Multiphase Flow in Resolved Porous Media Using Lattice Boltzmann Methods

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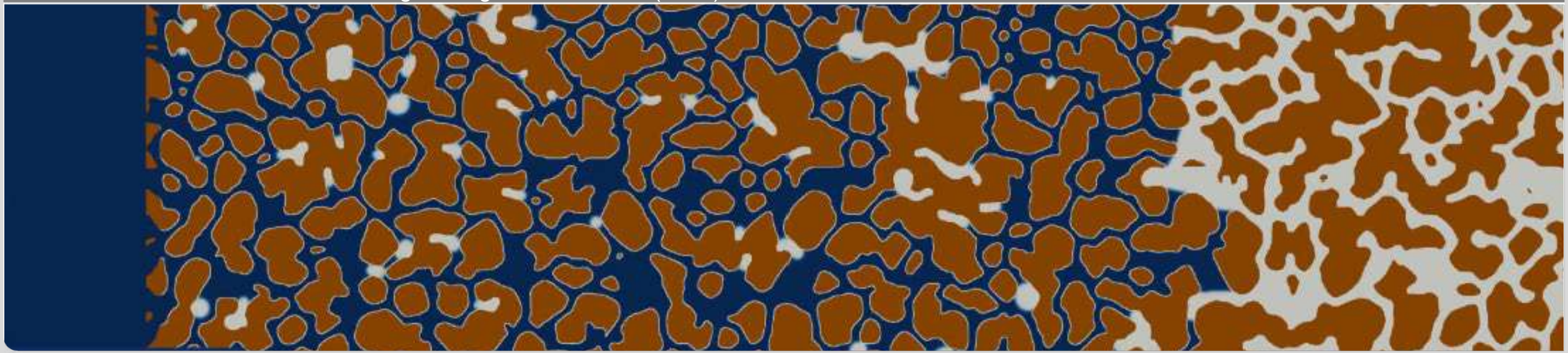
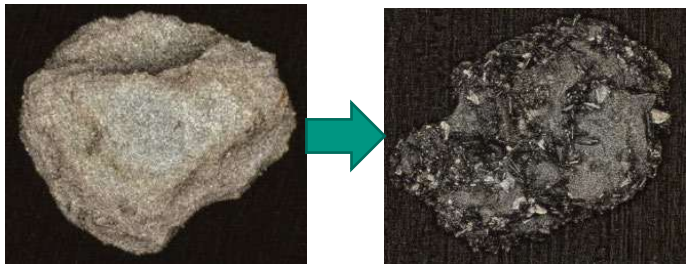


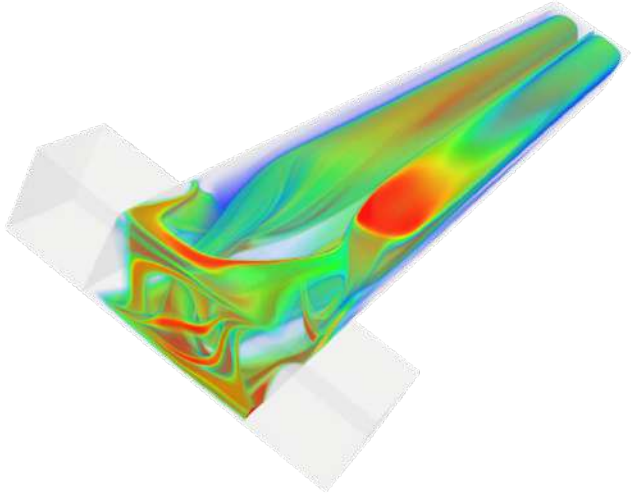
Possible simulation cases

- Saturation & crystallization



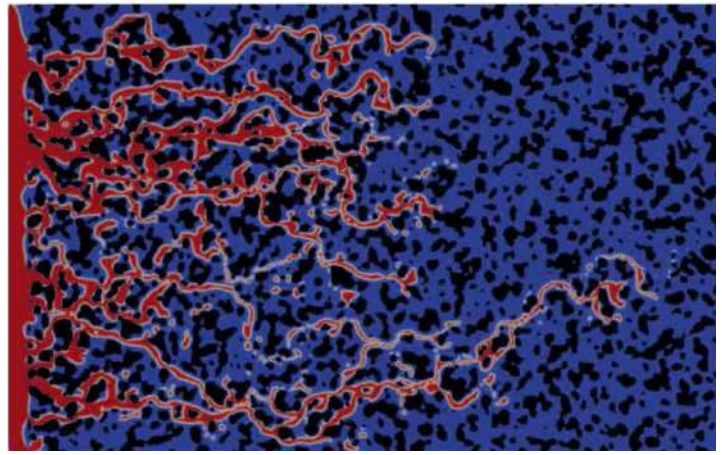
Unloaded CSH particle loaded CSH particle [Schröter17]

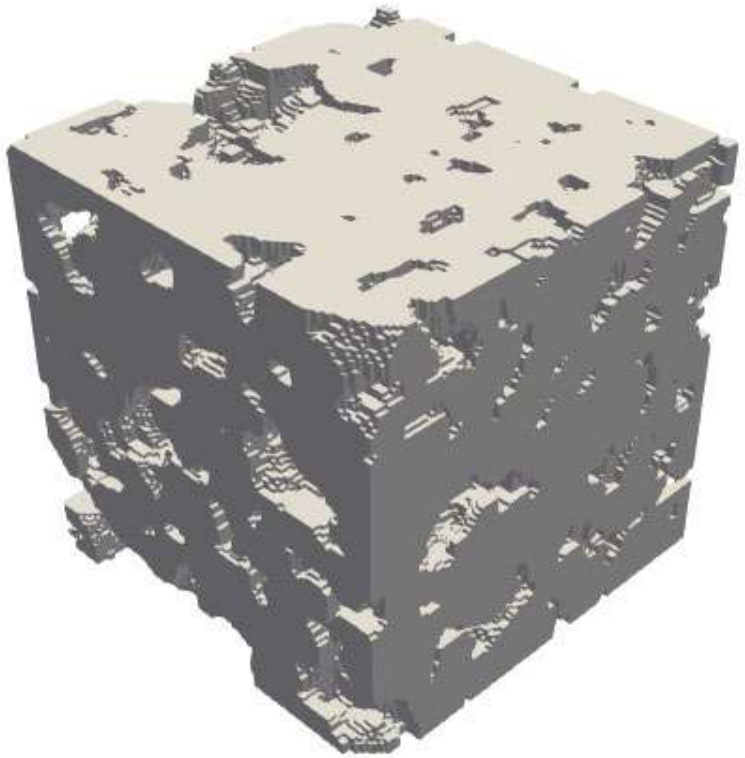
- Reactive micromixing

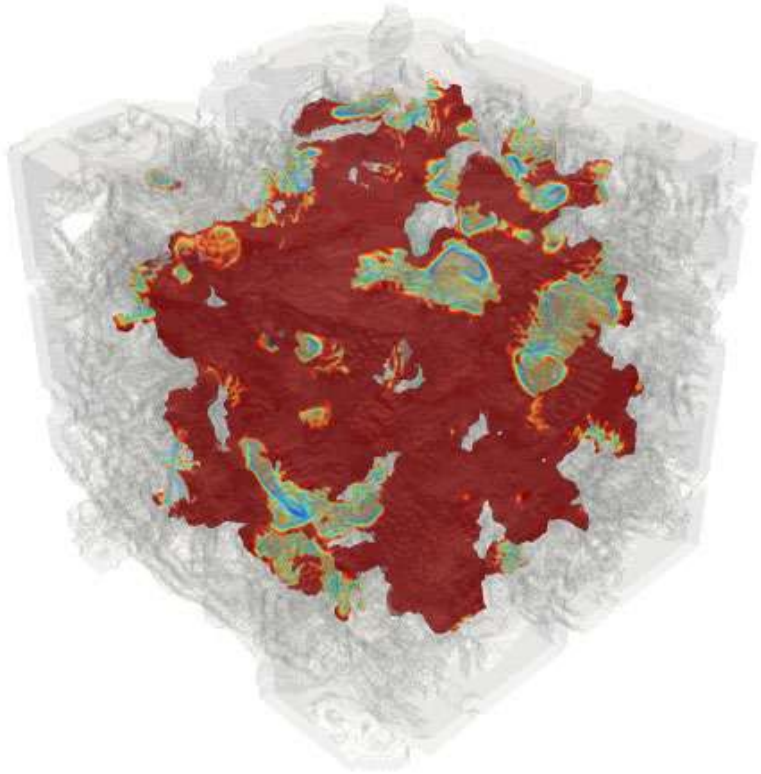


- Resolving nanoparticles & changing surfaces

- Multiphase flows





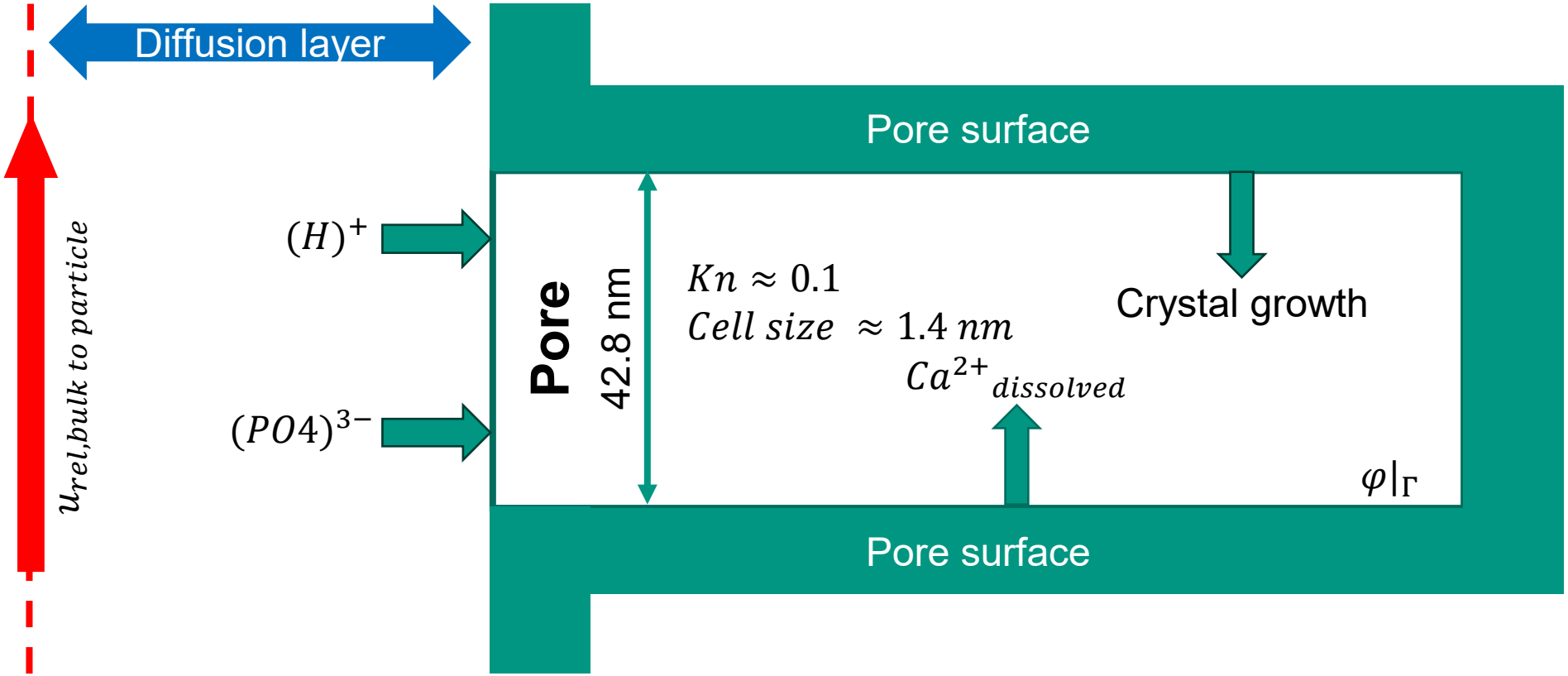


SATURATION & CRYSTALLIZATION

Bukreev et al., Part I, (2025). Accepted by Engineering with Computers.

