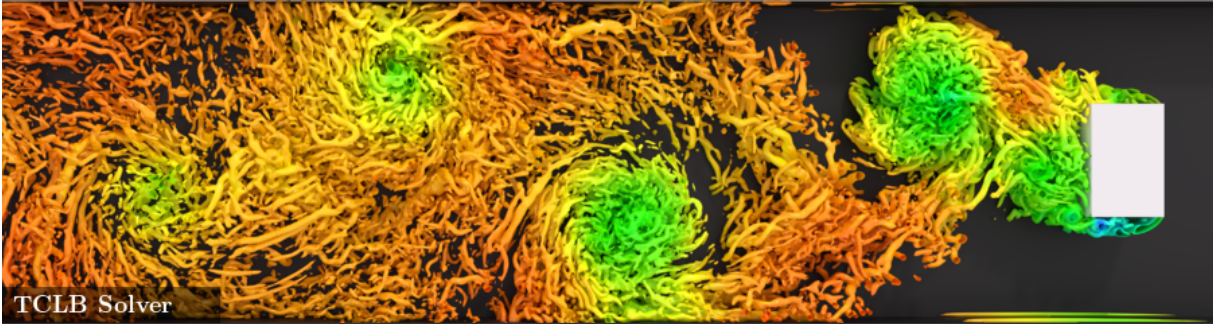


LBM Workshop

Role of diffusion-reaction equations in epidemic modelling

Warsztaty finansowane w ramach projektu IDUB Against COVID, Politechnika Warszawska

Michał Dzikowski (ICM UW), Grzegorz Gruszczyński (ICM UW, PW)

Wrocław 2021

Presentation plan

- What is LBM
- How it is implemented
- What is TCLB
- What we do
    - Multiphase & multicomponent flows
    - Heat transfer
    - Nonlinear diffusion-reaction systems of equations

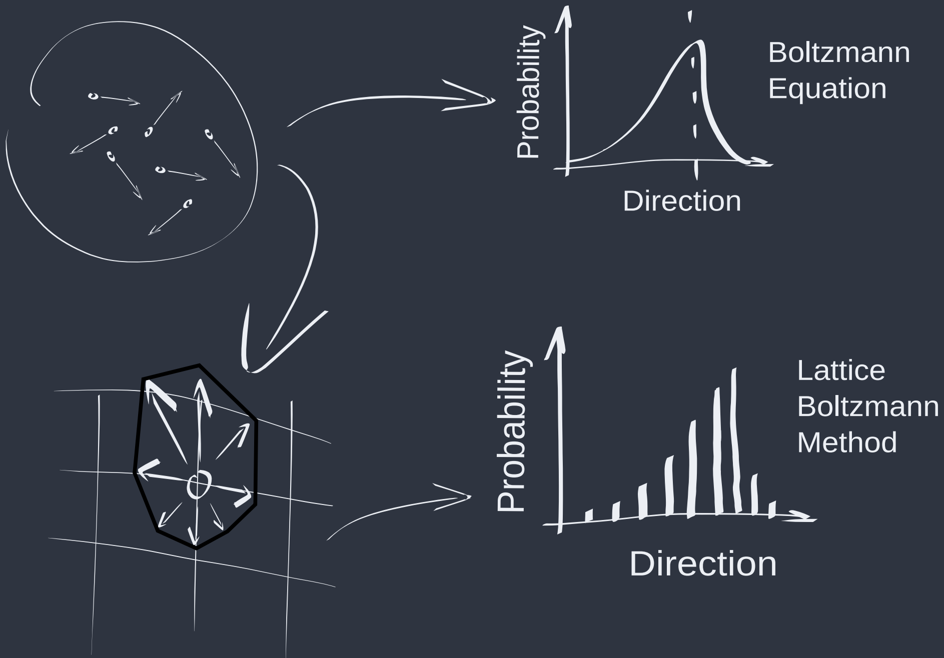
What is LBM

What is LBM?

