Modelling Multiphase and Interfacial Flows with Complex Geometries using LBM

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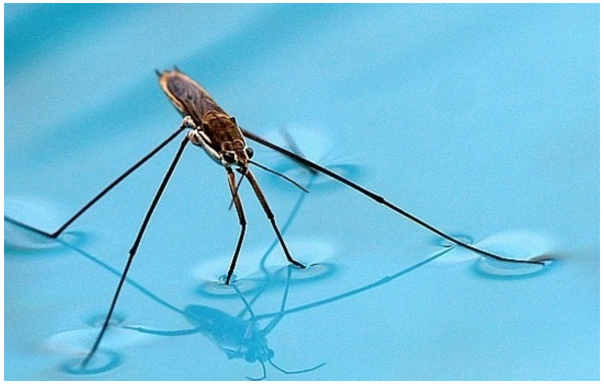
Slides with unpublished results have been removed.

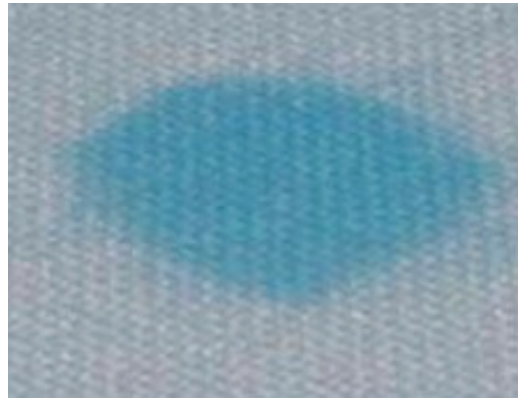
Wetting Phenomena as Underpinning Science

Biology



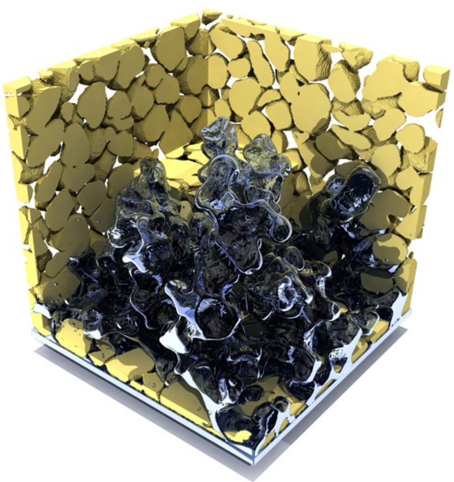
Water Strider

Fabrics



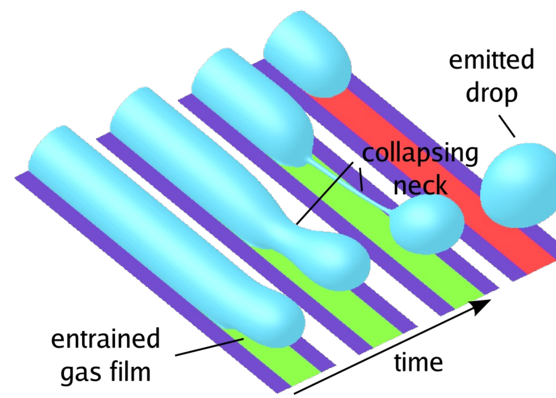
Electronics

Oil Recovery



Paints & Coatings

Microfluidics



Ternary Fluid Flows

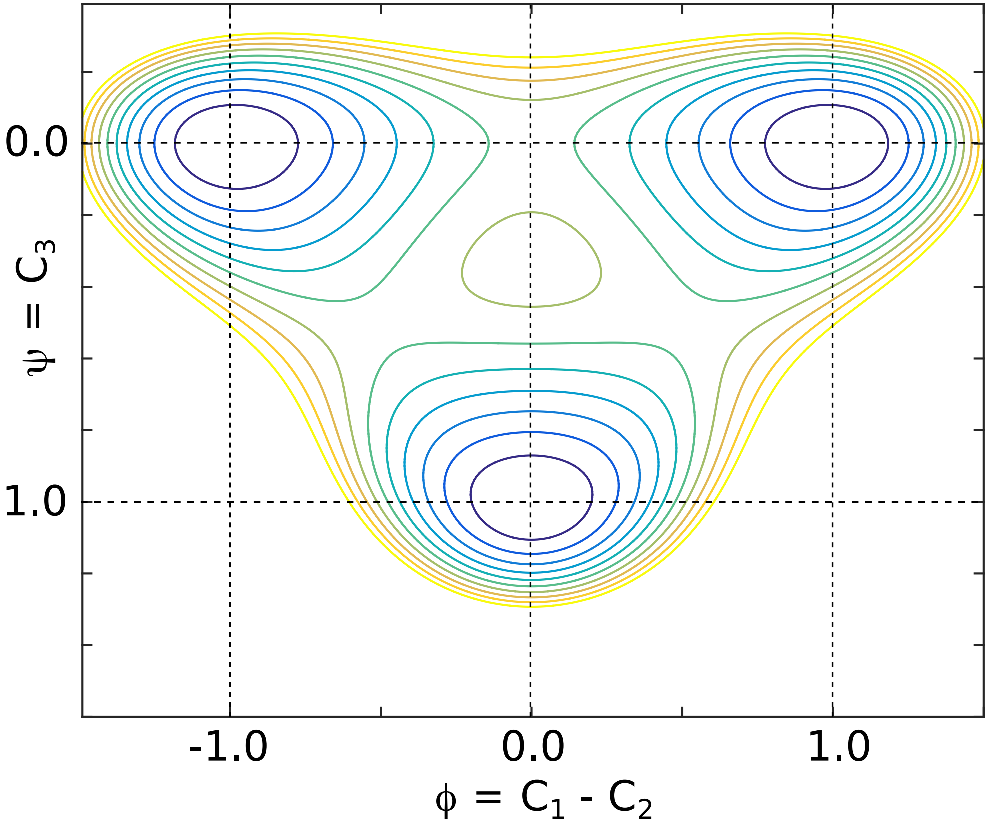
Free Energy LBM

Free energy (similar to diffuse interface / phase field model)

$$F = \int_\Omega \left[\frac{\kappa_1}{2} C_1^2 (1 - C_1)^2 + \frac{\kappa_2}{2} C_2^2 (1 - C_2)^2 + \frac{\kappa_3}{2} C_3^2 (1 - C_3)^2 \right] dV$$ ← **Double wells**

$$+ \int_\Omega \left[\frac{\alpha^2 \kappa_1}{2} (\vec{\nabla} C_1)^2 + \frac{\alpha^2 \kappa_2}{2} (\vec{\nabla} C_2)^2 + \frac{\alpha^2 \kappa_3}{2} (\vec{\nabla} C_3)^2 \right] dV$$ ← **Gradients**

e.g. Semprebon, Krüger, **HK**, PRE (2016); Boyer & Lapuerta, ESAIM (2006)



Given constraint $C_1 + C_2 + C_3 = 1$

Three independent energy minima

$$C_1 = 1, \quad C_2 = 0, \quad C_3 = 0;$$
$$C_1 = 0, \quad C_2 = 1, \quad C_3 = 0;$$
$$C_1 = 0, \quad C_2 = 0, \quad C_3 = 1.$$

Interface width α

Surface tension $\gamma_{mn} = \frac{\alpha}{6}(\kappa_m + \kappa_n)$

Equations of Motion – Numerical Scheme

The **macroscopic equations** we solve are:

