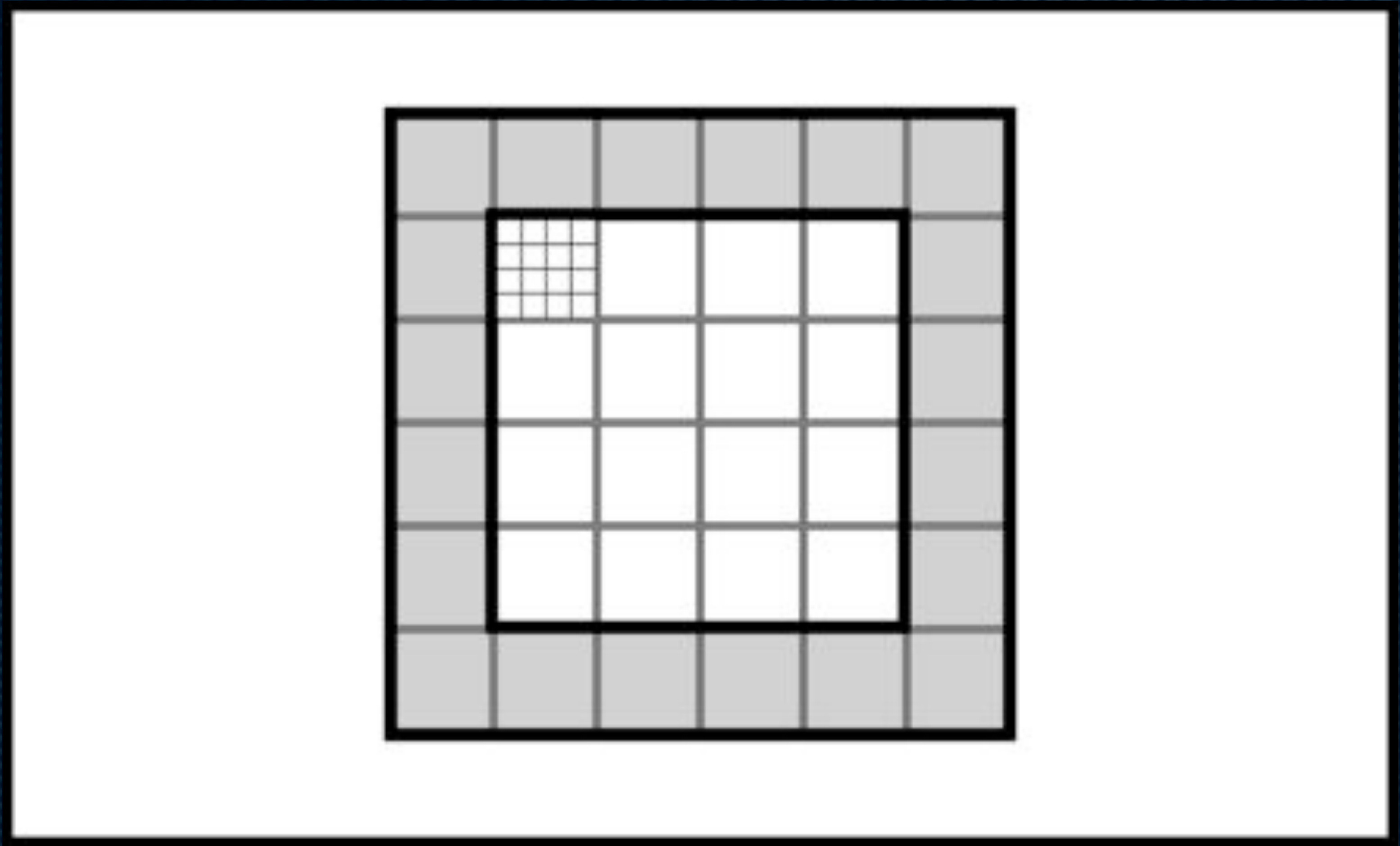


- Densely packed particles
- 264 331 905 rigid spherical objects

Performance Engineering

LBM on Clusters with GPUs

Domain Partitioning and Parallelization



Pure LBM Performance on Tsubame 2

- MLUPS: Mega Lattice Updates per Seconds
- Pure LBM performance is limited by bandwidth
- Implementation in CUDA
- Scenario: Lid Driven Cavity