> LBM is a CFD numerical method derived as an analogue to Boltzmann equation

- Boltzmann equation describes, using statistical mechanics/physics, the state of the rarefied gas in local equilibrium.
- Boltzmann equation desribes state of a gas using spatial variables plus probability distribution of the particles velocity
- LBM is build by imposing discretisation of the paticles "allowed" velocity field, resulting model is an N-S approximation

What is LBM?



Probability
Direction
Boltzmann
Equation
Probability
Direction
Lattice
Boltzmann
Method

What is LBM

> LBM is not for everything

The lattice Boltzmann method (LBM) is a relatively new (~30yrs), widely used numerical scheme for solving both the Navier-Stokes equation (NSE) and advection-diffusion problems. Its popularity has significantly risen in the recent three decades due to its ability to handle complex boundary shapes and its relative ease of implementation and parallelization.

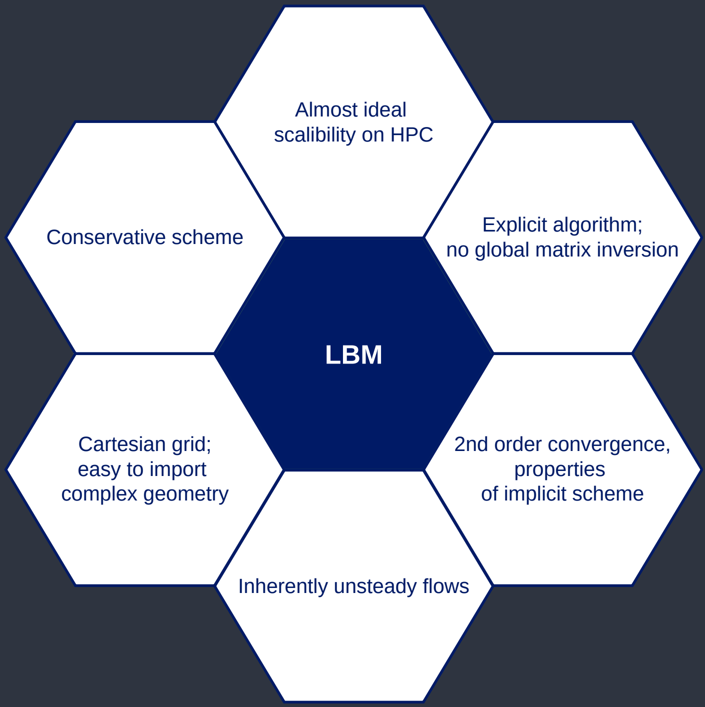
Commercial LMB software:

- SIMULIA PowerFLOW
- ProLB
- Cadence (Numeca) Omnis/LB
- SimScale

No-commercial LMB software is also available:

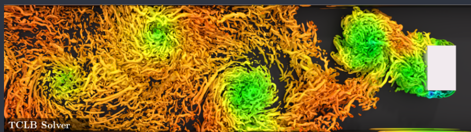
- Palabos (AGPLv3)
- OpenLB (GPLv3)
- waLBerla (GPLv3)
- VirtualFluids (GPLv3)
- TCLB (GPLv3)
- others not yet found ;-)

Why LBM?


Almost ideal scalibility on HPC
Conservative scheme
Explicit algorithm; no global matrix inversion
LBM
Cartesian grid; easy to import complex geometry
2nd order convergence, properties of implicit scheme
Inherently unsteady flows

What is TCLB

Templated CUDA LBM solver (TCLB)



TCLB began development in 2012 with the aim at providing a framework for efficient CFD computations with LBM, mainly for research.

