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Wetting Problems Using Advanced Mesoscale Modeling

AQTIVATE Conference

01-Oct-2026

Funded by the European Union

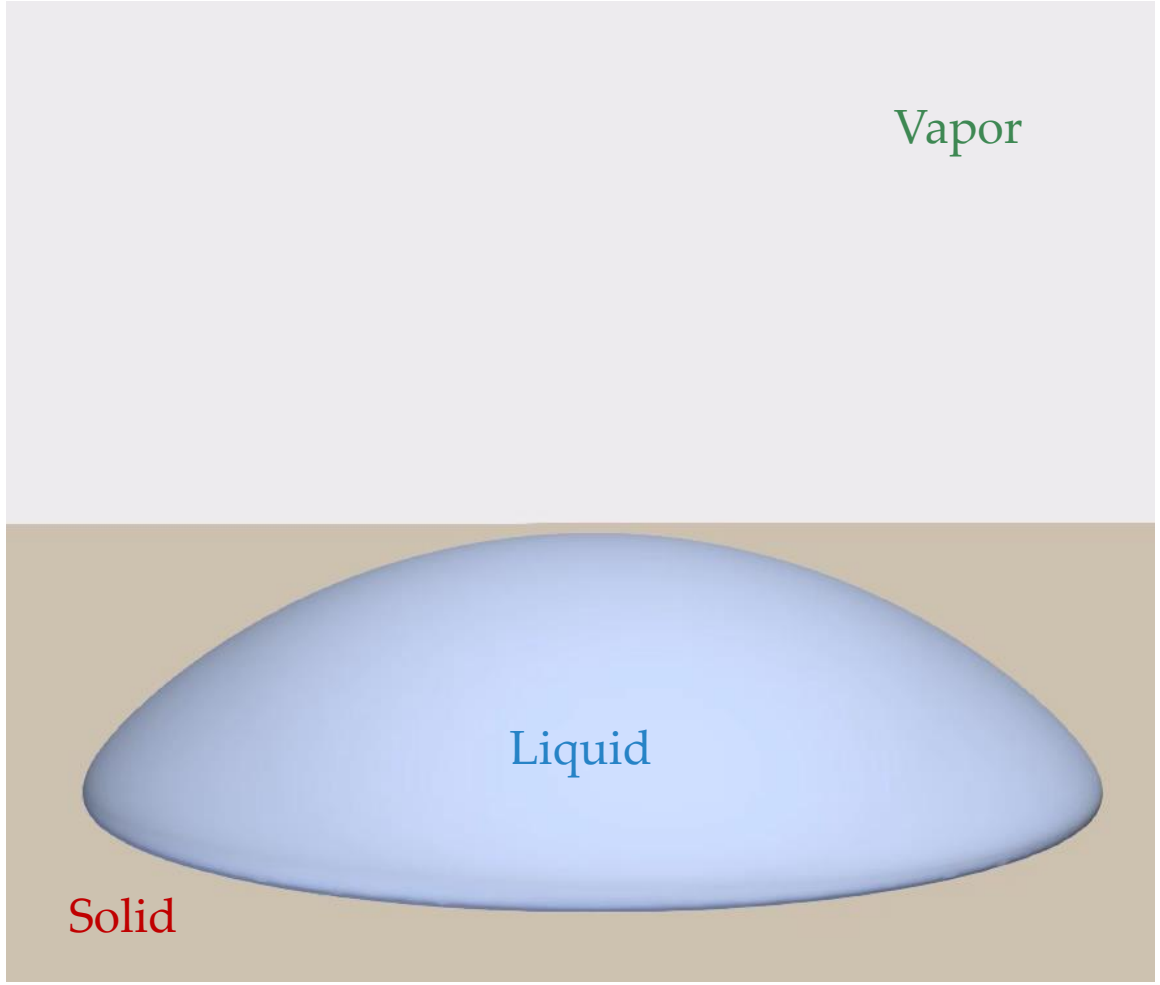
AQTIVATE

AQTIVATE has received funding from the European Union's research and innovation programme under the Marie Skłodowska-Curie Doctoral Networks action and Grant Agreement No 101072344.

Wetting: a Complex Problem

The interaction between a droplet and a solid is a complex multiscale problem involving multiple phases relevant to many industrial processes like coating, inkjet printing, microfluidics, biology, …

To tackle it, we employ numerical simulations and reproduce droplet statics configuration and spreading using a mesoscale, sharp interface approach



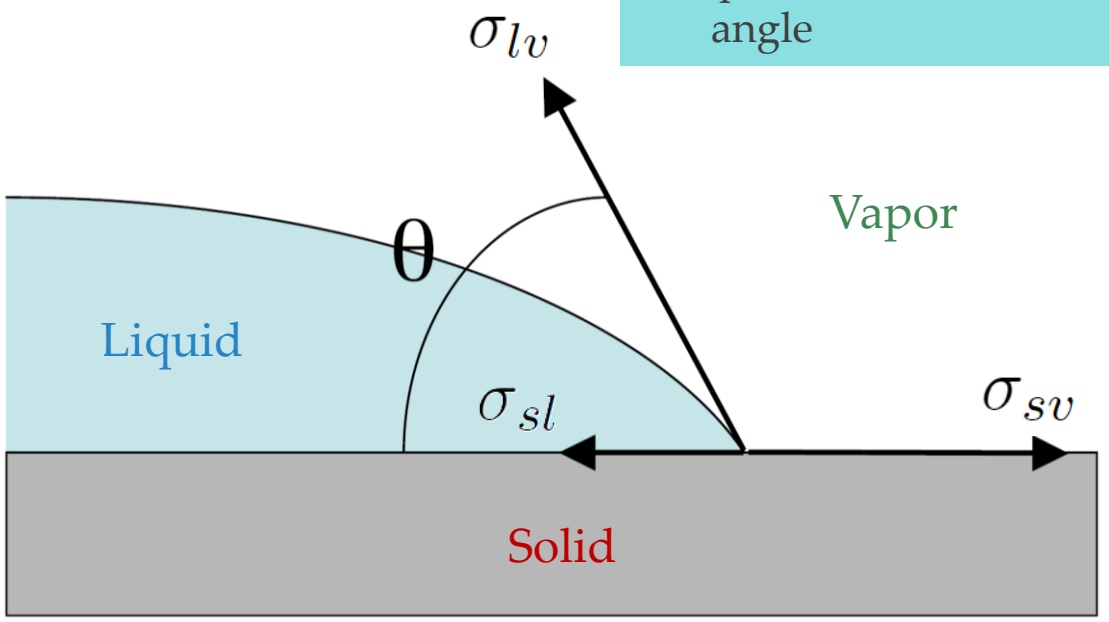
Spreading of a droplet on a solid surface using the IBLB method

Why is Wetting Complex?

Macroscale:

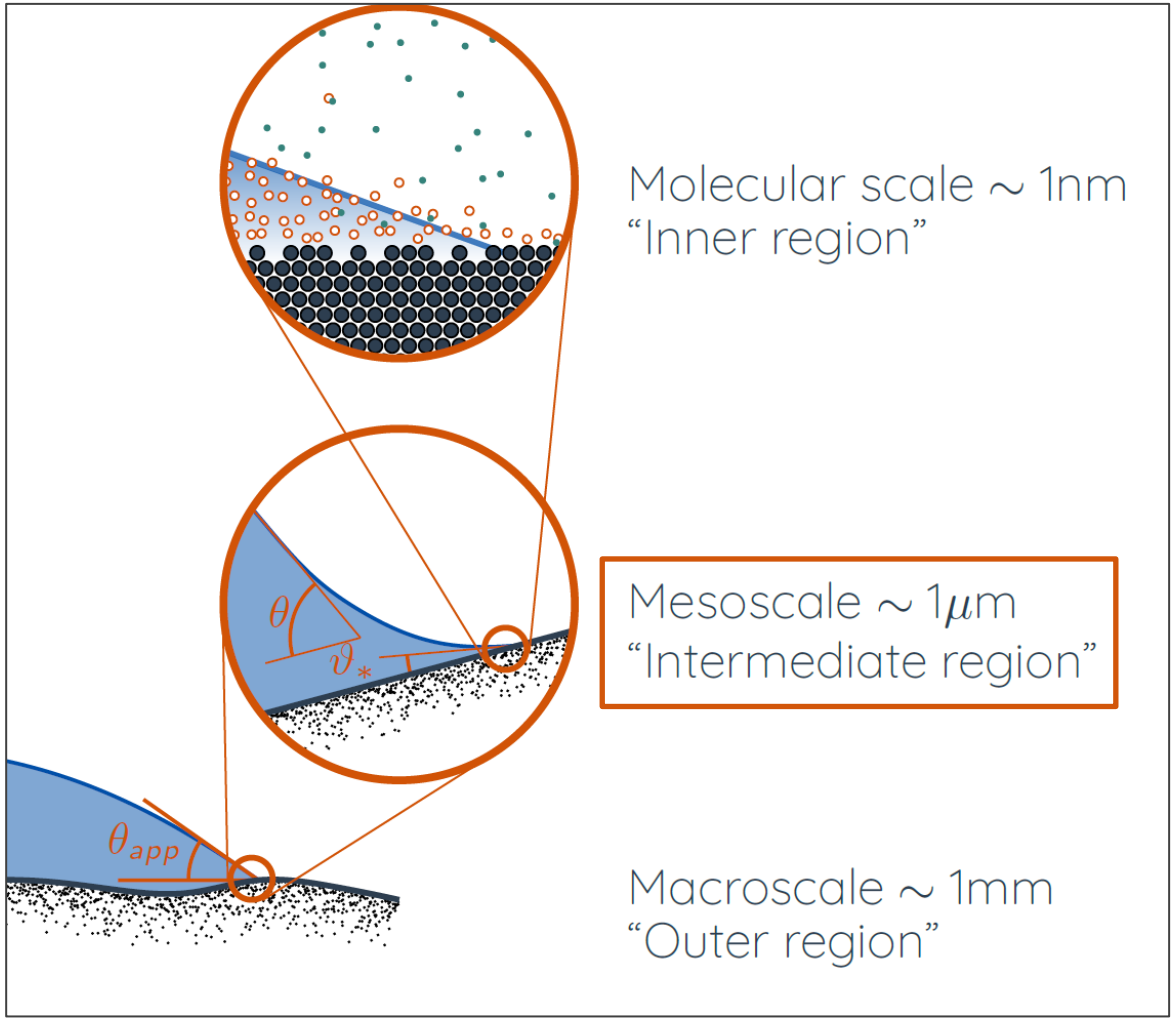
σ_{ij}:surface tension between phase i and j

θ: equilibrium contact angle



Young's Equation:

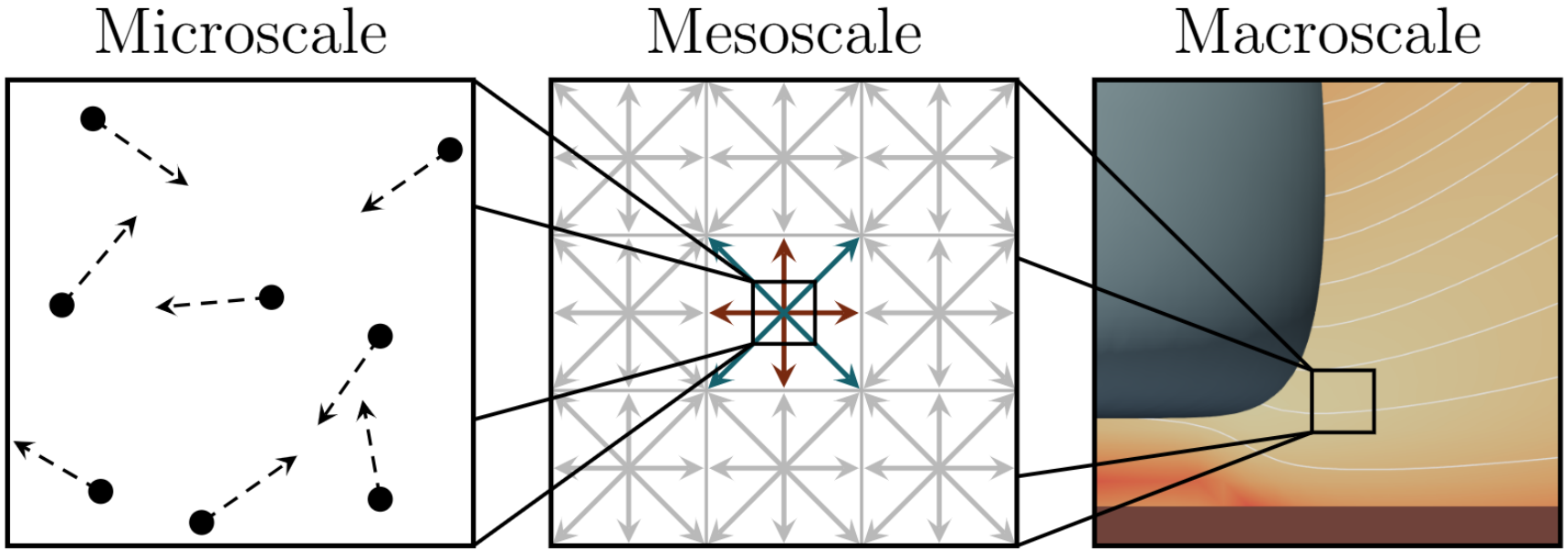
$$\sigma_{sv} = \sigma_{sl} + \sigma_{lv}\cos\theta$$



[1] Bonn D., Eggers J., Indekeu J., Meunier J. and Rolley E., *Rev. Mod. Phys.*, 81 (2009) 739

