Lattice Boltzmann Methods on the way to exascale

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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**
     2.8×10^{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

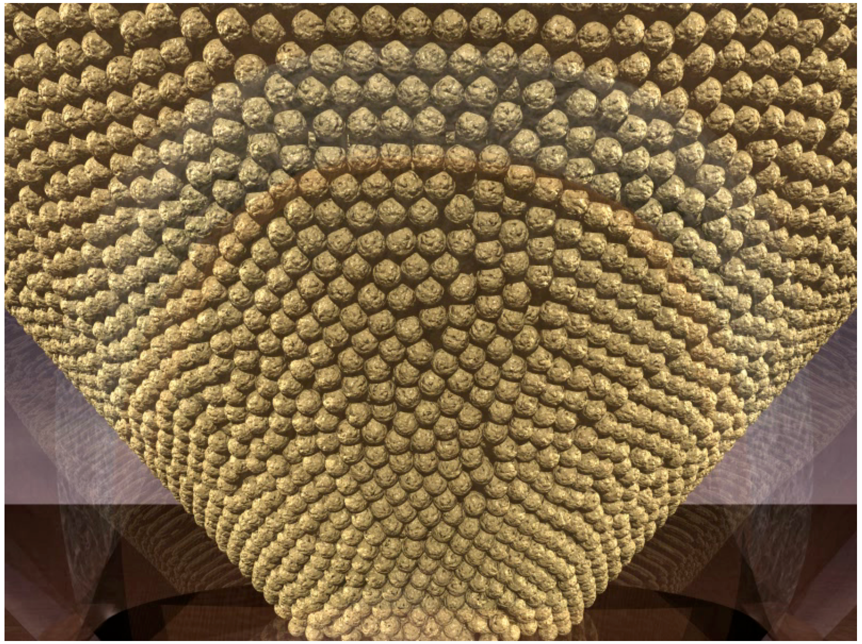
- Intel Xeon architecture
- 147,456 cores
- 16 cores (2.7 GHz) per node
- 32 GiB RAM per node
- Pruned tree interconnect
- 3.2 PFlops Peak
- TOP 500: #27

Building block I:

The Lagrangian View:

Granular media simulations

with the physics engine



1 250 000 spherical particles
256 processors
300 300 time steps
runtime: 48 h (including data output)
texture mapping, ray tracing

Pöschel, T., & Schwager, T. (2005). *Computational granular dynamics: models and algorithms*. Springer Science & Business Media.

Nonlinear Complementarity and Time Stepping

			Non-penetration conditions	Coulomb friction conditions
continuous	forces		$\xi \geq 0 \perp \lambda_n \geq 0$	$\|\boldsymbol{\lambda}_{to}\|_2 \leq \mu \lambda_n$
		$\xi = 0$	$\dot{\xi}^+ \geq 0 \perp \lambda_n \geq 0$	$\|\boldsymbol{\delta v}^+_{to}\|_2 \boldsymbol{\lambda}_{to} = -\mu \lambda_n \boldsymbol{\delta v}^+_{to}$
		$\dot{\xi}^+ = 0$	$\ddot{\xi}^+ \geq 0 \perp \lambda_n \geq 0$	($\|\boldsymbol{\delta v}^+_{to}\|_2 = 0$) $\|\dot{\boldsymbol{\delta v}}^+_{to}\|_2 \boldsymbol{\lambda}_{to} = -\mu \lambda_n \dot{\boldsymbol{\delta v}}^+_{to}$
	impulses		$\xi \geq 0 \perp \Lambda_n \geq 0$	$\|\boldsymbol{\Lambda}_{to}\|_2 \leq \mu \Lambda_n$
		$\xi = 0$	$\dot{\xi}^+ \geq 0 \perp \Lambda_n \geq 0$	$\|\boldsymbol{\delta v}^+_{to}\|_2 \boldsymbol{\Lambda}_{to} = -\mu \Lambda_n \boldsymbol{\delta v}^+_{to}$
discrete			$\frac{\xi}{\delta t} + \delta v'_n(\boldsymbol{\lambda}) \geq 0 \perp \lambda_n \geq 0$	$\|\boldsymbol{\lambda}_{to}\|_2 \leq \mu \lambda_n$ $\|\boldsymbol{\delta v}'_{to}(\boldsymbol{\lambda})\|_2 \boldsymbol{\lambda}_{to} = -\mu \lambda_n \boldsymbol{\delta v}'_{to}(\boldsymbol{\lambda})$

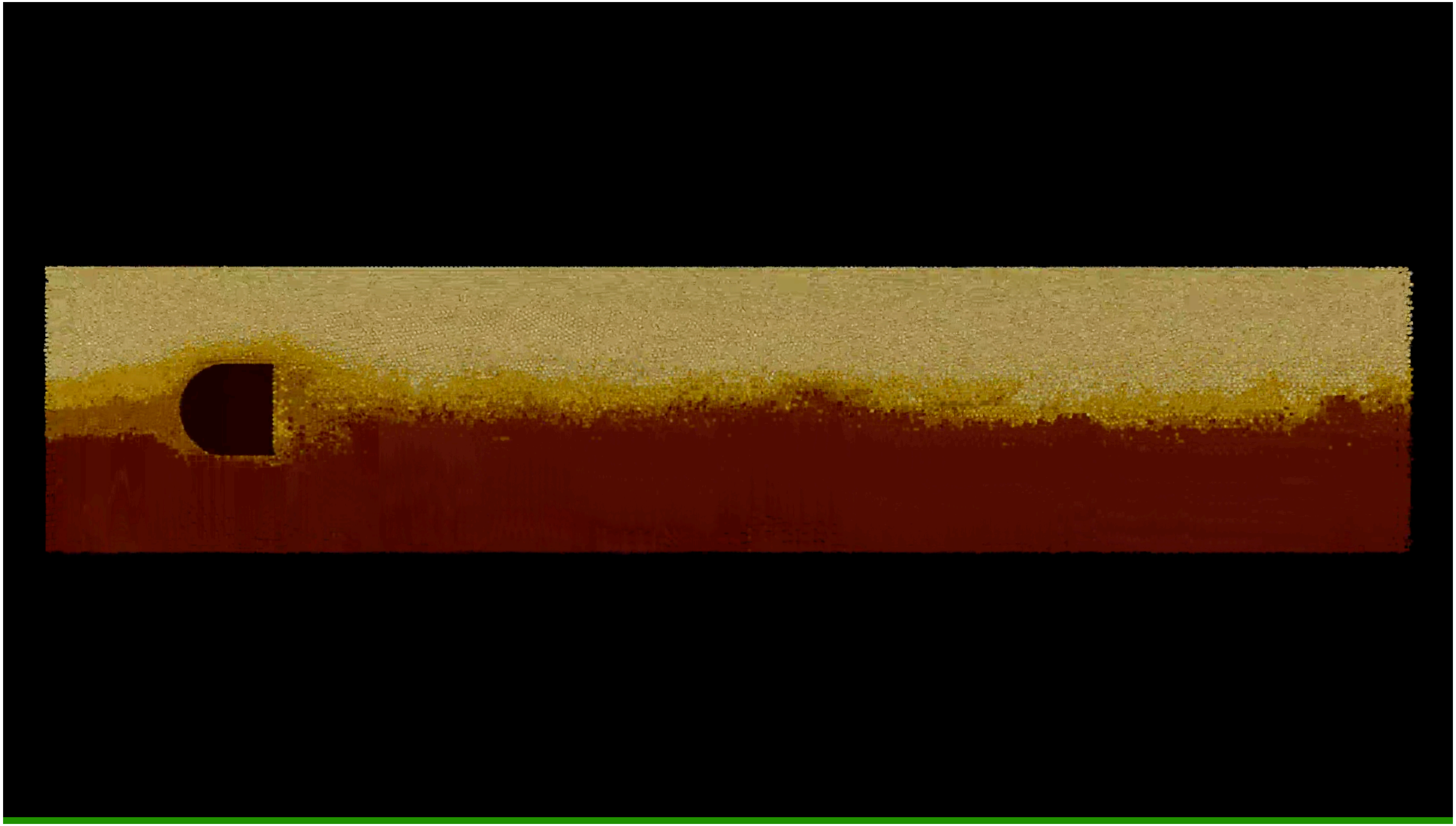
Signorini condition — impact law — friction cone condition — frictional reaction opposes slip

Moreau, J., Panagiotopoulos P. (1988): Nonsmooth mechanics and applications, vol 302. Springer, Wien-New York

Popa, C., Preclik, T., & UR (2014). Regularized solution of LCP problems with application to rigid body dynamics. *Numerical Algorithms*, 1-12.

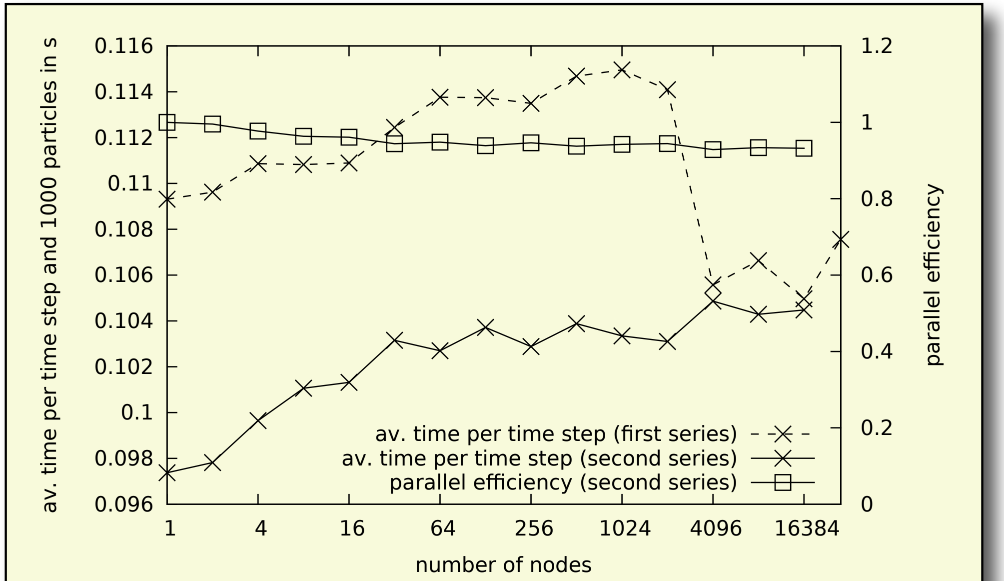
Preclik, T. & UR (2015). Ultrascale simulations of non-smooth granular dynamics; Computational Particle Mechanics, DOI: 10.1007/s40571-015-0047-6

Dense granular channel flow with crystallization



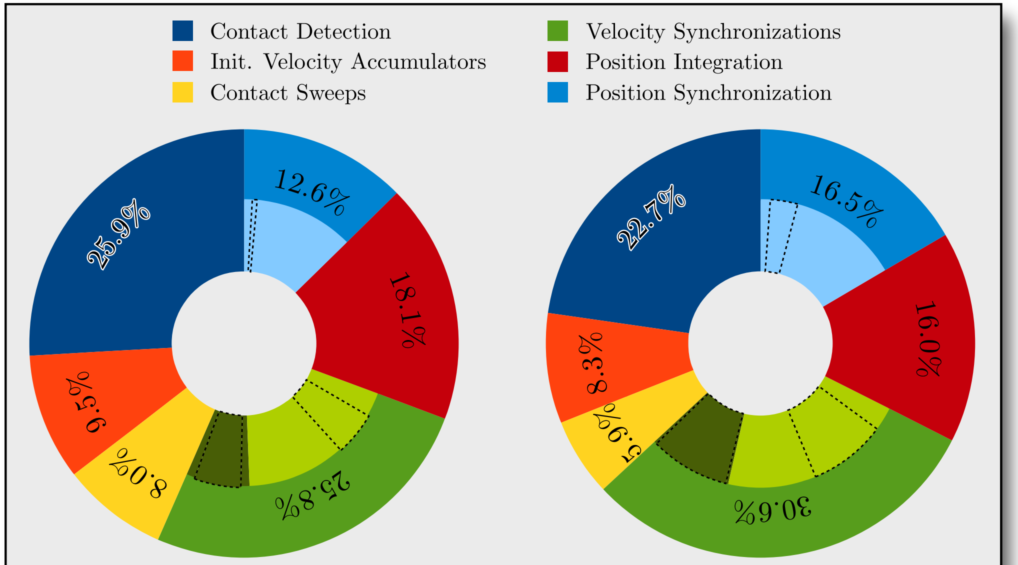
Scaling Results

- 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
  - **2.8×10^{10} non-spherical particles**
  - **1.1×10^{10} contacts**
- granular gas: scaling results



