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Gauß-Allianz

Performance Engineering for Computational Science

U. Ruede

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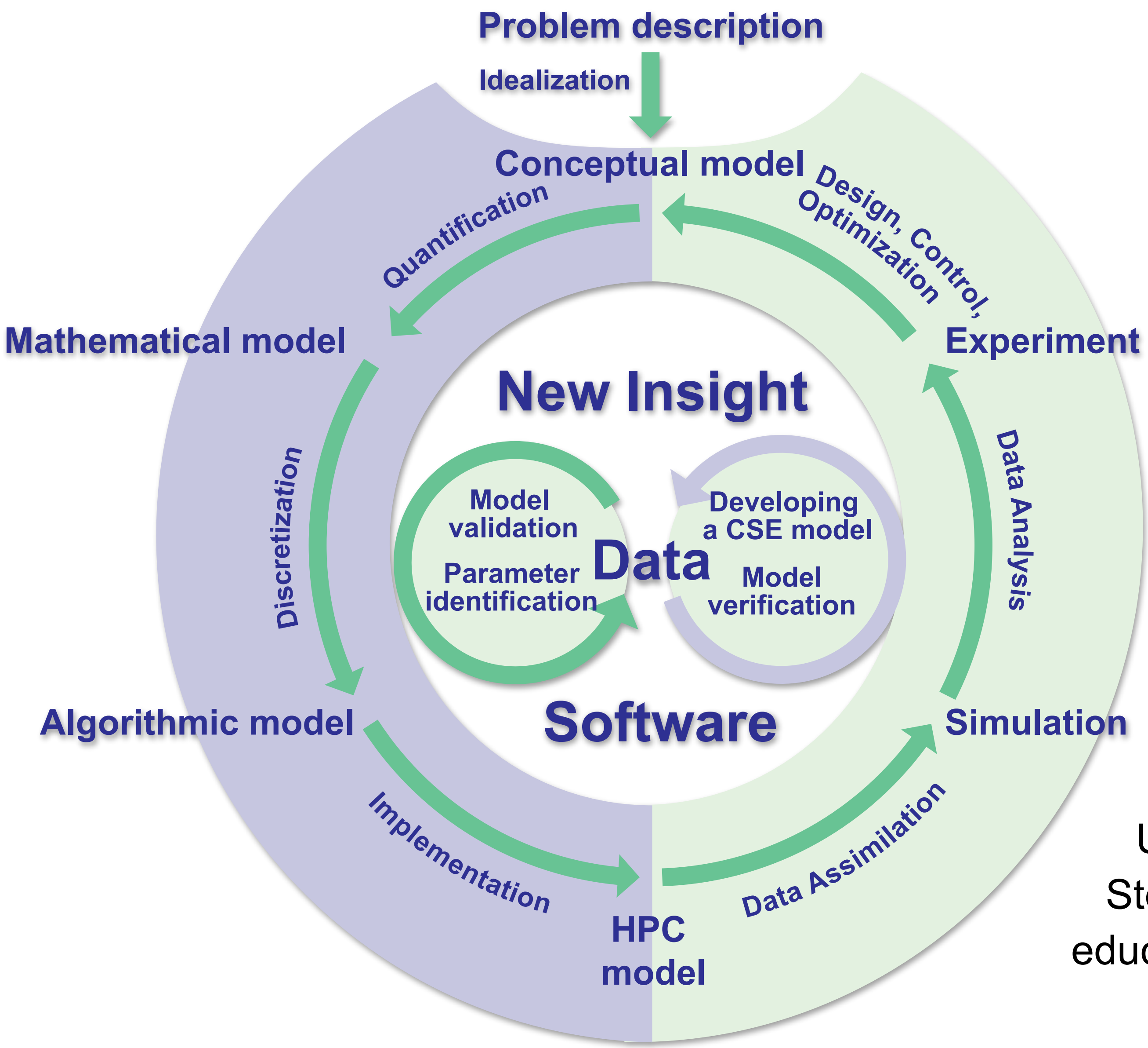
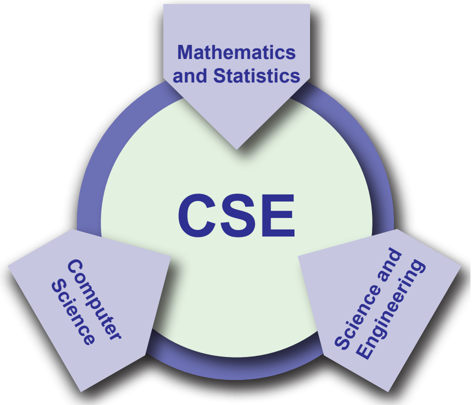
Outline

- ExaScale computing
  - node efficiency, scalability, and algorithmic complexity
- TerraNeo
  - HHG
  - HyTeG
- waLBerla
  - Lattice Boltzmann
  - Rigid Body Dynamics
- Conclusions

Part I: Extreme Scale Computing

What is it about

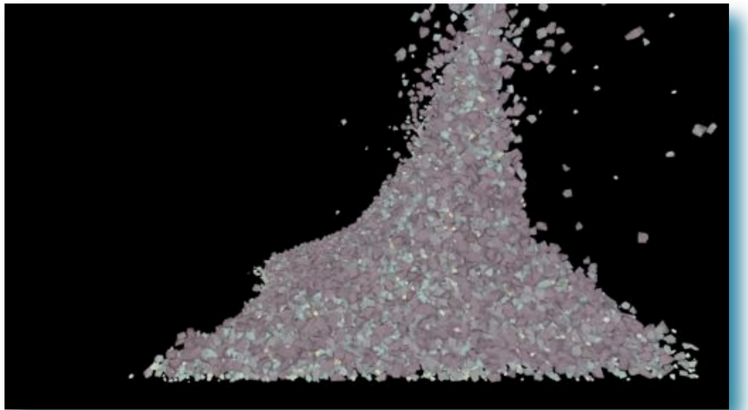




UR, Willcox, K., McInnes, L. C., & Sterck, H. D. (2018). Research and education in **computational science and engineering**. *Siam Review*, *60*(3), 707-754.

What is ExaScale possibly good for?

- ExaScale: 10^{18} FLOPS (floating point operations per second)
- When we have
  - 1000
  - x 1000
  - x 1000 particles (or pores)
  - each resolved by 1000 cells
- then we still can still execute 1 Mflop per each cell
  - 1 MFLPOS = 10^6 FLOPS = the performance of PC in 1990



Simulation performed with in-house multi-physics framework waLBerla/PE

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

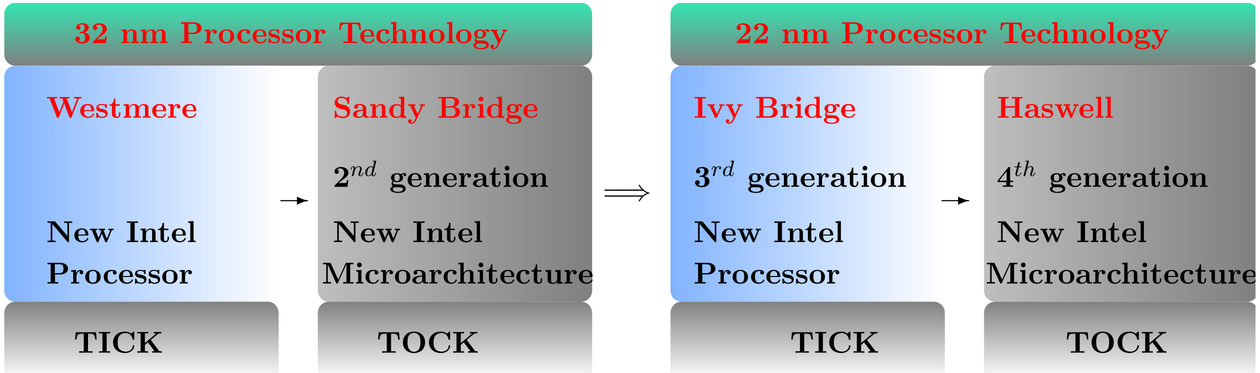
10^{18} FLOPS …

- At clock rates of 1 Ghz a single stream of operands will produce results at 10^9/sec
  - degree of concurrency= 10^9
- This will be achieved hierarchically
  - 10^4 nodes
  - 10^3 cores/node
  - 10^2 instructions on the fly/core (vectorization, pipelining, …)
- We must use them all!
- Energy: 1nJ/Flop
  - 1 GW for Exascale
- Resilience: MTBF of 100 years per cell phone (= 10 Gflop)
  - 10^8 cell phones: MTBF for Exascale = 30 sec

Energy consumption of floating point operations

based on: Ayesha Afzal: *The Cost of Computation: Metrics and Models for Modern Multicore-based Systems in Scientific Computing*, Master Thesis, FAU Erlangen, 2015

Clock rates of 2-3 GHz correspond to cycle times of 0.3-0.5 nsec.



Metrics	Energy cost				
	ε_{flop}	$\varepsilon_{byte}^{L1-REG}$	$\varepsilon_{byte}^{L2-L1}$	$\varepsilon_{byte}^{L3-L2}$	$\varepsilon_{byte}^{MEM-L3}$
Flop only	830 pJ/F	0	0	0	0
Load only	0	227 pJ/B	314 pJ/B	256 pJ/B	1880 pJ/B
Store only	0	377 pJ/B	300 pJ/B	340 pJ/B	2977 pJ/B

8 core Sandy Bridge System - measured through systematic benchmarking
see also Georg Hager's talk at PACO 2015

Best values on Green 500 currently convert to 0.1 nJ/Flop:
equivalent to 100 MW for ExaFlops performance

The first performance question:

What is the minimal cost of solving a PDE?

(such as Poisson's or Stokes' equation in 3D)

- asymptotic results of the form

  $$\text{Cost} \leqq C\, N^p \qquad \text{(Flops?)}$$

  with unspecified constant C are inadequate to predict performance

The key goal of numerical analysis:

relate accuracy and cost!

How do we quantify true cost?

(i.e. resources needed)

- Number of flops?
- Memory consumption?
- Memory bandwidth? (aggregated?)
- Communication bandwidth?
- Communication latency?
- Power consumption?

How do we predict cost?

- What is the cost of solving the discrete Poisson equation?
  - C'mon: it's the mother of all PDE!
  - Yep, there are O(N) algorithms:
    wavelet, fast multipole, multigrid, …
  - but what is the **best constant** published?
- for Poisson 2D, second order:

  #Flops = **30 N** (Stüben, 1982)

- Intel Haswell CPU: 1030.4 GFlops single precision performance
  - $N=10^6$
  - expected time to solution: **$3*10^{-5}$ sec** (microseconds!)
- standard computational practice in 2017 misses this by **many orders of magnitude**!
- why do we have this enormous **gap** between theory and practice?
- **no**, it cannot be explained by „cache effects" alone.
- This talk tries to contribute to the failure analysis.

What is the largest system that we can solve today?

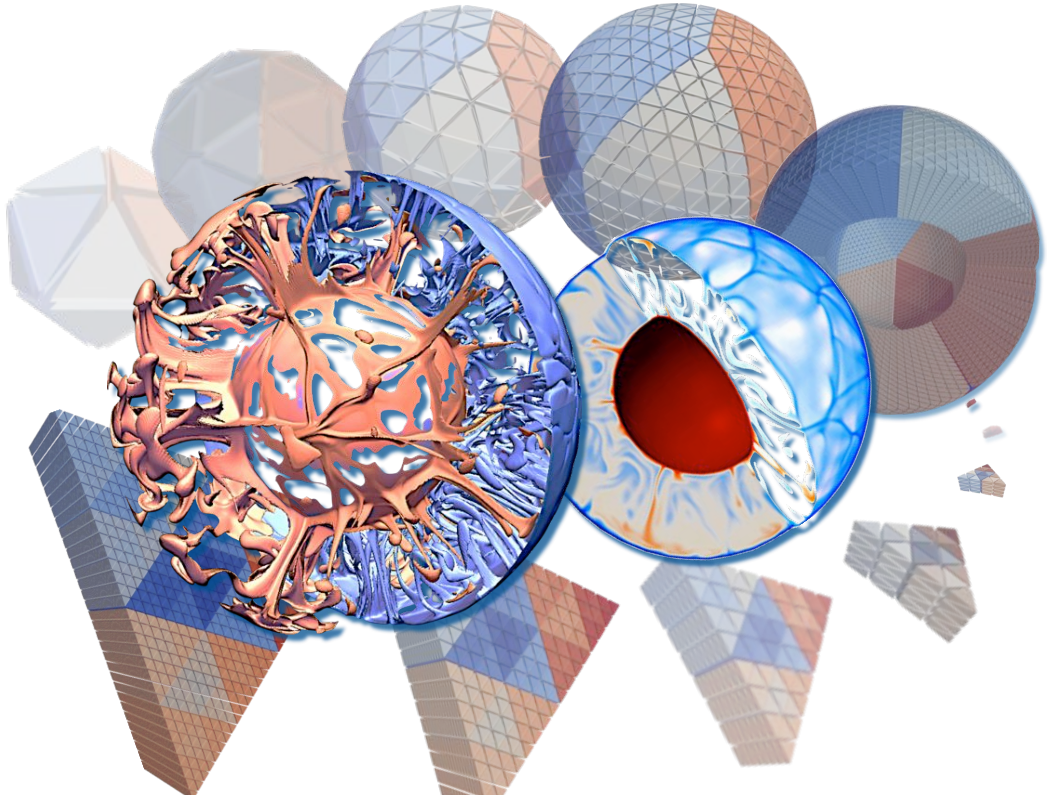
Bergen, B, Hülsemann, F, UR (2005): Is $1.7 \cdot 10^{10}$ unknowns the largest finite element system that can be solved today? Proceedings of SC'05.

- and now, 13 years later?
- we have 400 TByte main memory = $4 \cdot 10^{14}$ Bytes = 5 vectors each with **$N=10^{13}$** double precision elements
- matrix-free implementation necessary
  - even with a sparse matrix format, storing a matrix of dimension **$N=10^{13}$** is not possible
- Which algorithm?
  - multigrid
  - Cost = C*N
  - C „moderate“, e.g. C=100.
- does it parallelize well on that scale?
- should we worry since $\kappa = O(N^{2/3})$?

