OpenLB

Open source Lattice Boltzmann code

NHR PerfLab Seminar – Erlangen, Germany -- October 2023

Facing Challenges in Computational Fluid Mechanics with Lattice Boltzmann Methods, OpenLB and High Performance Computers

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LBRG

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Institute for Applied and Numerical Mathematics (IANM)
Institute of Mechanical Process Engineering an Mechanics (MVM)
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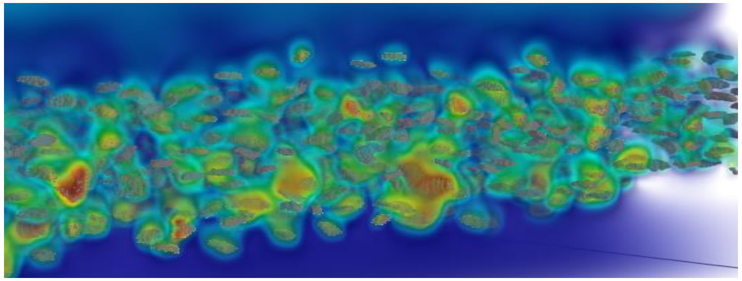
Challenges in (Computational) Fluid Mechanics

Challenge 1: Turbulence

- capture small scales
- models inaccurate or expensive

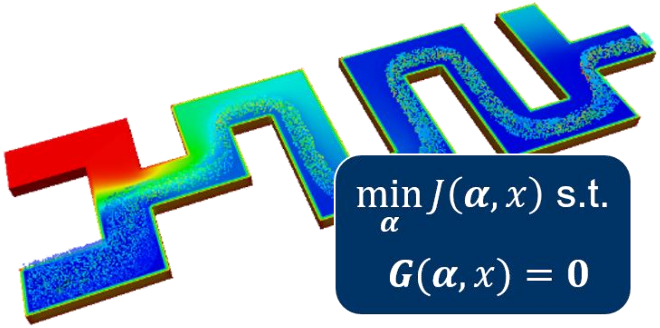
Challenge 2: Suspensions

- capture effects of small particles
- models inaccurate or expensive



Challenge 3: Optimal Control / Optimization

- enable model calibration & optimization
- formulation problem dependent, expensive

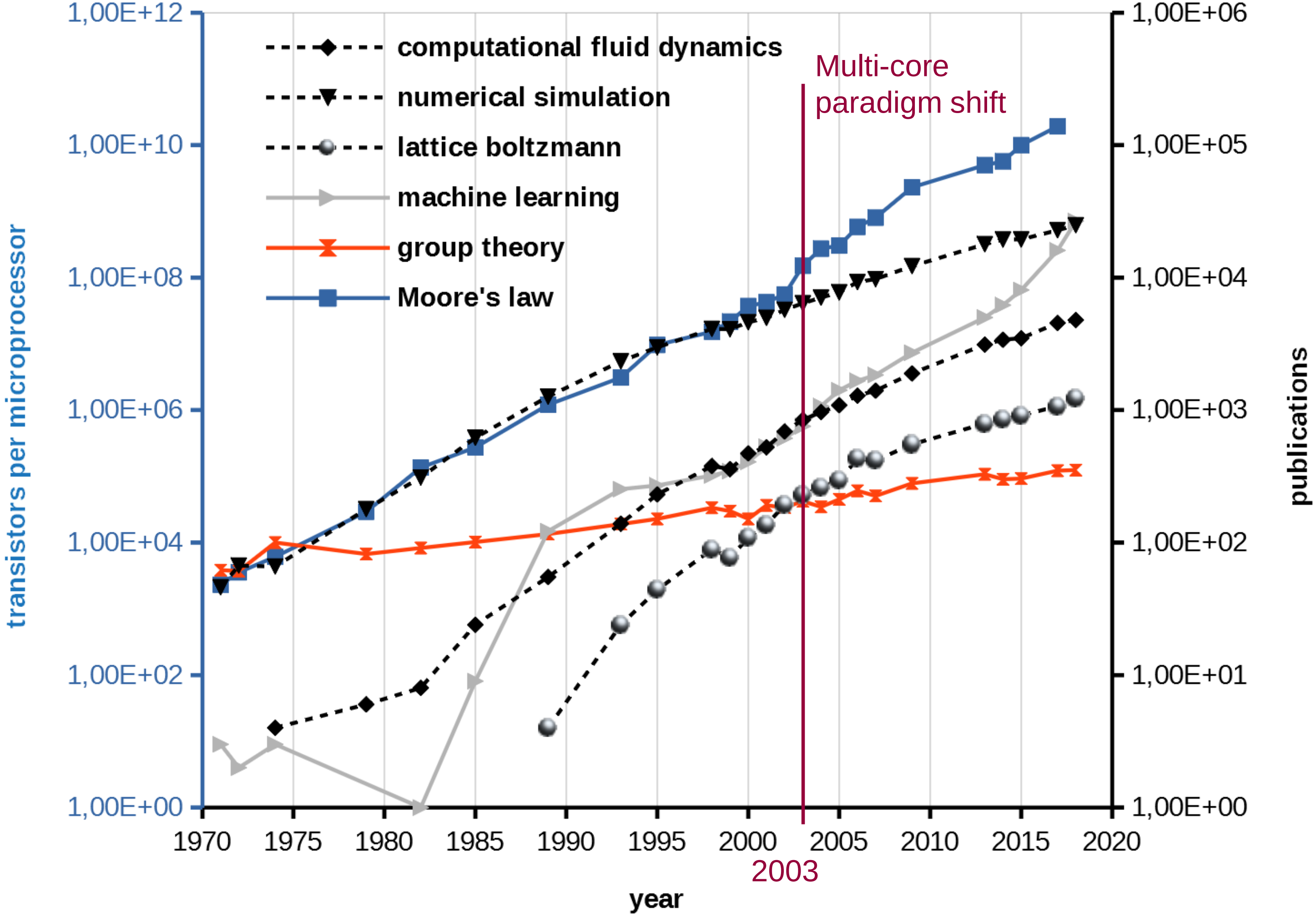


$$\min_{\boldsymbol{\alpha}} J(\boldsymbol{\alpha}, x) \text{ s.t. } \boldsymbol{G}(\boldsymbol{\alpha}, x) = \boldsymbol{0}$$

Kwak, D., Kiris, C., Kim, C. S. (2005) Comput Fluids, 34(3), pp.283-299

Slotnick, J., Khodadoust, A., Alonso, J. *et al.* (2014). NASA *TR*, no. NASA/CR-2014-218178

Facing the Challenges: Compute Power Available



Facing the Challenges: LBRG's Solution Approach

Parallel Homogenized Lattice Boltzmann Methods (HLBM)

- physical mesoscopic model
- algorithmic properties / parallelism
- LB approach as PDE solver

Sustainable Research & Education

- beyond one PhD cycle
- open (source) community
- method AND application view
- interdisciplinary
- modern C++, CI, GIT, ..

Challenge 1:

DNS/LES instead of RANS

Challenge 2:

resolve particles' shape, force, …

Challenge 3:

algorithmic differentiation & adjoints, combine measurement & simulation

Lattice Boltzmann Research Group (Research Fields)

Process Engineering

Medical Engineering

...

...

Scientific Computing on High Performance Computers

Optimal Control and Optimization

Mathematical Modelling and Numeric

Lattice Boltzmann Research Group (Team)

Agenda

Overview LBM & *OpenLB*

Challenge I -- Turbulence

Challenge II -- Suspensions

Challenge III -- Optimization

Summary

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Overview LBM & *OpenLB*

Challenge I -- Turbulence

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Summary

LBM as Generic PDE Solver [4]

macroscopic:

Navier-Stokes equation
$\boldsymbol{u}, p$ in $I \times \Omega$

$h \to 0$

[1]

mesoscopic:

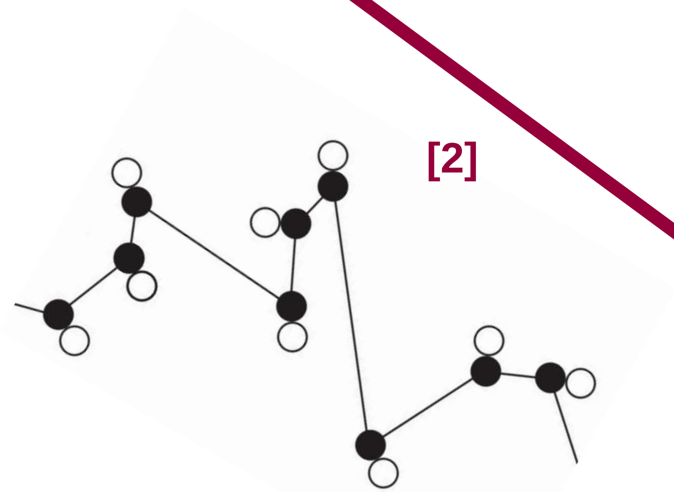
Boltzmann equation /
BGK-Boltzmann equation
f in $I \times \Omega \times \mathbb{R}^d$

$h \in \mathbb{R}_{>0}$

$\omega \sim h^2, \; l_f \sim h, \; c_s \sim 1/h$

[3] **Consistent discretisation: LBM**

[2]



$\Delta t = h^2, \; \Delta r_k = h, \; v_i \sim 1/h$

lattice Boltzmann equation
f_i in $I_h \times \Omega_h \times Q$

- explicit scheme
- efficient parallelisation

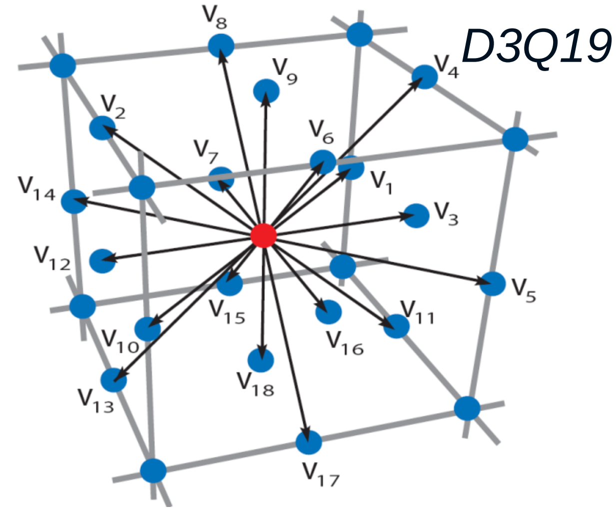
[1] Saint-Raymond (2003) ASENS (4) 36, 271-317. [2] Junk, Klar, Luo (2005) JCP 210(2), 676-704.

[3] Krause (2010) KIT Karlsruhe.

[4] Simonis, Frank, Krause (2020). PTRSA 378: 201904.

Lattice Boltzmann Methods (LBM)

Idea: coupling model parameter $h \in \mathbb{R}_{>0}$ with discretisation parameter: *Lattice DdQq*



Macroscopic moments:

density $\rho = \sum_{i=0}^{q-1} f_i$, velocity $\rho \boldsymbol{u} = \sum_{i=0}^{q-1} \boldsymbol{v_i} f_i$

Time loop $t = t_0, t_0 + h^2, t_0 + 2h^2, ..., t_1$

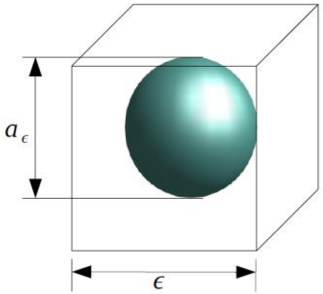
Position space loop $\boldsymbol{r} \in \Omega_h$

(1) Collision $\tilde{f}_i(t, \boldsymbol{r}) = f_i(t, \boldsymbol{r}) - \frac{1}{3\nu + 1/2}\left(f_i(t, \boldsymbol{r}) - M^{eq}_{f_i}(t, \boldsymbol{r})\right)$

(2) Streaming $f_i(t + h^2, \boldsymbol{r} + h^2 \boldsymbol{v_i}) = \tilde{f}_i(t, \boldsymbol{r})$

Homogenization Limits of Stationary Navier-Stokes Equations for Porous Media Fluid Flows

Theorem [Allaire]: Three homogenization limits of stationary Navier-Stokes equations (dependent on scaling of obstacles (ratio σ_ϵ) being small/critical/large):



1. If $\lim_{\epsilon \to 0} \sigma_\epsilon = +\infty$, $\boldsymbol{u}$ and p converge strongly to solution of stationary NSE:

$$\begin{cases} \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} - \mu \boldsymbol{\Delta} \boldsymbol{u} = \boldsymbol{F} - \boldsymbol{\nabla} p & \text{in } \Omega, \\ \operatorname{div} \boldsymbol{u} = 0 & \text{in } \Omega. \end{cases}$$

2. If $\lim_{\epsilon \to 0} \sigma_\epsilon = \sigma > 0$, $\boldsymbol{u}$ and p converge weakly to solution of Brinkman-type law (BTL)

$$\begin{cases} \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} - \mu \boldsymbol{\Delta} \boldsymbol{u} + \frac{\mu}{\sigma^2} \mathbf{M} \boldsymbol{u} = \boldsymbol{F} - \boldsymbol{\nabla} p & \text{in } \Omega, \\ \operatorname{div} \boldsymbol{u} = 0 & \text{in } \Omega. \end{cases}$$

3. If $\lim_{\epsilon \to 0} \sigma_\epsilon = 0$, $\boldsymbol{u}$ and p converge strongly to solution of Darcy‘s law (DL)

$$\begin{cases} \mu \mathbf{M} \boldsymbol{u} = \boldsymbol{F} - \boldsymbol{\nabla} p & \text{in } \Omega, \\ \operatorname{div} \boldsymbol{u} = 0 & \text{in } \Omega. \end{cases}$$

Allaire (1991). Archive for Rational Mechanics and Analysis, 113, 209-259

Homogenization Limits of Non-stationary Navier-Stokes Equations for Porous Media Fluid Flows

Hypothesis: Three homogenization limits of non-stationary Navier-Stokes equations (dependent on scaling of obstacles (ratio σ_ϵ) being small/critical/large):

1. If $\lim_{\epsilon\to 0}\sigma_\epsilon = +\infty$, $\boldsymbol{u}$ and p converge weakly to solution of non-stationary NSE:

$$\begin{cases} \partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} - \mu\boldsymbol{\Delta}\boldsymbol{u} = \boldsymbol{F} - \boldsymbol{\nabla}p & \text{in } \Omega, \\ \operatorname{div}\boldsymbol{u} = 0 & \text{in } \Omega. \end{cases}$$

2. If $\lim_{\epsilon\to 0}\sigma_\epsilon = \sigma > 0$, $\boldsymbol{u}$, p converge weakly to solution of evolutionary Brinkman-type law (eBTL)

$$\begin{cases} \partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} - \mu\boldsymbol{\Delta}\boldsymbol{u} + \frac{\mu}{\sigma^2}\mathbf{M}\boldsymbol{u} = \boldsymbol{F} - \boldsymbol{\nabla}p & \text{in } \Omega, \\ \operatorname{div}\boldsymbol{u} = 0 & \text{in } \Omega. \end{cases}$$

3. If $\lim_{\epsilon\to 0}\sigma_\epsilon = 0$, $\boldsymbol{u}$ and p converge weakly to solution of time-dependent Darcy's law (tDL)

$$\begin{cases} \partial_t \boldsymbol{u} + \mu\mathbf{M}\boldsymbol{u} = \boldsymbol{F} - \boldsymbol{\nabla}p & \text{in } \Omega, \\ \operatorname{div}\boldsymbol{u} = 0 & \text{in } \Omega. \end{cases}$$

Simonis, Hafen, Jeßberger, Dapelo, Krause (2023). Submitted.

- If porosity structure is approx. isotropic, we can reduce $\mathbf{M}$ to its eigenvalue K (permeability).
- Use homogenized lattice Boltzmann equation to approximate eBTL (case 2).

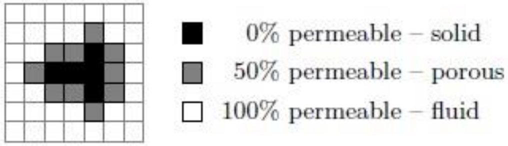
$$f_i^h(t+h^2) - f_i^h(t) = -\frac{1}{3\nu+\frac{1}{2}}\left[f_i^h(t) - M^{eq}_{f_i^h}(n_{f_i^h}, d_h \boldsymbol{u}_{f_i^h})(t)\right]$$

- with porous Maxwellian

$$M^{eq}_{f_i^h}(n_{f_i^h}, d_h\boldsymbol{u}_{f_i^h}) = \frac{w_i}{w} n_{f_i^h}\left[1+3h^2 d_h \boldsymbol{v}_i\cdot\boldsymbol{u}_{f_i^h} - \frac{3}{2}h^2 d_h^2 \boldsymbol{u}_{f_i^h}^2 + \frac{9}{4}h^4 d_h^2 \left(\boldsymbol{v}_i\cdot\boldsymbol{u}_{f_i^h}\right)^2\right]$$

- and lattice porosity $d_h = 1-\left(3\nu+\frac{1}{2}\right)\nu h^2 K^{-1}$
- Compute moments of f_i^h:

$$n_{f_i^h} = \sum_i f_i^h \text{ and } \boldsymbol{u}_{f_i^h} = \sum_i \boldsymbol{v}_i f_i^h$$



Theorem: If f_i^h, its material derivatives up to order three and its zeroth and first moment are of zeroth order in h, the homogenized lattice BGK Boltzmann equations (HLBGKBE) are **a limit consistent discretization of order $O(h^2)$ (i.e. two in space, one in time)** of the eBTL (case 2: critical obstacle size)

Simonis, Hafen, Jeßberger, Dapelo, Krause (2022). Submitted.

Simonis, Krause (2022). arXiv preprint (under review), doi: 10.48550/arXiv.2208.06867.

Aims and Focus

OpenLB for ..