Bukreev et al., Part II, (2025). Accepted by Engineering with Computers.

Surface reaction model in a CSH nanopore



[Bukreev25_I]

[Bukreev25_II]

Dissolution: $CSH + 1.66H^+ \rightarrow 0.83Ca^{2+} + SiO_2 + 4H_2O$

Crystallization: $8Ca^{2+} + 2H^+ + 6{PO_4}^{3-} \rightarrow Ca_8H_2(PO_4)_6 \cdot 5H_2O \downarrow$

Outer Helmholtz plane (Γ) considered as surface (according to Electric Triple Layer Theory)

Governing equations

Reacting ions

Nernst-Planck reactive equations:

$$\partial_t C_i + \nabla \cdot \left(C_i \left(\boldsymbol{u}_{\mathrm{fl}} + \boldsymbol{u}_{\mathrm{el},i} \right) \right) = D_i \Delta C_i + \sum_k R_{k,i}$$

$$\boldsymbol{u}_{\mathrm{el},i} = -D_i \frac{z_i e}{k_{\mathrm{B}} T} \nabla \psi$$

Carrier fluid

Navier-Stokes:

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{\nabla p}{\rho} + \nu \Delta \boldsymbol{u} + \frac{\boldsymbol{F}_{\mathrm{el}}}{\rho}$$

$$\boldsymbol{F}_{\mathrm{el}} = -\nabla \psi \sum_i F z_i C_i$$

$\boldsymbol{u}$

C_i

C_i

ψ

Electric potential

Poisson equation:

$$\Delta \psi = -\frac{F}{\epsilon} \sum z_i C_i$$

ψ

Constants

Goal variables

Reactions in the bulk in boundary cells

Reaction rate: $R_i = \upsilon_i \dot{r}_k$

Ion activity: $a_i = C_i \gamma_i$

$$lg(\gamma_i) = -\frac{A z_i^2 \sqrt{I}}{1 + B \cdot a\sqrt{I}}$$

$$I = \frac{1}{2}\sum_i C_i z_i^2$$

Unloaded CSH particle

loaded CSH particle

[BA K. Schröter]

Dissolution: $CSH + 1.66H^+ \rightarrow 0.83Ca^{2+} + 4H_2O + SiO_2$

$$\dot{r}_{diss} = k_{diss}\left(\frac{a_{H^+}{}^{-1.66} a_{Ca^{2+}}^{0.83}}{K_{sp,CSH}} - 1\right)$$

Crystallization: $8Ca^{2+} + 2H^+ + 6PO_4{}^{3-} \rightarrow Ca_8H_2(PO_4)_6 \cdot 5H_2O \downarrow$

$$\dot{r}_{cryst} = \frac{1}{\Delta x} k_{cryst}\left(\left(\frac{a_{Ca^{2+}}^8 a_{PO_4{}^{3-}}^2 a_{H^+}^6}{K_{sp,OCP}}\right)^{1/16} - 1\right)^4$$

OCP

Ω

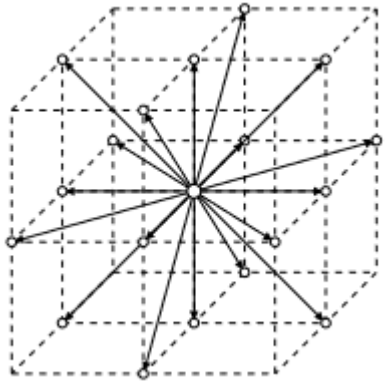
Reactions in bulk in the boundary cells

Discretization: Lattice Boltzmann Methods

$$f_i(\boldsymbol{x} + \boldsymbol{\xi_i}\Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = \Delta t\left(\Omega_i^C + \Omega_i^S\right)$$

$$\Omega_i^{C,BGK} = \frac{f_i^{eq}(\boldsymbol{x}, t) - f_i(\boldsymbol{x}, t)}{\tau}$$

Equation	$f_j^{\mathrm{eq}}(\boldsymbol{x}, t)$	$\Omega_j^S(\boldsymbol{x}, t)$
PE	$w_j \psi$	$\left(1 - \frac{\triangle t}{2\tau}\right) w_j S_{\mathrm{PE}}$
RNPE	$w_j C_i \left(1 + \frac{\boldsymbol{\xi_j} \cdot (\boldsymbol{u}_{\mathrm{fl}} + \boldsymbol{u}_{\mathrm{el}})}{c_{\mathrm{s}}^2}\right)$	$\left(1 - \frac{\triangle t}{2\tau}\right) w_j S_{\mathrm{RNPE}}$
NSE	$w_j \rho \left(1 + \frac{\boldsymbol{\xi_j} \cdot \boldsymbol{u}}{c_{\mathrm{s}}^2} + \frac{(\boldsymbol{\xi_j}\boldsymbol{\xi_j} - \delta_{\alpha\beta} c_{\mathrm{s}}^2) : \boldsymbol{u}\boldsymbol{u}}{2c_{\mathrm{s}}^4}\right)$	$\left(1 - \frac{\triangle t}{2\tau}\right) w_j \left(\frac{\boldsymbol{\xi_j}}{c_{\mathrm{s}}^2} + \frac{(\boldsymbol{\xi_j}\boldsymbol{\xi_j} - \delta_{\alpha\beta} c_{\mathrm{s}}^2) \cdot \boldsymbol{u}}{c_{\mathrm{s}}^4}\right) \cdot \boldsymbol{F}$



D3Q19

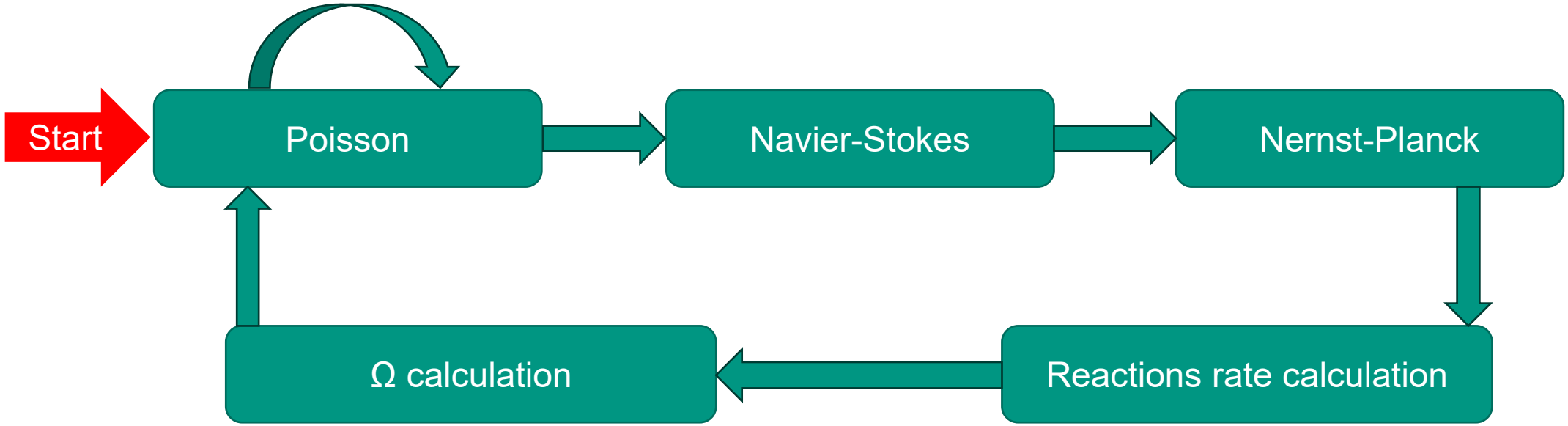
f_i - Probability Distribution Function (PDF)

Fully local → GPU + MPI in ***OpenLB***

Macro-variables as PDF moments:

Equation	0th order	1st order
PE	$\psi = \sum_j f_{j,\mathrm{PE}} + \frac{1}{2} S_{\mathrm{PE}}$	$\nabla\psi = -\frac{1}{\tau_{\mathrm{PE}} c_{\mathrm{s}}^2 \triangle x} \sum_j \boldsymbol{\xi_j} f_{j,\mathrm{PE}}$
RNPE	$C_i = \sum_j f_{j,\mathrm{RNPE}} + \frac{1}{2} S_{\mathrm{RNPE}}$	-
NSE	$\rho = \sum_j f_{j,\mathrm{NSE}}$	$\boldsymbol{u} = \sum_j \boldsymbol{\xi_j} f_{j,\mathrm{NSE}} + \frac{1}{2}\boldsymbol{F}$

Discretization: full simulation loop



Assumption: Strang splitting

➢ Constant variables during each step

Automatic differentiation (AD)