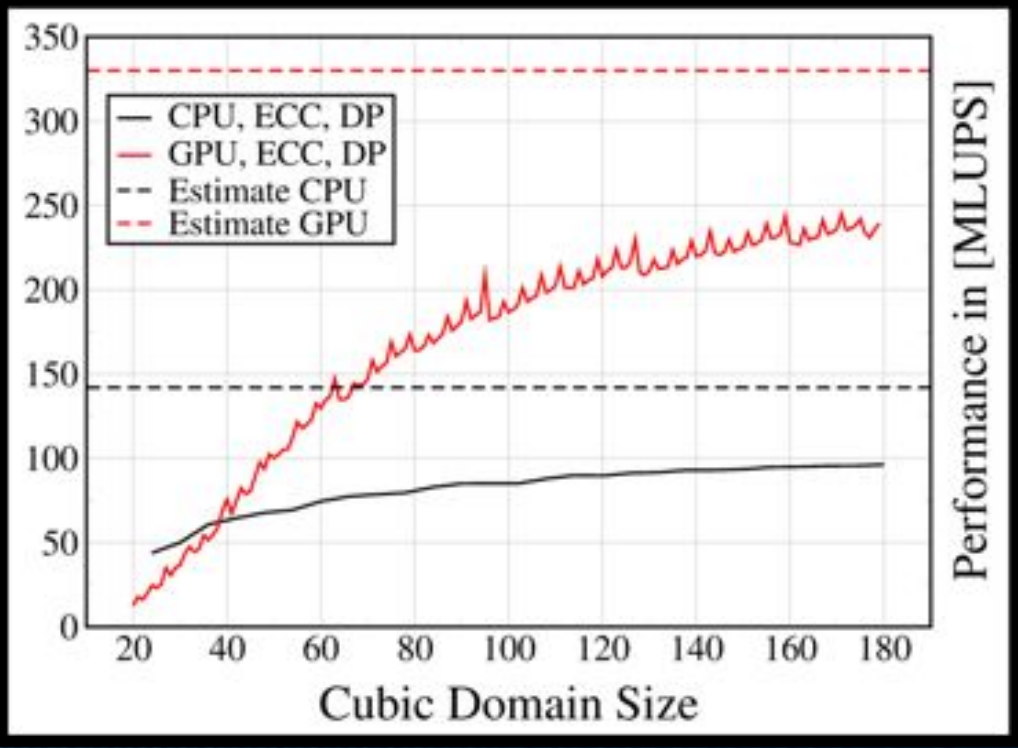
	NVIDIA Tesla M2050	Xeon X5670 „Westmere“	Factor
		2 sockets 12 cores	
Flops [TFlop/s]	1.0 / 0.5	0.25/0.13	x 4
Theoretical Peak Bandwidth [GB/s]	148	64	x 2-3
Stream Copy Bandwidth [GB/s]	100(+ECC)/ 115(-ECC)	43	x 2-3

