OpenLB

Open source Lattice Boltzmann code

Groupe de travail: Schémas de Boltzmann sur réseau, *March 24th, 2021*

OpenLB -- Fluid Flow Simulation and Control on High Performance Computers

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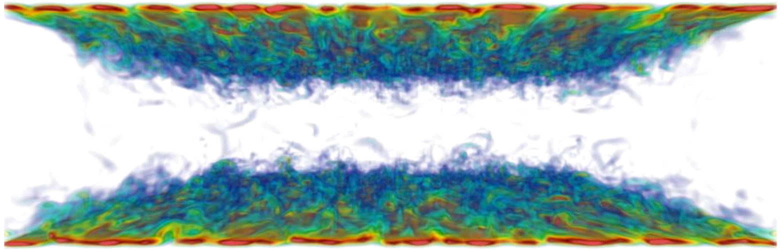
Challenges in (Computational) Fluid Mechanics

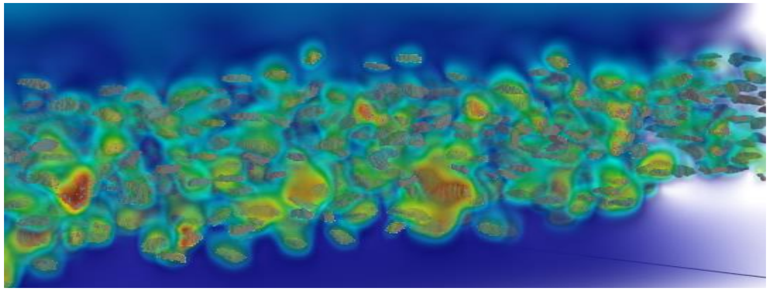
Challenge 1: Turbulence

- capture small scales
- models inaccurate or expensive



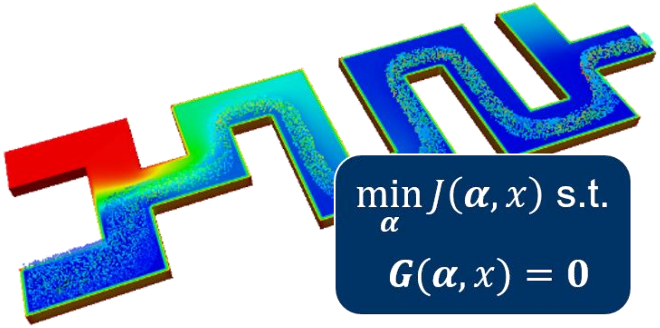
Challenge 2: Suspensions

- capture effects of small particles
- models inaccurate or expensive



Challenge 3: Optimal Control / Optimization

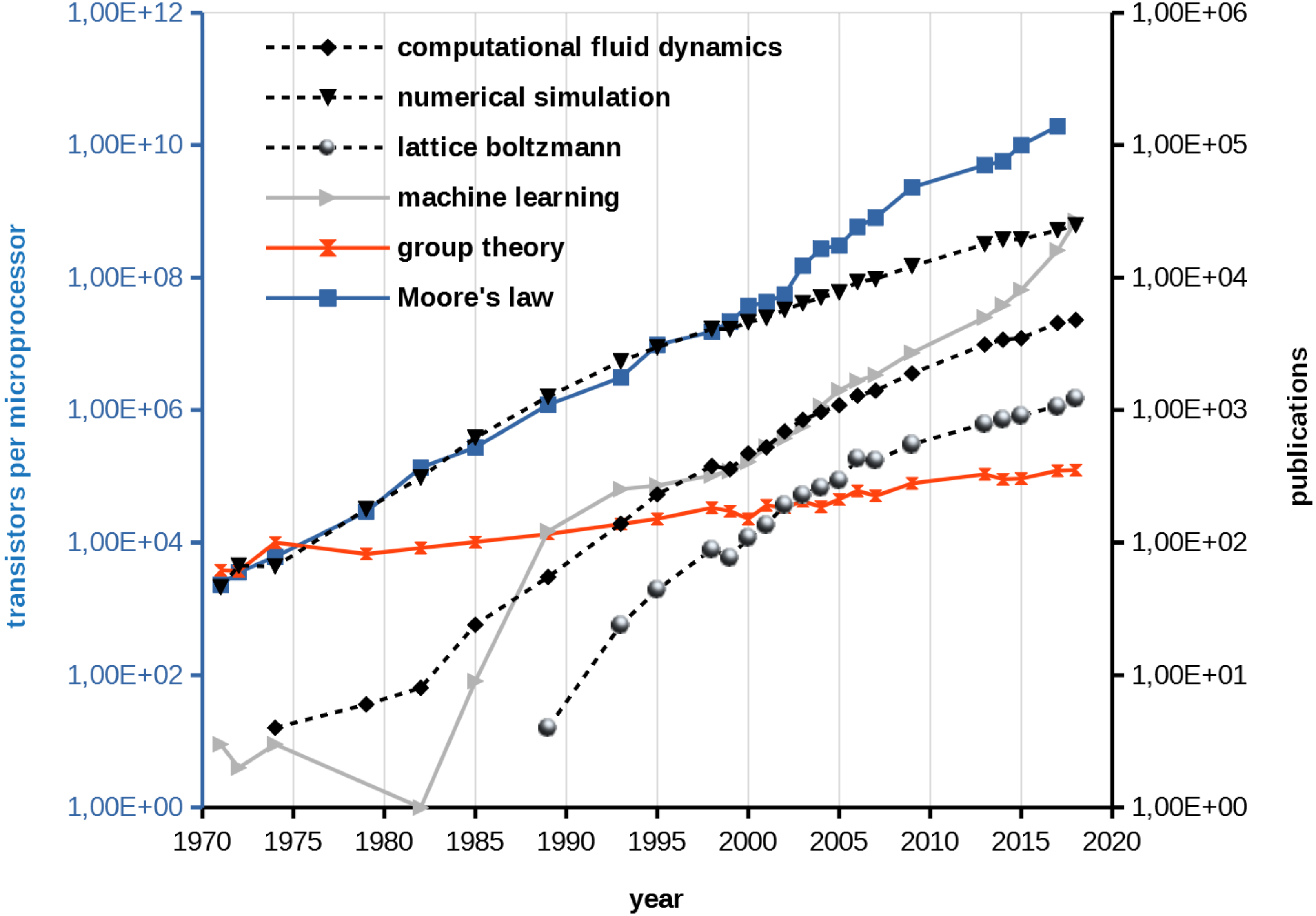
- enable model calibration & optimization
- formulation problem dependent, expensive



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 Lattice Boltzmann Methods (LBM)

- 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

Agenda

Overview *OpenLB*

Challenge I -- Turbulence

Challenge II -- Suspensions

Challenge III -- Optimization

Summary

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Summary

Modelling Flows of Incompressible Newtonian Fluids

macroscopic:

Navier-Stokes equation

$\boldsymbol{u}, p$ in $I \times \Omega$

$h \to 0$

[Saint-Raymond 2003]

mesoscopic:

Boltzmann equation /
BGK-Boltzmann equation $h \in \mathbb{R}_{>0}$

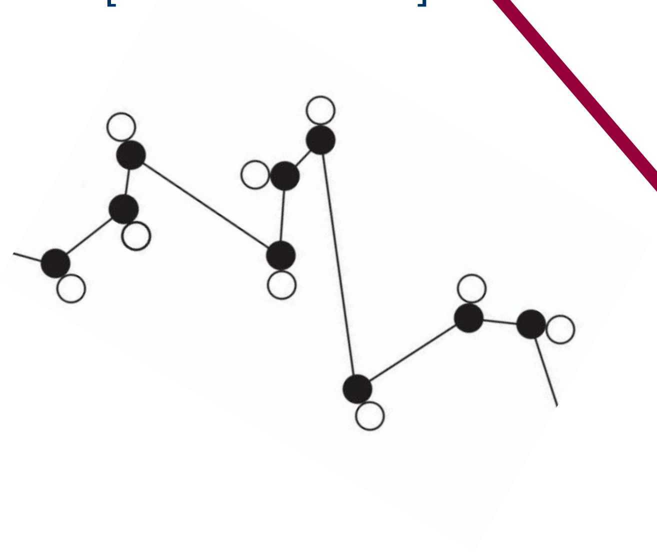
f in $I \times \Omega \times \mathbb{R}^d$

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

[K. 2010]

consistent discretisation: LBM

[Junk et al. 2005]