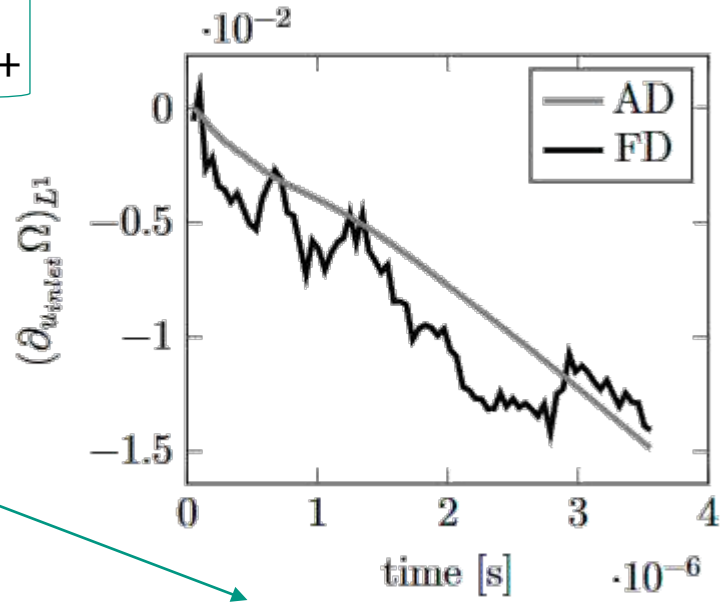
Vector-populations in ***OpenLB***

Operator overloading

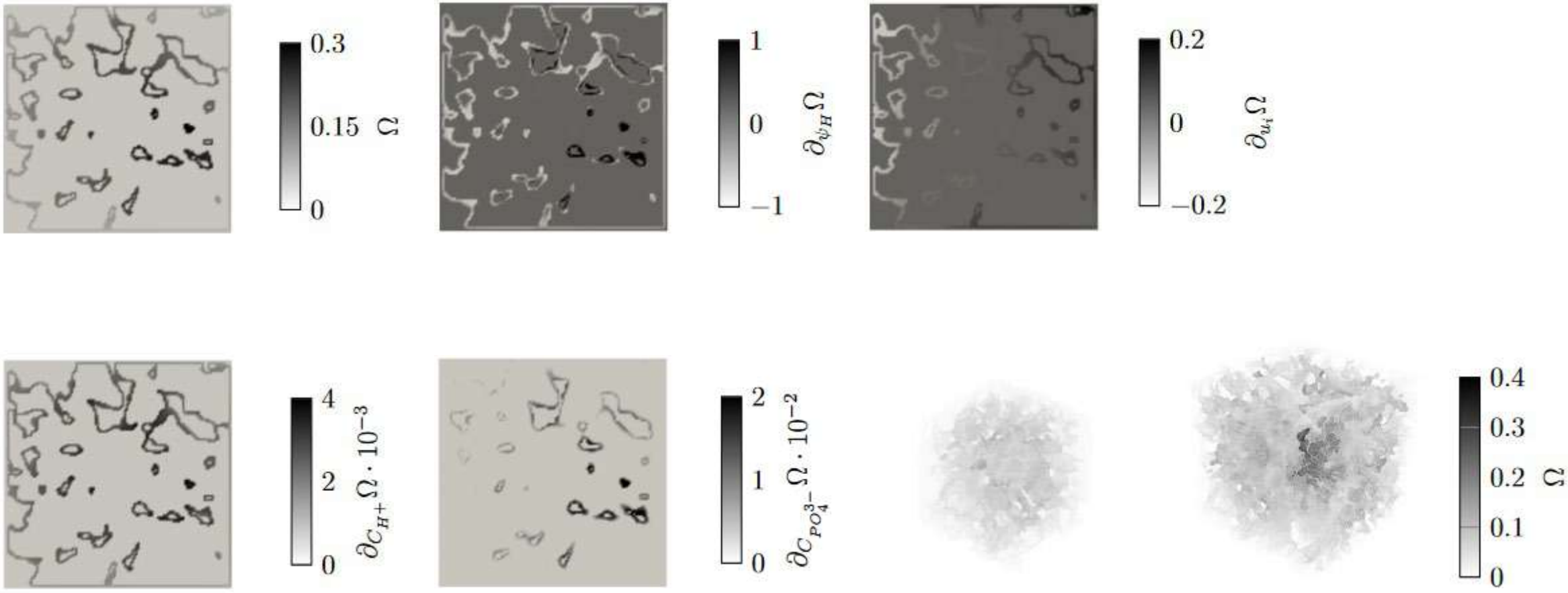
$$\begin{bmatrix} f_{i,C_{H^+}} \\ \partial_k f_{i,C_{H^+}} \end{bmatrix} \quad \begin{bmatrix} f_{i,C_{PO_4^{3-}}} \\ \partial_k f_{i,C_{PO_4^{3-}}} \end{bmatrix} \quad \begin{bmatrix} f_{i,C_{Ca^{2+}}} \\ \partial_k f_{i,C_{Ca^{2+}}} \end{bmatrix}$$

$$\boldsymbol{\partial_k \Omega_{OCP}}$$

$$\frac{\partial \Omega_{OCP}}{\partial \psi_H} \quad \frac{\partial \Omega_{OCP}}{\partial \|\boldsymbol{u}\|_{inlet}} \quad \frac{\partial \Omega_{OCP}}{\partial C_{H^+,inlet}} \quad \frac{\partial \Omega_{OCP}}{\partial C_{PO_4^{3-},inlet}} \quad \frac{\partial \Omega_{OCP}}{\partial d_{pore}} \quad \frac{\partial \Omega_{OCP}}{\partial l_{pore}}$$



Realistic 3D geometry



Work in progress: crystal growth

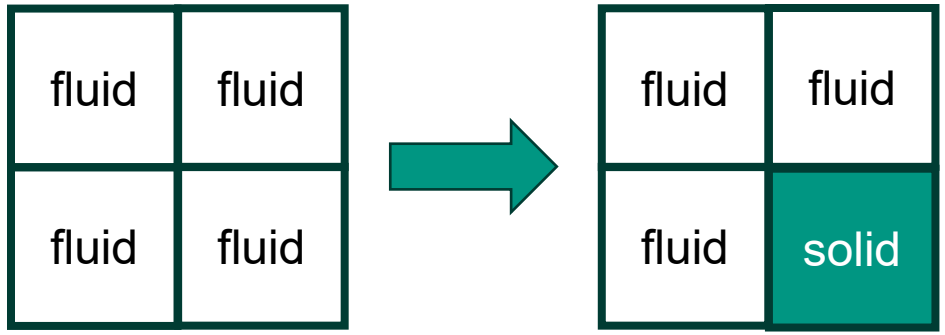
1. Nucleation:

$$\partial_t N = A_N exp\left[-\frac{16\pi\sigma^3 v^2}{3k_B T(k_B T(ln\Omega))^2}\right]$$

$$\sigma = \Delta x(p_n - p_t)$$

2. Crystal layer growth ($N \geq 1/V_{cell}$)

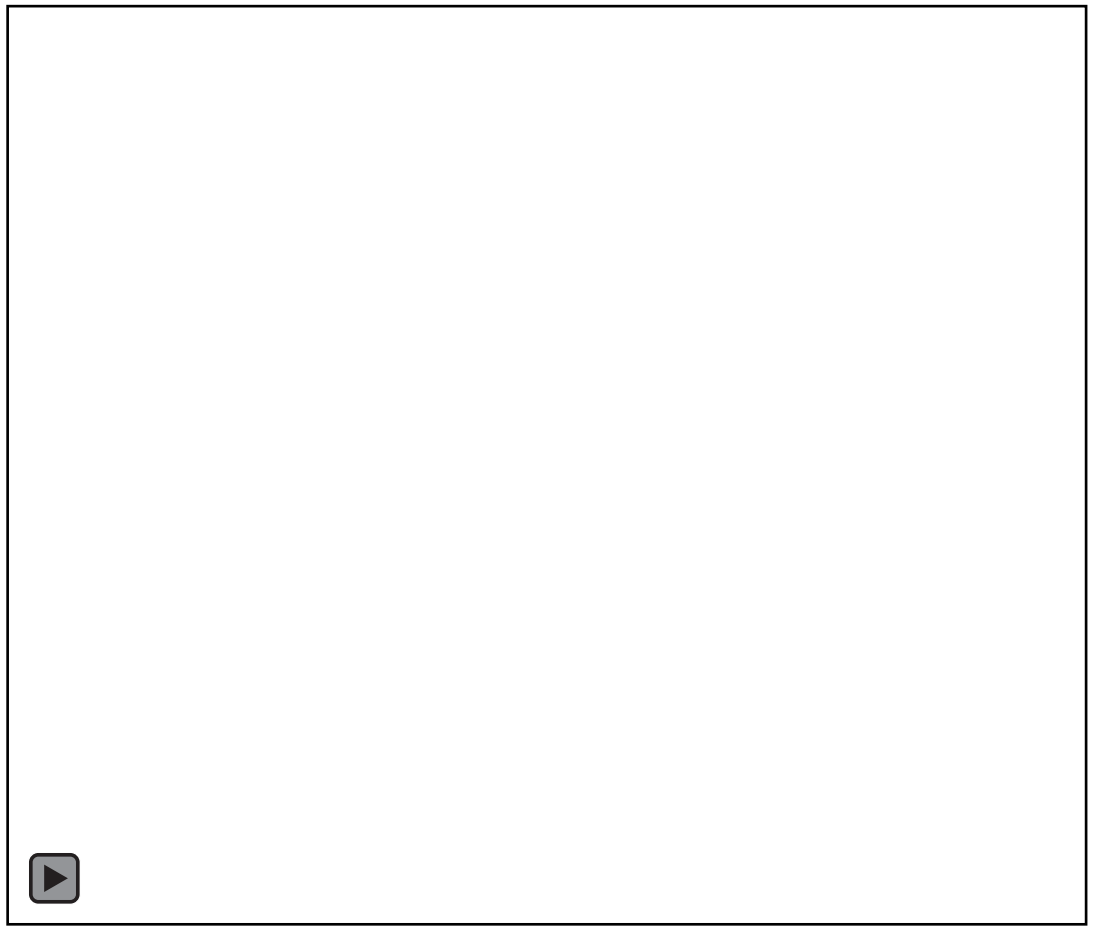
$$\partial_t x_{cr} = r_{cr}\frac{M_{cr}}{\rho_{cr}}$$



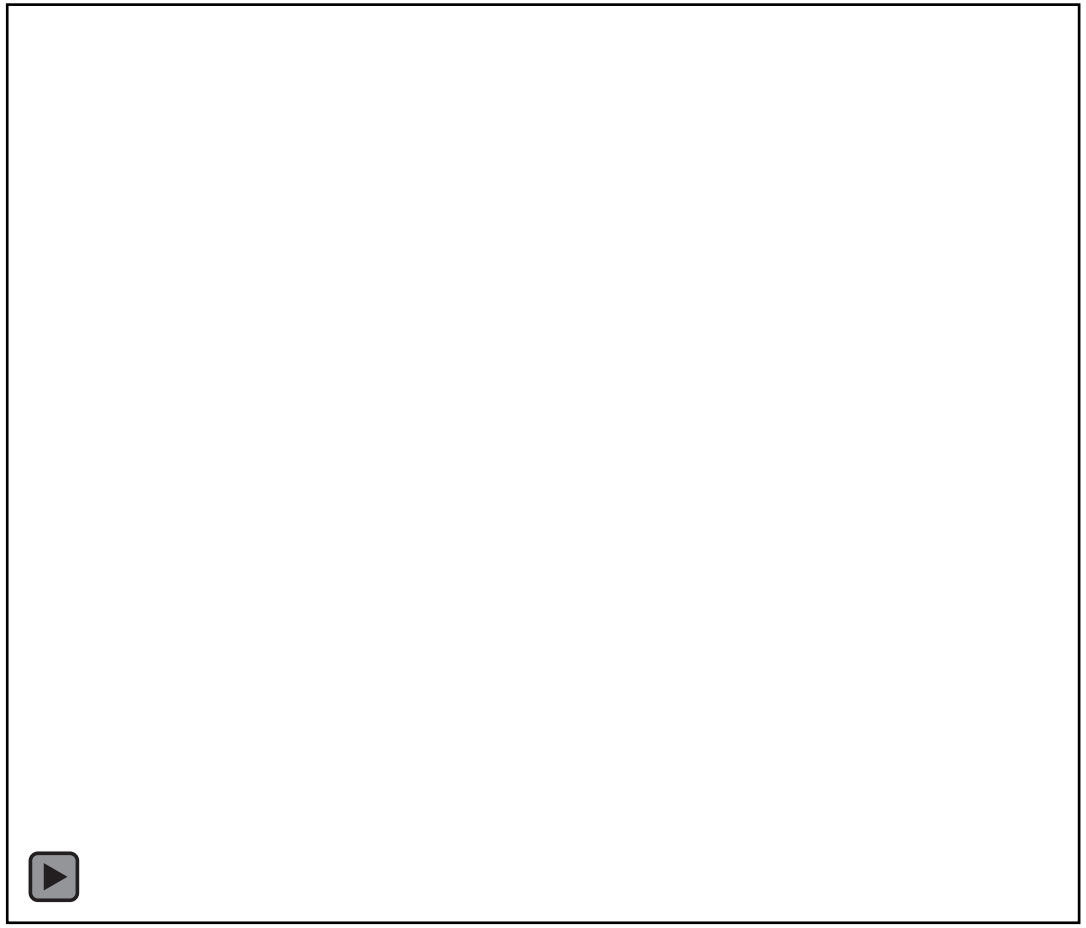
The crystal layer height h is equal to the crystal structure unit cell height.

Crystal structure unit cell height is almost equal to the lattice cell.