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

Breakup up of compute times on Erlangen RRZE Cluster Emmy

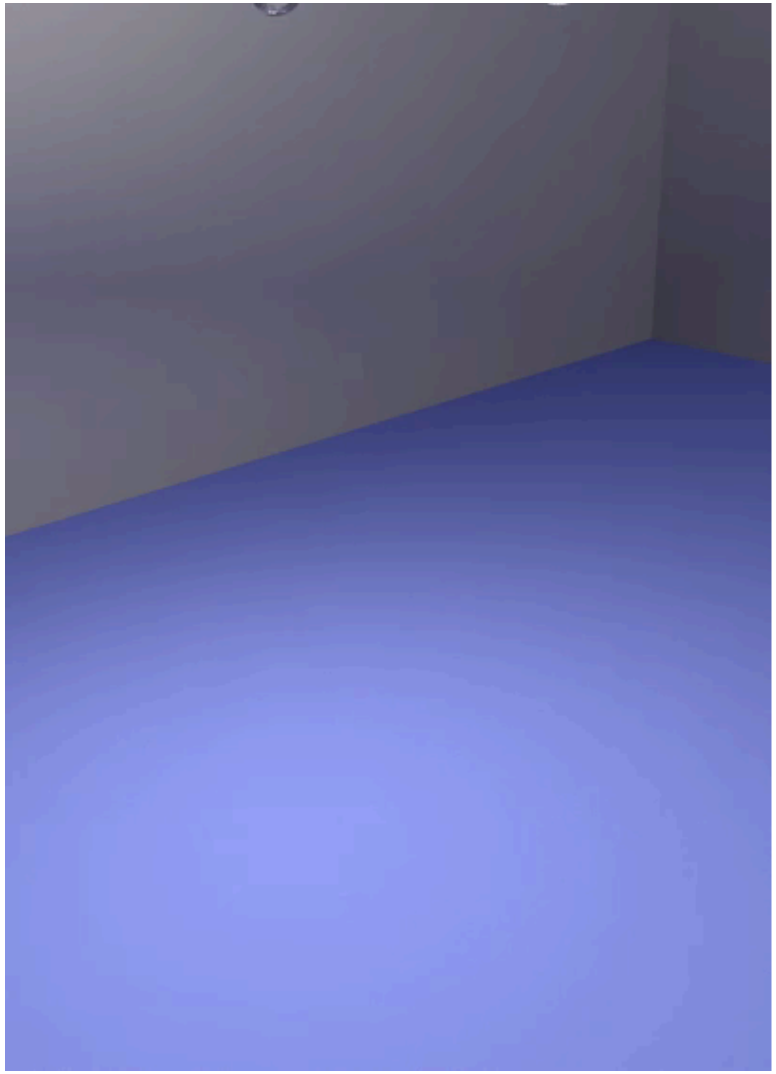


(a) Time-step profile of the granular gas executed with $5 \times 2 \times 2 = 20$ processes on a single node.

(b) Time-step profile of the granular gas executed with $8 \times 8 \times 5 = 320$ processes on 16 nodes.

Building Block III:

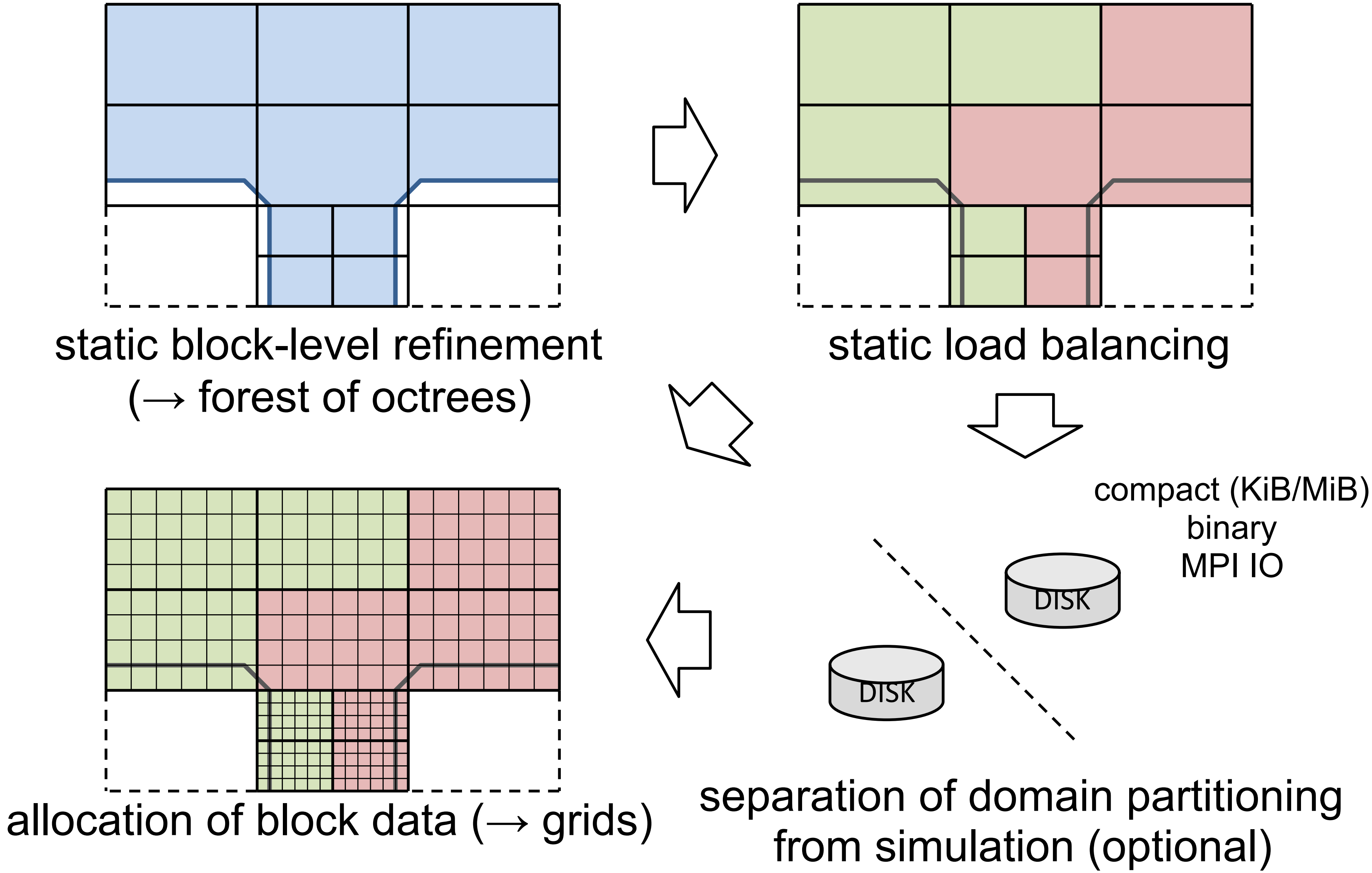
Scalable Flow Simulations with the Lattice Boltzmann Method



Succi, S. (2001). *The lattice Boltzmann equation: for fluid dynamics and beyond*. Oxford university press.

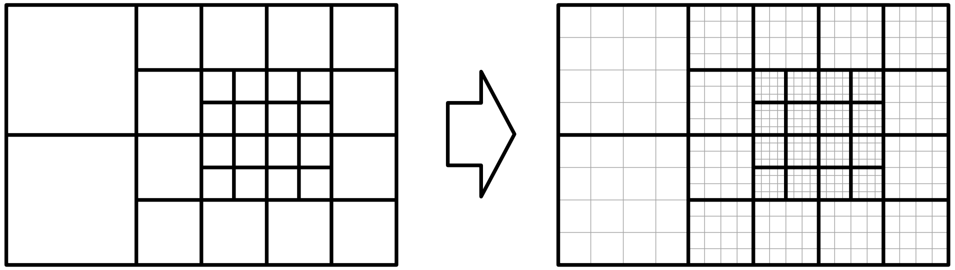
Feichtinger, C., Donath, S., Köstler, H., Götz, J., & Rüde, U. (2011). WaLBerla: HPC software design for computational engineering simulations. *Journal of Computational Science*, *2*(2), 105-112.

Partitioning and Parallelization

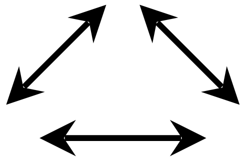


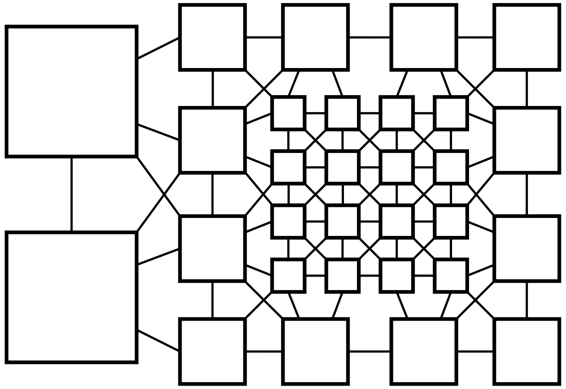
Parallel AMR load balancing

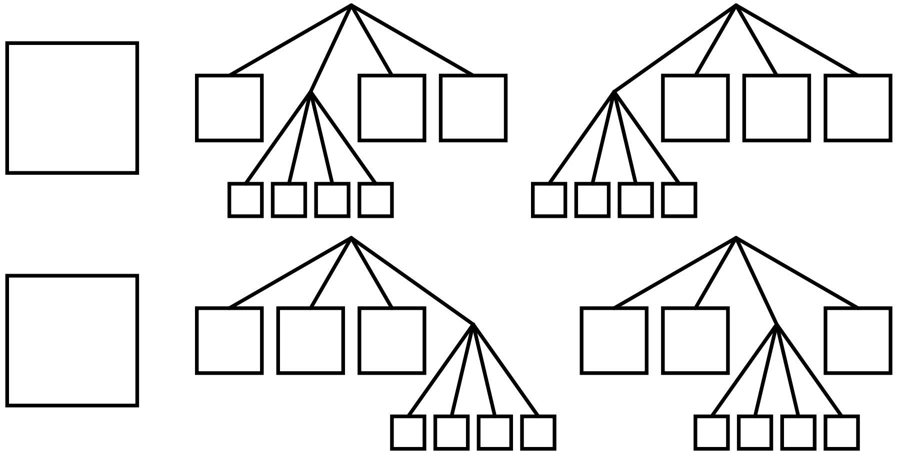
different views on
domain partitioning



2:1 balanced grid
(used for the LBM)