.. **teachers**

- practical classes
- workshops

.. **applicants** and **developers**

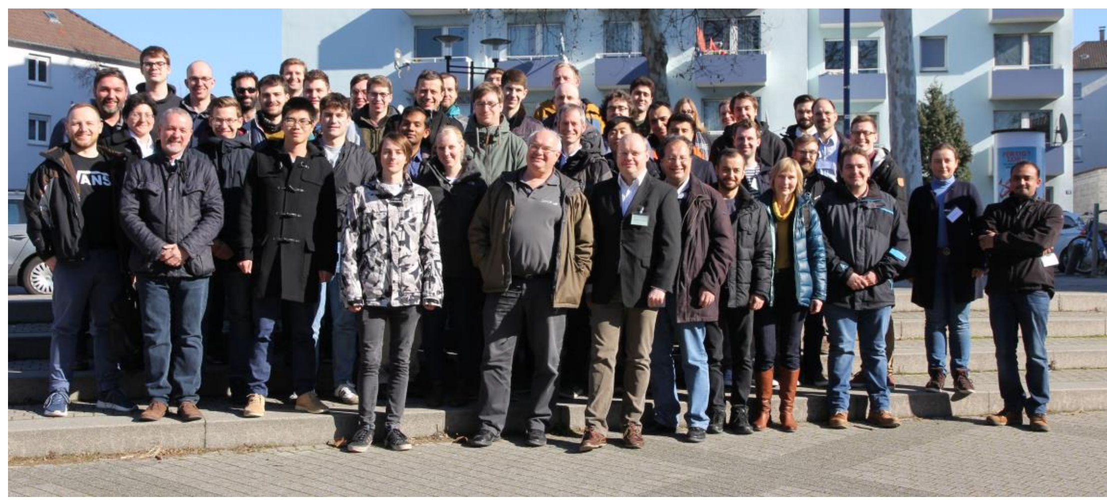
- industry
- academia

in order to establish

a strong LBM community.

Current Key Aspects

- Complex geometries
- Cloud computing/ HPC
- Optimisation
- Particle flows
- Turbulent Flows



3rd Spring School 2019, Mannheim, Germany

OpenLB Community

OpenLB Community..

.. aims at

- continuous development and maintenance
- on current standard HPC-Hardware
- based on state-of-the-art LBM

.. offers

- annually **spring schools**
- maintenance of the **forum**
- maintenance of the OpenLB website
- **support for installation for members** (maximum 1 HPC-Cluster p.a., 2 Desktops p.a.)
- an online annual meeting, for the first time in 2023, with the following program:
  - presentation and discussion of **new research results** LBM (2 hours incl. slides as report)
  - discussion and naming of OpenLB refactoring priorities
  - discussion and naming of **priorities of new OpenLB features**
  - discussion and naming of priorities of new LBM developments
- **individual consulting for members**, duration: 2 h p.a.
- initiating the publication of the member's logo on the OpenLB "Partners & Friends" website

OpenLB: Facts and Figures

openlb.net

2D and 3D fluid flow and transport simulations based on LBM

Realisation

- Started in 2006 by Jonas Latt & Mathias J. Krause
- Open source (GPL2)
- C++, object oriented, **template-based**, modular, extensible
- **Hybrid parallelisation:** SISD & SIMD using MPI, OpenMP & CUDA

Features in latest release 1.6

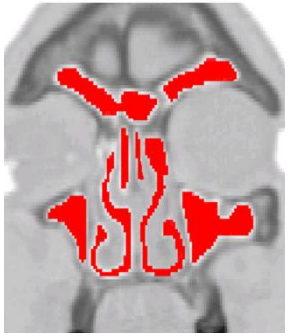
- Various lattice types: D2Q9, D3Q15, D3Q19, ...
- Local, non-local, on- and off-lattice boundary conditions
- Collision models: BGK, MRT, Entropic, Cumulant, LES, multi-phase, multi-component, thermal, reactions, adjoints, free surface, …
- Many examples on benchmark cases & applications
- **Build-in pre-processing from e.g. STL-files, geometry primitives**
- Unit conversion for problem set-up in SI-units
- XML interface for input parameters
- Visualization (built-in and VTK), error norms and analysis tools

2011

2009

2007

Built-in Geometry Creation and Meshing



CT/MRT

Step 1a): Segmentation, Smoothing

Materialise driving your innovations

VMTK, ITK, …

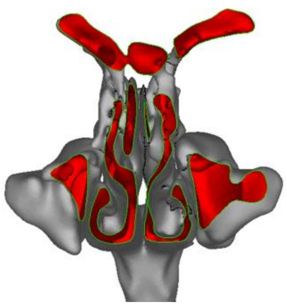
CAD

Step 1b): Import

Indicator Functors

Step 1c): Built-in

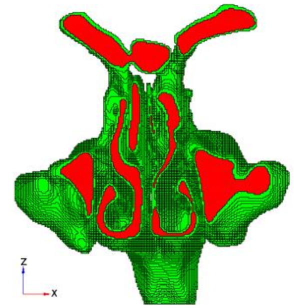
openlb.net



STL Surface Mesh **and/or** Geometry Primitives

Step 2: Built-in voxelizing

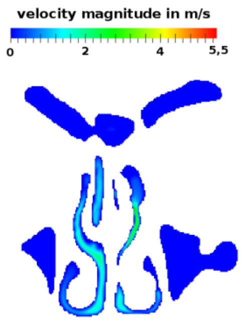
openlb.net



Voxel Mesh

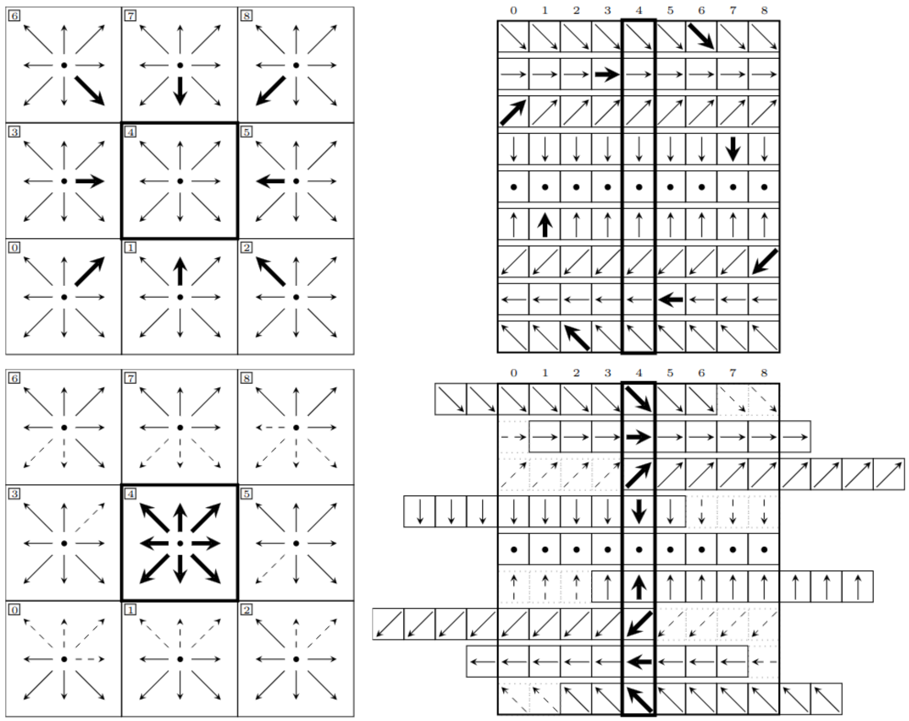
openlb.net

Step 3: Setting of material-dependent boundary conditions



Simulation Results

LBM Algorithm: Data Structure & Periodic Shift Pattern



Functors & operators **templated** enables

- platform specific data structures
- code generation using **CSE**

Block structured data

- stored as **Structure Of Arrays**
- addressable as fields

enables

- vectorization of collision (step)
- implicit propagation by rotation of population columns **(Periodic Shift Pattern** [1]**)**

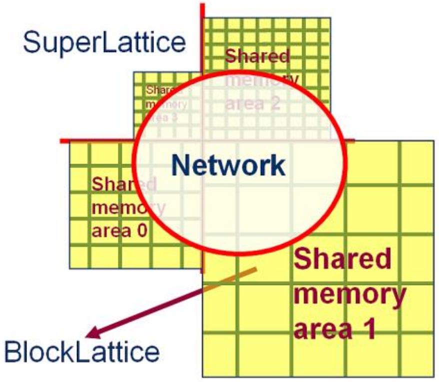
➔ transparent support for bandwidth-saturating, vectorized executions

[1] Kummerländer et al. (2023). Concurrency and Computation. doi: 10.1002/cpe.7509.

Parallelisation: Hybrid Concept

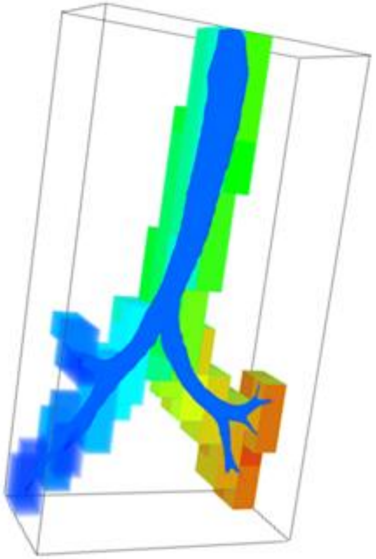
Spatial domain decomposition

- **Sparse multi-block** for complex geometries
- **Inter-block: (CUDA-aware) MPI**
- **Intra-block: OpenMP, AVX512, CUDA, …**



Performance optimization

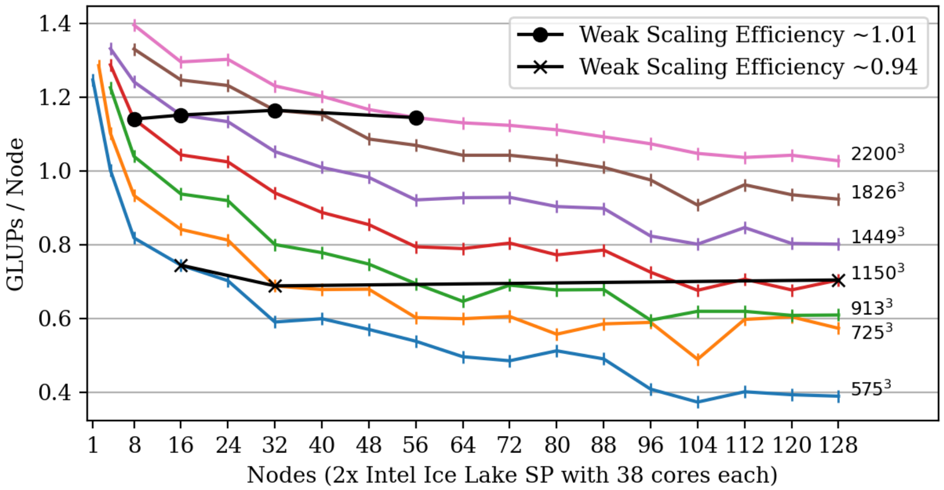
- C++ templates, CSE with PU-dependent kernel generation
- PU-block assignments:
  - modelled via cost functions depending on
    decomposition, boundary conditions, bulk model
      used heterogenous PU, network, ..
  - solved by **heuristic** [2] and **graph-based** [1] **algorithm**



[1] Fietz, et al. (2012). Euro-Par 2012 Parallel Processing.

[2] Kummerländer, et al. (2023). in preparation.

Efficient LBM on Heterogeneous HPC Systems



Scalability benchmarks on HoreKa

(#73 / TOP500, November 2022 – 8 PFLOPs peak)

- OpenLB Release 1.5
- LDC benchmark case
- Hybrid MPI / OpenMP execution utilizing AVX-512 on CPU Partition
- Hybrid MPI / CUDA on GPU partition

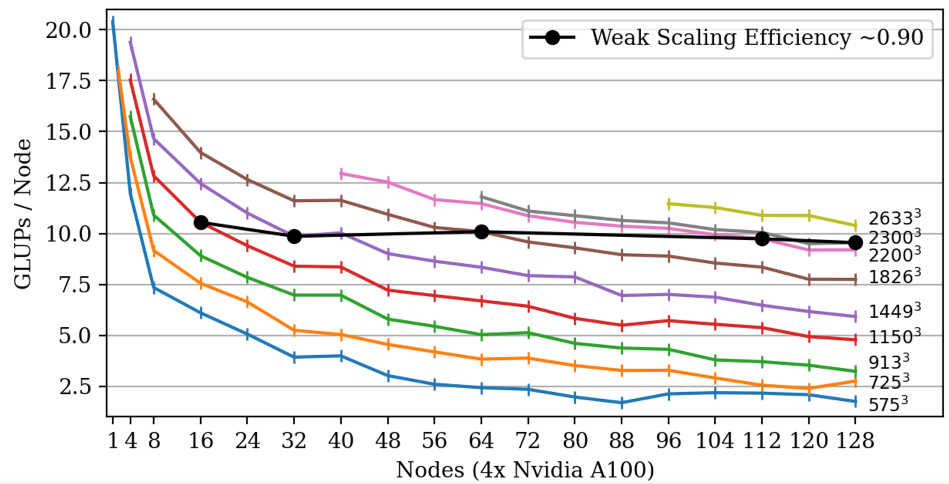
Up to **18 billion (10^9) cells**

Up to **1.33 trillion (10^{12}) cell updates / second**

~0.25 PFLOPs

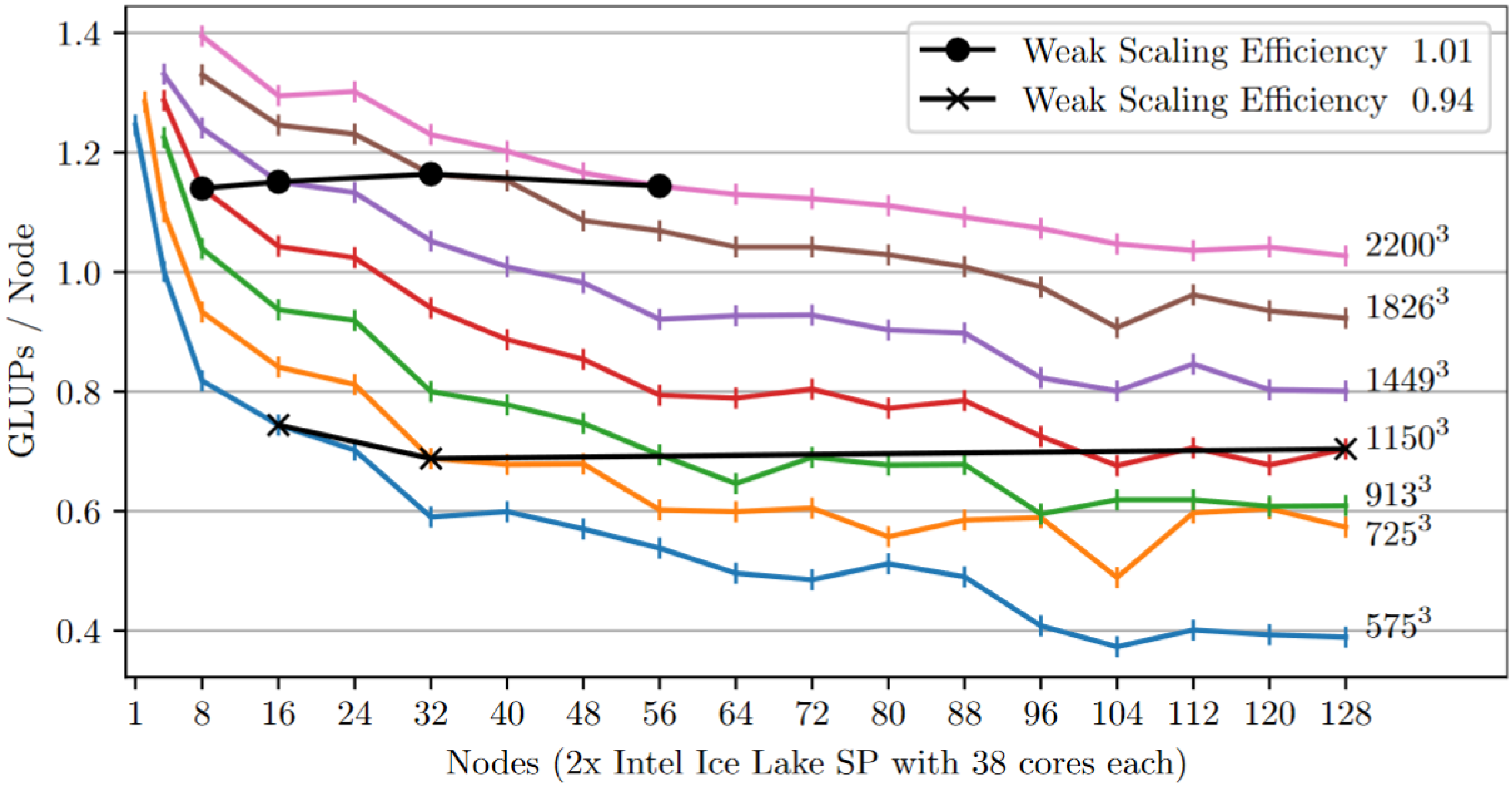
Translates well to application cases e.g. 600 billion cell updates / second for the turbulent nozzle flow case on 56 GPU nodes.