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

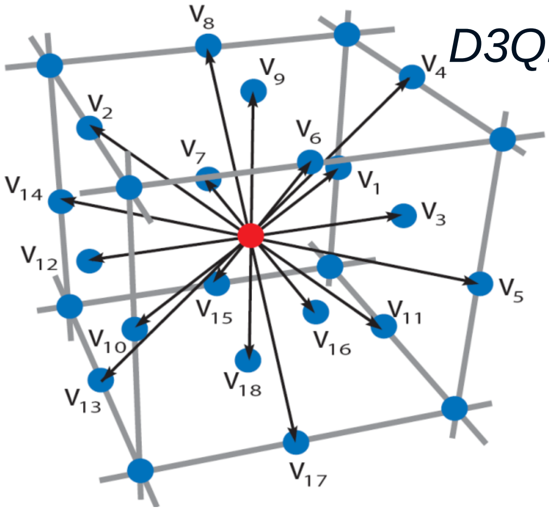
lattice Boltzmann equation

f_i in $I_h \times \Omega_h \times Q$

- explicit scheme
- efficient parallelisation

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

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

Facts and Figures

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

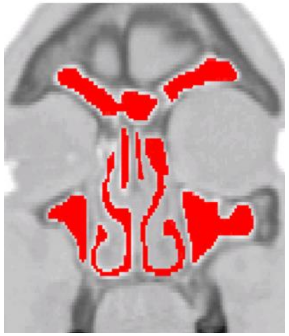
Realization

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

Features in latest release 1.4

- Various lattice types: D2Q9, D3Q15, D3Q19, ...
- Local, non-local, on- and off-lattice boundary conditions
- Collision models: BGK, MRT, LES, multiphase, thermal
- **Build-in pre-processing from e.g. STL-files**
- Unit conversion for problem set-up in SI-units
- XML interface for input parameters
- Visualization (built-in and VTK)

Built-in Geometry Creation and Meshing



CT/MRT

***Step 1a)*:**

Segmentation,
Smoothing

Materialise
driving your innovations

VMTK, ITK, …

CAD

Step 1b):

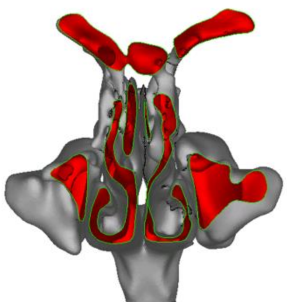
Import

Indicator Functors

Step 1c):

Built-in

openlb.net

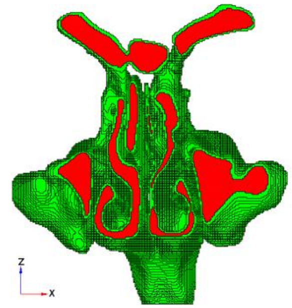


STL Surface Mesh **and/or**
Geometry Primitives

Step 2:

Built-in voxelizing

openlb.net

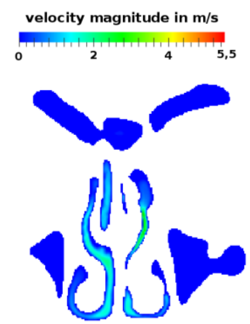


Voxel
Mesh

openlb.net

Step 3:

Setting of
material-
dependent
boundary
conditions

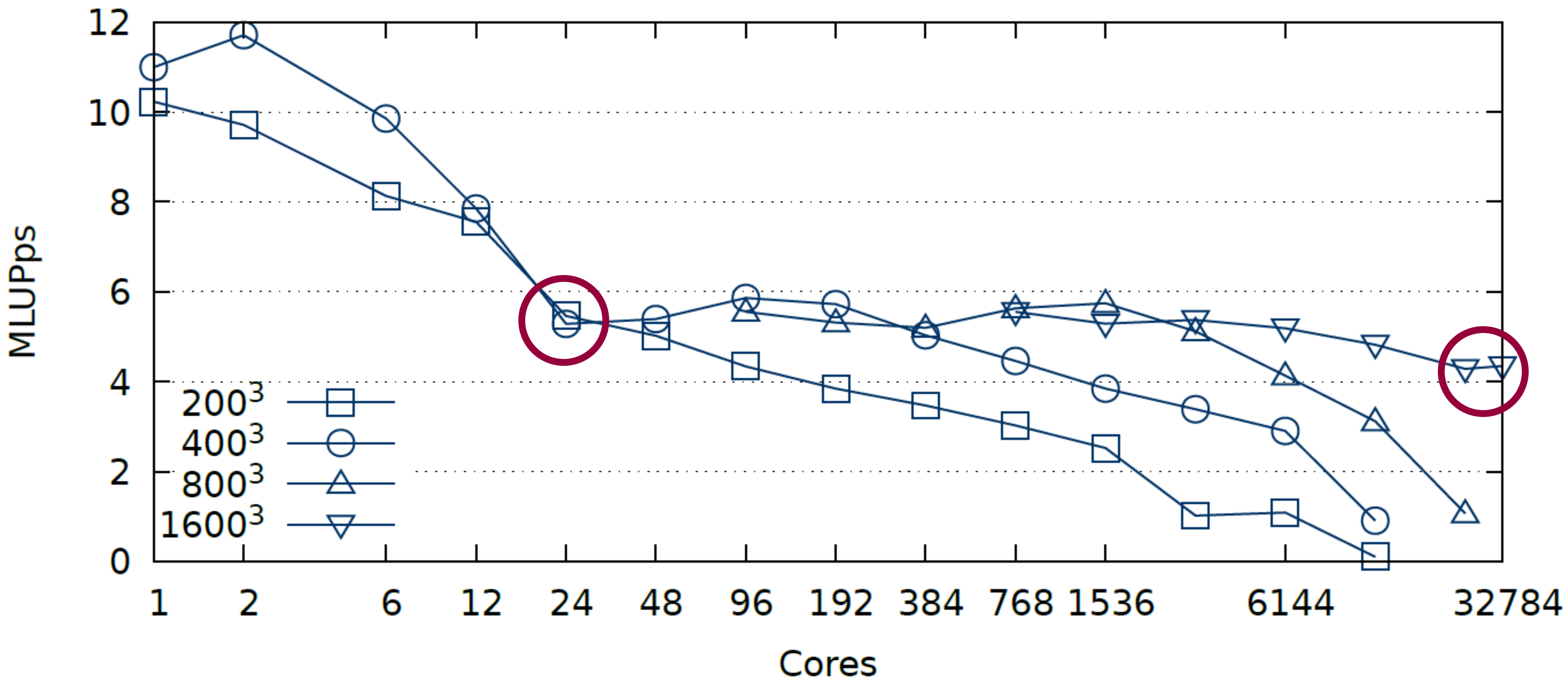


Simulation
Results

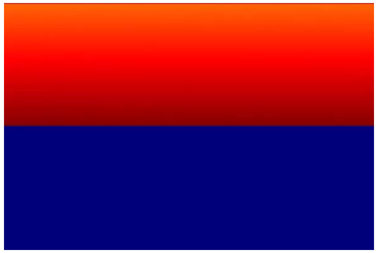
Parallel Performance @ Magnus, Curtin, Australia

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

PAWSEY supercomputing centre

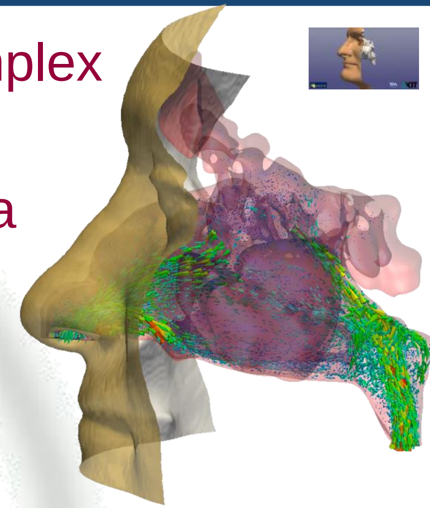


Applications

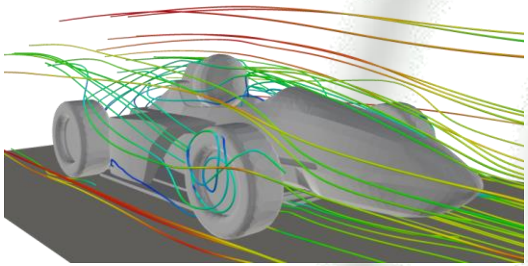


Multiphase flows

Flows in complex geometries, porous media

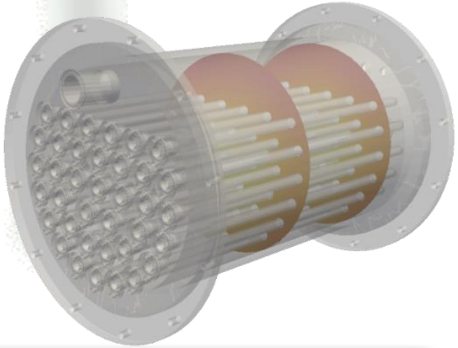


Turbulent flows

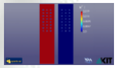


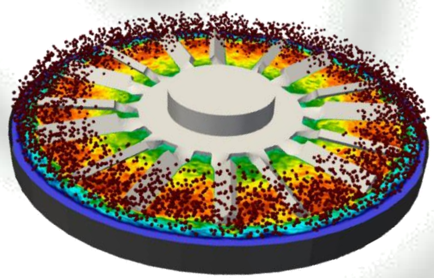
OpenLB Applications

Radiative transport

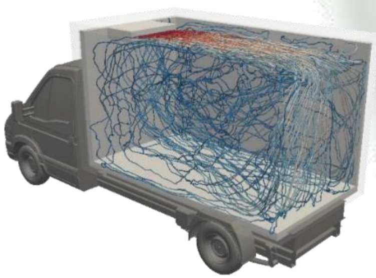


Particle flows





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. (2020). Comput Math Appl, in Press.