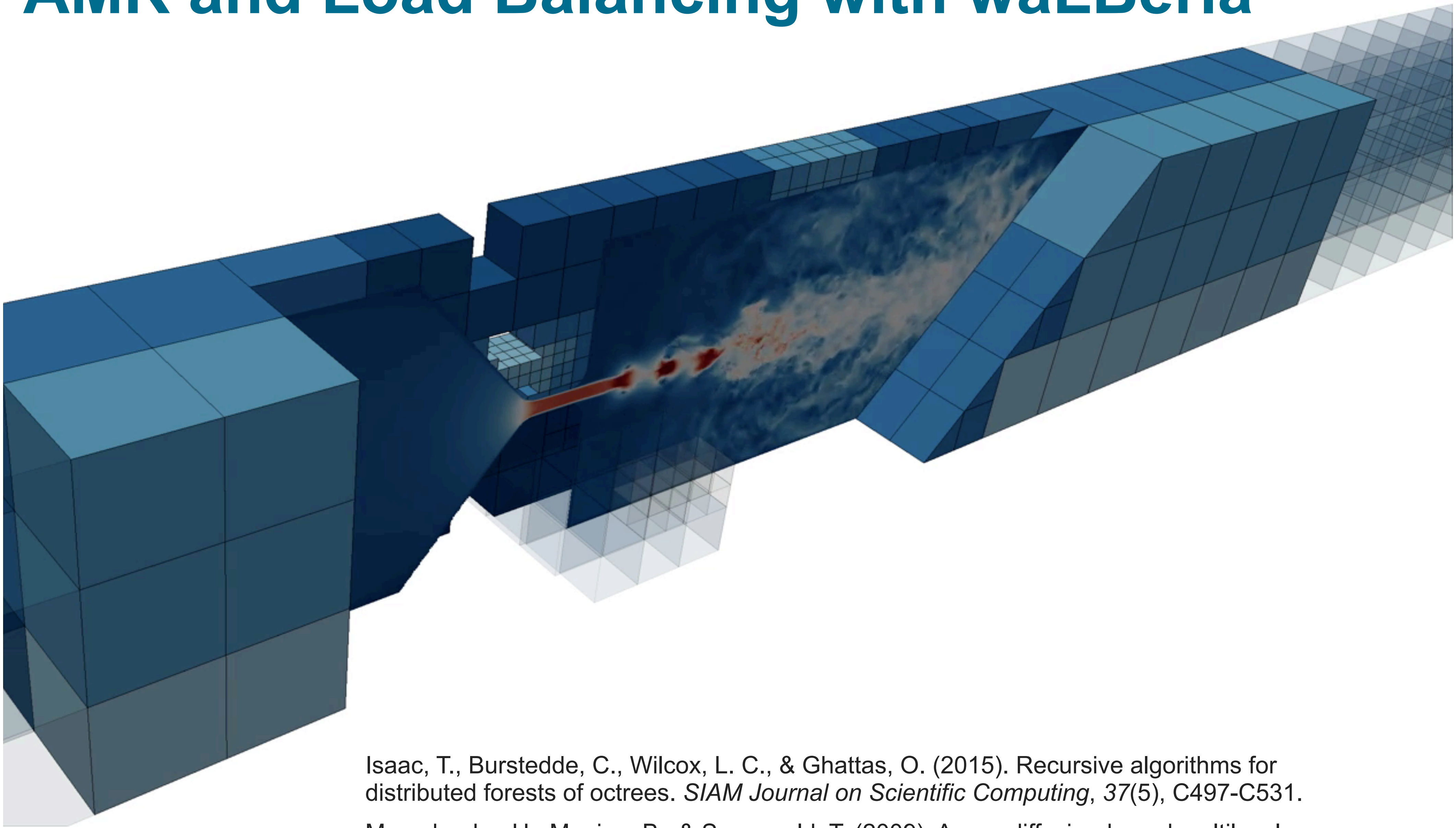




distributed graph:
nodes = blocks
edges explicitly stored as
<block ID, process rank> pairs

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

AMR and Load Balancing with waLBerla



Isaac, T., Burstedde, C., Wilcox, L. C., & Ghattas, O. (2015). Recursive algorithms for distributed forests of octrees. *SIAM Journal on Scientific Computing*, *37*(5), C497-C531.

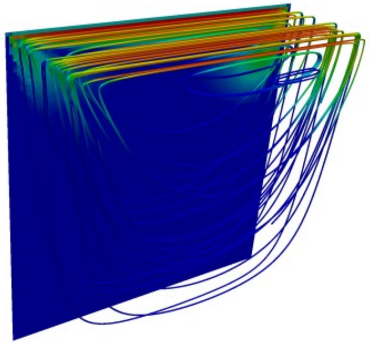
Meyerhenke, H., Monien, B., & Sauerwald, T. (2009). A new diffusion-based multilevel algorithm for computing graph partitions. *Journal of Parallel and Distributed Computing*, *69*(9), 750-761.

Schornbaum, F., & Rüde, U. (2016). Massively Parallel Algorithms for the Lattice Boltzmann Method on NonUniform Grids. *SIAM Journal on Scientific Computing*, *38*(2), C96-C126.

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):



avg. blocks/process (max. blocks/proc.)

level	initially	after refresh	after load balance
0	0.383 (1)	0.328 (1)	0.328 (1)
1	0.656 (1)	0.875 **(9)**	0.875 **(1)**
2	1.313 (2)	3.063 **(11)**	3.063 **(4)**
3	3.500 (4)	3.500 **(16)**	3.500 **(4)**

AMR Performance

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

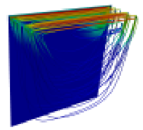
- Benchmark (LBM D3Q19 TRT):