- Continuity equation

$$\partial_t \rho + \partial_\alpha \left(\rho u_\alpha \right) = 0$$

- Navier-Stokes equation

$$\partial_t \left(\rho u_\alpha \right) + \partial_\beta \left(\rho u_\alpha u_\beta \right) = -\partial_\beta P_{\alpha\beta} + \partial_\beta \eta \left(\partial_\beta u_\alpha + \partial_\alpha u_\beta \right) + F_\alpha$$

MRT scheme with Guo forcing / Exact Difference Method

Chemical force $F_\alpha = -\phi \partial_\alpha \mu_\phi$

- Cahn-Hilliard equation

$$\partial_t \phi + \partial_\alpha \left(\phi u_\alpha \right) = M_\phi \nabla^2 \mu_\phi$$

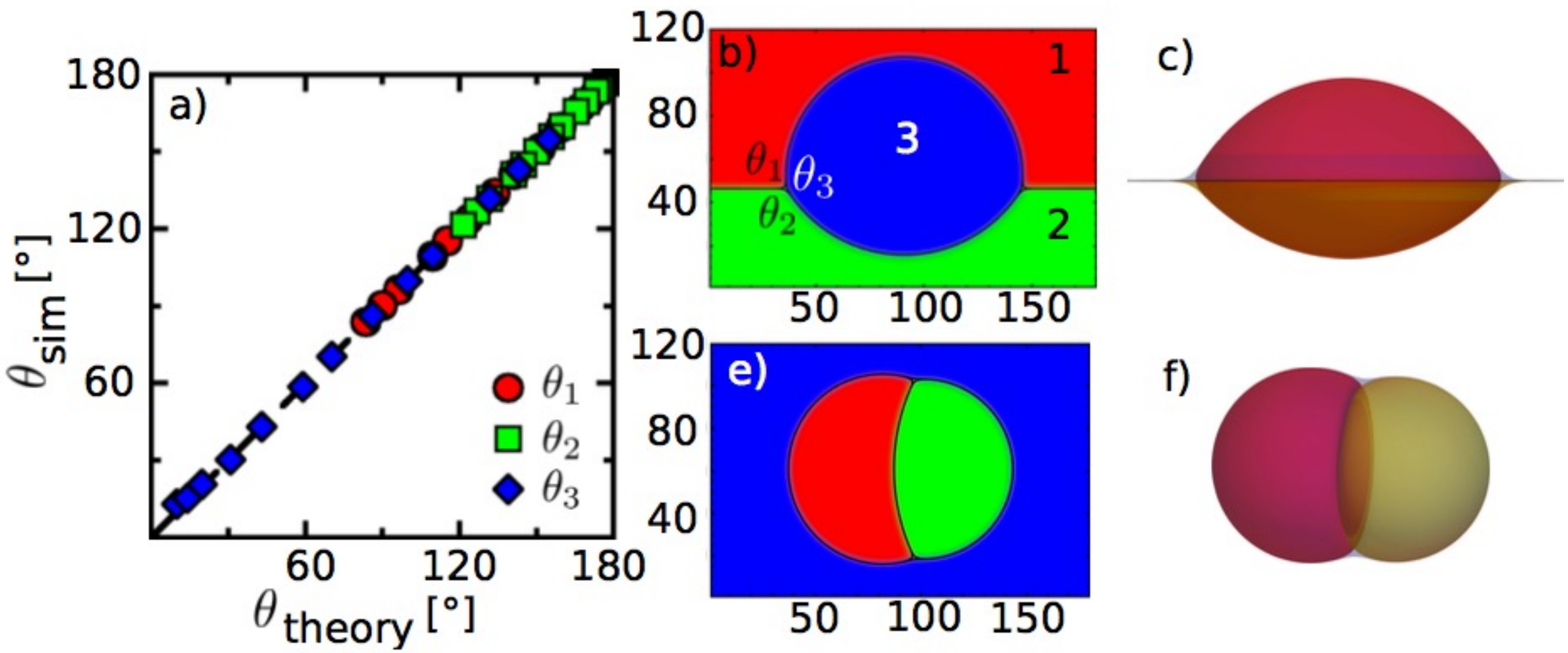
→ BGK scheme

Chemical potential $\mu_\phi = \dfrac{\delta F}{\delta \phi}$

Need more than one Cahn-Hilliard equation if we have > 2 components

Neumann Triangle

Semprebon, Krüger, **HK**, PRE (2016)



Balance of surface tension

$$\Rightarrow \quad \vec{\gamma}_{12} + \vec{\gamma}_{23} + \vec{\gamma}_{31} = 0$$

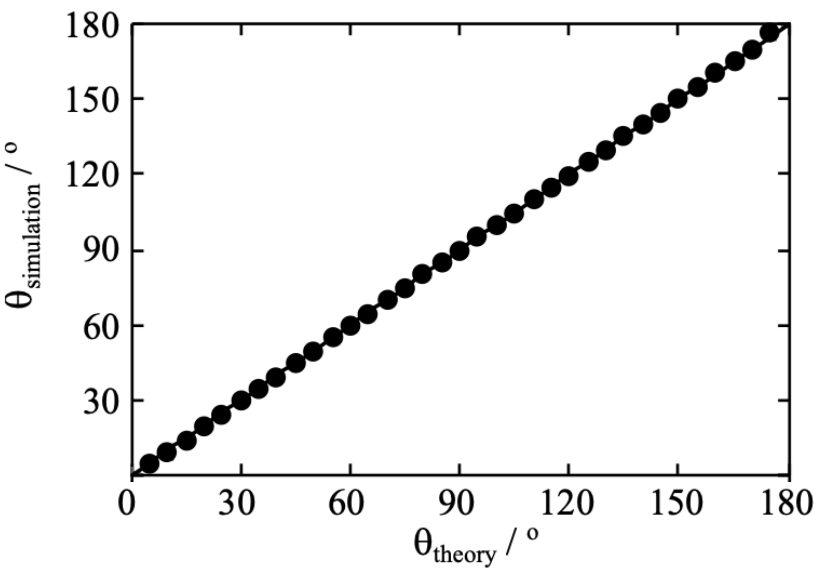
$$\Rightarrow \quad \frac{\gamma_{23}}{\sin\theta_1} = \frac{\gamma_{31}}{\sin\theta_2} = \frac{\gamma_{12}}{\sin\theta_3}$$