Agenda

Overview *OpenLB*

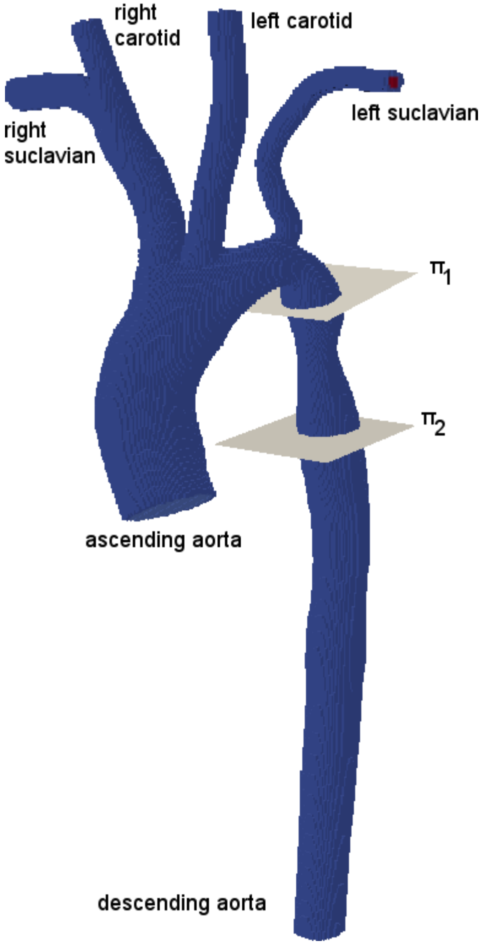
Challenge I -- Turbulence

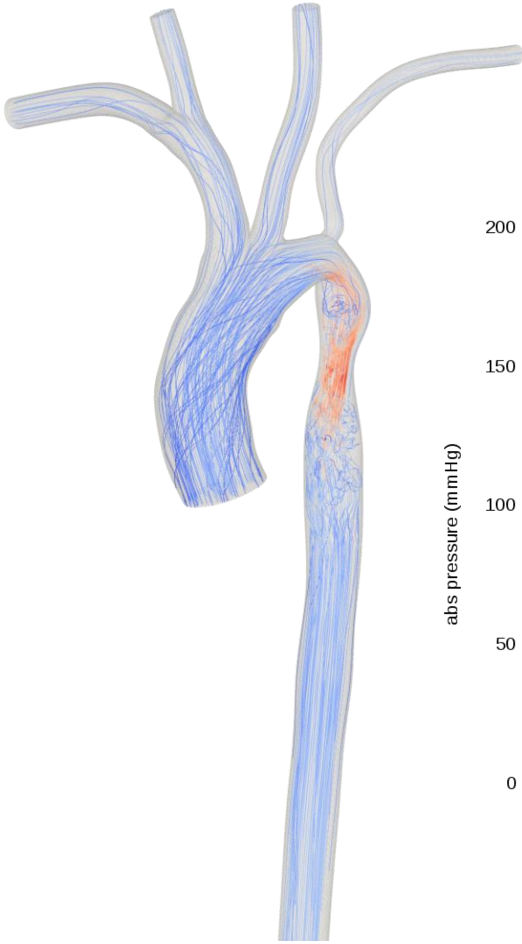
Challenge II -- Suspensions

Challenge III -- Optimization

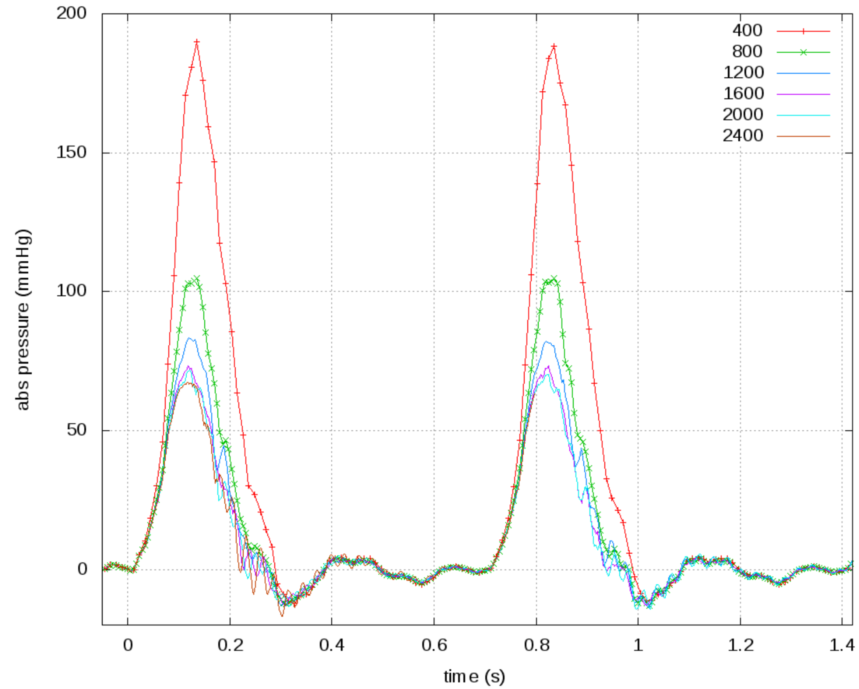
Summary

Aorta Benchmark, DNS





Goal: Validate DNS LBM

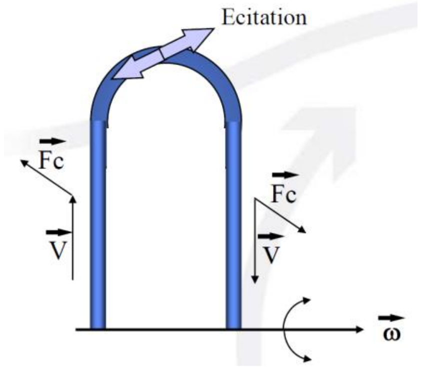


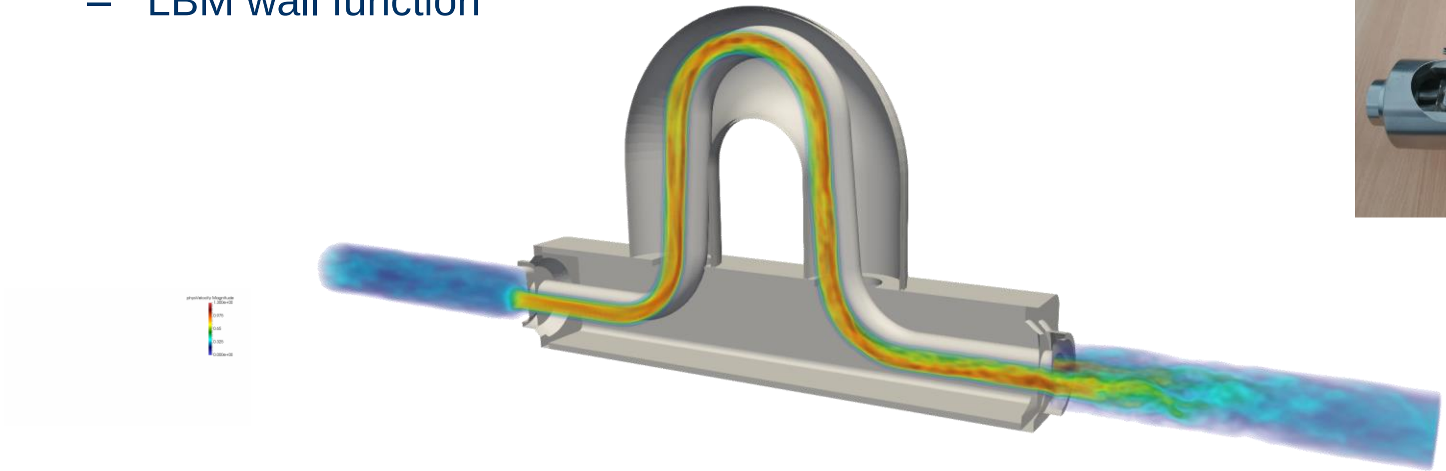
Henn, T., Krause, M. J. *et al.* (2012). In proceedings MICCAI12 STACOM12 7746, 34.