Example: strong scaling efficiency 0.8 for 575³, 64 - 128 nodes

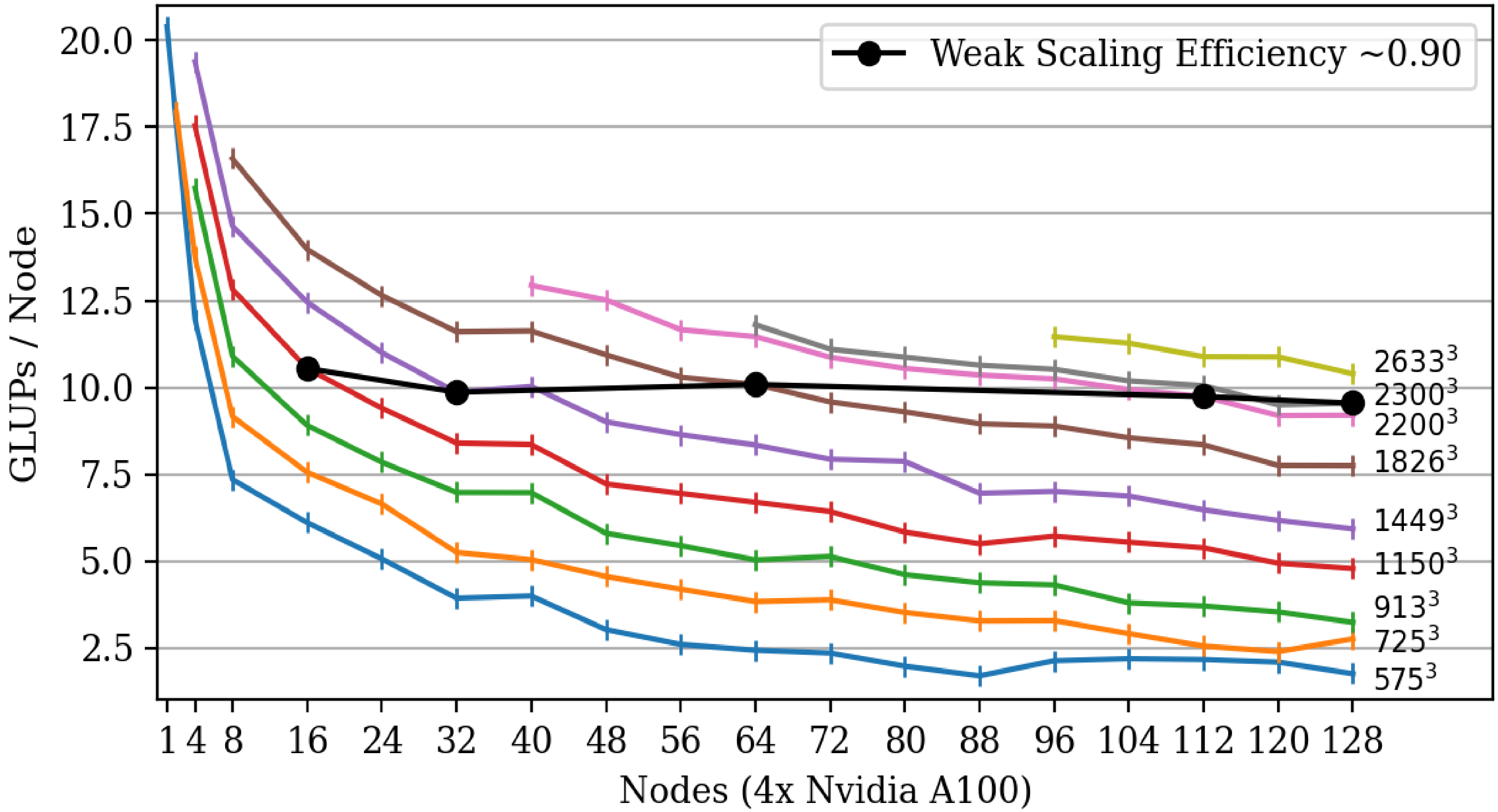


Kummerländer, Bukreev, et al. (2022). High Perf Comp in Science and Eng ’21 (accepted).

Parallel Performance (CPU, MPI+OpenMP+AVX512) @ HoreKa, KIT, Germany

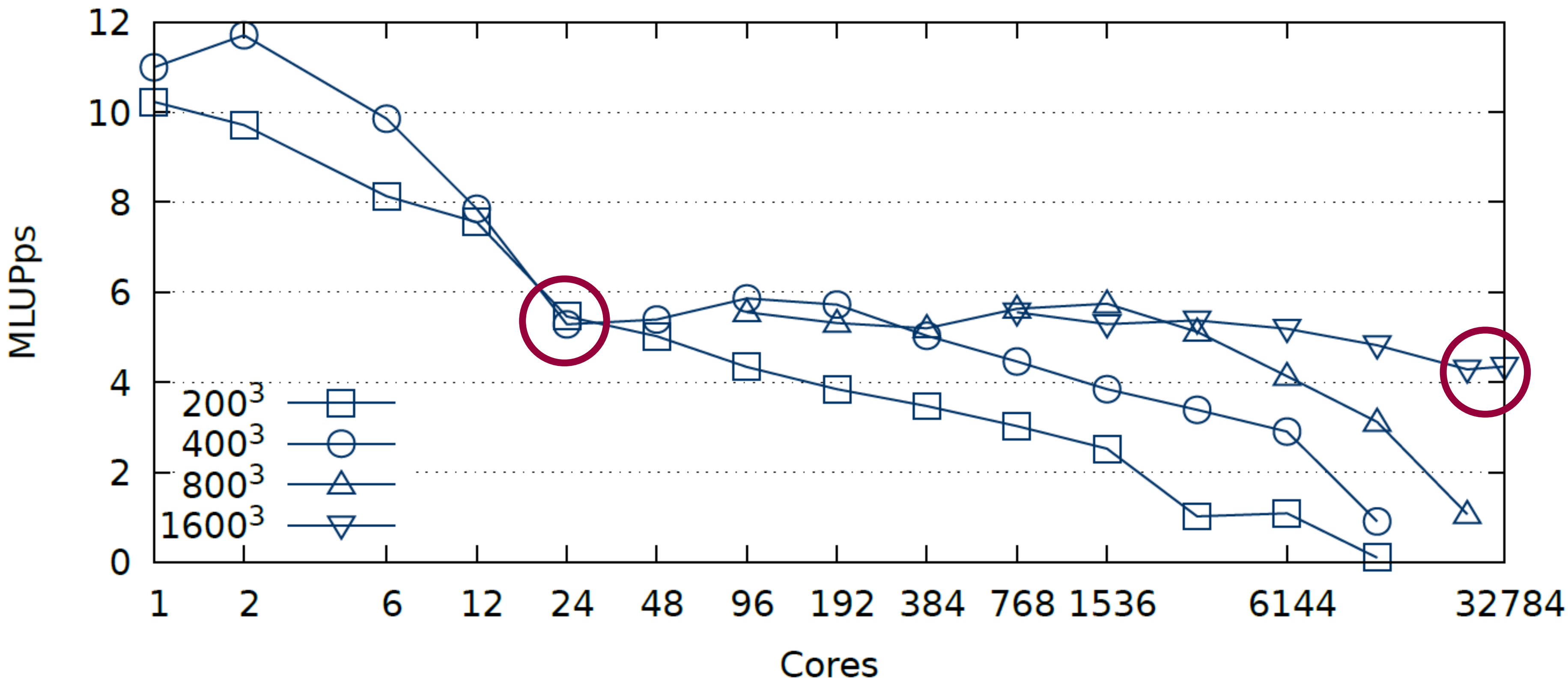


Parallel Performance (GPU, CUDA & MPI) @ HoreKa, KIT, Germany

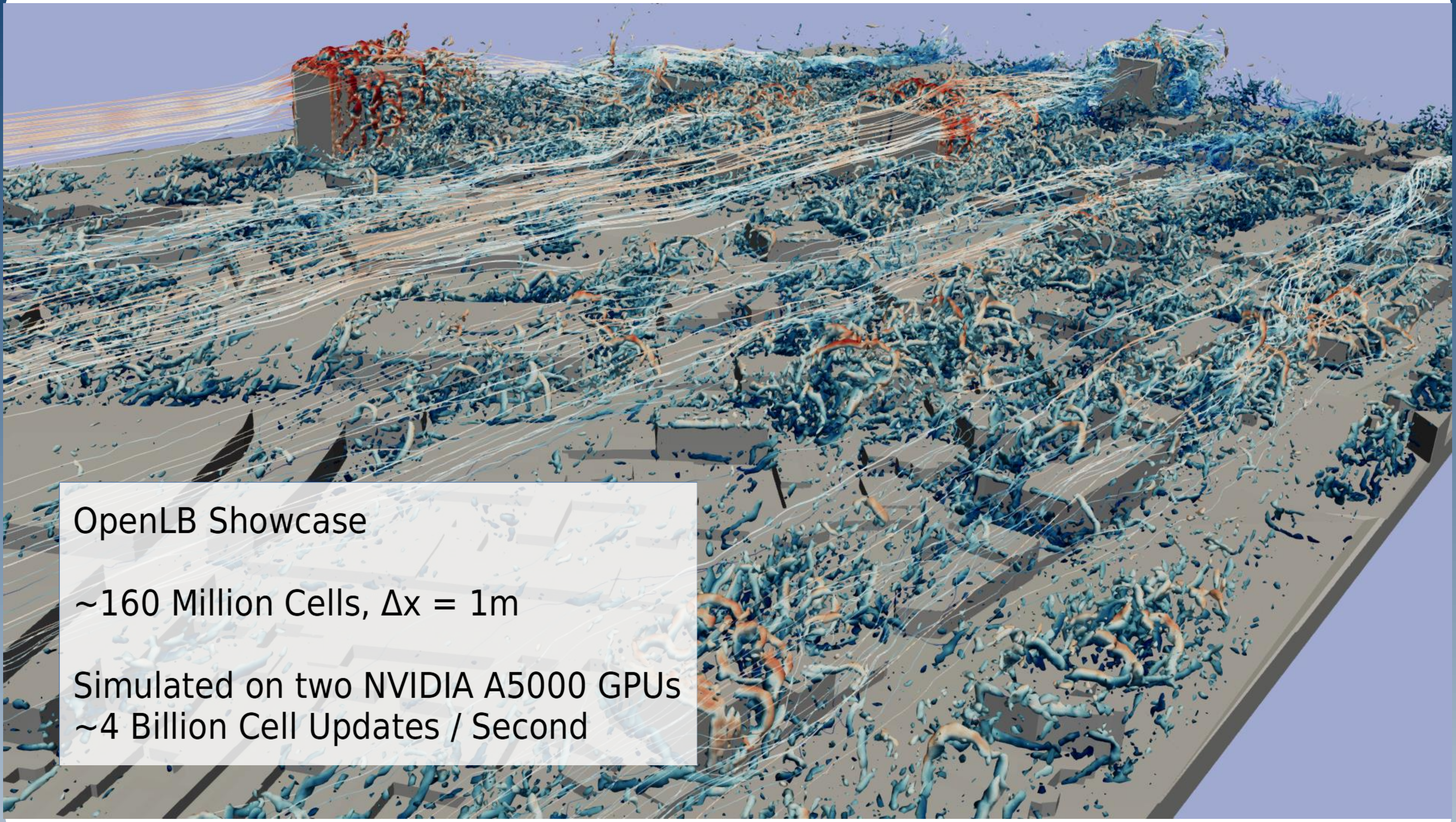


Parallel Performance @ Magnus, Curtin, Australia

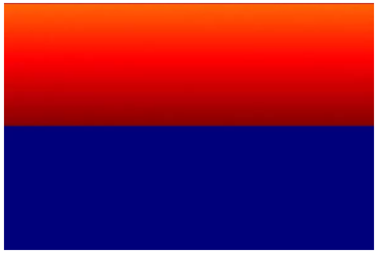
Approximately 80% efficiency
1 node ~ 1 cluster (1366 nodes)
46 days ~ 1 hour



Simulation under your Desk

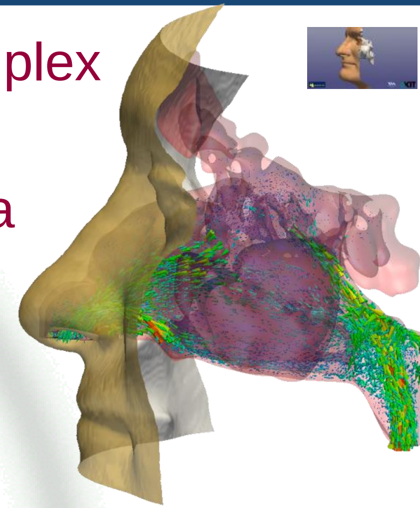


Applications

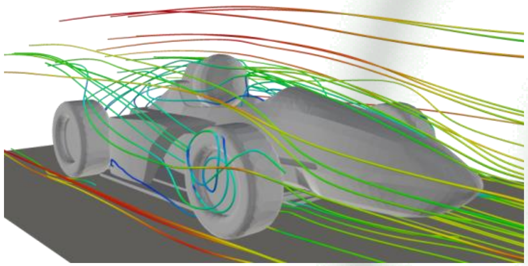


Multiphase flows

Flows in complex geometries, porous media

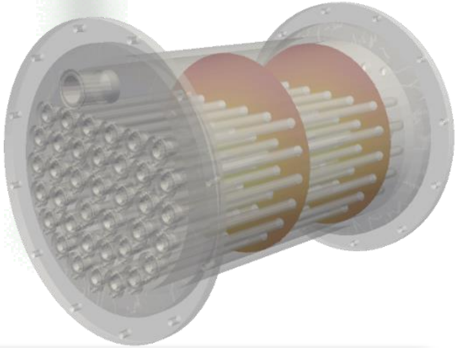


Turbulent flows

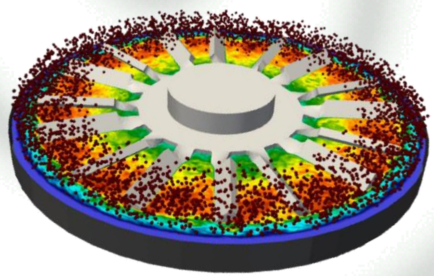


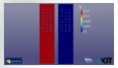
OpenLB Applications

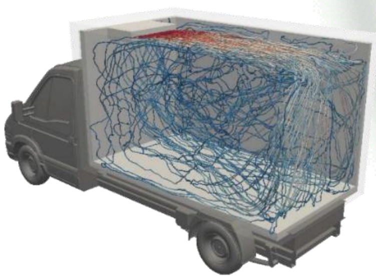
Radiative transport



Particle flows







Thermal flows

Krause, M. J., Kummerländer, A., Avis, S. J., Kusumaatmaja, H., Dapelo, D., Klemens, F., Gaedtke, M., Hafen, N., Mink, A., Trunk, R., Marquardt, J. E., Maier, M.-L., Haussmann, M., Simonis, S. (2021). Comput Math Appl. 81, 258-288.