Implementing Contact Angles

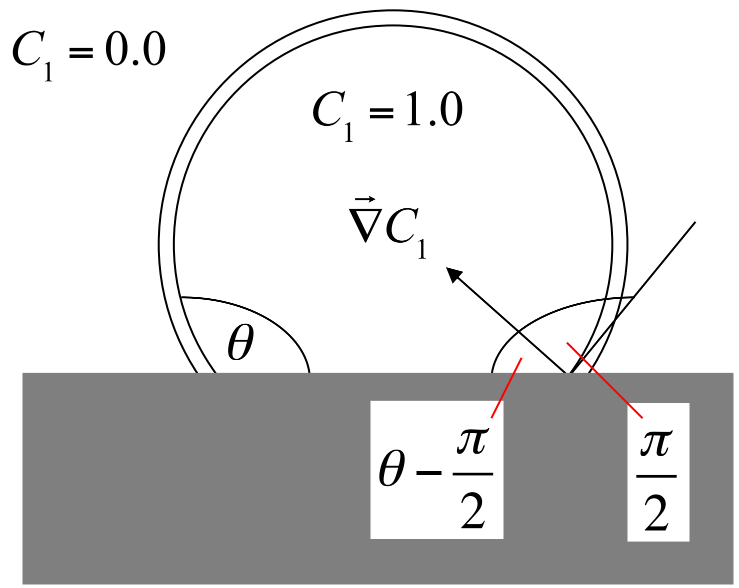
Cubic Wetting Boundary Condition

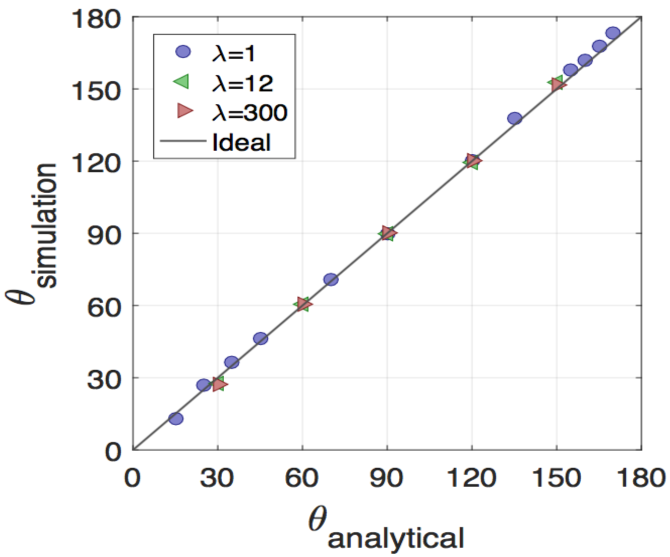
$$\mathbf{n}\cdot\nabla C_m|_S = \sum_{m=1}^{N} \xi_{mn} C_m C_n$$

$$\xi_{mn} = \frac{4}{\varepsilon}\cos\theta_{mn}$$



Geometric boundary condition:

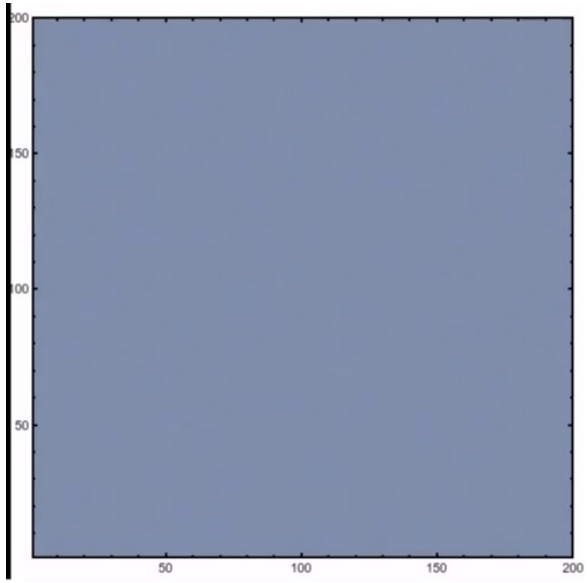


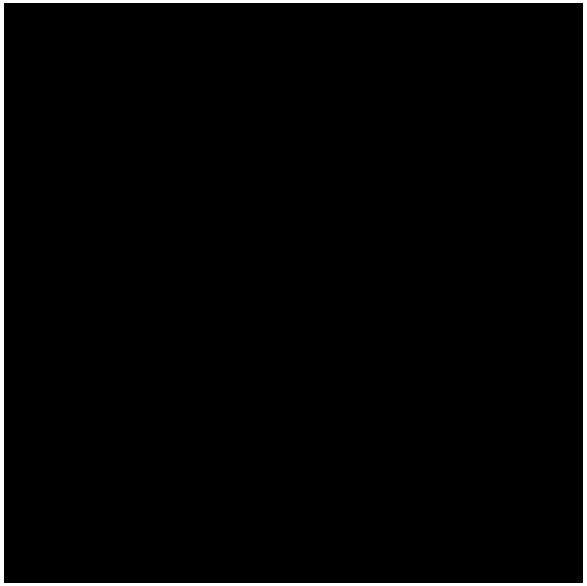


Baala, Pepona, Karlin, **HK**, Semprebon, PRE (2019)

