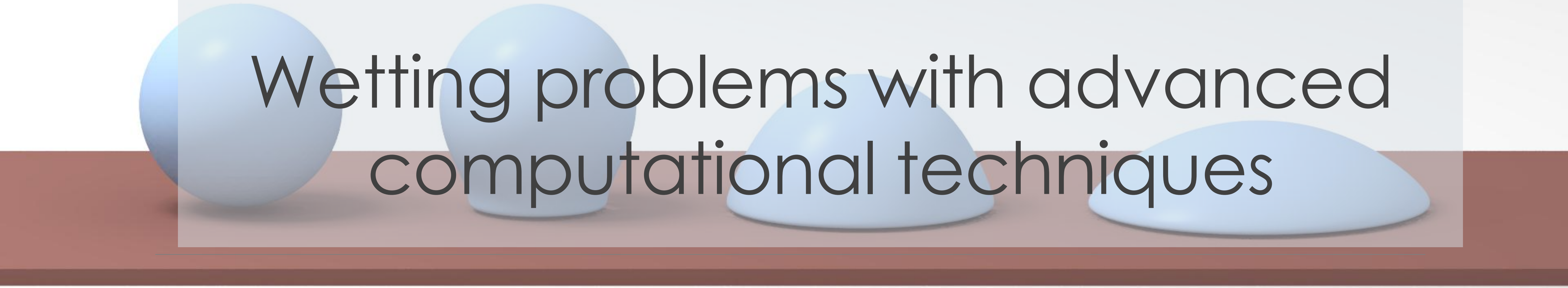
Wetting problems with advanced computational techniques



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Elisa Bellantoni – 39th Cycle

bellanto@roma2.infn.it

Funded by the European Union

AQTIVATE

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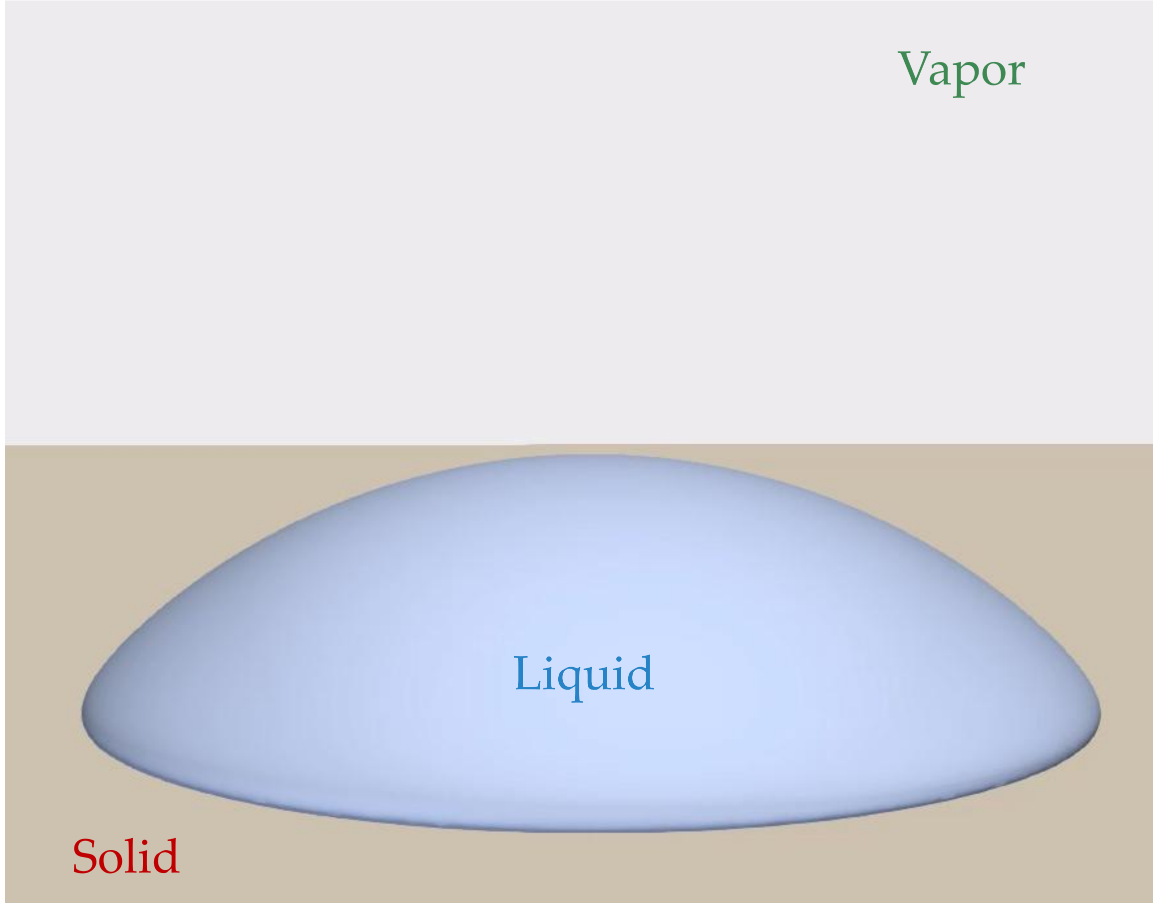
Second-year Overview

- MSCA European Joint Doctorate programme (AQTIVATE, https://aqtivate.ucy.ac.cy/)
- 1st year at The Cyprus Institute
  2nd year at Tor Vergata University of Rome
  3rd year at Télécom Paris
- Paper published on *Physical Review E*
- 3 talks and 2 poster presentations at international conferences & workshops
- Three month secondment at Hewlett-Packard Enterprise HPC/AI EMEA research lab

Talk at the EFDC2 conference
(Dublin, August 2025)

Research project



Spreading of a droplet on a flat surface

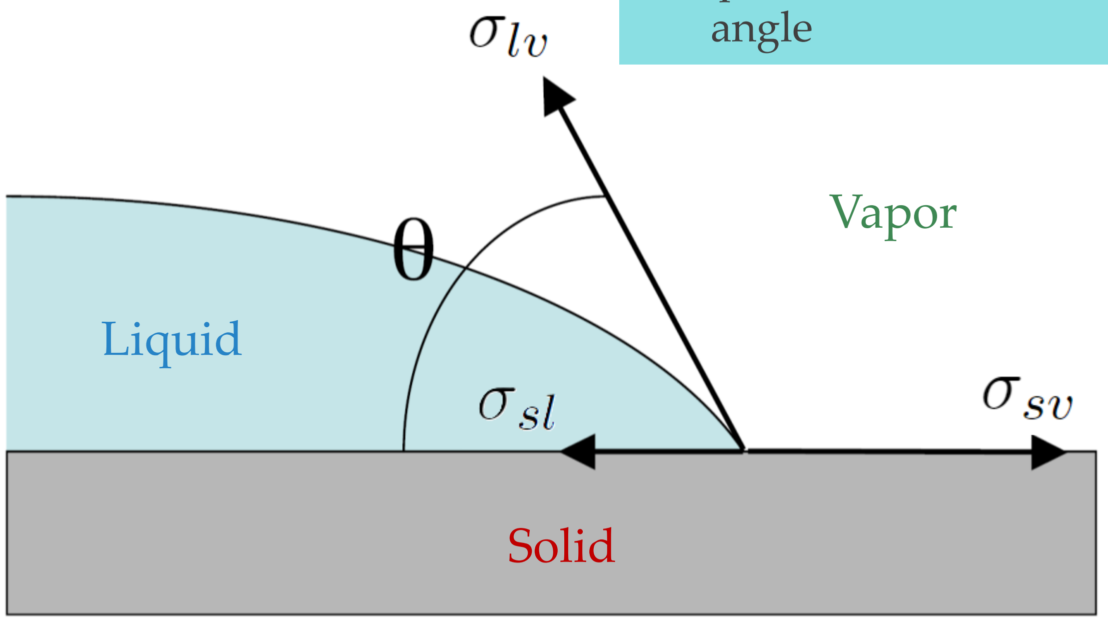
Complex Wetting Problems Using Neural Networks:
Study of complex wetting phenomena using computational fluid dynamics (CFD) simulations + machine learning

We are interested in reproducing results for complex fluid flows and complex interfaces