Algorithms Matter!

- Solution of Laplace equation in 3D wit $N=n^3$ unknowns
- Direct methods:
  - banded: $\sim n^7 = N^{2.33}$
  - nested dissection: $\sim n^6 = N^2$
- Iterative Methods:
  - Jacobi: $\sim 50\ n^5 = 50\ N^{1.66}$
  - CG: $\sim 100\ n^4 = 100\ N^{1.33}$
  - Full Multigrid: $\sim 200\ n^3 = 200\ N$

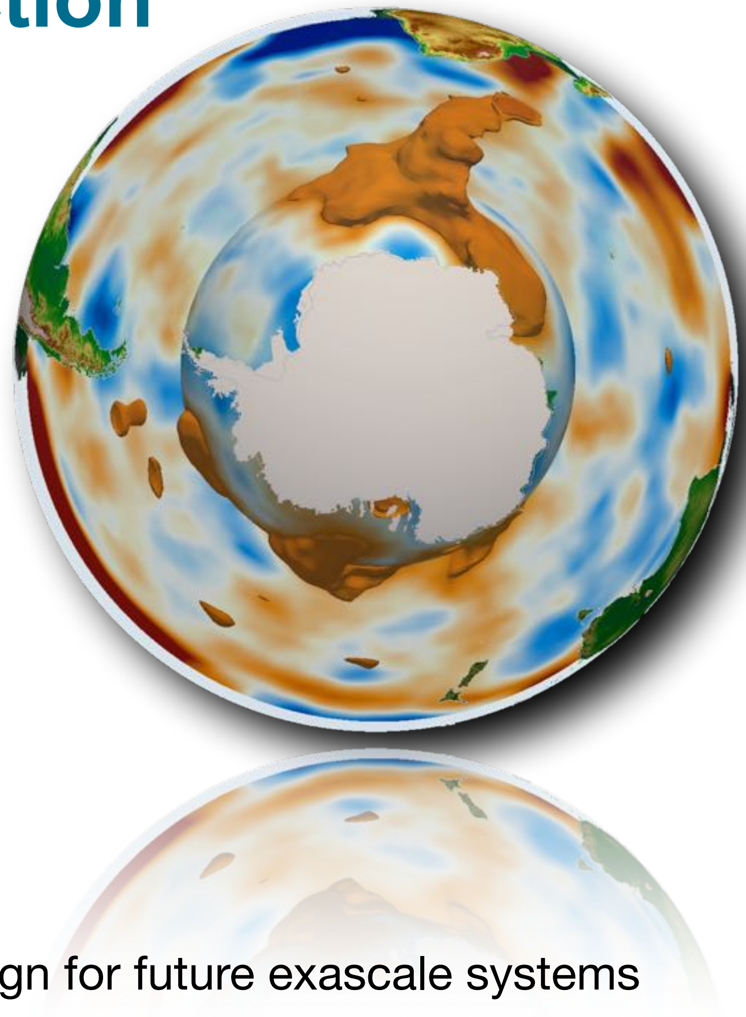
Energy per FLOP: 1nJ				
Computer Generation	gigascale: 10^9	terascale: 10^{12}	petascale: 10^{15}	exascale: 10^{18}
problem size: DoF=N	10^6	10^9	10^{12}	10^{15}
Direct method: $1*N^2$	0.278 Wh	278 kWh	278 GWh	278 PWh
Krylov method: $100*N^{1.33}$	10 Ws	28 Wh	278 kWh	2.77 GWh
Full Multigrid: 200 N	0.2 Ws	0.056 Wh	56 Wh	56 kWh
TerraNeo prototype (est. for Juqueen)	0.13 Wh	30 Wh	27 kWh	?



Part II: Hierarchical Hybrid Grids

TERRANEO

Example: Earth Mantle Convection



Why Mantle Convection?

- driving force for plate tectonics
- mountain building and earthquakes

Why Exascale?

- mantle has 10^{12} km^3
- inversion and UQ blow up cost

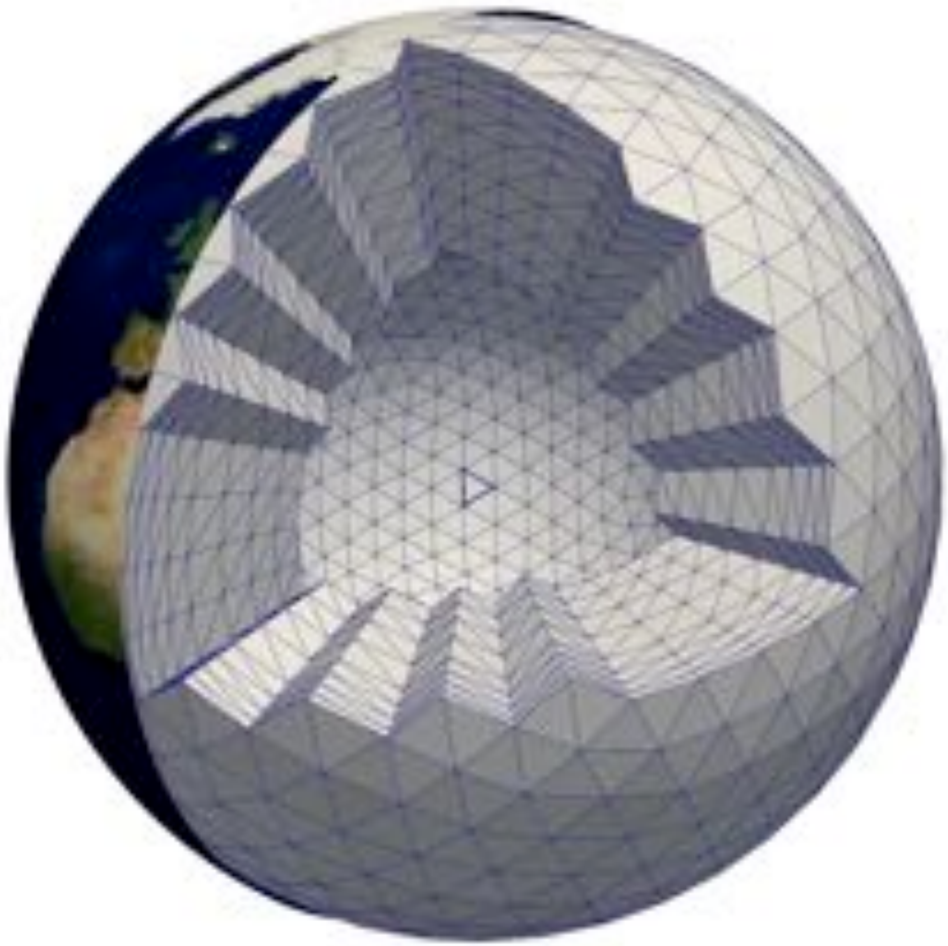
Why TerraNeo?

- ultra-scalable and fast
- sustainable framework

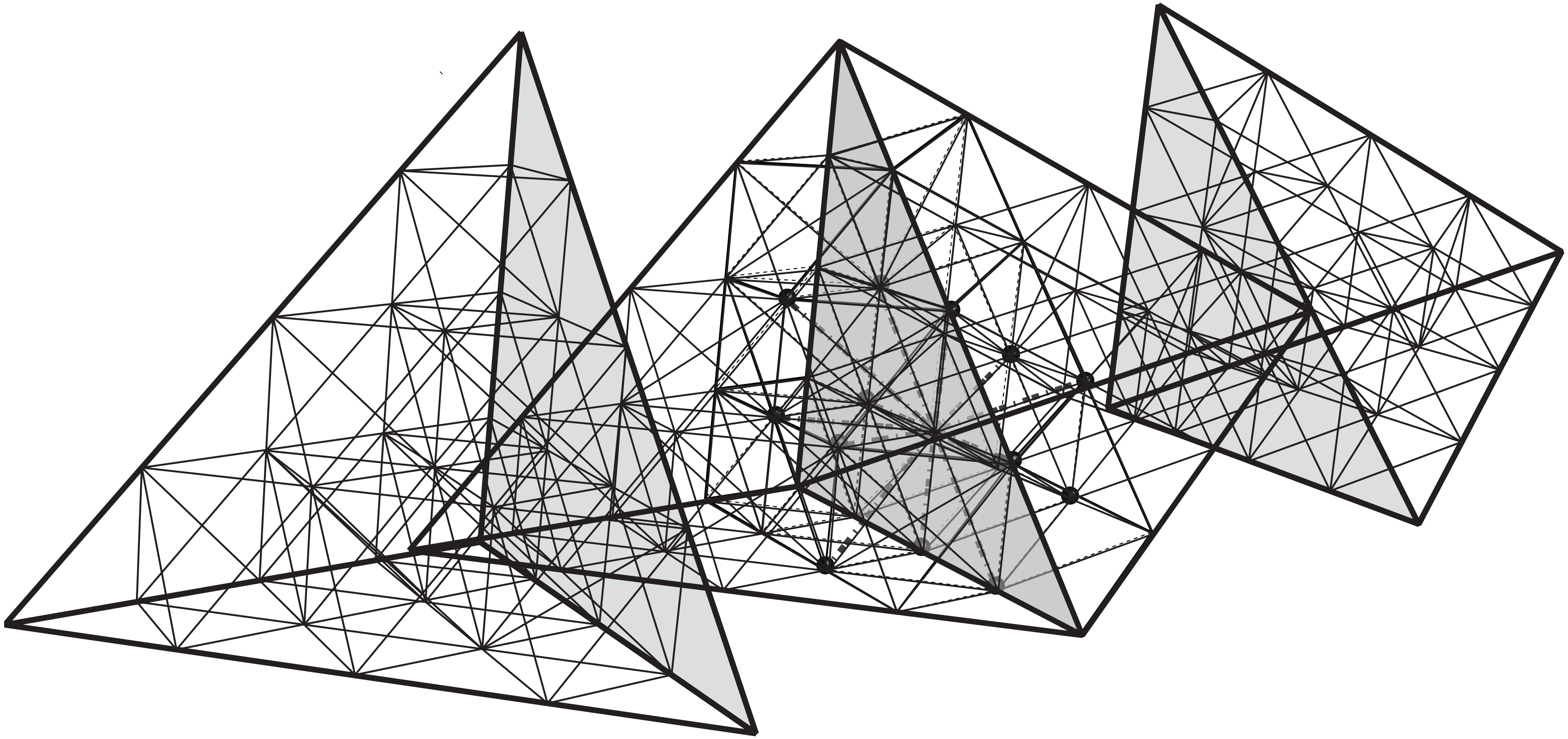
Challenges

- **computer sciences:** software design for future exascale systems
- **mathematics:** HPC performance oriented metrics
- **geophysics:** model complexity and uncertainty
- **bridging disciplines:** integrated co-design

Meshing of the Mantle with Tets



HHG: A modern mesh-free architecture for FE

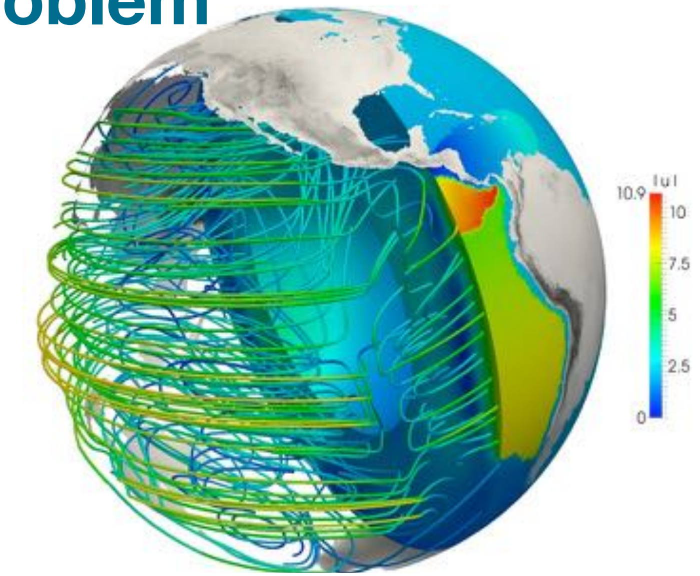


Structured refinement of an unstructured base mesh

Geometrical Hierarchy: Volume, Face, Edge, Vertex

HHG Solver for Stokes System
Motivated by Earth Mantle convection problem

Gmeiner, Waluga, Stengel, Wohlmuth, UR: Performance and Scalability of Hierarchical Hybrid Multigrid Solvers for Stokes Systems, SISC, 2015.



$$
\begin{aligned}
-\nabla \cdot (2\eta\epsilon(\mathbf{u})) + \nabla p &= \rho(T)\mathbf{g}, \\
\nabla \cdot \mathbf{u} &= 0, \\
\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T - \nabla \cdot (\kappa \nabla T) &= \gamma.
\end{aligned}
$$

$\mathbf{u}$	velocity
p	dynamic pressure
T	temperature
ν	viscosity of the material
$\epsilon(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$	strain rate tensor
ρ	density
$\kappa, \gamma, \mathbf{g}$	thermal conductivity, heat sources, gravity vector

Scale up to ~10^{13} nodes/ DOFs

⇒ resolve the whole Earth Mantle globally with 1km resolution

Stokes equation: $-\mathrm{div}(\nabla \mathbf{u} - p\mathbf{I}) = \mathbf{f}, \quad \mathrm{div}\,\mathbf{u} = 0$

FEM Discretization:

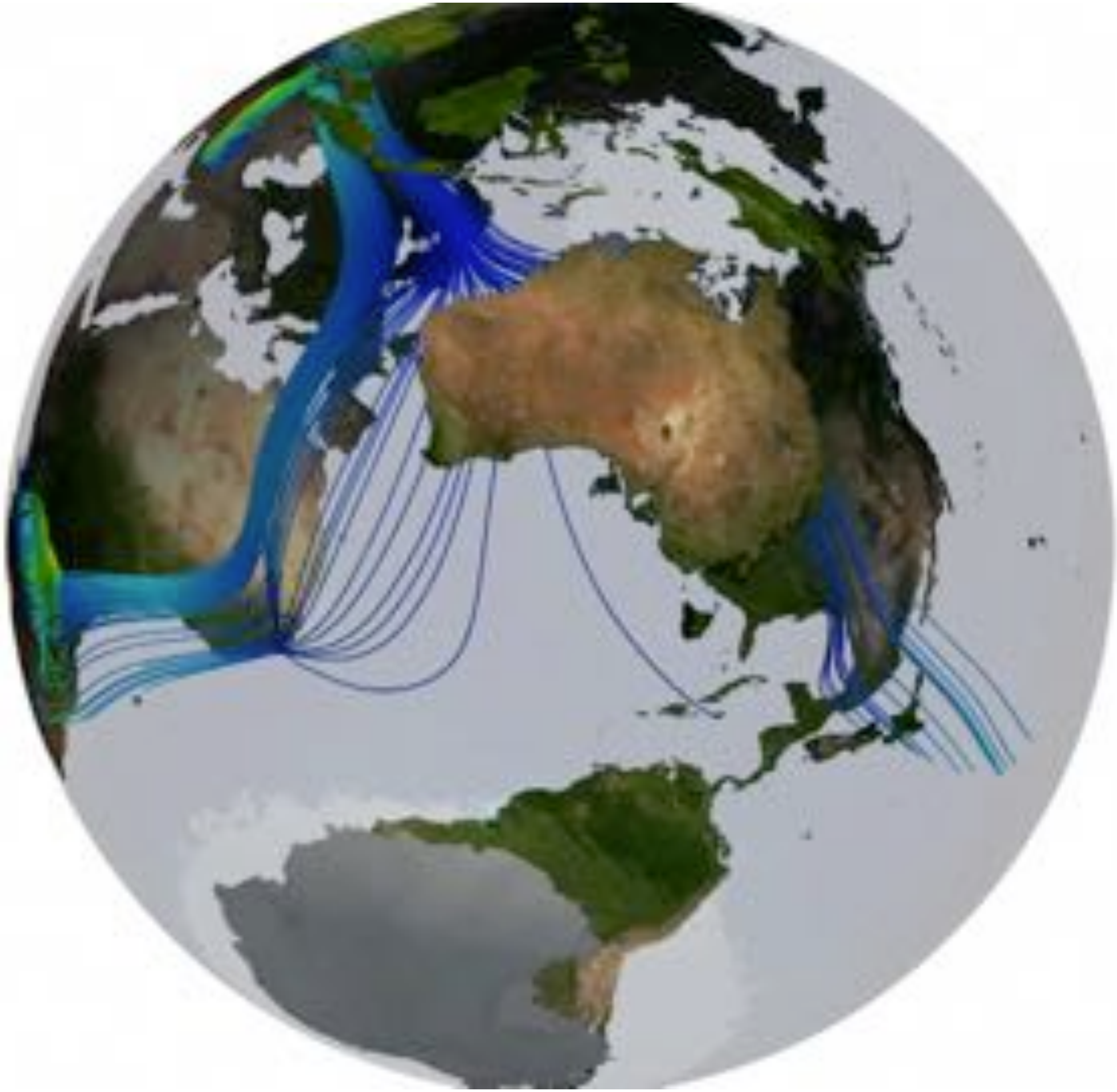
$$
\begin{aligned}
\mathbf{a}(\mathbf{u}_l, \mathbf{v}_l) + \mathbf{b}(\mathbf{v}_l, p_l) &= \mathbf{L}(\mathbf{v}_l) && \forall\, \mathbf{v}_l \in \mathbf{V}_l, \\
\mathbf{b}(\mathbf{u}_l, q_l) - \mathbf{c}(p_l, q_l) &= 0 && \forall\, q_l \in Q_l,
\end{aligned}
$$

with: $\mathbf{a}(\mathbf{u}, \mathbf{v}) := \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v}\, dx, \quad \mathbf{b}(\mathbf{u}, q) := -\int_\Omega \mathrm{div}\,\mathbf{u} \cdot q\, dx$

Schur-complement formulation:

$$
\begin{bmatrix} \mathbf{A}_l & \mathbf{B}_l^\top \\ 0 & \mathbf{C}_l + \mathbf{B}_l \mathbf{A}_l^{-1} \mathbf{B}_l^\top \end{bmatrix} \begin{bmatrix} \underline{\mathbf{u}}_l \\ \underline{p}_l \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{f}}_l \\ \mathbf{B}_l \mathbf{A}_l^{-1} \underline{\mathbf{f}}_l \end{bmatrix}
$$

Stationary Flow Field



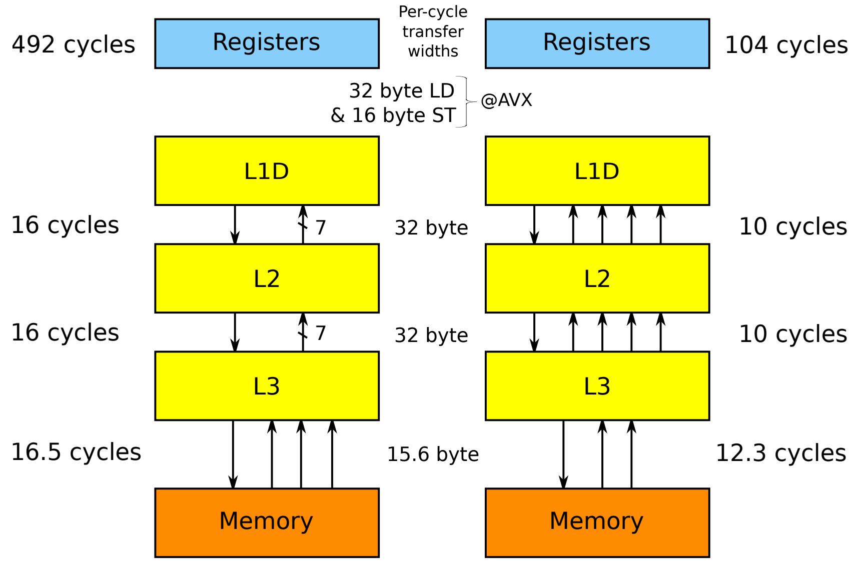
Exploring the Limits …

Gmeiner B., Huber M, John L, UR, Wohlmuth, B: A quantitative performance study for Stokes solvers at the extreme scale, Journal of Computational Science, 2016.

- Multigrid with Uzawa smoother
- Optimized for minimal memory consumption
  - 10^{13} Unknowns correspond to 80 TByte for the solution vector
  - Juqueen has 450 TByte Memory
  - matrix free implementation essential

is this the largest FE system solved to date?

nodes	threads	DoFs	iter	time	time w.c.g.	time c.g. in %
5	80	$2.7 \cdot 10^9$	10	685.88	678.77	1.04
40	640	$2.1 \cdot 10^{10}$	10	703.69	686.24	2.48
320	5 120	$1.2 \cdot 10^{11}$	10	741.86	709.88	4.31
2 560	40 960	$1.7 \cdot 10^{12}$	9	720.24	671.63	6.75
20 480	327 680	$1.1 \cdot 10^{13}$	9	776.09	681.91	12.14



ECM Analysis of multigrid smoother for variable/constant coefficient performance

Towards systematic performance engineering:

Parallel Textbook Efficiency
as guiding design principle

Brandt, A. (1998). Barriers to achieving **textbook multigrid efficiency** (TME) in CFD.

Thomas, J. L., Diskin, B., & Brandt, A. (2003). **Textbook Multigrid Efficiency** for Fluid Simulations*. Annual review of fluid mechanics, 35(1), 317-340.

Gmeiner, UR, Stengel, Waluga, Wohlmuth: Towards **Textbook Efficiency for Parallel Multigrid**, Journal of Numerical Mathematics: Theory, Methods and Applications, 2015

Gmeiner, Huber, John, UR, Wohlmuth, A quantitative **performance study for Stokes solvers** at the extreme scale, Journal of Computational Science, Volume 17, 2016, Pages 509-521

Textbook Multigrid Efficiency (TME)

„Textbook multigrid efficiency means solving a discrete PDE problem with a computational effort that is only a small (less than 10) multiple of the operation count associated with the discretized equations itself." [Brandt, 98]

- work unit (**WU**) = single elementary relaxation
  classical ***algorithmic*** TME-factor:
  ops for solution/ ops for work unit
- Here we introduce a new
  parallel TME-factor:
  - algorithmic efficiency
  - scalability & node efficiency

ParTME paradigm for parallel performance analysis

- Analyse **cost of an elementary** relaxation to define cost of work unit (WU) depending on idealized HW
  - micro-kernel benchmarks
  - measure aggregate performance
- Measure **parallel solver performance**
- Compute ParTME factor as quotient

Parallel TME

μ_{sm} # of elementary relaxation steps on single core/sec

U # cores

$U\mu_{\mathrm{sm}}$ aggregate peak relaxation performance

$T_{\mathrm{WU}}(N,U) = \frac{N}{U\mu_{\mathrm{sm}}}$ **idealized** time for a work unit

$T(N,U)$ time to solution for N unknowns on U cores

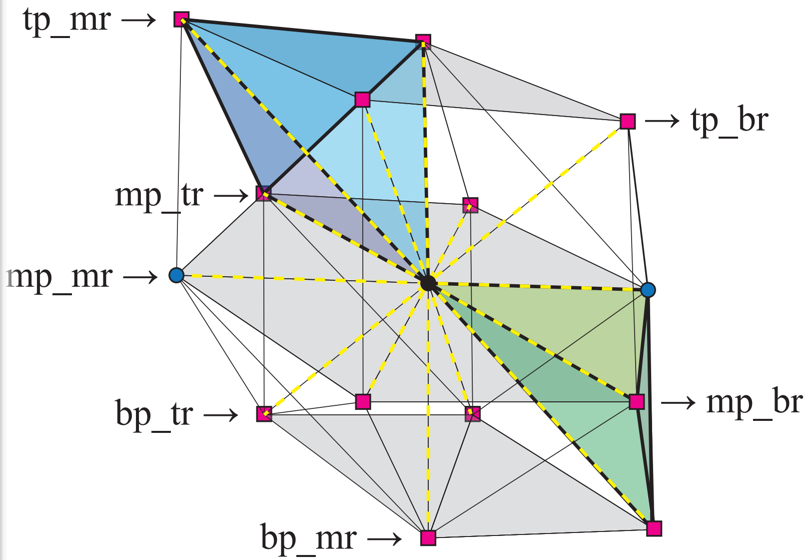
Parallel textbook efficiency factor

$$\boxed{E_{\mathrm{ParTME}}(N,U) = \frac{T(N,U)}{T_{\mathrm{WU}}(N,U)} = T(N,U)\frac{U\mu_{\mathrm{sm}}}{N}}$$

combines **algorithmic** and **implementation** efficiency.

TME Efficiency Analysis: RB-GS Smoother

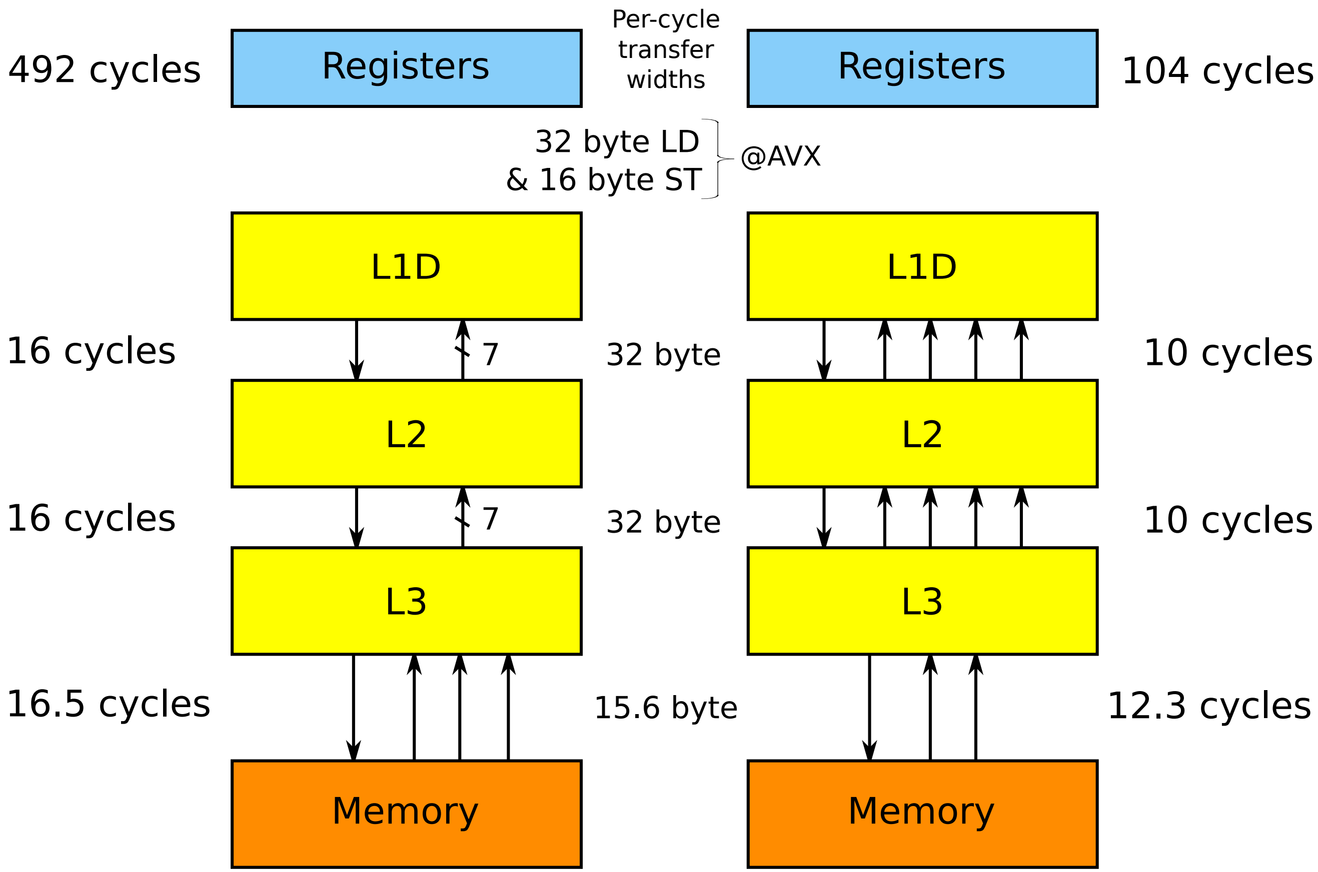
```
for (int i=1; i < (tsize-j-k-1); i=i+2) {
   u[mp_mr+i] = c[0] * (
    -c[1] *u[mp_mr+i+1] - c[2] *u[mp_tr+i-1] -
     c[3] *u[mp_tr+i]   - c[4] *u[tp_br+i]   -
     c[5] *u[tp_br+i+1] - c[6] *u[tp_mr+i-1] -
     c[7] *u[tp_mr+i]   - c[8] *u[bp_mr+i]   -
     c[9] *u[bp_mr+i+1] - c[10]*u[bp_tr+i-1] -
     c[11]*u[bp_tr+i]   - c[12]*u[mp_br+i]   -
     c[13]*u[mp_br+i+1] - c[14]*u[mp_mr+i-1] +
     f[mp_mr+i] );
```



- This loop should be executed on **single SuperMuc core** at
  - 720 M updates/sec (*in theory* - peak performance)
  - μ_{sm} = **176 M** updates/sec (*in practice* - memory access bottleneck; RB-ordering prohibits vector loads)
- Thus **whole SuperMuc** should perform
  - $U\mu_{\mathrm{sm}}$ = 147456*176M ≈ **26 T** (updates/sec)

Execution-Cache-Memory Model (ECM)

Hager et al. Exploring performance and power properties of modern multi−core chips via simple machine models. Concurrency and Computation: Practice and Experience, 2013.