Immersed Boundary Lattice Boltzmann for Wetting Problems

LBM: Mesoscopic Fluid Description



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

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

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

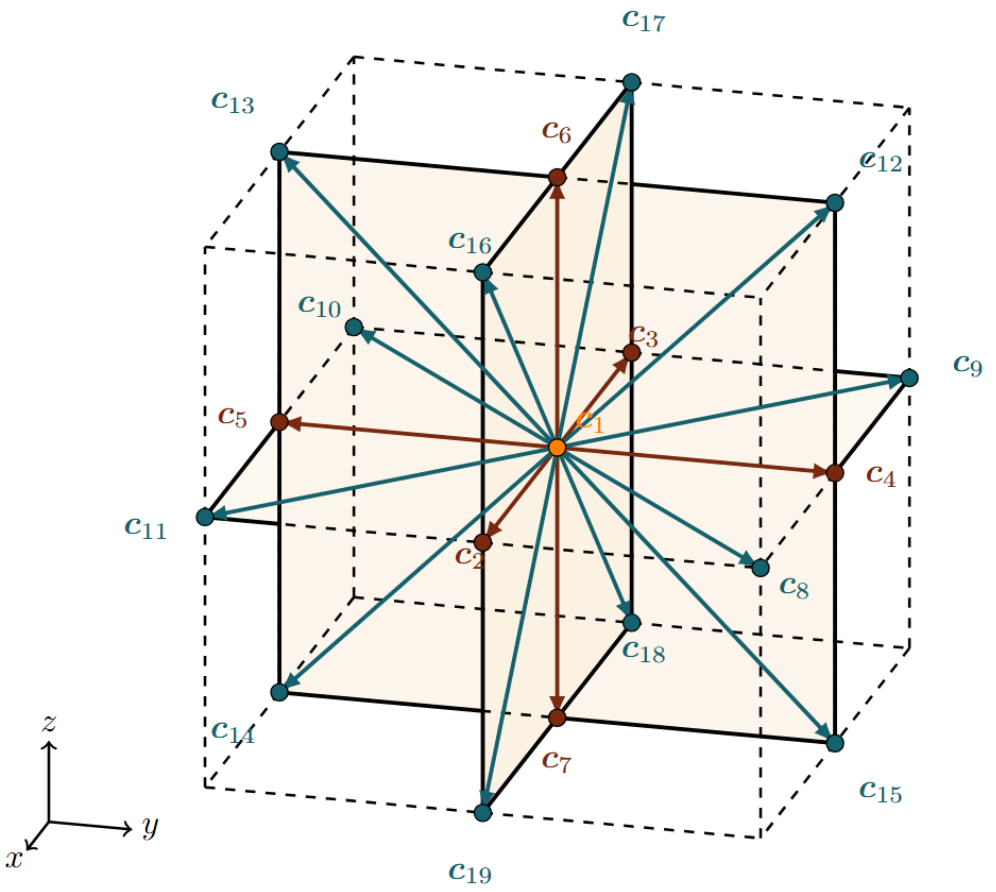
The macroscopic variables are recovered exactly as the moments of f via a **Gauss-Hermite quadrature**:

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

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

Equilibrium is given by a second-order truncation of the **Maxwell-Boltzmann distribution** in Hermite polynomials:

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



D3Q19 velocity stencil employed in our model

Lattice Boltzmann Equation

Discretizing time, coordinate and velocity space, we get:

Streaming

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

Collisions (viscosity)

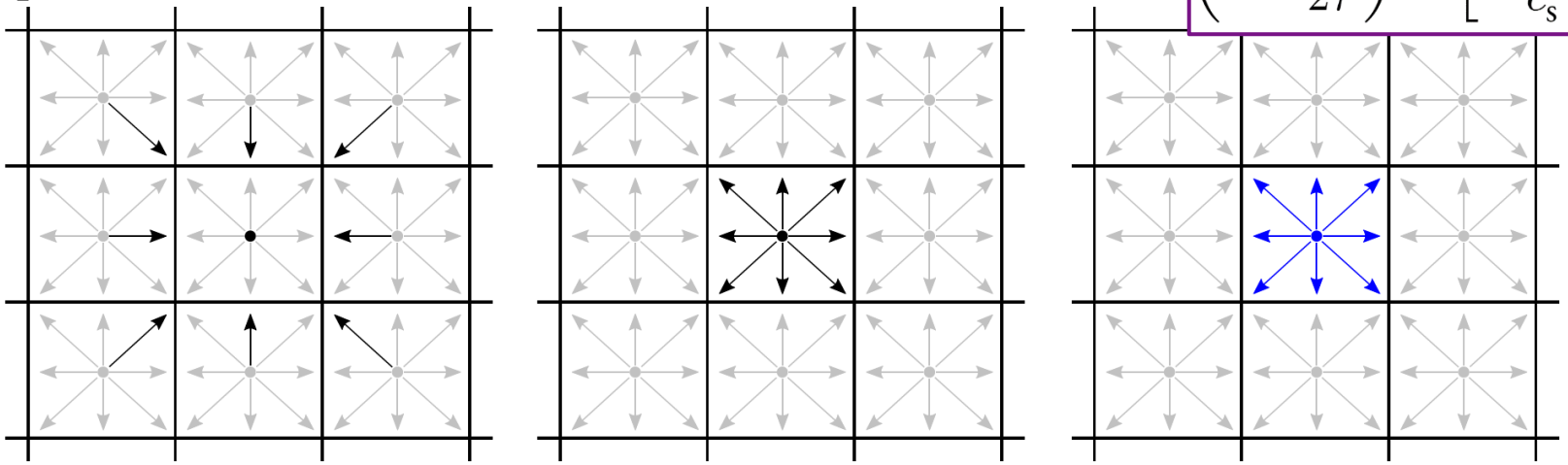
$$-\frac{1}{\tau}\left[f_k(\boldsymbol{x},t) - f_k^{(\mathrm{eq})}(\boldsymbol{x},t)\right]$$

BGK Operator

Source term (surface tension, wetting)

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.

Notice: the representation on the side is 2D for visualization purposes, **our model is fully 3D**

IBLB: Coupling Interface and Fluid

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):

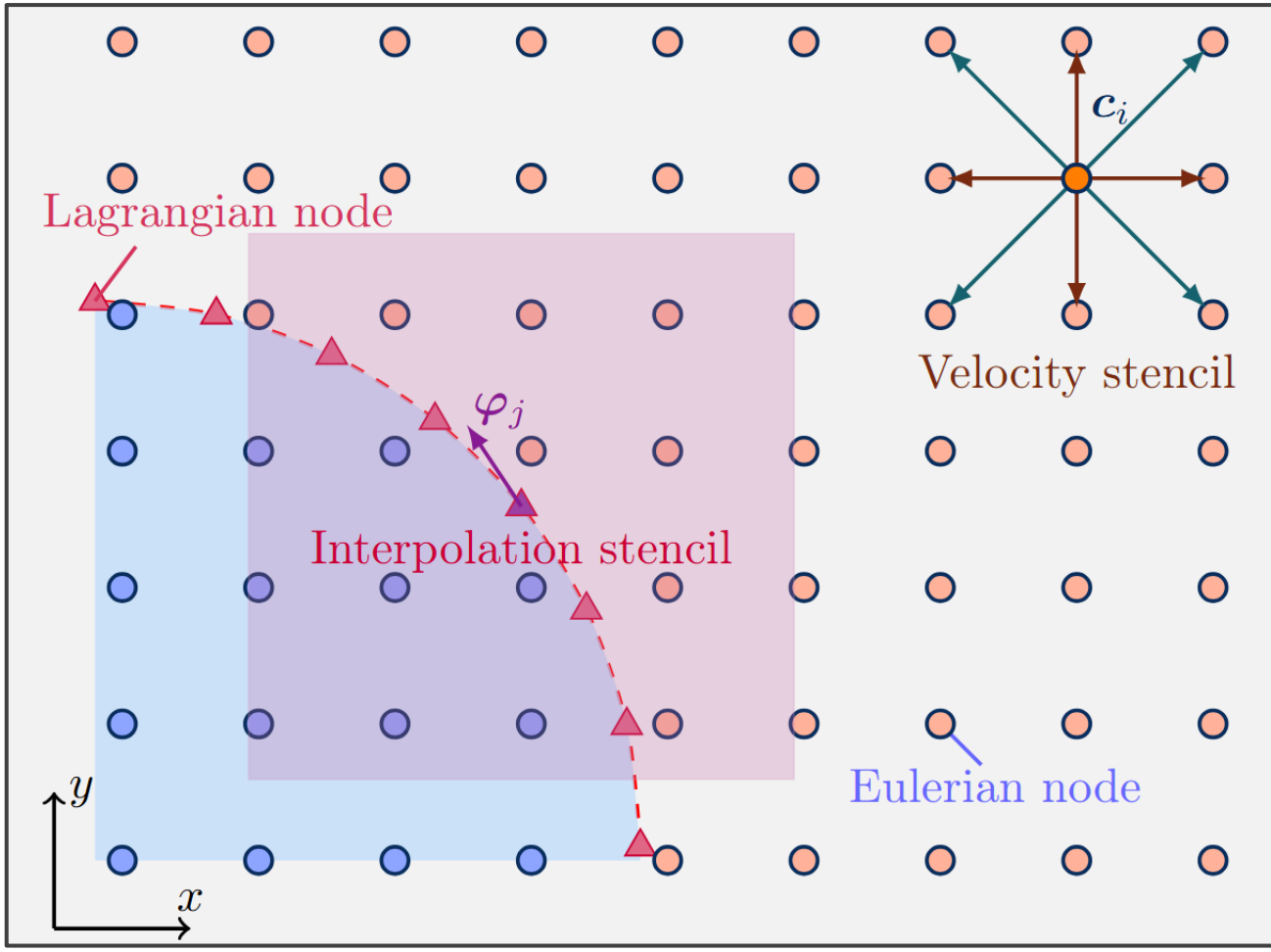
$$\dot{\boldsymbol{r}}(t) = \boldsymbol{u}(\boldsymbol{r}(t), t) = \int \mathrm{d}^3 x \, \boldsymbol{u}(\boldsymbol{x}, t) \delta(\boldsymbol{x} - \boldsymbol{r}(t))$$

and interface-fluid momentum exchange (force spreading):

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

Fluid force

Marker force



Immersed boundary lattice Boltzmann

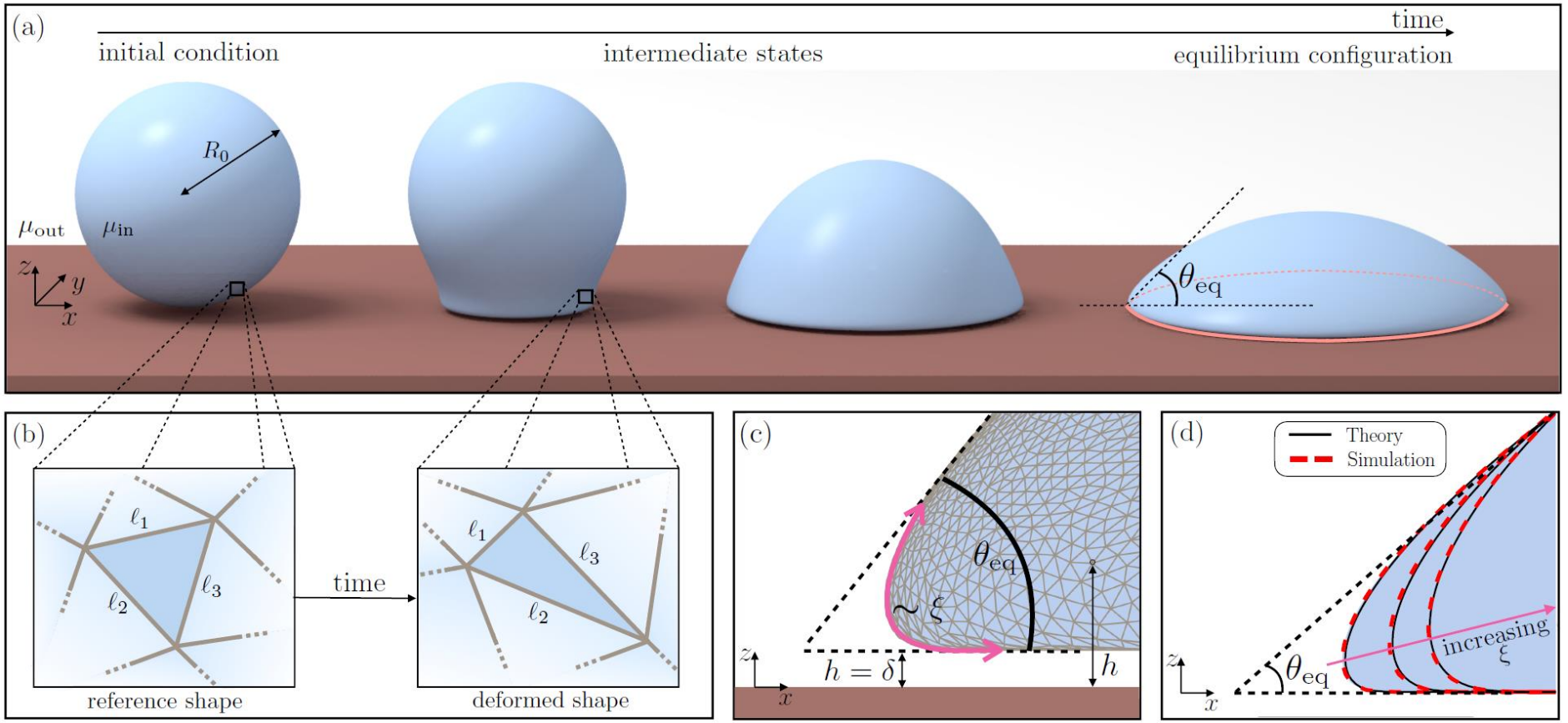
IBLB for Wetting: Extension

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

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

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

Set contact angle a priori



δ: Drop-solid separation

ξ: Wall interaction length

[2] **Bellantoni E.**, Guglietta F., Pelusi F., Desbrun M., Um K., Nicolaou M., Savva N. and Sbragaglia M., *Physical Review E*, 2025 **112** 025305.