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





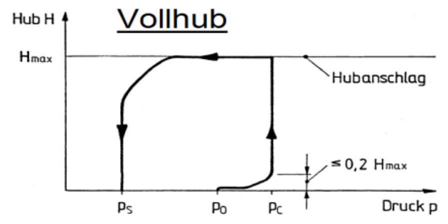
Haussmann, M., Reinshaus, P., Simonis, S. *et al.* (2020). Preprint arXiv:2005.04070 [physics.comp-ph].

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

Safety Valve Simulation, LES

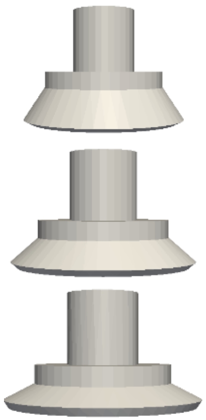
Goal: avoid chatter

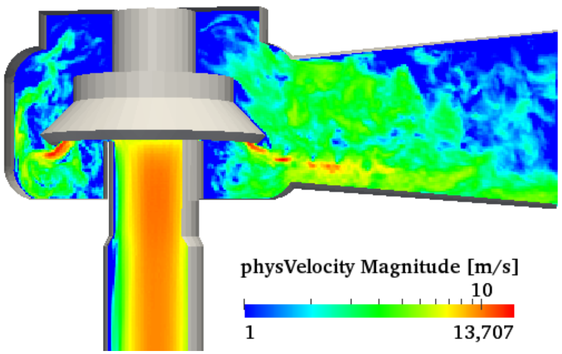
➔ vary shape of disk

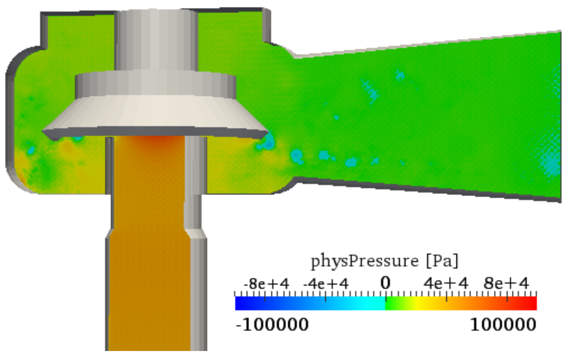


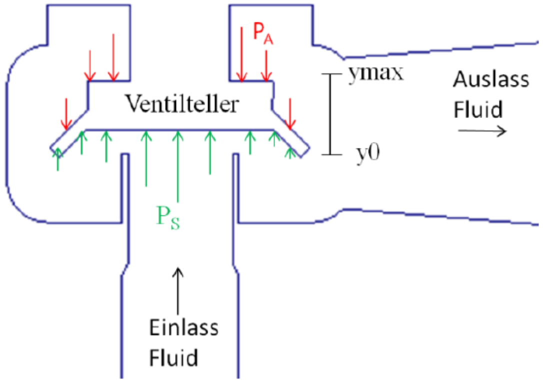
- 3D transient turbulent simulation
- 1 billion degrees of freedom
- parallelization: 30 days ➔ 1 day
  64 cores ➔ 2.048 cores
- optimize shape of disk

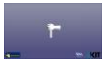
different disk angle









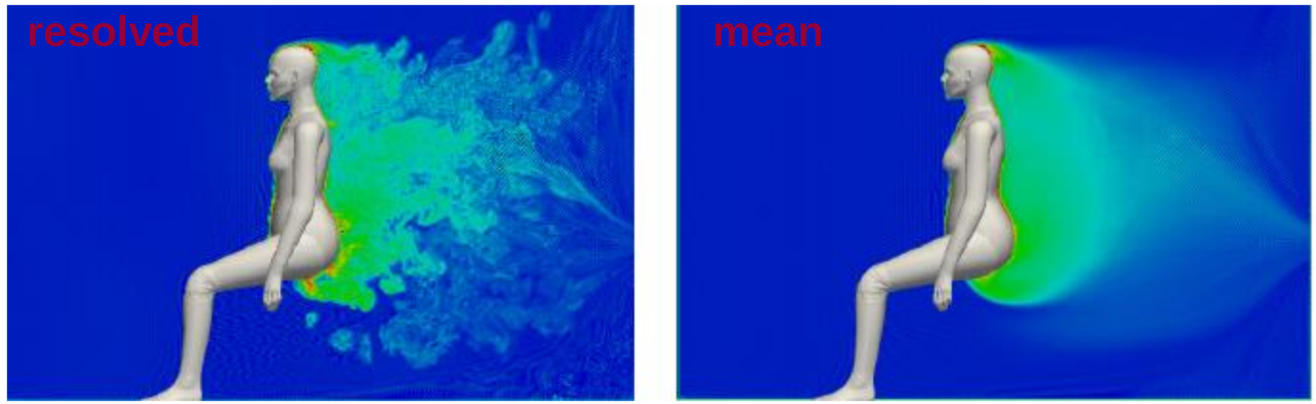


Thermal Flow for Thermal Comfort, LES

Goal: Improve thermal comfort

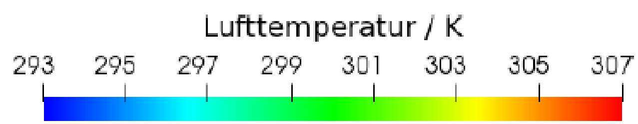
control flow patterns by change of design and flow conditions of

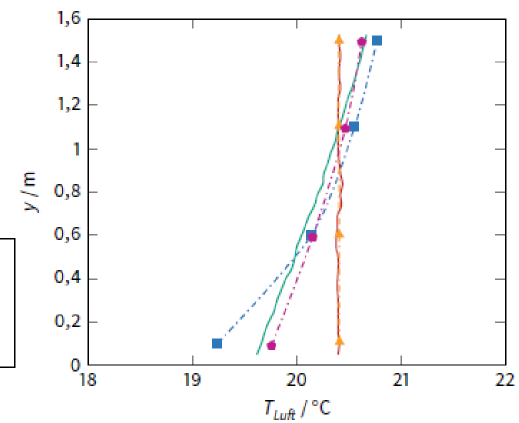
- Heating
- Air condition
- Ventilator



Benchmark study:

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



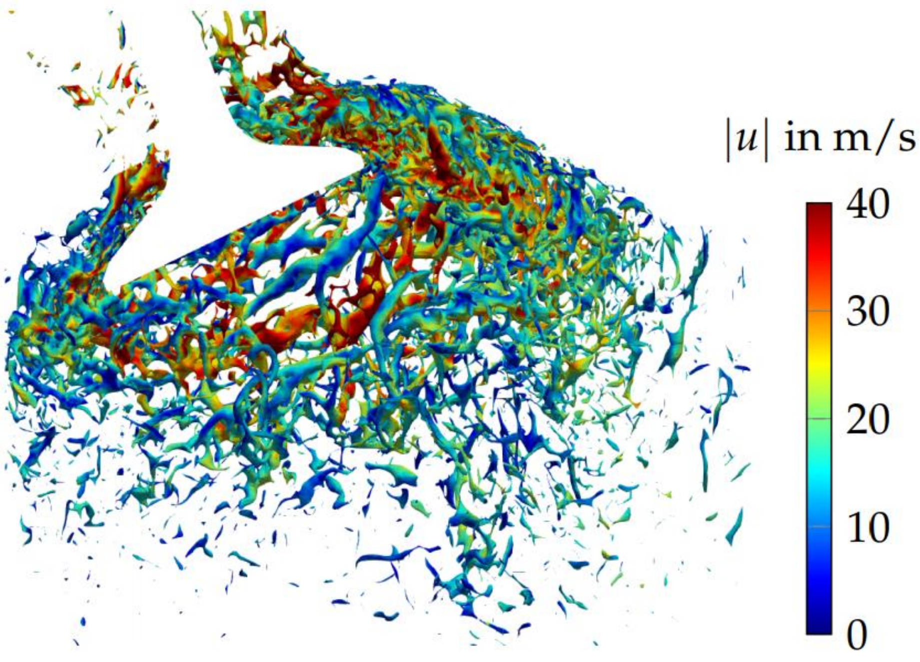


Siodlaczek, M., Gaedtke, M., Simonis S. *et al.* (2020). Submitted to Build Environ.