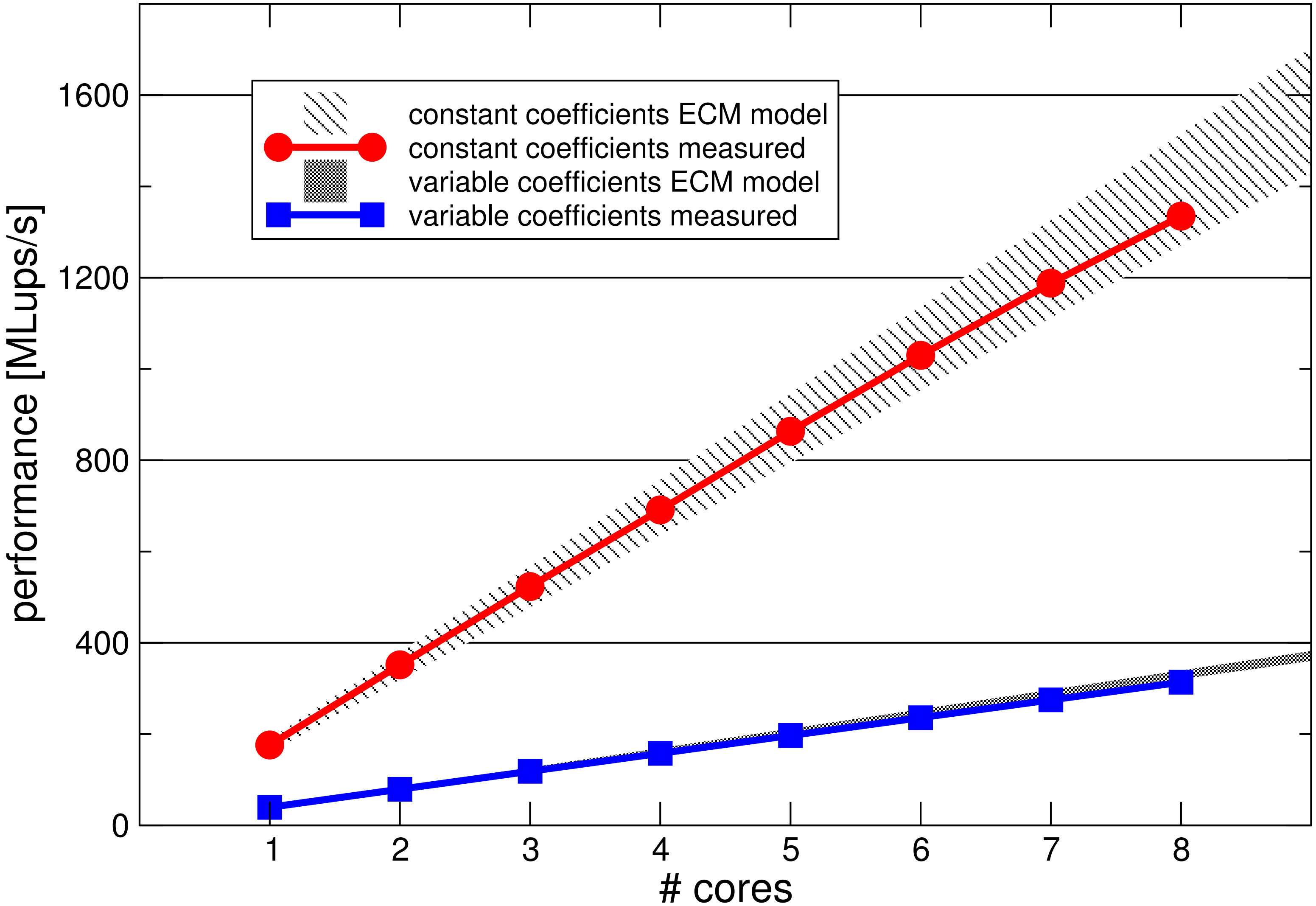
Variable coefficients   Constant coefficients

ECM model for the 15-point stencil on SNB core.

Arrow indicates a 64 Byte cache line transfer.

Run-times represent 8 elementary updates.

ECM: single-chip prediction vs. measurement



Sandy Bridge single-chip performance scaling of the stencil smoothers on 256^3 grid points. Measured data and ECM prediction ranges shown.

ParTME results for Stokes system

Gmeiner, Huber, John, UR, Wohlmuth, A quantitative performance study for Stokes solvers at the extreme scale, Journal of Computational Science, vol.17, 2016, pp. 509-521

Drzisga, D., John, L., UR, Wohlmuth, B., & Zulehner, W. (2018). On the Analysis of Block Smoothers for Saddle Point Problems. *SIAM Journal on Matrix Analysis and Applications*, *39*(2), 932-960.

	TME	ParTME				
DoFs		8.2×10^6	5.3×10^8	4.3×10^9	3.4×10^{10}	2.7×10^{11}
cores		1	192	1536	12288	98304
FMG-1V(2,2)	9.07	43.43	150	200	278	500

- variable V-cycle, Uzawa-type smoother
- TME factor <10
- ParTME factor >200
- coarse grid solver becomes a bottleneck

Nevertheless we are reaching **10^{13}** unknowns.

Redesigning the HHG prototype
Hybrid Tetrahedral Grids - HyTeG

- Geometric and algebraic multigrid solvers with scalable complexity
  - Scalable solvers
  - Robust higher order discretization (Fast4HHO, EoCoE)
  - Scalable & Robust Coarse Grid solvers, MUMPS, …
  - …
- Advanced algorithms with potential for exascale computing
  - Matrix-free Methods (EoCoE)
  - Algorithm Based Fault Tolerance, ABFT
  - …
- Software for ExaScale Computing
  - TerraNeo Project
  - HyTeG Software (HHG)
  - …

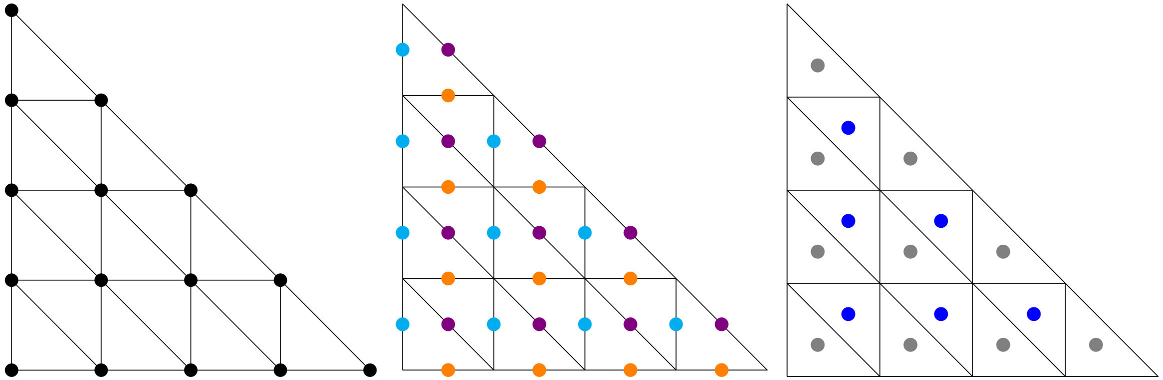
Bauer, S., Mohr, M., UR, Weismüller, J., Wittmann, M., & Wohlmuth, B. (2017). A two-scale approach for efficient **on-the-fly operator assembly** in massively parallel high performance multigrid codes. *Applied Numerical Mathematics*, *122*, 14-38.

Bauer, S., Drzisga, D., Mohr, M., UR, Waluga, C., & Wohlmuth, B. (2017). A stencil scaling approach for accelerating **matrix-free** finite element implementations. *arXiv preprint arXiv:1709.06793 (submitted to SISC)*

Kohl, N., Thönnes, D., Drzisga, D., Bartuschat, D., UR (2018). The **HyTeG** finite-element software framework for scalable multigrid solvers. *International Journal of Parallel, Emergent and Distributed Systems*, 1-20.

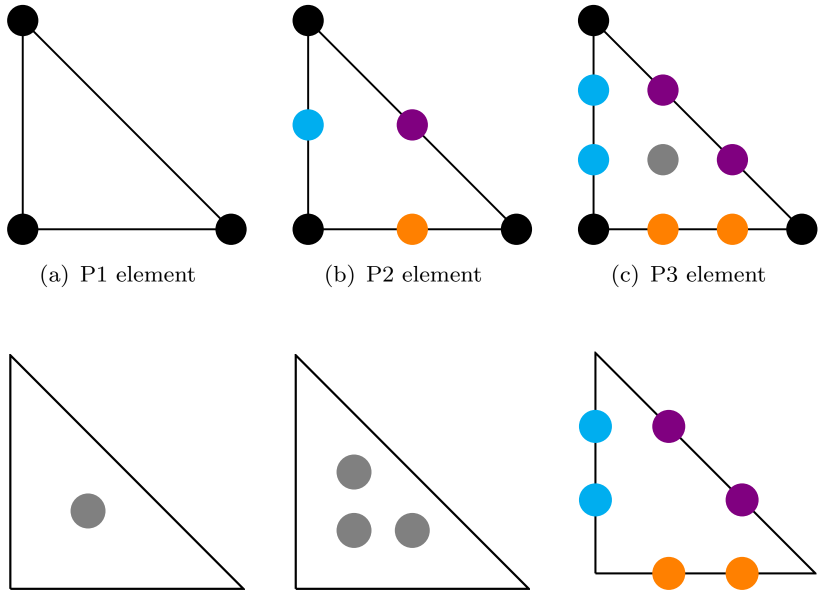
HyTeG: Hybrid tetrahedral grids

- Generalizes HHG mesh structures for arbitrary discretizations
- Structured-within-unstructured mesh



(a) vertex DoFs (b) edge DoFs (c) face DoFs

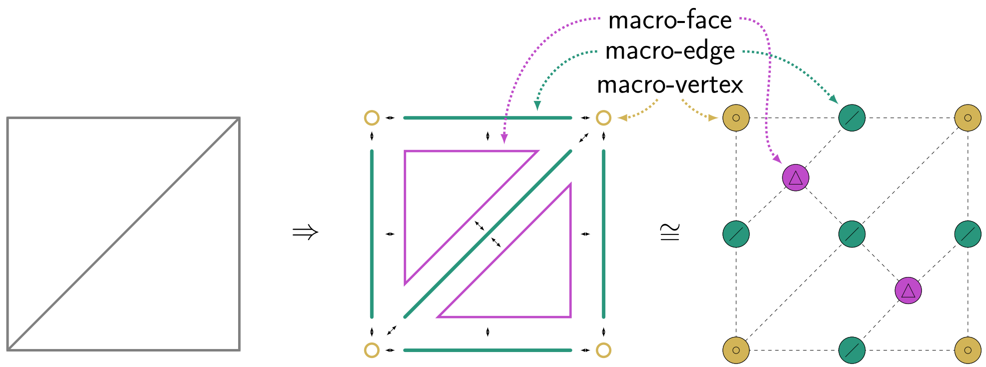
Geometric structure



(a) P1 element (b) P2 element (c) P3 element

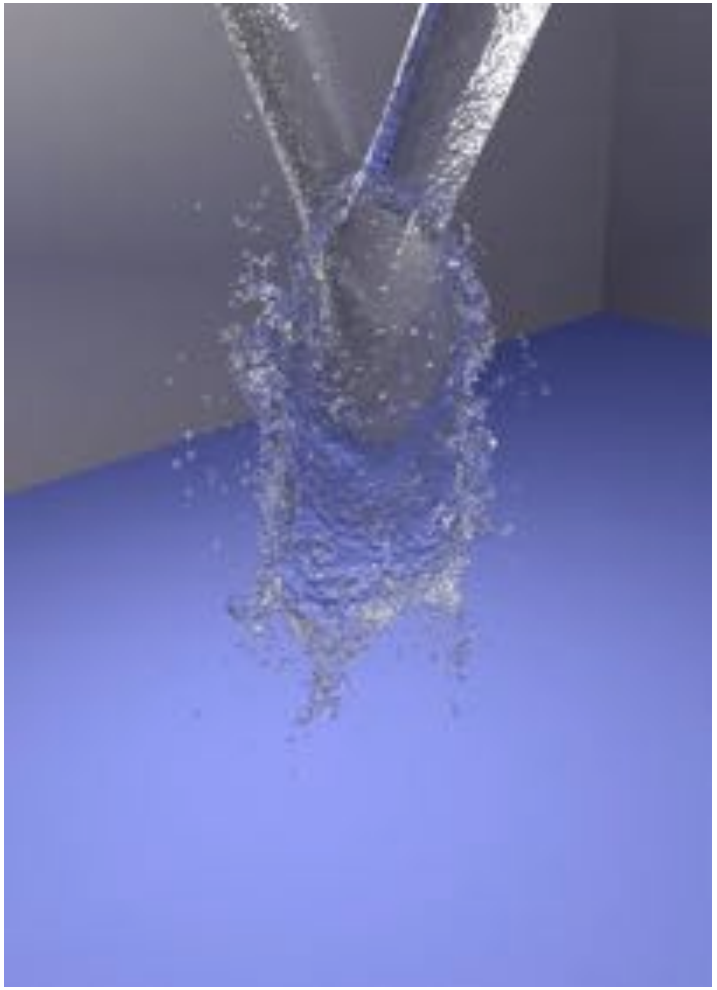
(d) FV/DG0 element (e) DG1 (C) element (f) DG1 (E) element