Multiscale Description

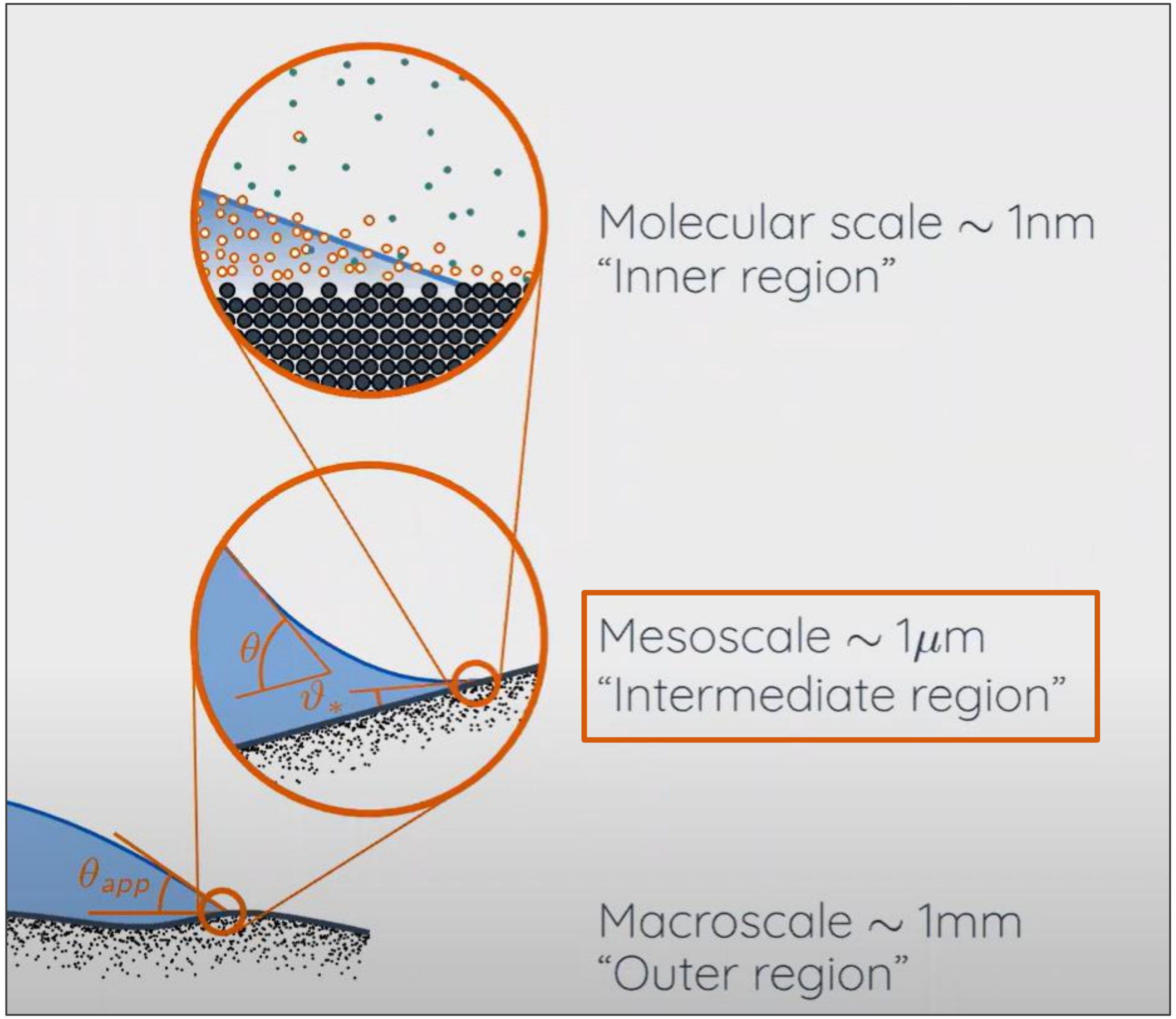
Macroscale:

σ_{ij}:surface tension between phase i and j
θ: equilibrium contact angle



Young's Equation:

$$\sigma_{sv} = \sigma_{sl} + \sigma_{lv} \cos\theta$$



[1] Bonn et al., "Wetting and spreading", 2009 (doi:10.1103/RevModPhys.81.739)

Immersed Boundary Lattice Boltzmann for Wetting Problems

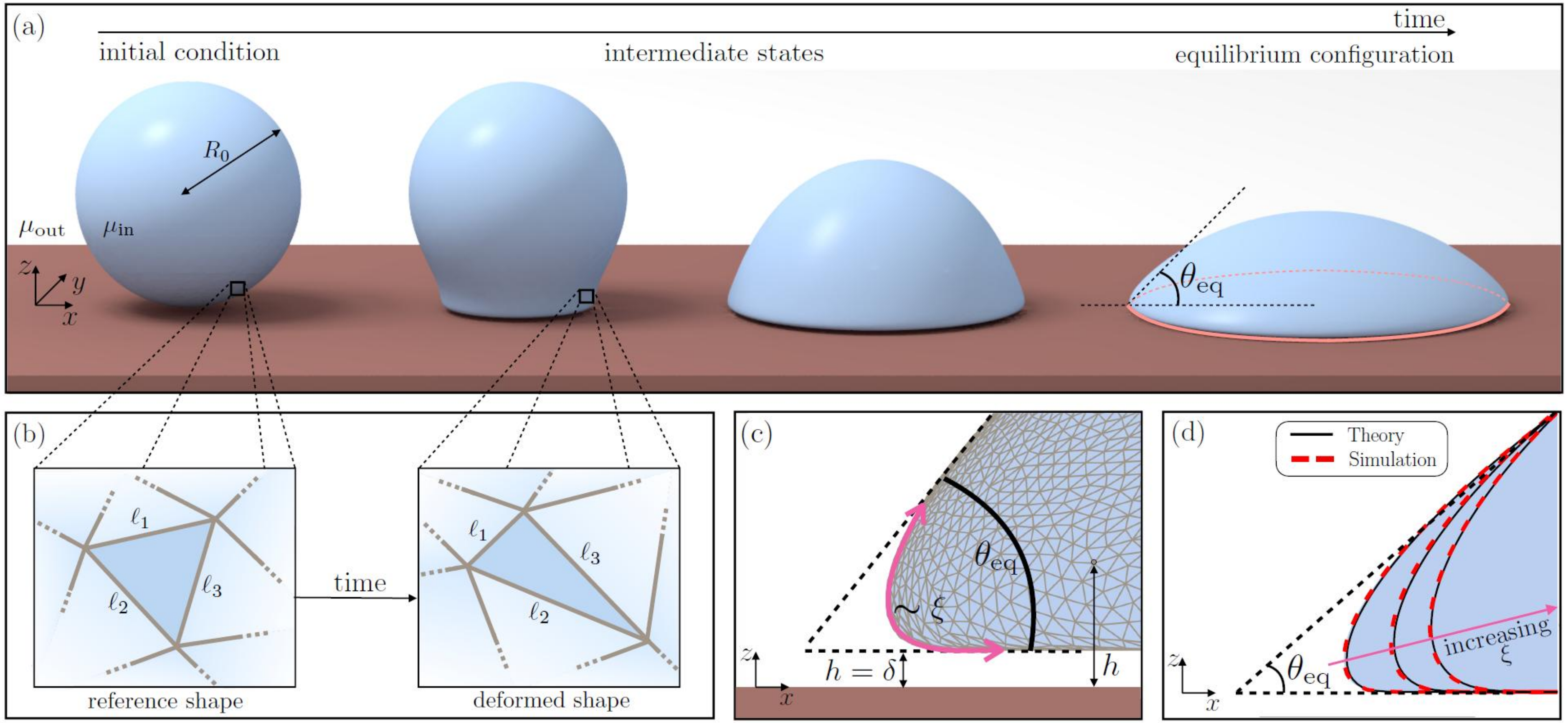
Modeling Wetting

$$A = S_{\text{node}} \frac{\sigma}{\xi} \frac{(m-1)(n-1)}{(n-m)} (1 + \cos\theta_{\text{eq}})$$

Surface tension: $$\boldsymbol{\varphi}^S = -\sigma \left(\boldsymbol{\nabla} \cdot \hat{\boldsymbol{n}} \right) \hat{\boldsymbol{n}}$$

Wetting: $$\boldsymbol{\varphi}^{\text{W}} = -\Pi \, \hat{\boldsymbol{n}} = A \left[\left(\frac{\xi}{h} \right)^n - \left(\frac{\xi}{h} \right)^m \right] \hat{\boldsymbol{n}}$$

