Modeling and ALE-based simulation of Dynamic Wetting

From fundamentals to some recent advancements

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TECHNISCHE UNIVERSITÄT DARMSTADT

CRC 1194 Interaction between Transport and Wetting Processes

Mathematical Modeling and Analysis

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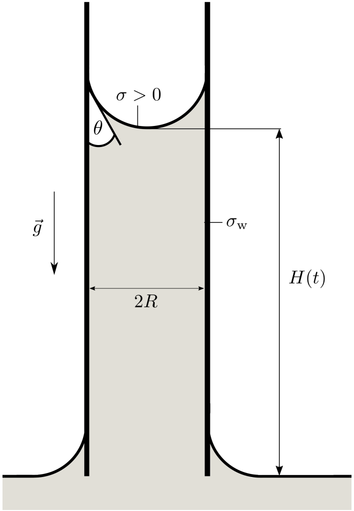
- **HHU Düsseldorf:** Matthias Köhne

Wetting of complex surfaces

Capillary rise: A prototypical (dynamic) wetting process



- A liquid column rises against gravity driven by capillarity.
- **Free energy** functional (including some approximations):

$$\mathcal{E}(h) = \pi R^2 \sigma + 2\pi R h \sigma_{\mathrm{w}} + \frac{\pi}{2} \rho g R^2 h^2 .$$

  σ_{w}: specific energy due to **wetting** of the solid
- Young equation for the equilibrium **contact angle**

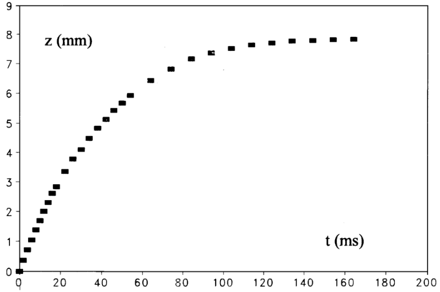
$$\sigma \cos \theta_0 + \sigma_{\mathrm{w}} = 0.$$

- Energy **minimization** yields Jurin's equation

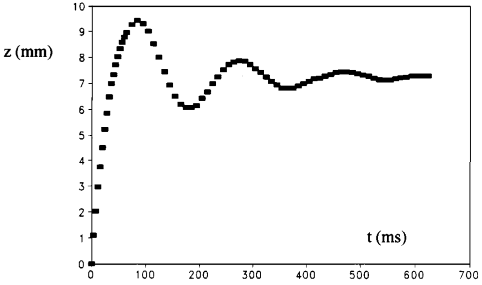
$$h_0 = -\frac{2\sigma_{\mathrm{w}}}{\rho g R} = \frac{2\sigma \cos \theta_0}{\rho g R}.$$

Dynamics of capillary rise

- There are different **regimes** for the rise **dynamics** observed in experiments.
- (Quéré, Europhys. Lett., 1997):
  Monotone rise for ethanol, **oscillatory** rise for ether (low viscosity).
- It is still very challenging to **predict** the dynamics.



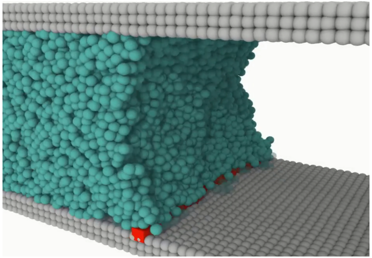
(a) Ethanol ($\eta = 1.17\text{mPa} \cdot \text{s}$).



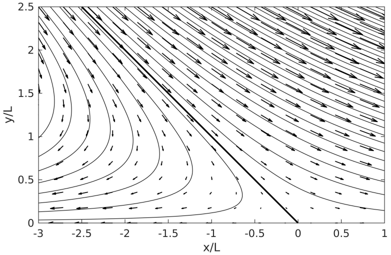
(b) Ether ($\eta = 0.3\text{mPa} \cdot \text{s}$).

Figure: Experimental data by Quéré (1997). Capillary rise in a glass tube ($R = 0.689\text{mm}$).

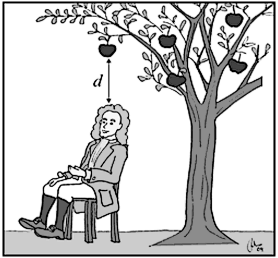
- **Molecular dynamics:** very accurate description of the local physics. Simulations are limited to short length and time scales.
- **Continuum mechanics:** capable of describing larger scales, small scale physics "encoded" in boundary conditions.
- **Simplified models:** Phenomenological models or models derived from continuum mechanics using some simplifying approximations.