Tsubame 2

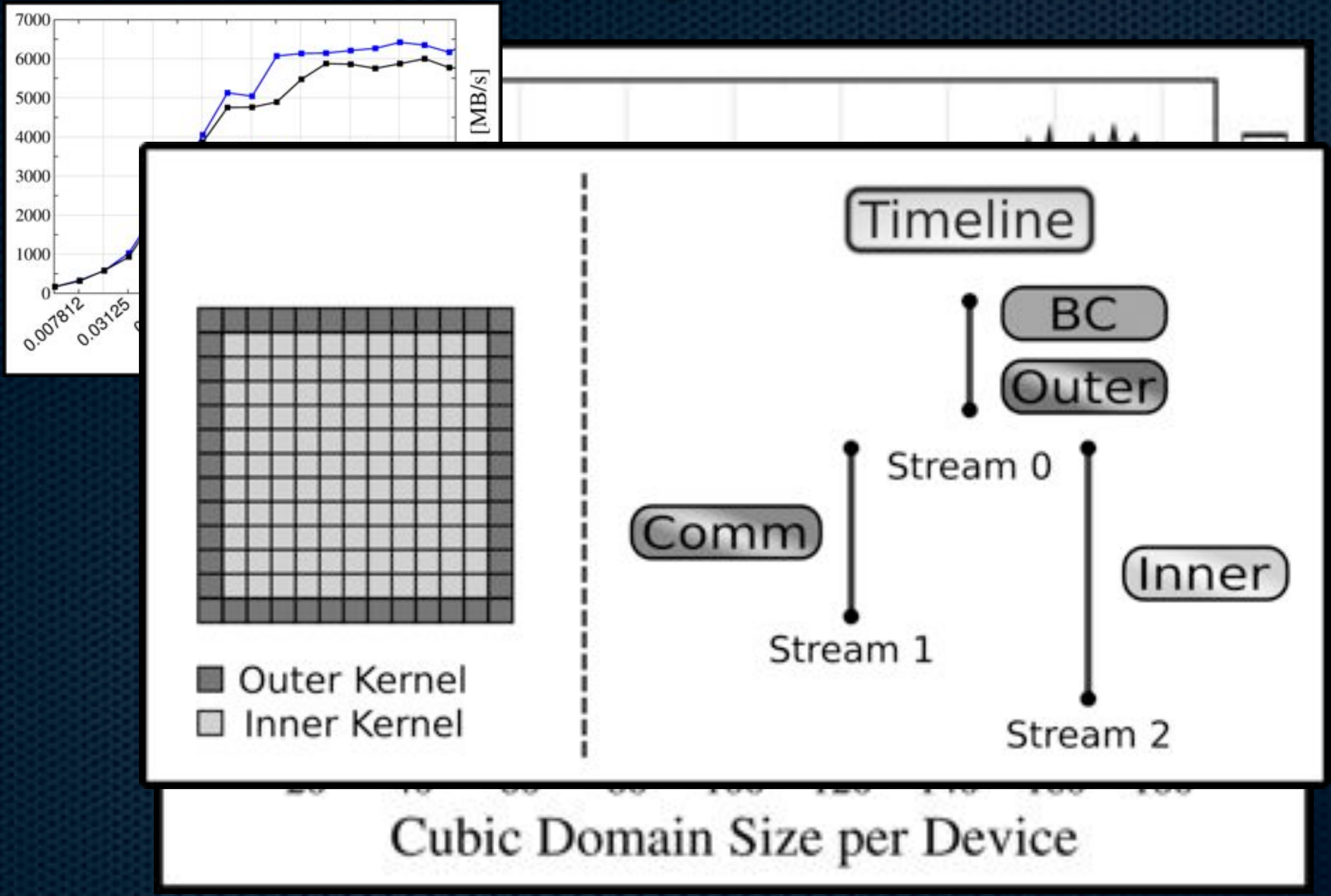
- 1408 compute nodes equipped with GPUs
- 3 NVIDIA Tesla M2050 per node
- Peak performance:
  - 2.2 PFlop/s
  - 633 TB/s memory bandwidth
- Total performance: 2.4 PFlops/s
- 14^{th} in the TOP500 list
- Located at Tokyo Institute of Technology, Japan
- Collaboration with Prof. Takayuki Aoki