Set contact angle a priori

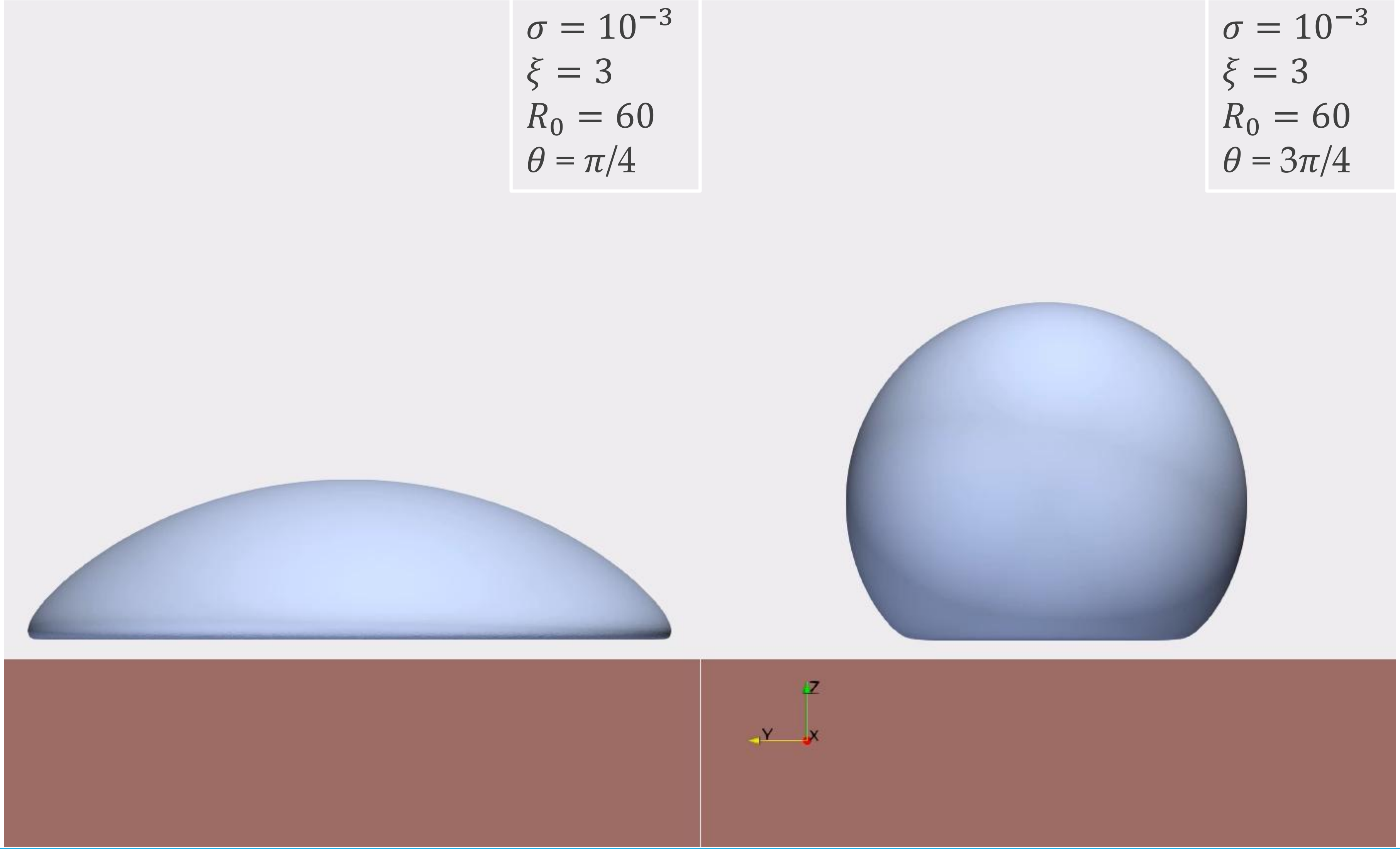


δ: Drop-solid separation
ξ: Wall interaction length

[2] Bellantoni et al., "Immersed boundary--lattice Boltzmann mesoscale method for wetting problems", PRE, 2025 (doi.org/10.1103/mp3p-8j22)

Hydrophilic vs Hydrophobic Droplets

$$\frac{t_f}{(\mu R_0/\sigma)} = 20$$



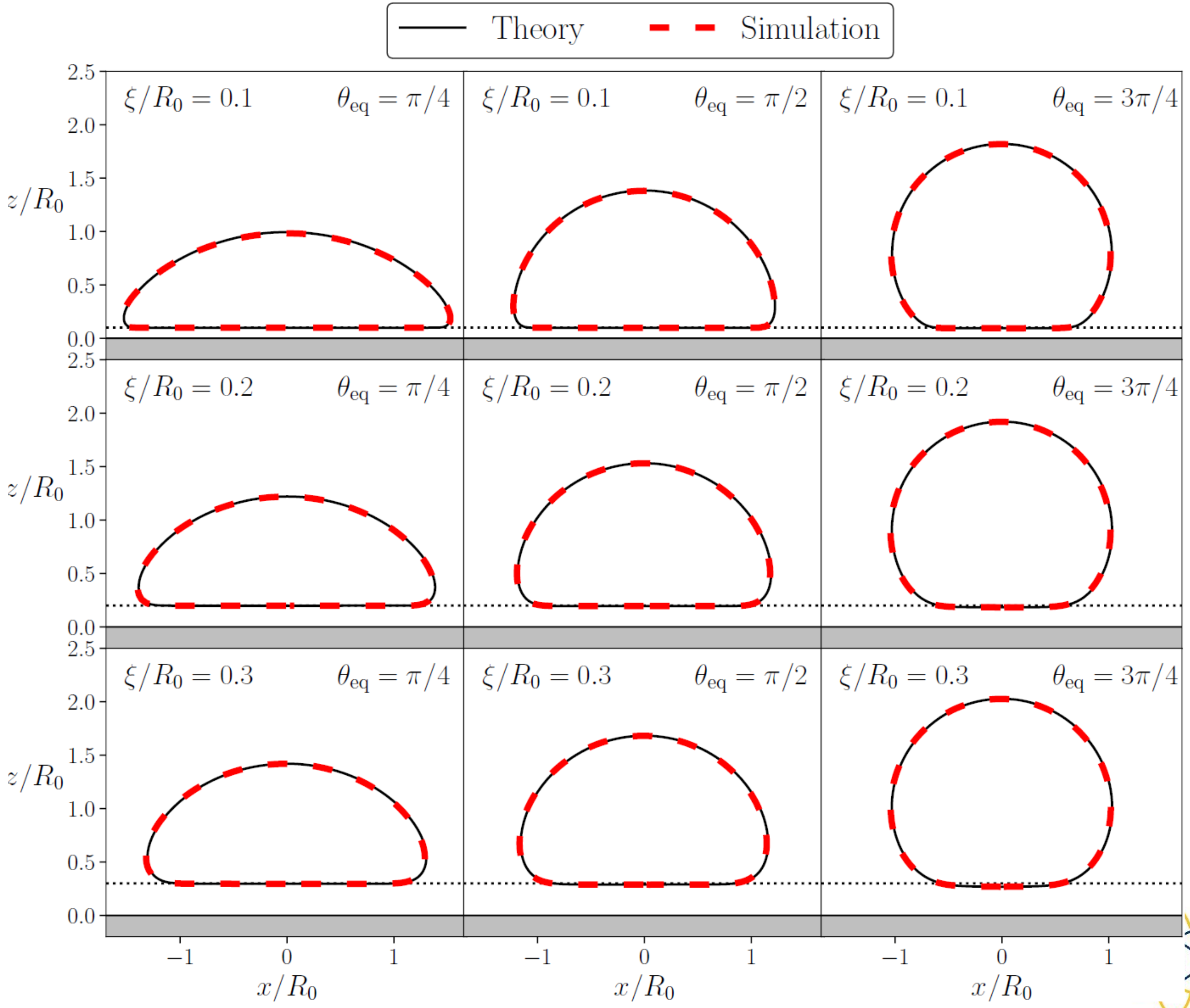
Equilibrium Shape

We consider Young-Laplace equation:

$$\Delta p = \sigma \nabla \cdot \hat{\boldsymbol{n}} + \Pi$$

and derive analytical solutions for droplet shapes at equilibrium

ξ / R_0 has a higher impact on more hydrophilic droplets, i.e. were curvature changes more abruptly



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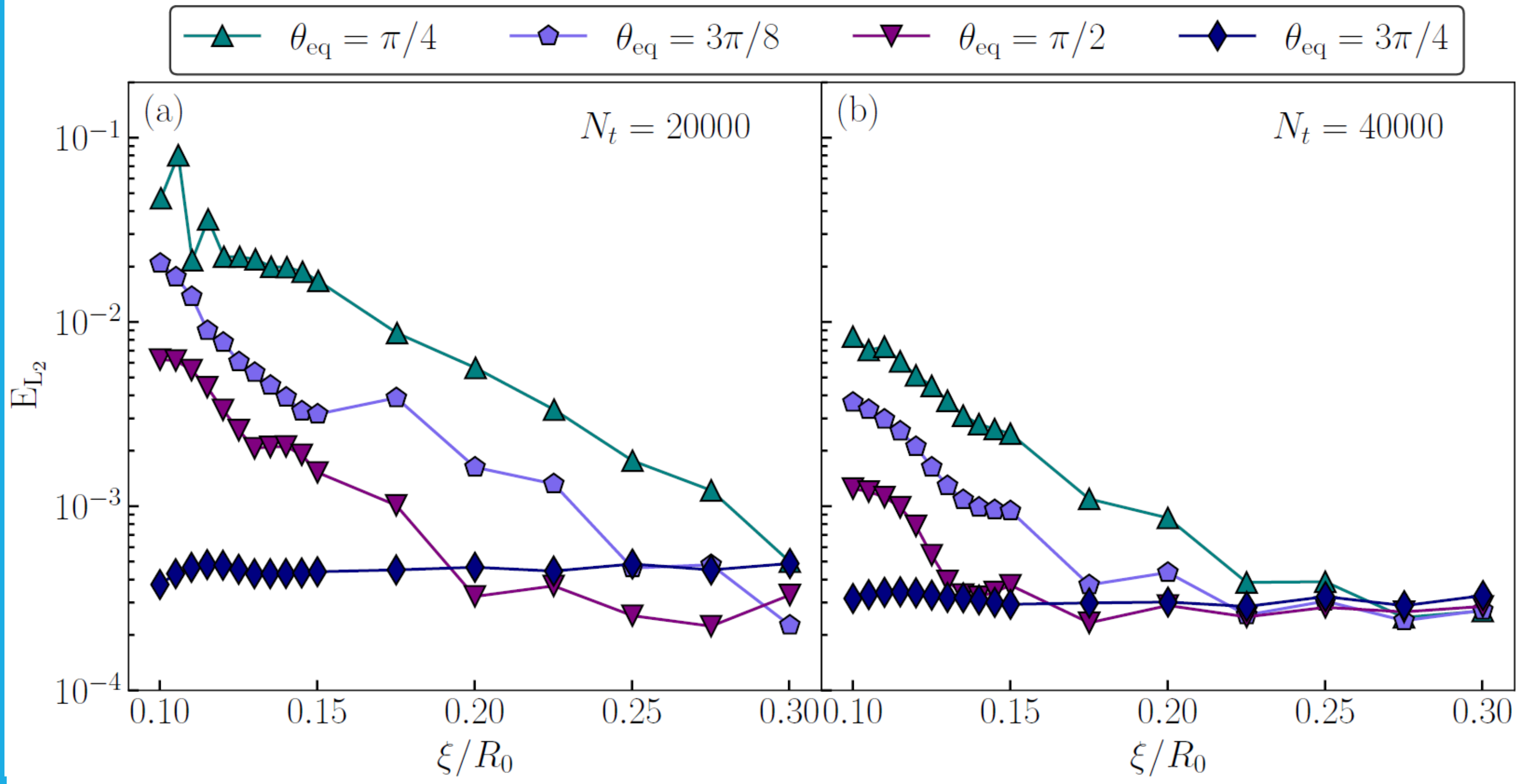
Equilibrium Shape – L2 Error