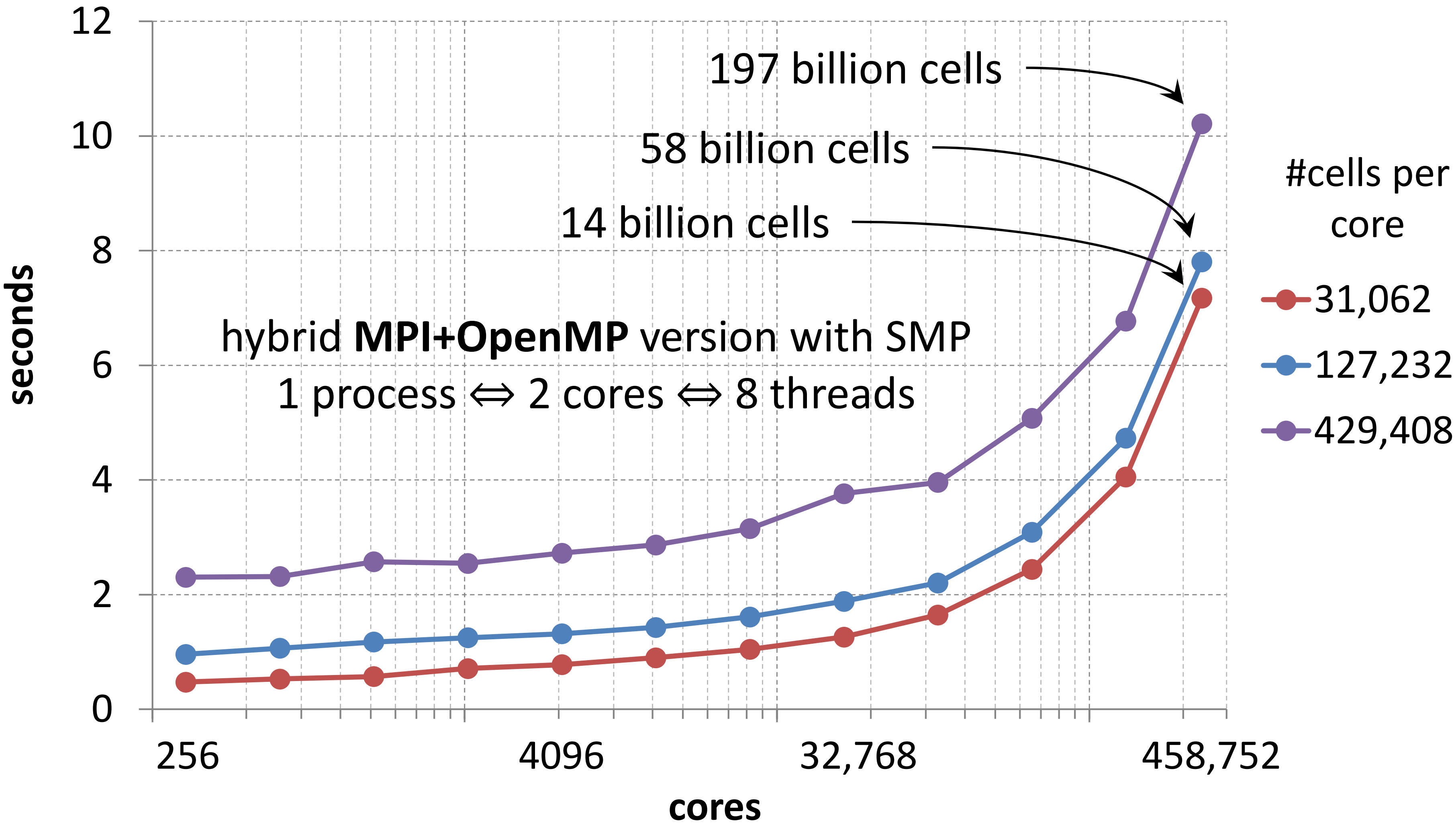
during this refresh process …

… 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

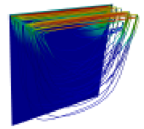
- JUQUEEN – space filling curve: Morton

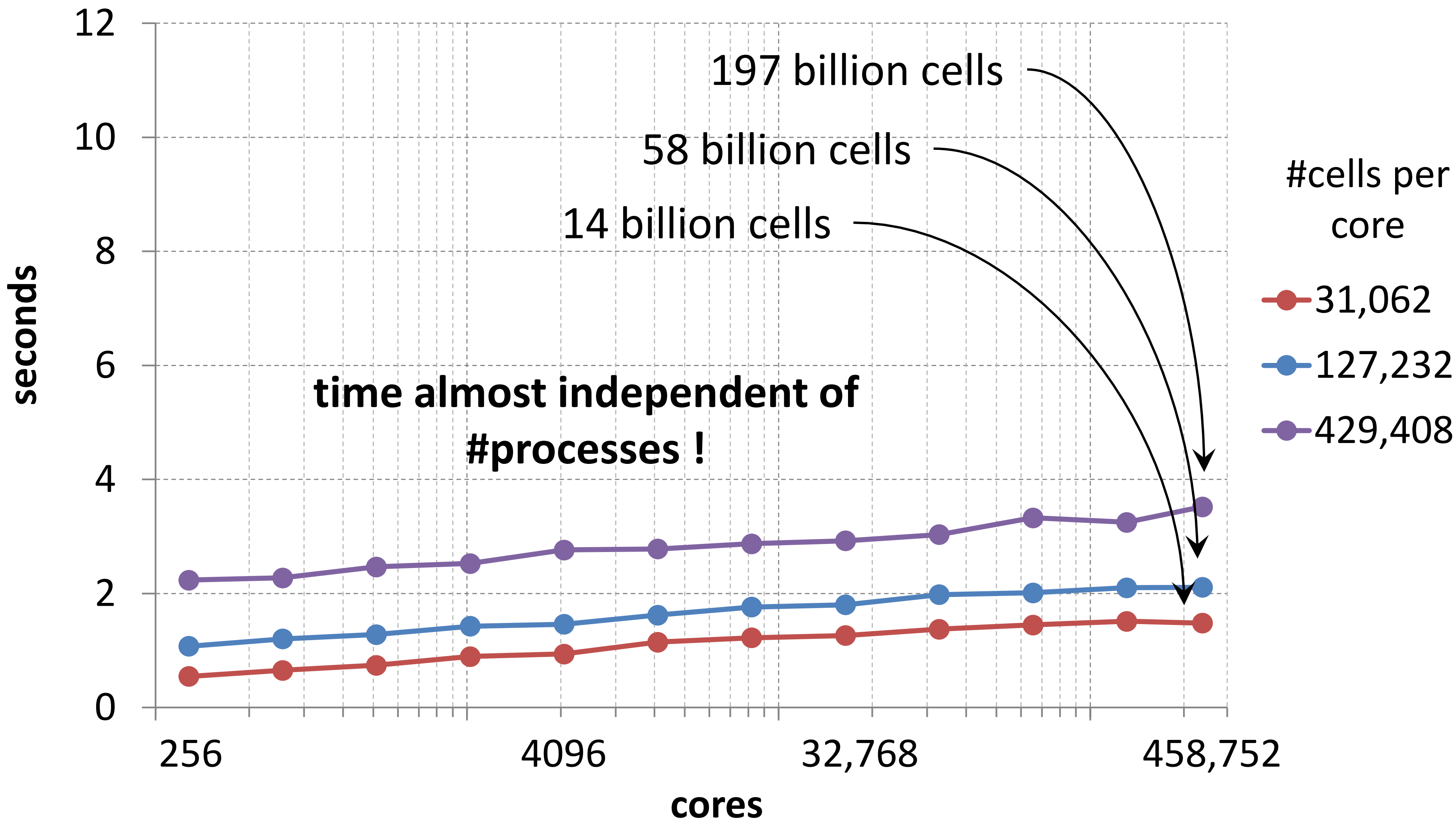




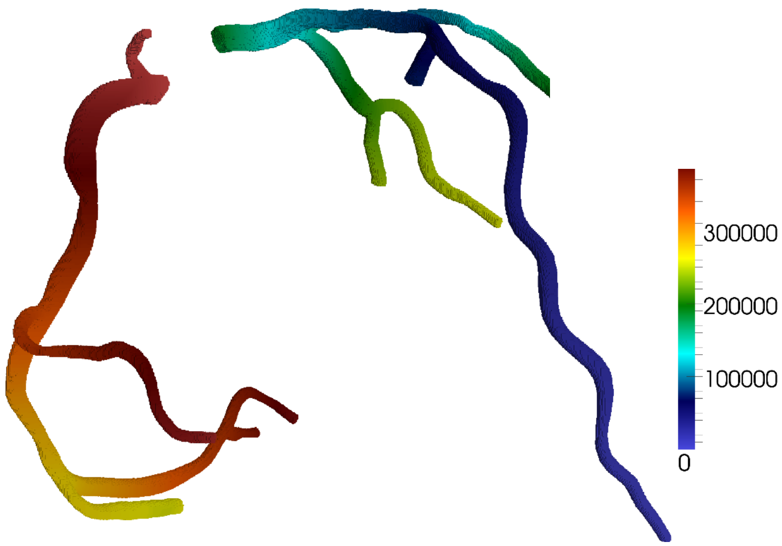
AMR Performance

- JUQUEEN – diffusion load balancing



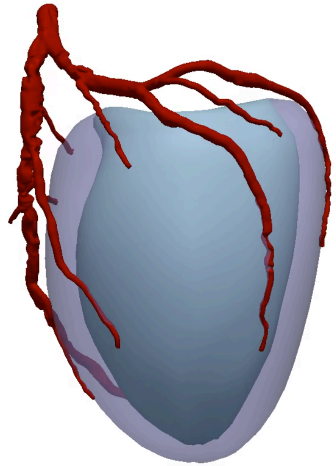


Performance on Coronary Arteries Geometry



Color coded proc assignment

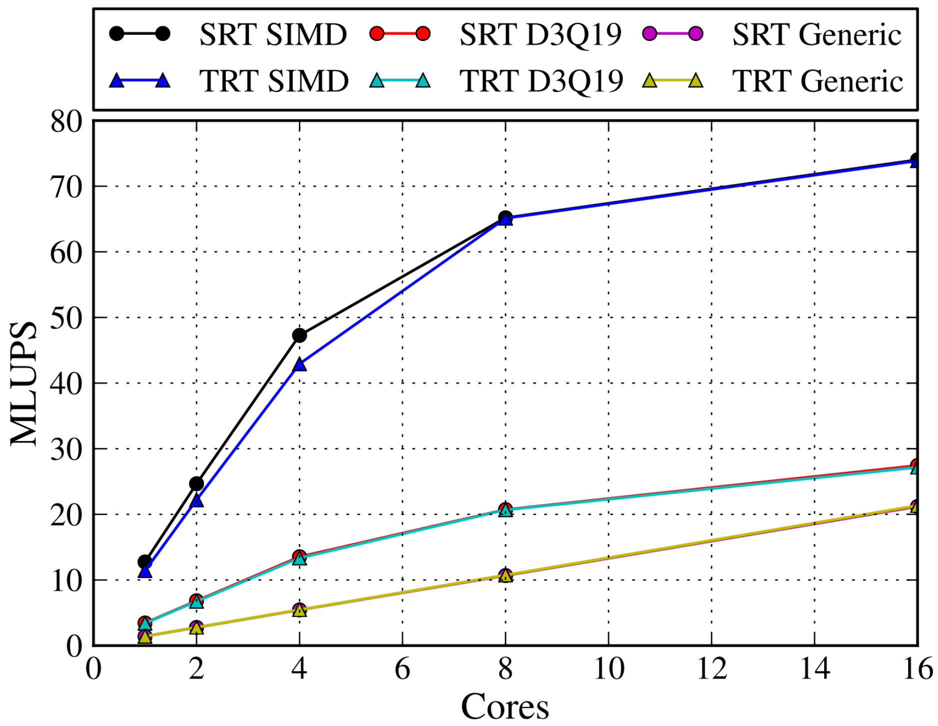
Godenschwager, C., Schornbaum, F., Bauer, M., Köstler, H., & UR (2013). A framework for hybrid parallel flow simulations with a trillion cells in complex geometries. In *Proceedings of SC13: International Conference for High Performance Computing, Networking, Storage and Analysis* (p. 35). ACM.



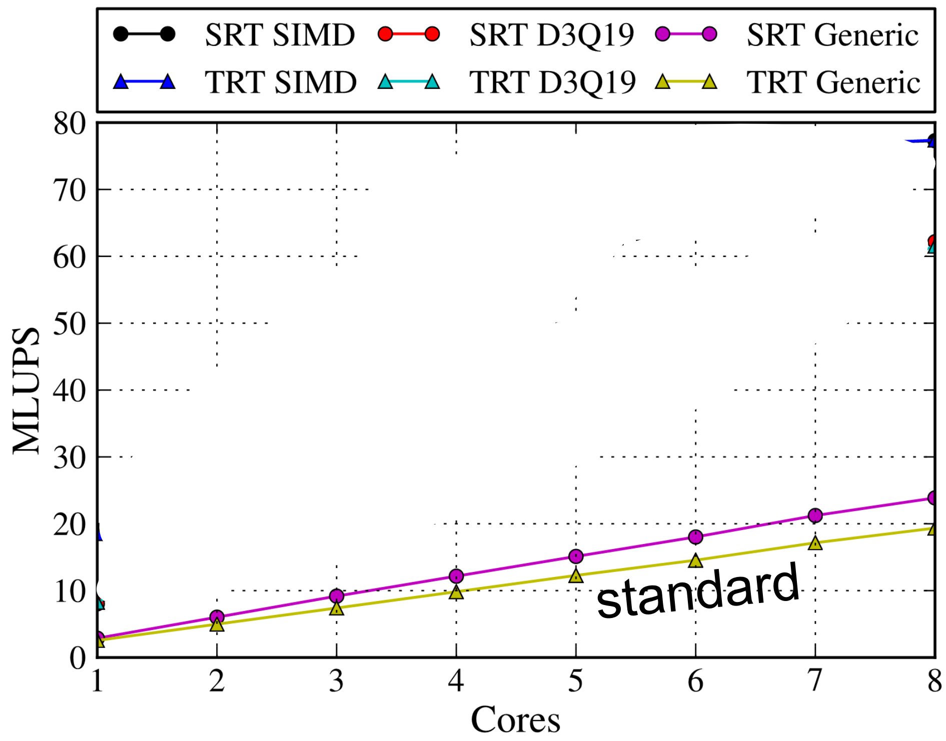
- **Weak scaling**
  458,752 cores of JUQUEEN
  over a trillion (10^{12}) fluid lattice cells
  - cell sizes 1.27µm
    diameter of red blood cells: 7µm
  - 2.1 10^{12} cell updates per second
  - 0.41 PFlops
- **Strong scaling**
  32,768 cores of SuperMUC
  - cell sizes of 0.1 mm
  - 2.1 million fluid cells
  - 6000+ time steps per second