Work in progress: crystal growth



Velocity [m/s]



Electric potential [V]

Work in progress: Knudsen slip

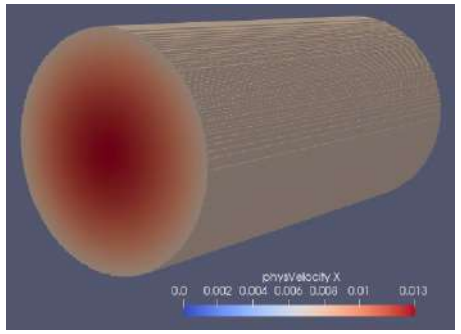
Mean Free Path (MFP)

$$u_s = \frac{2-\sigma_v}{\sigma_v}\left[\frac{\lambda}{1+bKn}\right]\left(\frac{\partial u_t}{\partial n}\right)_w$$

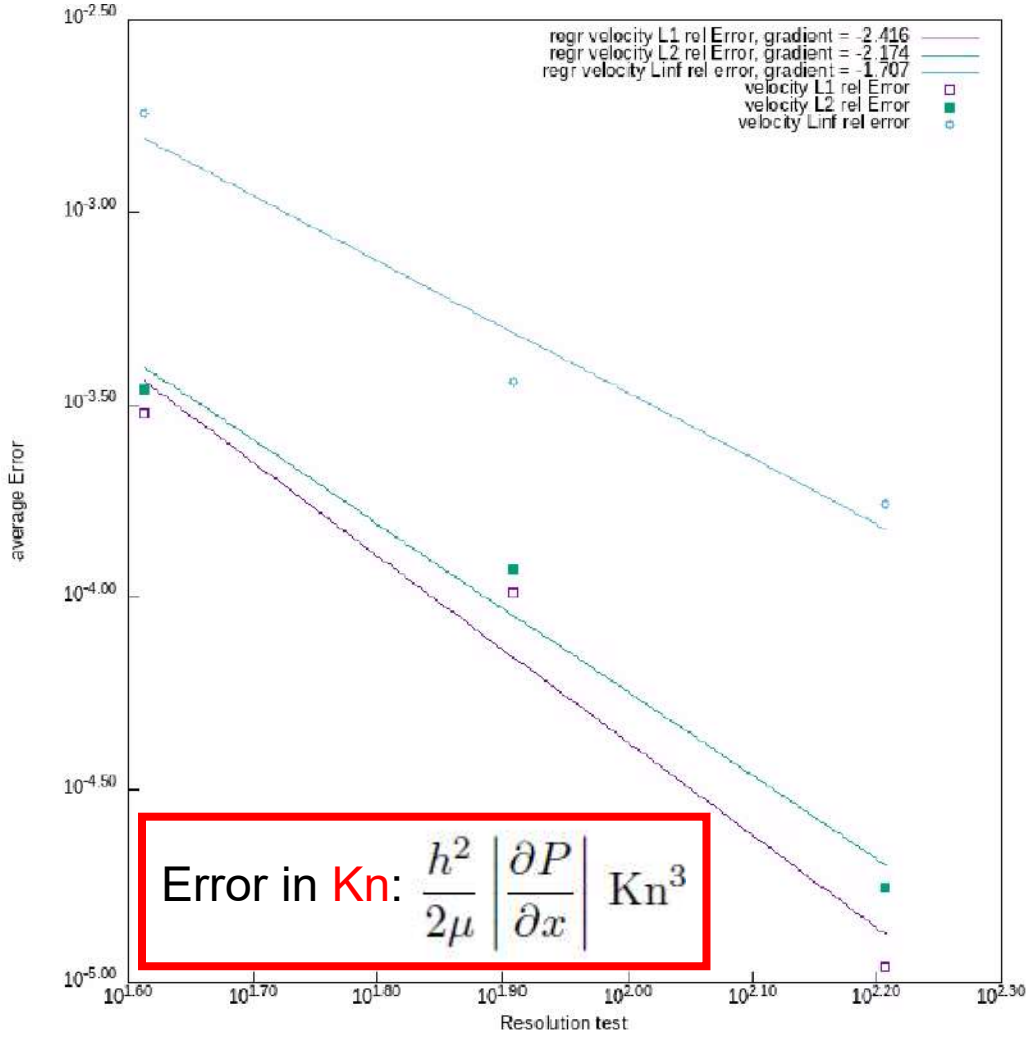
Accomodation coeff.

General slip coeff., different for each Kn number

- Velocity inlet
- Pressure outlet
- Length = 2*diameter
- Rel. time = 1,4
- Kn = 0,45



$$u(r) = \frac{R^2}{4\mu}\frac{\partial P}{\partial x}\left(1-\frac{r^2}{R^2}-4\frac{2-\sigma_v}{\sigma_v}\left[\frac{Kn}{1+bKn}\right]\right)$$



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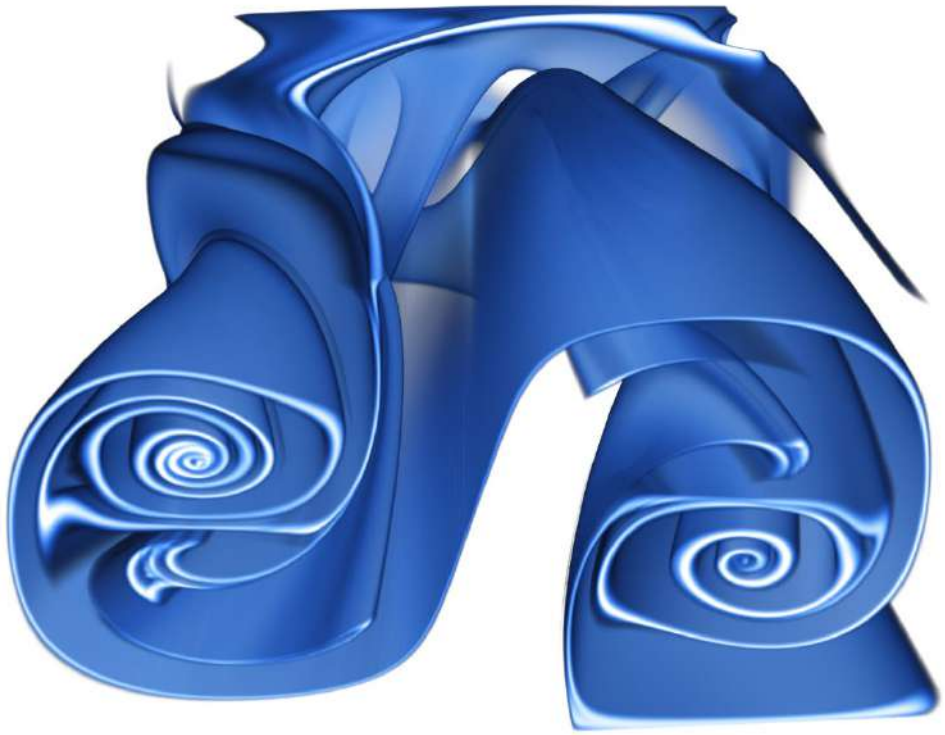
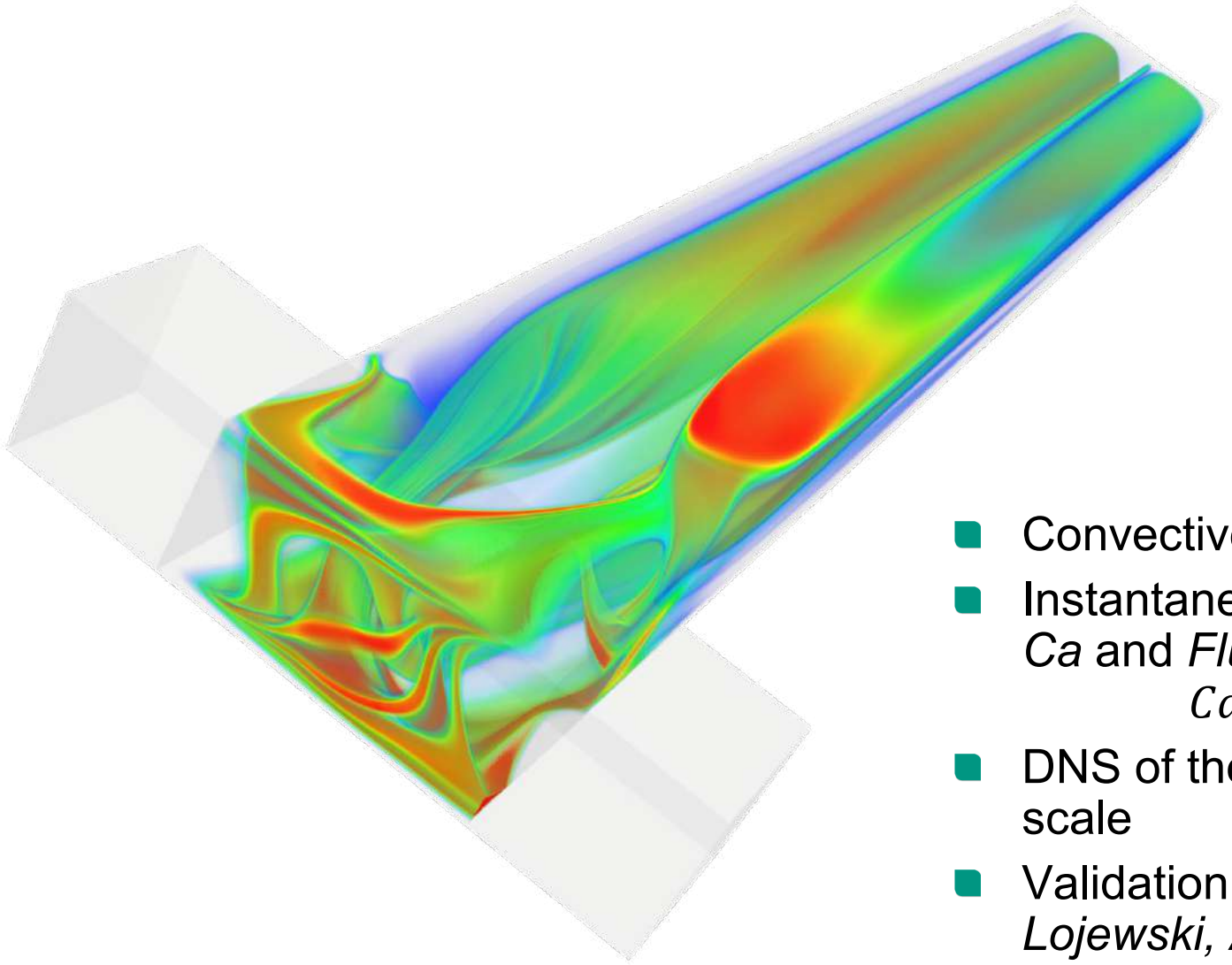


REACTIVE MICROMIXING

Bukreev, Kummerländer, Jeßberger, Teutscher, Simonis,Bothe, Krause (2025). AIAA-J 63:4.

Kummerländer, Bukreev, Teutscher, Dorn, Krause (2025). JPDC 206, 105169.