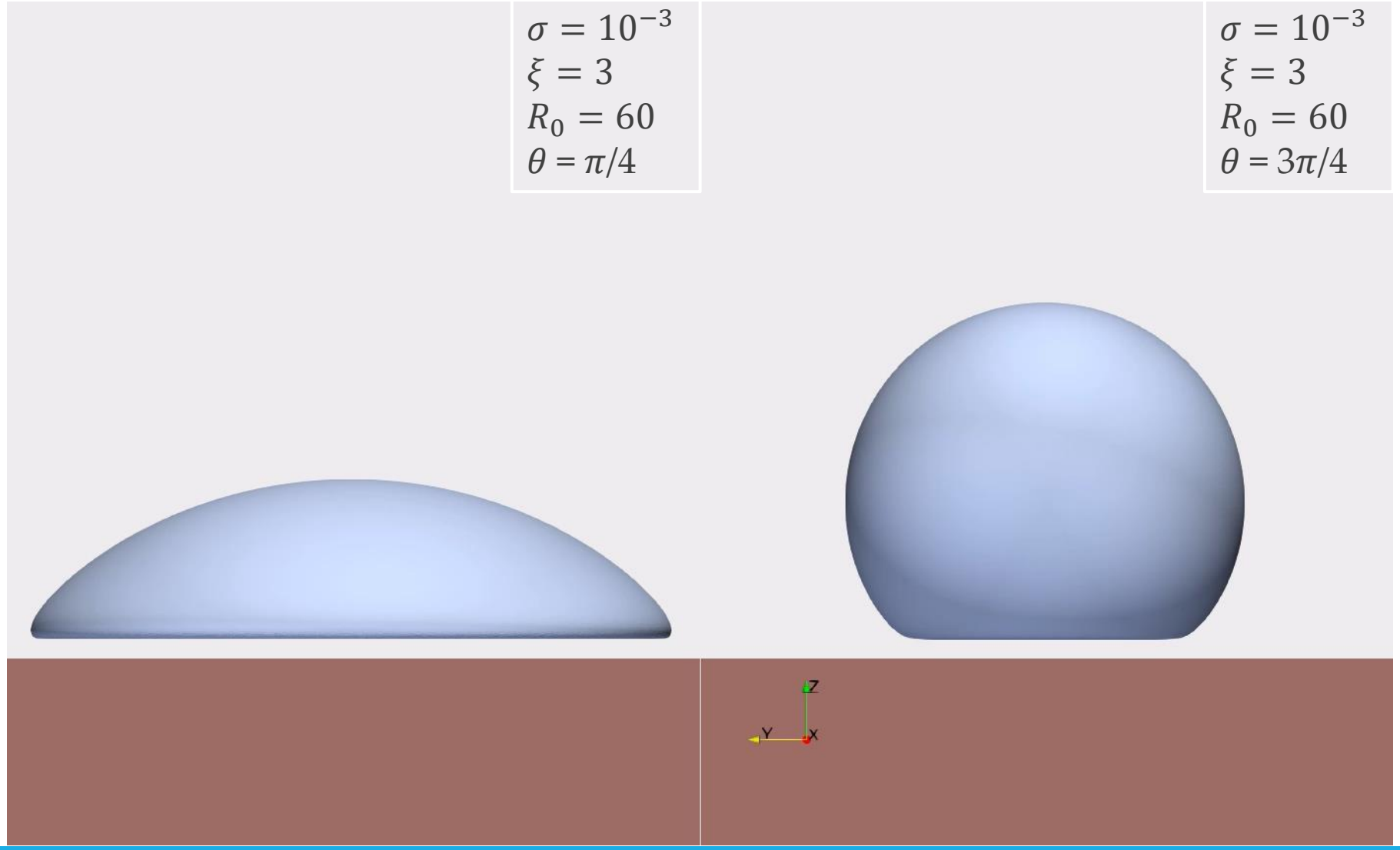
Method's validation

Hydrophilic vs Hydrophobic Droplets

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

$\sigma = 10^{-3}$
$\xi = 3$
$R_0 = 60$
$\theta = \pi/4$

$\sigma = 10^{-3}$
$\xi = 3$
$R_0 = 60$
$\theta = 3\pi/4$



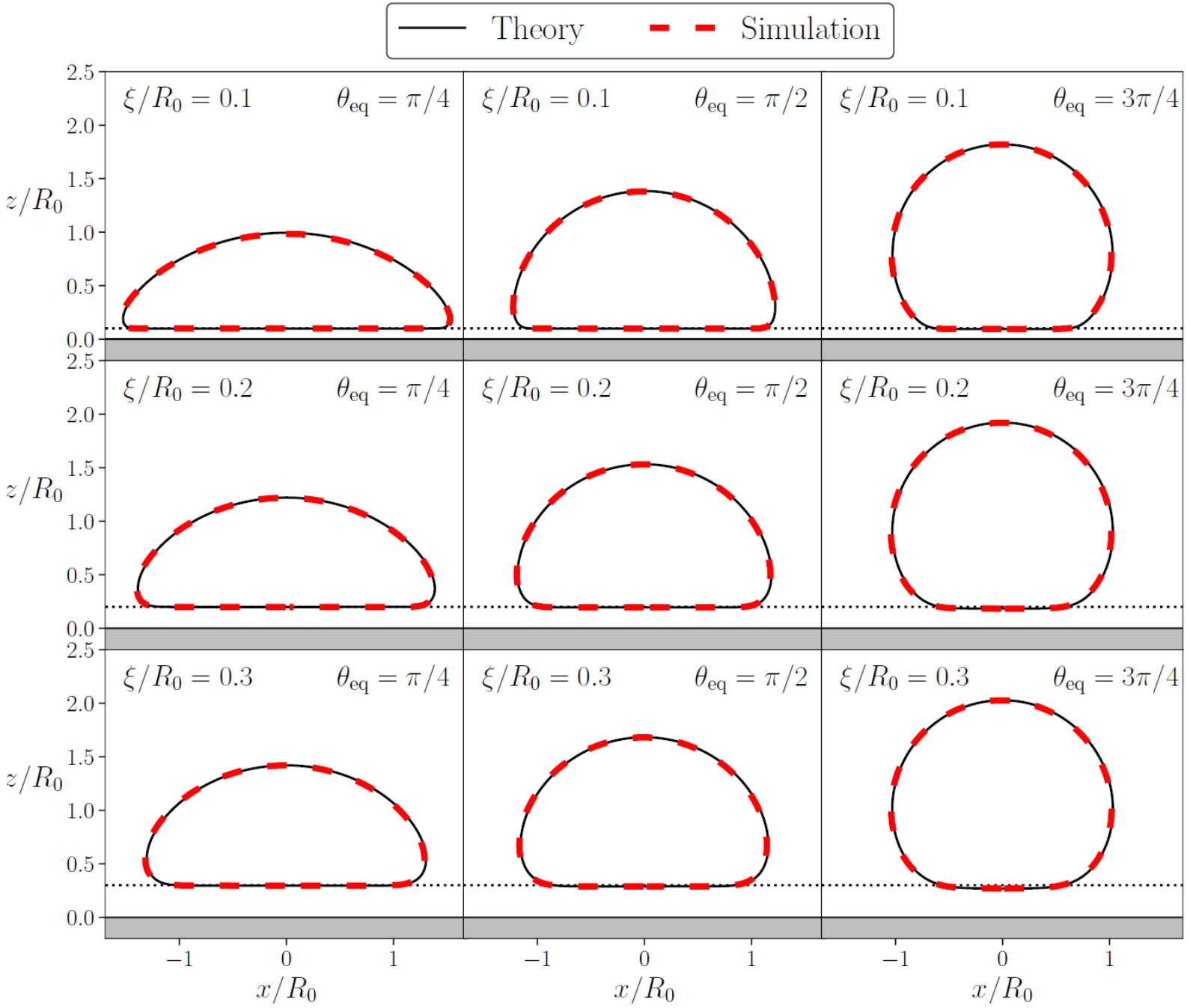
Equilibrium Shape

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



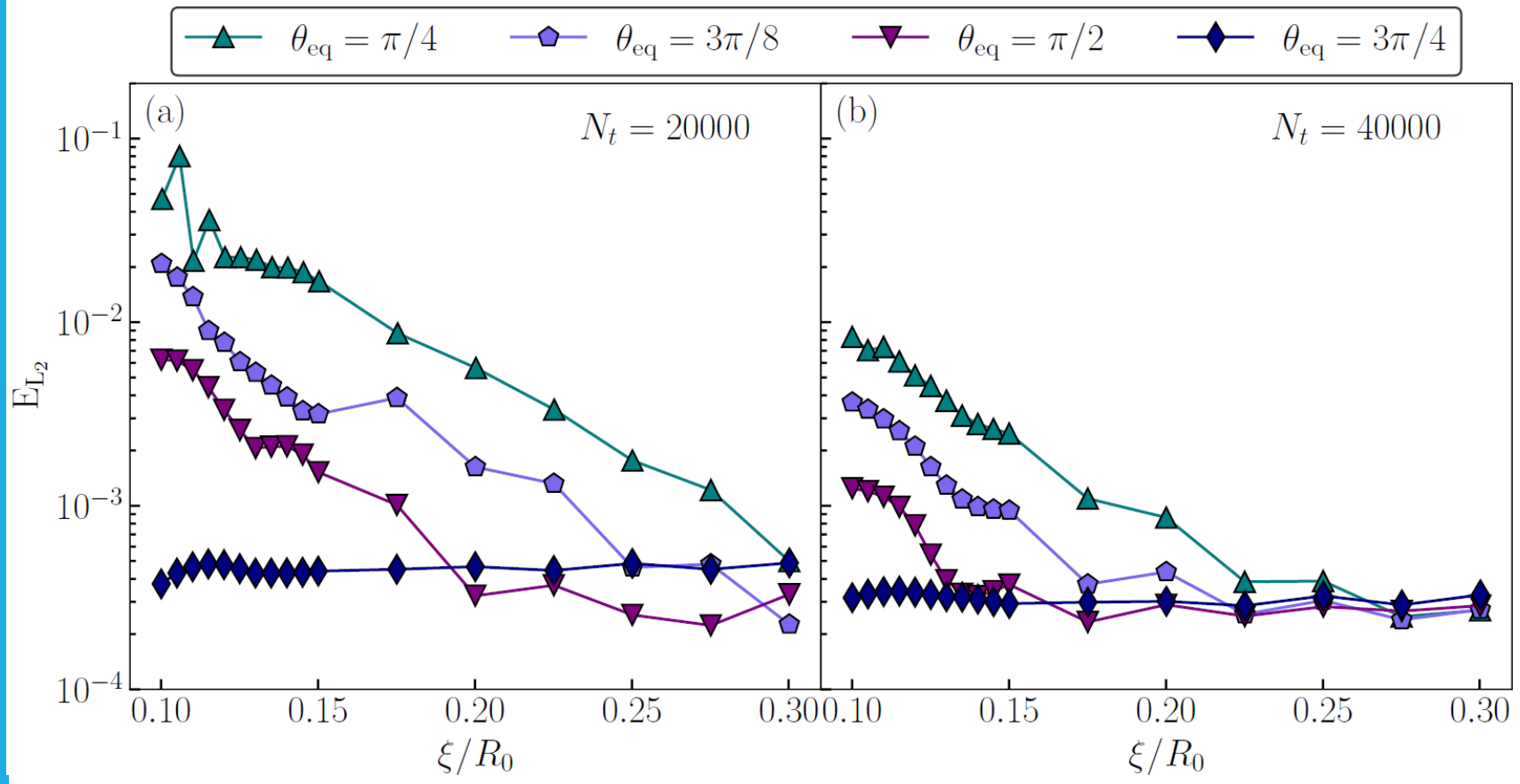
Equilibrium Shape – L2 Error

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:

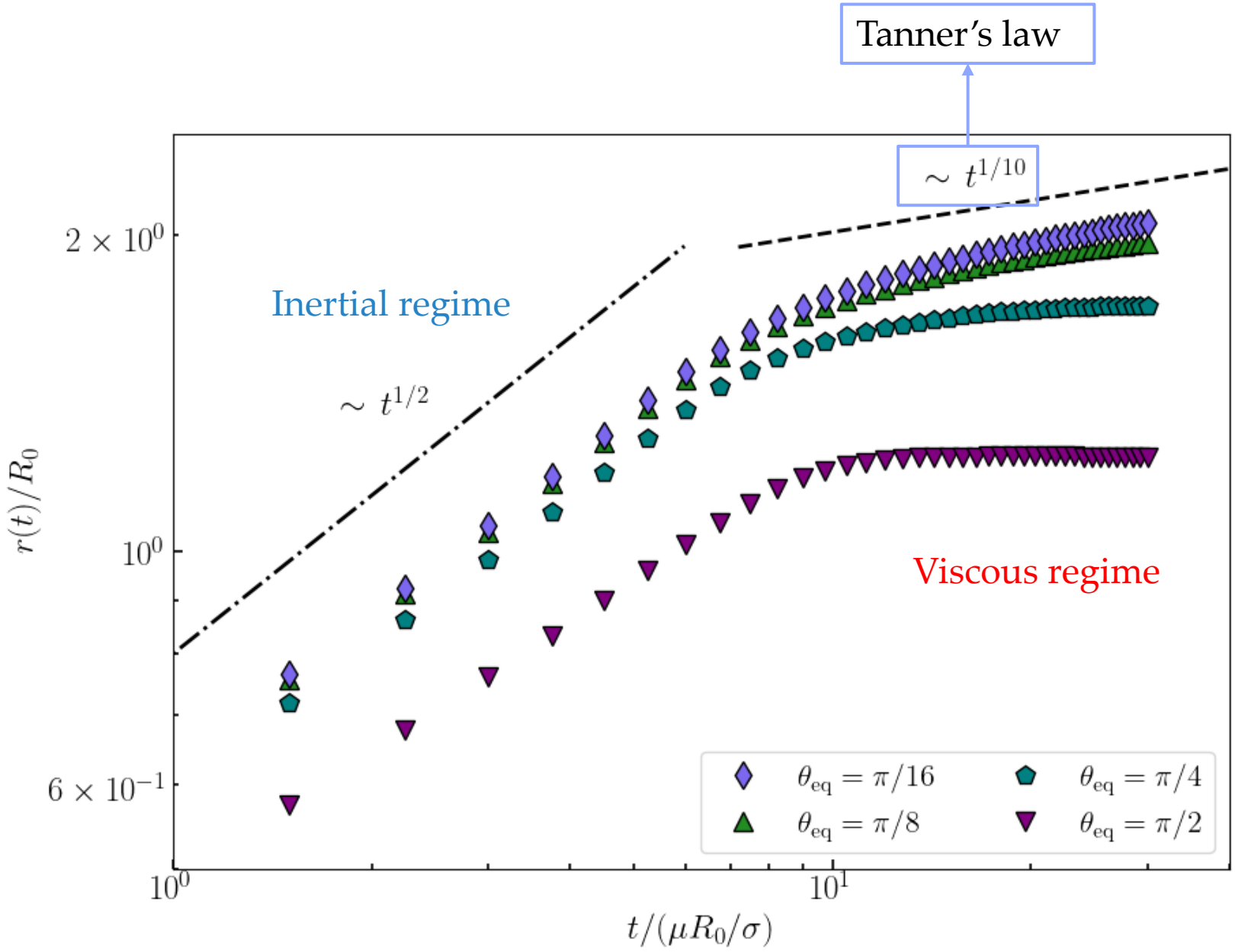
$$E_{L2} = \sqrt{\frac{\int_0^{\pi} |G_{\text{sim}}(\phi) - G_{\text{theo}}(\phi)|^2 \mathrm{d}\phi}{\int_0^{\pi} |G_{\text{theo}}(\phi)|^2 \mathrm{d}\phi}}$$