Example: Phase Separation

c1 = c2 = c3

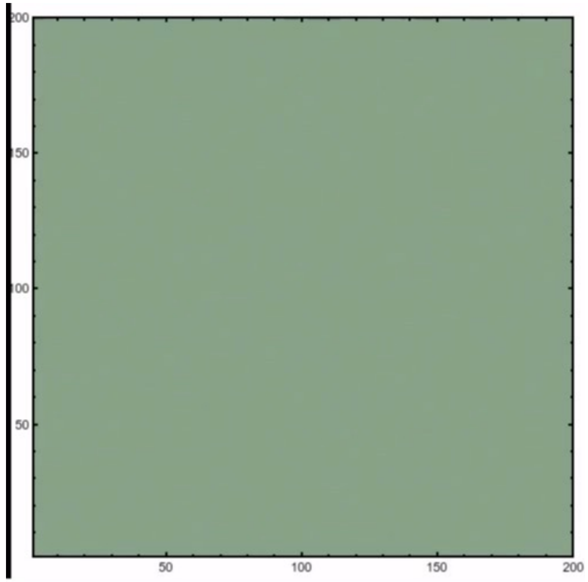


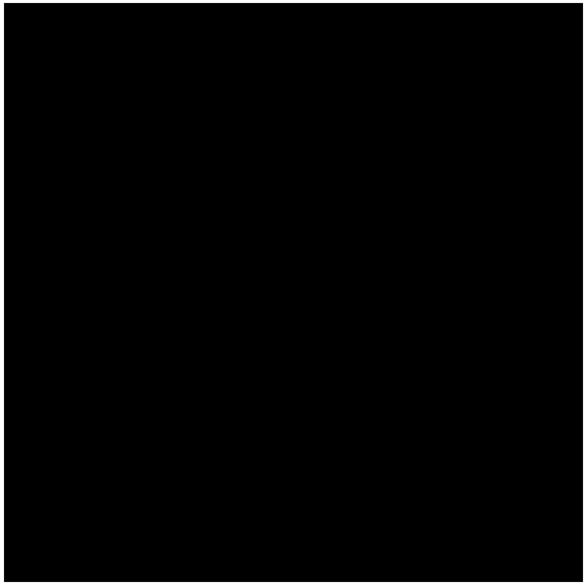


c1 = c2

c1 + c2 < c3

c1 = c2 >> c3

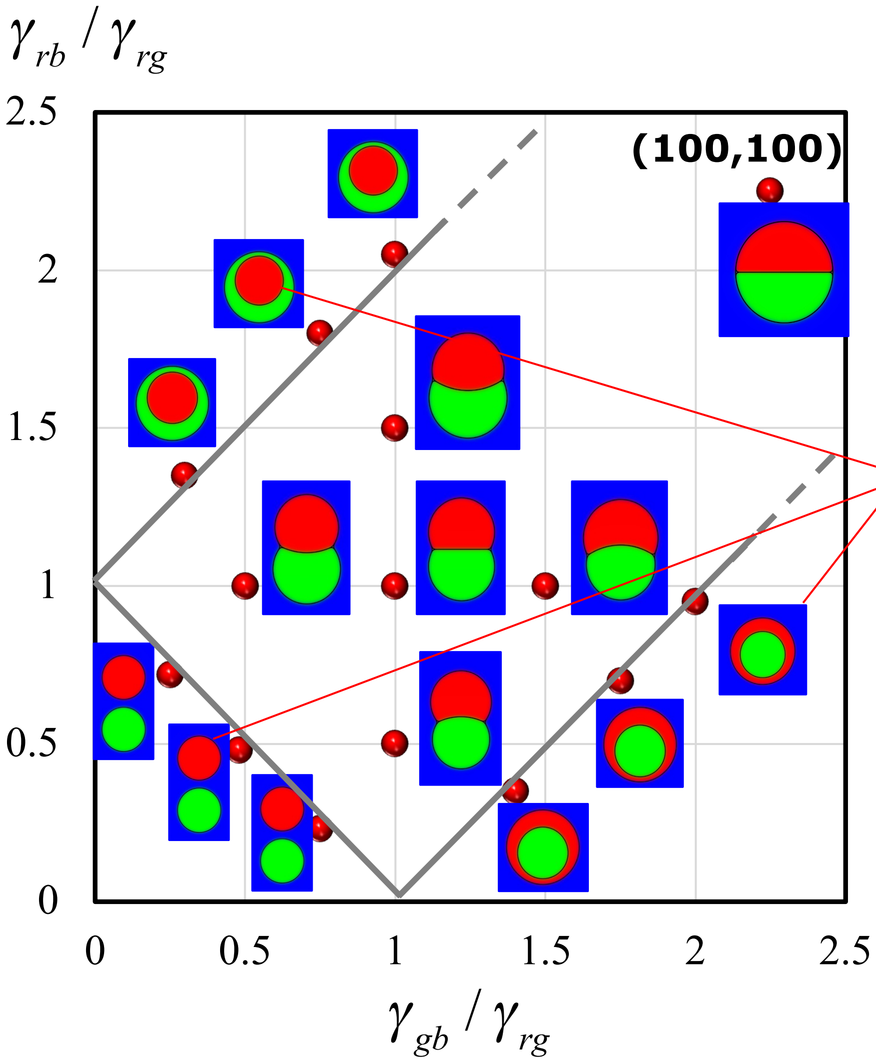




c1 = c2

c1 + c2 > c3

Problem: Droplet Cloaking



Free energy

$$F = \int_{\Omega} \left[\frac{\kappa_1}{2} C_1^2 (1-C_1)^2 + \frac{\kappa_2}{2} C_2^2 (1-C_2)^2 + \frac{\kappa_3}{2} C_3^2 (1-C_3)^2 \right] dV$$
$$+ \int_{\Omega} \left[\frac{\alpha^2 \kappa_1}{2} (\vec{\nabla} C_1)^2 + \frac{\alpha^2 \kappa_2}{2} (\vec{\nabla} C_2)^2 + \frac{\alpha^2 \kappa_3}{2} (\vec{\nabla} C_3)^2 \right] dV$$

Surface tension $\quad \gamma_{mn} = \frac{\alpha}{6} (\kappa_m + \kappa_n)$

Requires negative values of kappa's.

Example:

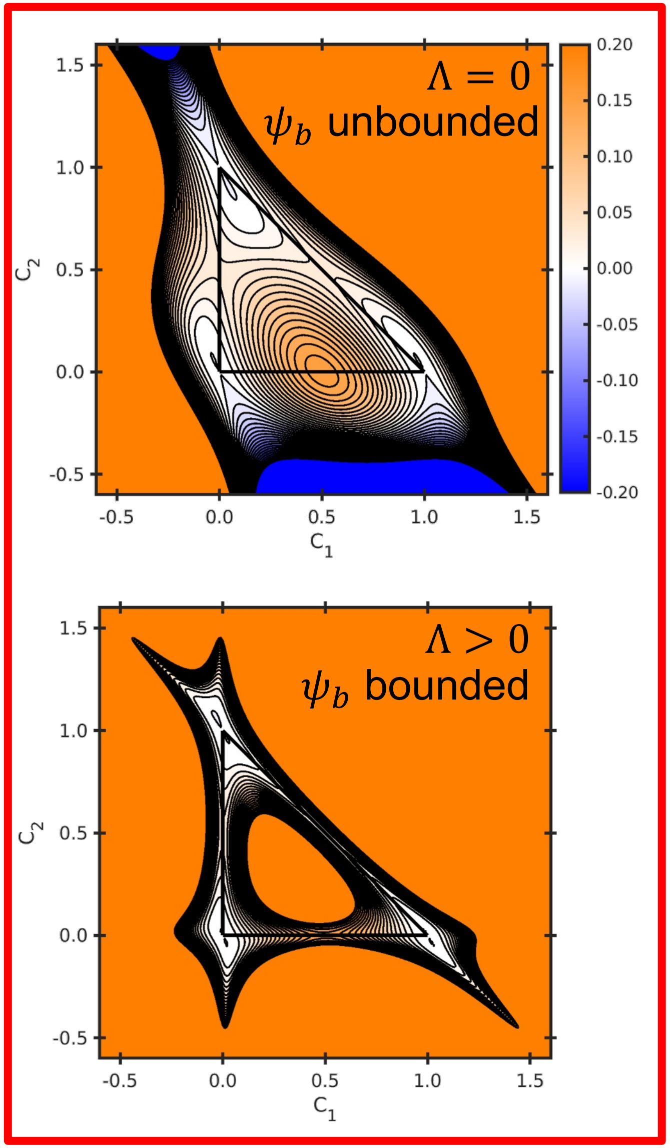
$\gamma_{rb} + \gamma_{gb} < \gamma_{rg}$

$(\kappa_r + \kappa_b) + (\kappa_g + \kappa_b) < (\kappa_r + \kappa_g)$

$2\kappa_b < 0$

The double well potential is unbounded

Problem: Droplet Cloaking



Free energy

$$F = \int_\Omega \left[\frac{\kappa_1}{2} C_1^2 (1 - C_1)^2 + \frac{\kappa_2}{2} C_2^2 (1 - C_2)^2 + \frac{\kappa_3}{2} C_3^2 (1 - C_3)^2 \right] dV$$
$$+ \int_\Omega \left[\frac{\alpha^2 \kappa_1}{2} (\vec{\nabla} C_1)^2 + \frac{\alpha^2 \kappa_2}{2} (\vec{\nabla} C_2)^2 + \frac{\alpha^2 \kappa_3}{2} (\vec{\nabla} C_3)^2 \right] dV$$

Surface tension $\gamma_{mn} = \frac{\alpha}{6}(\kappa_m + \kappa_n)$

Requires negative values of kappa's.

Need to add "penalty term"

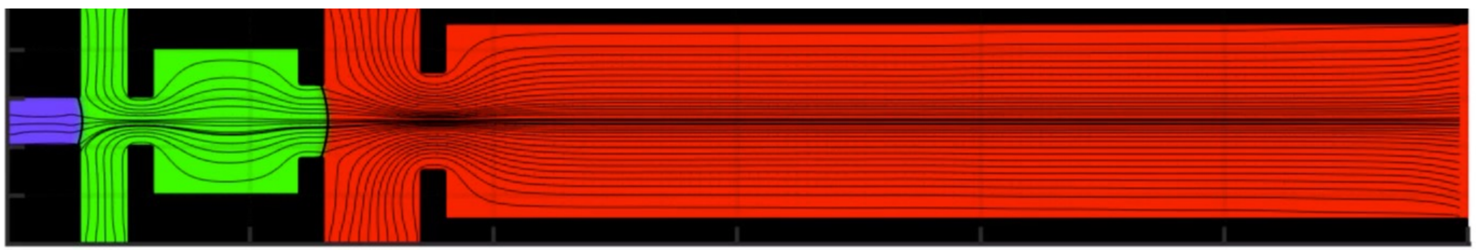
$$\Delta F_b = \Lambda C_1^2 C_2^2 C_3^2$$