Example element types



unstructured mesh macro-primitives graph representation

Topological structure



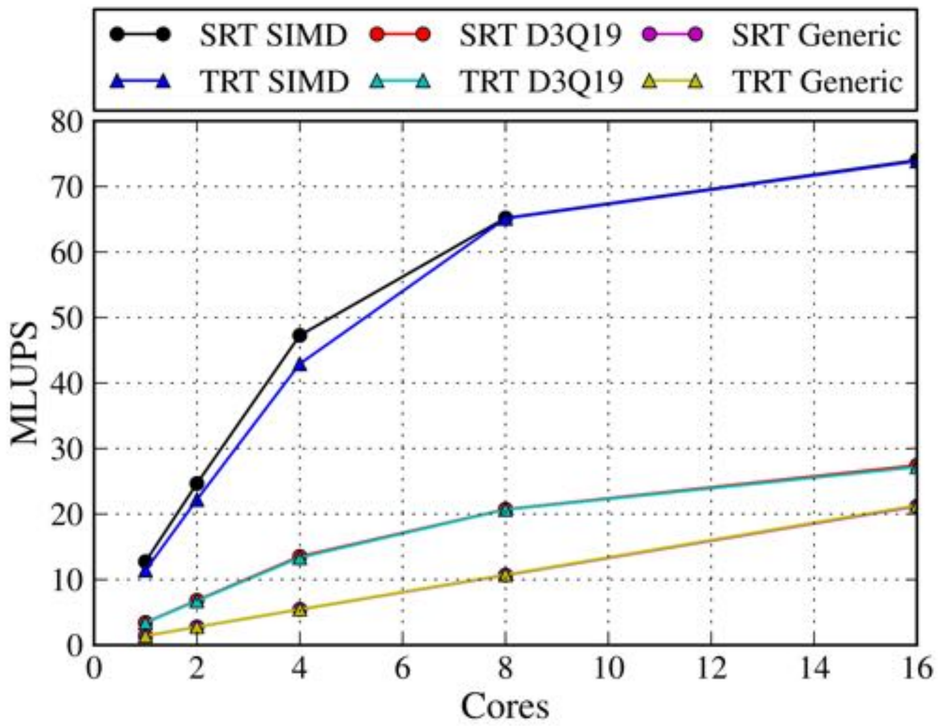
Part III: Lattice Boltzmann

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

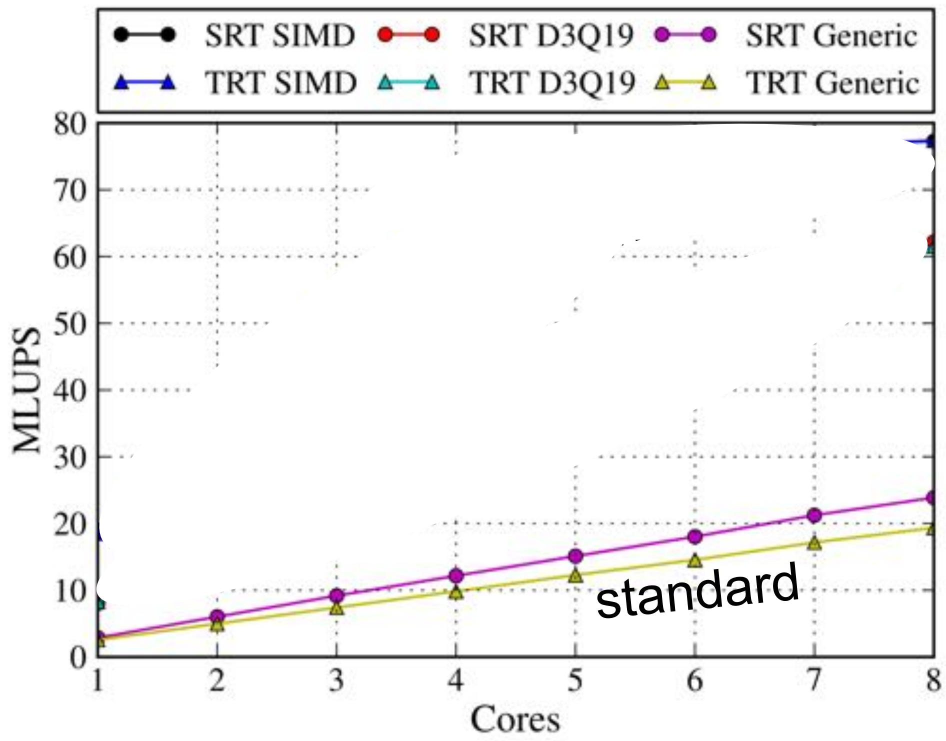
Feichtinger, C., Donath, S., Köstler, H., Götz, J., & Rüde, U. (2011). WaLBerla: HPC software design for computational engineering simulations. *Journal of Computational Science*, *2*(2), 105-112.

Single Node Performance

JUQUEEN



SuperMUC

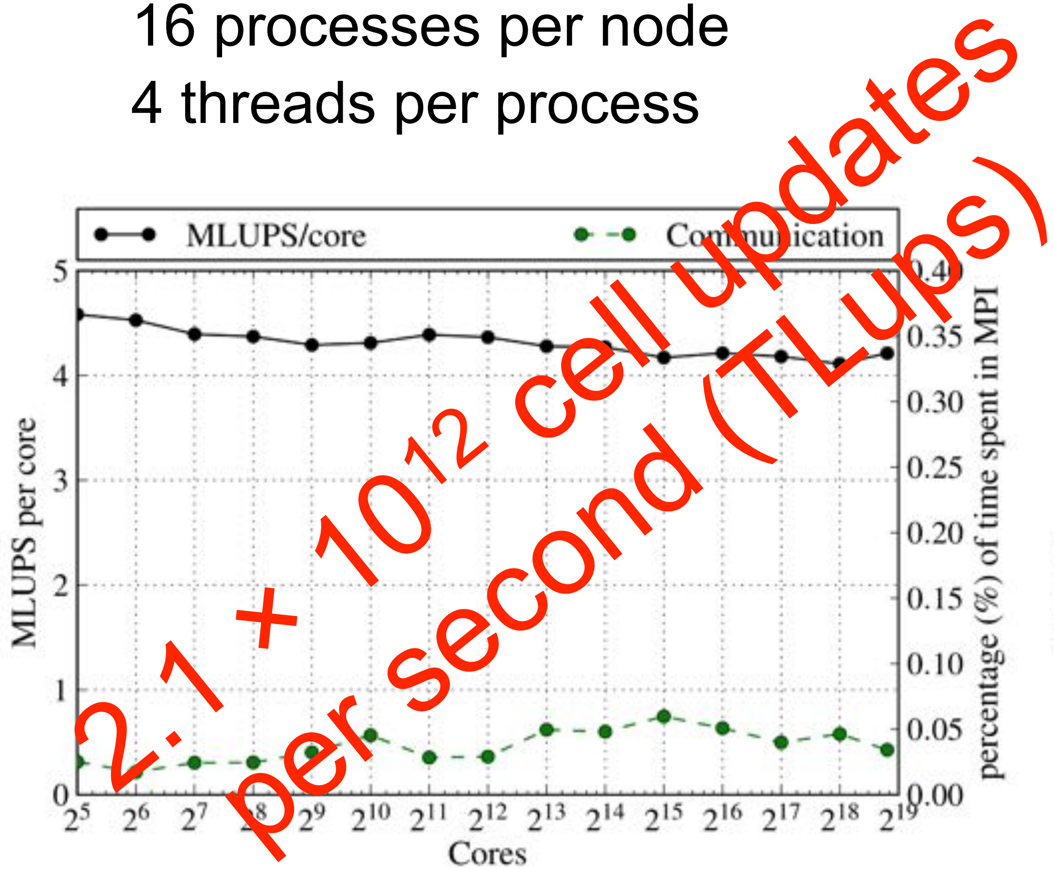


Pohl, T., Deserno, F., Thürey, N., UR, Lammers, P., Wellein, G., & Zeiser, T. (2004). Performance evaluation of parallel large-scale lattice Boltzmann applications on three supercomputing architectures. *Proceedings of the 2004 ACM/IEEE conference on Supercomputing* (p. 21). IEEE Computer Society.

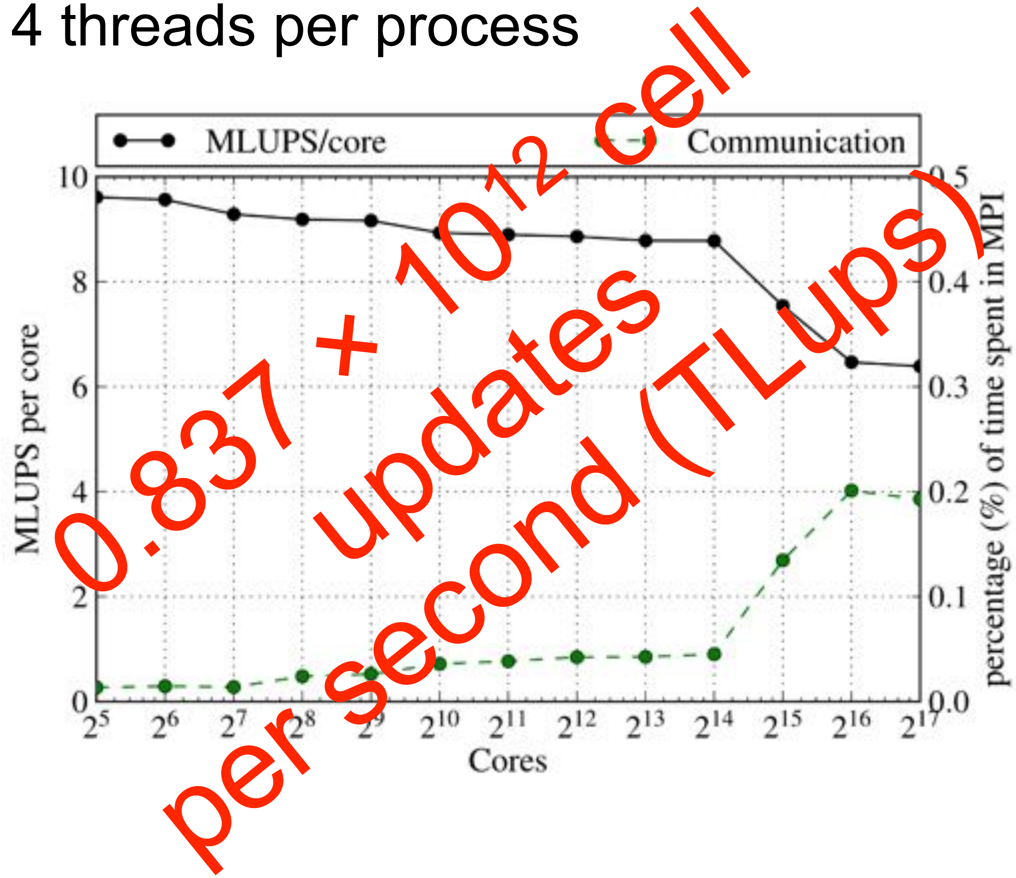
Donath, S., Iglberger, K., Wellein, G., Zeiser, T., Nitsure, A., & UR (2008). Performance comparison of different parallel lattice Boltzmann implementations on multi-core multi-socket systems. *International Journal of Computational Science and Engineering*, *4*(1), 3-11.