Agenda

Overview LBM & *OpenLB*

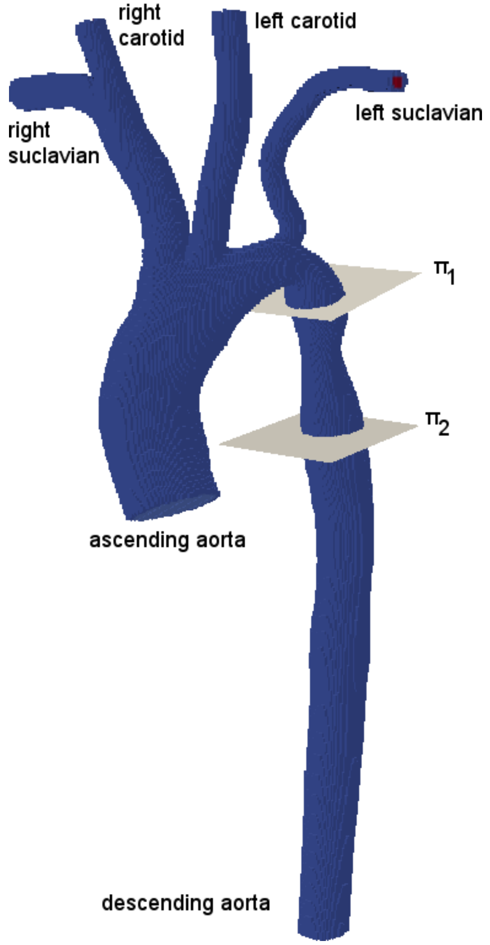
Challenge I -- Turbulence

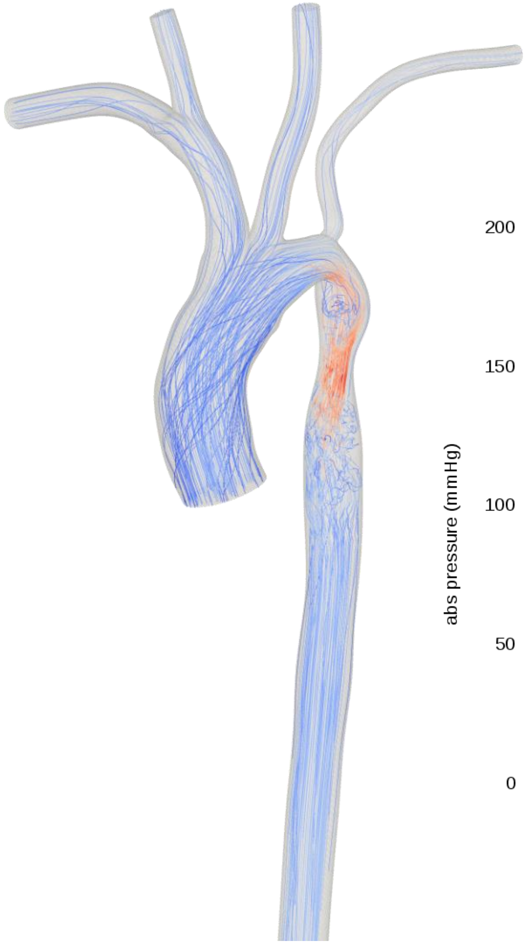
Challenge II -- Suspensions

Challenge III -- Optimization

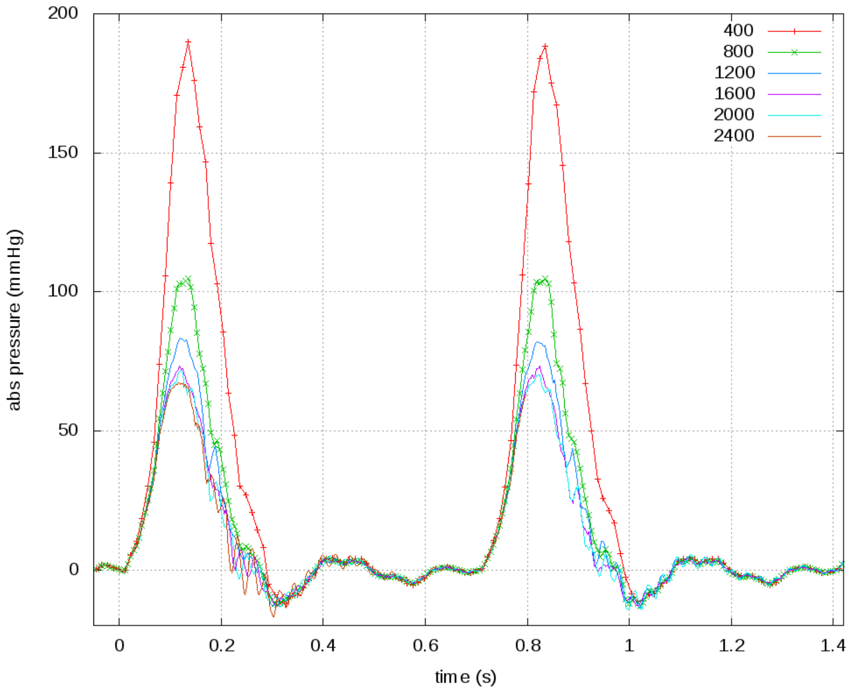
Summary

Aorta Benchmark, DNS



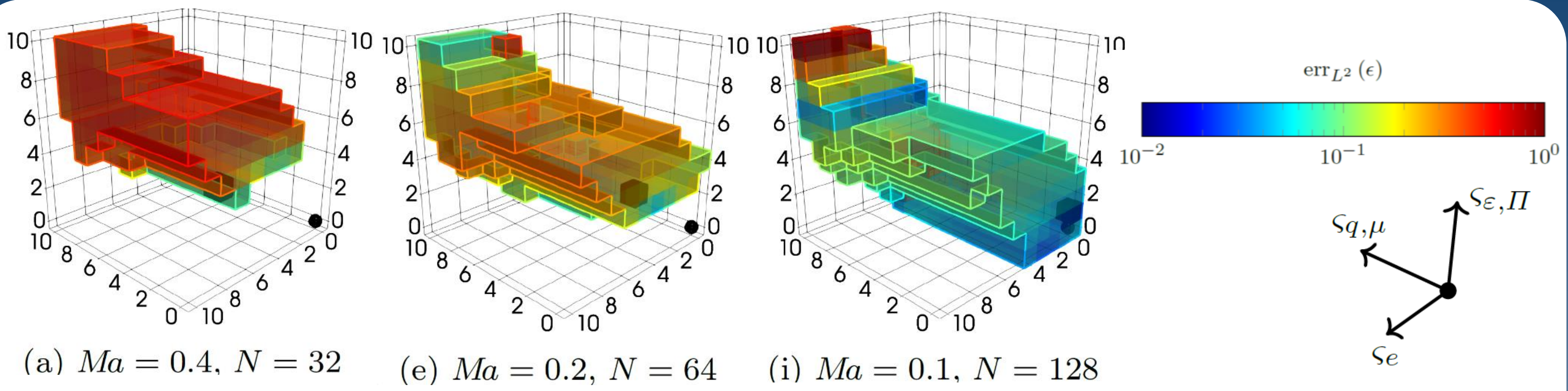


Goal: Validate DNS LBM



Henn, T., Krause, M. J. *et al.* (2012). In proceedings MICCAI12 STACOM12 7746, 34.

Brute Force Stability / Accuracy [3], BGK for DNS!



Taylor-Green vortex benchmark $Re = 1600$, diffusive scaling $N \to \infty\ (Ma \to 0)$

Axes: Prefactors of kinetic relaxation times. Colormap: Dissipation rate error (wrt. [1]) until $t = 10\ [s]$

Finding 1: Stability volume moves towards BGK point (black sphere) with resolution

Finding 2: Error minimal MRT [2] configuration (black cube) near to BGK

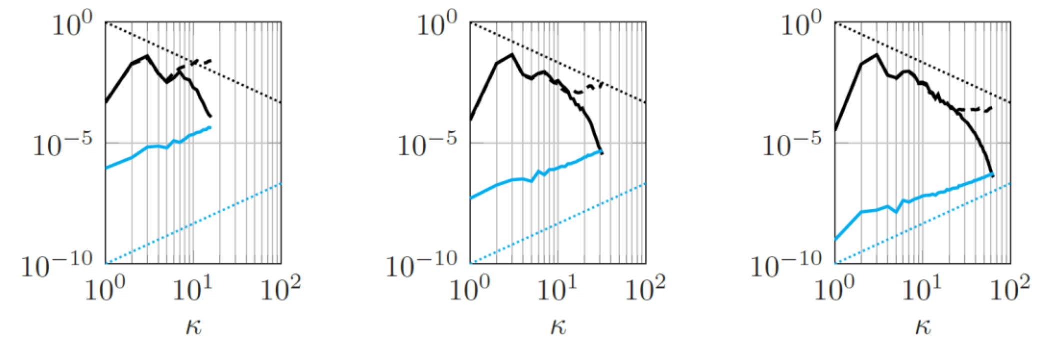
Finding 3: MRT acts as implicit turbulence model (numerical dissipation)

[1] Brachet et al. (1983) JFM 130: 411-452.

[2] D'Humières et al. (2002) PTRSA 360 (1792): 437-451.

[3] Simonis, Haussmann, Kronberg, Dörfler, Krause (2021). PTRSA 379: 2020405.

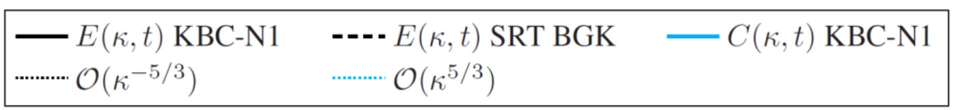
Spectral Brute-force Analysis of KBC LBM

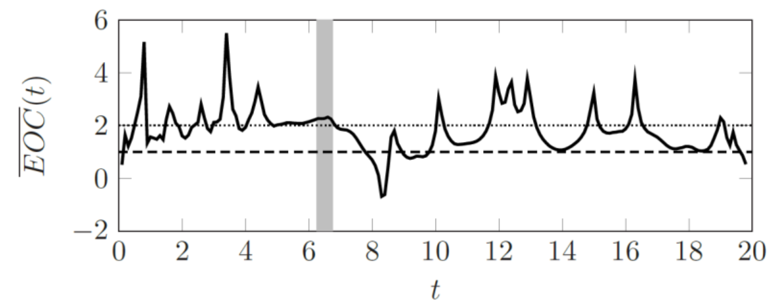


(g) $Re = 6000$, $Ma = 0.2$, $N = 32$, $t \approx 7.37$

(h) $Re = 6000$, $Ma = 0.1$, $N = 64$, $t \approx 6.45$

(i) $Re = 6000$, $Ma = 0.05$, $N = 128$, $t \approx 6.60$





Artificial turbulence (stochastic Taylor–Green vortex)

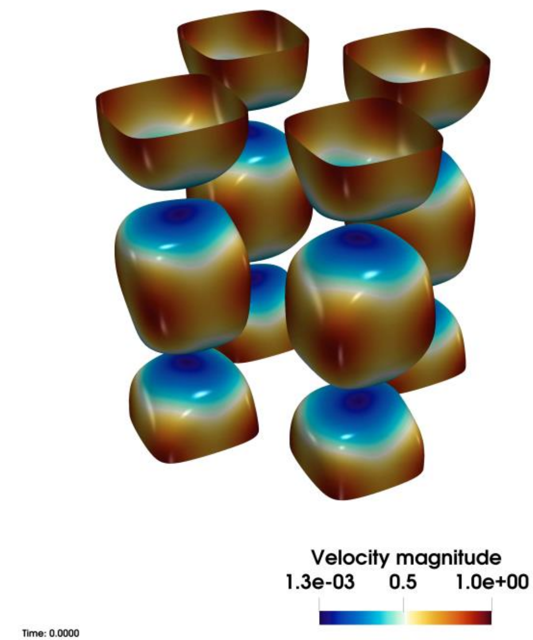
$Re < 11000$, diffusive scaling $N \to \infty$ ($Ma \to 0$)

Finding 1: Average EOC $\approx$ **2** (diss. rate psDNS until $t = 20$ [s])

Finding 2: Relaxation spectrum $+5/3$**-law** (turbulence K41)

Finding 3: Entropic relaxation frequenncy limits SRT EOC $\approx$ **1.3**

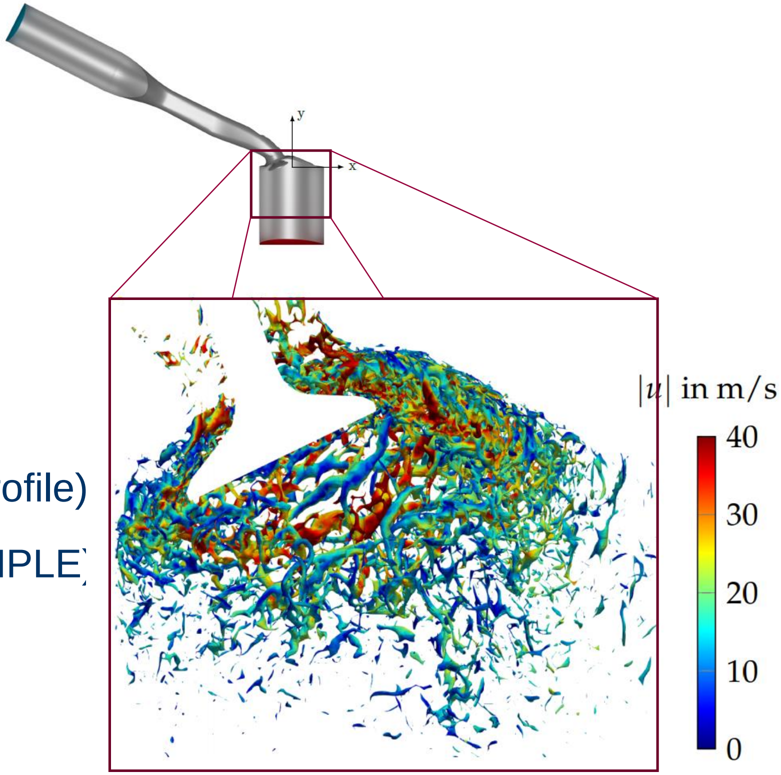
$\Rightarrow$ **KBC is limit consistent, implicit hyperviscosity model**



Simonis (2023). PhD thesis. KIT.

Turbulent Flows with LBM LES: Combustion Chamber

- **Messurement: PIV**
  - Silicon droplets ~500 nm
  - xy-symmetriy plane $< U >, < U_{RMS} >$
  - error ~1% for target $< U >$



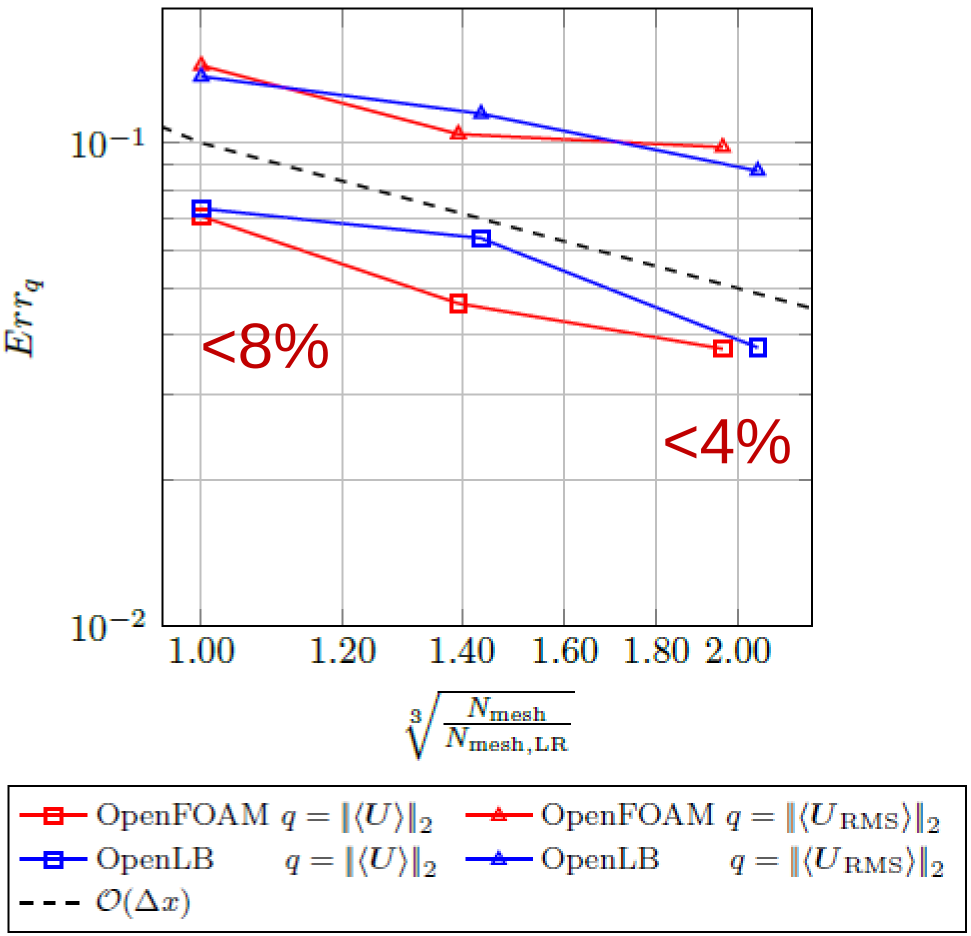
- **Simulation: Wall-modelled LES**
  (Smagorinsky–Lilly, van Driest damping, Musker-profile)
  - OpenFOAM (FVM, pimpleFOAM ← PISO&SIMPLE)
  - OpenLB (LBM, SRT)

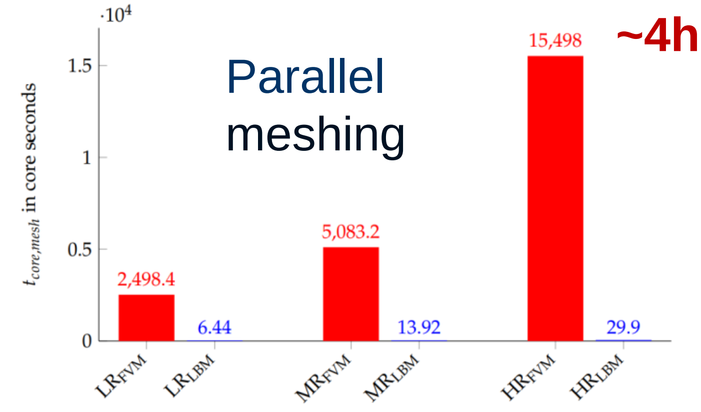
- **Comparison of OpenFOAM and OpenLB** w.r.t.: capability of **prediction accuracy (4% to 8%), computational cost, ease of use**.

Haussmann, Barreto, Kouyi *et al. (2019). Comput. Math. App. 78, 3285– 3302.*

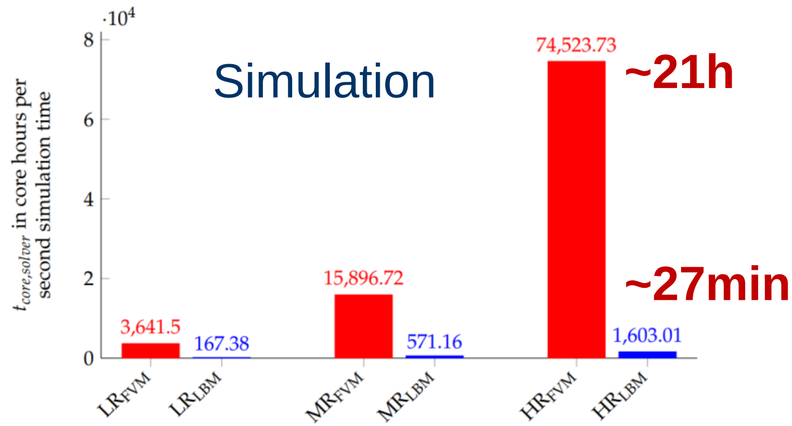
Haussmann, Ries, Jeppener-Haltenhoff *et al.* (2020). Computation 2020, 8(2), 43.

OpenLB (LBM) vs OpenFOAM (FVM)





➔ OpenLB is 424x faster

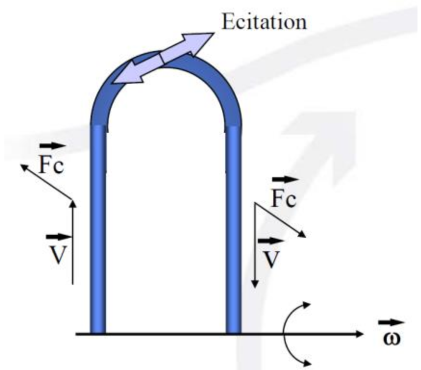


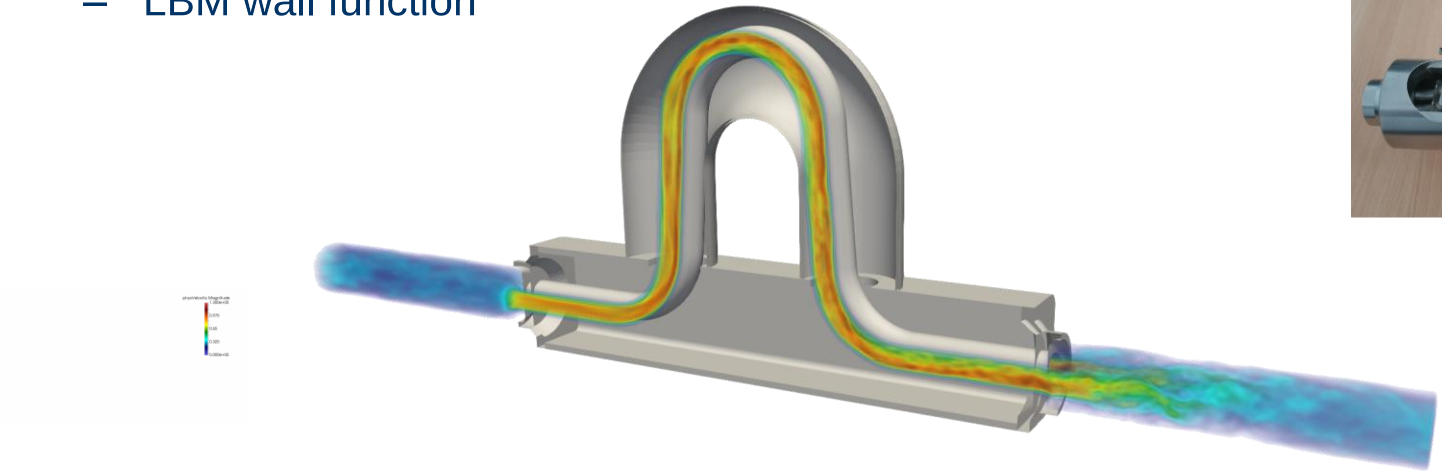
➔ OpenLB is 32x faster

Coriolis Mass Flowmeter Simulation, LES

Goal: Improve measurement accuracy

- Investigation of pressure drop
  - Comparison with experimental data
- Investigation of vortex phenomena
  - LBM Large Eddy Simulation Smagorinsky model
  - LBM wall function





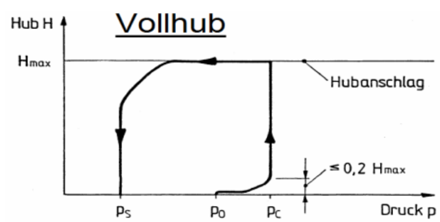
Haussmann, M., Reinshaus, P., Simonis, S. *et al.* (2020). Preprint arXiv:2005.04070 [physics.comp-ph].