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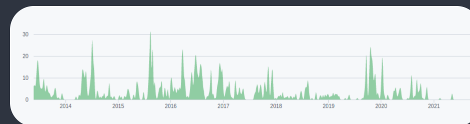
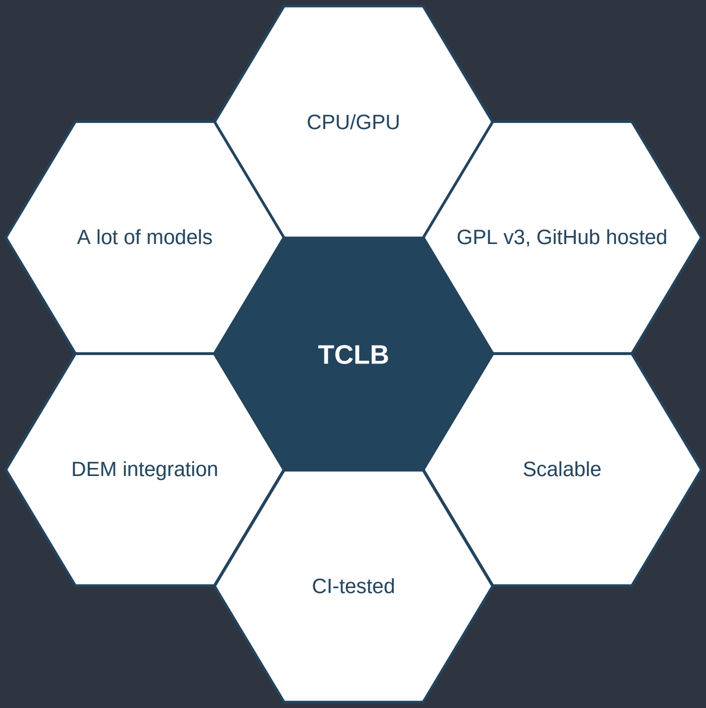
- Zbigniew Gawłowicz
- Mariusz Rutkowski
- Dmytro Sashko
- Travis Mitchell
- Paweł Obrępalski
- Grzegorz Gruszczyński



Developed at:

- Zakład Aerodynamiki at Politechnika Warszawska (Warsaw University of Technology)
- School of Mechanical & Mining Engineering at University of Queensland
- Interdyscyplinarne Centrum Modelowania Matematycznego i Komputerowego at University of Warsaw

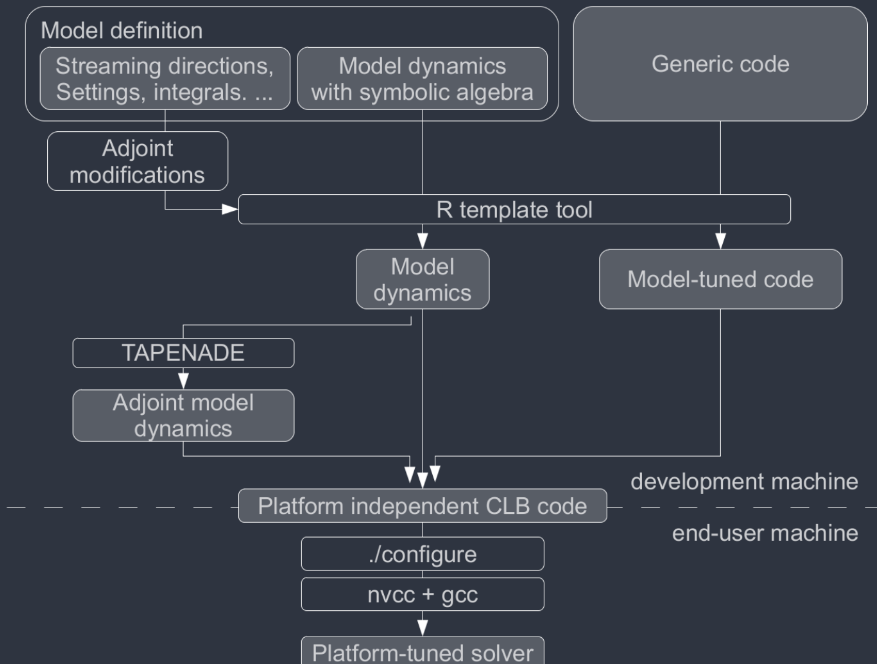
What is TCLB?