(a) Molecular dynamics.



(b) Continuum mechanics.



(c) Simplified models.

Figure (c) taken from www.aps.org/publications/apsnews/200908/zerogravity.cfm.

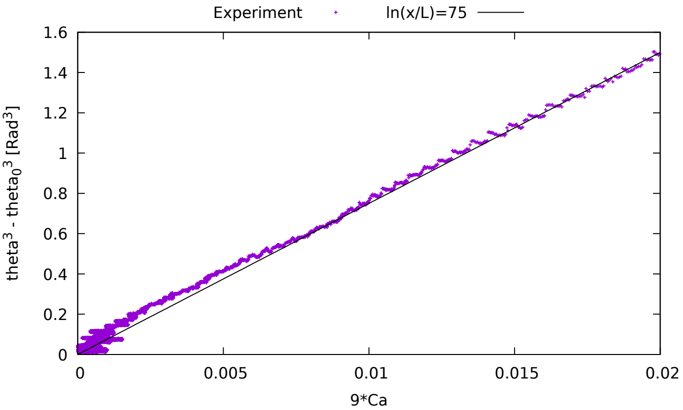
Fitting parameters vs. predictive models

- A **spreading** glycerol-water droplet is described fairly well by Cox-Voinov, i.e.

$$\theta_{app}^3 - \theta_m^3 = 9\,\text{Ca}\,\ln\left(\frac{x}{l}\right), \qquad (1)$$

for the (obviously **unphysical**) choice

$$\ln\left(\frac{x}{l}\right) \approx 75 \quad \Leftrightarrow \quad \frac{x}{l} \approx 10^{32.5}.$$



Outline

Outline

Static wetting and the Young equation

Goal: Determine the stationary shape of a wetting droplet on an ideal surface.

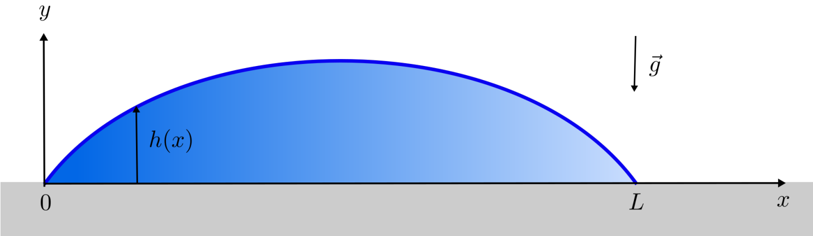
- Some (technical) simplifications: 2D geometry, small contact angle ($\theta < 90^\circ$).
- **Height function** representation of the free surface

$$\Sigma = \{(x, h(x)) : 0 \leq h \leq L\}.$$

- Potential energy functional:

$$\mathcal{E} = \sigma|\Sigma| + \sigma_{\mathrm{w}}|W| + \mathcal{E}_g.$$

- Liquid-Gas surface tension σ, specific **wetting energy** $\sigma_{\mathrm{w}} = \sigma_{\mathrm{sl}} - \sigma_{\mathrm{sg}}$, gravitational energy $\mathcal{E}_g$.



Static wetting and the Young equation (II)

- Energy functional $\mathcal{E} = \mathcal{E}(L, h)$ (neglecting gravity for simplicity)

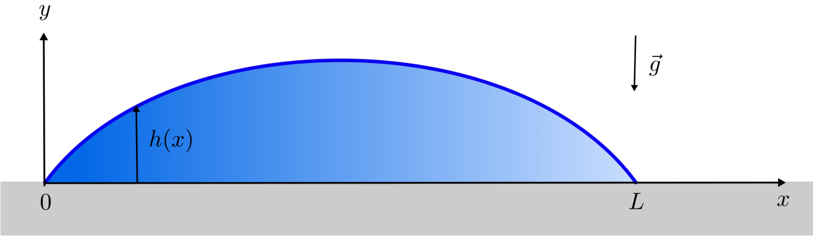
$$\boxed{\mathcal{E}(L,h) = \sigma \int_0^L \sqrt{1 + h'(x)^2}\, dx + L\, \sigma_{\mathrm{w}}}$$

has to be **minimized** over the configuration space

$$L \geq 0, \quad h \in C^2(0, L) \quad \text{with} \quad h \geq 0,\ h(0) = h(L) = 0$$

subject to the **volume conservation** constraint

$$\int_0^L h(x) dx = V_0.$$



Static wetting and the Young equation (III)