Haussmann, M., Barreto, A. C., Kouyi, G. L. *et al.* (2019). Comput. Math. with Appl., 78(10), 3285.

Safety Valve Simulation, LES

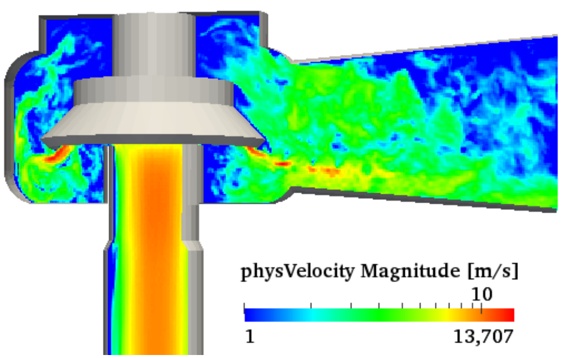
Goal: avoid chatter

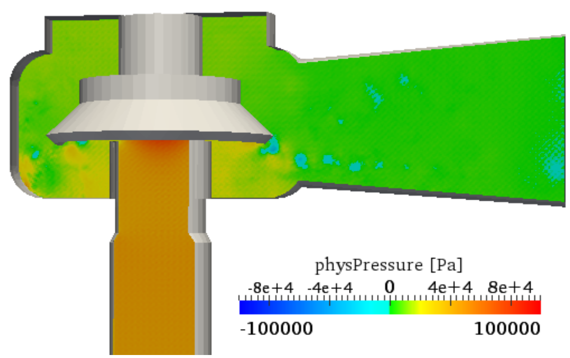
➔ vary shape of disk

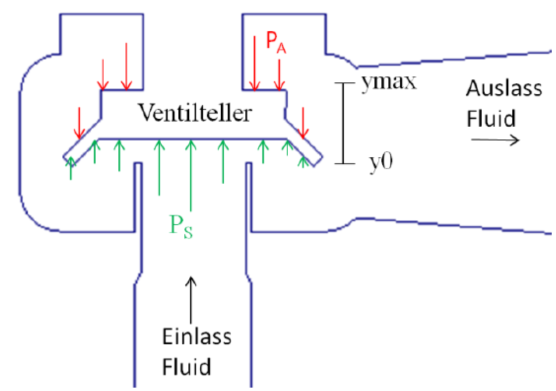


- 3D transient turbulent simulation
- 1 billion degrees of freedom
- parallelization: 30 days ➔ 1 day
  64 cores ➔ 2.048 cores
- optimize shape of disk

different disk angle





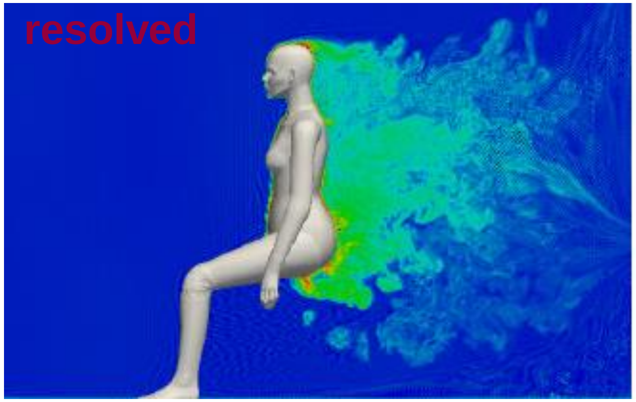


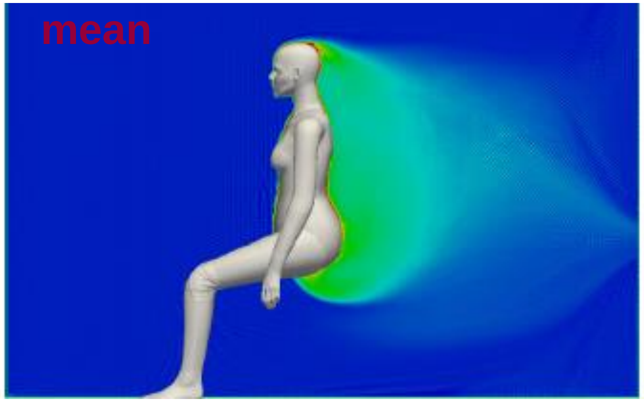
Thermal Flow for Thermal Comfort, LES

Goal: Improve thermal comfort

control flow patterns by change of design and flow conditions of

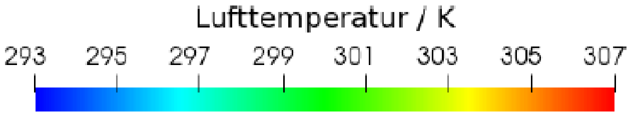
- Heating
- Air condition
- Ventilator

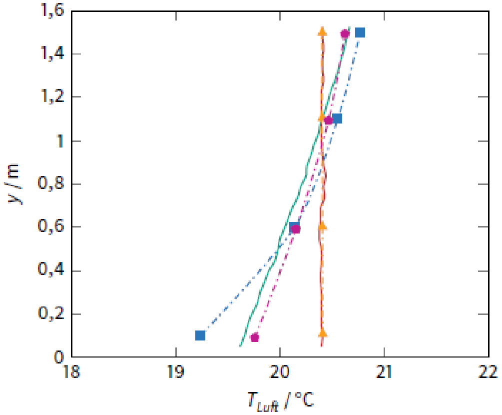




Benchmark study:

- Re=29,000
- Pe=20,600
- LES - Smagorinsky type
- 130 mio. grid cells



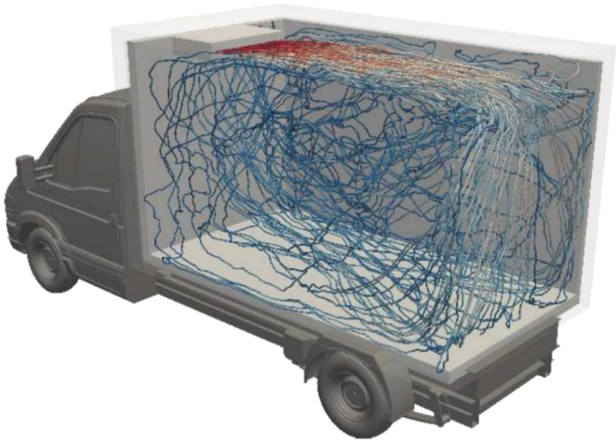


Siodlaczek, M., Gaedtke, M., Simonis S. *et al.* (2020). Submitted to Build Environ.

Thermal Flow in Refrigerated Vehicles, LES

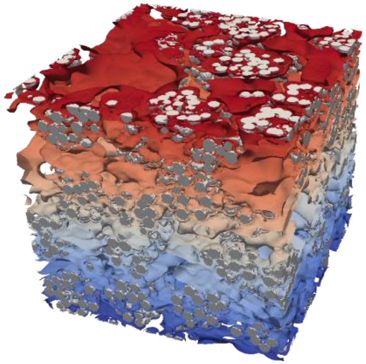
Goal: Improve the insulation efficiency

➔ exchange insulation material
- extruded polysterol (XPS) by
- vacuum insulation panels (VIP)



Convection in vehicle's cooling chamber:

- Air conditioning volume flow of $990\,\frac{m^3}{h}$
- Turbulent free jet, $\mathrm{Re} = 28{,}000$
- Large eddy simulation (LES) Smagorinsky
- Resolved heat flux through insulation walls
- Utilizing conjugated heat transfer implementation



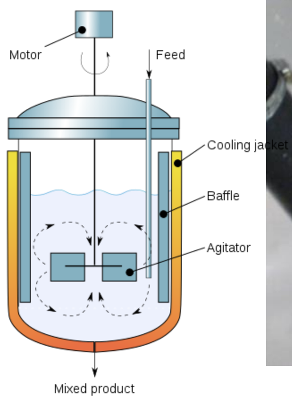
Gaedtke, M., Wachter, S., Kunkel, S. *et al.* (2019). Heat and Mass Transfer, 1-13.

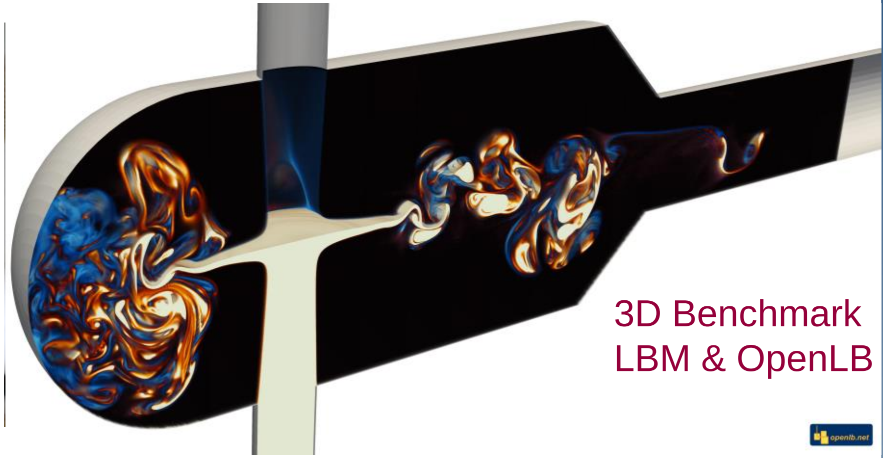
Gaedtke, M., Wachter, S., Raedle, M. *et al.* (2018). Comput. Math. with Appl., 76(10), 2315-2329.

Ross-Jones, J., Gaedtke, M., Sonnick, S. *et al.* (2019). Comput. Math. with Appl., 77(1), 209-221.

Optimal Mixing & Reactions

Goal: **Optimize design & process parameters for better mixing, to save costs or energy**





Challenge: **Mixing at Batchelor scale (< Kolmogorov length) vs. process scale (~1m)**

Model: **Optimization problem with a PDE system as side condition**

Agenda

Overview LBM & *OpenLB*

Challenge I -- Turbulence

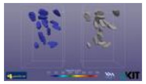
Challenge II -- Suspensions

Challenge III -- Optimization

Summary

Fine Particle Fractionation, Particle

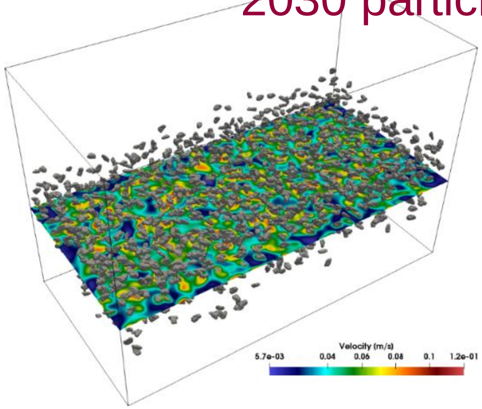
Challenge: Low selectivity in the range from $100\ nm$ to $10\ \mu m$



Goal: Improvement of separation processes

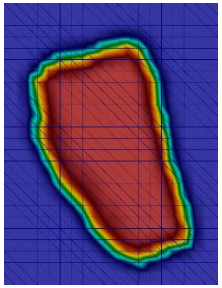
➔ Simulation of a large number of **arbitrary shaped particles**

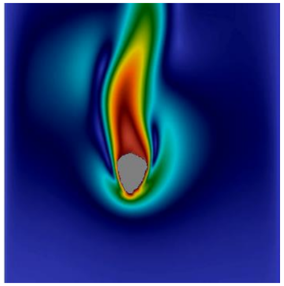
2030 particles

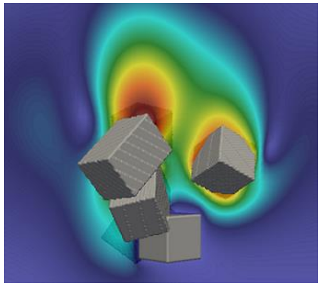


Method needs to account for surface structure

Contact treatment for non-spherical particles is complex







HLBM for Resolved Particle Simulations

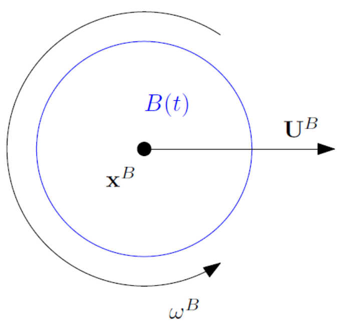
$$\tilde{\boldsymbol{u}} = d\boldsymbol{u}_f + (1-d)\boldsymbol{U}^B$$

Case 1: $d = 1$ $\quad \tilde{\boldsymbol{u}} = \boldsymbol{u}_f$ → standard LBM

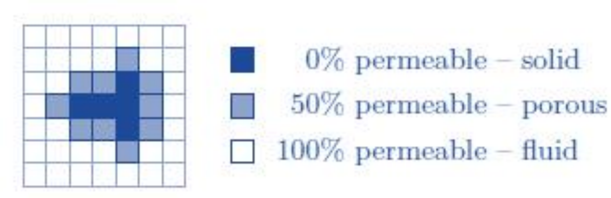
Case 2: $d = 0$ $\quad \tilde{\boldsymbol{u}} = \boldsymbol{U}^B$ → rigid body motion

Case 3: $d \in [0,1], \boldsymbol{U}^B = 0$ $\quad \tilde{\boldsymbol{u}} = d\boldsymbol{u}_f$ → porous media LBM → eBTL

Case 4: $d \in [0,1]$ $\quad \tilde{\boldsymbol{u}} = d\boldsymbol{u}_f + (1-d)\,\boldsymbol{U}^B$ → HLBM for particle



$$\begin{cases} d = 0 \\ d \in (0,1) \\ d = 1 \end{cases}$$



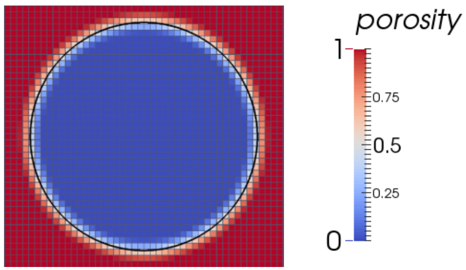
Trunk, Marquardt, Thäter *et al.* (2018). Comput Fluids, 172, 621-631.

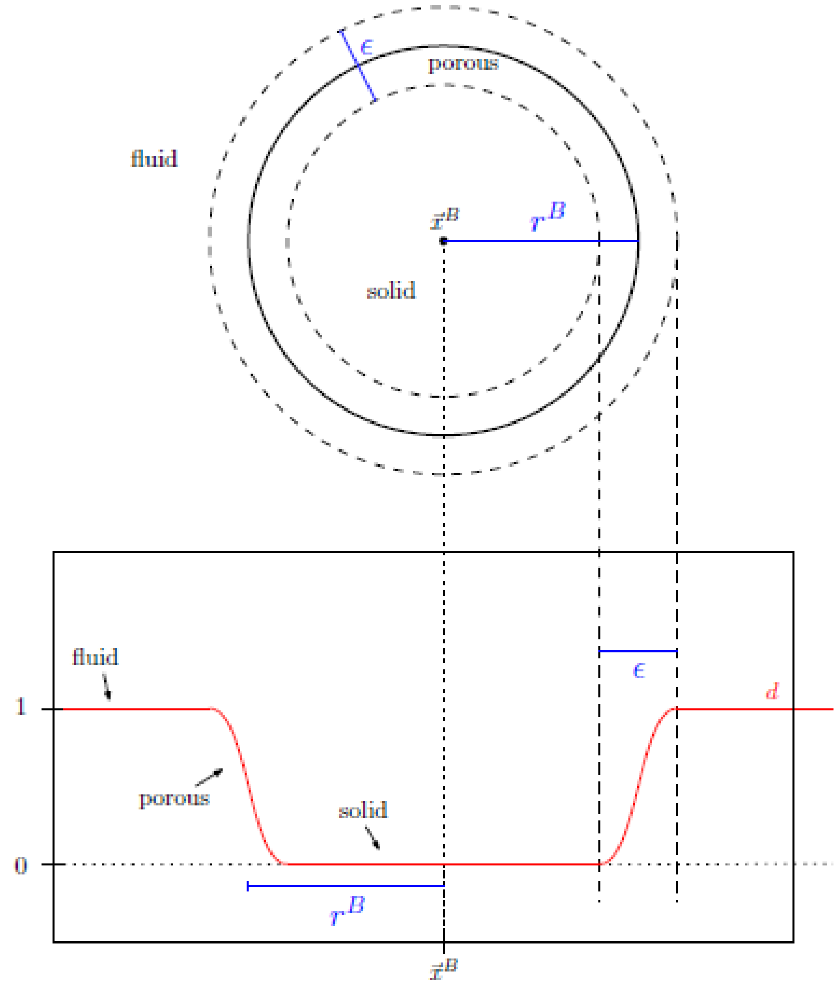
Krause, Klemens, Henn *et al.* (2017). Particuology, 34, 1-13.