Single Node Performance

JUQUEEN



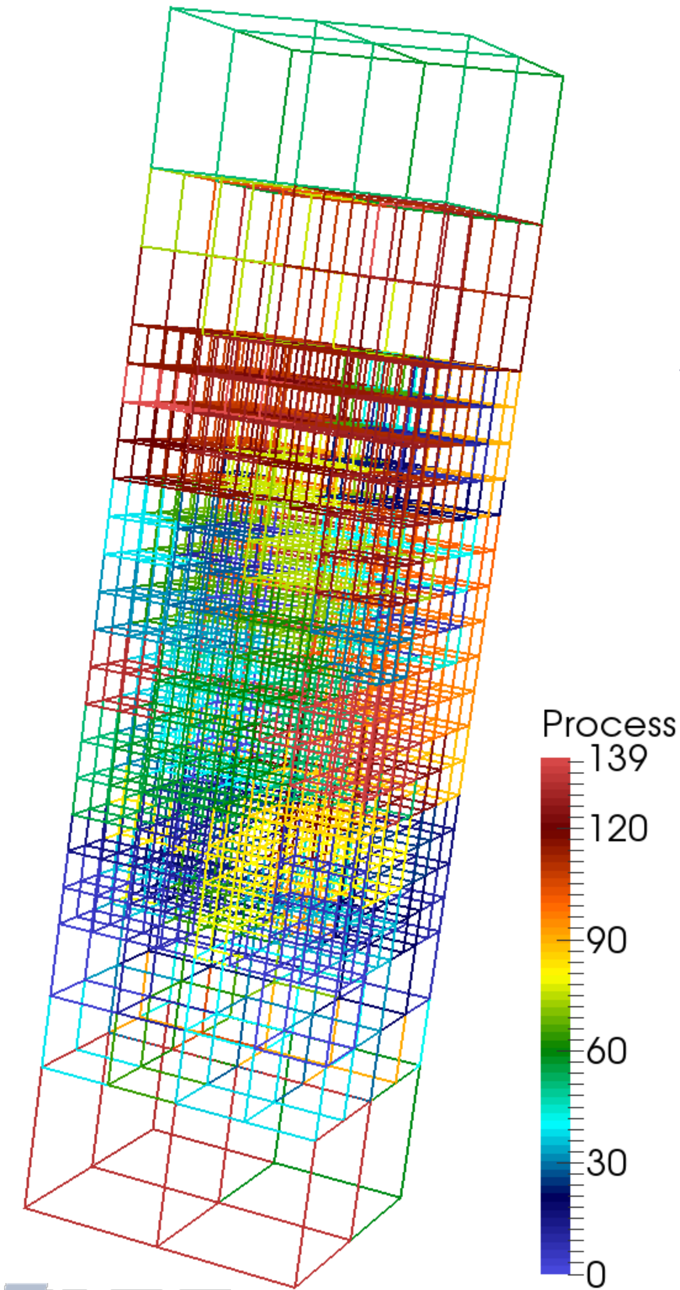
SuperMUC

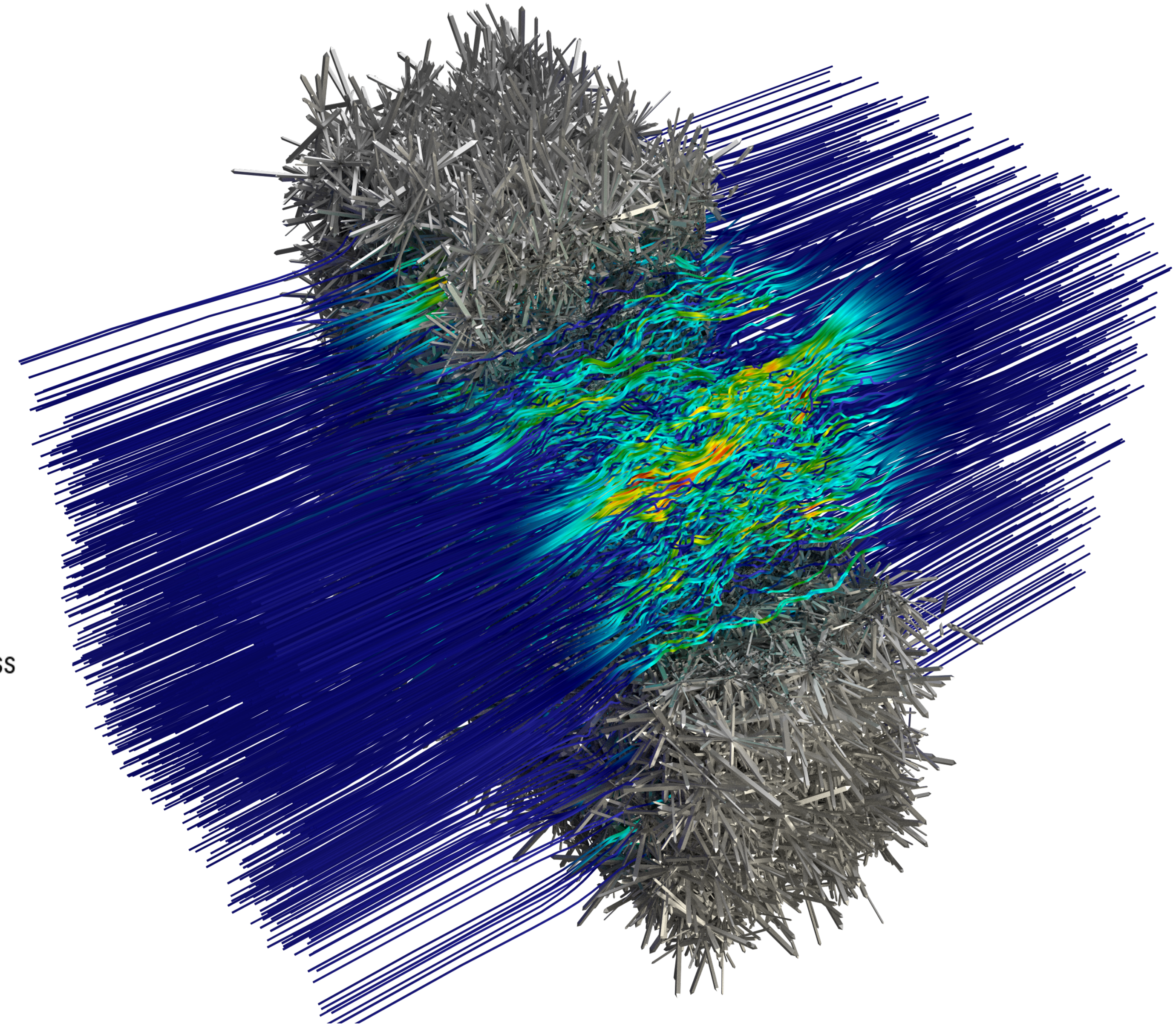


Pohl, T., Deserno, F., Thürey, N., UR, Lammers, P., Wellein, G., & Zeiser, T. (2004). Performance evaluation of parallel large-scale lattice Boltzmann applications on three supercomputing architectures. *Proceedings of the 2004 ACM/IEEE conference on Supercomputing* (p. 21). IEEE Computer Society.

Donath, S., Iglberger, K., Wellein, G., Zeiser, T., Nitsure, A., & UR (2008). Performance comparison of different parallel lattice Boltzmann implementations on multi-core multi-socket systems. *International Journal of Computational Science and Engineering*, *4*(1), 3-11.

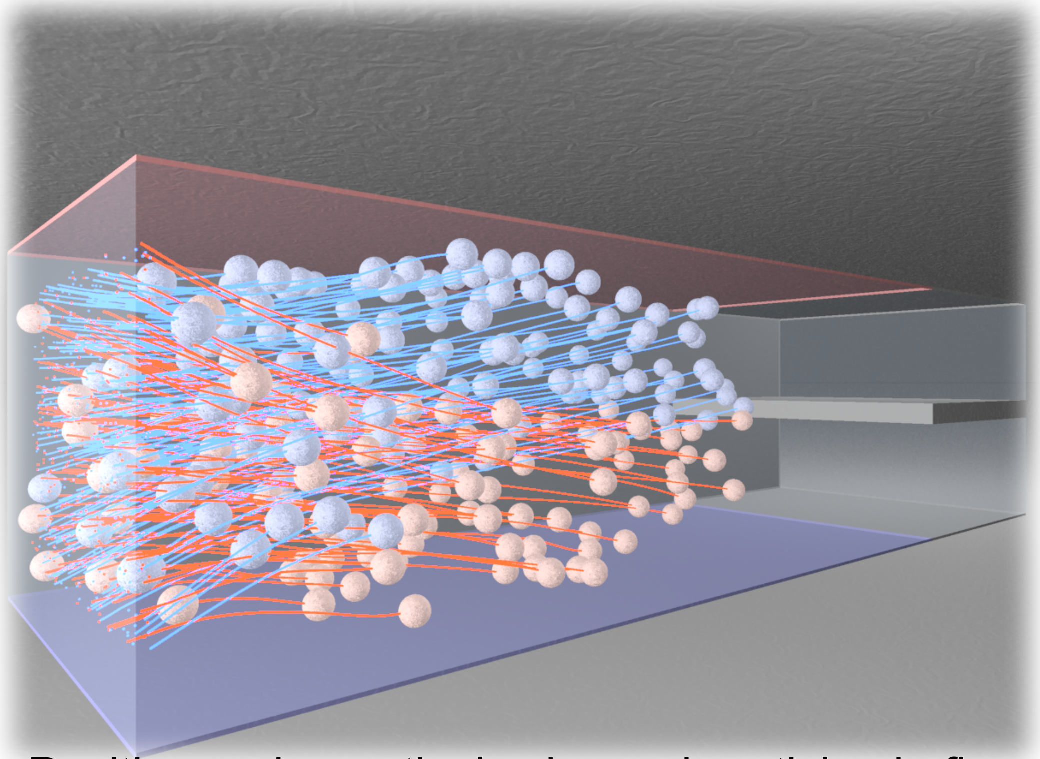
Flow through structure of thin crystals (filter)





work with Jose Pedro Galache and Antonio Gil
CMT-Motores Termicos, Universitat Politecnica de Valencia

Building Block IV (electrostatics)



Positive and negatively charged particles in flow subjected to transversal electric field

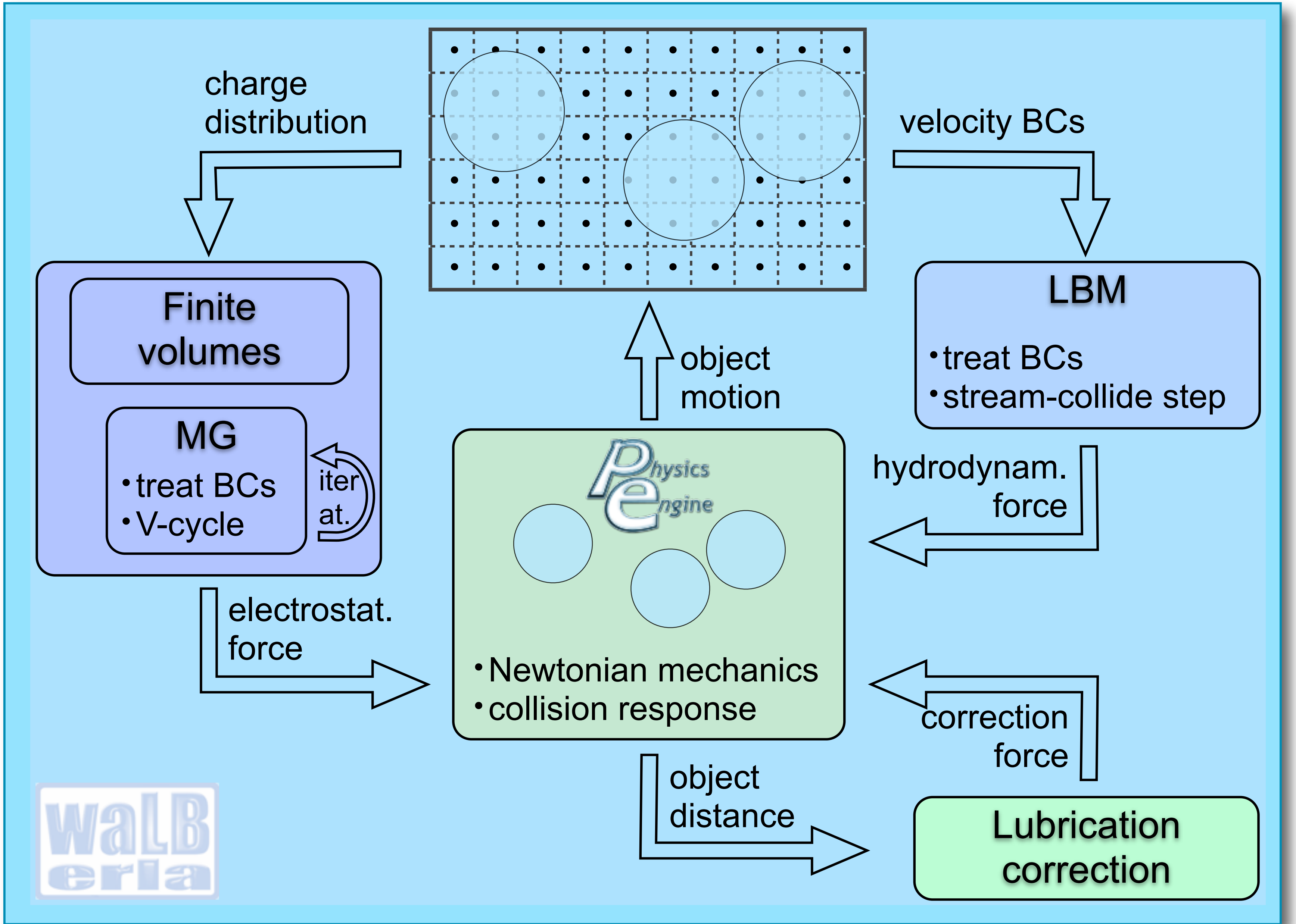
Direct numerical simulation of charged particles in flow

Masilamani, K., Ganguly, S., Feichtinger, C., & UR (2011). Hybrid lattice-boltzmann and finite-difference simulation of electroosmotic flow in a microchannel. *Fluid Dynamics Research*, *43*(2), 025501.