Reactive Mixing in a T-Micromixer



- Convective and diffusive mixing of two components
- Instantaneous, irreversible neutralization reaction of *Ca* and *Fluo4* ions

$$Ca^{2+} + Fluo4^{5-} \rightarrow [CaFluo4]^{3-}$$

- DNS of the T-micromixer resolved till the Batchelor scale
- Validation on results of *Bothe et al. 2006,2011; Lojewski, A. 2010*

Mathematical model

- Incompressible Navier-Stokes equations (NSE) for carrier flow

$$\partial_t u - \frac{1}{Re}\Delta u + u \cdot \nabla u + \nabla p = 0, \qquad \nabla \cdot u = 0.$$

- Advection-Diffusion Reactive equation (ADRE) for species dynamics

$$\partial_t c_i + u \cdot \nabla c_i + \nabla \cdot (D_i(c_i, u)\nabla c_i) = R_i, \qquad R_i = \pm k c_A c_B$$

$$D_i(c_i, u) = D_{i,mol}(c_i) + D_{i,turb}(u),$$

$$D_{i,turb} = \frac{\nu_{turb}}{Sc_{i,turb}}, \quad \textit{[Gaedtke, M. 2020]}$$

$$\nu_{turb} = \left(C_{Smago}\Delta x\right)^2 |S_{mn}|$$

S_{mn} - shear rate

$Sc_{i,turb}$ - chosen turbulent Schmidt number

LBM discretization

- NSE-LBM:

$$f_i(x+\xi_i dt, t+dt) = f_i(x,t) + \frac{1}{\tau}\left(f_i^{eq}(x,t) - f_i(x,t)\right)$$

$$f_i^{eq}(x,t) = w_i \rho \left(1 + \frac{\xi_i u}{c_s^2} + \frac{(\xi_{i\alpha}\xi_{i\beta} - c_s^2 \delta_{\alpha\beta}) u_\alpha u_\beta}{2c_s^4}\right)$$

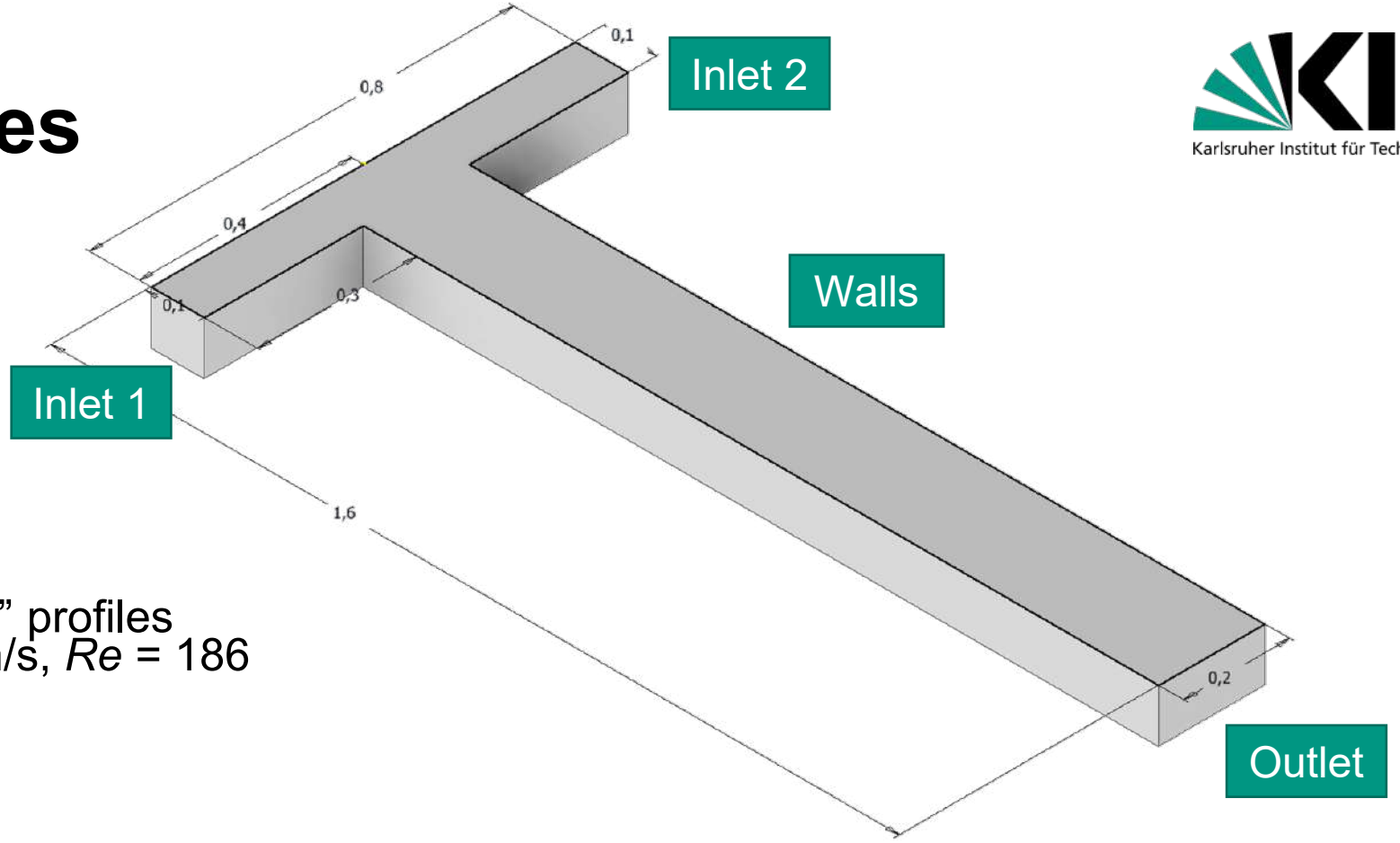
- ADRE-LBM

$$g_i(x+\xi_i dt, t+dt) = g_i(x,t) + \frac{1}{\tau_j(x,D_j)}\left(g_i^{eq}(x,t) - g_i(x,t)\right) + \left(1 - \frac{1}{2\tau_j(x,D_j)}\right) w_i R_j$$

$$g_i^{eq}(x,t) = w_i c_j \left(1 + \frac{\xi_i u}{c_s^2}\right);\ \text{Artefacts cutoff: } if\left(c_j < 10^{-8}\right) \rightarrow c_j = 10^{-8}$$

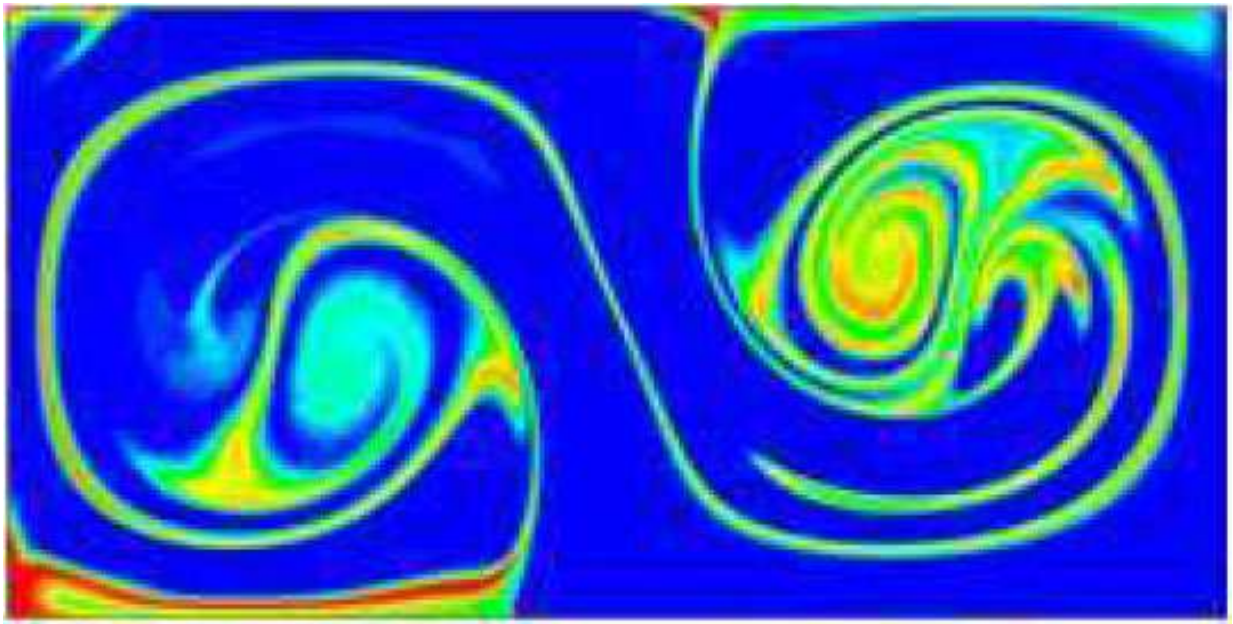
$$R_i = \pm k c_A c_B$$

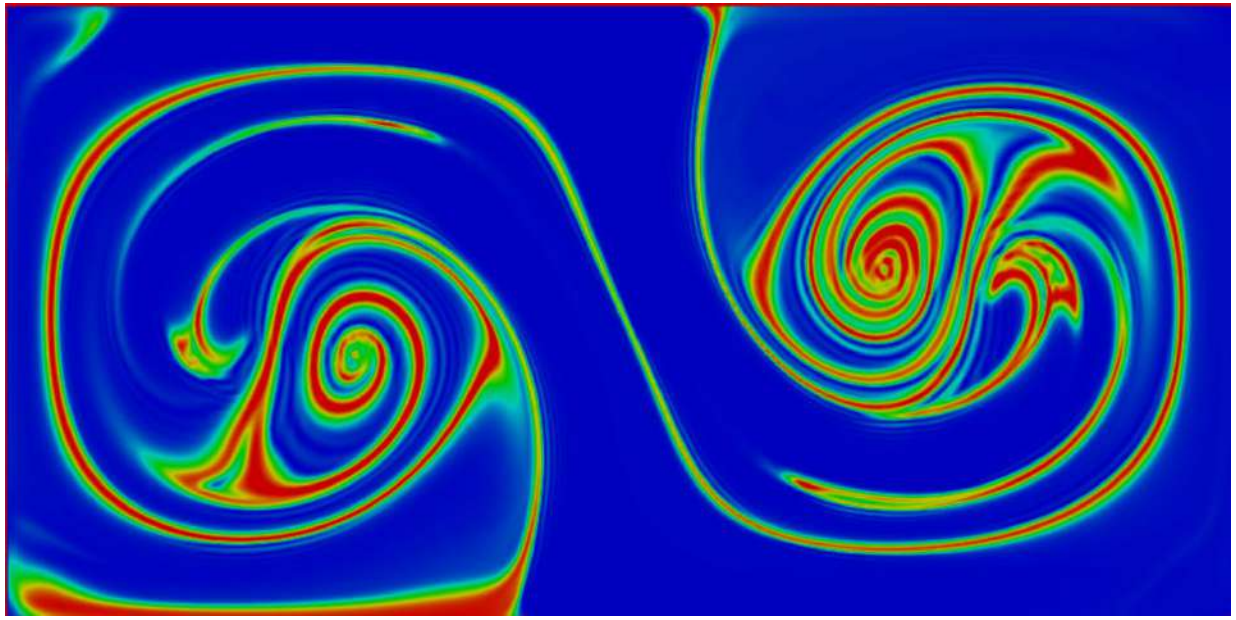
Setup. Boundaries



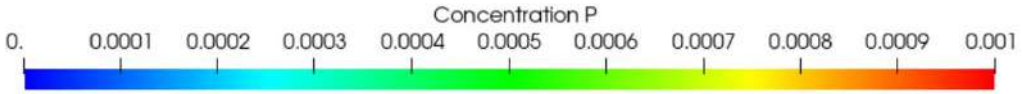
- NSE:
  - Inlets: rectangle “Poiseuille” profiles with average velocity 1,4 m/s, *Re* = 186
  - Outlet: pressure outlet
  - Walls: bounce-back
  - Simulated time: 0,038 s
- ADRE:
  - Inlets: Dirichlet concentrations $10^{-8}([CaFluo4]^{3-})$, $1(Ca^{2+})$ and $0{,}001(Fluo4^{5-})$ [mol/m³]
  - Outlet: Neumann BC
  - Walls: bounce-back
  - Simulated time: 0,01 s

$[CaFluo4]^{3-}$ at the axis length 550 µm



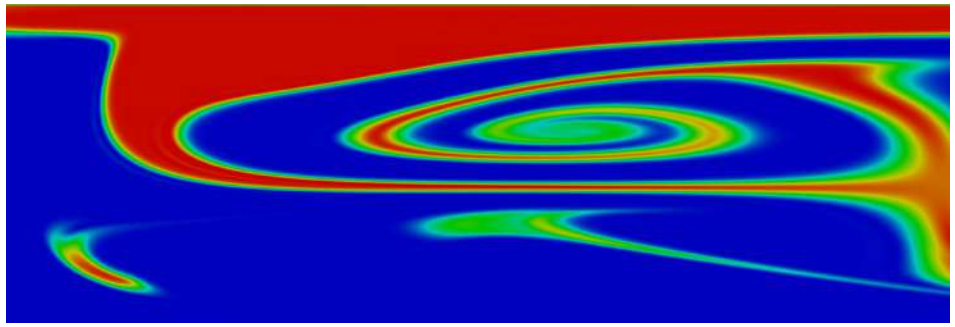


FVM simulation
[Lojewski, A. 2010]