N_t: #triangles in the mesh
$G(\phi)$: droplet's radial profile

A more quantitative comparison shows very low errors between theoretical and simulated shape for the drop

Reference formula:

$$E_{L2} = \sqrt{\frac{\int_0^\pi |G_{sim}(\phi) - G_{theo}(\phi)|^2 d\phi}{\int_0^\pi |G_{theo}(\phi)|^2 d\phi}}$$



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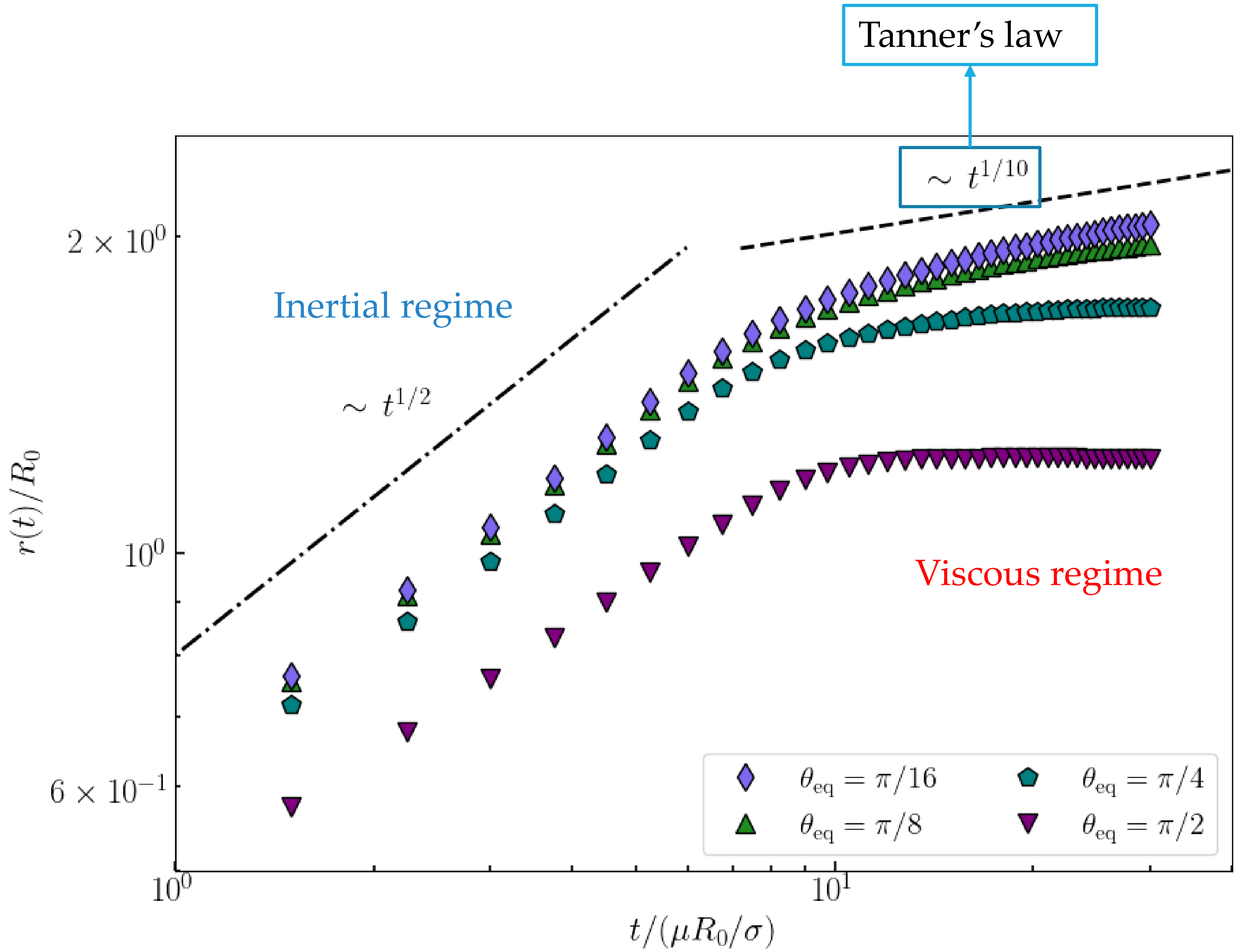
Spreading Dynamics

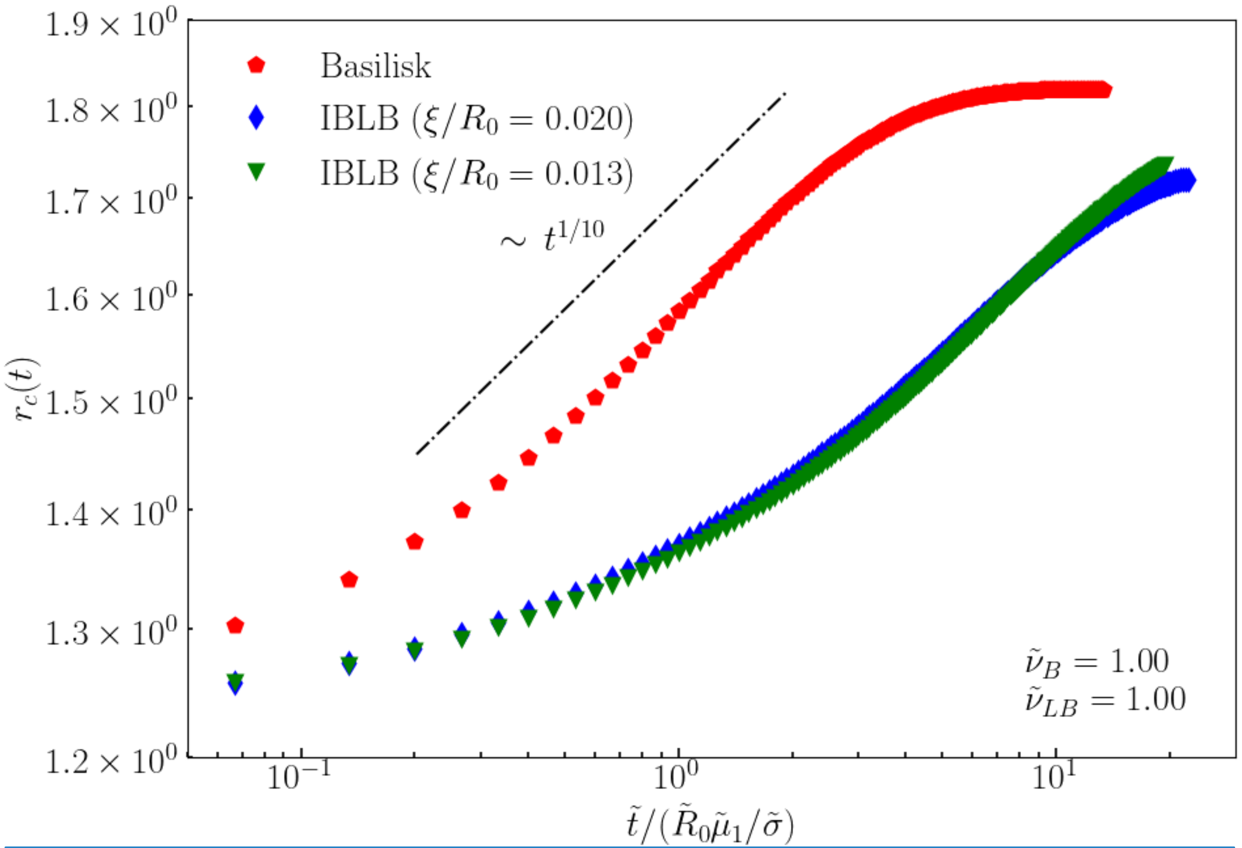
Analytical and experimental studies describe power-law scalings for the contact radius dynamics $r(t)$ in different regimes