Weak scaling for TRT lid driven cavity - uniform grids

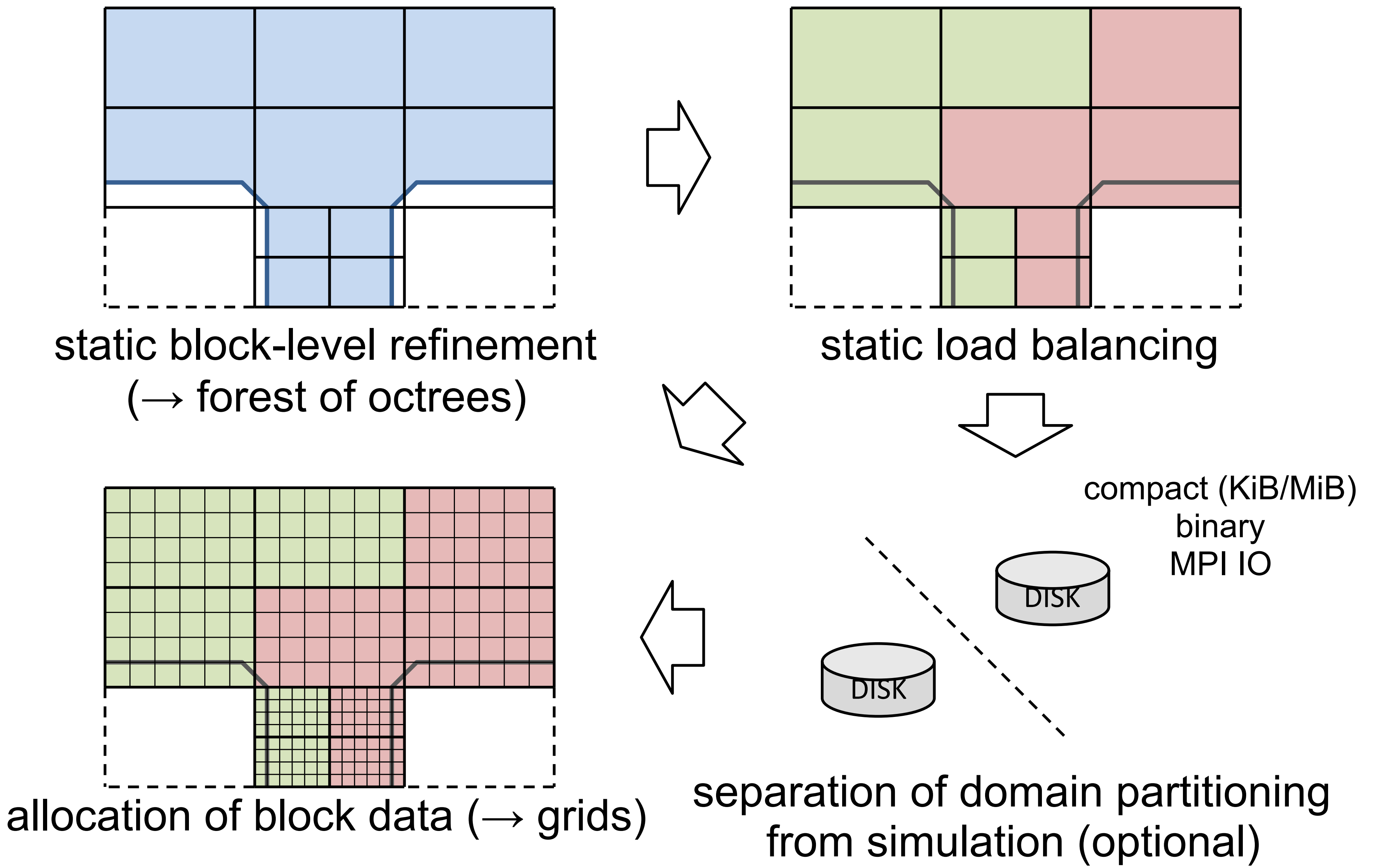
JUQUEEN
16 processes per node
4 threads per process



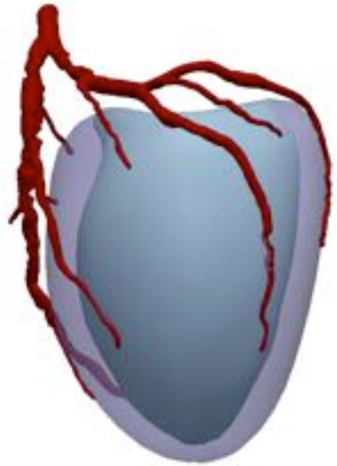
SuperMUC
4 processes per node
4 threads per process



Domain Partitioning and Parallelization



Performance on Coronary Arteries Geometry



Color coded proc assignment

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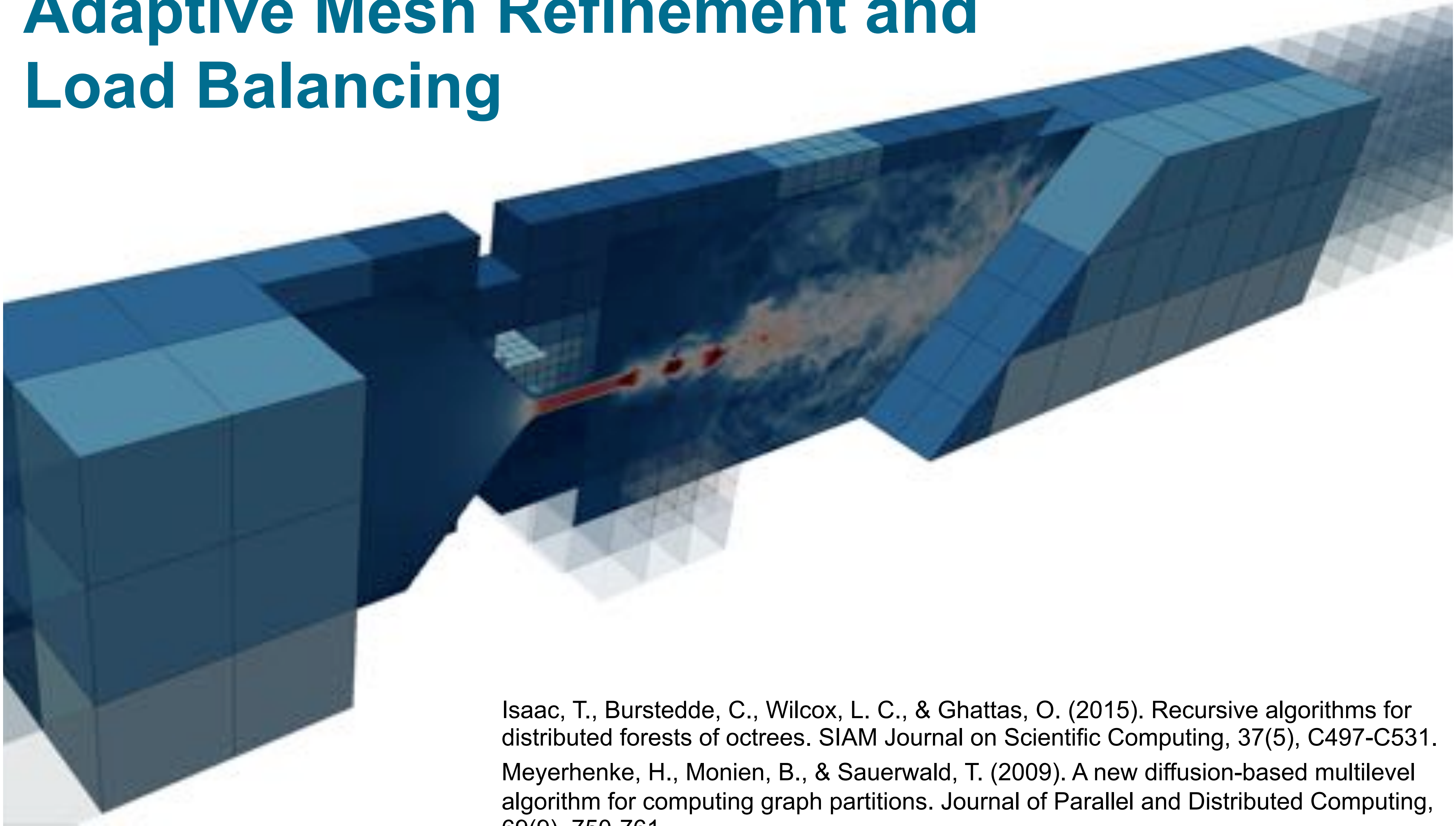
- **Weak scaling**
  458,752 cores of JUQUEEN
  over a trillion (10^{12}) fluid lattice cells
- **Strong scaling**
  32,768 cores of SuperMUC
  - cell sizes of 0.1 mm
  - 2.1 million fluid cells
  - 6000 time steps per second

Adaptive Mesh Refinement and Load Balancing



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

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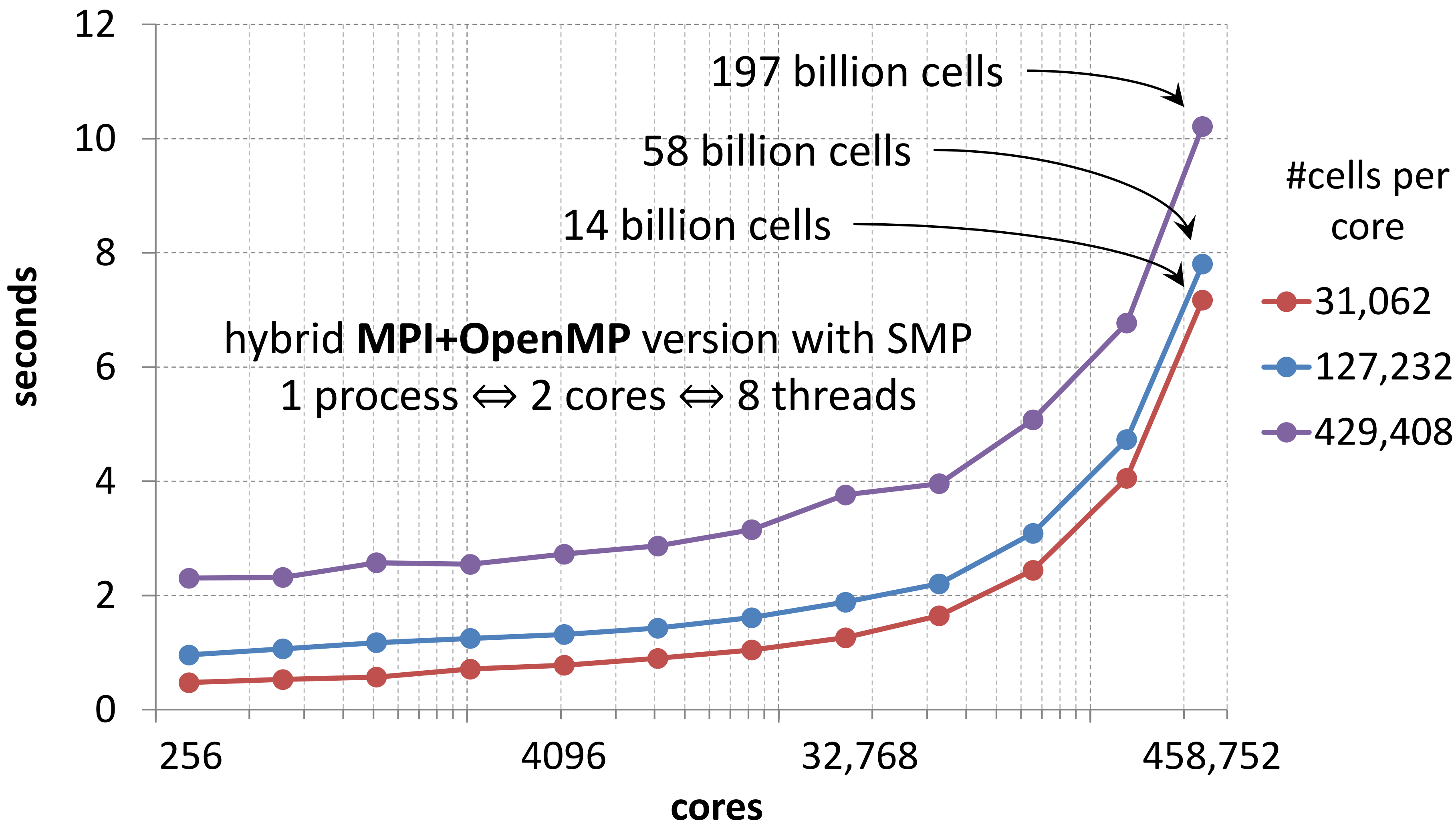
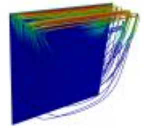
AMR Performance