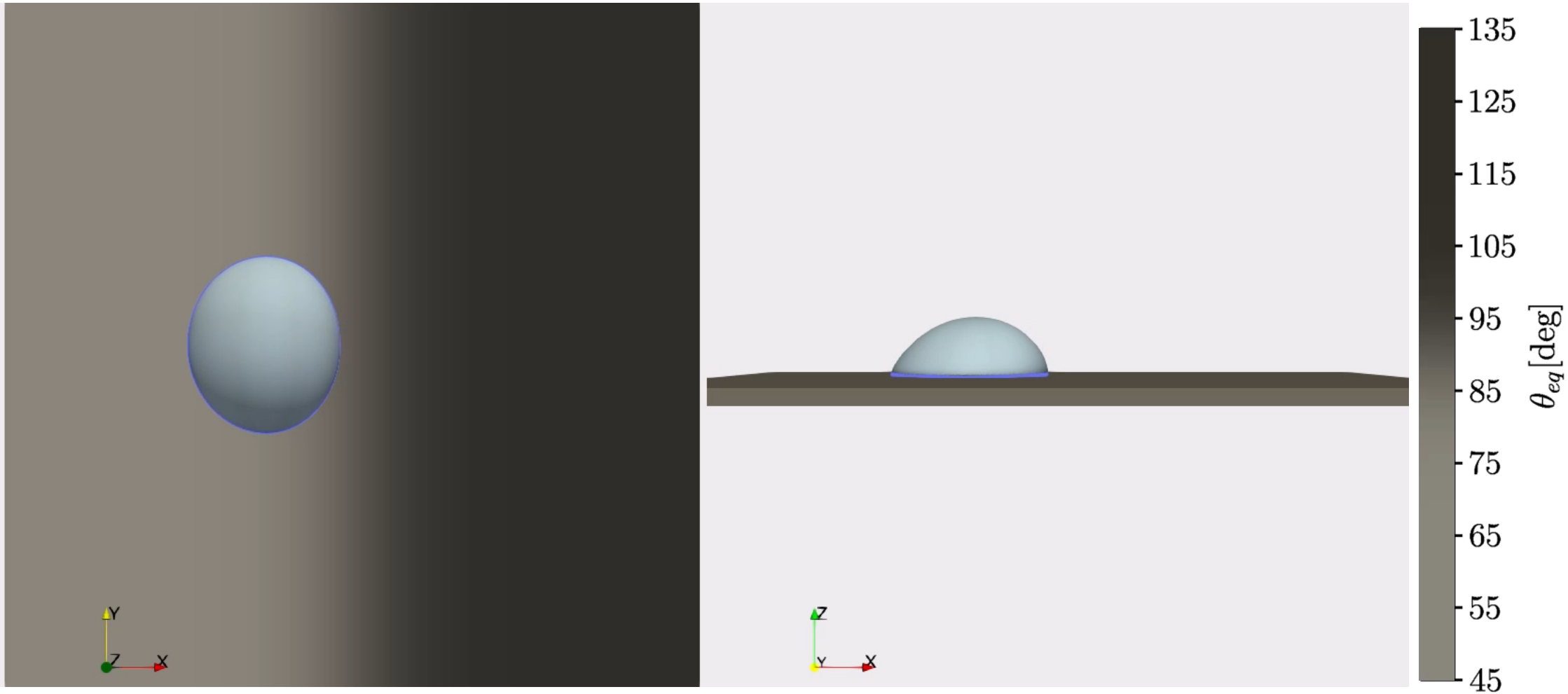
Spreading Dynamics

We consider the evolution of the **contact radius** $r(t)$

Analytical and experimental studies describe power-law scalings for the contact radius dynamics in the **inertial** and **viscous regimes**



Contact Angle Hysteresis



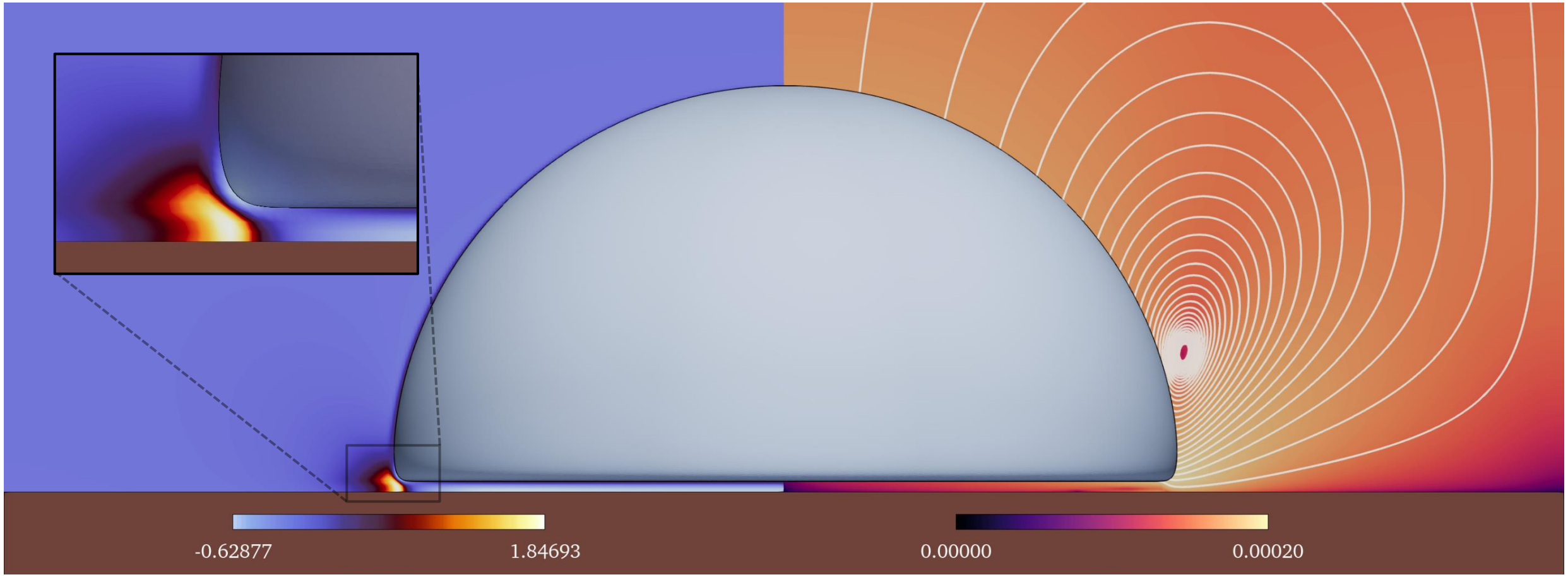
Top view

Side view

All good – but what about the thin film?

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?**



Physical system: soft pastes & emulsions

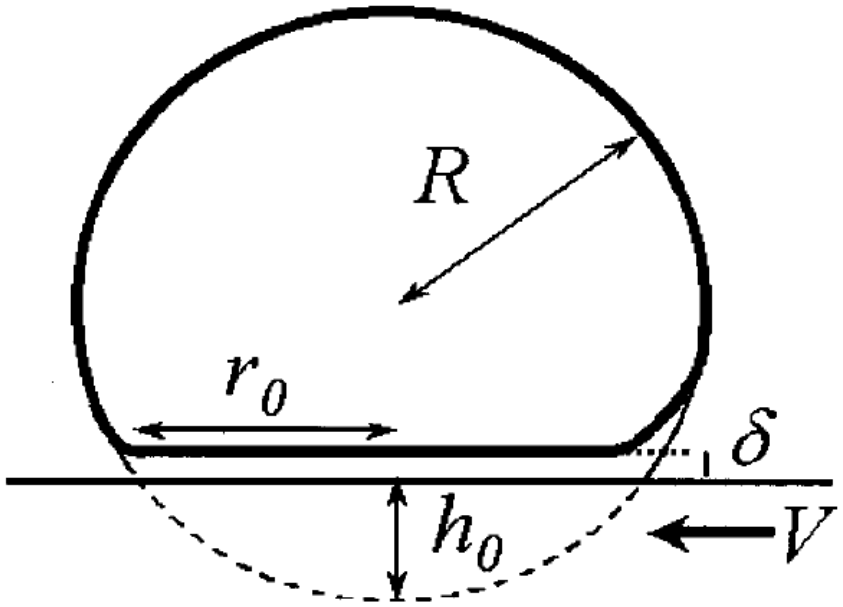


FIG. 5. Schematic of an elastohydrodynamically lubricated soft particle squeezed against a translating wall. [3]

The extra pressure in thin film layers, is similar to, e.g., the description of the slip and flow of **soft pastes** and **emulsions** [3]

The IBLB method could provide a numerical framework to study this kind of phenomena

[3] Meeker S. P., Bonnecaze R. T., and Cloitre M., *Physical Review Letters* **92** (2004) 198302

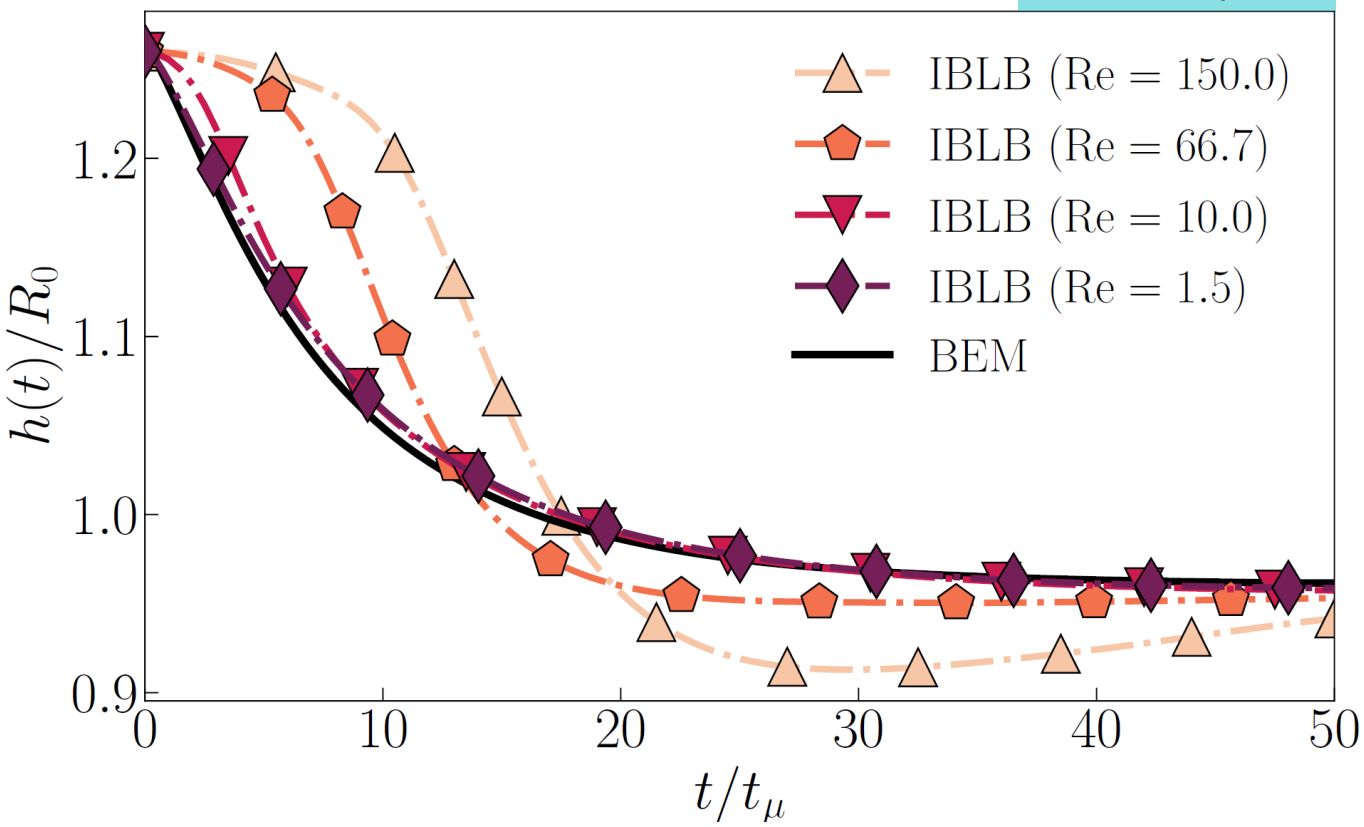
Comparison with BEM: Stokes Regime

We compare our results with independent hydrodynamic solvers

For a **Stokes' flow**, the problem can be casted as a boundary integral to determine the fluid velocity at the interface