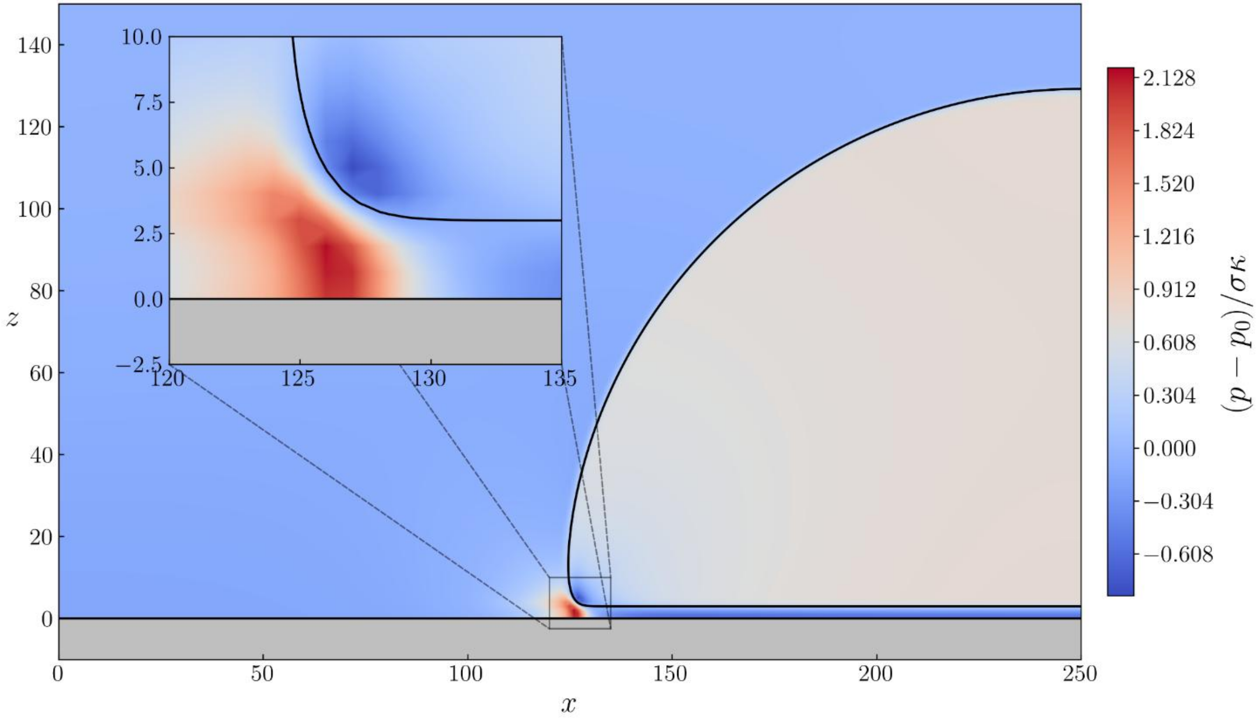
Comparison with other Numerical Methods

Investigating the Thin Film Physics

Our method recovers macroscopic results where no thin film layer between the droplet and the substrate is observed ($\xi/R_0 \ll 1$). **What is the influence of the thin film on spreading?**



Comparison with Basilisk CFD solver (https://basilisk.fr/)

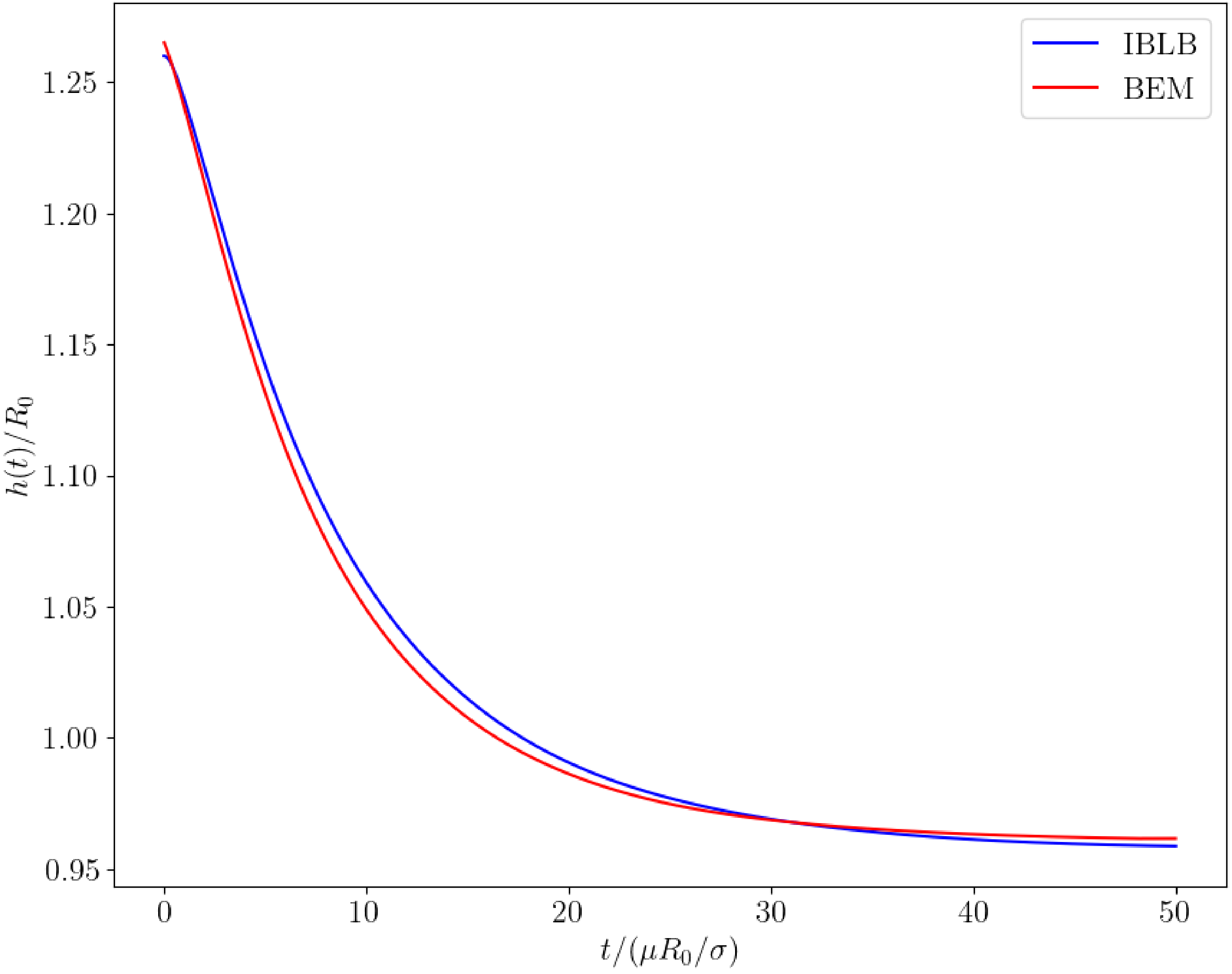


The film causes **drag** due to extra pressure

Comparison with a Stokes' Solver

We are investigating a similar comparison with a boundary element method (BEM) accounting for the presence of a thin film but no inertia (Stokes' flow)

Work in preparation

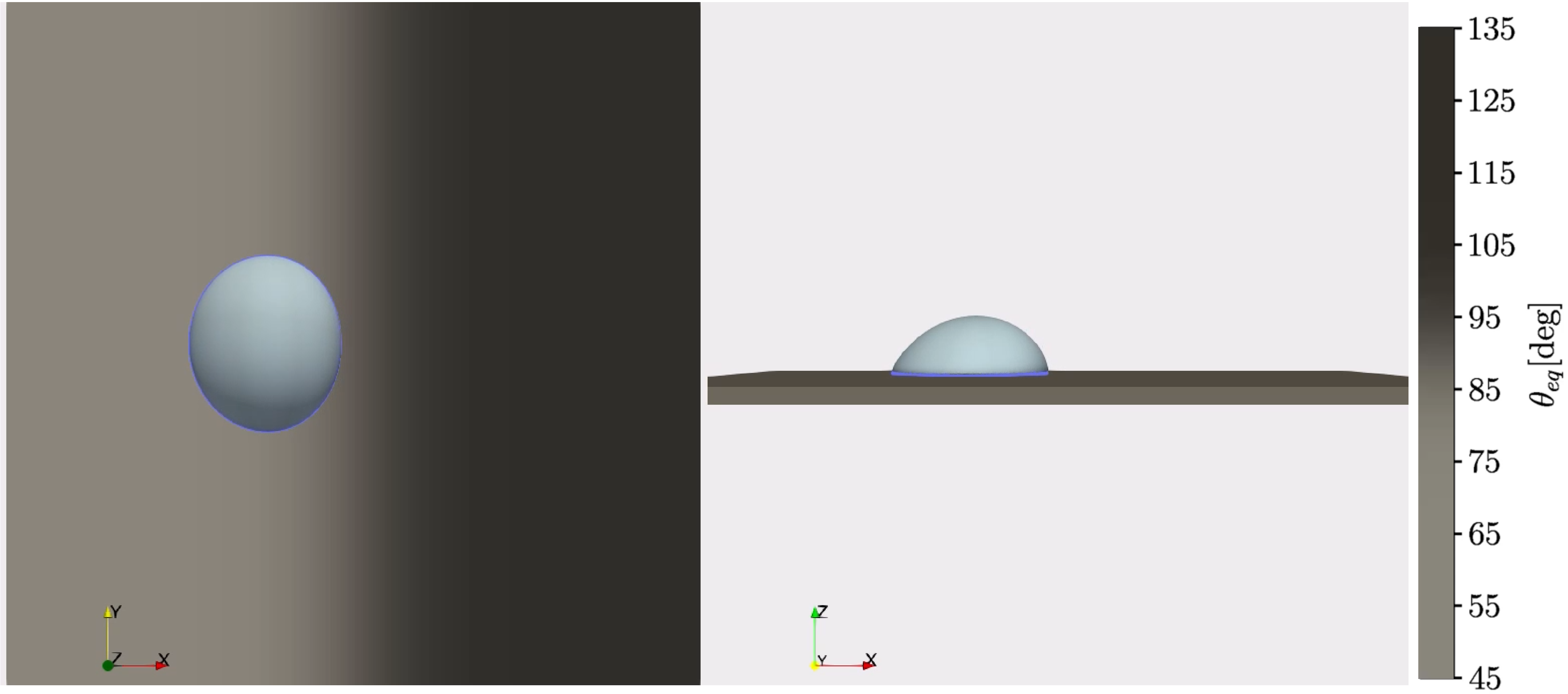


Machine Learning Applications

Current Plan for ML Implementation

1. Generate data with the IBLB
2. Train Neural Network with generated data to learn simple spreading dynamics
3. Introduce complexities in wetting process:
   a) visco-elasticity (interface)
   b) surface heterogeneities (substrate) → straightforward in the IBLB setup
4. Wrap everything together

Chemical Heterogeneity Patterns



Top view

Side view

Proposed Approach

We are putting our focus on a model aimed at predicting the droplet's shape evolution during spreading.