- **Non-dimensional** form $\tilde{x} := x/L, \quad \tilde{h}(\tilde{x}) := h(\tilde{x}L)/L, \quad 0 \le \tilde{x} \le 1$ allows for an **independent variation** of L and $\tilde{h}$.
- Minimize

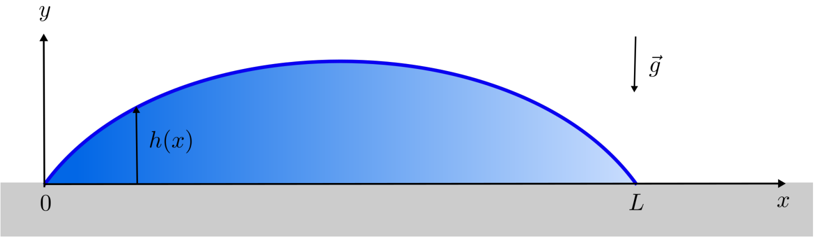
$$\mathcal{E}(L, \tilde{h}) = L\left(\sigma \int_0^1 \sqrt{1 + \tilde{h}'^2}\, d\tilde{x} + \sigma_w\right)$$

over the configuration space

$$L \ge 0, \quad \tilde{h} \in C^2(0,1) \quad \text{with} \quad \tilde{h} \ge 0,\ \tilde{h}(0) = \tilde{h}(1) = 0$$

subject to

$$\int_0^1 \tilde{h}\, d\tilde{x} = \frac{V_0}{L^2}.$$



Static wetting and the Young equation (IV)

- Introduce a **Lagrange multiplier** for the volume constraint:

$$\mathcal{E}(L,\tilde{h},\lambda) = L\left(\sigma \int_0^1 \sqrt{1+\tilde{h}'^2}\, d\tilde{x} + \sigma_w\right) + \lambda\left(\int_0^1 \tilde{h}\, d\tilde{x} - \frac{V_0}{L^2}\right)$$

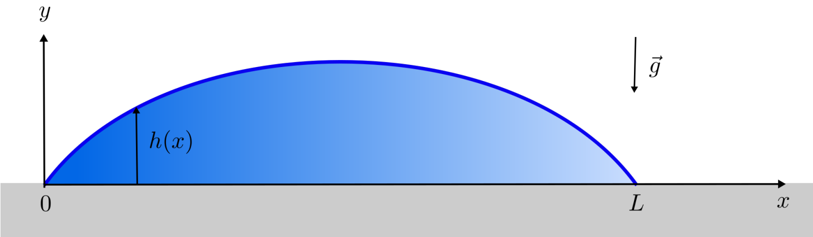
- Configuration space:

$$L \geq 0, \quad \tilde{h} \in C^2(0,1) \quad \text{with} \quad \tilde{h} \geq 0,\ \tilde{h}(0) = \tilde{h}(1) = 0$$

- **Stationarity** conditions:

$$0 = \frac{\partial \mathcal{E}}{\partial L} \quad \text{and} \quad 0 = \frac{\partial}{\partial \varepsilon}\mathcal{E}(L, \tilde{h} + \varepsilon\,\varphi, \lambda)\Big|_{\varepsilon=0}$$

for all smooth test functions $\varphi \in C_c^\infty(0,1)$.



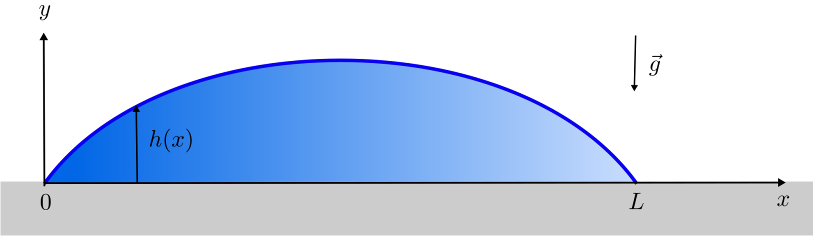
Static wetting and the Young equation (V)

- Stationarity **with respect to length** L leads to

$$0 = \sigma \int_0^1 \sqrt{1+\tilde{h}'^2}\, d\tilde{x} + \sigma_w + \frac{2\lambda\sigma V_0}{L^3}. \tag{2}$$

- Stationarity **with respect to shape** $\tilde{h}$ leads to ("Euler-Lagrange equation"):

$$\boxed{\left(\frac{\tilde{h}'}{\sqrt{1+\tilde{h}'^2}}\right)' = \frac{\lambda}{L\sigma} = \text{const.}} \tag{3}$$



Static wetting and the Young equation (VI)