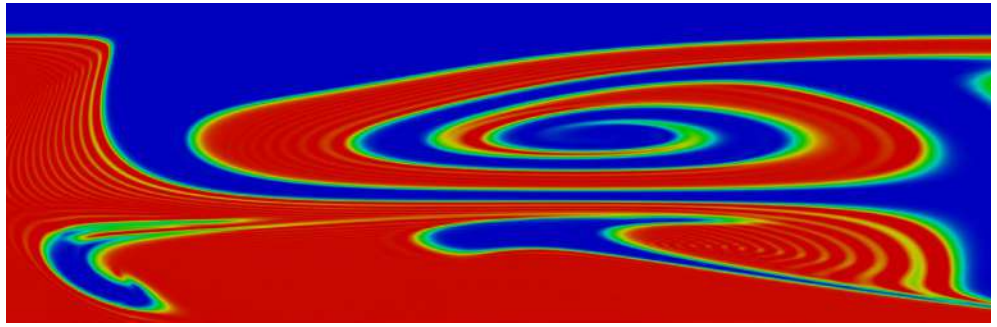


OpenLB
simulation

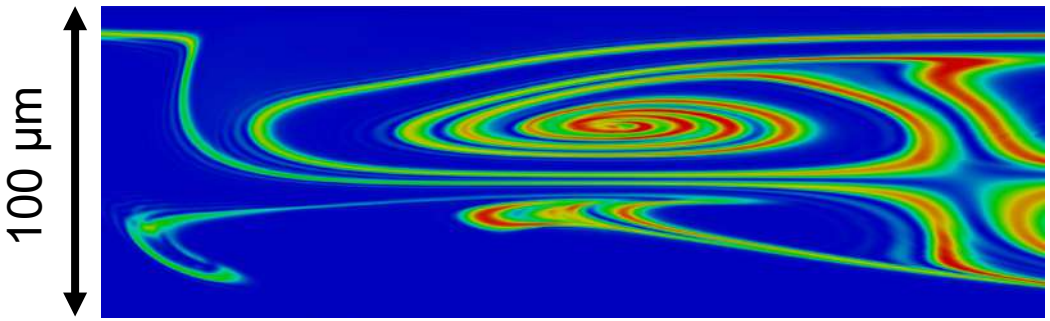
Dean vortices



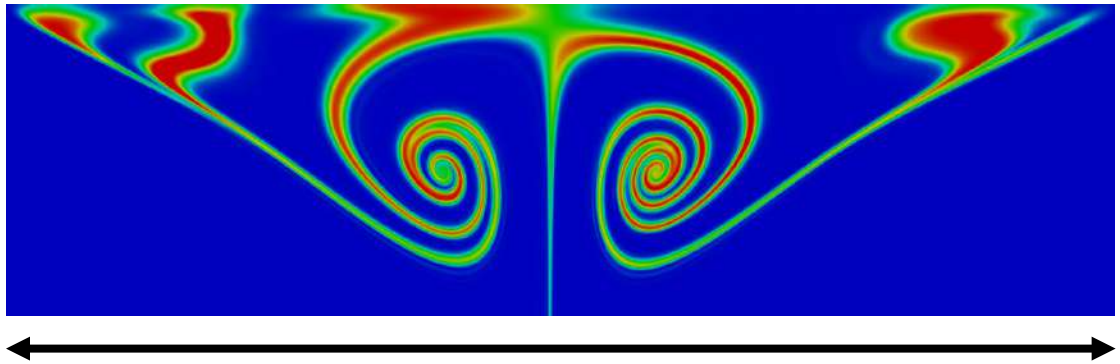
Ca^{2+}



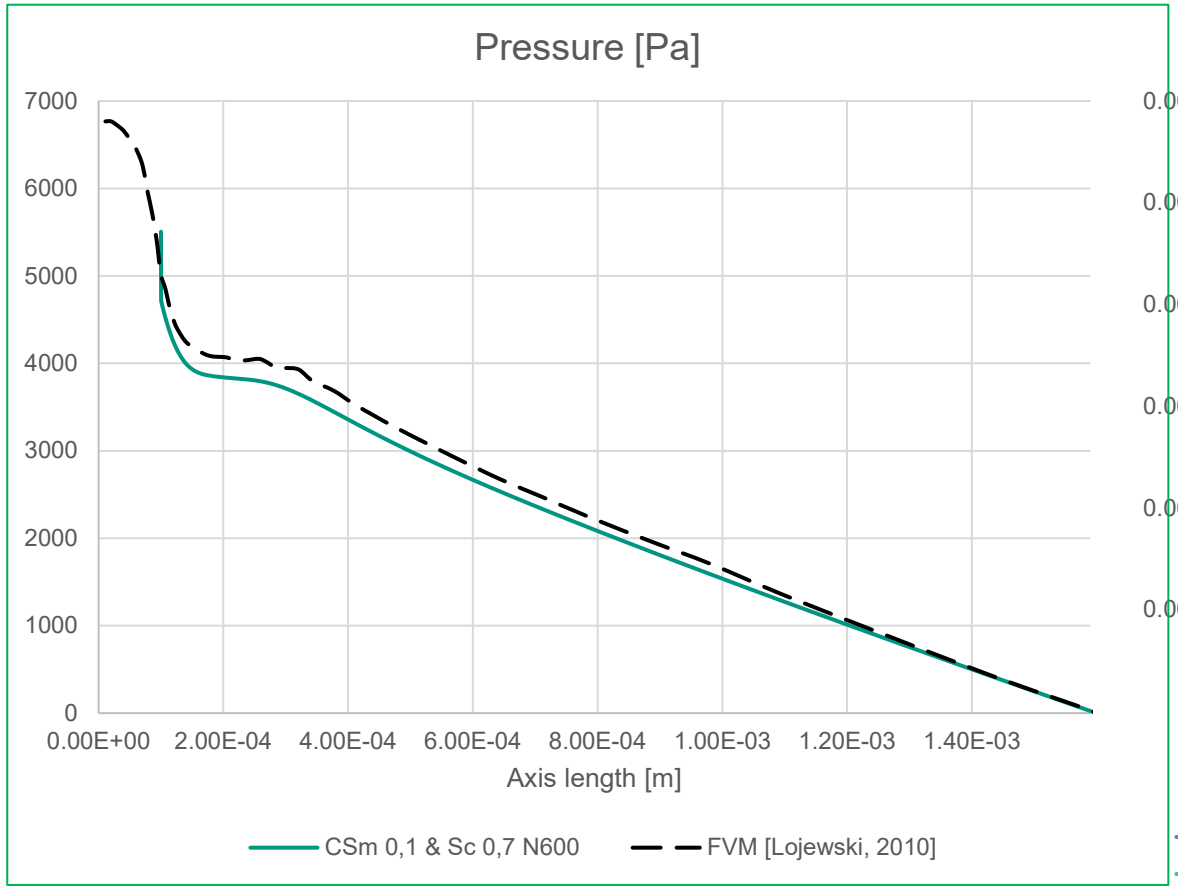
$Fluo4^{5-}$

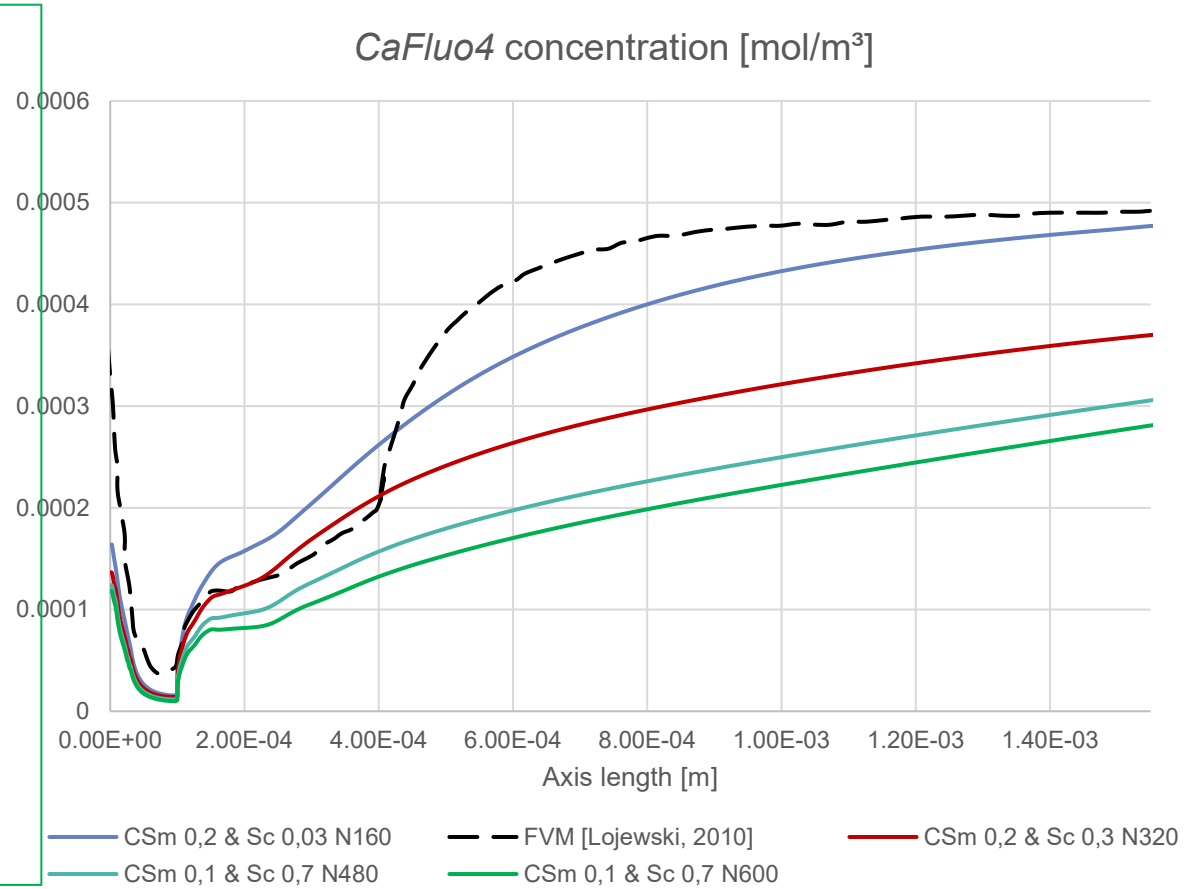


$[CaFluo4]^{3-}$

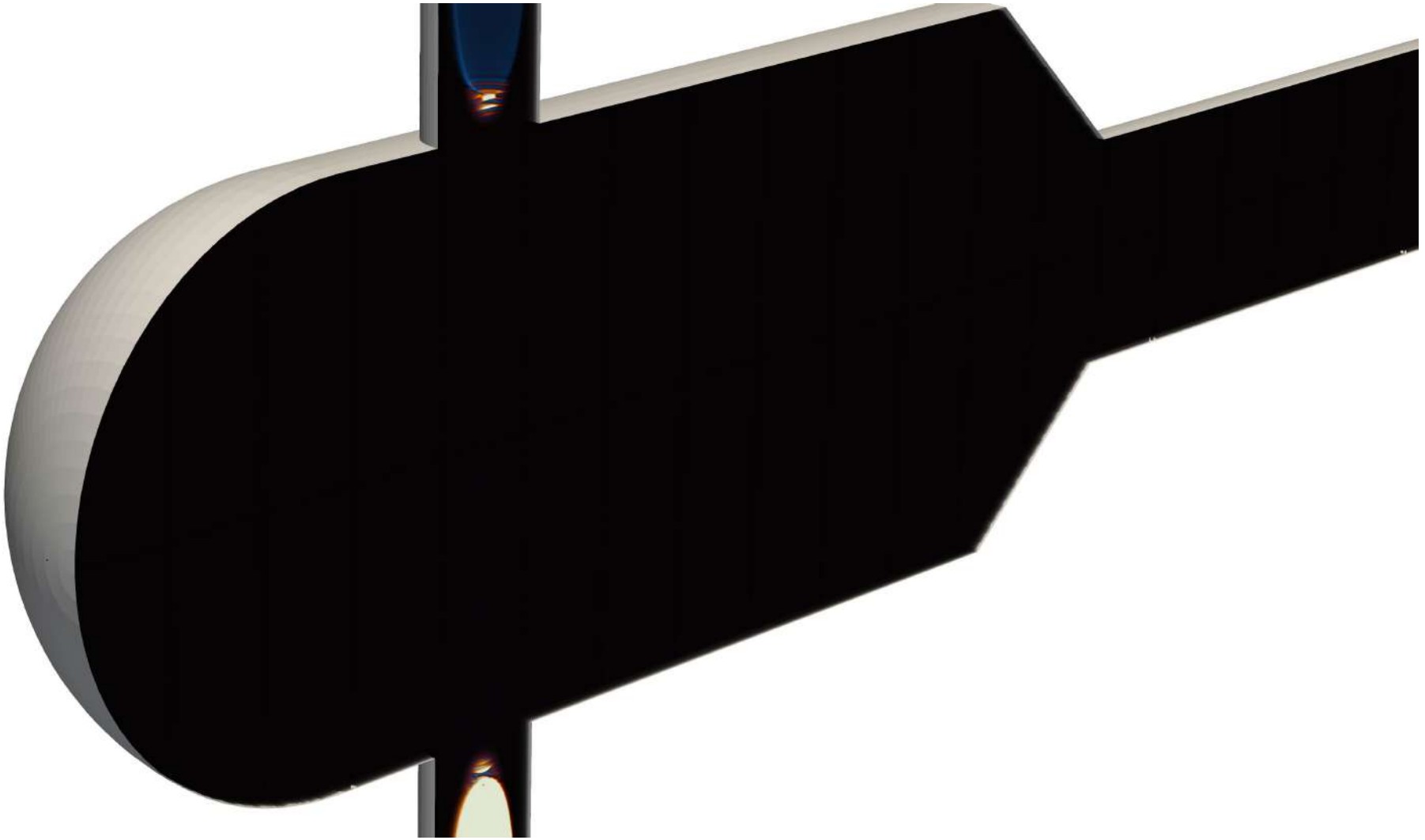


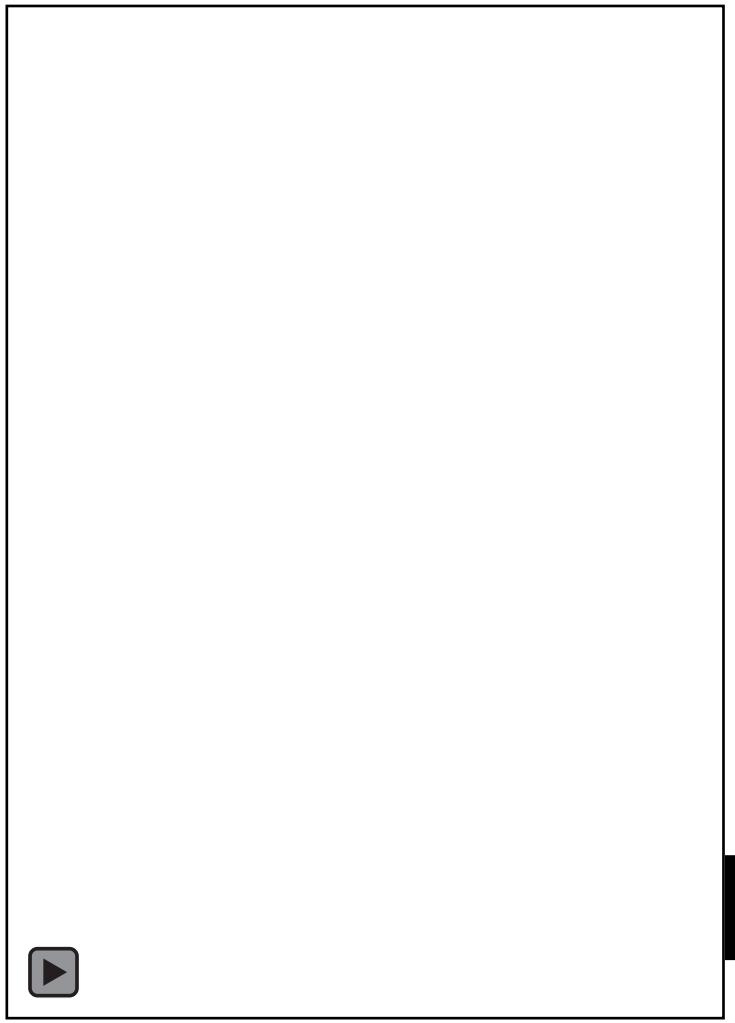
Comparision of LBM and FVM





Outlook: turbulent micromixer





MULTIPHASE FLOWS

Raeli,Borello, Serazio, Czelusniak, Bingert, Krause, Viberti (2025). ISDN 978-88-946678-2-0.

Approaching dual-equation Models

Shifting the order parameter to Allen-Cahn equations

Less physics, more modeling

1.Incompressible pressure evolution LBE:

$$f_i(x_\alpha + c_{i\alpha}\Delta t, t + \Delta t) = f_i(x_\alpha, t) + \frac{1}{\tau}\left(f_i^{\mathrm{eq}} - f_i\right) + S_i$$

New equilibrium for pressure evolution:

$$f_i^{\mathrm{eq}} = \frac{\omega_i}{c_s^2}\left(p + \rho\left(\boldsymbol{c}_i \cdot \boldsymbol{u} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^2} - \boldsymbol{u} \cdot \boldsymbol{u}\right)\right), i \neq 0$$

Phase Field Thermodynamics:

Separating Force – FD order parameter

$\boldsymbol{F} = \mu_\phi \nabla\phi$ → easier gradient

Thermodyn. Information – no cubic EoS

$$\mu_\phi = \left(\frac{\partial F}{\partial \phi}\right)_{T,\rho} - \kappa\Delta\phi$$

Surface Tension

$\sigma \propto \phi(\boldsymbol{x})\nabla\Delta\phi(\boldsymbol{x})$

2.Interface-tracking order parameter equation:

Phase densities and phase viscosities all $f(\phi), \phi \in [0; 1]$