Example: Droplet Microfluidics

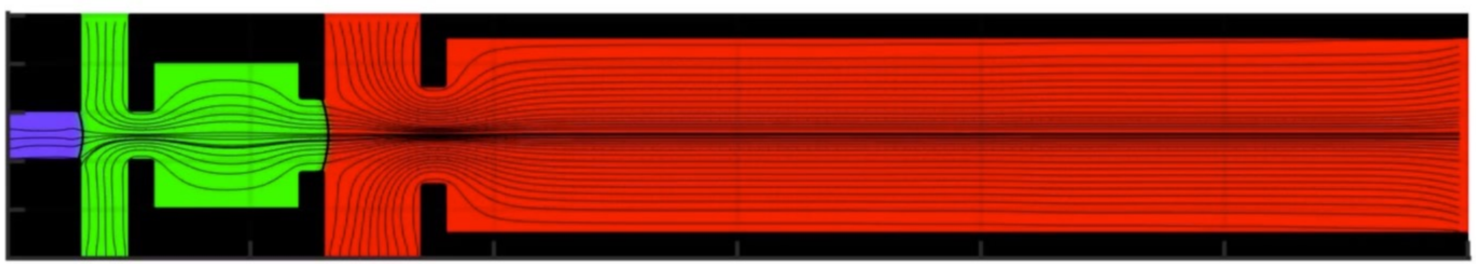
- Wang et al., J. Fluid Mech. 895, A22 (2020)

Full Wetting

Neutral Wetting



Non Wetting



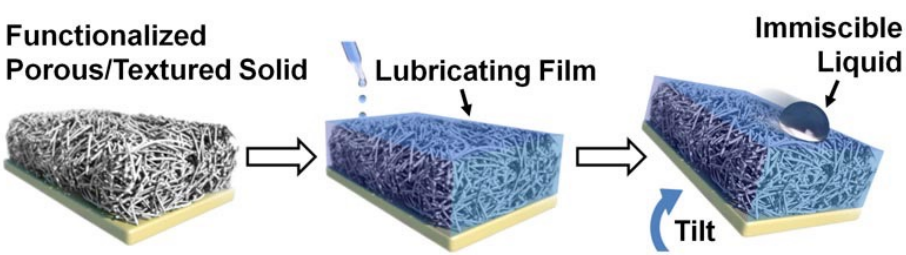
Example: Liquid Infused Surfaces

Dry

Wet

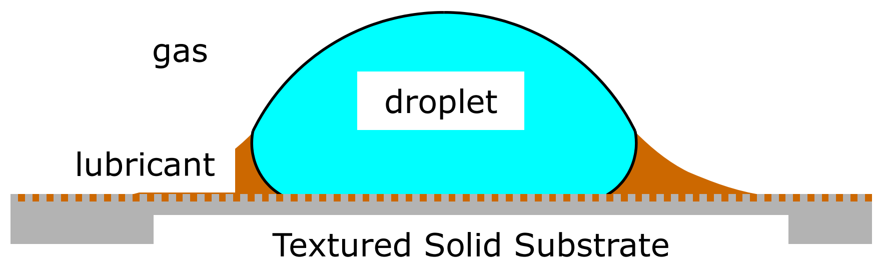
Youtube

Preparation



Wong et al., Nature (2011); Lafuma & Quere, Europhys. Lett. (2011); and many others…