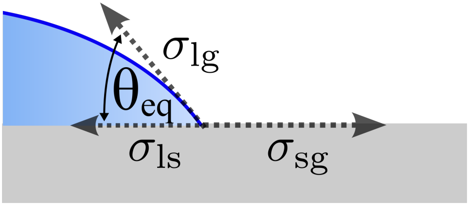
- Equation (3) shows that the shape is a **spherical cap** (curvature κ is constant).
- Combining equation (2) and (3) leads to

$$0 = \frac{\sigma}{L}\left(|\Sigma| + 2\kappa V_0\right) + \sigma_{\mathrm{w}}.$$

- With some elementary geometry (i.e. $|\Sigma| + 2\kappa V_0 = L\cos\theta$), we arrive at the **Young-Dupre equation**

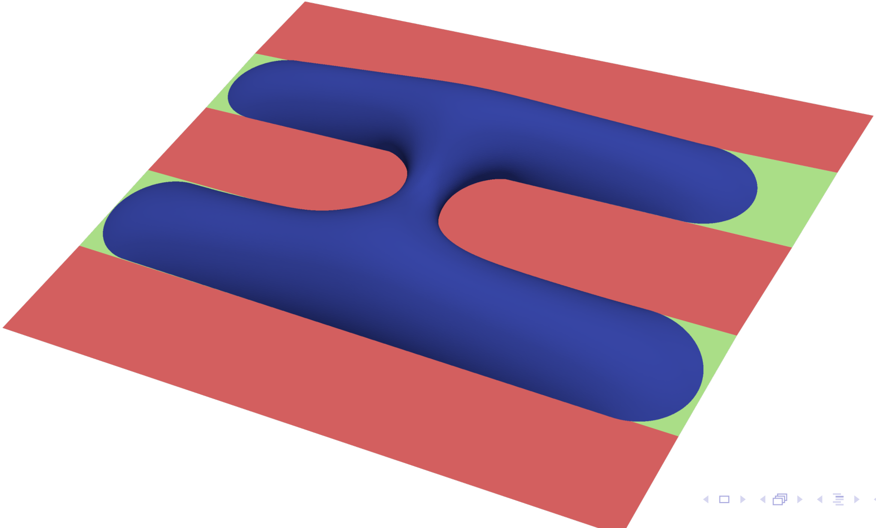
$$\boxed{\sigma\cos\theta + \sigma_{\mathrm{w}} = 0.} \tag{4}$$

- For more details, see Chapter 1 of [Fri21].

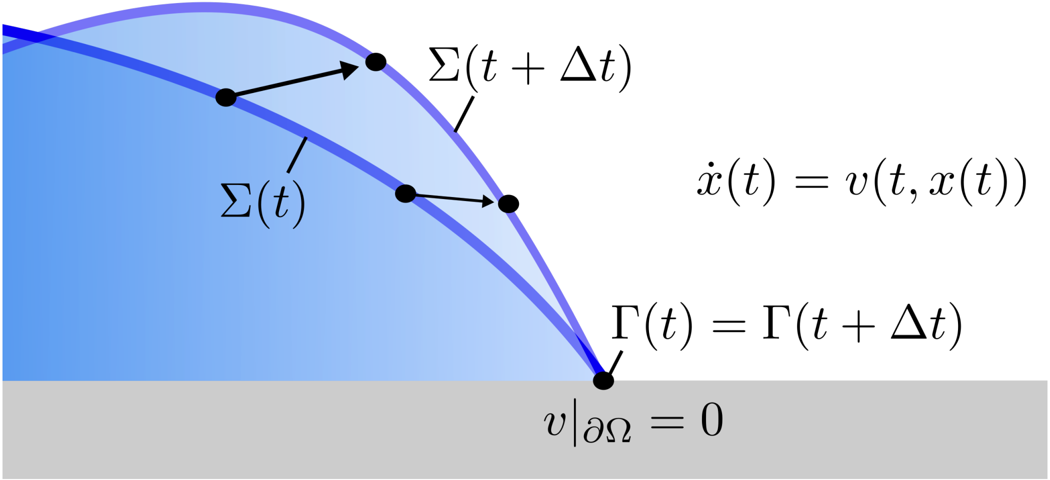


Stationary shapes for structured surfaces

- The variational approach can also be applied numerically for more complex cases.
- We used **Surface Evolver** [BB12] to compute the (nearly critical) shape of a droplet on a chemically structured surface [Har+21].
- This allowed us to study the subsequent **dynamic breakup process** in great detail.



The dynamics of wetting and the Huh-Scriven paradox



- The no slip boundary condition at the solid is incompatible with a moving contact line [HS71].