CPU/GPU
A lot of models
GPL v3, GitHub hosted
TCLB
DEM integration
Scalable
CI-tested

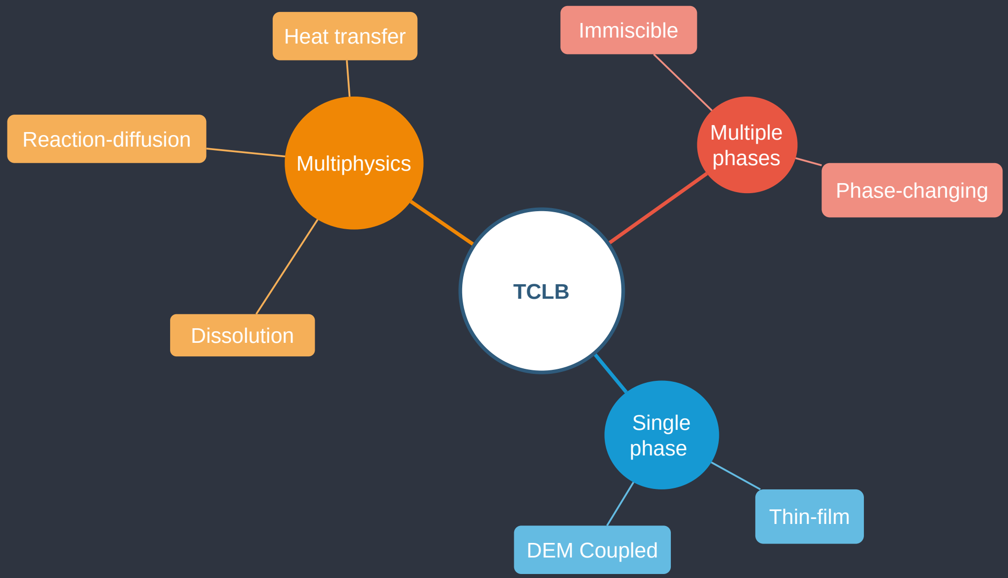
Templated CUDA LBM solver

- Main component of TCLB are templated models, that define collision kernels, boundary condytions etc.
- Models could be written in C, or in C/Rtemplate which allows high-level definition of mathematical operations
- Model define also number of variables, stencils etc.

Templated CUDA LBM solver

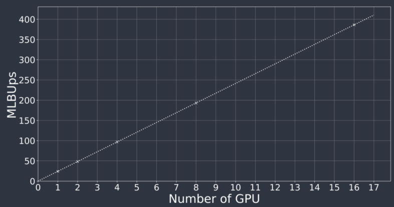


Models in TCLB



Multi-GPU performance & scaling

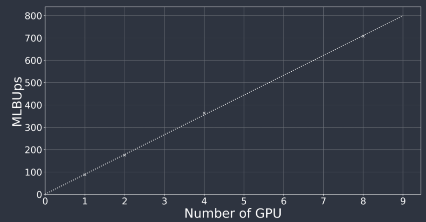
Weak scaling on K40



(h) Prometheus: $\{32768, 32768, 32768, 32768, 32768\}x\{80, 160, 320, 640, 1280\}x\{3, 3, 3, 3, 3\}$

Same load per single nVIDIA K40 GPU (Prometeusz)

Weak scaling on V100



(g) Rysy: $\{32768, 32768, 32768, 32768\}x\{80, 160, 320, 640\}x\{3, 3, 3, 3\}$

Same load per single nVIDIA V100 GPU (ICM)

Keep in mind that this LBM benchmark used D3Q27Q27 lattice with 54 LBM DOFS per node