Typical Geometry Considered

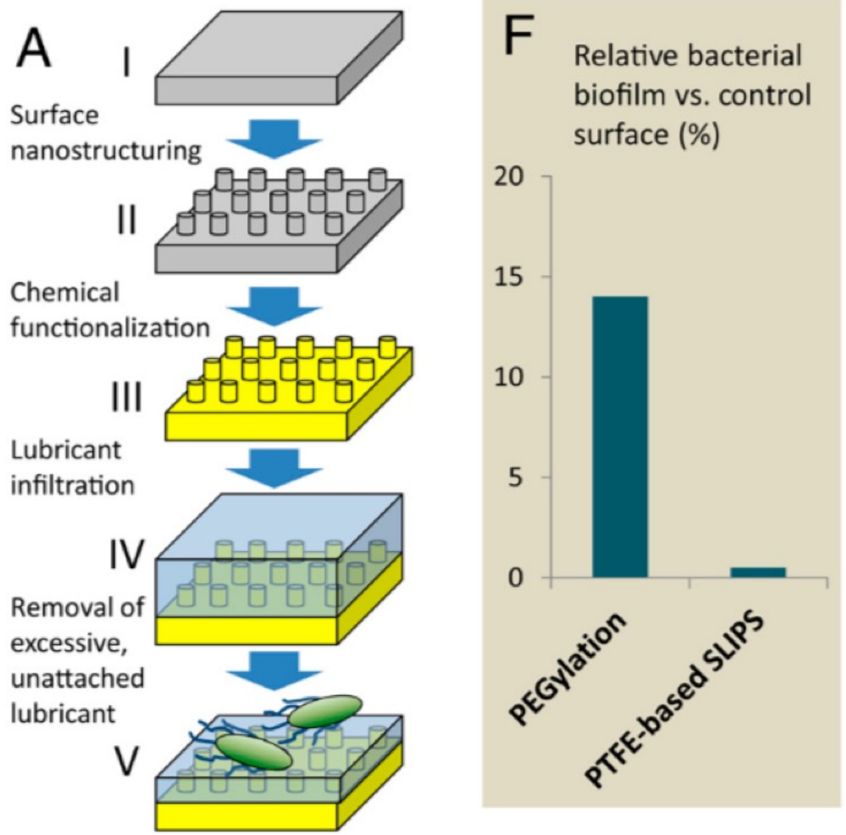


Applications of LIS

Packaging

Paint

Anti Biofouling

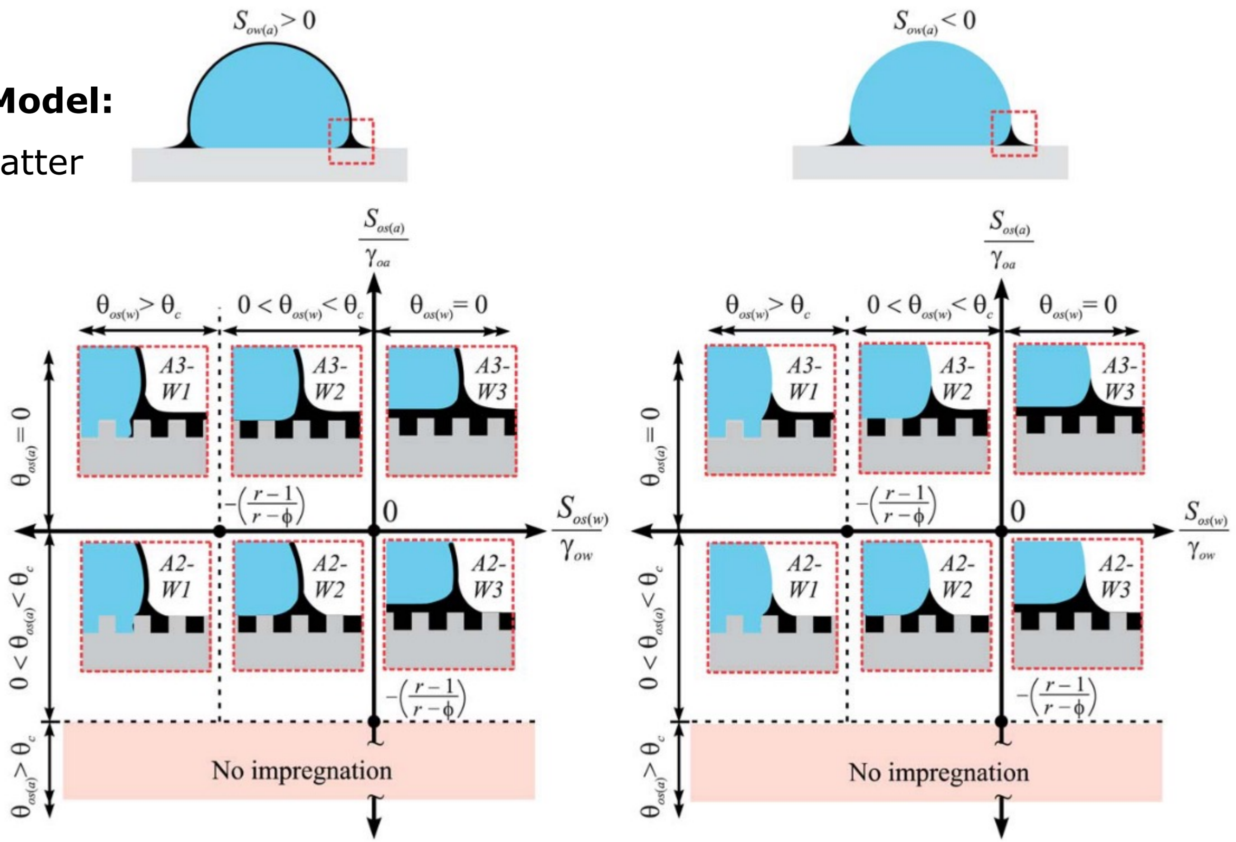


Epstein et al., PNAS (2012)

Possible Wetting States

Thermodynamic Model:

Smith et al., Soft Matter (2013)



Spreading Coefficient: $S_{ij(k)} = \gamma_{jk} - \gamma_{ij} - \gamma_{ik}$ →

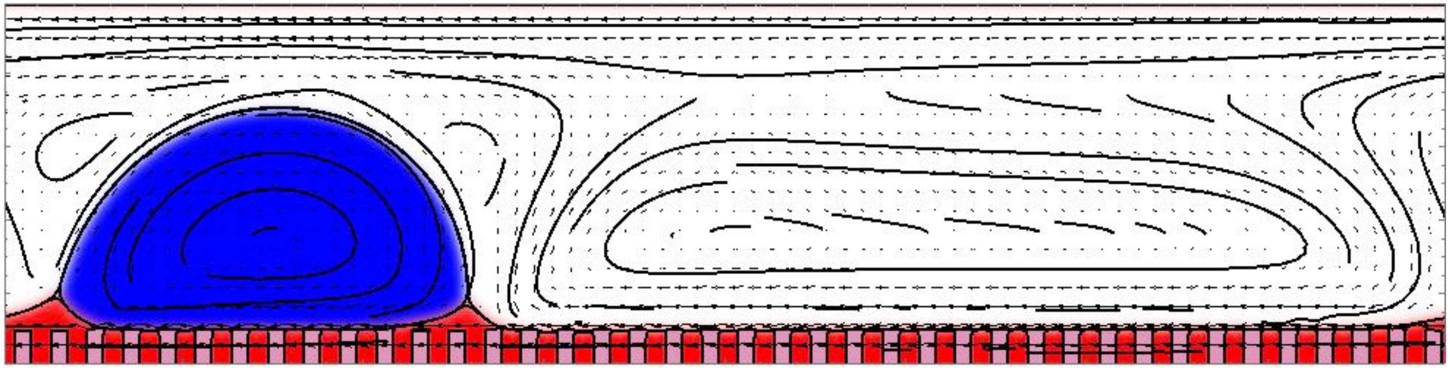
If $S_{ij(k)} > 0$, cloaking takes place.

$\gamma_{jk} > \gamma_{ij} + \gamma_{ik}$

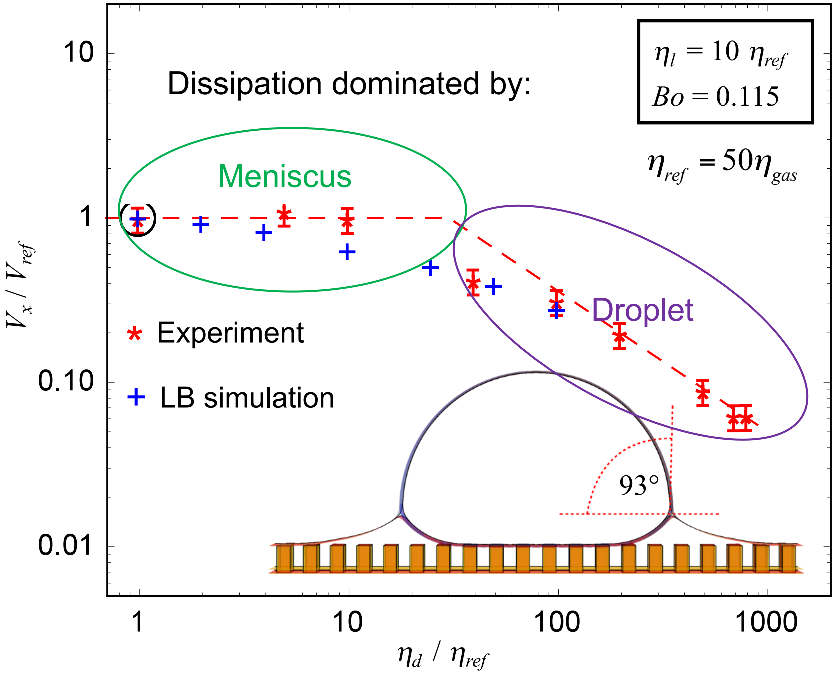
jk interface is unfavourable.

Drop Dynamics

❑ Sadullah et al., Langmuir 34, 8112 (2018); Naga et al., in preparation (2023)

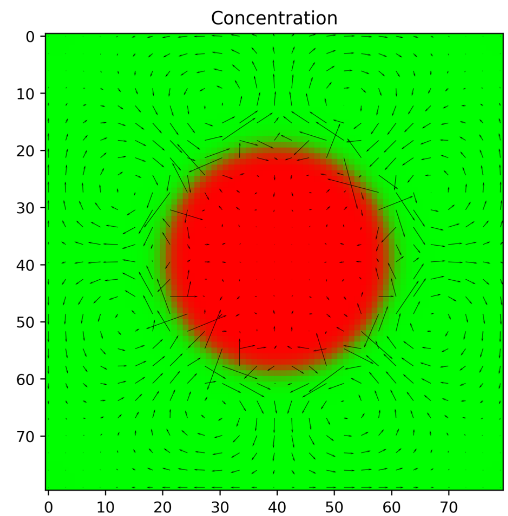


Experimental data: Keiser et al., Soft Matter (2017)

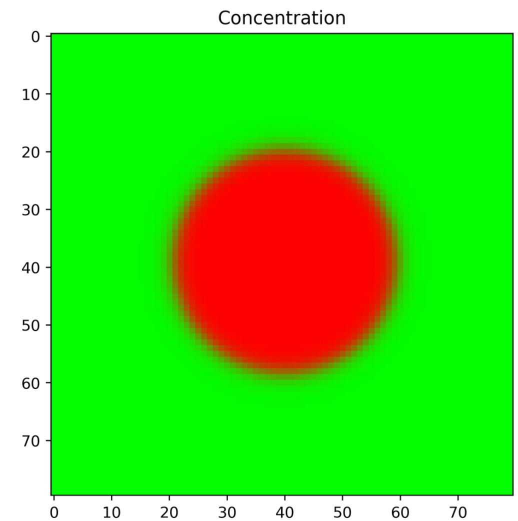


But can we look into the dissipation profile?