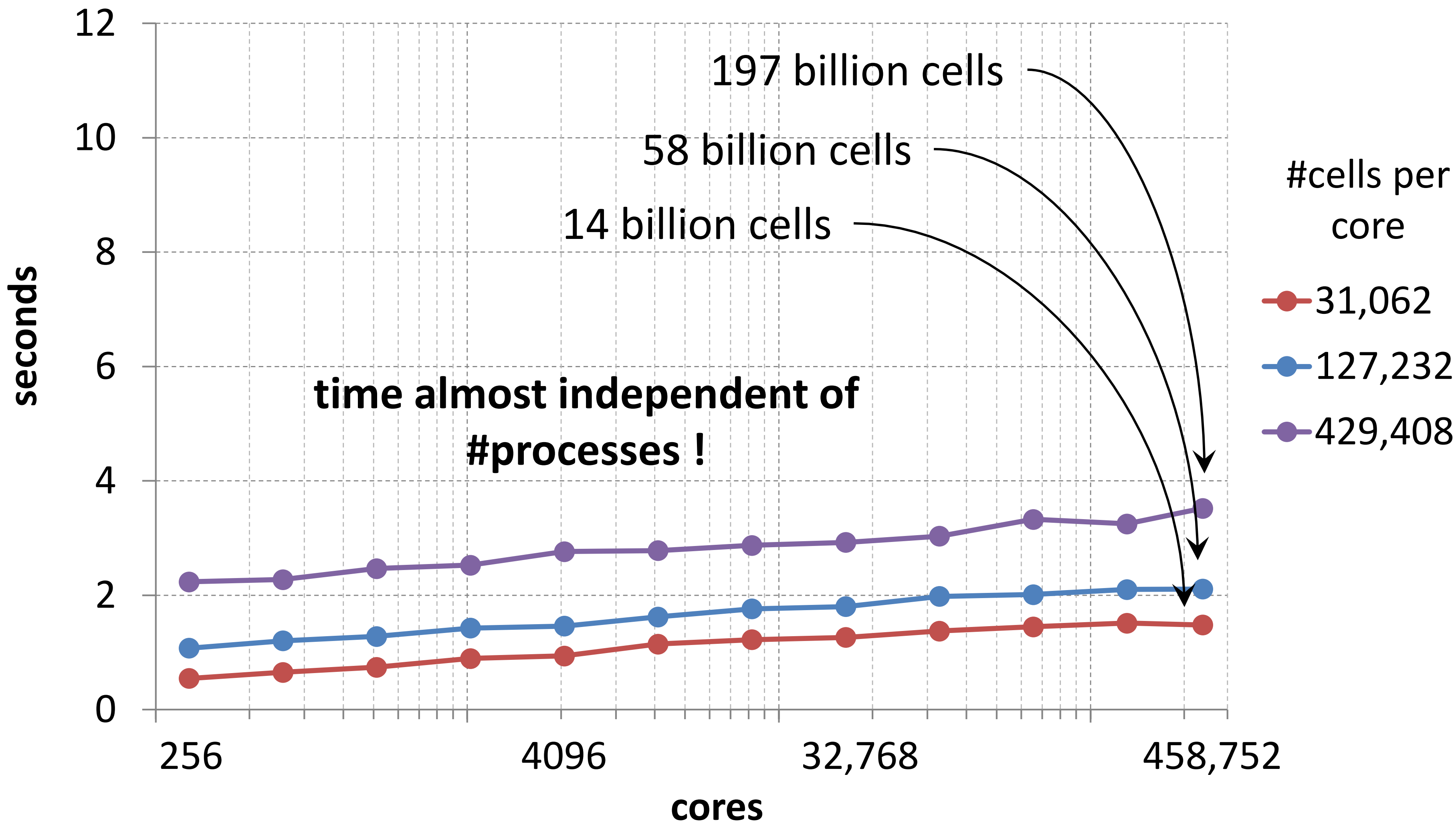
- JUQUEEN – space filling curve: Morton



AMR Performance

- JUQUEEN – diffusion load balancing

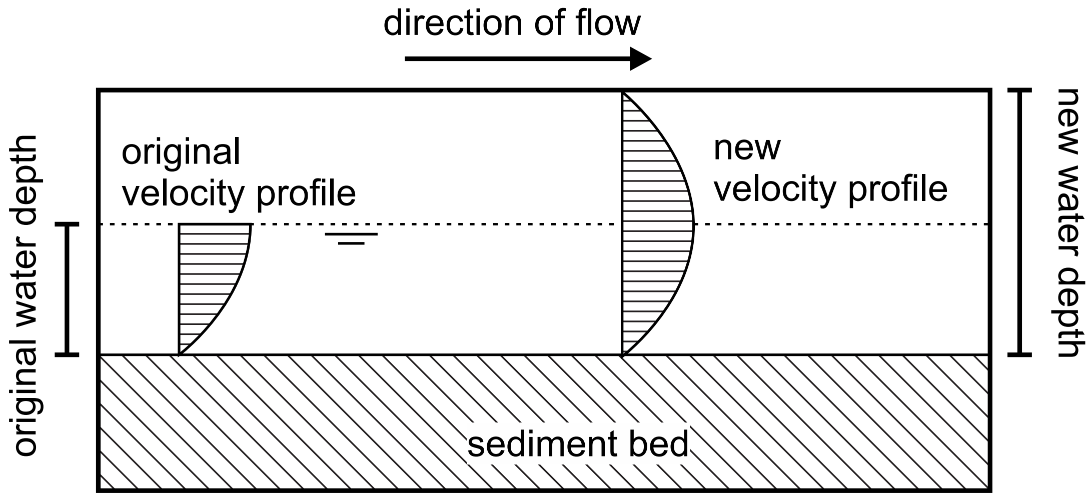


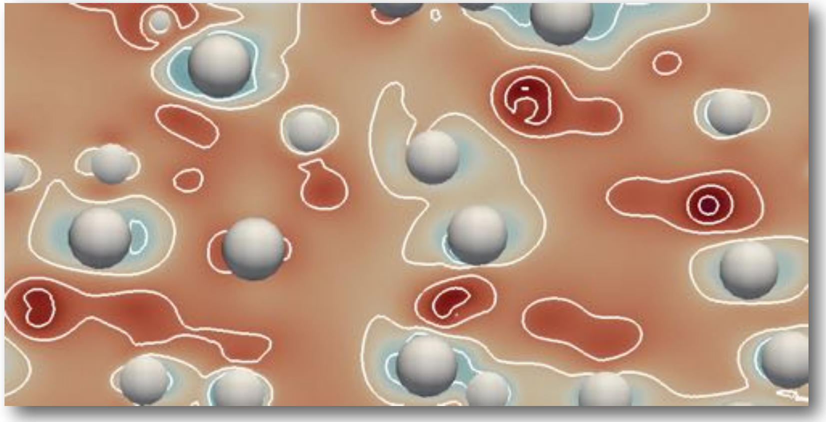


Application Example:

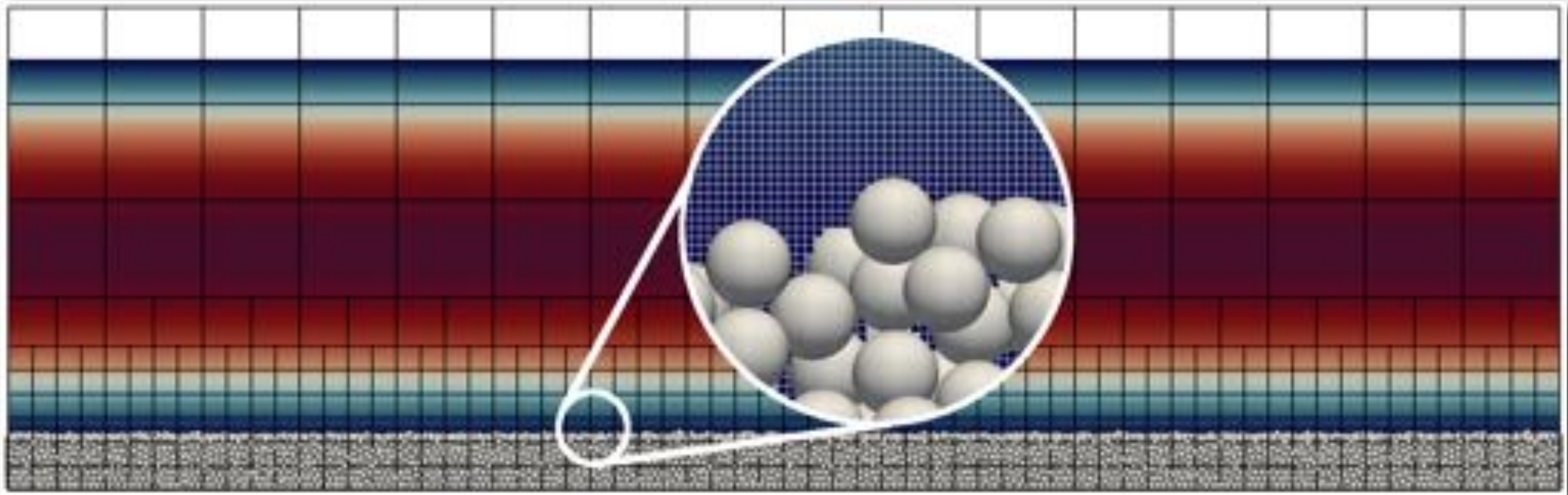
Direct simulation of complex fluids

Simulation of suspended particle transport





shear stress at bed surface



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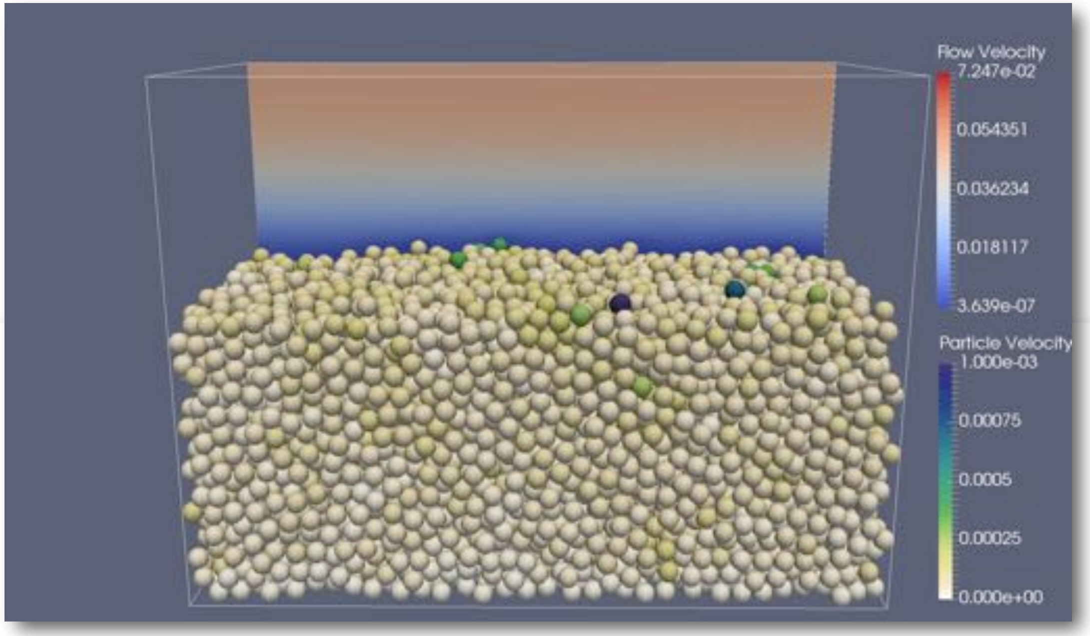
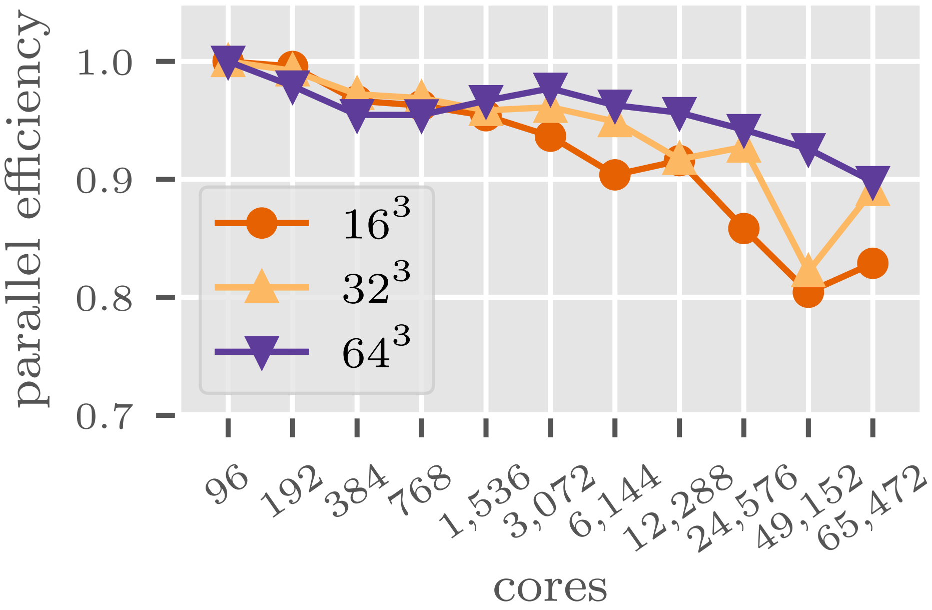
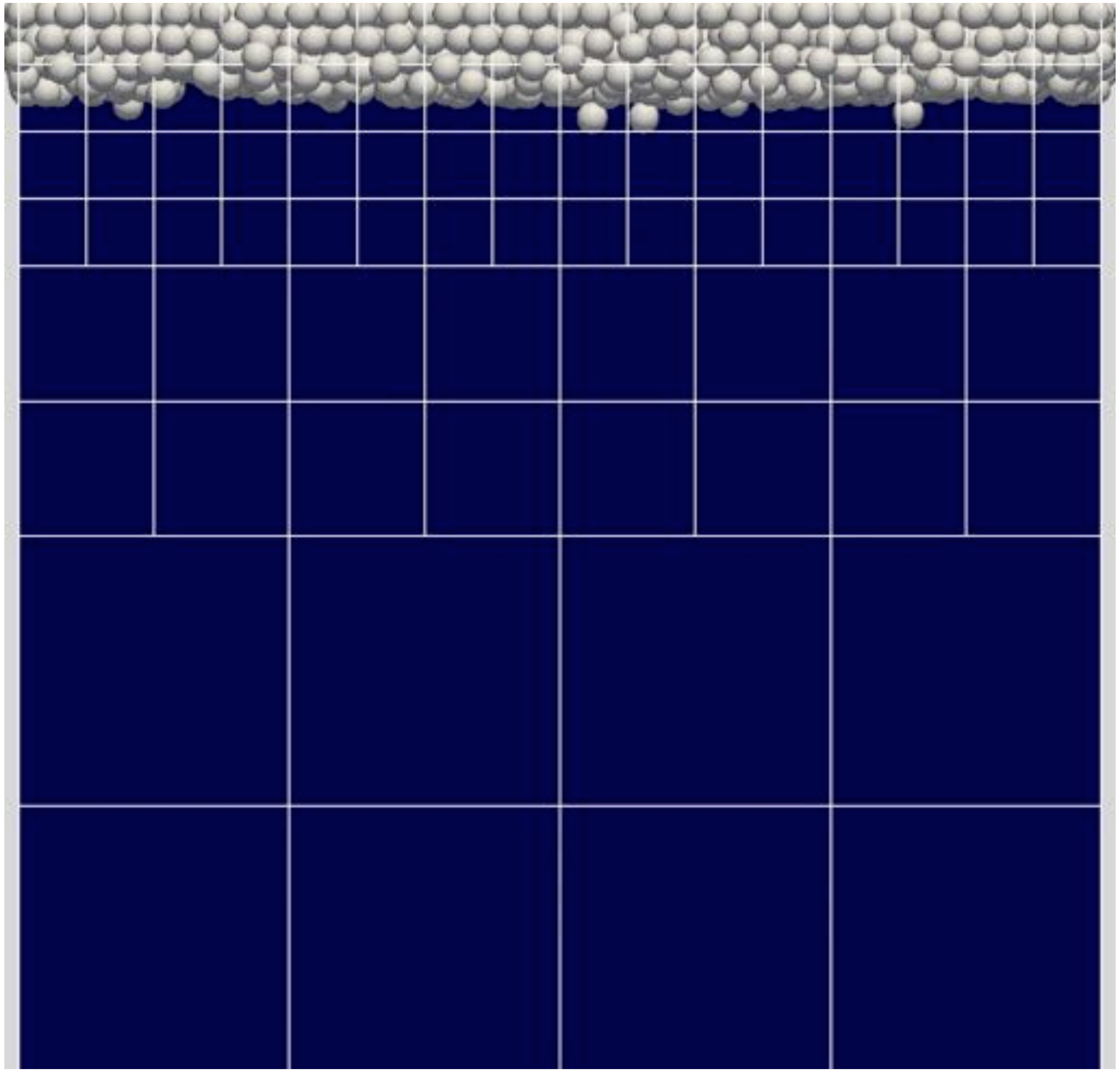
Simulation of suspended particle transport