Single GPU and CPU Node Performance

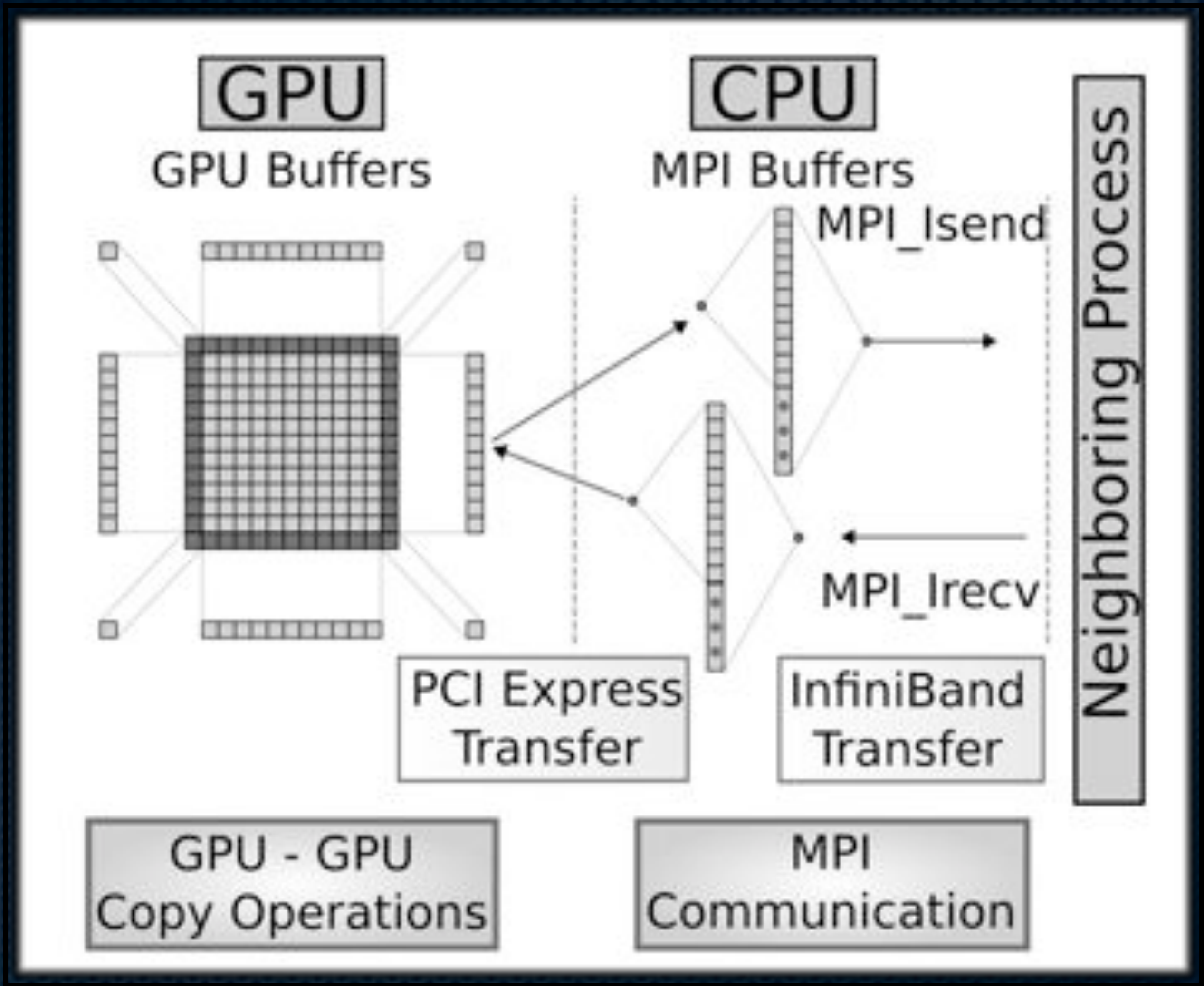
- Performance estimates based in Stream bandwidth:
  - CPU: 142 MLUPS (ECC, DP, -BC)
  - GPU: 330 MLUPS (ECC, DP, -BC)
- Resulting performance 75 % of estimate (+BC)
- CPU Kernel:
  - SSE Intrinsics