Problems with Spurious Velocities



Max velocity ~10^-5



Max velocity ~10^-15

Scheme from T. Lee and L. Liu, J. Comput. Phys. (2010)

Incompressible Multiphase Scheme

Key Scheme: Use approach proposed by Lee and Liu, JCP 2010

- Incompressible 2-component flow: Boltzmann equation for pressure and momentum
- Mixed stencils for the spatial gradients: Required for the macroscopic variables
- Wetting boundary conditions for the chemical potential and order parameters (concentrations)

Extension to 3-component has been done

- Similar to work by Abadi et al., PRE 97, 033312 (2018) and several others from this group
- 2-D and no solid boundaries

Additional Extension Required

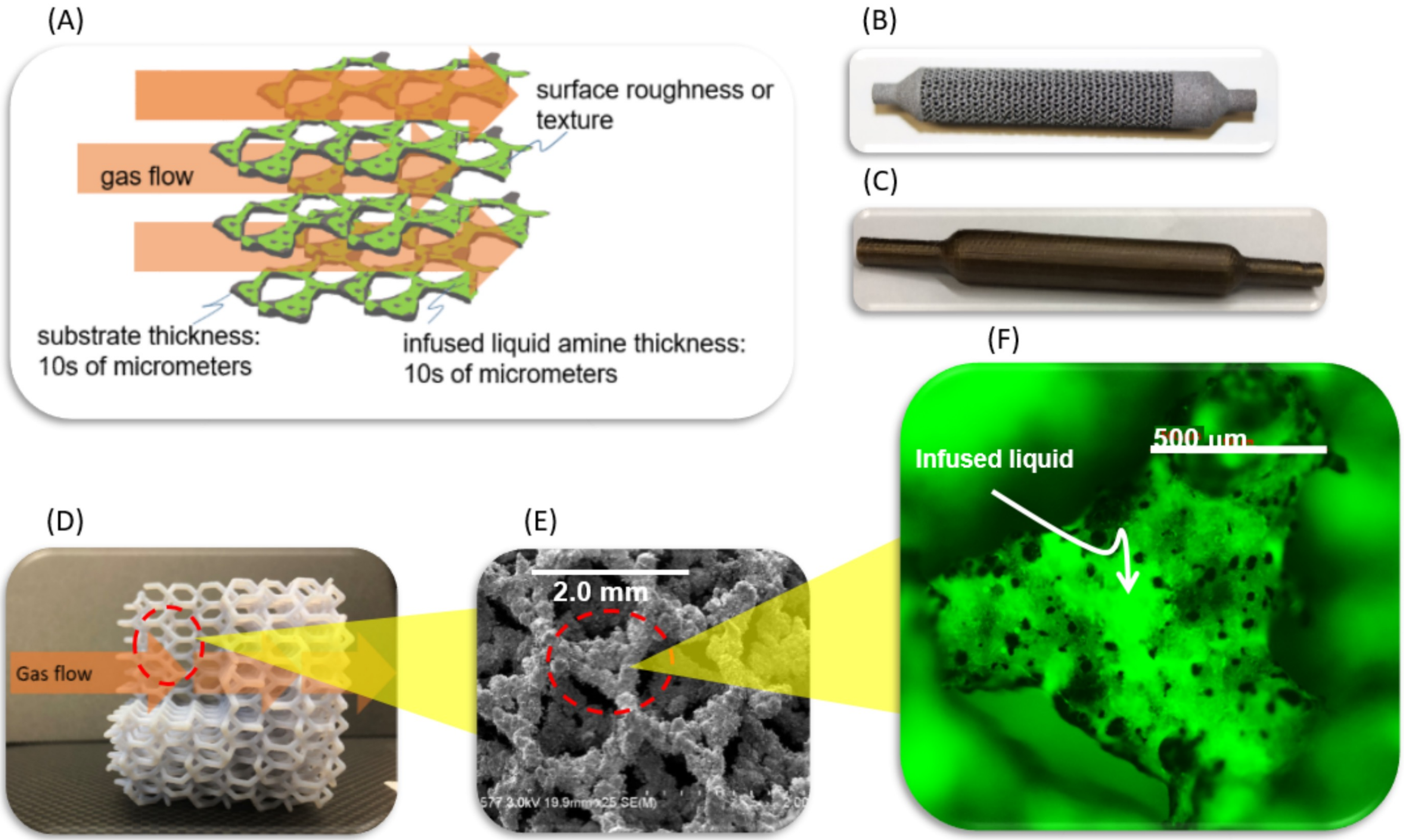
- 3D using D3Q19
- Solid boundaries

Evaporation on Structured Surfaces

Solid with Infused Reactive Liquid

- M. S. Yeganeh et al., Science Advances (2022)

Application: carbon capture



Model

Continuity & Navier Stokes

$$\frac{\partial}{\partial t}(\rho) + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}\mathbf{u}) = -\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot [\mu(\boldsymbol{\nabla}\mathbf{u} + \boldsymbol{\nabla}\mathbf{u}^{\mathrm{T}})] + \mathbf{F},$$

Modified Cahn-Hilliard

As source term

$$\frac{\partial C}{\partial t} + \boldsymbol{\nabla} \cdot (\mathbf{u}C) = \boldsymbol{\nabla} \cdot (M\boldsymbol{\nabla}\mu) \longrightarrow \frac{\partial C}{\partial t} + \boldsymbol{\nabla} \cdot (\mathbf{u}C) = \boldsymbol{\nabla} \cdot (M\boldsymbol{\nabla}\mu) - \boxed{\frac{\dot{m}'''}{\rho_l}}$$

$$\dot{m}'' = \frac{\rho_{\mathrm{g,I}} D}{1 - Y_{\mathrm{v}}} \boldsymbol{\nabla} Y_{\mathrm{v}} \cdot \mathbf{n}. \longrightarrow \dot{m}''' = \frac{\rho_{g,I} D}{1 - Y_v} \nabla Y_v \cdot \nabla C$$

Lee & Liu scheme, JCP (2010)

Advection-Diffusion

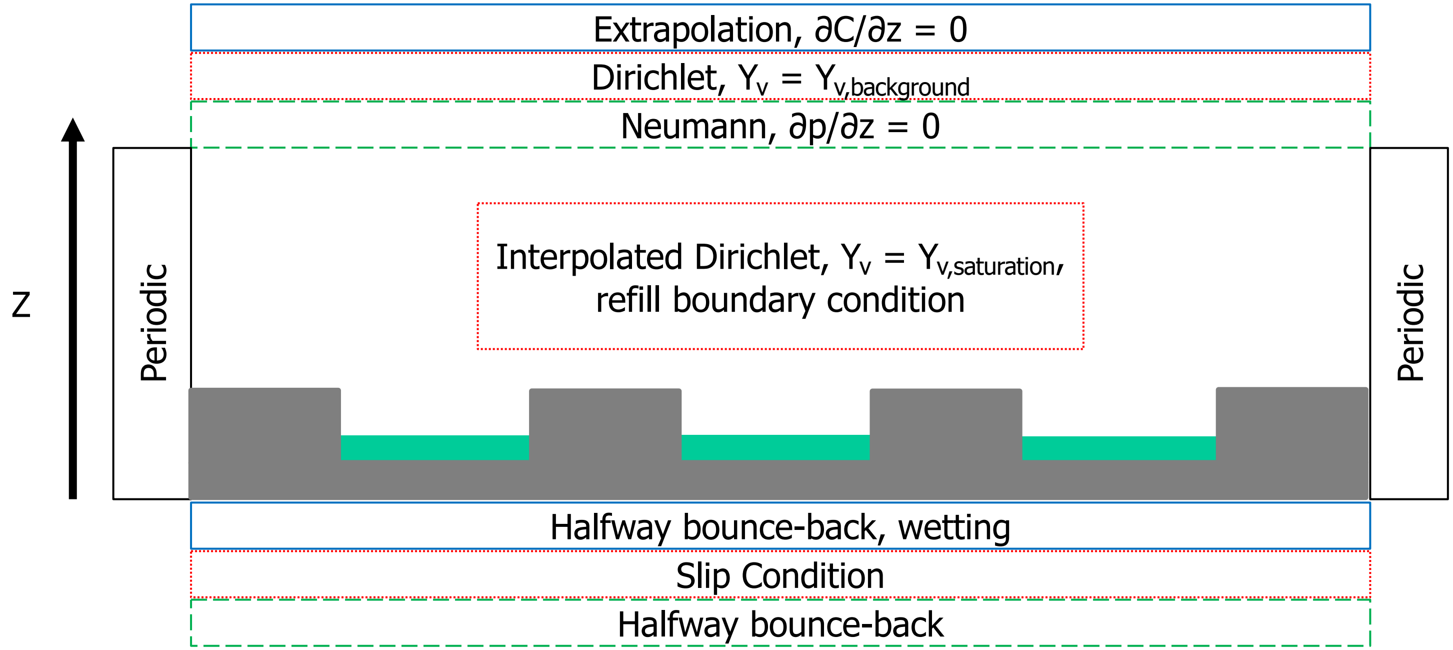
$$\frac{\partial Y_{\mathrm{v}}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} Y_{\mathrm{v}} = \boldsymbol{\nabla} \cdot (D\boldsymbol{\nabla} Y_{\mathrm{v}}). \longrightarrow \text{BGK scheme}$$