Turbulent Flows with LBM LES: Applications

- **Wall models** for LBM LES, e.g.:
  Near-wall-models (NWM)
  with SRT LBM

- **NWM-LES LBM for**
  Complex turbulent flows
  relevant to
  internal combustion engines

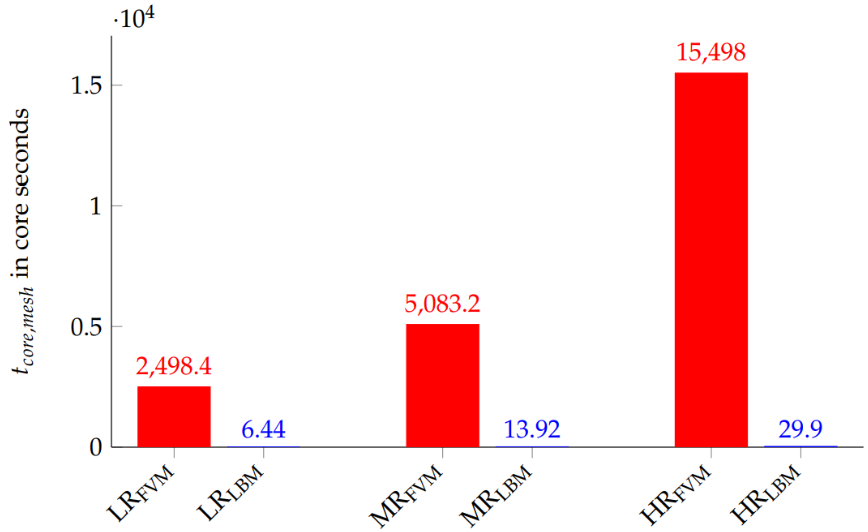


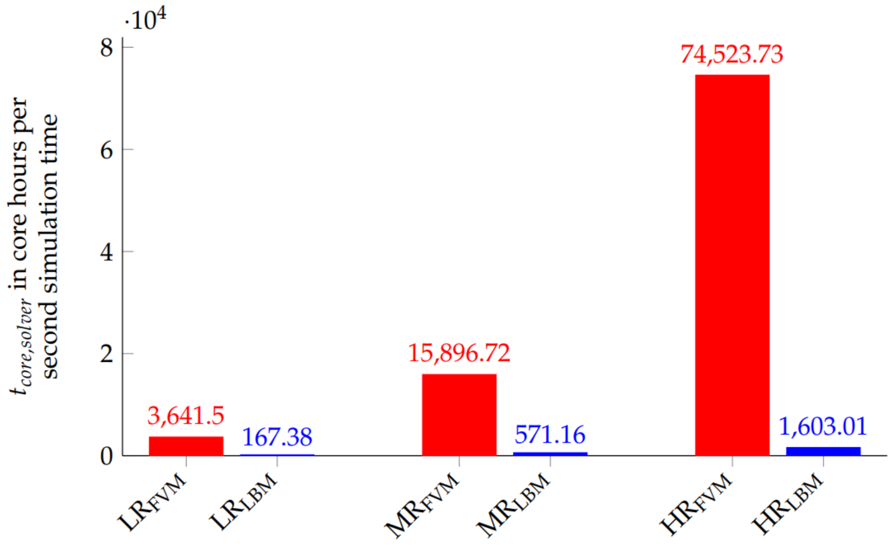
- **Comparison of OpenFOAM and OpenLB** w.r.t.:
  capability of **prediction accuracy, computational cost, ease of use**.

Haussmann, M., Barreto, A. C., Kouyi, G. L. *et al. (2019). Comput. Math. App. 78, 3285– 3302.*

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

OpenLB (LBM) vs OpenFOAM (FVM)

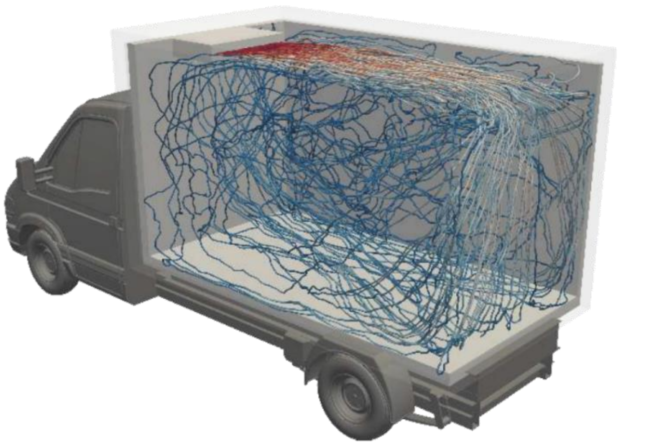




- Similar **NWM-LES**:
  Smagorinsky–Lilly, van Driest damping, Musker wall function
- Similar **prediction accuracy**
- **computational cost for the present setup**:
  meshing with OpenLB is 424x faster than with OpenFOAM
  simulation with OpenLB is 32x faster than with OpenFOAM

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

Thermal Flow in Refrigerated Vehicles, LES



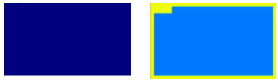
Goal: Improve the insulation efficiency

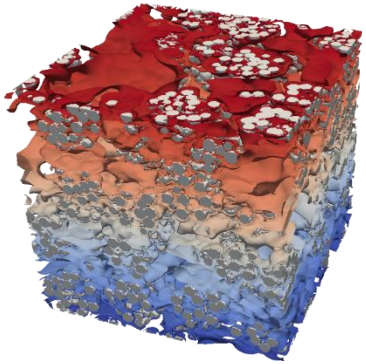
➔ exchange insulation material

- 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.

Agenda

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Challenge III -- Optimization

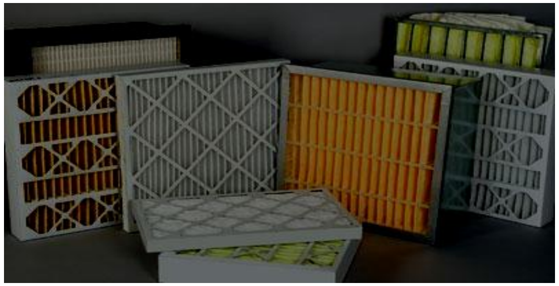
Summary

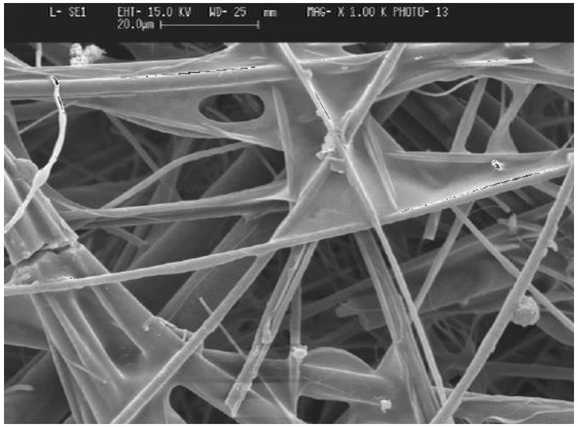
Micro Filtration, Particle

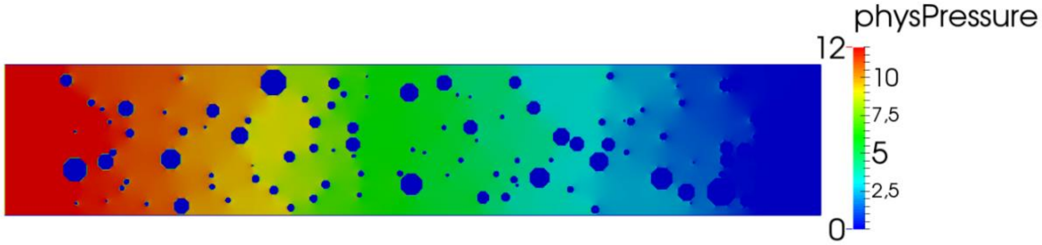
Goal: design of an efficient filter

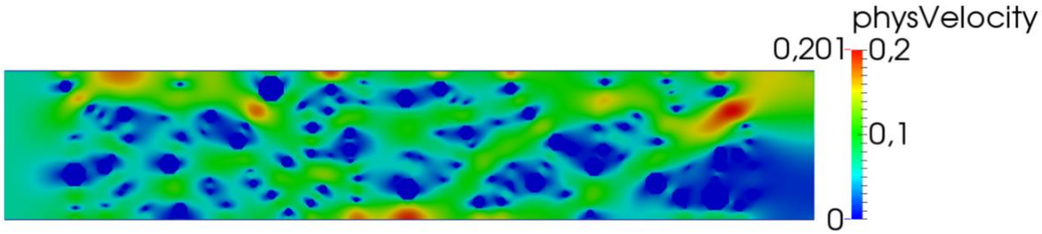
➔ vary shape of filter and flow conditions

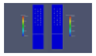
- geometry from µCT scans
- 2D and 3D transient simulation slip flow
    - particles (Lagrange)
    - air as density (Euler)







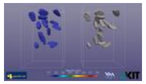




Augusto, L. D. L. X., Ross-Jones *et al.* (2018). Commun Comput Phys, 23, 910-931.