HLBM – Particle Representation

- No need for second grid
- No interpolation
- Smooth transition, e.g. $\varepsilon \coloneqq 2h$

- Example for a sphere:
  - With: $\varphi(\boldsymbol{x}) = \left\|\boldsymbol{x} - \boldsymbol{x}^B\right\|_2 - r^B + \frac{\varepsilon}{2}$
  - $d(\boldsymbol{x}) = \begin{cases} 0, & \text{for } \varphi(\boldsymbol{x}) \le 0 \\ \sin^2\left(\frac{\pi\varphi(\boldsymbol{x})}{2\varepsilon}\right), & \text{for } \varphi(\boldsymbol{x}) \in (0, \varepsilon) \\ 1, & \text{for } \varphi(\boldsymbol{x}) \ge 0 \end{cases}$





Shape Parameter (Pearson Correlation Coefficient)

a_S	Shortest half axis	ρ_p	Particle density	κ_{con}	Convexity	λ_{CSF}	Corey shape factor
a_I	Intermediate half axis	E	Elongation	ψ	Sphericity	λ_H	Hofmann shape entropy
a_L	Longest half axis	F	Flatness	κ_{rnd}	Roundness	λ_{LR}	Le Roux shape factor

	a_L	a_I	a_S	ξ_1	ξ_2	ρ_p	E	F	κ_{con}	ψ	$\psi_\perp$	κ_{rnd}	λ_{CSF}	λ_H	λ_{LR}
a_L	1.0	0.55	0.04	0.41	0.17	0.03	0.74	0.51	0.65	0.52	0.64	0.68	0.67	0.73	0.75
a_I	0.55	1.0	0.57	0.39	0.47	0.08	0.13	0.13	0.63	0.61	0.47	0.85	0.05	0.04	0.02
a_S	0.04	0.57	1.0	0.18	0.57	0.03	0.44	0.72	0.41	0.45	0.31	0.61	0.73	0.64	0.65
ξ_1	0.41	0.39	0.18	1.0	0.02	0.08	0.19	0.15	0.47	0.44	0.31	0.57	0.18	0.21	0.21
ξ_2	0.17	0.47	0.57	0.02	1.0	0.03	0.16	0.36	0.07	0.05	0.23	0.34	0.34	0.32	0.31
ρ_p	0.03	0.08	0.03	0.08	0.03	1.0	0.02	0.1	0.03	0.05	0.04	0.05	0.08	0.02	0.03
E	0.74	0.13	0.44	0.19	0.16	0.02	1.0	0.45	0.33	0.2	0.47	0.17	0.72	0.85	0.84
F	0.51	0.13	0.72	0.15	0.36	0.1	0.45	1.0	0.07	0.01	0.0	0.01	0.94	0.79	0.83
κ_{con}	0.65	0.63	0.41	0.47	0.07	0.03	0.33	0.07	1.0	0.93	0.75	0.86	0.17	0.22	0.23
ψ	0.52	0.61	0.45	0.44	0.05	0.05	0.2	0.01	0.93	1.0	0.73	0.86	0.08	0.1	0.12
$\psi_\perp$	0.64	0.47	0.31	0.31	0.23	0.04	0.47	0.0	0.75	0.73	1.0	0.74	0.18	0.2	0.23
κ_{rnd}	0.68	0.85	0.61	0.57	0.34	0.05	0.17	0.01	0.86	0.86	0.74	1.0	0.06	0.08	0.11
λ_{CSF}	0.67	0.05	0.73	0.18	0.34	0.08	0.72	0.94	0.17	0.08	0.18	0.06	1.0	0.92	0.95
λ_H	0.73	0.04	0.64	0.21	0.32	0.02	0.85	0.79	0.22	0.1	0.2	0.08	0.92	1.0	0.99
λ_{LR}	0.75	0.02	0.65	0.21	0.31	0.03	0.84	0.83	0.23	0.12	0.23	0.11	0.95	0.99	1.0

Measured: ~**70.000 CPU-hours**
~ **8 CPU-years**

➔ Thanks to HPC done in a few days

Novel Shape-Modell

Drag correlation $(R_a^2 = 0.96)$

- Found most important parameters
  - Elongation E
  - Roundness κ_{rnd}
  - Reynolds number Re
  - Hofmann shape entropy λ_H

- Mean deviation
  - Current (training): 2.84%
  - Current (test): 2.65%
  - Ganser: 86.26%
  - Hölzer & Sommerfeld: 23.65%
  - Bagheri & Bonadonna: 17.70%
  - Dioguardi & Mele: 26.97%

Terminal settling velocity $(R_a^2 = 0.86)$

- Found most important parameters
  - Particle density ρ_p
  - Roundness κ_{rnd}
  - Sphericity ψ
  - Hofmann shape entropy λ_H

- Mean deviation
  - Current (training): 5.50%
  - Current (test): 4.63%
  - Haider & Levenspiel: 57.85%
  - Dellino: 27.85%

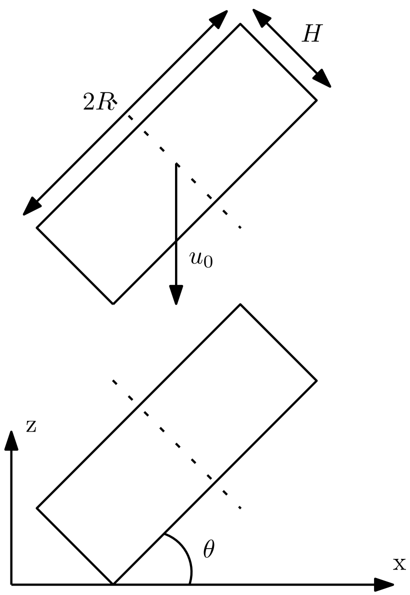
Discrete contact model

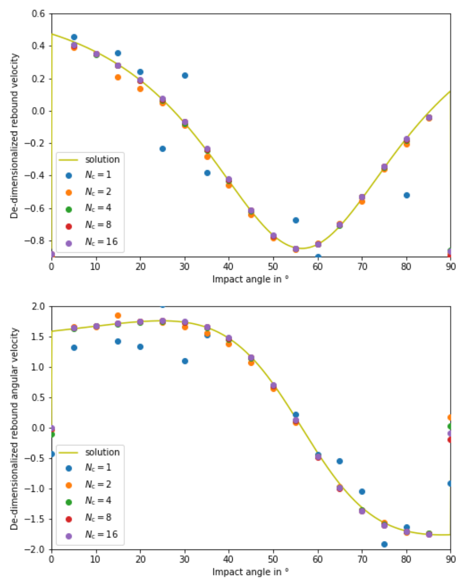
Goal: Shape-dependent contact forces

➔ Normal force $\boldsymbol{F}_n = E^* k \boldsymbol{n}_c \sqrt{Vd}(1 + c\dot{d})$

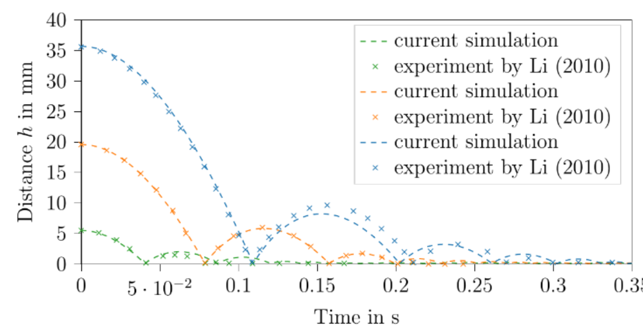
Non-constant parameters derived from mesh-based algorithm

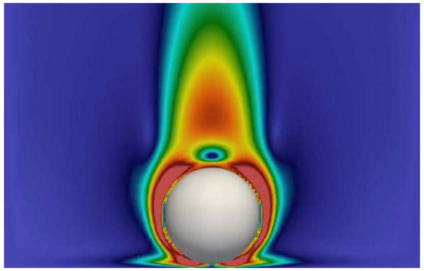
Cylinder-wall impact (without fluid)





Rebounding sphere in viscous fluid





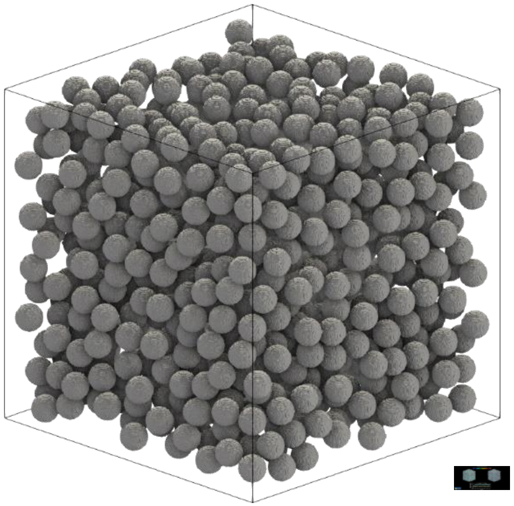
Marquardt, J. E., Römer, U. J., Nirschl, H. & Krause, M. J.. Particuology 80, 180–191 (2023).

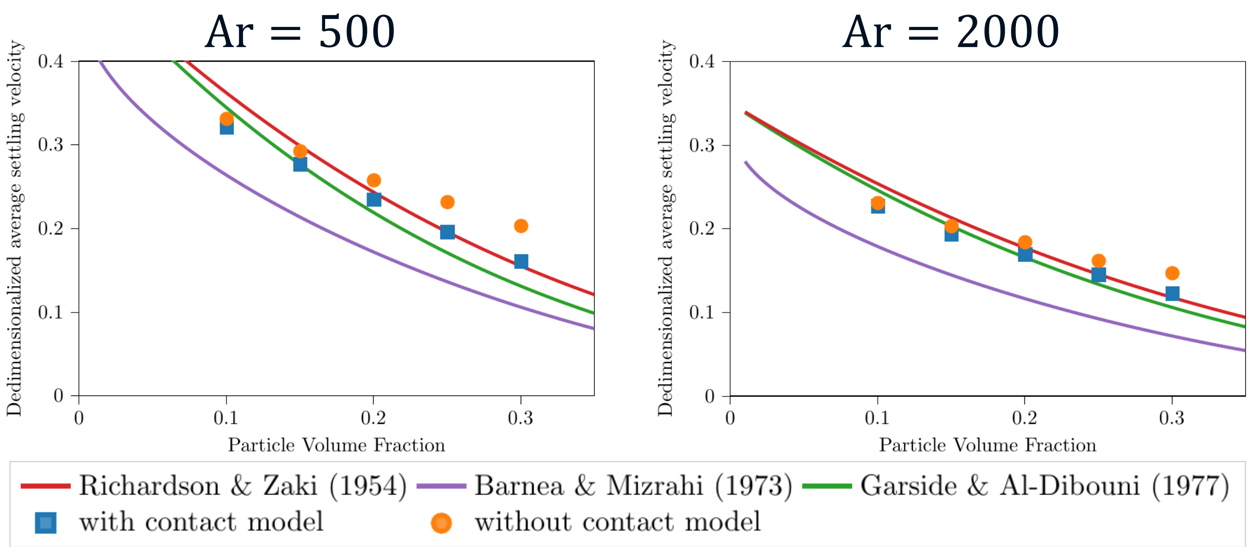
Application to hindered settling

Goal: Examine shape-dependency of settling particle collectives

➔ Challenges: Arbitrary shapes, computational effort

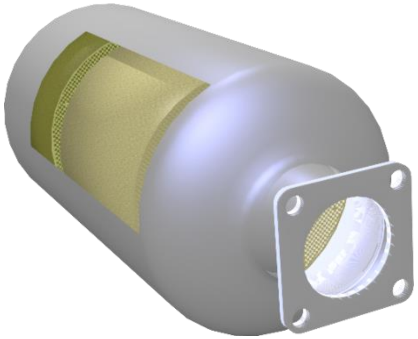
- High particle volume fractions (up to 30%)
- Hundreds/Thousands of surface resolved particles
- Shape-dependent four-way coupling





Marquardt et al. (2023). In preparation

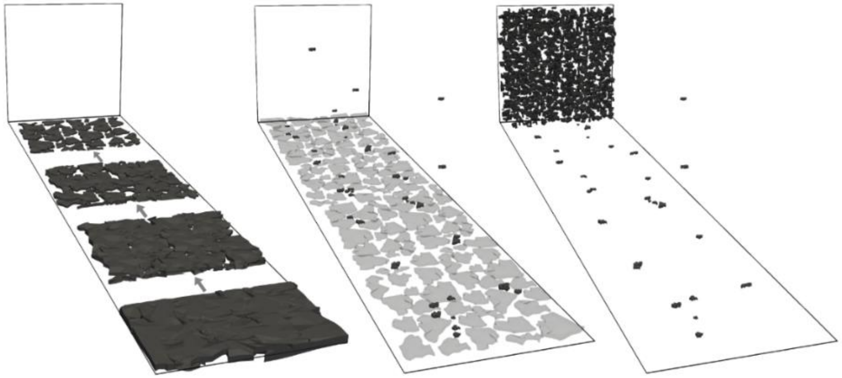
Exhaust Treatment by Wall-flow Filters, Particle

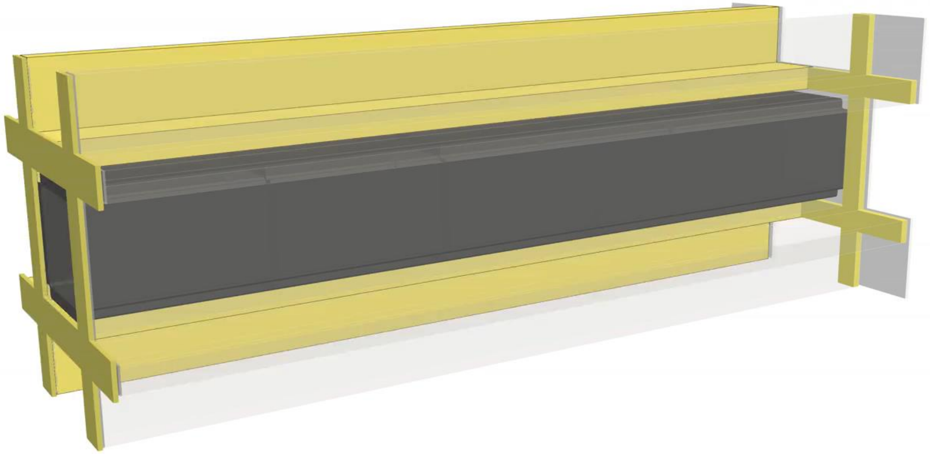


Goal: Investigation of particle-layer rearrangement

➔ simulation of resolved particulate flows

- Ash accumulates, forms specific deposition patterns
- Patterns evolve due to oxidation during the filter regeneration
- Effect of deposition patterns:
    - change in filter efficiency
    - increase of pressure loss



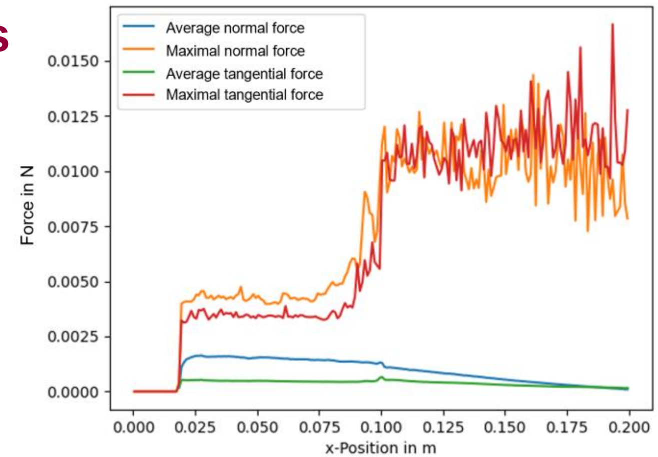


Hafen, N., Dittler, A., Krause, M. J. (2020). Submitted to Philos. Trans. R. Soc. A.