CPU/GPU Performance & scaling

Strong scaling on Cray Cluster

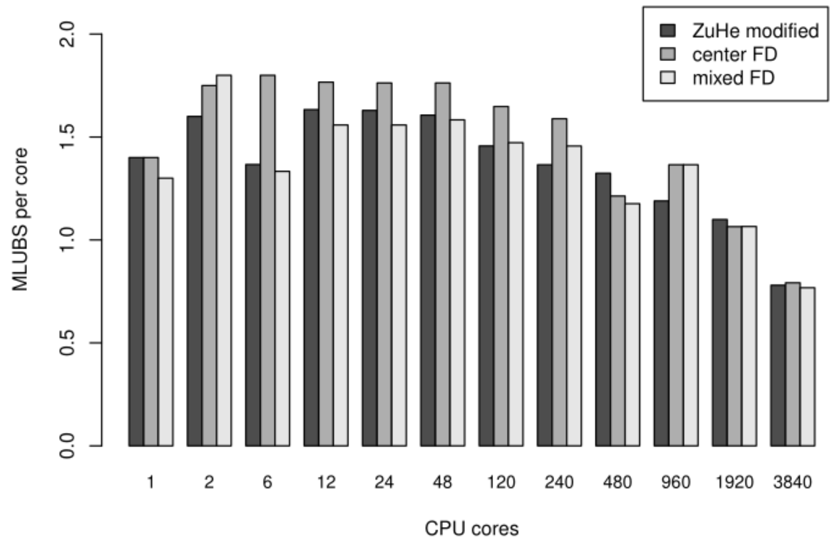


Figure 1: Strong scaling of the TCLB solver on CPU.

CPU/GPU Performance & scaling

Peak & measured performance

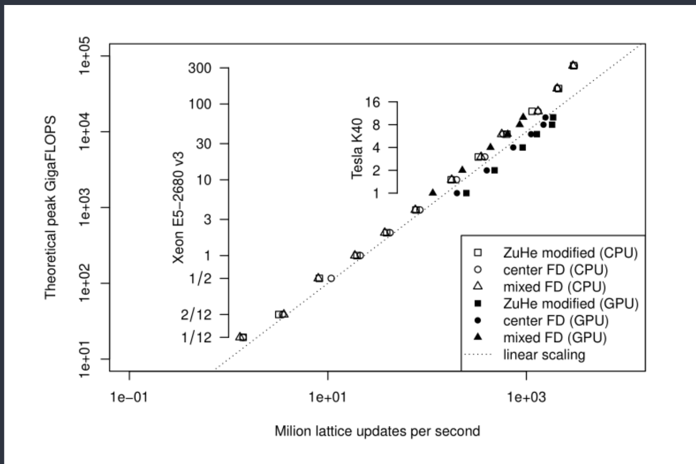


Figure 3: Comparison of solver performance and peak GPU/CPU performance. One is measured in millions of lattice elements updated in a second (MLUPS) and the latter in billions of floating point operations per second (GFLOPS)

Actual performance vs. theoretical one

Take home message: TCLB scales well with theoretical peak power

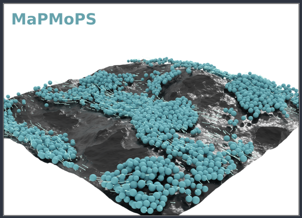
Projects involving TCLB

ShaleSeq

(finished)

Multidisciplinary project for carbon capture and storage analysis for Pomeranian shales

MaPMoPS



Pre-Exascale project for particle simulations at University of Queensland and POWSEY supercomputing center.

QuickerSim CFD Solver

(finished)

R&D project in CFD software house and consulting company QuickerSim - involved thermal LBM developments.

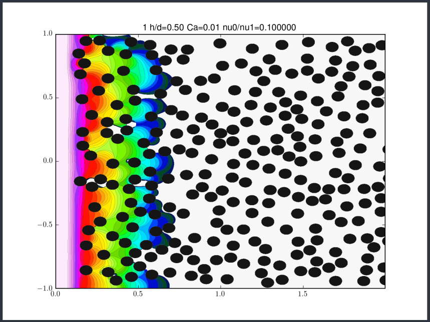
Inne

- IDUB Against COVID, Politechnika Warszawska
- IDUB: Nowe Idee - Wyzwania Petabajtów, Uniwersytet Warszawski