Right now, two routes seem promising:

1. **Input**: $h(t), \lambda, \theta_{\mathrm{eq}}$ (IBLB data)
   Derive a rough estimate of the shape of the drop (e.g. assuming equilibrium config)
   Use AI to correct the dynamics (e.g. LNO architecture or similar neural operator)
   Exploit $\mathrm{d}h/\mathrm{d}t$ as our predictor (e.g. similar to the approach followed in [3])
   Output: full shape evolution

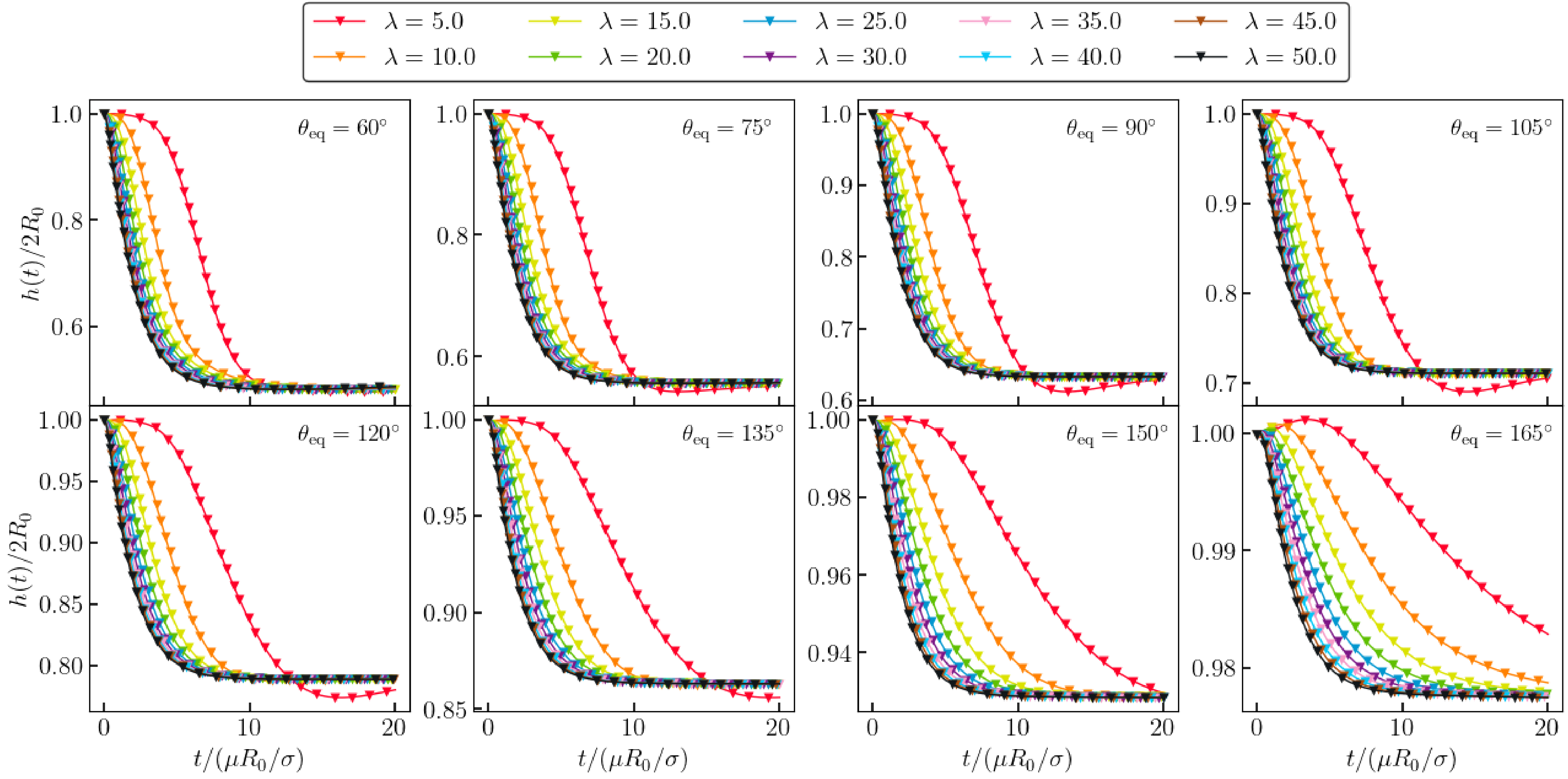
2. **Input**: $h(t), \lambda, \theta_{\mathrm{eq}}$ (IBLB data)
   Take profile shape from simplified, analytical solver (e.g. Stokes flow)
   Train AI model to learn how to add inertia (e.g. transformer or LSTM)
   Output: full shape evolution

Use case: Faster surrogate for wettable surface design, helpful for microfluidics applications

[3] Demou & Savva; "AI-assisted modeling of capillary-driven droplet dynamics", 2023 (doi:10.1017/dce.2023.19)

IBLB-generated dataset

Multiple simulations with a range of viscosities and equilibrium contact angles



Conclusions & Outlook

Conclusions

- Thorough validation of an IBLB method for wetting, published in *Physical Review E*
- Comparison of the method with other solvers
- Several conferences and workshops attended (*Smart-Turb Smart-Heart Workshop, HSR 2025, Droplets 2025, Complex Flows & Complex Fluids Workshop, EFDC2*)
- Strategy for the development of an ML application using IBLB data
- Secondment on the parallel implementation of a lattice Boltzmann code

Outlook for 2025/26

- Wrap up work on thin film role in spreading physics
- Maybe compare IBLB results with MD simulations (separate work)
- Implement and test data-driven tools for complex wetting problems
- Write thesis and prepare for defense (autumn/winter 2026)

Thank you for your attention!

[1] D. Bonn, J. Eggers, J. Indekeu, J. Meunier, E. Rolley; “Wetting and spreading”, *Rev. Mod. Phys.*, vol. 81, p. 739–805, 2009. doi:10.1103/RevModPhys.81.739

[2] **E. Bellantoni**, F. Guglietta, F. Pelusi, M. Desbrun, K. Um, M. Nicolaou, N. Savva, M. Sbragaglia, “Immersed boundary - lattice Boltzmann mesoscale method for wetting problems”, *Physical Review E*, 2025 (doi.org/10.1103/mp3p-8j22)

[3] A. D. Demou & N. Savva; “AI-assisted modeling of capillary-driven droplet dynamics,” *Data-Centric Engineering*, vol. 4, p. e24, 2023. doi:10.1017/dce.2023.19