Fine Particle Fractionation, Particle

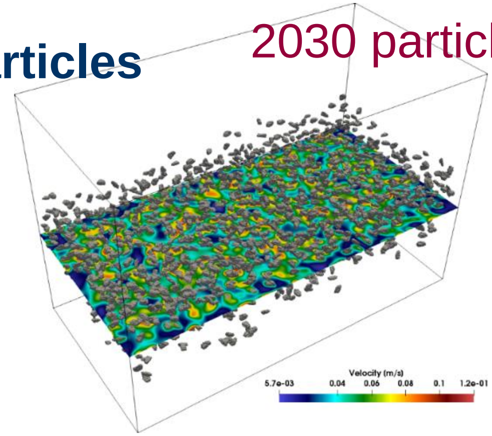
Challenge: Low selectivity in the range from $100\ nm$ to $10\ \mu m$



Goal: Improvement of separation processes

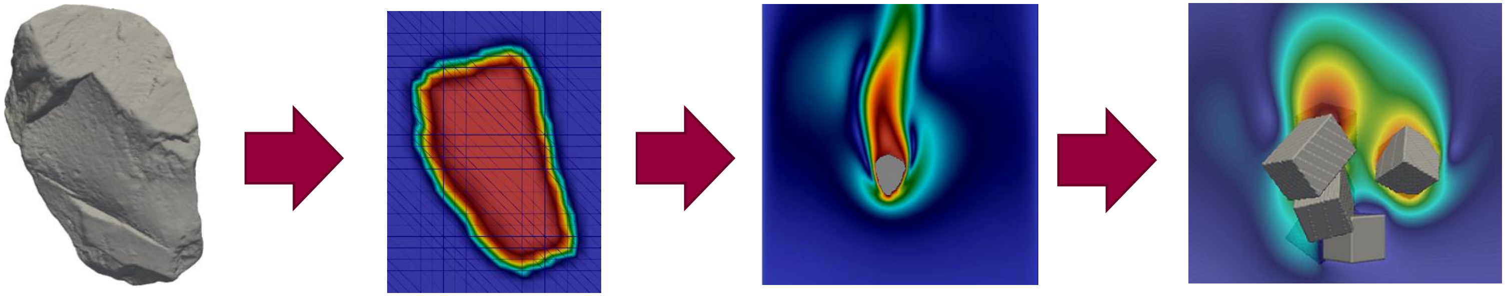
➔ Simulation of a large number of **arbitrary shaped particles**

2030 particles



Method needs to account for surface structure

Contact treatment for non-spherical particles is complex



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

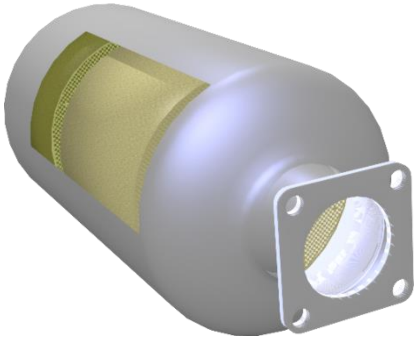
Krause, M. J., Klemens, F., Henn, T. *et al.* (2017). Particuology, 34, 1-13.

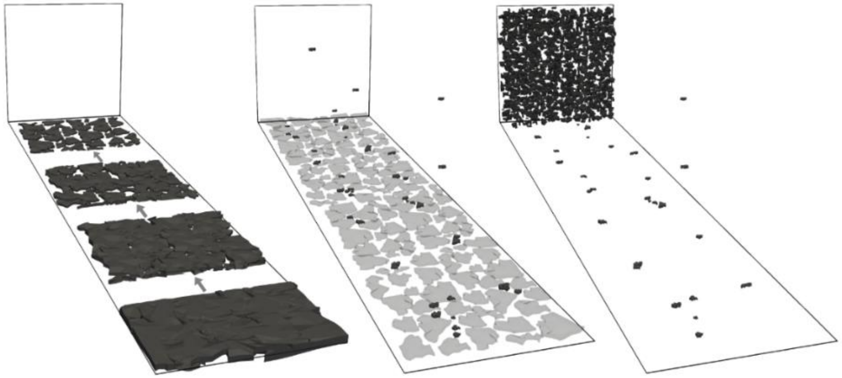
Exhaust Treatment by Wall-flow Filters, Particle

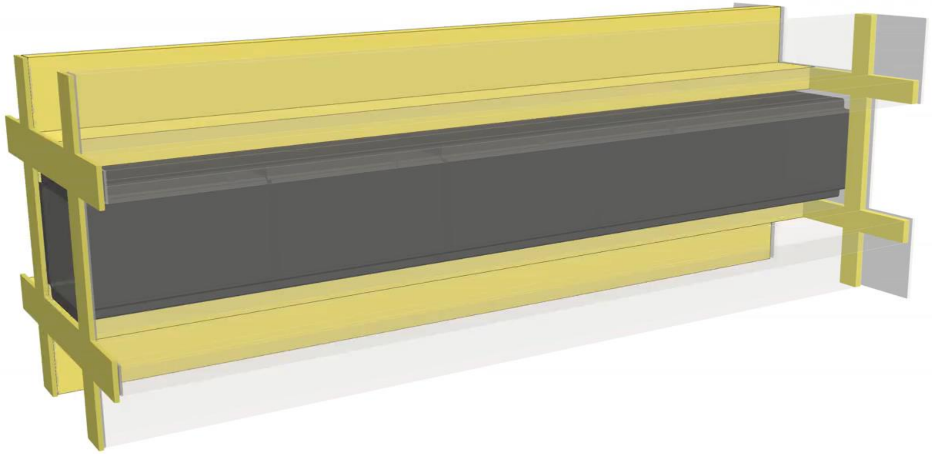
Goal: Investigation of particle-layer rearrangement

➔ 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





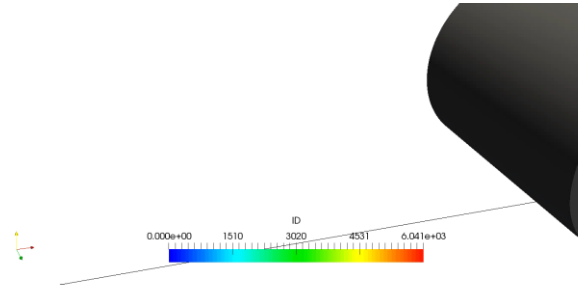


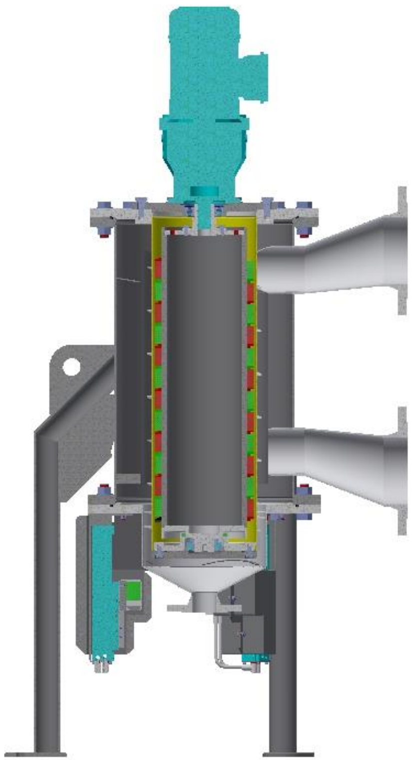
Hafen, N., Dittler, A., Krause, M. J. (2020). Submitted to Philos. Trans. R. Soc. A.