  - Non-temporal stores
  - Padding
- GPU Kernel:
  - Register usage optimized
  - Memory layout: SoA
  - Padding
- Kernels implemented by Johannes Habich



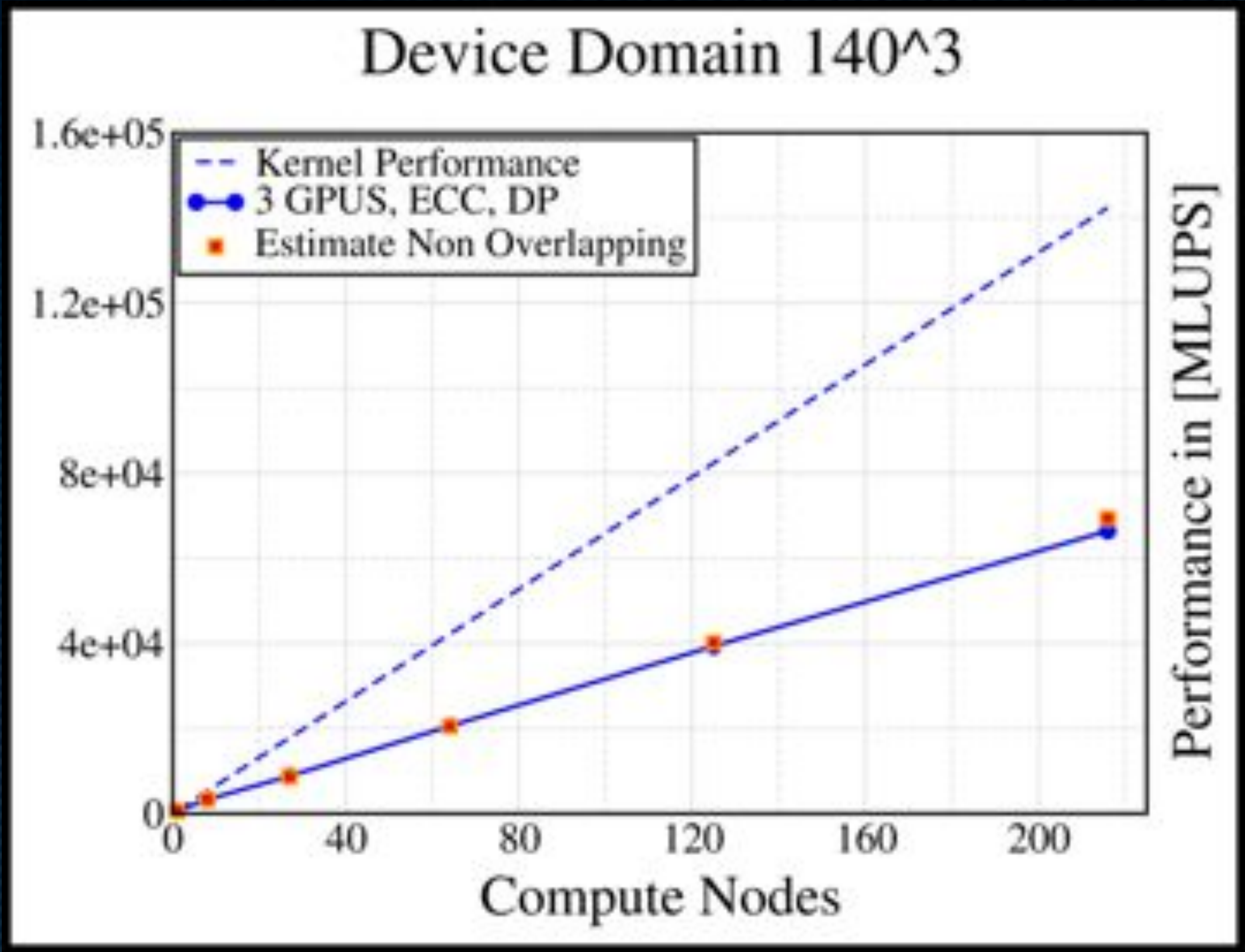
Single Node (3 GPU) Performance
Overlapping Communication