We solve this using a boundary element method (**BEM**) and consider the droplet height evolution to compare results

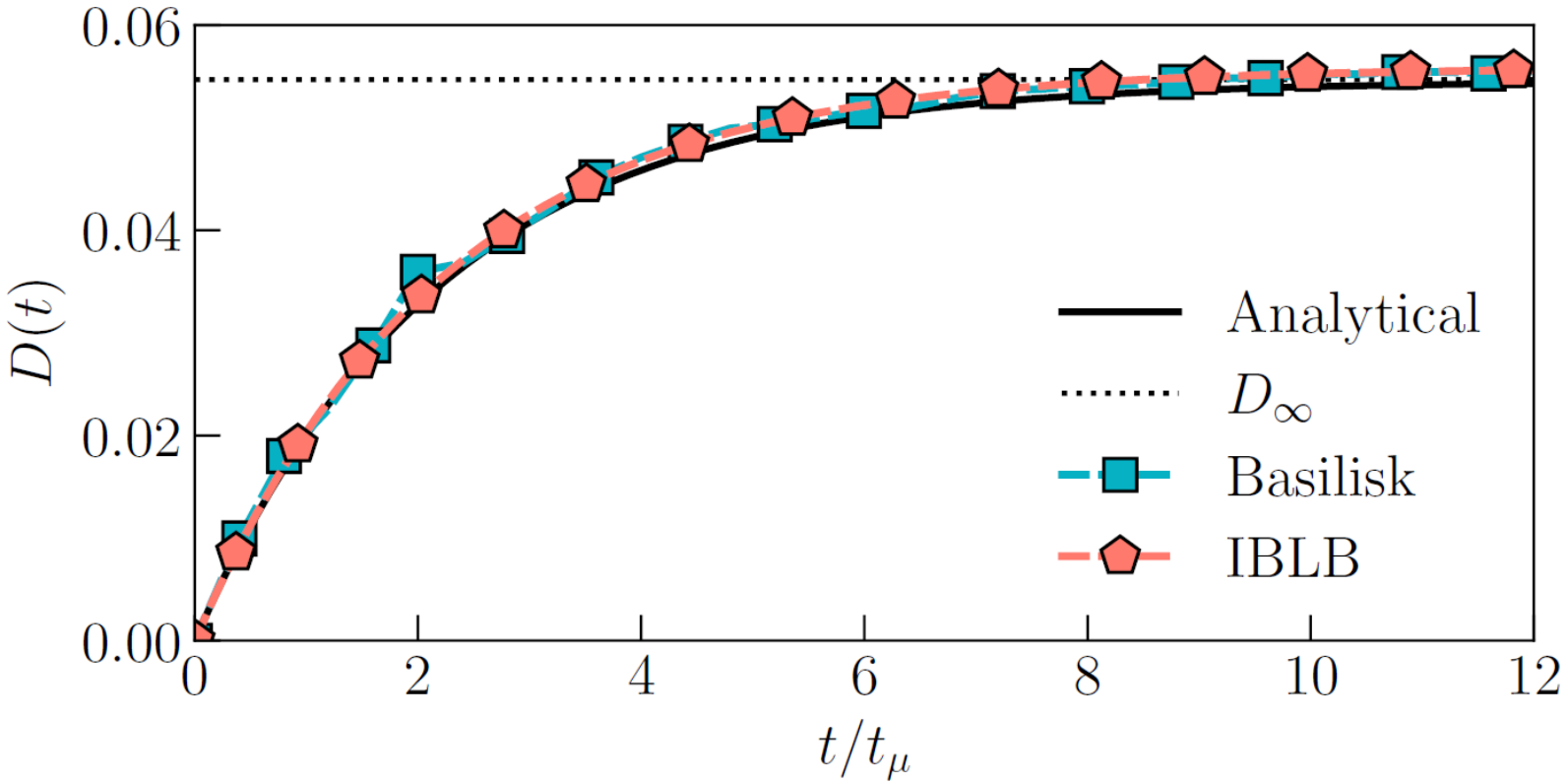
$$\mathrm{Re} := \frac{\rho U R_0}{\mu}$$



[4] **Bellantoni E.**, Guglietta F., Demou A., Pelusi F., Um K., Nicolaou M., Desbrun M., Sbragaglia M., & Savva N., 2026 *EPL* **155** 63002

Comparison with *Basilisk*: Drop under Shear

To compare results when inertia is present in the system, we further compare against *Basilisk* volume of fluid (VoF) solver [5,6]



Deformation index:

$$D(t) := \frac{r_1(t) - r_3(t)}{r_1(t) + r_3(t)}$$

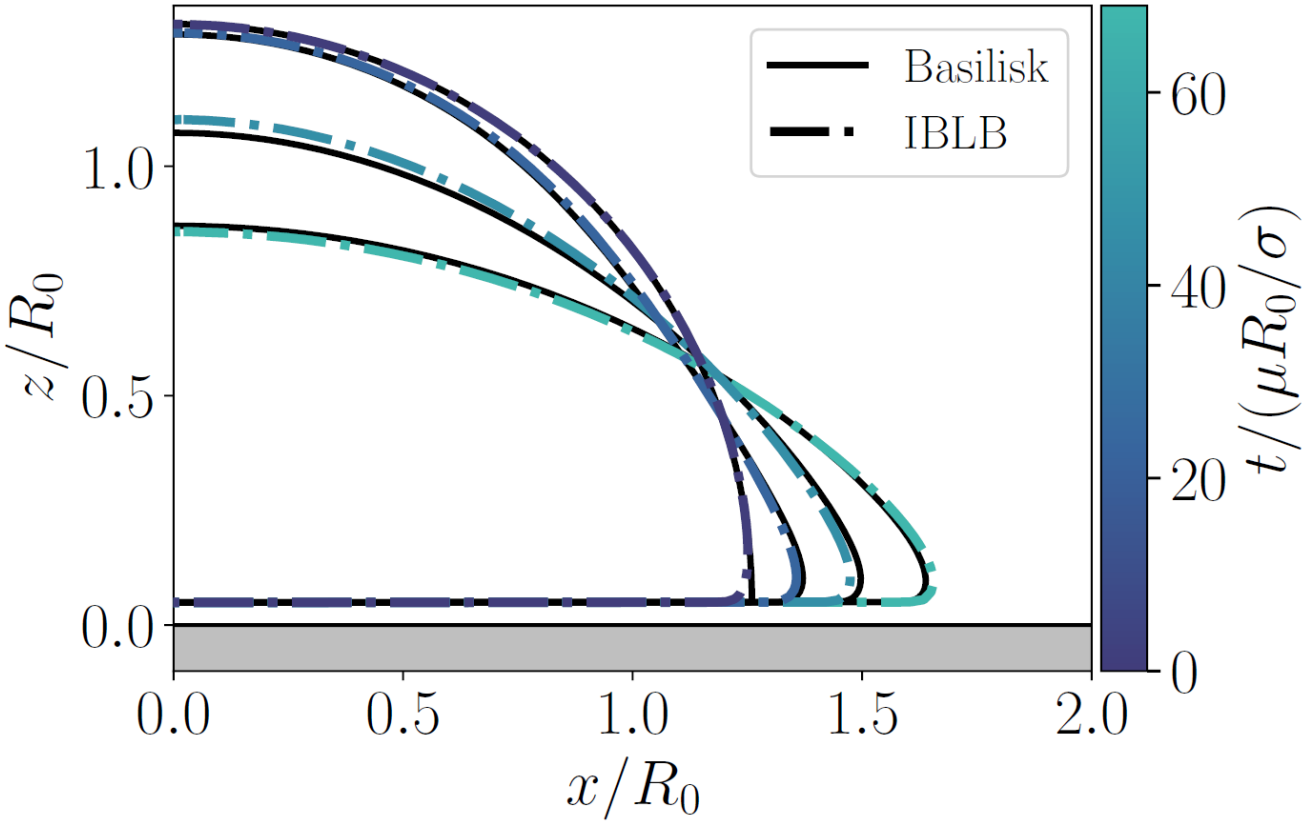
$$t_\mu := \frac{\mu R_0}{\sigma}$$

[5] Popinet S., *Journal of Computational Physics*, **190** (2003) 572.
[6] Popinet S., *Journal of Computational Physics*, **302** (2015) 336.

Comparison with *Basilisk*: Stokes Regime

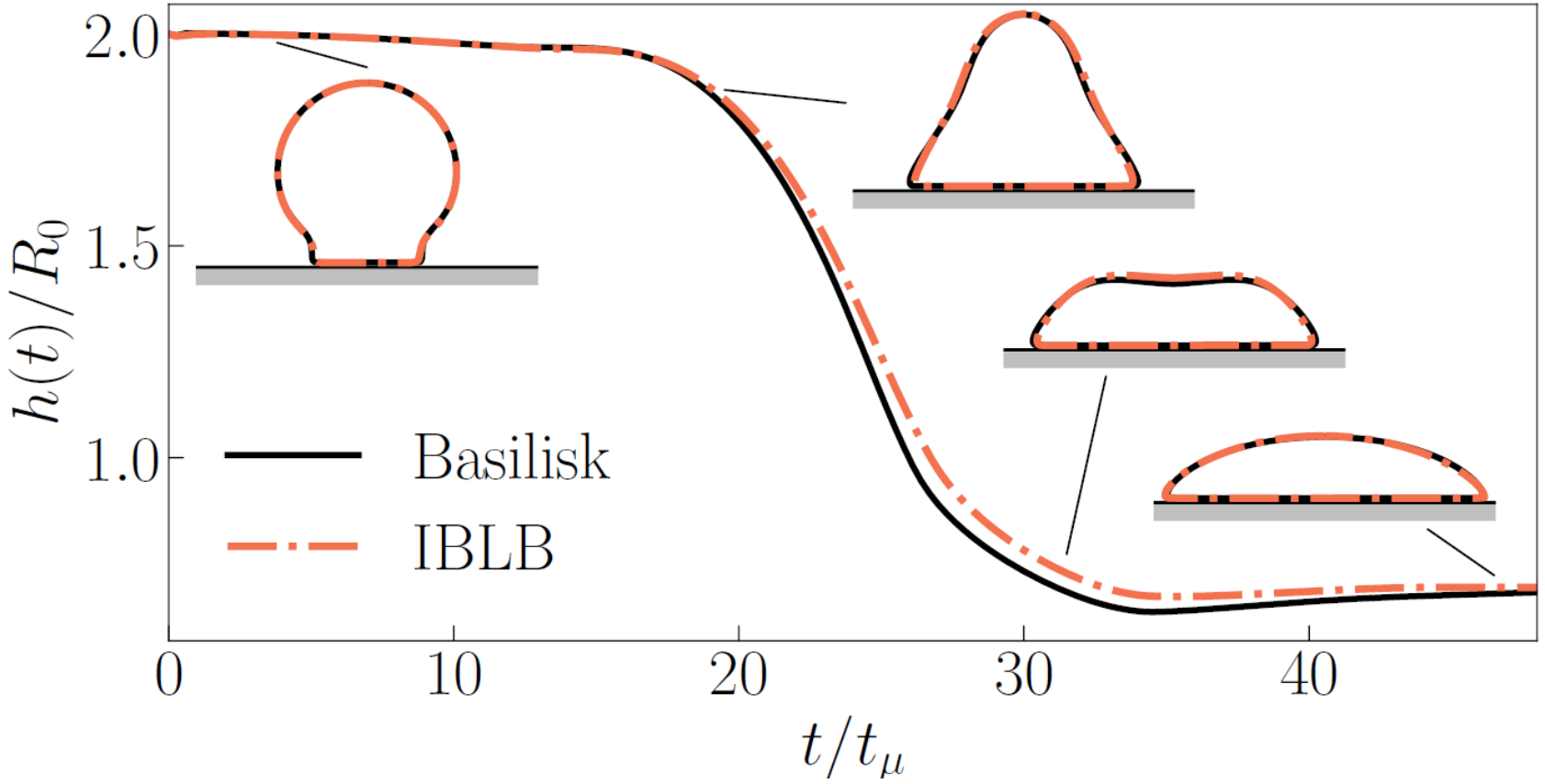
To compare results when inertia is present in the system, we further consider the *Basilisk* volume of fluid (VoF) solver

This allows to control what's happening to the droplet shape throughout the spreading process