What we do

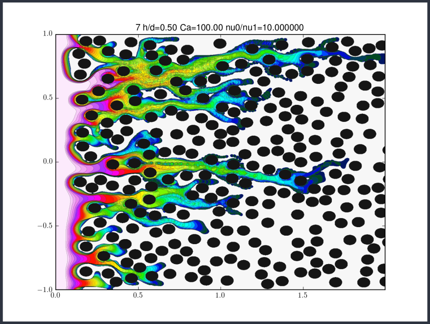
Two-component immiscible flow

Strong capilar effects



During invasion pores are invided one-by-one in almost discontinous manner

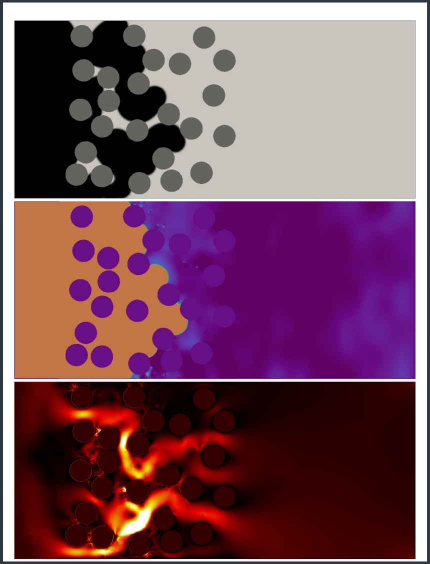
Weak capilary effects



Viscous dominated regime - low viscosity fluid fingers into high density one

Two-component immiscible flow

Strong capilar effects



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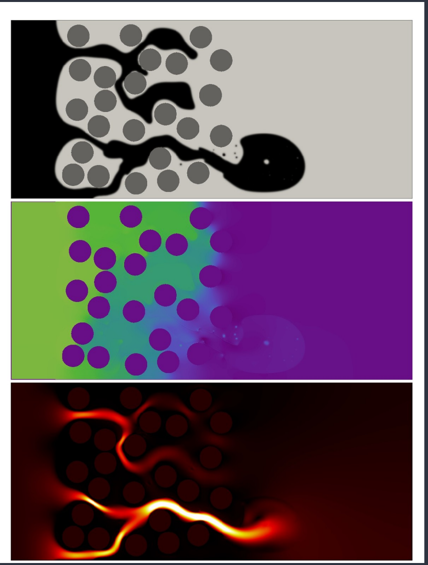
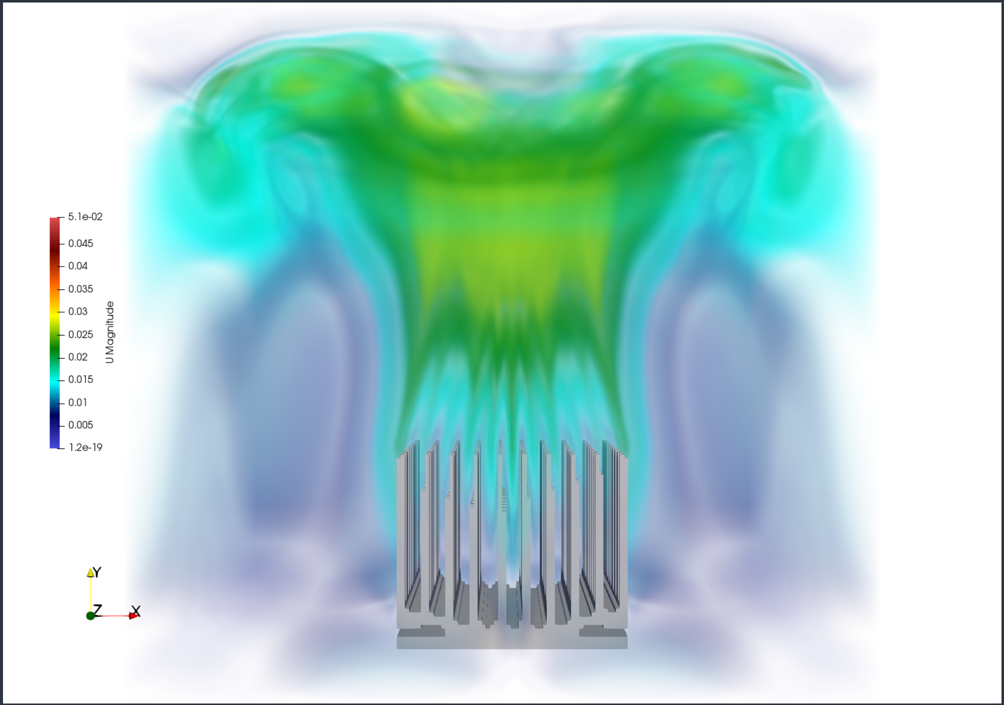