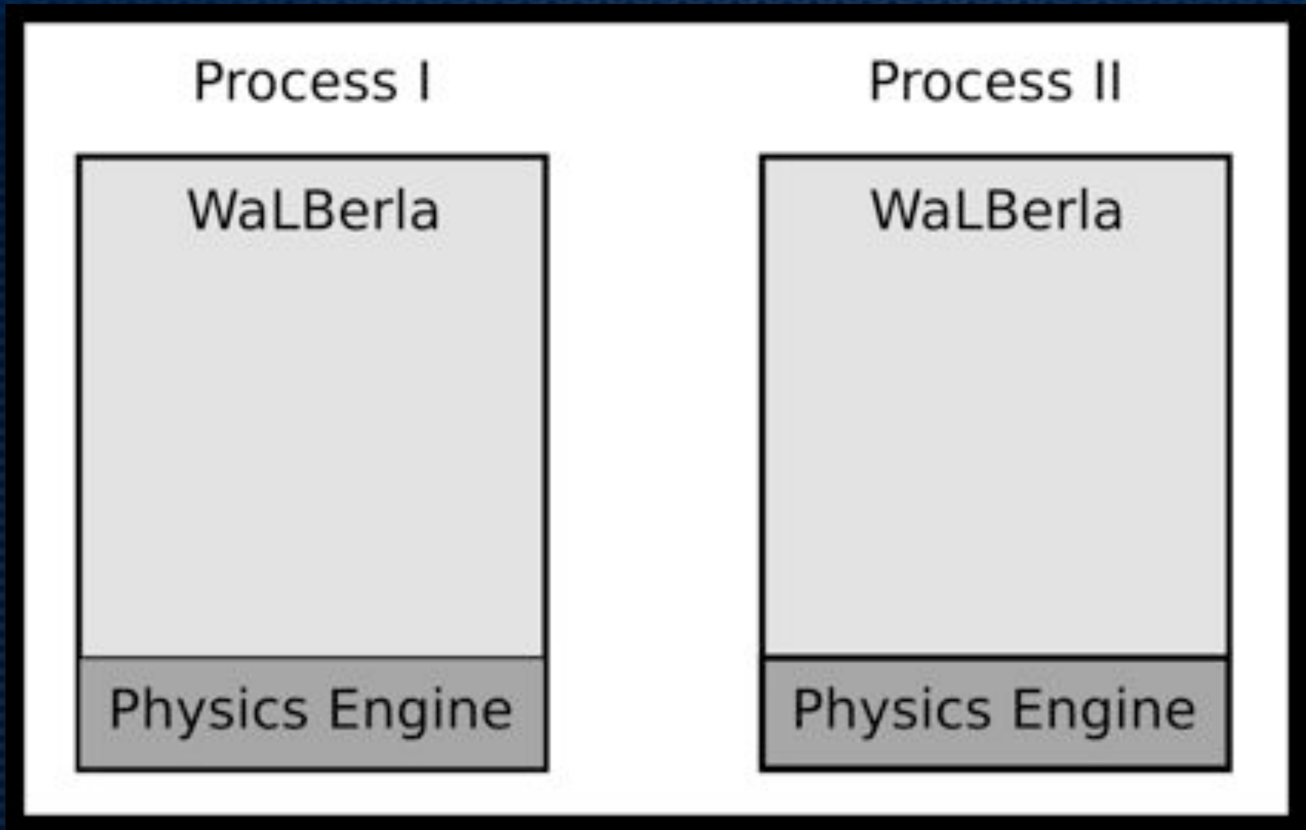
Weak Scaling Performance



Weak Scaling Performance

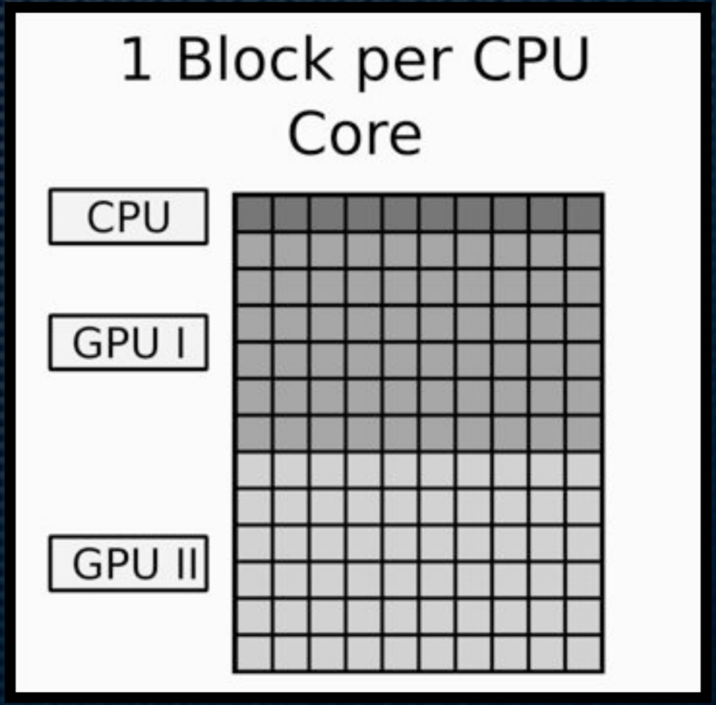



Time Loop
Rigid Body Mapping
Fluid Flow Computation
Communication
Force Calculation
Rigid Body Dynamics
Communication


Process I
Process II
WaLBerla
Physics Engine
WaLBerla
Physics Engine

Heterogeneous (GPU+CPU) LBM

- Requirements:
  - Different data structures
  - Different kernels
  - Common communication interface
  - Load balancing
  - Node Setup:
    - 1 MPI Process per Core
    - 1 MPI Process per Socket
    - 1 MPI Process per Node