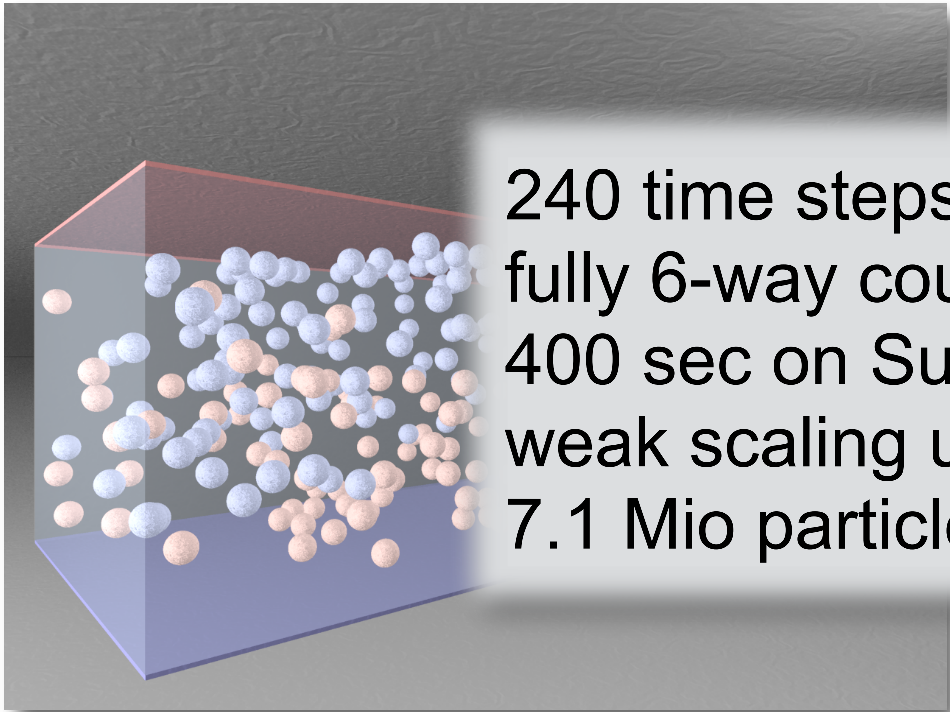
Bartuschat, D., Ritter, D., & UR (2012). Parallel multigrid for electrokinetic simulation in particle-fluid flows. In *High Performance Computing and Simulation (HPCS), 2012 International Conference on* (pp. 374-380). IEEE.

Bartuschat, D. & UR (2015). Parallel Multiphysics Simulations of Charged Particles in Microfluidic Flows, *Journal of Computational Science*, Volume 8, May 2015, Pages 1-19

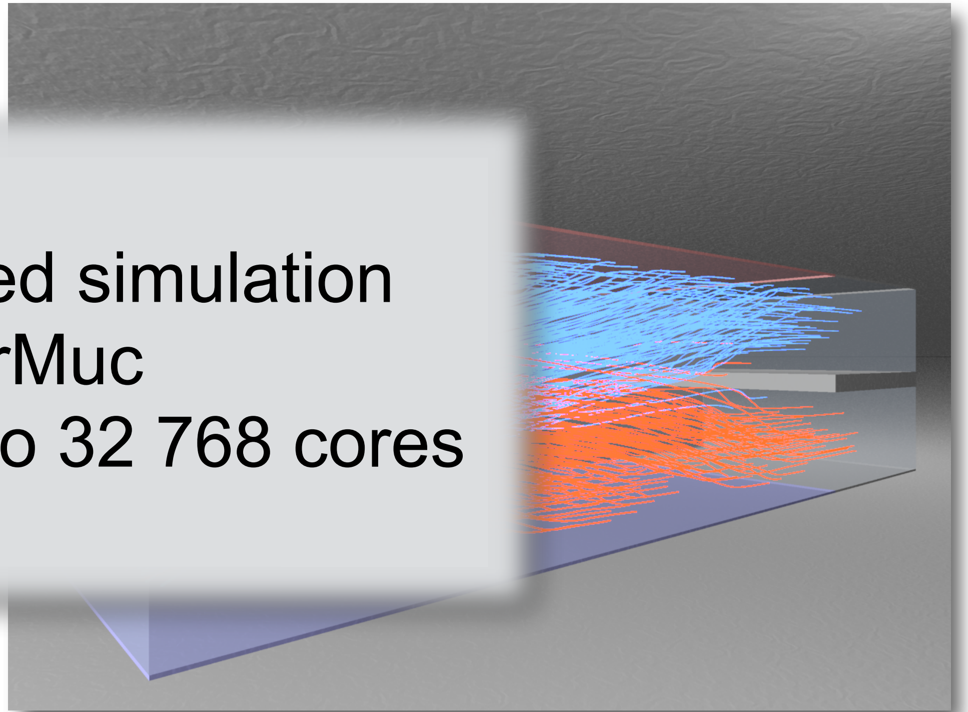
6-way coupling

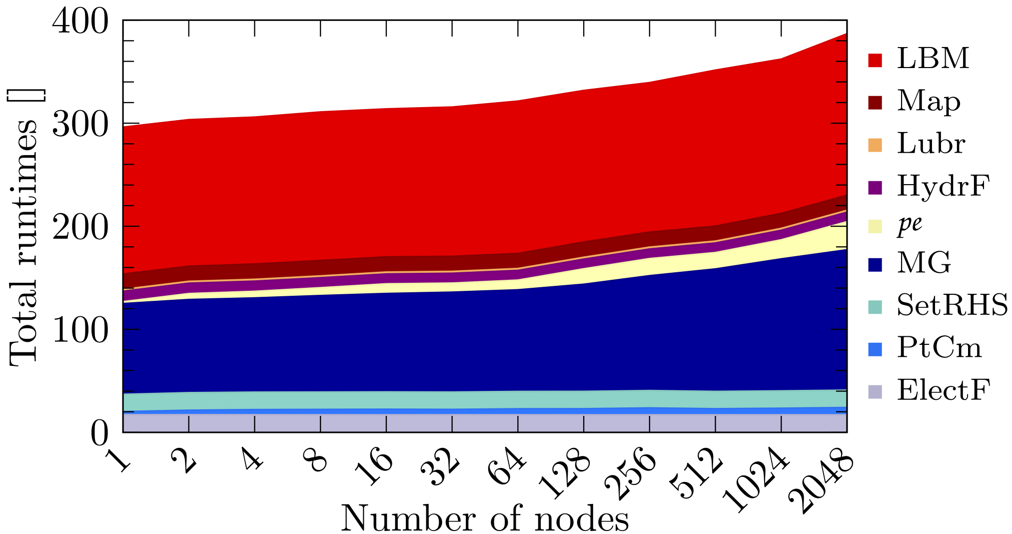


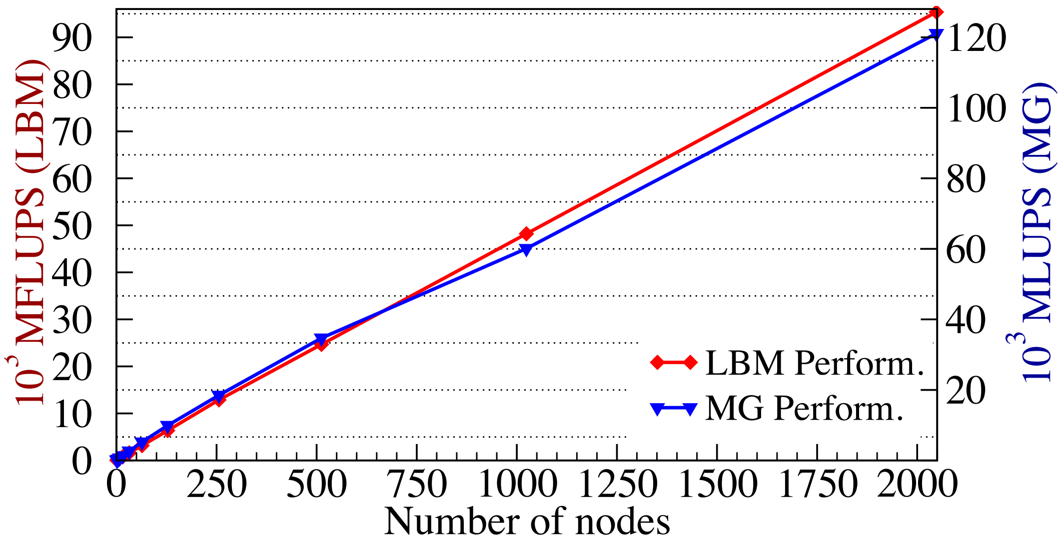
Separation experiment



- 240 time steps
- fully 6-way coupled simulation
- 400 sec on SuperMuc
- weak scaling up to 32 768 cores
- 7.1 Mio particles







Building Block V

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

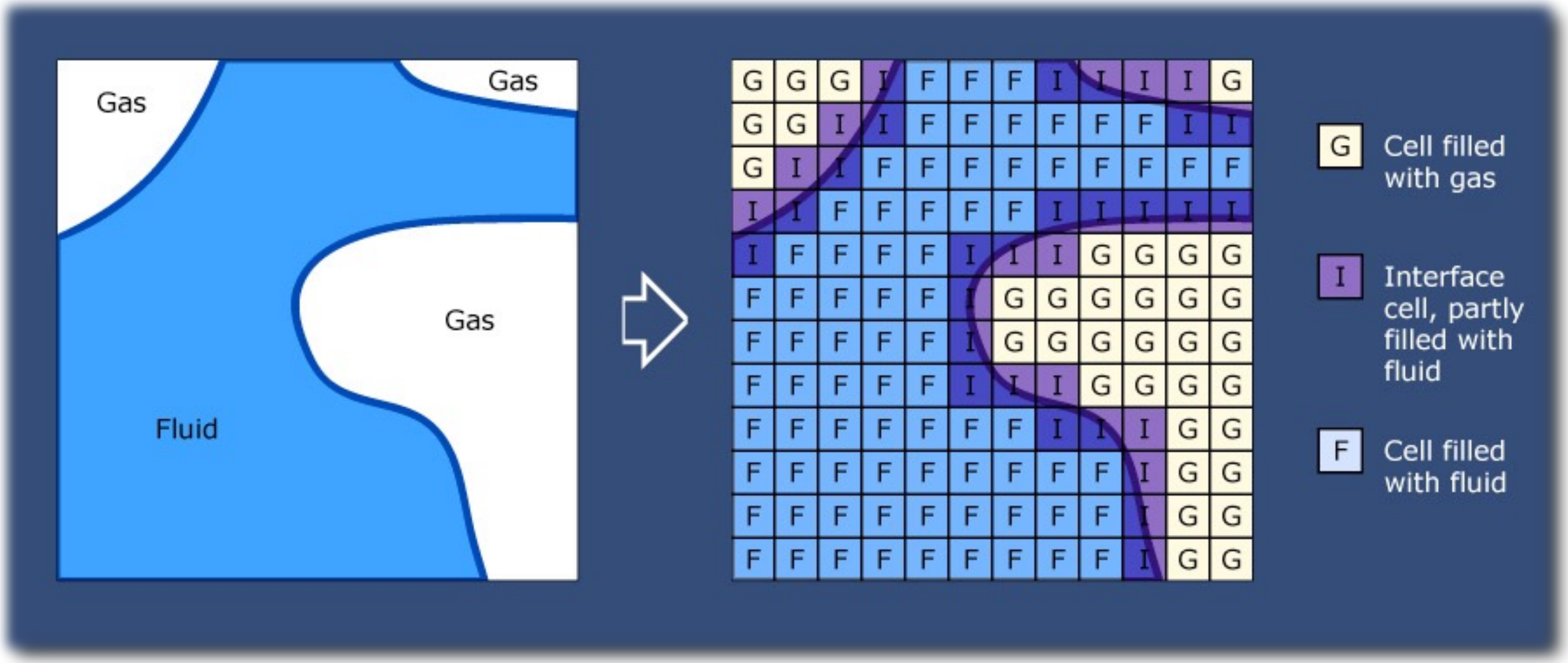
Körner, C., Thies, M., Hofmann, T., Thürey, N., & UR. (2005). Lattice Boltzmann model for free surface flow for modeling foaming. *Journal of Statistical Physics*, *121*(1-2), 179-196.

Donath, S., Feichtinger, C., Pohl, T., Götz, J., & UR. (2010). A Parallel Free Surface Lattice Boltzmann Method for Large-Scale Applications. *Parallel Computational Fluid Dynamics: Recent Advances and Future Directions*, 318.

Anderl, D., Bauer, M., Rauh, C., UR, & Delgado, A. (2014). Numerical simulation of adsorption and bubble interaction in protein foams using a lattice Boltzmann method. *Food & function*, *5*(4), 755-763.