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AQTIVATE

Conferences & workshops 2025

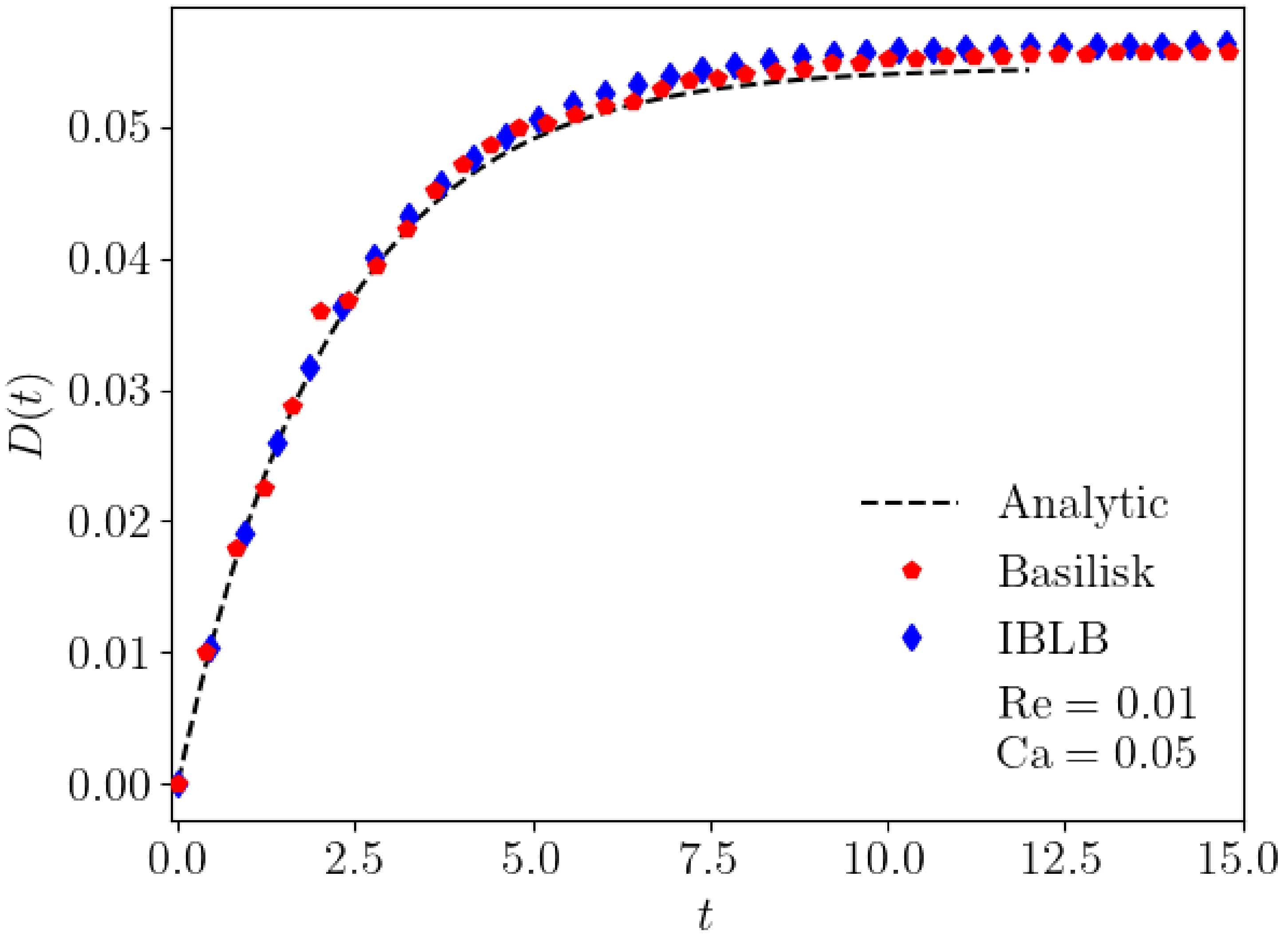
- **Smart-Turb Smart-Heart Workshop**, 19-23 May 2025, in Castro (LE, **Italy**) – III Bilateral Workshop Smart-Turb Smart-Heart organized by Prof. Luca Biferale → **Talk**
- **HSR 2025**, 11-14 June 2025, in Syros (Greece) - 11th International Meeting of the Hellenic Society of Rheology in (https://mathweb.aegean.gr/hsr2025/index.php) → **Talk**
- **Droplets 2025**, 1-3 July 2025, in Liège (Belgium) - 6th International Conference on Droplets (https://droplets2025.org/) → **Poster**
- **Complex Flows & Complex Fluids Workshop**, 8-11 July 2025, Rome (Italy) - Satellite StatPhys29 (https://biferale.web.roma2.infn.it/ComplexFlowsComplexFluids/) → **Poster**
- **EFDC2**, 26-29 August 2025, Dublin (Ireland) - 2nd European Fluid Dynamics Conference (https://www.efdc2.com/) → **Talk**

Basilisk-IBLB: Droplet under Shear

For a free droplet under shear, analytical solutions for the deformation index $D(t)$ are available

Quantity	Basilisk	IBLB
ρ_{in}	4.6×10^{-6}	1.0
λ	1	1
μ_{in}	$0.16\bar{6}$	$0.16\bar{6}$
σ	63.3	0.001
R_0	19	19
Re	0.01	0.01
Ca	0.05	0.05

Report on the comparison available at:
https://www.overleaf.com/8895627552rqddhfxttwqx#08c397



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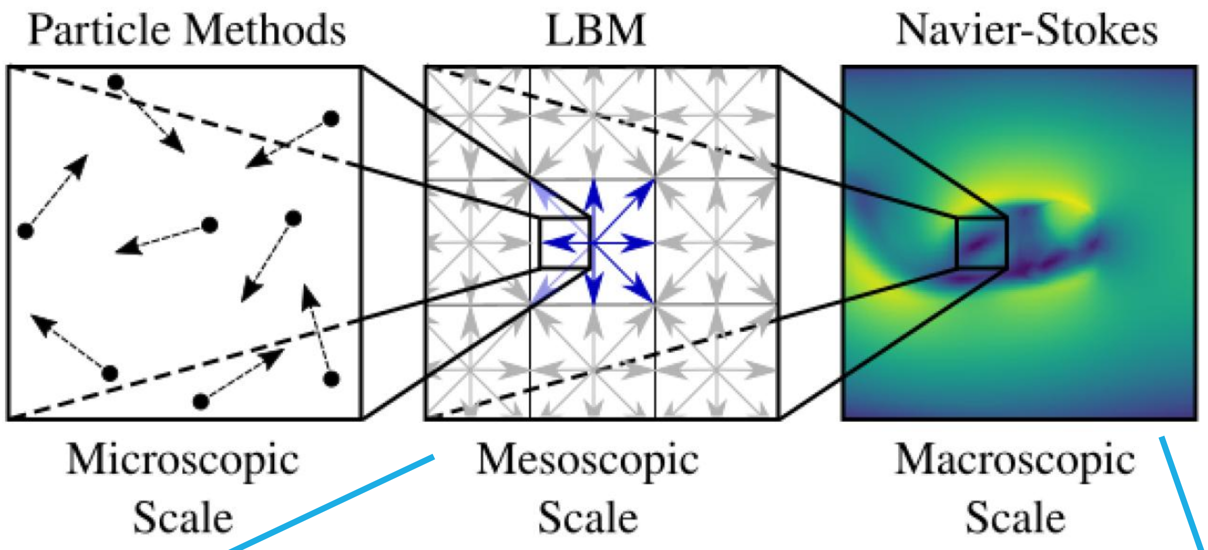
How do we describe the fluids?



ρ: fluid density
$\boldsymbol{u}$: fluid velocity
$\boldsymbol{F}$: body force
μ: fluid viscosity
f: particle distribution function (PDF)
$\boldsymbol{v}$: particle velocity

Boltzmann Equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} f + \frac{1}{\rho}\boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = \Omega[f]$$

Lattice Boltzmann Method

Continuity and NSE:

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

$$\rho \left[\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} \right] = -\boldsymbol{\nabla} p + \mu \nabla^2 \boldsymbol{u} + \boldsymbol{F}$$

Meso to Macro

ω_k: lattice weights
c_s: lattice speed of sound

$$\mathbf{c}_k = \frac{\mathbf{v}_k}{c_s}$$

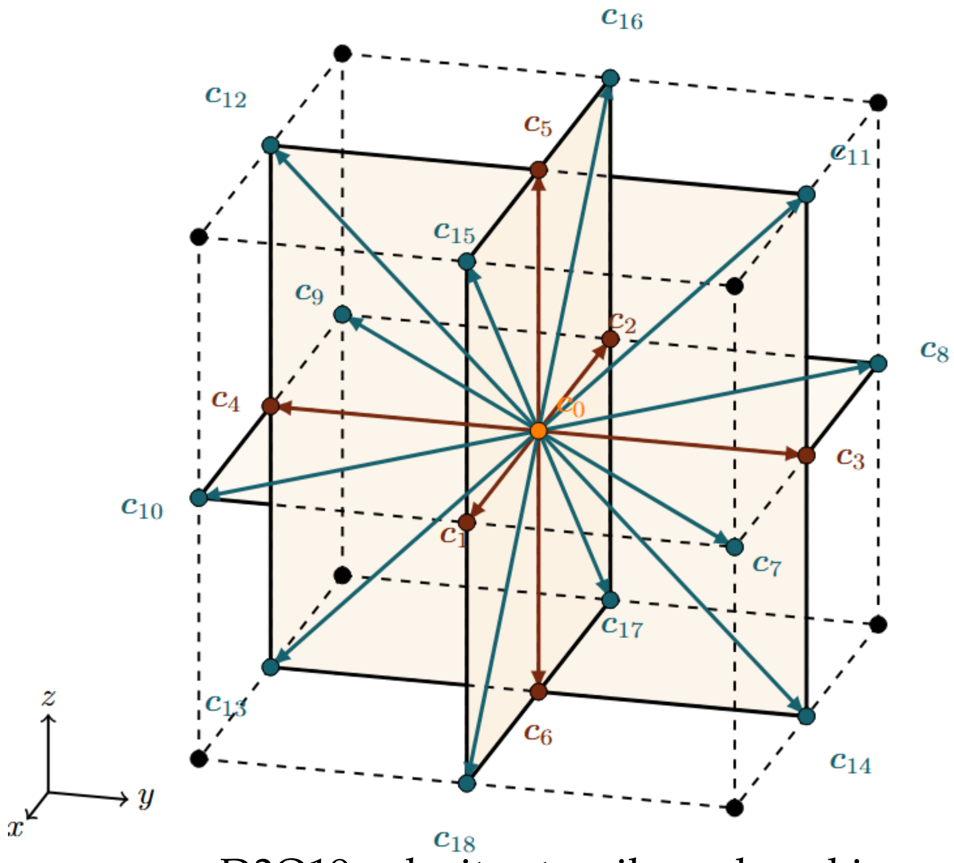
A finite set of velocity vectors suffices to recover the moments of f via a Gauss-Hermite quadrature:

$$\rho(\boldsymbol{x},t) = m\int d\boldsymbol{v} f(\boldsymbol{x},\boldsymbol{v},t) = m\sum_{k=1}^{19} f_k$$

$$\rho(\boldsymbol{x},t)\boldsymbol{u}(\boldsymbol{x},t) = m\int d\boldsymbol{v} f(\boldsymbol{x},\boldsymbol{v},t)\boldsymbol{v} = m\sum_{k=1}^{19} f_k\boldsymbol{v}_k$$