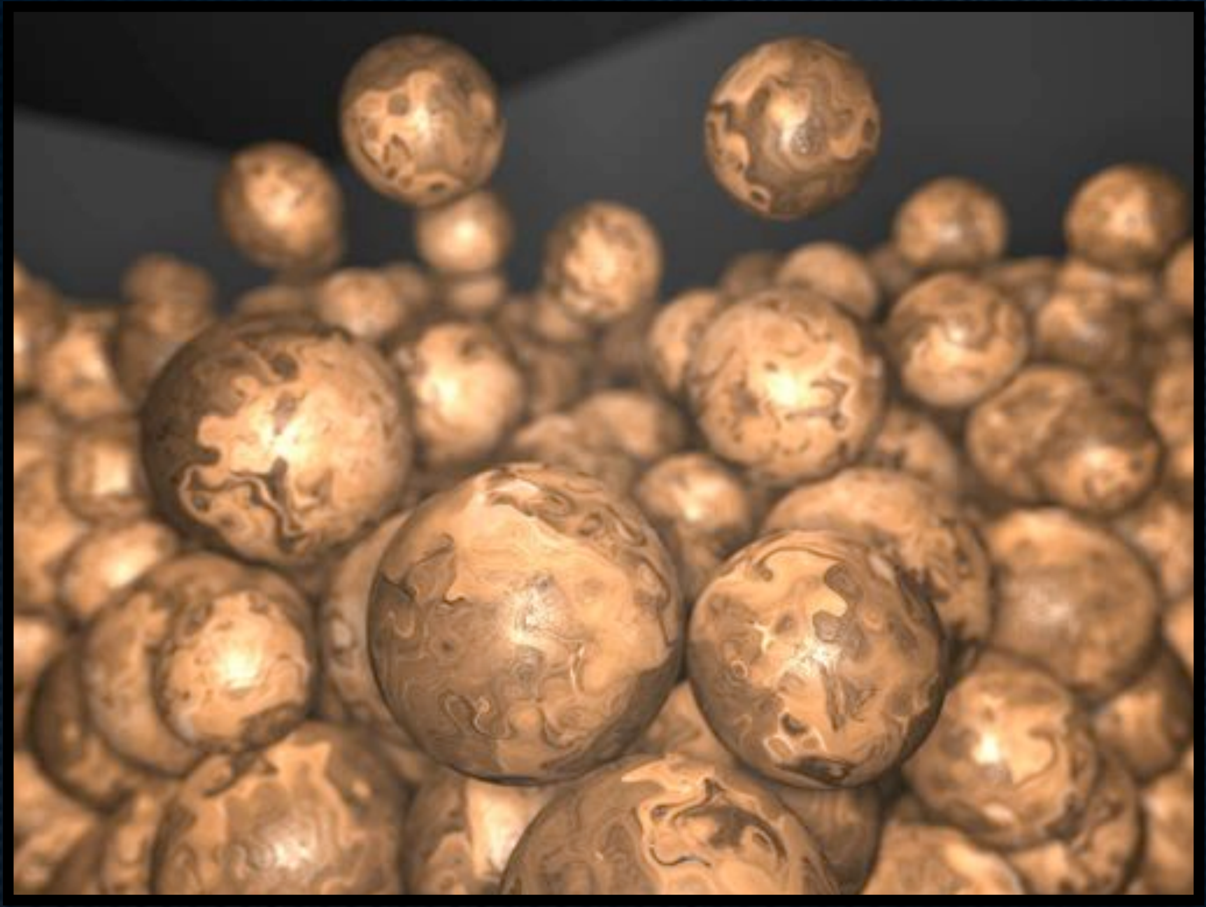
CPU vs GPU: LBM Implementation Effort

- Subjective evaluation
- Valid for the pure LBM implementation
- Partly for stencil based methods