Free energy F, such that interface is hyperbolic tangent

Local Allen-Cahn: $\partial_t\phi + \partial_\alpha(\phi u_\alpha) = \partial_\alpha(M(\partial_\alpha\phi - \boldsymbol{n}\frac{4\phi(1-\phi)}{W}))$

Achieves phys. surface tension

Martins, Ivan Talão, Pablo Fariñas Alvariño, and Luben Cabezas-Gómez. "Dimensional lattice Boltzmann method for transport phenomena simulation without conversion to lattice units." arXiv preprint arXiv:2302.04120 (2023).

Achieving high surface tension for high Δx

Lattice σ and dimensional analysis

- The equilibrium properties such as (lattice) **interface thickness** w and (lattice) **surface tension** σ can be **chosen a priori** as they influence the system‘s thermodynamics in an **analytically known** way:

$$\mu_\phi = 4\beta(\phi - 1)(\phi - 0.5)\phi - \kappa\nabla^2\phi$$

with $\beta = \frac{12\sigma}{w}$ and $\kappa = \frac{3\sigma w}{2}$ ➡ $\sigma \uparrow$: $\beta \uparrow$: $\mu_\phi \uparrow$: $\boldsymbol{F} \uparrow$ → instability

- Under diffusive scaling with a constant value for the conversion factor of density $C_\rho = C_m/\Delta x^3$ and the units $[\sigma_{phys}] = MT^{-2}$, the following holds for σ_L when doubling Δx:

$$\sigma_L = \frac{\sigma_{phys}}{(C_m C_t^{-2})} = \frac{\sigma_{phys}}{(C_\rho \Delta x^3 \Delta x^{-4})} = \frac{\sigma_{phys}\Delta x}{C_\rho} \text{ with } 2\Delta x \rightarrow \sigma_L \text{ doubles!}$$

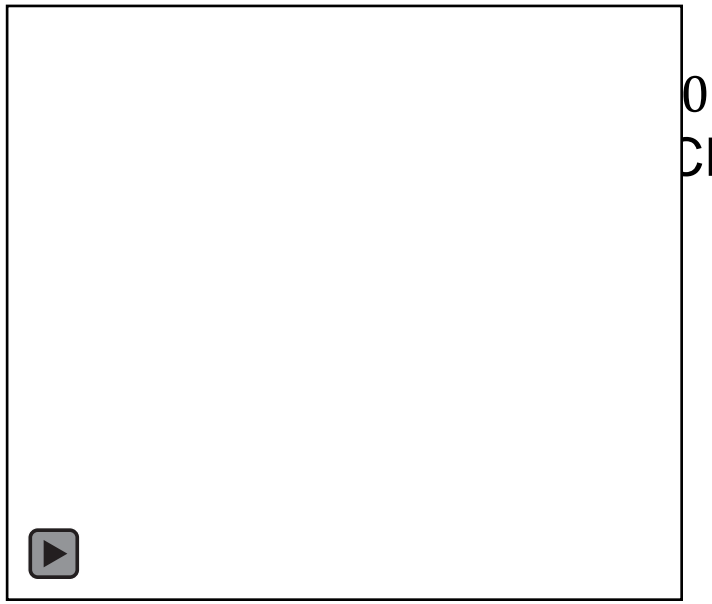
Numerical dispersion in local ACE for high σ_L

Introduction to the hybrid Allen-Cahn formulation

Why hybrid?!