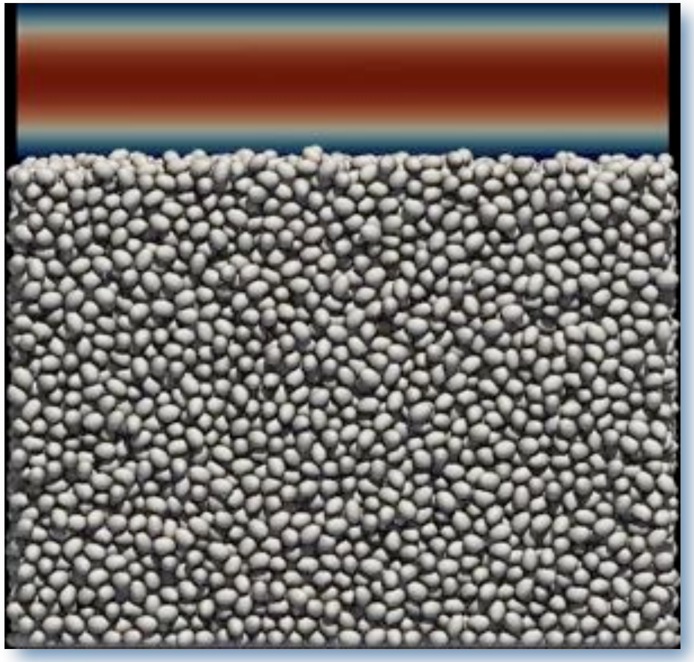
$0.864*10^9$ LBM cells; 350 000 spherical particles

Sedimentation and fluidized beds

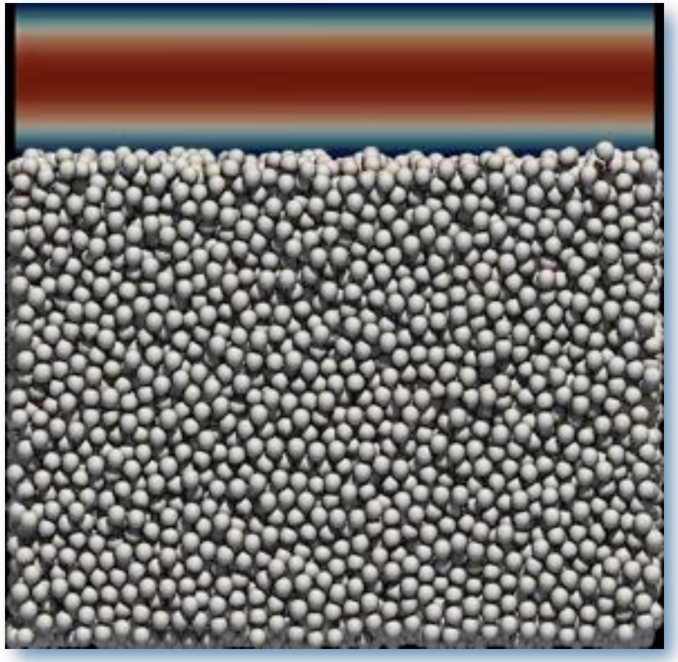


- 3 levels mesh refinement
- 3800 spherical particles
- Galileo number 50
- 128 processes
- 1024-4000 blocks
- Block size 32^3

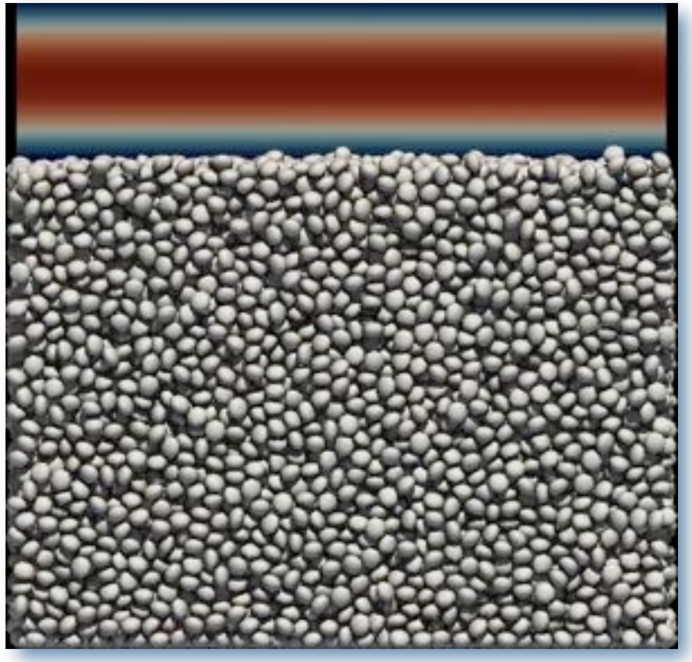
Study of particle shape effects



prolate



spherical



oblate

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Rettinger, C., UR (2018). A coupled lattice Boltzmann method and discrete element method for discrete particle simulations of **particulate flows**. *Computers & Fluids*.

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Eibl, S., UR (2018). A Systematic Comparison of Dynamic **Load Balancing** Algorithms for Massively Parallel Rigid Particle Dynamics. *arXiv preprint arXiv:1808.00829*.

Why are these codes so fast?

~~Optimizing~~ Pessimizing the Performance

with greetings from D. Bailey's: *Twelve Ways to Fool the Masses...*

Pessimize ↓

- traverse memory in unfavorable order, ignore caches, use many small MPI messages
  - **$10^{13} \rightarrow 10^{12}$ unknowns**
- Do not use a matrix-free implementation: a single multiplication with the mass and stiffness matrix can easily cost 50 memory accesses
  - **$10^{12} \rightarrow 10^{11}$ unknowns**
- Write „generic code“: implement unstructured grids, pointers, using extensively indirect memory access
  - **$10^{11} \rightarrow 10^{10}$ unknowns**
- algorithmic overhead: check convergence redundantly, use an expensive error estimator, etc.
  - **$10^{10} \rightarrow 10^{9}$ unknowns**
    (... still a large system ...)

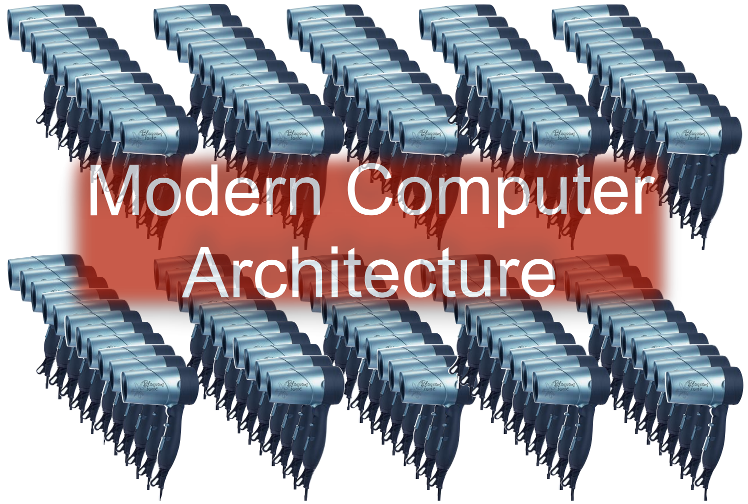
Optimize ↑

Why is optimization hard?

Would you want to propel a Superjumbo

with four strong jet engines

or with 1,000,000 blow dryer fans?



The End of Moore's Law

We are used to 1000x improvement per decade through:

- Transistor Scaling - this will come to a halt

We must change strategy:

- Architectural „improvements“ (GPU, manycore)
- Algorithms
- Implementation

Moore's *deflation of computational cost* has dictated the economics of computing - and now this will gradually change.

In the coming decade …

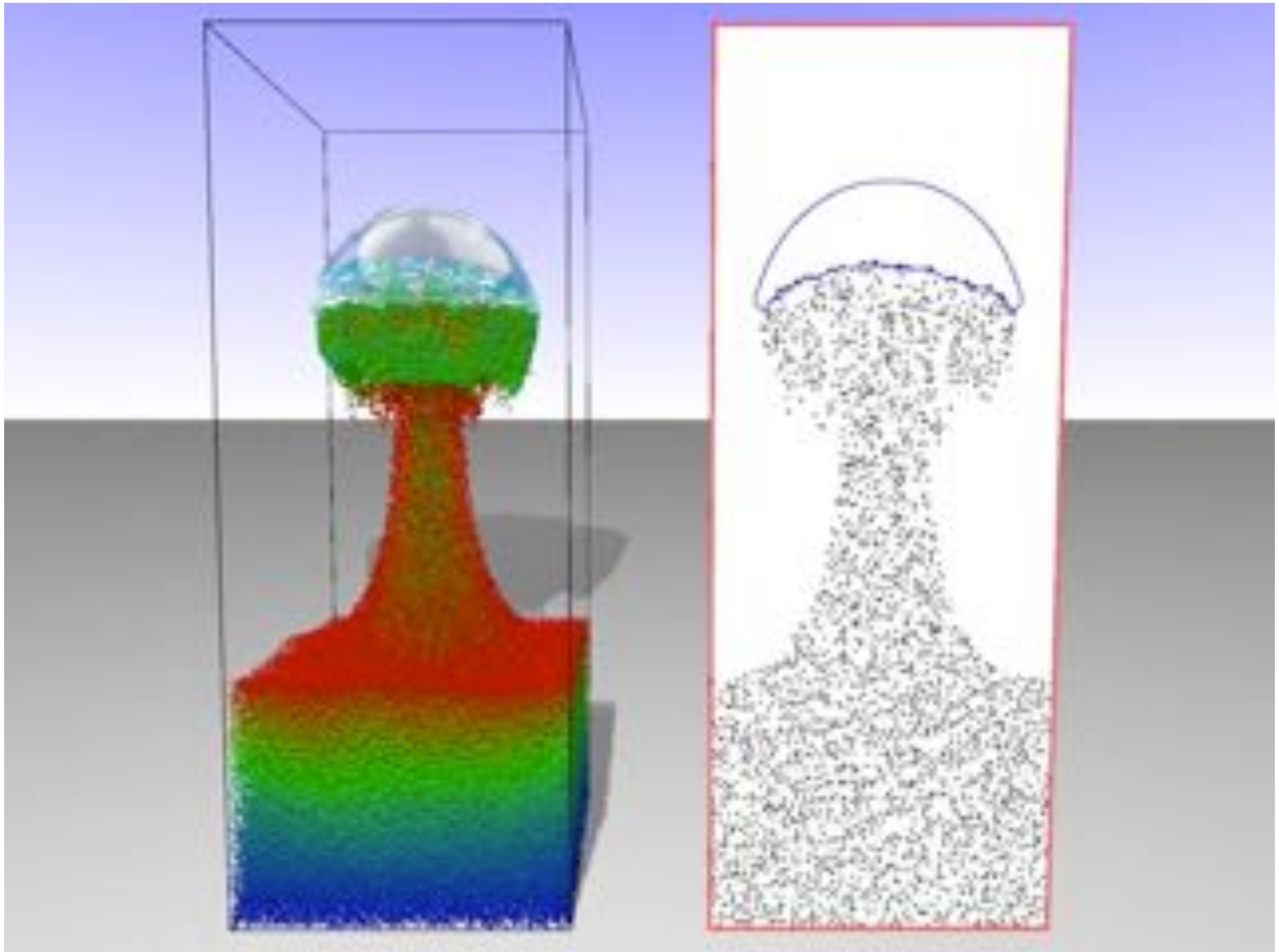
- absolute „performance“ instead of „scalability“
- We will gradually refactor/redesign many of today’s application codes
  - it is not a question of cost but of development time
- Gradual shift of investments from HW to SW
  - slowdown of HW investment cycles
  - performance improvements through „performance engineering“

Computational Science is done in Teams

- Dr.-Ing. Dominik Bartuschat
- Martin Bauer, M.Sc. (hons)
- Dr. Regina Degenhardt
- Sebastian Eibl, M. Sc.
- Dipl. Inf. Christian Godenschwager
- Marco Heisig, M.Sc.(hons)
- PD Dr.-Ing. Harald Köstler
- Nils Kohl, M. Sc.
- Sebastian Kuckuk, M. Sc.
- Christoph Rettinger, M.Sc.(hons)
- Jonas Schmitt, M. Sc.
- Dipl.-Inf. Florian Schornbaum
- Dominik Schuster, M. Sc.
- Dominik Thönnes, M. Sc.

- Dr.-Ing. Benjamin Bergen
- Dr.-Ing. Simon Bogner
- Dr.-Ing. Stefan Donath
- Dr.-Ing. Jan Eitzinger
- Dr.-Ing. Uwe Fabricius
- Dr. rer. nat. Ehsan Fattahi
- Dr.-Ing. Christian Feichtinger
- Dr.-Ing. Björn Gmeiner
- Dr.-Ing. Jan Götz
- Dr.-Ing. Tobias Gradl
- Dr.-Ing. Klaus Iglberger
- Dr.-Ing. Markus Kowarschik
- Dr.-Ing. Christian Kuschel
- Dr.-Ing. Marcus Mohr
- Dr.-Ing. Kristina Pickl
- Dr.-Ing. Tobias Preclik
- Dr.-Ing. Thomas Pohl
- Dr.-Ing. Daniel Ritter
- Dr.-Ing. Markus Stürmer
- Dr.-Ing. Nils Thürey

Thank you for your attention!



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