Difficulty	CPU	GPU
Kernel	✶✶	✶ / ✶✶✶
Intra Node	✶	✶✶
Inter Node	✶✶	✶✶✶

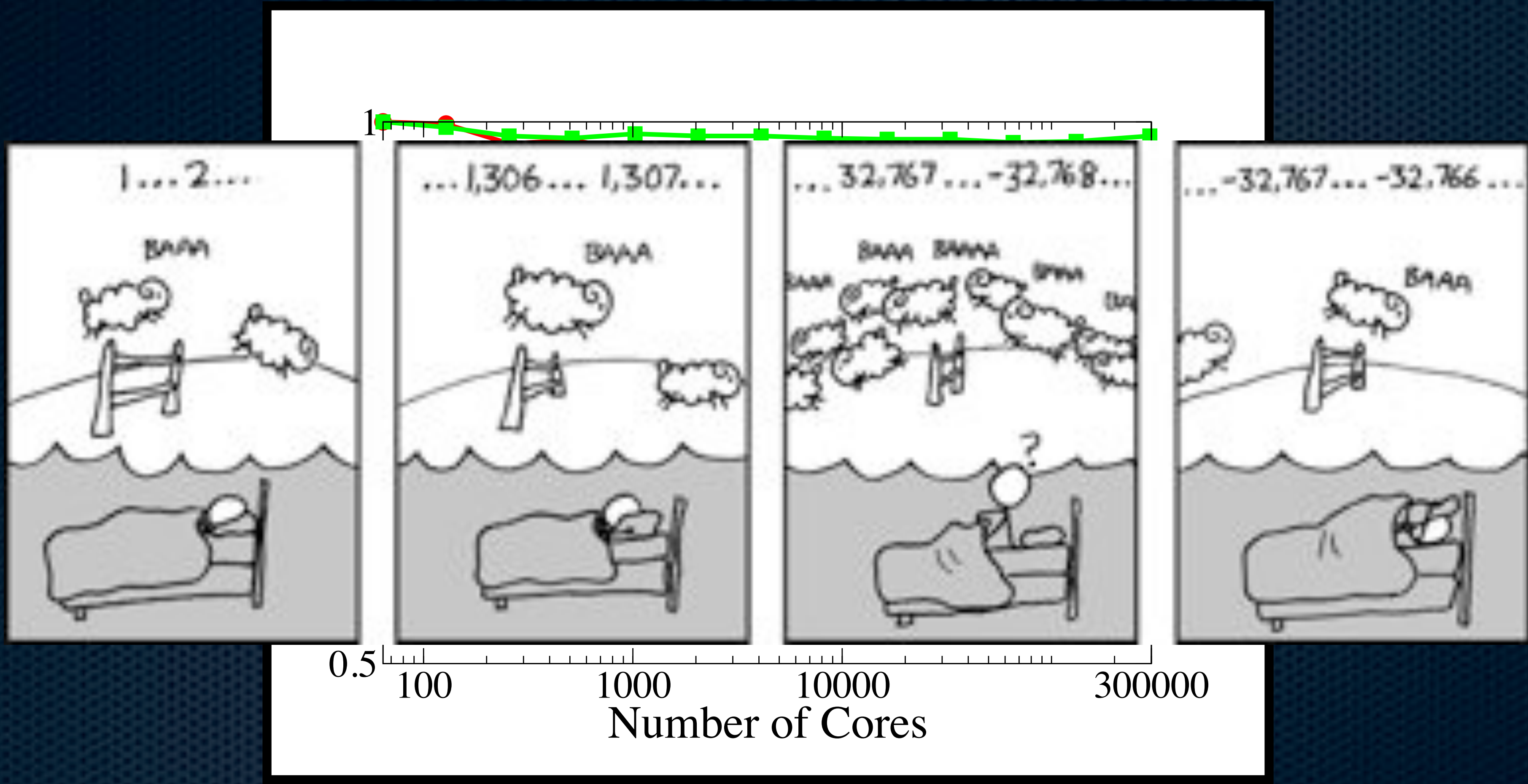
Fluidization

Heterogenous CPU-GPU Simulation



Particles: 31250 Domain: 400x400x200 Timesteps: 400 000
Devices: 2 x M2070 + 1 Intel „Westmere“ Runtime: 17.5 h

Fluidization: Weak Scaling on CPUs



- Scaling 64 to 294 912 cores
- Densely packed particles
- 1.5e[11] lattice cells
- 2.6e[8] rigid spherical objects

Conclusions

Simulations with Fluid Control

The ~~Two~~ Three 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, LTM, LSTM, LGDV, RRZE, LME, Neurozentrum, Radiologie, Applied Mathematics, Theoretical Physics, etc. Especially for foams: C. Körner (WTM) & A. Delgado (LSTM)
  - International: Utah, Technion, Constanta, Ghent, Boulder, München, CAS, Zürich, Delhi, Tokyo, ...
- Dissertationen Projects
  - N. Thürey, T. Pohl, S. Donath, S. Bogner, C. Godenschwager (LBM, free surfaces, 2-and 3-phase flows)
  - M. Mohr, B. Bergen, U. Fabricius, H. Köstler, C. Freundl, T. Gradl, B. Gmeiner (Massively parallel PDE-solvers)
  - M. Kowarschik, J. Treibig, M. Stürmer, J. Habich (architecture aware algorithms)
  - K. Iglberger, T. Preclik, K. Pickel (rigid body dynamics)
  - J. Götz, C. Feichtinger, F. Schornbaum (Massively parallel LBM software, suspensions)
  - C. Mihoubi, D. Bartuschat (Complex geometries, parallel LBM)
- (Long Term) Guests in summer/fall 2009-12:
  - Dr. S. Ganguly, Prof. S. Chakraborty, IIT Kharagpur (Humboldt) - Electro-osmotic 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. Steve Roberts, Prof. Linda Stals, Australian National University
  - Prof.s Hanke, Oppelstrup, Edsberg, Gustavsson KTH Stockholm (DAAD), Mathematical Modelling
- >35 Diplom- /Master- Thesis, ~35 Bachelor Thesis
- Funding by KONWIHR, DAAD, DFG, BMBF, EU, Elitenetzwerk Bayern

Thank you for your attention!

Slides, reports, thesis, animations available for download at:

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