Trick: Solve the **local ACE** in the region of the interface with $-2w \leq \psi \leq 2w$ for the **signed distance ψ** to have the locality property and solve the **non-local ACE** in the rest of the domain (bulk) for killing off the numerical dispersion

Non-local Allen-Cahn: $\partial_t \phi + \partial_\alpha(\phi u_\alpha) = M\left[\partial_\alpha^2 \phi - \frac{4\beta}{\kappa}(\phi - 1)(\phi - 0.5)\phi + \beta_0(t)(1-\phi)\phi\right]$



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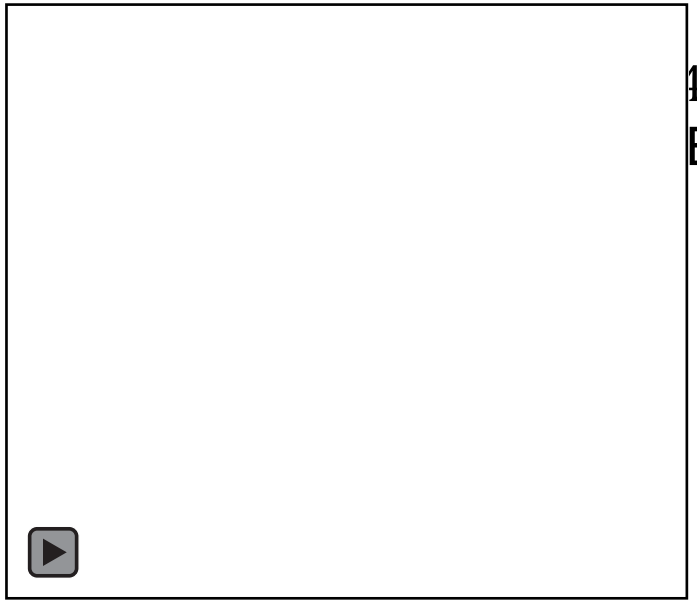

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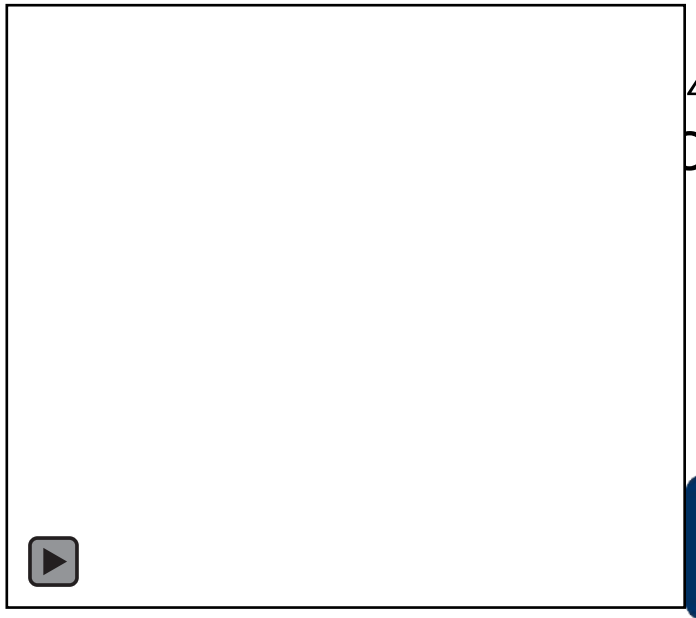

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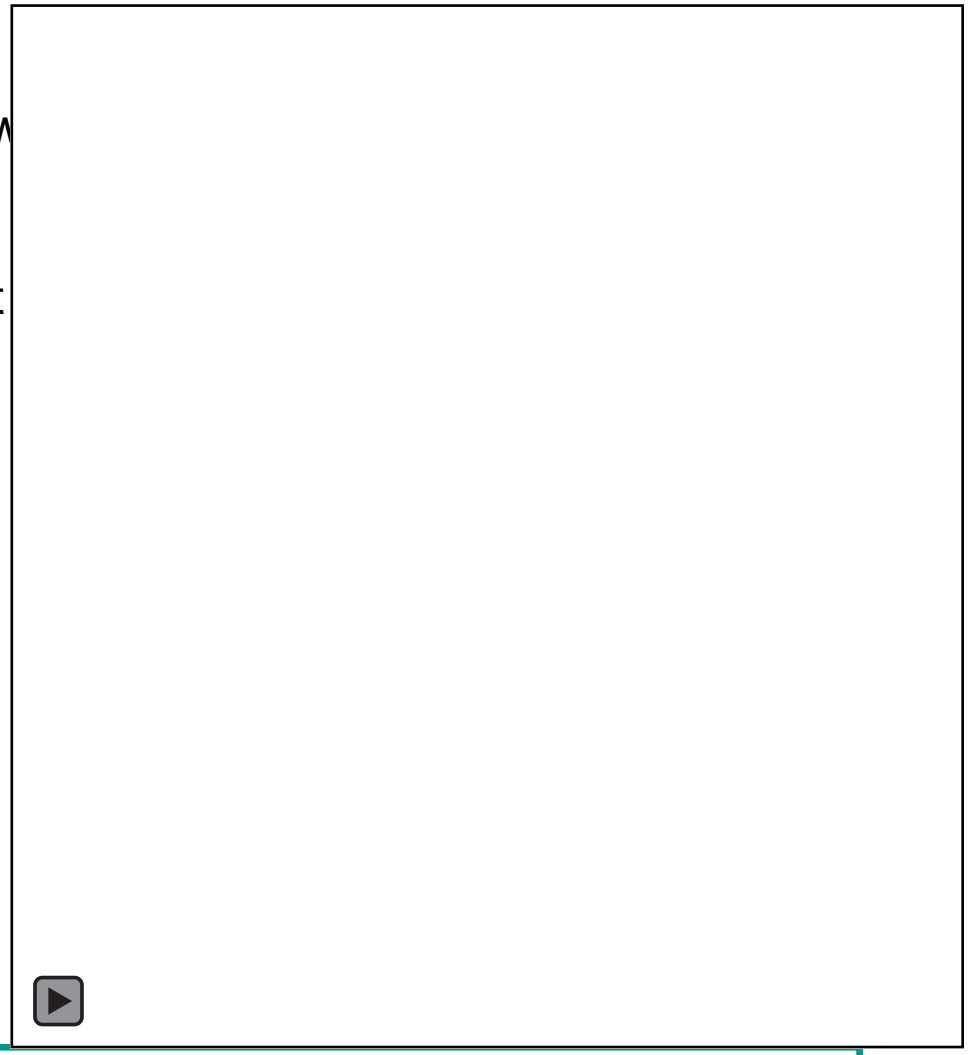
First model usage and OpenLB refactoring

Attempting bubble generation to introduce in situ bubbles

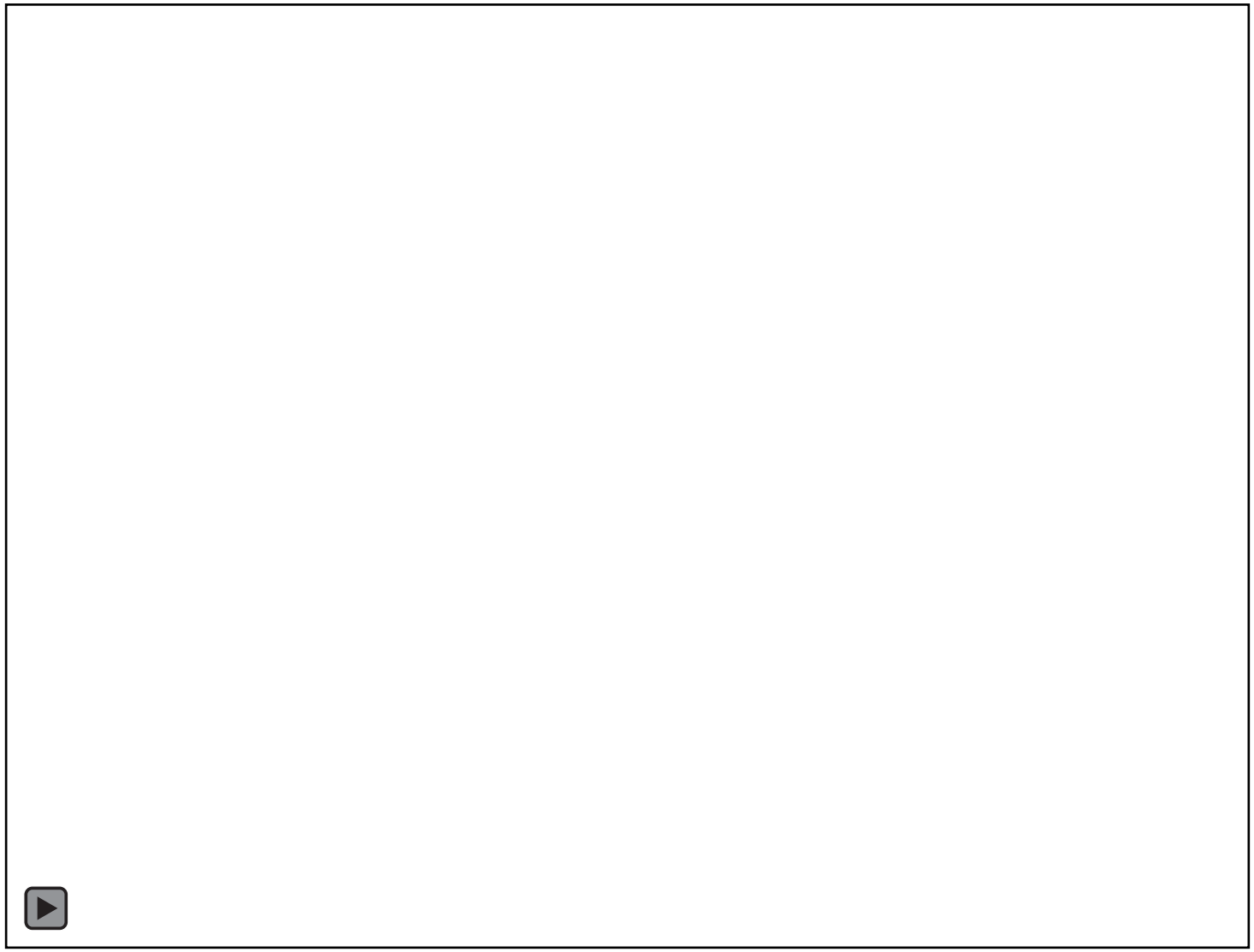
- Bubble generator prototype:
  - Apply all boundary conditions to have constant inflow of gas bubbles, although the physical properties of the water-air system are not met here
  - Pressure oscillations from bubbles leaving the outlet which is the main problem of the implementation so far
- Huge OpenLB core source code Refactoring:
  - Initialize multiphase models (others too) with an arbitrary number of macroscopic variables in equilibrium populations (density, pressure, velocity!)
  - First tests for moving interface with density ratio successful
  - >30 files to be refactored, platform specific code
  - Performed in Hackathon 2024



Bubble Generator Prototype

First applications: Showcase of gas storage

Complex porous geometry: gasStorage2d in OpenLB1.8

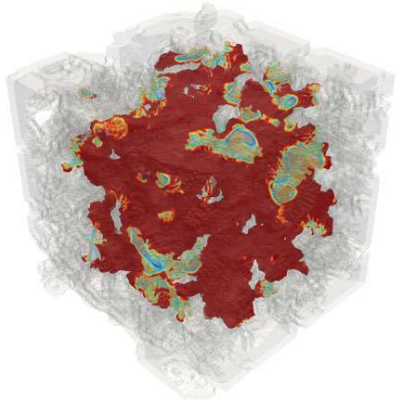


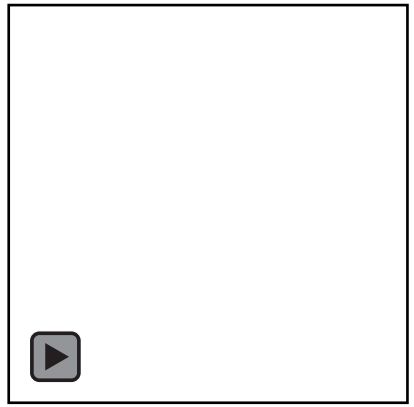
Water pushing gas and vice versa, Water pushing much harder because of higher momentum!

Physical surface tension ~ 0.01 of water air, with $\Delta x = \sim 1\ \mu m$, density ratio of 70 bar hydrogen and water

Conclusion

- OpenLB allows efficient CPU-GPU implementation and simulation of
  - Resolved porous structures with high Knudsen numbers
  - Surface and bulk chemistry
  - Multiphase flows with resolved phasic interface inside of pores





Thank you for your attention!

9th Spring School

Lattice Boltzmann Methods with OpenLB Software Lab

Liverpool, England, UK, 23. – 27. March 2026

- For scientists and industrial users
  - **Option B**eginners: comprehensive theoretical lectures on LBM, mentored training on case studies using *OpenLB*
  - **Option A**dvanced: bring your own problem
- Knowledge exchange & networking at poster session, lunches, dinner, coffee breaks, excursion
- More Info: www.openlb.net/spring-school

Executive committee:
John Bridgeman, Davide Dapelo, Mohaddeseh Musavi Nezhad, Mathias J. Krause, Shota Ito, Stephan Simonis

Invited speakers:
Timm Krüger, Halim Kusumaatmaja, Timothy Reis, Pierre Boivin, Julien Favier

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