Damage Potential of Fruit Pieces

Goal: Investigation of coarsely dispersed suspens with high particle volume fractions

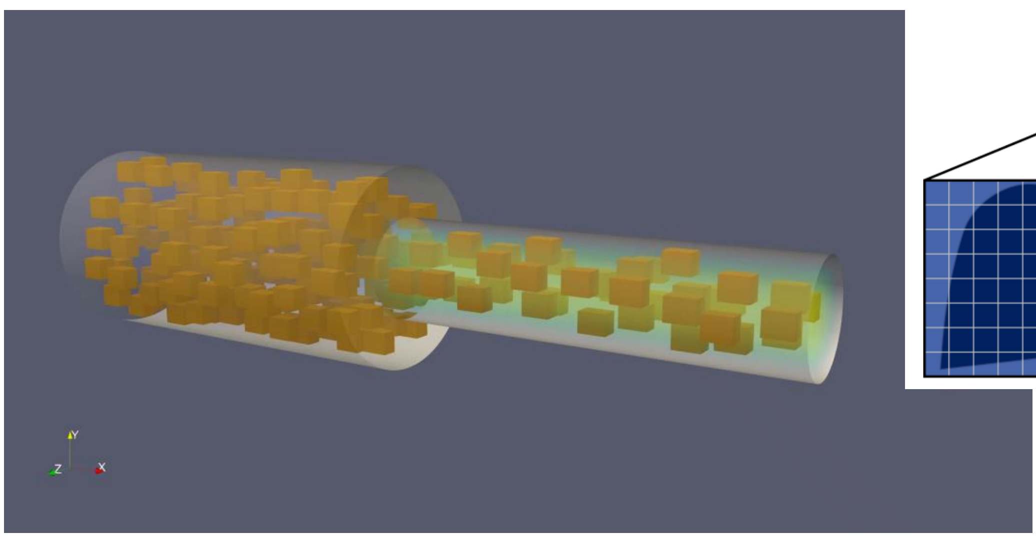
➔ realistic shapes are important for accurate results

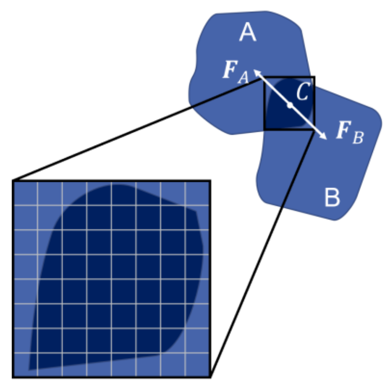


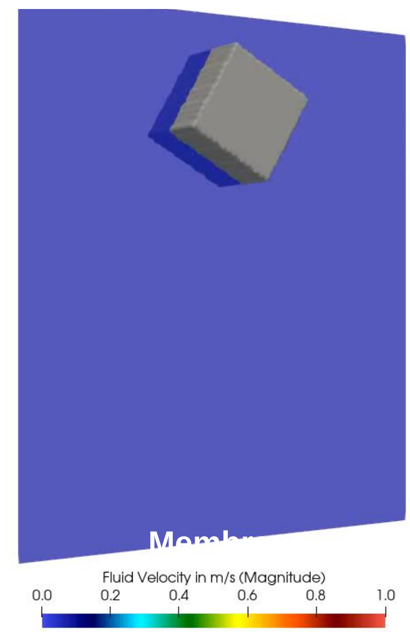
Challenges:

- Modelling (four-way coupling, phys. properties, …)
- High computational effort

Solutions: (HLBM + discrete contact treatment via overlap volume





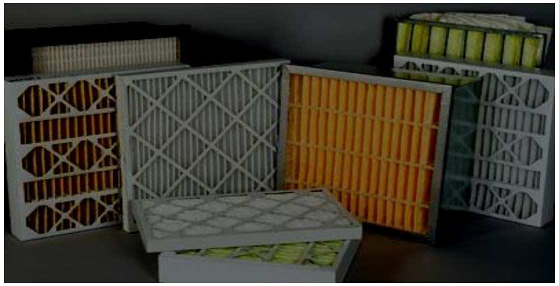


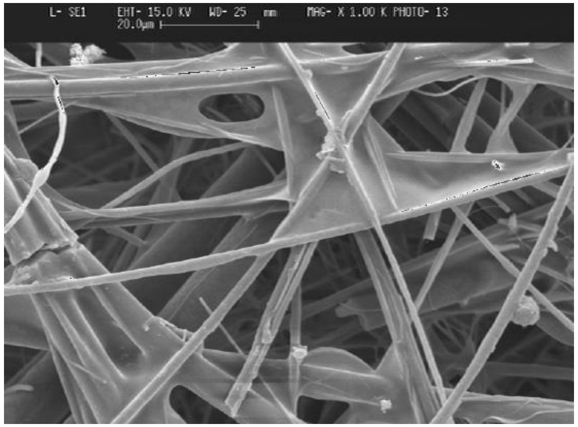
Micro Filtration, Particle

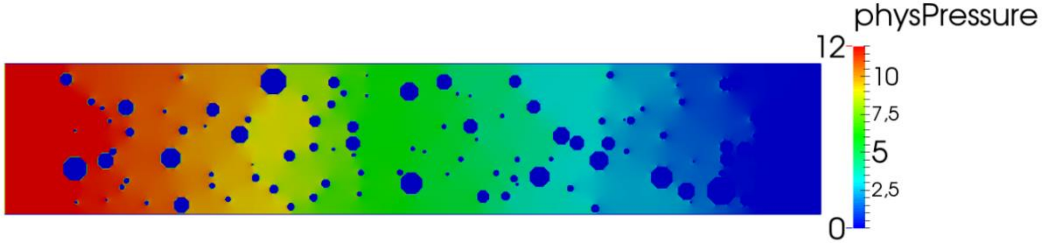
Goal: design of an efficient filter

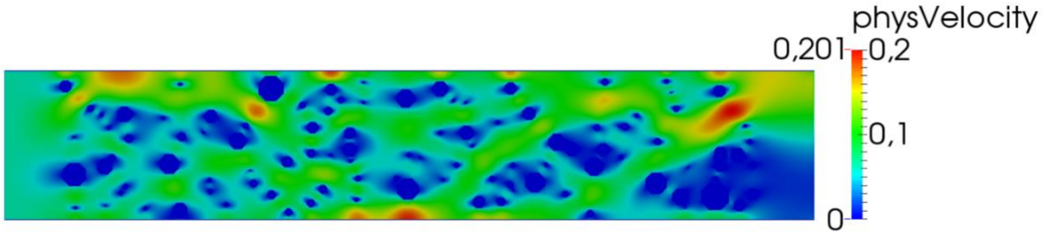
➔ vary shape of filter and flow conditions

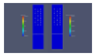
- geometry from µCT scans
- 2D and 3D transient simulation slip flow
    - particles (Lagrange)
    - air as density (Euler)









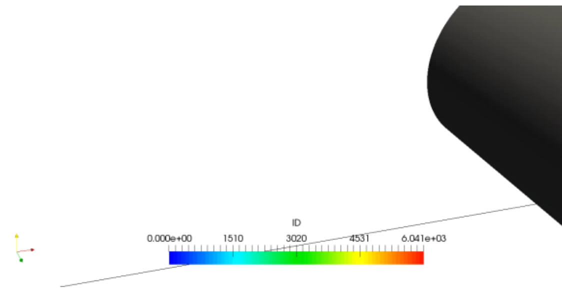


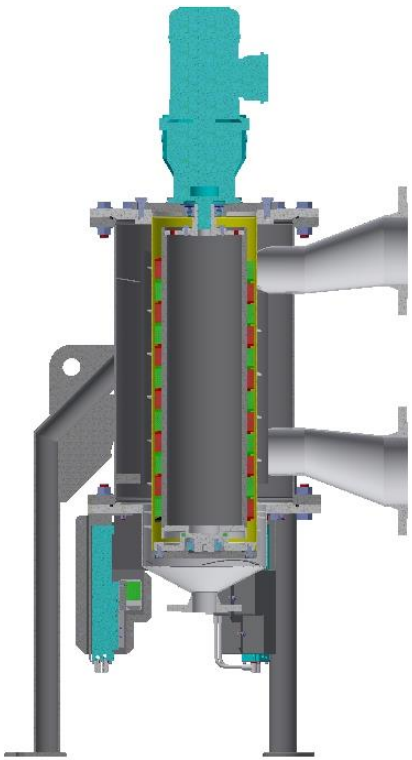
Augusto, L. D. L. X., Ross-Jones *et al.* (2018). Commun Comput Phys, 23, 910-931.

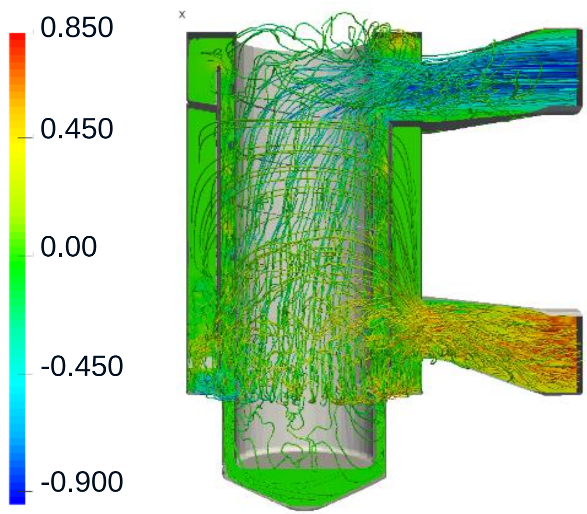
Magnetic Spiral Separator, Particle

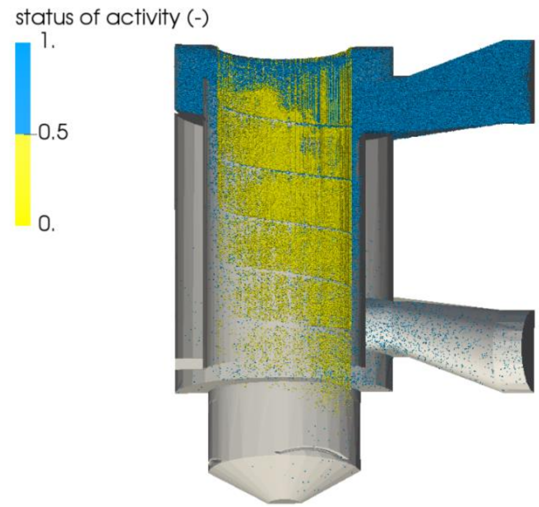
Goal: basic understanding, increase efficiency

3D simulation with LBM
- carrier fluid (Euler)
- magnetic field (Euler)
- magnetic particles (Lagrange)









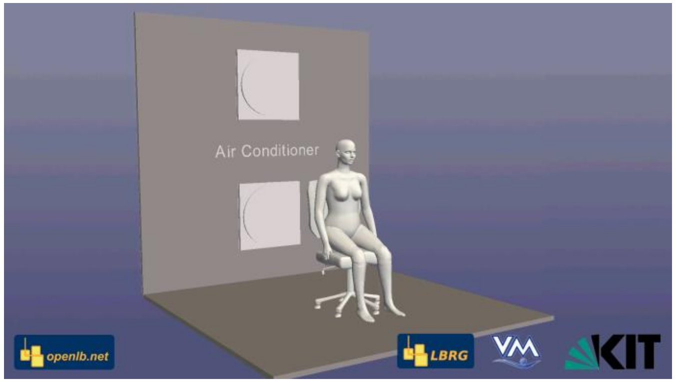
Maier, M. L., Milles, S. *et al.* (2018). Comput. Math. with Appl., 76(11-12), 2744-2757.

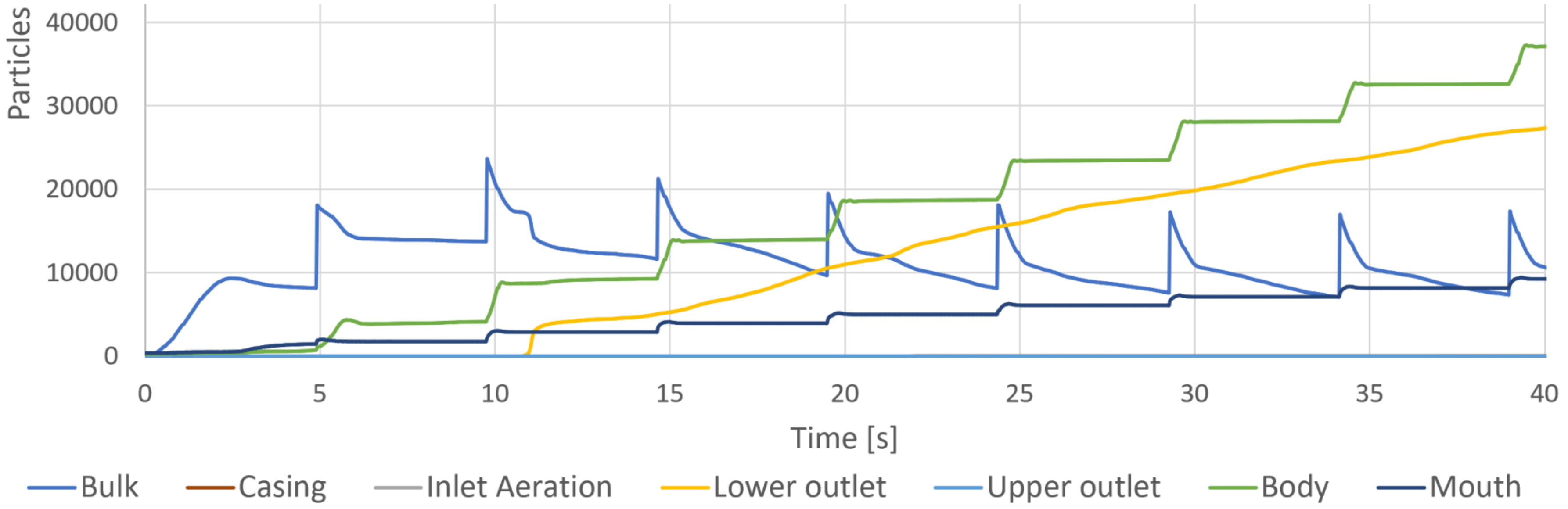
Maier, M. L., Henn, T., Thaeter, G. *et al.* (2017). Chem Eng Technol, 40(9), 1591-1598.

Particulate Flows in Buildings, Particle & LES

Goal: Understand and control virus risk in buildings

➔ combine sub-grid particle model & LES
- evaluate situations
  - window open
  - person moving
- aeration system design
- control aeration using sensors





Photobioreactor Simulation, Complex System

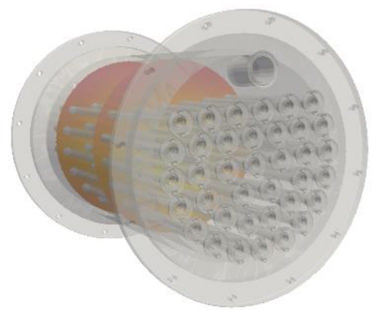
Goal: optimize energy balance

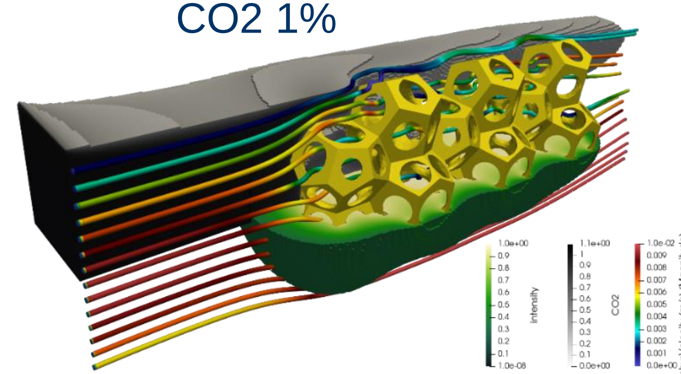
(energy input / bio mass output)

➔ change shape, position, inflow

- 3D suspension simulation
  - algae as particles (Lagrange)
  - CO_2 , Water as density (Euler)
  - algae consume CO_2
- 3D light simulation

next: vary pipe shape, sun position





absorption **out-scattering** **emission** **in-scattering**

Mink, A., McHardy, C. *et al.* (2020). J Quant Spectrosc Radiat Transf, 243, 106810.

Mink, A., Thäter, G., Nirschl, H. *et al.* (2016). J Comput Sci, 17, 431-437.

Agenda

Overview LBM & *OpenLB*

Challenge I -- Turbulence

Challenge II -- Suspensions

Challenge III -- Optimization

Summary

Optimal Control Solution Strategies

Problem: $\left.\begin{array}{l}\text{find control } \alpha \text{ and state } f \text{ such that} \\ J(f,\alpha) \text{ is minimised and } \; G(f,\alpha)=0 \text{ holds}\end{array}\right\}$

Side condition G governed by e.g. a BGK-Boltzmann equation

Two solution strategies [3]

- Iterative, gradient-based (Steepest Descent, LBFGS)
- Discretization: LBM
- Parallel

Approach I

First-discretize-then-optimize

- (Discrete) adjoint-based [1, 2]
- Algorithmic Differentiation [3]

Approach II [3]

First-optimize-then-discretize

- Adjoint-based

[1] Pingen, Evgrafov, Maute (2007). Struct Multidisc Optim 34(6), 507-524.

[2] Tekitek, Bouzidi, Dubois *et al.* (2006). Comput Fluids, 35(8-9), 805-813.

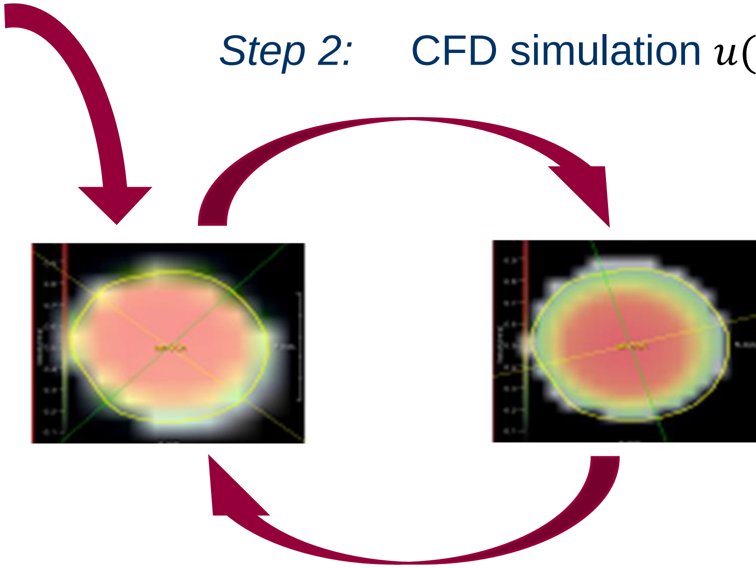
[3] Krause (2010). Dissertation, KIT Karlsruhe.