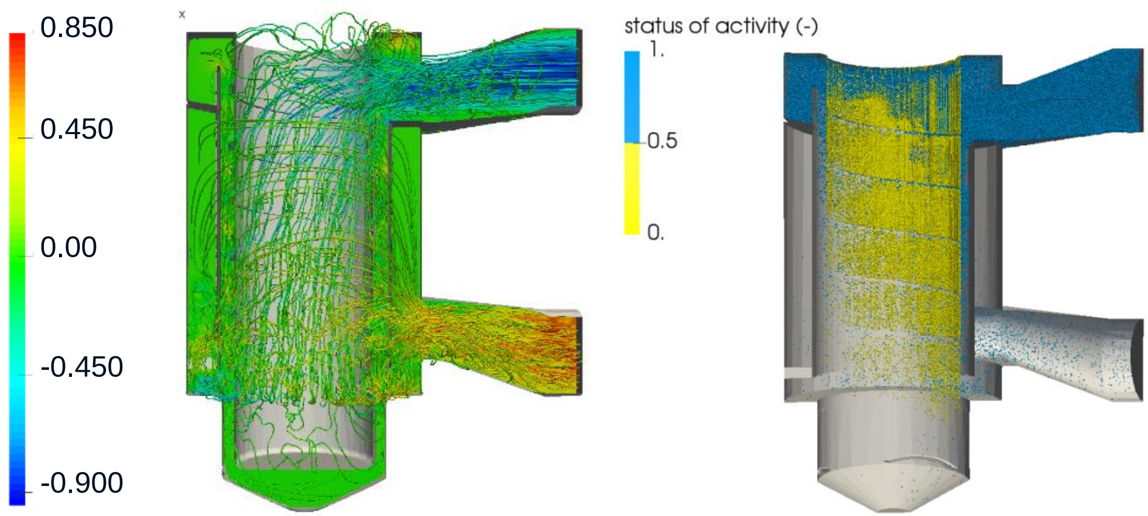
Magnetic Spiral Separator, Particle

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.

Photobioreactor Simulation, Complex System

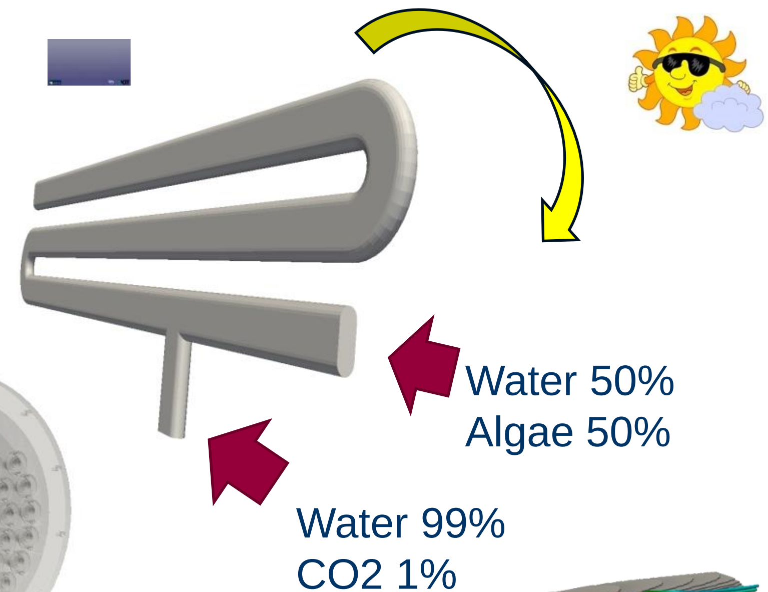
Goal: optimize energy balance

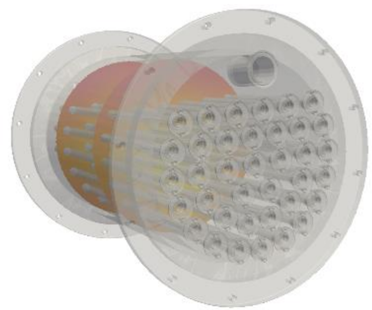
(energy input / bio mass output)

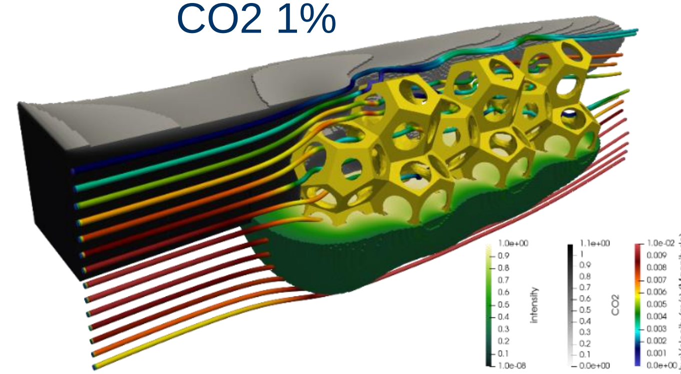
➔ change shape, position, inflow

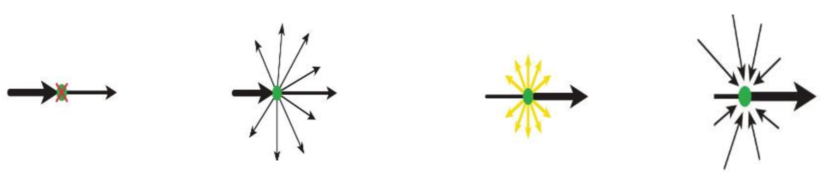
- 3D suspension simulation
  - algae as particles (Lagrange)
  - CO_2 , Water as density (Euler)
  - algae consume CO_2
- 3D light simulation

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 *OpenLB*

Challenge I -- Turbulence

Challenge II -- Suspensions

Challenge III -- Optimization

Summary

Optimal Control Solution Strategies

Problem: find control α and state f such that $J(f,\alpha)$ is minimised and $G(f,\alpha)=0$ holds

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, G., Evgrafov, A., Maute, K. (2007). Struct Multidisc Optim 34(6), 507-524.

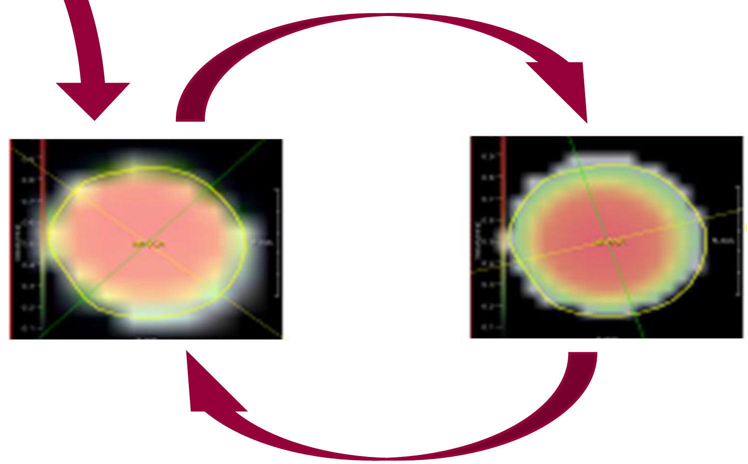
[2] Tekitek, M. M., Bouzidi, M., Dubois, F. *et al.* (2006). Comput Fluids, 35(8-9), 805-813.

[3] Krause, M. J. (2010)., KIT Karlsruhe.