Comparison with *Basilisk*: Navier-Stokes Regime

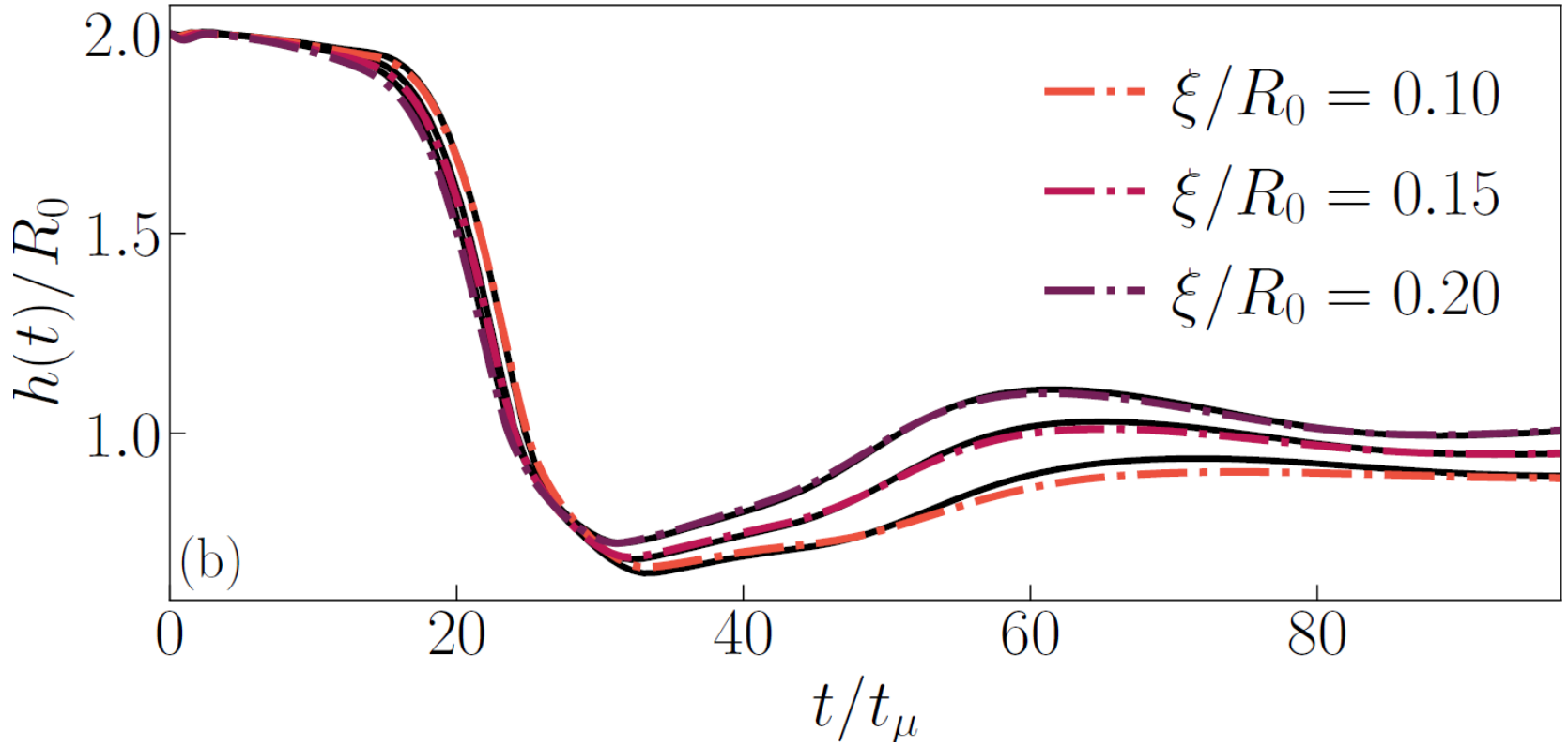
We can also analyze cases where inertia plays a significant role, highlighted by the "neck" formation in early stages of spreading and oscillations happening later on



$$t_\mu := \frac{\mu R_0}{\sigma}$$

Comparison with *Basilisk*: Oscillating Drop Shape

The oscillations are more prominent when ξ/R_0 is higher



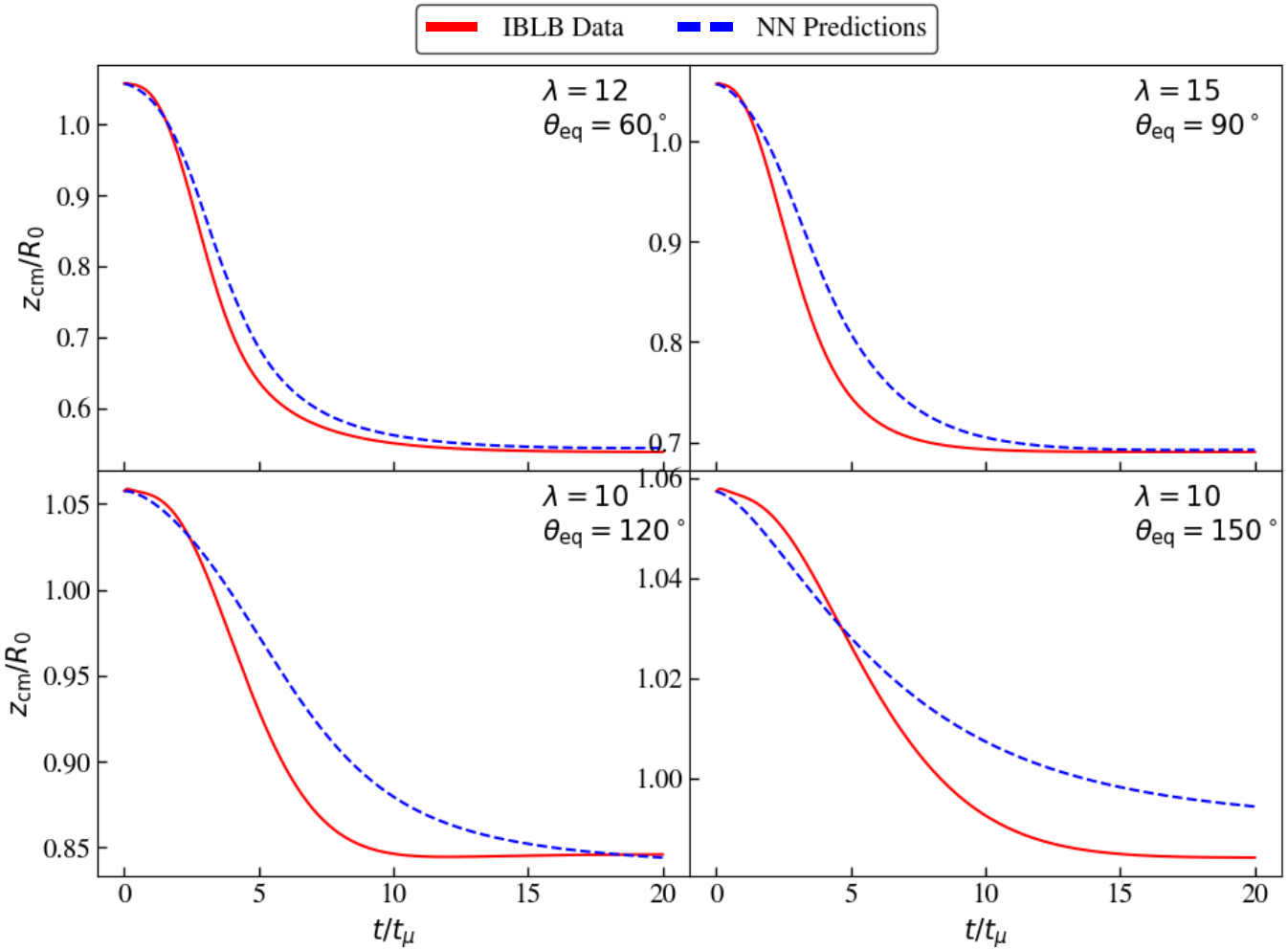
$$t_\mu := \frac{\mu R_0}{\sigma}$$

Conclusions & Outlook

Perspectives: ML tools from IBLB data

The IBLB is efficient for data production (GPU implementation) with several possible applications such as:

1. Predicting droplet shape evolution from some snapshots of the droplet during spreading (i.e. knowing shape at some t)
2. Equation discovery for droplet shape evolution (getting more insight into spreading driving mechanism)
3. Extracting interfacial properties given a few snapshots of the droplet under shear (a sort of ML rheometer)



Prediction of droplet CM evolution

Conclusions & Outlook

Conclusions:

- We have implemented a mesoscopic numerical method to simulate various wetting scenarios using a sharp interface approach
- The simulations agree well with theory and experiments for both droplet statics and dynamics
- The thin film physics is consistent with the description of independent hydrodynamic solvers

Further work:

- Add complexities to the interface (e.g. elasticity, viscoelasticity)
- Study systems with additional substrate complexities (e.g. more elaborate chemical heterogeneities, roughness, …)
- Develop ML tools to predict droplet shape evolution and/or extract droplet interfacial properties

Thank you for your attention!

References:

[1] Bonn D., Eggers J., Indekeu J., Meunier J. and Rolley E., *Review Modern Physics*, **81** (2009) 739

[2] **Bellantoni E.**, Guglietta F., Pelusi F., Desbrun M., Um K., Nicolaou M., Savva N. and Sbragaglia M., *Physical Review E*, **112** (2025) 025305

[3] Meeker S. P., Bonnecaze R. T., and Cloitre M., *Physical Review Letters* **92** (2004) 198302

[4] **Bellantoni E.**, Guglietta F., Demou A., Pelusi F., Um K., Nicolaou M., Desbrun M., Sbragaglia M., & Savva N., *EPL* **155** (2026) 63002

[5] Popinet S., *Journal of Computational Physics*, **190** (2003) 572.

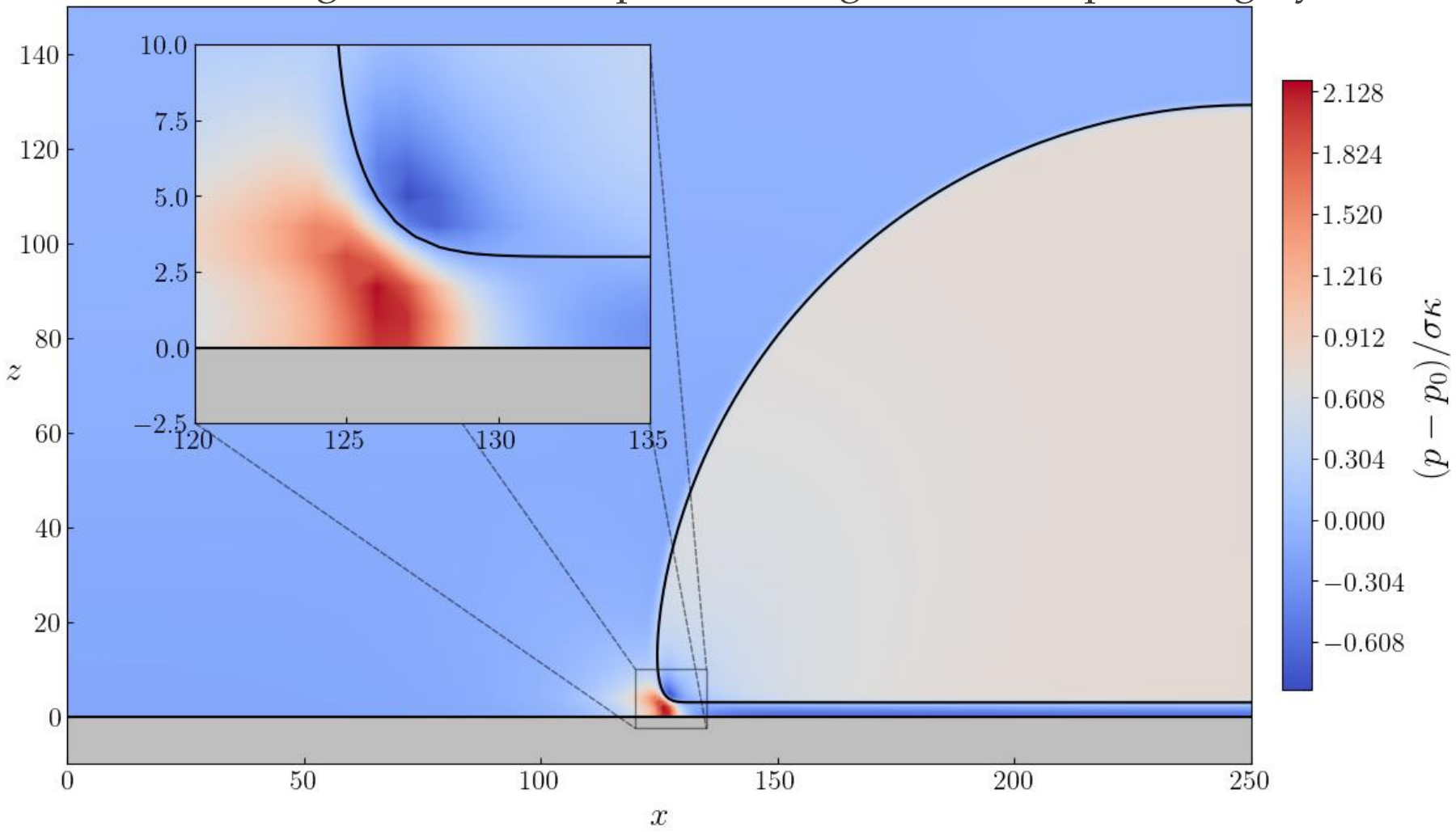
[6] Popinet S., *Journal of Computational Physics*, **302** (2015) 336.