CFD-MRI: Basic Algorithm, Optimization

Step 1: Noisy MRI scan velocity u^*,
boundary ➔ start "porosity" d_0

Step 2: CFD simulation $u(d_i)$

Goal:
Reduce noise,
identify flow topology

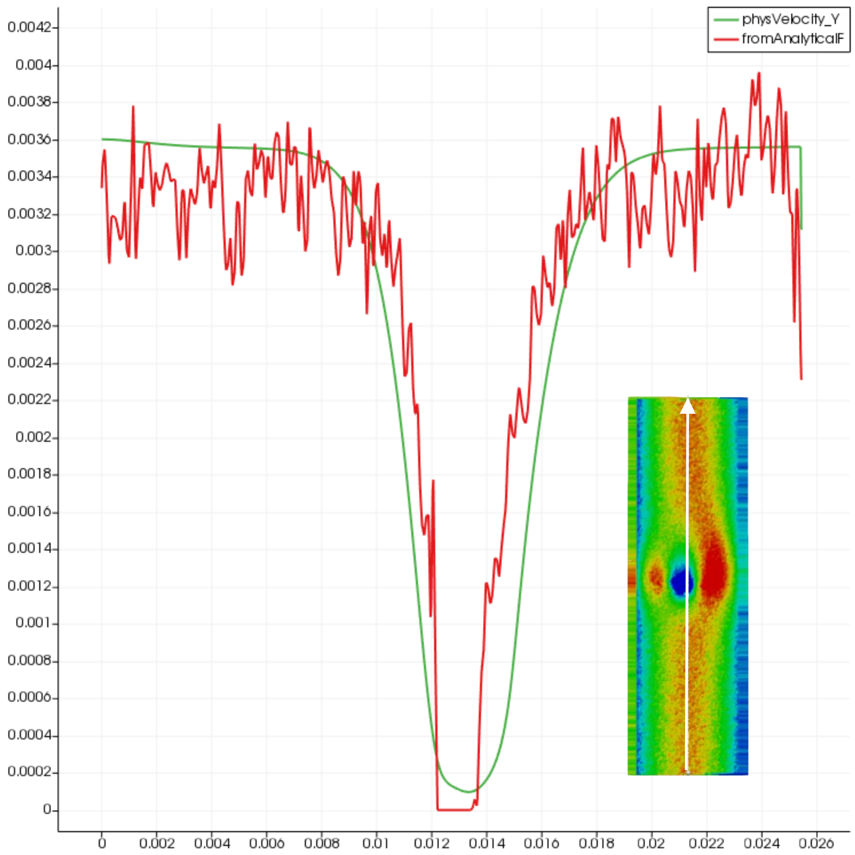


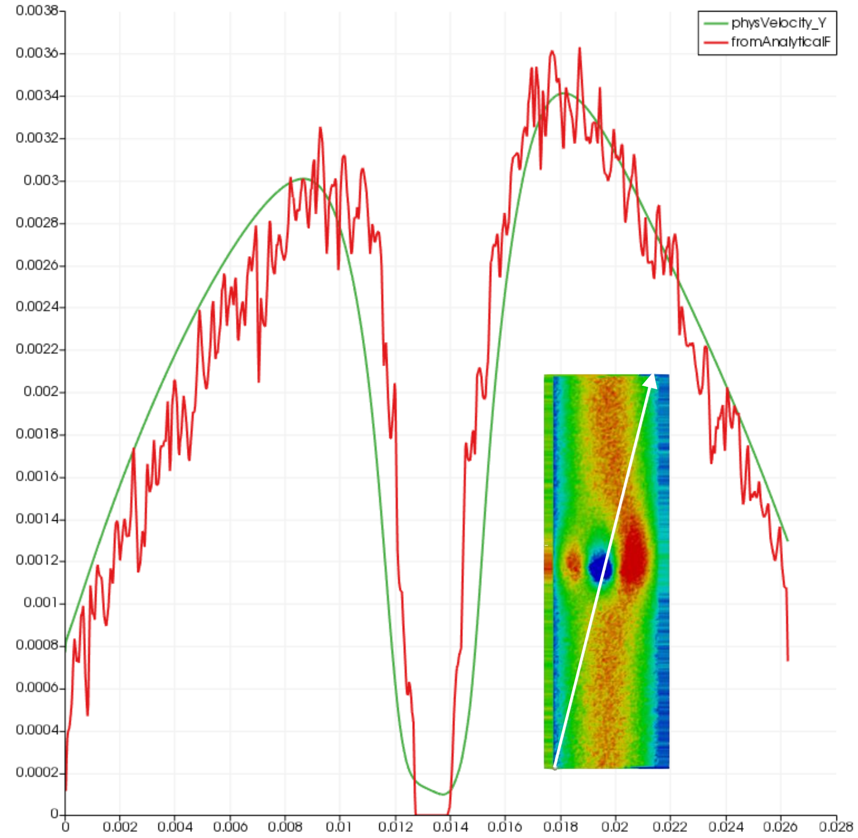
Step 3: Calculate *a)* difference between CFD and MRI $J = \int_\Omega (u(d_i) - u^*)^2$,
b) gradient dJ and with this,
c) new parameter for porosity d_{i+1}

Krause, Förster, Mink *et al.* (2016). In *HPC in Sci and Eng 16* (pp. 337-353).

Validation II: Qualitative Study - MRI Data (2)

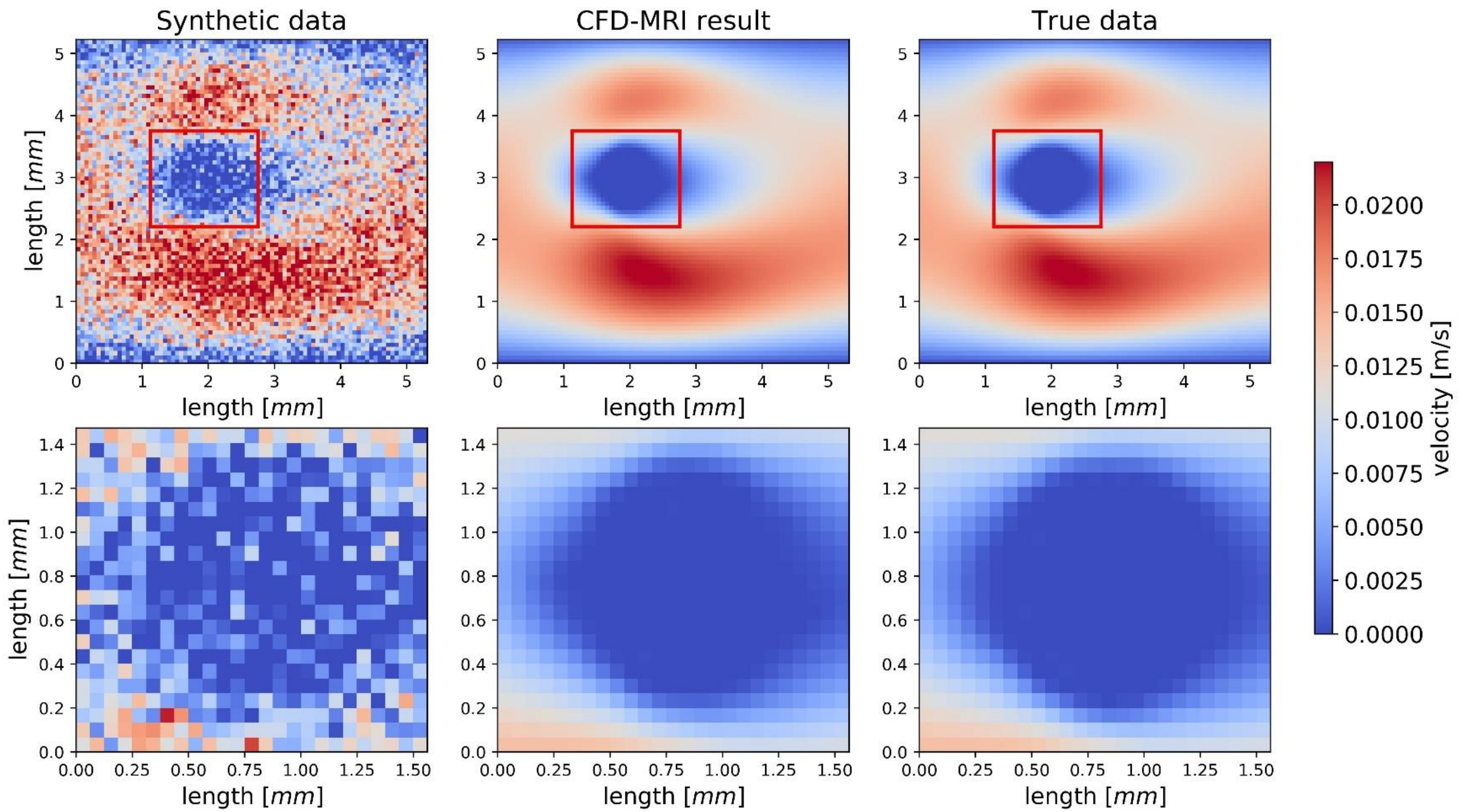
Velocity profile for different lines through the plane





→ Measurement noise drastically reduced

Validation III: Quantitative Study - Synthetic Data (1)

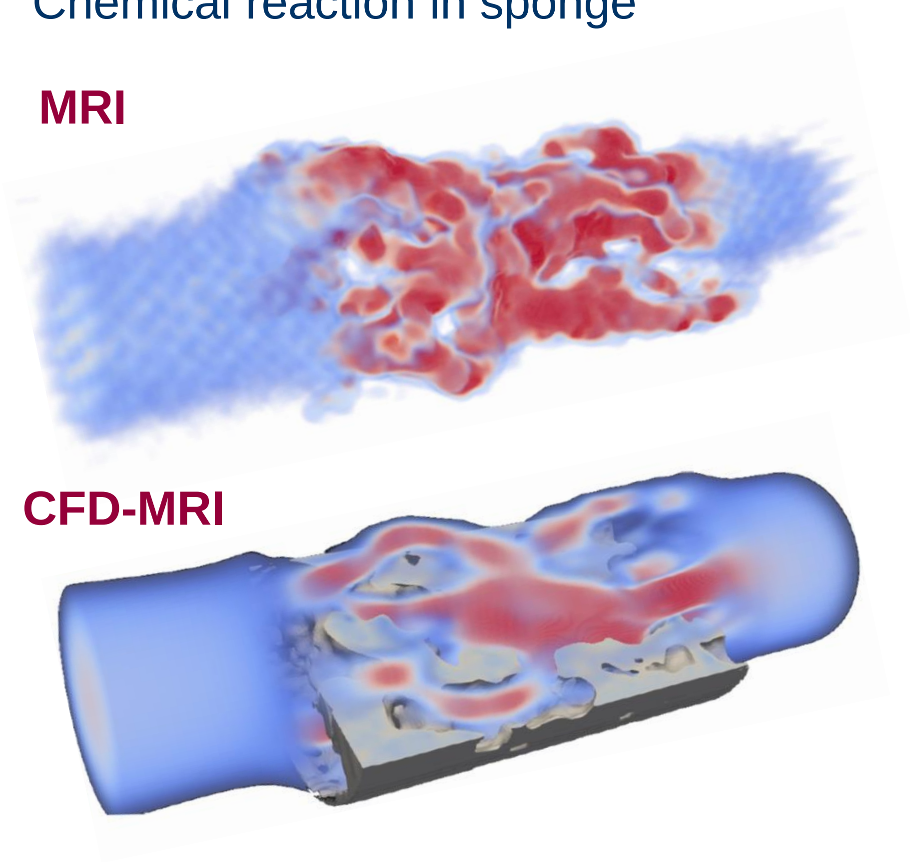


→ **Synthetic Measurement vs. True Data: rel. error 61.5%**

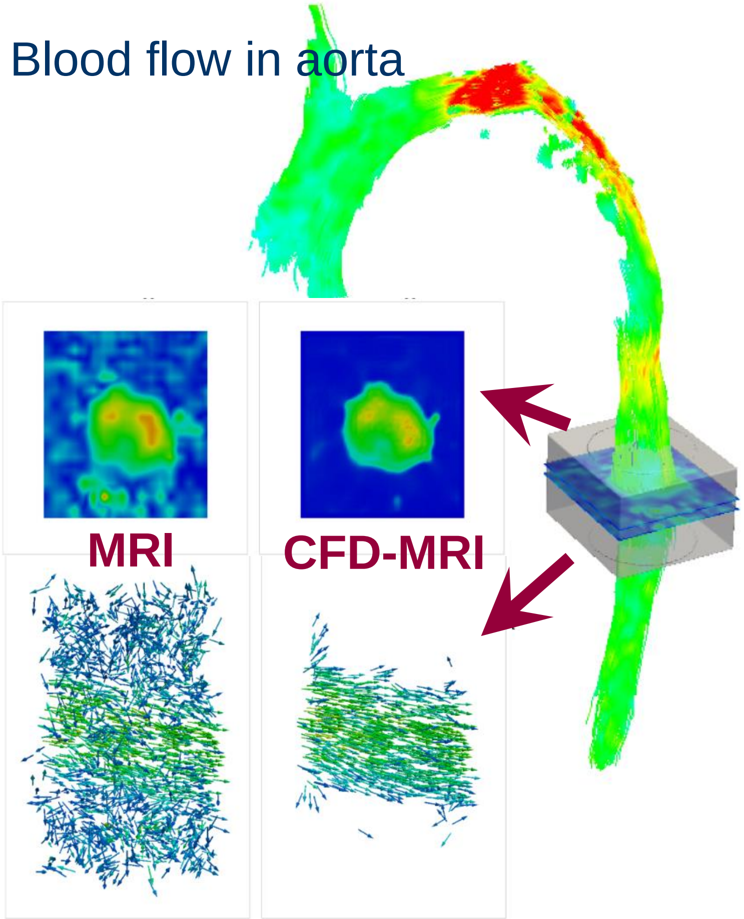
→ **CFD-MRI Data (Synthetic M.) vs. True Data: rel. error 0.68%**

CFD-MRI: Applications Sponge & Aorta, Optimization

Chemical reaction in sponge



Blood flow in aorta



Klemens, Schuhmann, Guthausen *et al.* (2018). Comput Fluids, 166, 218-224.

Klemens, Schuhmann, Balbierer *et al.* (2020). Comput Fluids, 197, 104391.

Agenda

Overview LBM & *OpenLB*

Challenge I -- Turbulence

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Summary

Summary: Facing Challenges in CFD

(H)LBM & *OpenLB* as Fast, Stable & Accurate Generic PDE Solver

Turbulence

DNS/LES/Implicit LB-based Modell instead of RANS

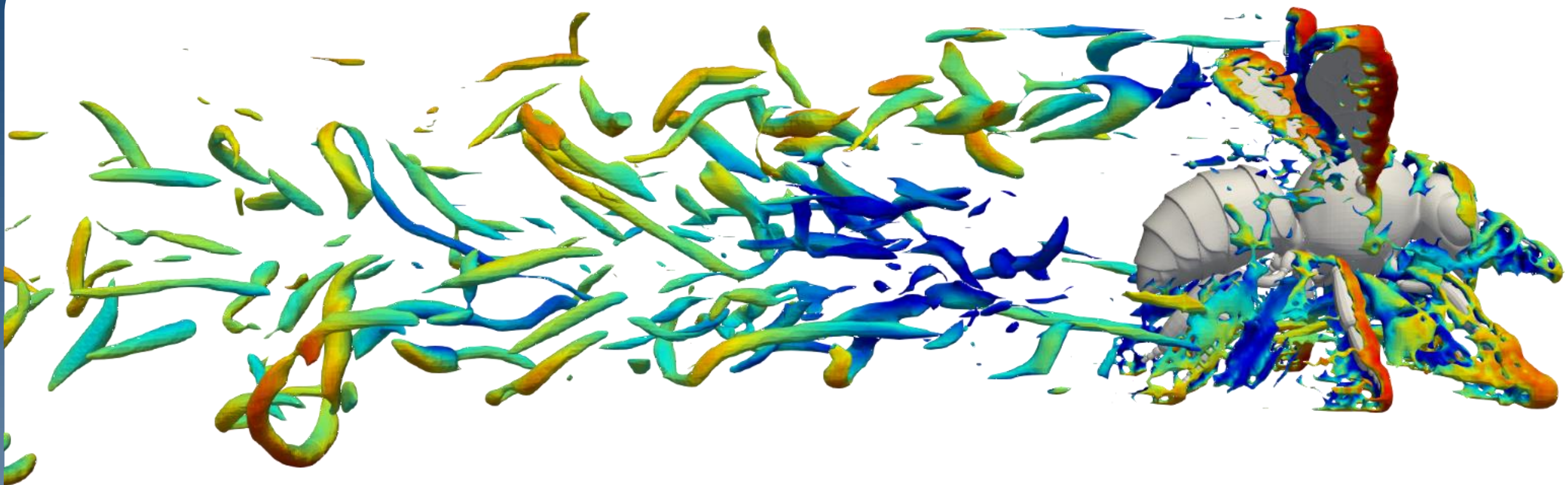
Suspensions

Resolve particles (shape, force, …)

Optimal Control/ Optimization

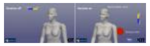
Algorithmic differentiation, adjoints

LBM & *OpenLB*: open source meshing and high performance at your fingertips!



Questions?

Download, try, participate…



Download **User Guide** **Forum**

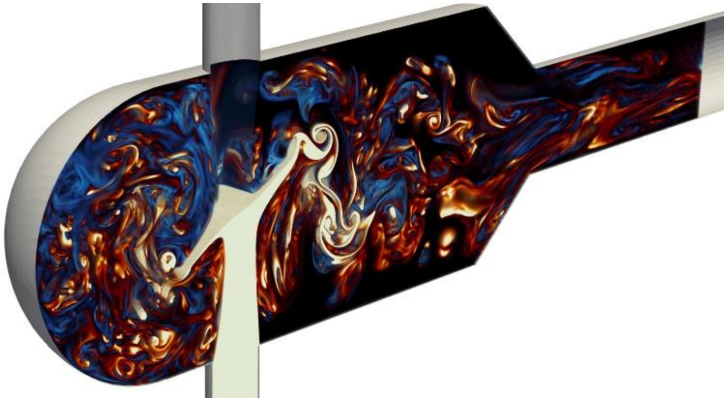
7th Spring School: LBM with OpenLB Software Lab

7th Spring School

Lattice Boltzmann Methods with OpenLB Software Lab

Heidelberg, Germany, March 4–8, 2024

- For scientists and industrial users
  Option Beginners: comprehensive theoretical lectures on LBM, mentored training on case studies using *OpenLB* (www.openlb.net),
  Option Advanced: bring your own problem
- Knowledge exchange, networking at poster session, coffee breaks and excursion



Academia 420 € / Industry 1.770 € for 5 days course including course material, 5x lunch, 2x dinner, coffee breaks and excursion

Karlsruhe Institute of Technology

HEIDELBERGER AKADEMIE DER WISSENSCHAFTEN
Akademie der Wissenschaften des Landes Baden-Württemberg

Executive committee
Stephan Simonis, Shota Ito, Kerstin Dick, Mathias J. Krause

Invited speakers
Timm Krüger, Halim Kusumaatmaja, Francois Dubois, Timothy Reis, Martin Frank