CFD-MRI: Basic Algorithm, Optimization

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

Step 2: CFD simulation $u(d_i)$



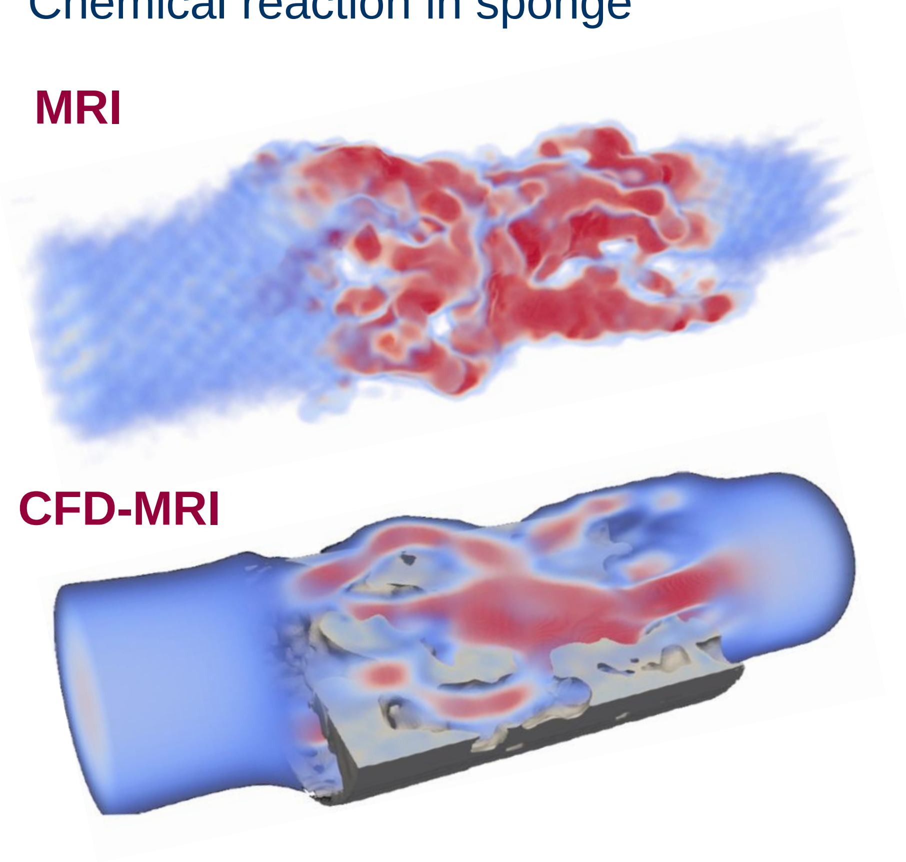
Goal:
Reduce noise,
identify flow topology

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}

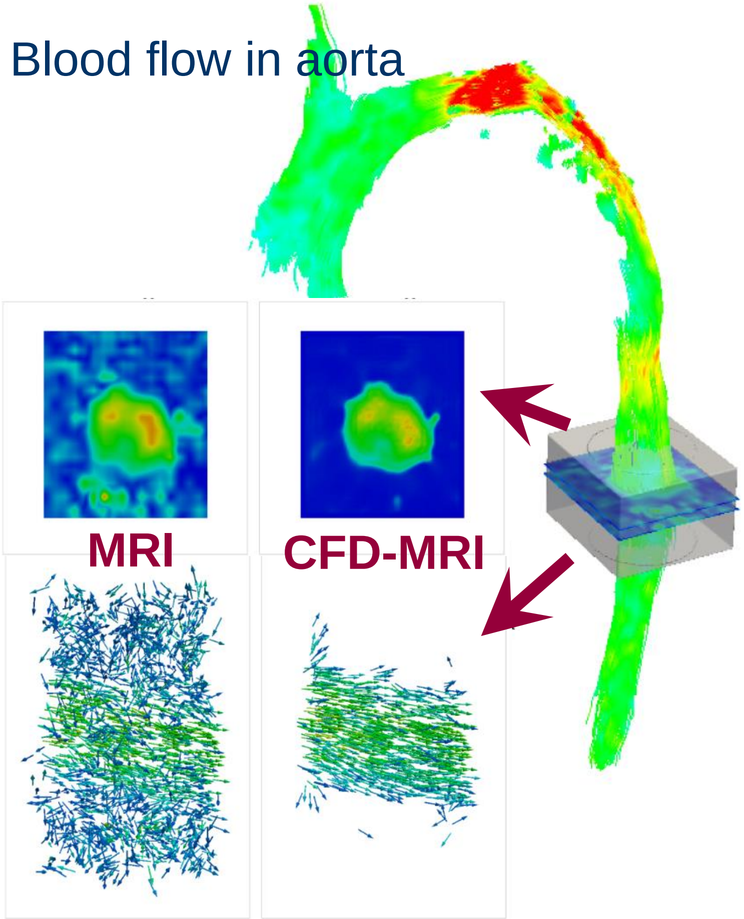
Krause, M. J., Förster, B., Mink, A. *et al.* (2016). In *HPC in Sci and Eng 16* (pp. 337-353).

CFD-MRI: Applications Sponge & Aorta, Optimization

Chemical reaction in sponge



Blood flow in aorta



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

Agenda

Overview *OpenLB*

Challenge I -- Turbulence

Challenge II -- Suspensions

Challenge III -- Optimization

Summary

Summary

Facing challenges in CFD:

Turbulence

DNS/LES instead of RANS

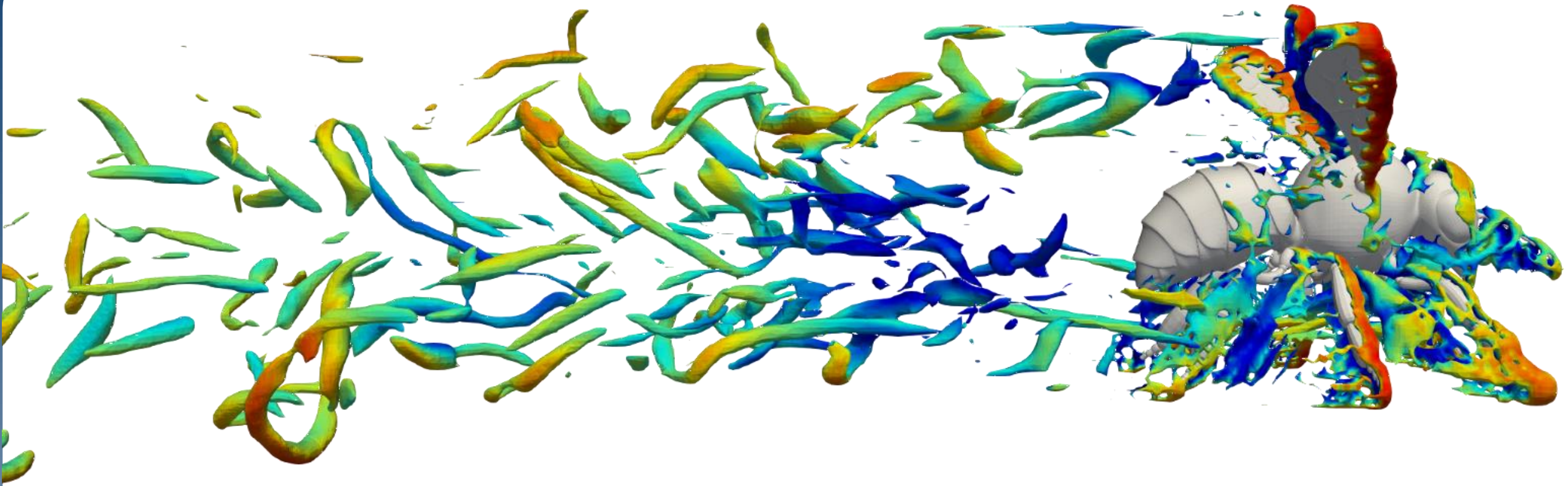
Suspensions

Resolve particles (shape, force, …)

Optimal Control/ Optimization

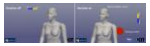
Algorithmic differentiation, adjoints, CFD-MRI

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



Questions?

Download, try, participate…



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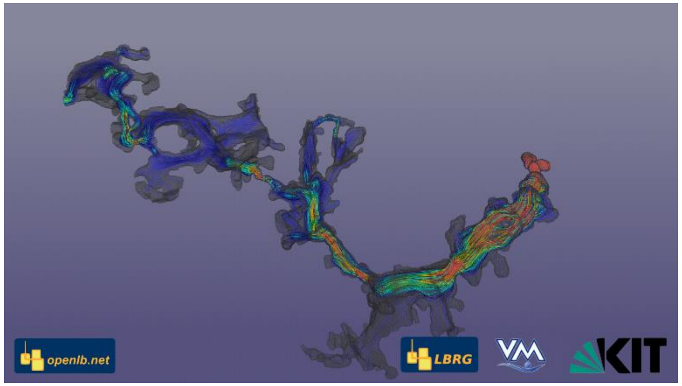
5th Spring School: LBM with OpenLB Software Lab

5th Spring School

Lattice Boltzmann Methods with OpenLB Software Lab

Kraków, Poland, 21st – 25th March 2022

- for scientists and industry, beginners level
- comprehensive **theoretical lectures on LBM**
- **mentored training** on case studies using *OpenLB*, **bring your own problem**
- knowledge exchange, networking at poster session, coffee breaks and excursion



350€ academia/1,700€ industry for 5 days course including course material, 5x lunch, 2x dinner, coffee breaks and excursion

Karlsruhe Institute of Technology

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POLISH NATIONAL AGENCY FOR ACADEMIC EXCHANGE

Executive committee

N. Hafen, **M. J. Krause**, J. E. Marquardt, **P. Madejski,** T. Kuś, N. Subramanian, M. Bujalski

Invited speakers

Timm Krüger, Tim Reis, Halim Kusumaatmaja, Francois Dubois