Funded by the European Union

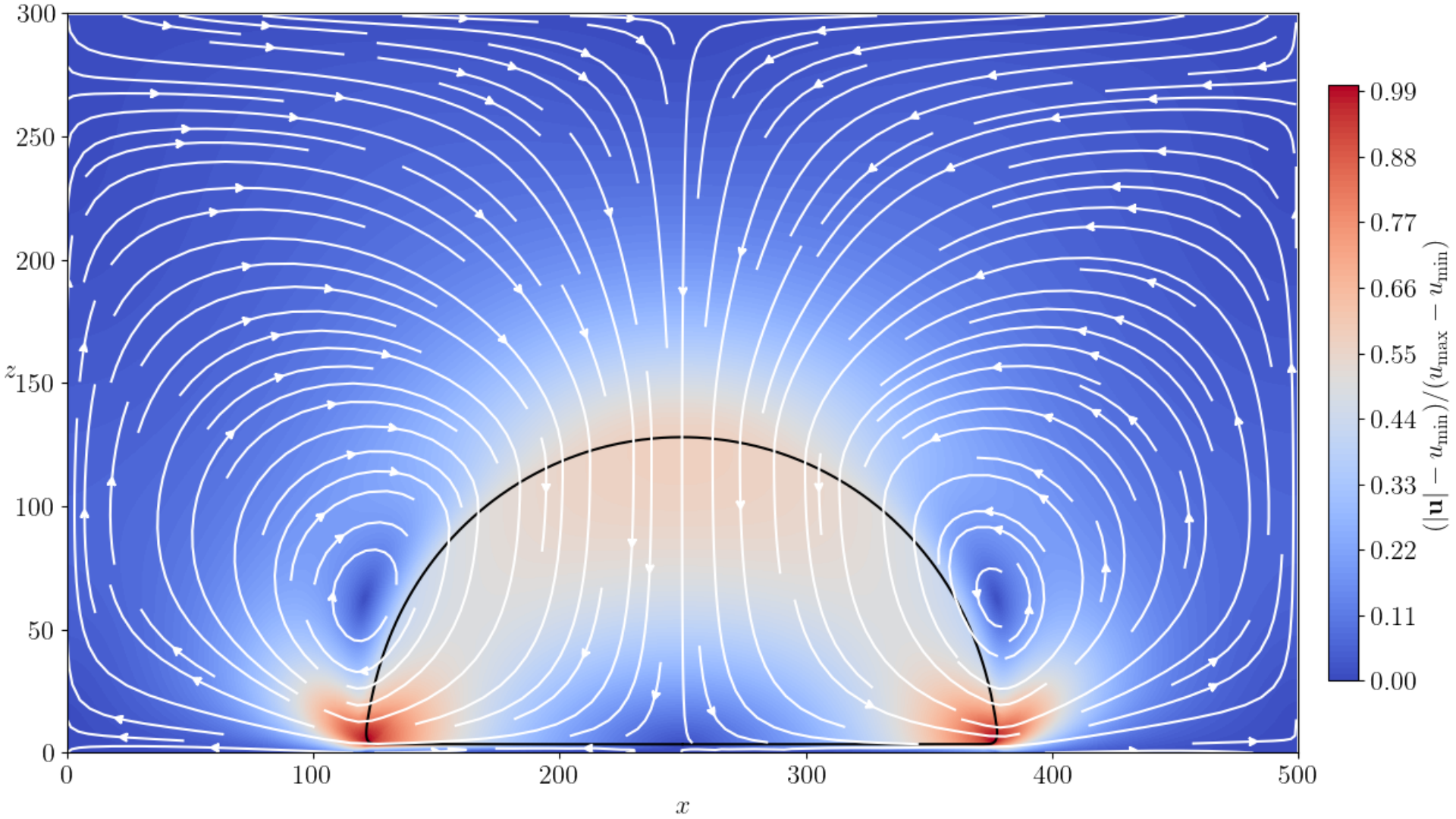
Backup

Effects of the Film on the Dynamics

The film creates an extra drag below the droplet, slowing down the spreading dynamics



Velocity Field



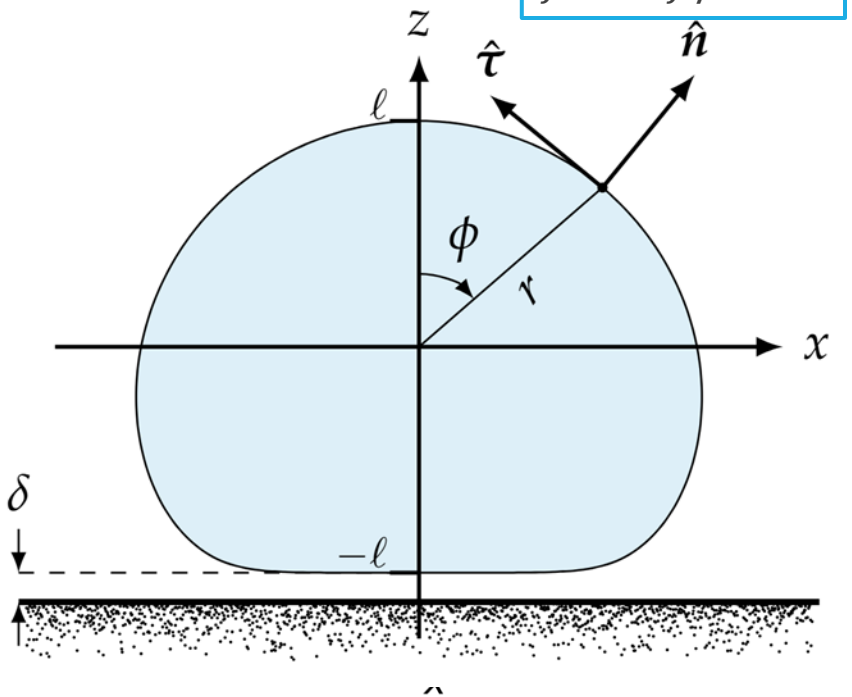
2. Droplet Interacting with the Wall

The droplet's profile shape can be obtained by solving the following ODE:

$$\frac{\Delta p}{\sigma} = \frac{2f^2 + 3\dot{f}^2(1-u^2) + f\left[u\dot{f} - (1-u^2)\ddot{f}\right]}{\left[(1-u^2)\dot{f}^2 + f^2\right]^{3/2}} + \frac{u\dot{f}}{f\sqrt{(1-u^2)\dot{f}^2 + f^2}} + \frac{A}{\sigma}\left[\left(\frac{\xi}{h}\right)^n - \left(\frac{\xi}{h}\right)^m\right]$$

This was solved numerically via Newton iteration, using Chebyshev pseudo-spectral collocation for discretization

$r \coloneqq f(\phi)$
$u \coloneqq \cos\phi$
$\dot{f} \coloneqq \mathrm{d}f/\mathrm{d}u$



Droplet contour at equilibrium (axisymmetric drop)

Droplet's Shape at Equilibrium

The shape of a droplet at equilibrium can be related to its curvature ($\nabla \cdot \hat{\boldsymbol{n}}$) and to the pressure jump (Δp) between the inner and outer fluid:

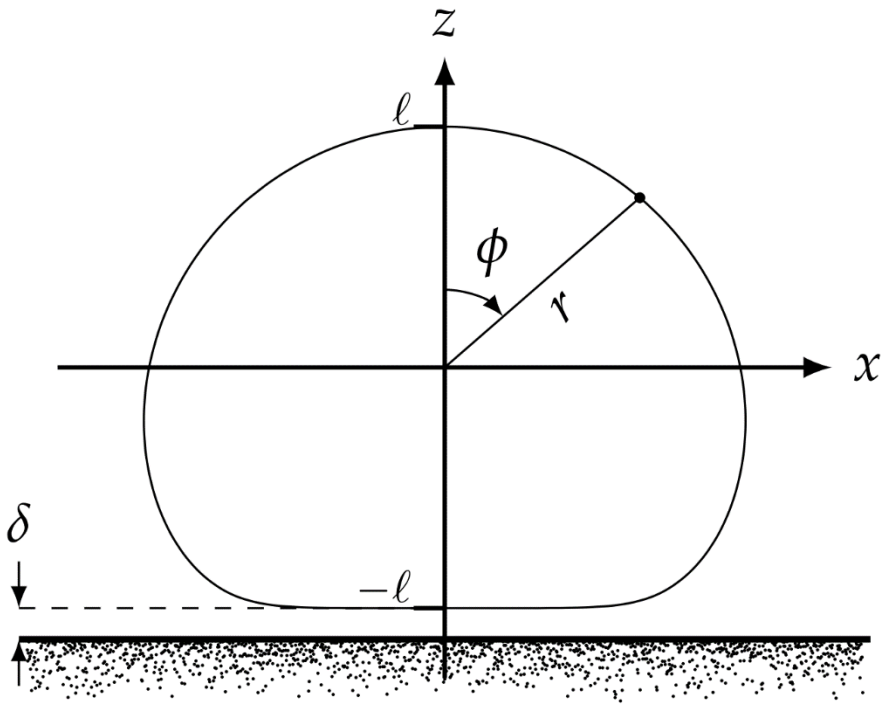
Young-Laplace Equation: $$\Delta p = \sigma \boldsymbol{\nabla} \cdot \hat{\boldsymbol{n}} + \Pi(h)$$

Disjoining pressure term: $$\Pi(h) = A\left[\left(\frac{\xi}{h}\right)^n - \left(\frac{\xi}{h}\right)^m\right]$$

With: $$A = \frac{\sigma}{\xi}\frac{(m-1)(n-1)}{(n-m)}(1+\cos\theta)$$

$\hat{\boldsymbol{n}}$: Outward normal to surface
h: Vertical distance from interface
ξ: Distance such that $\Pi(h=\xi)=0$

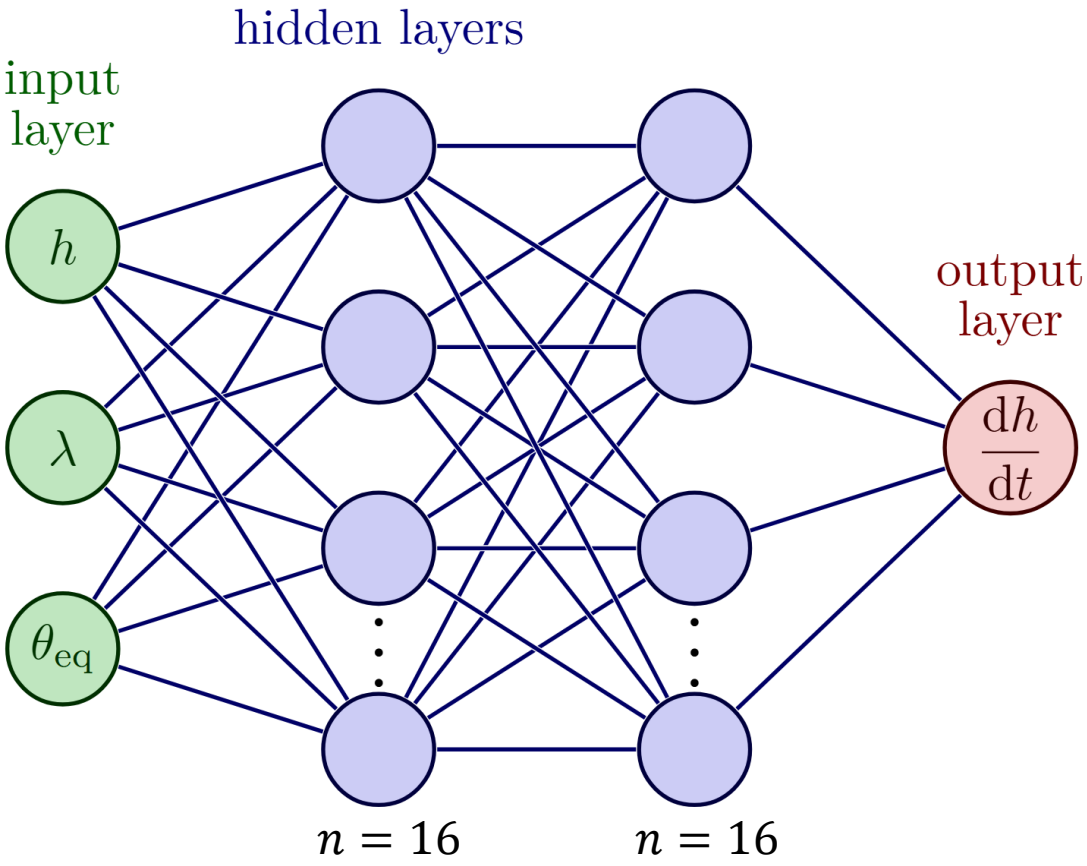
Set contact angle a priori



Droplet contour at equilibrium (axisymmetric drop)

AI tools from IBLB data

First NN experiment with IBLB data



Goal: predicting droplet's shape evolution during spreading

Proof-of-concept: simple NN learning the height's rate of change

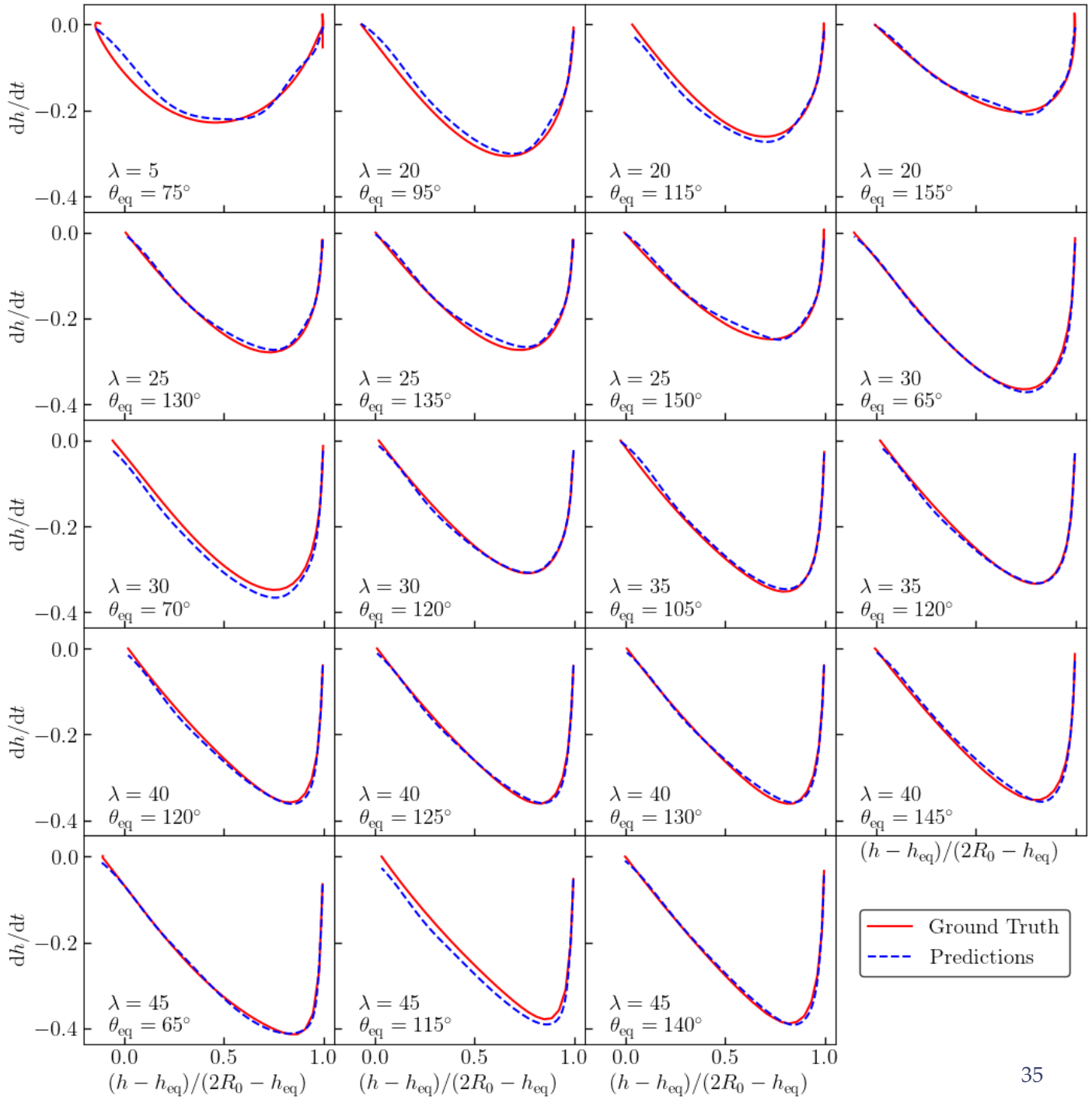
Input: $h(t), \lambda, \theta_{\mathrm{eq}}$ (IBLB data)

Output: $\mathrm{d}h/\mathrm{d}t$ (dynamical variable)

Use case: Faster surrogate for inverse design?