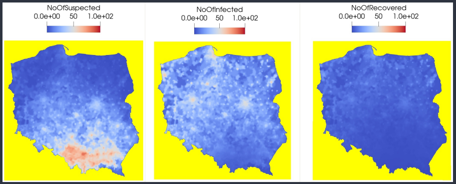
Viscous dominated regime - low viscosity fluid fingers into high density one

What we do: thermal flow

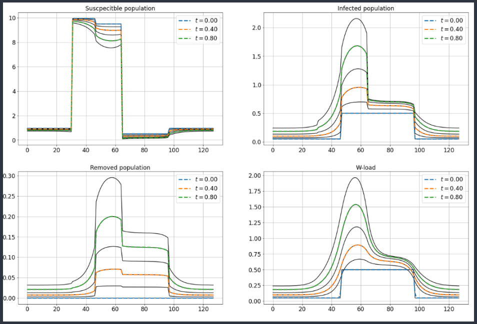


Reaction-diffusion generic models

Spatially variable SIR model



Proof of concept model developed to provide high throughput solver for optimization loop in epidemic parameter identification.



Model was build to be able to handle - system of reaction-diffusion equations using LBM and coupled to LBM N-S solution if needed. Such model represents wide range of non-epidemic problems like dissolution modeling.

Scientific Journal Publications

- W. Regulski et al., Pressure drop in flow across ceramic foams—A numerical and experimental study, Chemical Engineering Science, 2015
- Ł. Łaniewski-Wołłk, J. Rokicki, Adjoint Lattice Boltzmann for topology optimization on multi-GPU architecture, Computers & Mathematics with Applications, 2016
- M. Dzikowski, Ł. Łaniewski-Wołłk, J. Rokicki, Single Component Multiphase Lattice Boltzmann Method for Taylor/Bretherton Bubble Train Flow Simulations, Communications in Computational Physics, 2016
- A. Fakhari et al., Improved locality of the phase-field lattice-Boltzmann model for immiscible fluids at high density ratios, Phys. Rev. E, 2017
- T. Mitchell, C. Leonardi, A. Fakhari, Development of a three-dimensional phase-field lattice Boltzmann method for the study of immiscible fluids at high density ratios, International Journal of Multiphase Flow, 2018
- M. Dzikowski, L. Jasinski, M. Dabrowski, Depth-averaged Lattice Boltzmann and Finite Element methods for single-phase flows in fractures with obstacles, Computers & Mathematics with Applications, 2018
- G. Gruszczyński et al., A cascaded phase-field lattice Boltzmann model for the simulation of incompressible, immiscible fluids with high density contrast, Computers & Mathematics with Applications, 2019
- M Rutkowski et al., Open-loop optimal control of a flapping wing using an adjoint Lattice Boltzmann method, Computers & Mathematics with Applications, 2020
- M Matyka, M Dzikowski, Memory-efficient Lattice Boltzmann Method for low Reynolds number flows, Computer Physics Communications, 2021

PhD Thesis:

Warsaw University of Technology

- M. Dzikowski, Wykorzystanie metody gazu sieciowego Boltzmanna do symulacji przepływów dwufazowych (promotor: J. Rokicki)
- Ł. Łaniewski-Wołłk, Topology Optimization and Optimal Control using Adjoint Lattice Boltzmann Method (promotor: J. Rokicki)
- W. Regulski, Investigation of hydrodynamic properties of structures with open porosity using the Lattice Boltzmann Method (promotor: J. Szumbarski)

The University of Queensland

- J. McCullough Numerical investigation of conjugate heat transfer and temperature-dependent viscosity in non-Brownian suspensions with application to hydraulic fracturing, (supervisor: C. Leonardi)
- T. R. Mitchell, Development of a multiphase lattice Boltzmann model for high-density and viscosity ratio flows in unconventional gas wells, 2019 (supervisor: C. Leonardi)

Thank you for your attention!

github.com/CFD-GO/TCLB