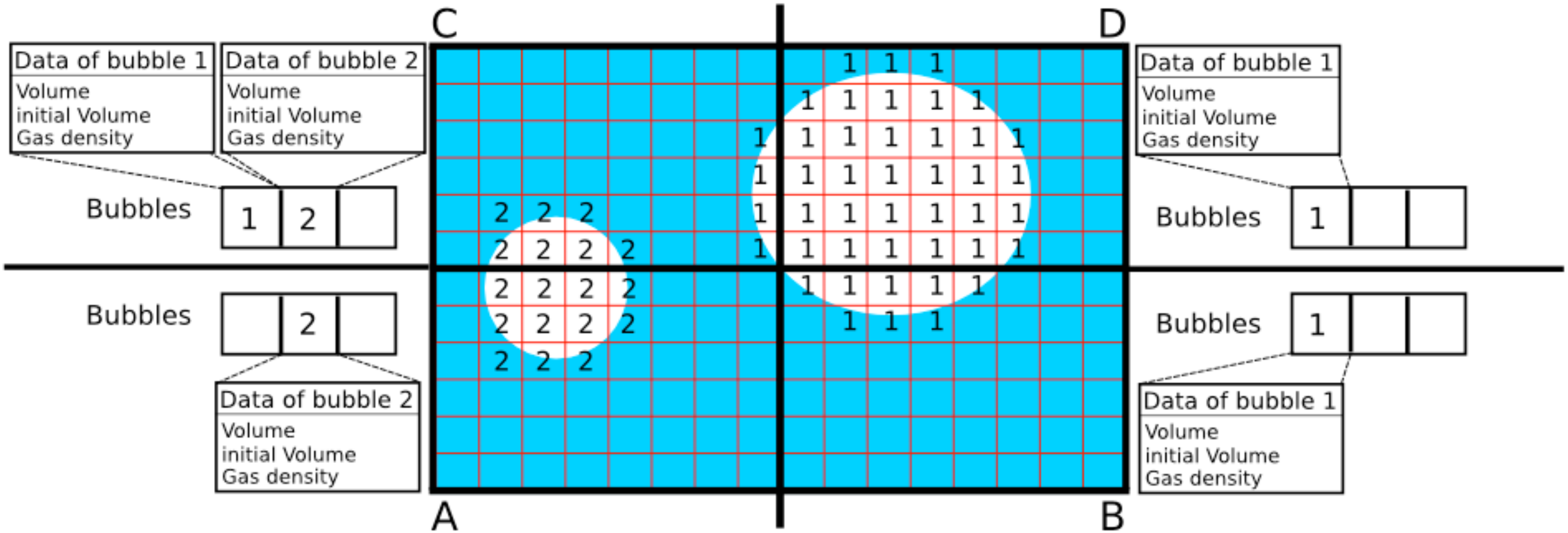
Free Surface Flows

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

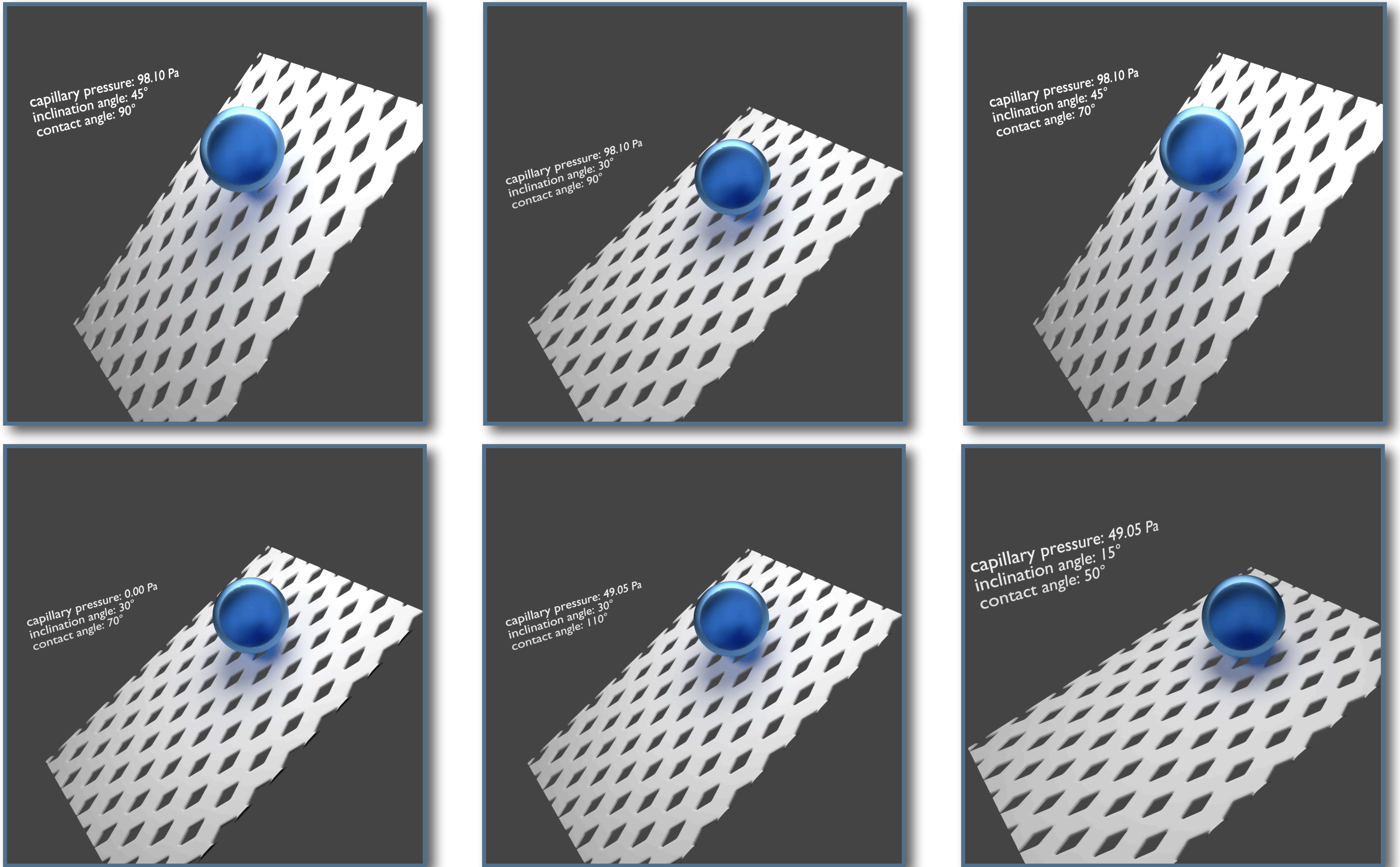


Free Surface Bubble Model

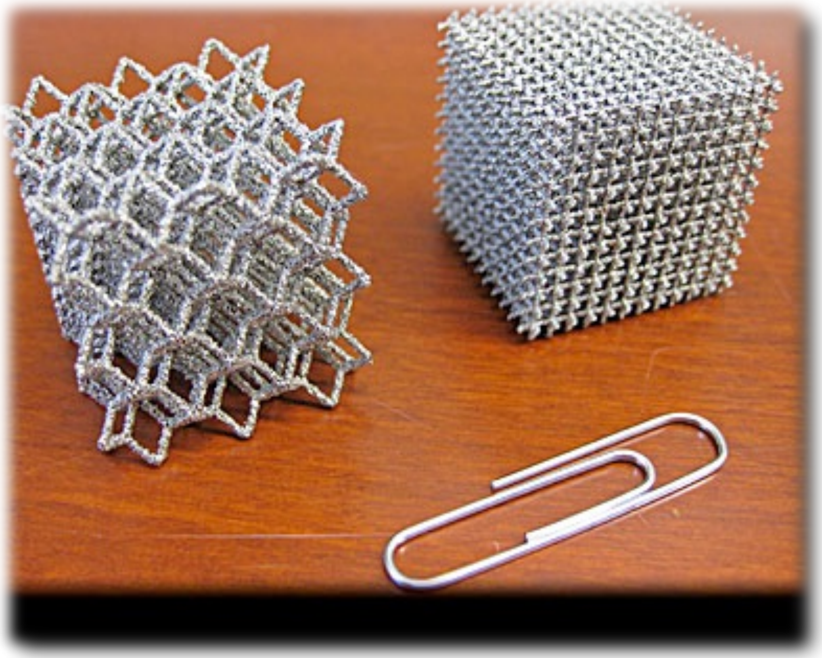
- Data of a Bubble:
  - Initial Volume (Density=1)
  - Current Volume
  - Density/Pressure = initial volume / current volume
- Update Management
  - Each process logs change of volume due to cell conversions (Interface – Gas / Gas – Interface) and mass variations in Interface cells
  - All volume changes 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

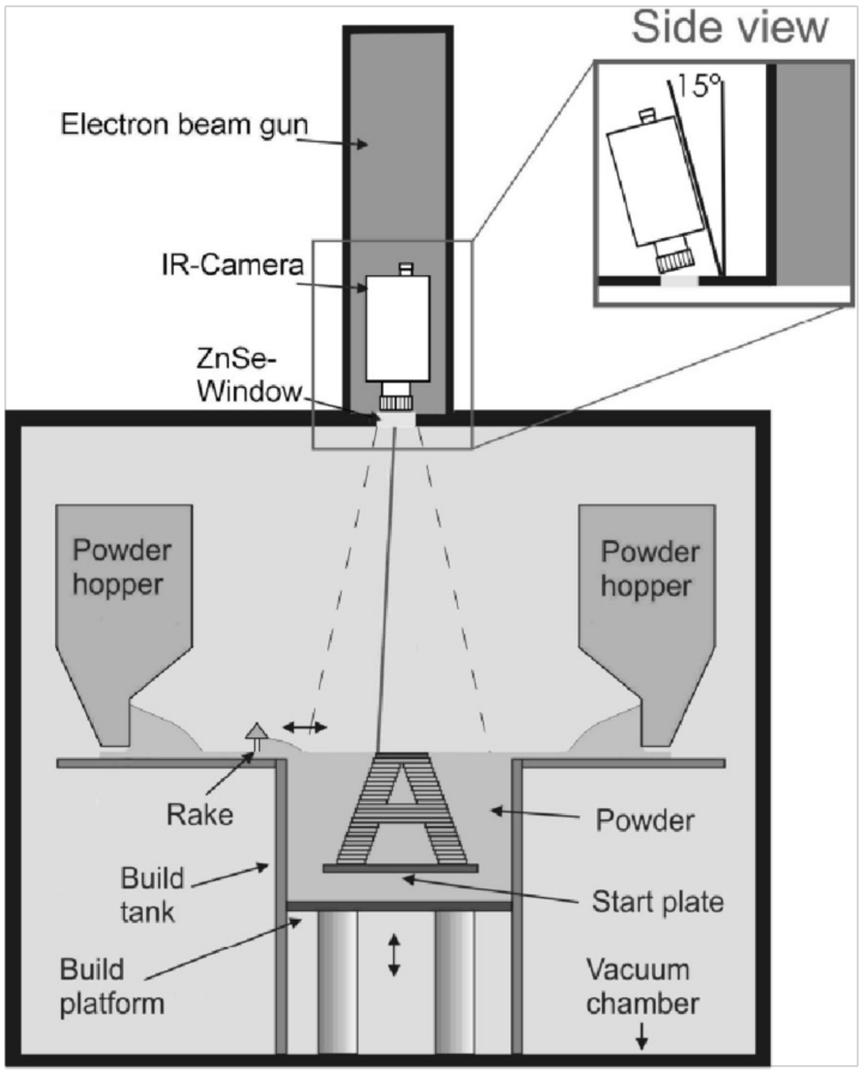


Additive Manufacturing
Fast Electron Beam Melting

Bikas, H., Stavropoulos, P., & Chryssolouris, G. (2015). Additive manufacturing methods and modelling approaches: a critical review. *The International Journal of Advanced Manufacturing Technology*, 1-17.