First NN experiment results:

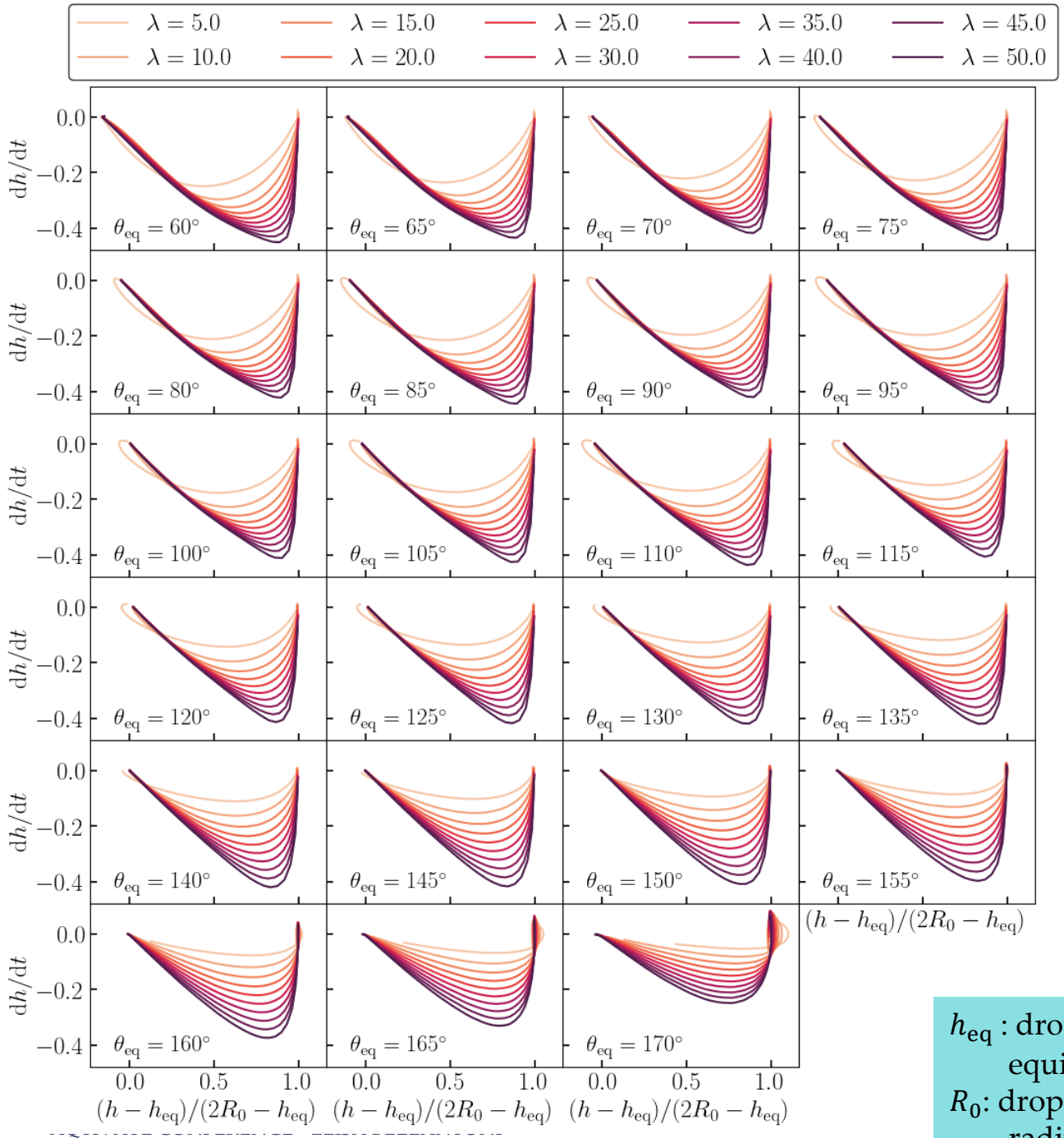
The network is able to learn something about the dynamics of a spreading droplet from the IBLB data, even with a relatively small dataset



First step: learn mapping $(h, \lambda, \theta_{eq}) \rightarrow dh/dt$

I have generated a datasets from a set of 230 simulations with different values of the **viscosity ratio** (λ) and equilibrium **contact angle** (θ_{eq})

For every simulation, I have 200 snapshots (i.e. full mesh data) of the spreading process



h_{eq} : droplet's height at equilibrium
R_0: droplet's initial radius

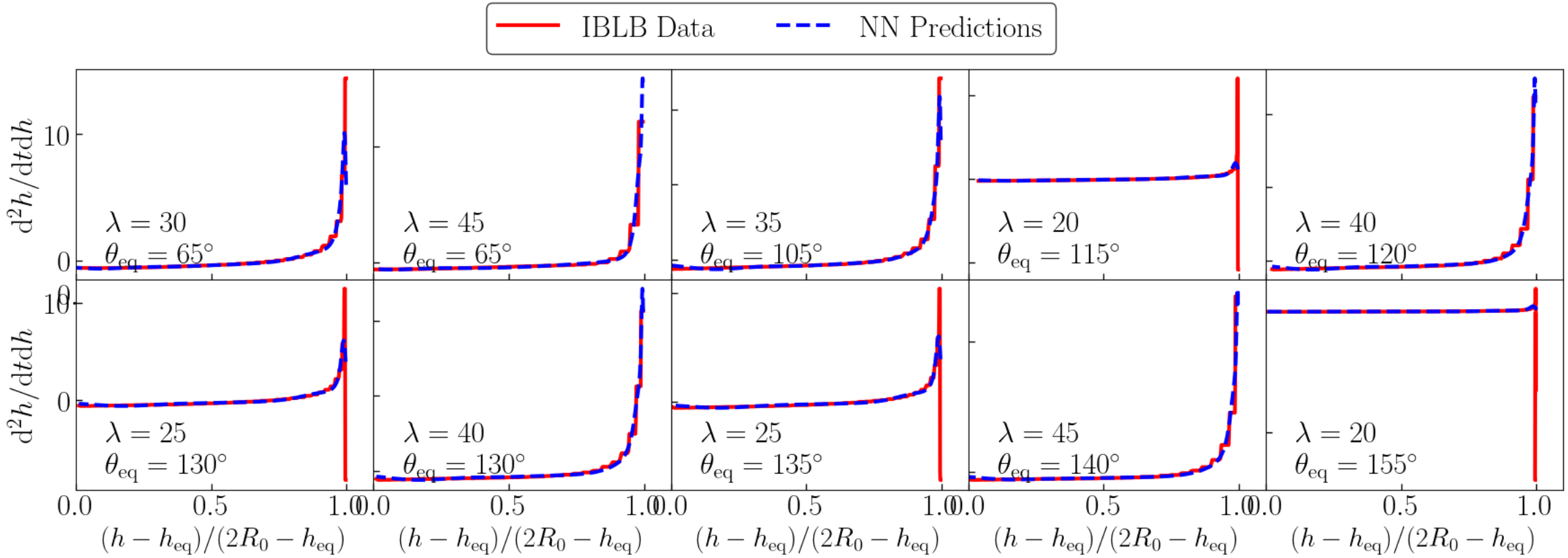
First NN Experiment Architecture

- Two hidden layers, fully connected
- ADAM optimizer
- MSE loss
- tanh activation function
- 5000 training epochs
- 230 independent spreading processes ("trajectories")
- Train-val-test split = 80%-12%-8%
- Train samples: 36821 (184 trajectories)
  Val samples: 5400 (27 trajectories)
  Test samples: 3800 (19 trajectories)
- Total trainable parameters: 353

```
Using device: cuda
+------------+------------+
| Modules    | Parameters |
+------------+------------+
| fc1.weight |      48    |
| fc1.bias   |      16    |
| fc2.weight |     256    |
| fc2.bias   |      16    |
| fc3.weight |      16    |
| fc3.bias   |       1    |
+------------+------------+
Total Trainable Params: 353
```

Current architecture's parameters

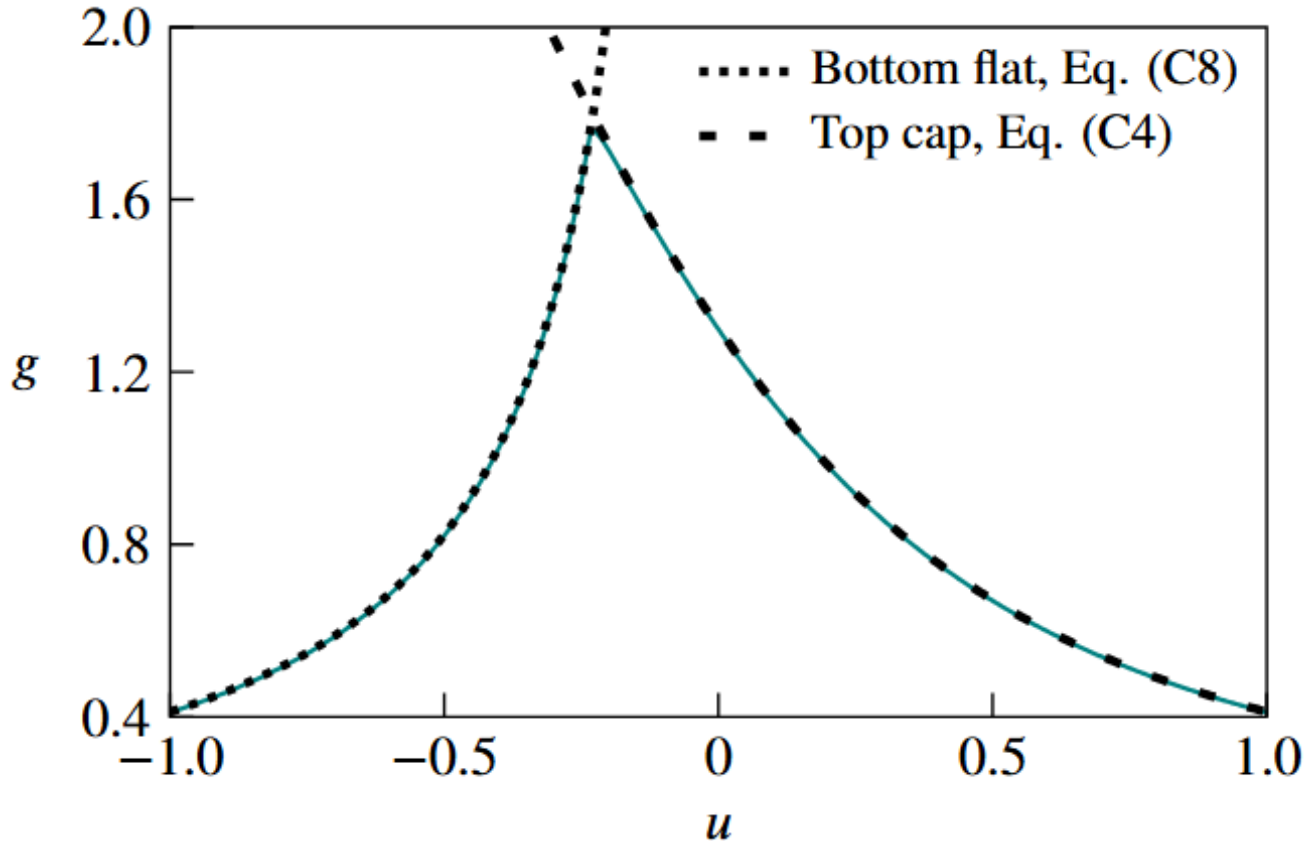
Predictions' Slope



Perspectives: AI tools from IBLB data

1. Predict droplet shape evolution from some snapshots of the droplet during spreading (i.e. knowing shape at some t)
2. Extract interfacial properties given a few snapshots of the droplet under shear (a sort of ML rheometer)

A convenient way to extract droplet shapes from our data is to use polar spherical coordinates wrt to the droplet center of mass and consider the radial coordinate $g = g(u) = g(\cos\phi)$ with ϕ polar angle



Asymptotical droplet shape