Equilibrium is given by a second-order truncation of the Maxwell-Boltzmann distribution:

$$f_k^{\text{eq}}(\boldsymbol{x},t) = \omega_k\rho\left(1 + \frac{\boldsymbol{u}\cdot\boldsymbol{c}_k}{c_s^2} + \frac{(\boldsymbol{u}\cdot\boldsymbol{c}_k)^2}{2c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right)$$



D3Q19 velocity stencil employed in our model

Lattice Boltzmann Method

Based on the Lattice Boltzmann Equation:

$$f_k(\boldsymbol{x}+\boldsymbol{c}_k\Delta t, t+\Delta t) - f_k(\boldsymbol{x},t) = \Delta t\,[\Omega_k(\boldsymbol{x},t) + S_k(\boldsymbol{x},t)]\ , \qquad k = 1,\ldots,Q$$

Streaming: $f_k(\boldsymbol{x}+\boldsymbol{c}_k\Delta t, t+\Delta t) - f_k(\boldsymbol{x},t)$

Collisions (viscosity): $\Omega_k(\boldsymbol{x},t)$

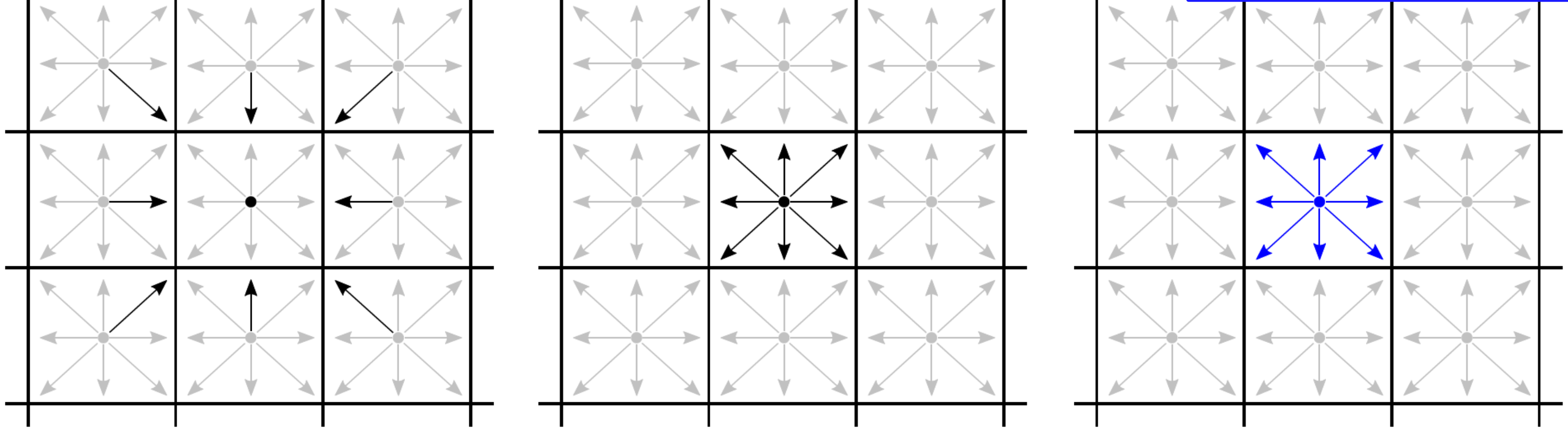
$$-\frac{1}{\tau}\left[f_k(\boldsymbol{x},t) - f_k^{(\mathrm{eq})}(\boldsymbol{x},t)\right]$$

BGK Operator

Source term (surface tension, wetting): $S_k(\boldsymbol{x},t)$

Guo Forcing scheme

$$\left(1-\frac{\Delta t}{2\tau}\right)\omega_i\left[\frac{\boldsymbol{c}_i-\boldsymbol{U}}{c_s^2} + \left(\frac{\boldsymbol{U}\cdot\boldsymbol{c}_i}{c_s^4}\right)\boldsymbol{c}_i\right]\cdot\boldsymbol{F}$$



Q: # velocity vectors
δt: time step size
τ: relaxation time
f^{eq}: equilibrium distr.

How do we describe the droplet?

Two reference frames:

- $\mathbf{x}$: Eulerian nodes (fluid nodes)
- $\mathbf{r}(t)$: Lagrangian nodes (boundary markers)

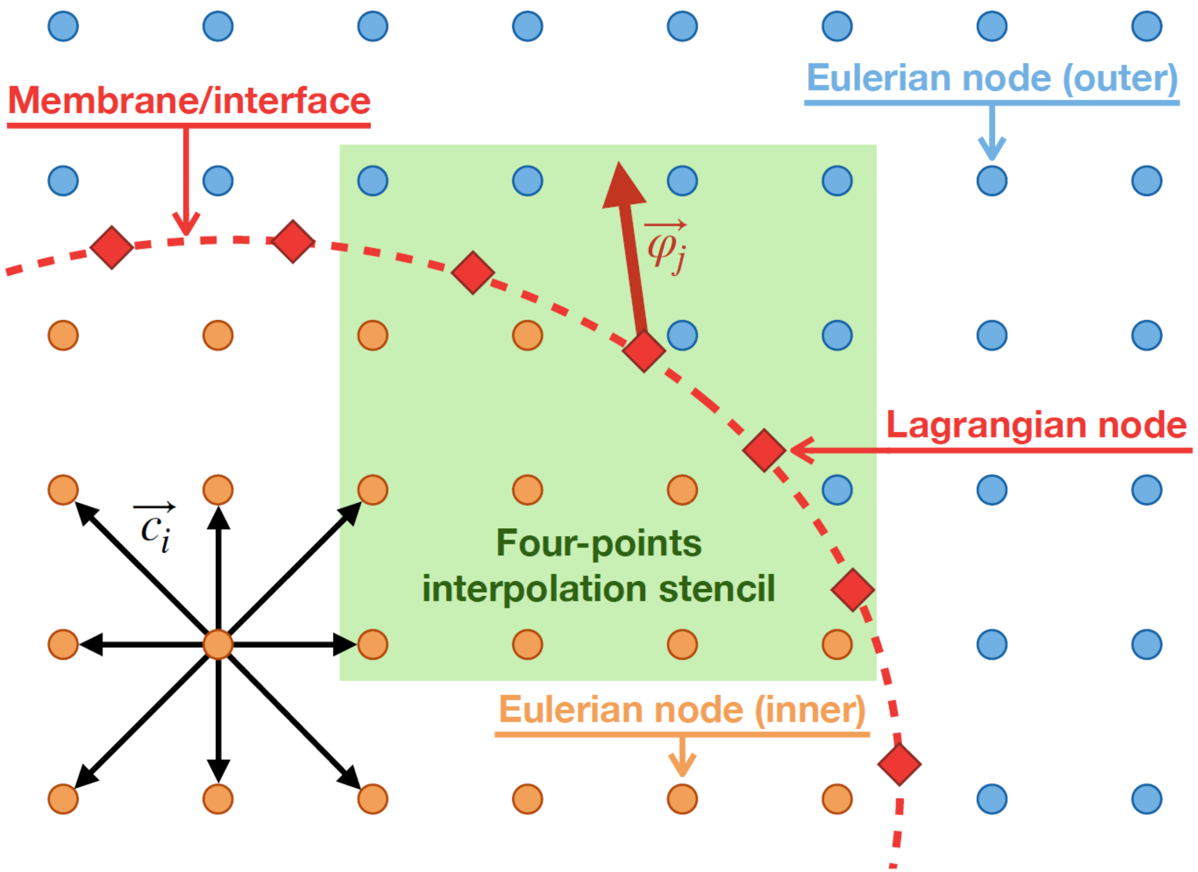
Two-way coupling via **no-slip** boundary condition (velocity interpolation):

$$\dot{\mathbf{r}}(t) = \mathbf{u}(\mathbf{r}(t), t) = \int \mathrm{d}^3x\, \mathbf{u}(\mathbf{x}, t)\delta(\mathbf{x} - \mathbf{r}(t))$$

and interface-fluid momentum exchange (force spreading):

$$\mathbf{F}(\mathbf{x}, t) = \int \mathrm{d}^2r\, \boldsymbol{\varphi}(\mathbf{r}, t)\delta(\mathbf{x} - \mathbf{r}(t))$$

Fluid force ($\mathbf{F}(\mathbf{x}, t)$) — Marker force ($\boldsymbol{\varphi}(\mathbf{r}, t)$)



Immersed boundary lattice Boltzmann [2]

[2] Guglietta, *Mesoscale investigations on the effects of membrane viscosity on transient red blood cell dynamics*, 2022 (doi:10.18154/RWTH-2022-05231)