Klassen, A., Scharowsky, T., & Körner, C. (2014). Evaporation model for beam based additive manufacturing using free surface lattice Boltzmann methods. *Journal of Physics D: Applied Physics*, *47*(27), 275303.

Electron Beam Melting Process
3D printing

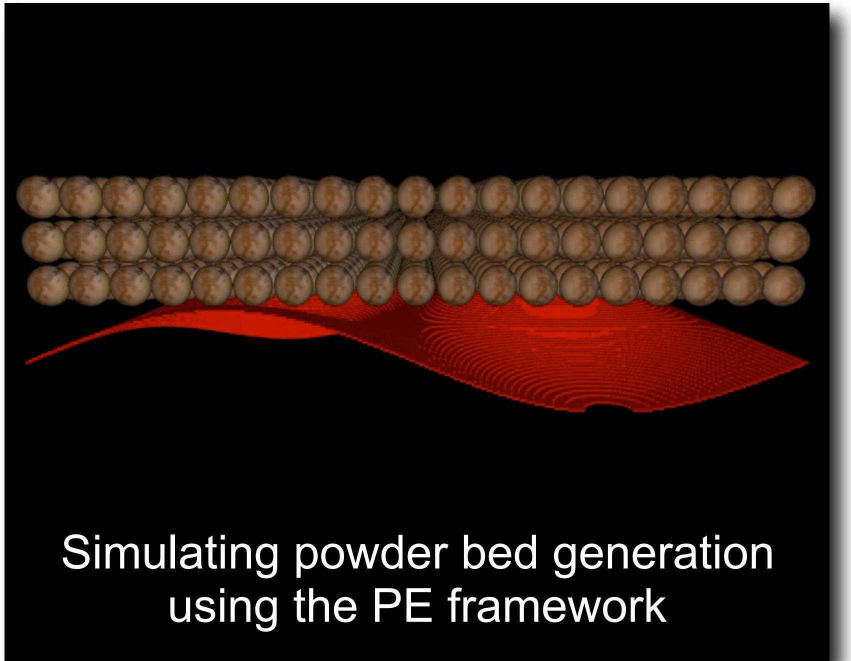


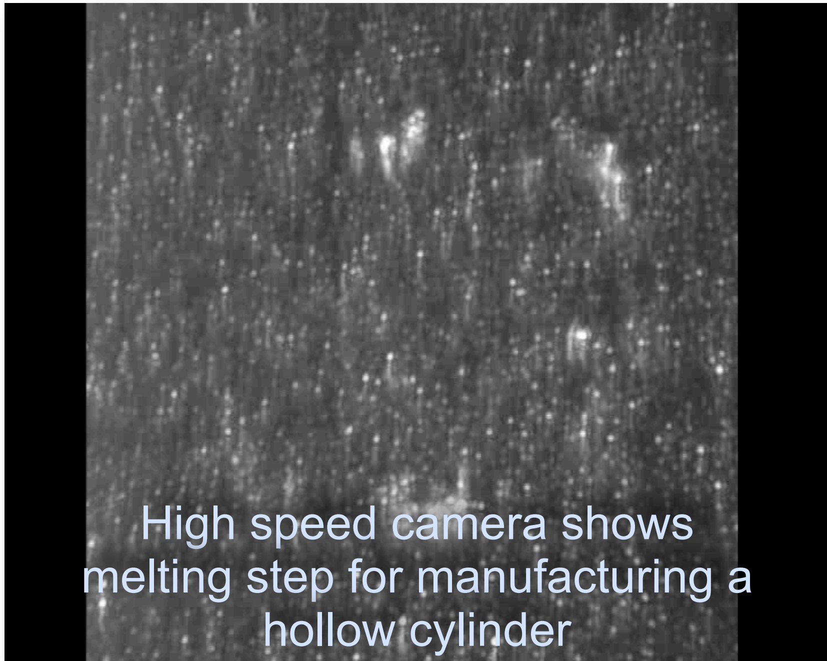
- EU-Project Fast-EBM
  - ARCAM (Gothenburg)
  - TWI (Cambridge)
  - FAU Erlangen
- Generation of powder bed
- Energy transfer by electron beam
  - penetration depth
  - heat transfer
- Flow dynamics
  - melting
  - melt flow
  - surface tension
  - wetting
  - capillary forces
  - contact angles
  - solidification

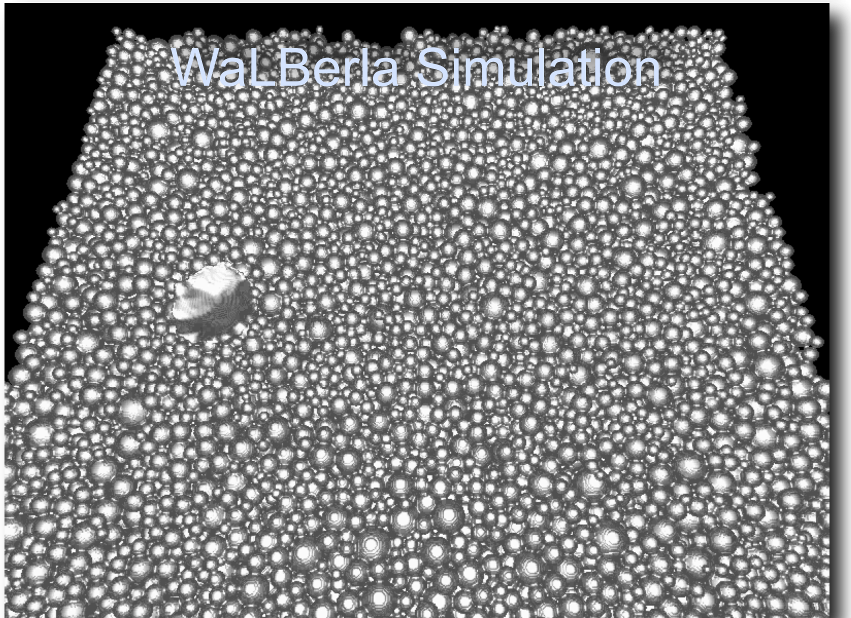
Ammer, R., Markl, M., Ljungblad, U., Körner, C., & UR (2014). Simulating fast electron beam melting with a parallel thermal free surface lattice Boltzmann method. *Computers & Mathematics with Applications*, *67*(2), 318-330.

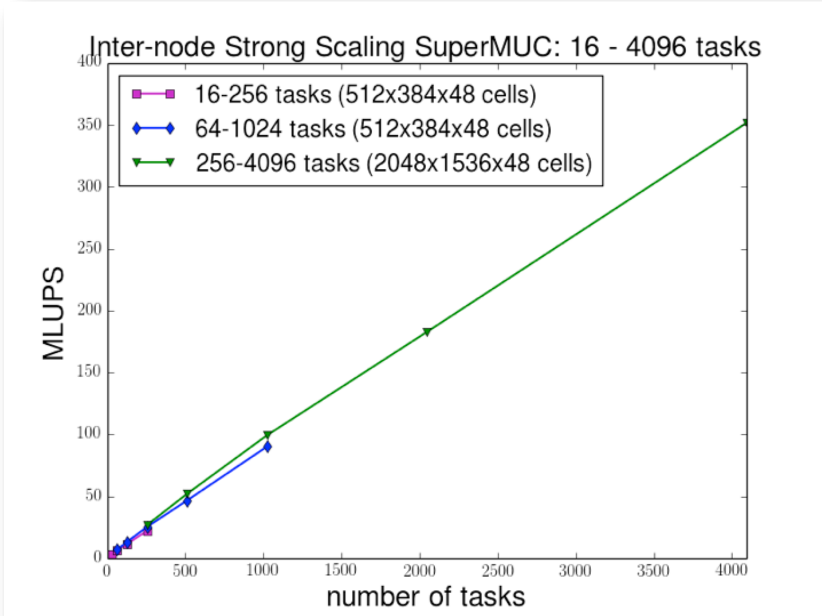
Ammer, R., UR, Markl, M., Jüchter V., & Körner, C. (2014). Validation experiments for LBM simulations of electron beam melting. *International Journal of Modern Physics C*.

Simulation of Electron Beam Melting





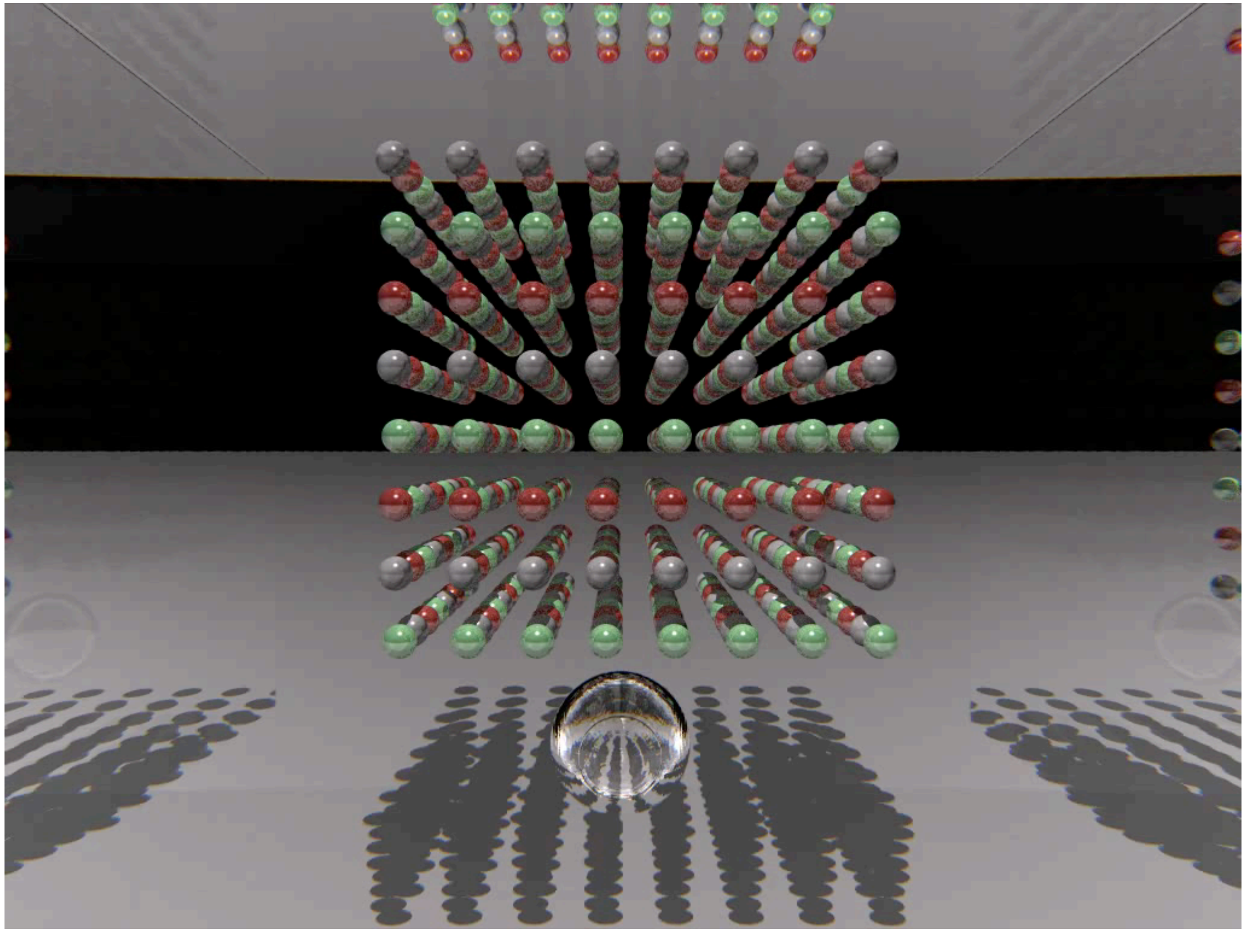




Conclusions

CSE research is done by teams

Thank you for your attention!



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