Sugimoto et al., Phys. Rev. E 103, 053307 (2021)

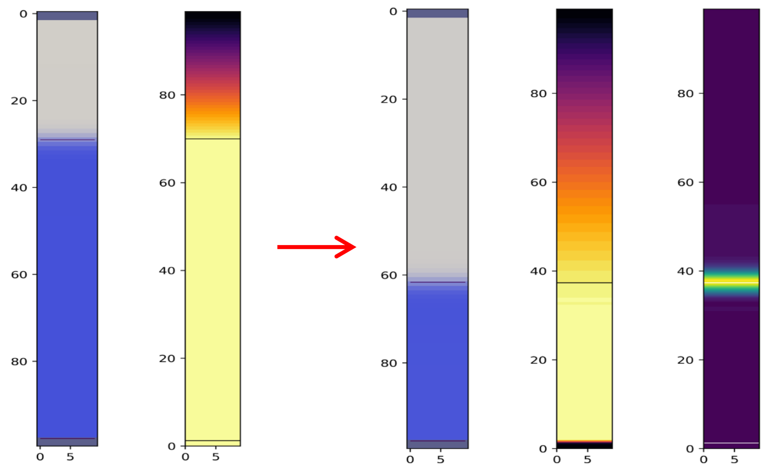
Typical Simulation Setup

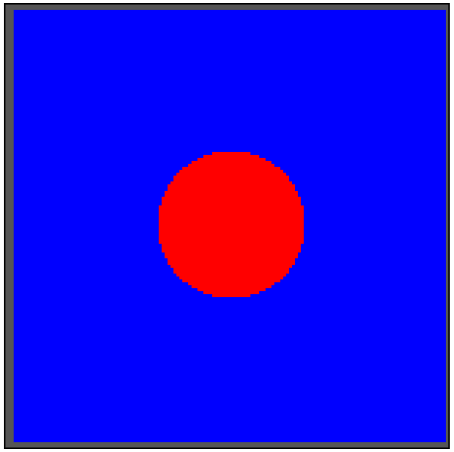
Boundary Conditions

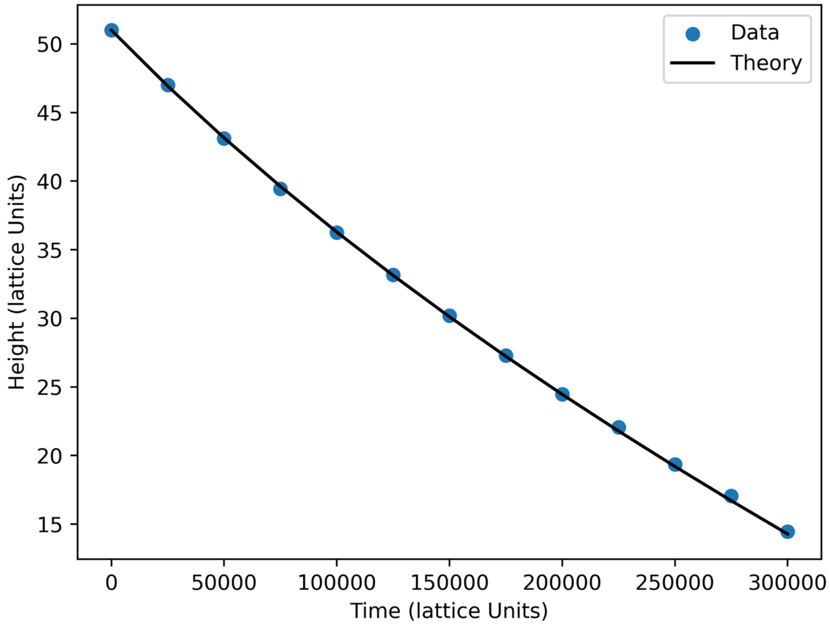
Navier Stokes | Advection-Diffusion for Vapor Concentration | Modified Cahn-Hilliard

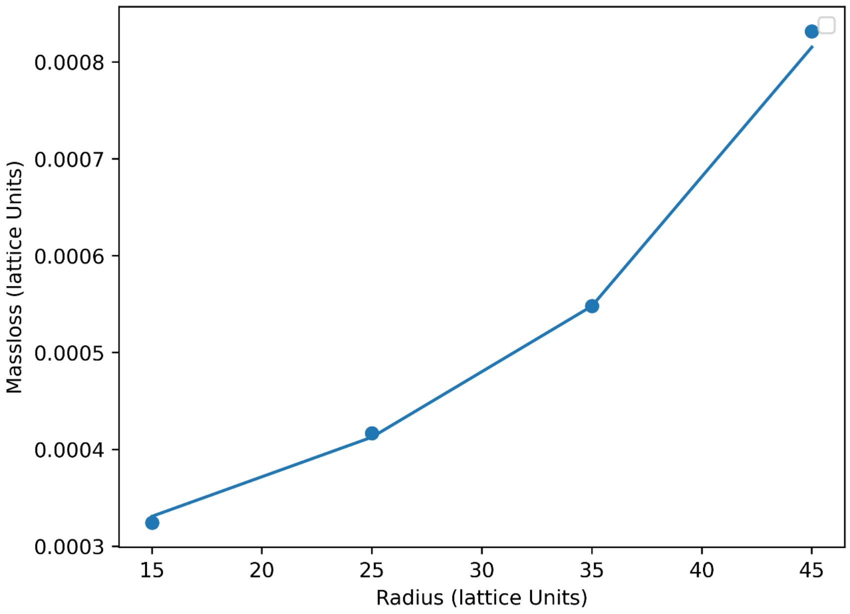


Benchmarks






Data
Theory
Height (lattice Units)
Time (lattice Units)


Massloss (lattice Units)
Radius (lattice Units)

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infineon

P&G

Summary

- LBM is a powerful approach to study complex multiphase and interfacial flows
- Challenge I: N > 2 components. We can capture accurate Neumann angles and Young's contact angles. Applications range from droplet microfluidics, liquid infused surfaces, and phase separation.
- Challenge II: Phase change phenomena (here, focussed on evaporation). We coupled multiphase LBM with humidity evolution. Multiphysics problems with complex boundary conditions.
- Challenge III: Complicated geometries. A different way to capture highly complex solid boundaries?

Thank you for listening!