Continuum mechanical modeling framework

- We apply the sharp interface two-phase Navier Stokes equations (see lecture by Dieter Bothe) for Newtonian fluids under isothermal conditions.

$$
\begin{aligned}
\rho \frac{Dv}{Dt} - \eta \Delta v + \nabla p = b, \quad \nabla \cdot v = 0, &\quad \text{in } \Omega \setminus \Sigma(t), \\
[\![v]\!] = 0, \quad [\![p\mathbb{1} - S]\!]\, n_\Sigma = \sigma \kappa n_\Sigma, &\quad \text{on } \Sigma(t), \\
v_\perp = 0 &\quad \text{on } \partial\Omega, \\
V_\Sigma = v \cdot n_\Sigma &\quad \text{on } \Sigma(t).
\end{aligned}
\tag{5}
$$

- Viscous stress tensor: $S = \eta(\nabla v + \nabla v^{\mathsf{T}})$
- **Goal:** Derive boundary conditions to model
  1. The **wettability** of the solid and
  2. the **mobility** of the contact line (i.e. the tangential velocity $v_{||}$ at the solid boundary).

Dissipative mechanisms in wetting

- We define the free energy functional

$$E(t) := \int_{\Omega\setminus\Sigma(t)} \frac{\rho v^2}{2}\, dV + \int_{\Sigma(t)} \sigma\, dA + \int_{W(t)} \sigma_w\, dA.$$

- We compute the rate of change $\dot{E}$ for a solution of (5) (for $b = 0$)

$$\boxed{\frac{dE}{dt} = -2\int_{\Omega\setminus\Sigma(t)} \eta D : D\, dV + \int_{\partial\Omega} v_{\|} \cdot (S n_{\partial\Omega})_{\|}\, dA + \sigma \int_{\Gamma(t)} (\cos\theta - \cos\theta_0)\, V_\Gamma\, dl.} \tag{6}$$

- For details of the proof of (6), see [Fri21] (Appendix A).
- **Closure relations** are required to satisfy the second law of thermodynamics $\dot{E} \leq 0$.

The Navier Slip condition

- **The Navier Slip Condition:** A linear closure relation for $\int_{\partial\Omega} v_{\|} \cdot (Sn_{\partial\Omega})_{\|}\, dA$ reads as

$$-\lambda v_{\|} = (Sn_{\partial\Omega})_{\|} \quad \Leftrightarrow \quad -v_{\|} = 2\frac{\eta}{\lambda}(Dn_{\partial\Omega})_{\|}, \tag{7}$$

  where $\lambda \geq 0$ is a constant (friction coefficient).
- The parameter $L := \eta/\lambda$ is called the "Navier slip length".

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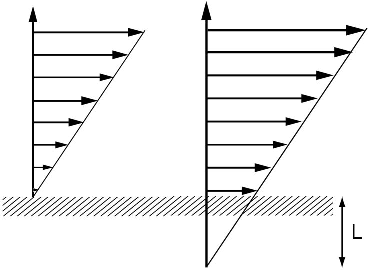

- The slip length controls the amount of tangential slip at a given shear rate.
- Finite slip (i.e. $L > 0$) (partially) regularizes the Huh Scriven singularity [HM77].
- A **logarithmic singularity** for the pressure and the curvature at the moving contact line remains (provided that $L < \infty$).
- The total dissipation rate is finite.
- Note: L is expected to be on the **nanometer scale** ($\rightarrow$ high computational costs!).

Contact line dissipation and contact angle models

- To complete the mathematical model, we need another **constitutive equation** which makes sure that

$$\sigma \int_{\Gamma(t)} (\cos\theta - \cos\theta_0)\, V_\Gamma \, dl \leq 0.$$

- V_Γ: normal speed of the contact line (positive for advancing contact line, negative for receding contact line).
- **Linear** closure relation (see Molecular Kinetic Theory of Wetting [BH69; Bla06])

$$\zeta V_\Gamma = \sigma(\cos\theta_0 - \cos\theta).$$

- More generally:

$$\theta = f(V_\Gamma)$$

  where f satisfies the inequality

$$V_\Gamma (f(V_\Gamma) - \theta_0) \geq 0.$$

Summary: "Standard Model" for Moving Contact Lines

- The "standard model"[1] based on the Navier slip condition reads as

$$
\begin{aligned}
\rho\frac{Dv}{Dt} - \eta\Delta v + \nabla p = b, \quad \nabla\cdot v = 0, &\quad \text{in } \Omega\setminus\Sigma(t),\\
[\![v]\!] = 0, \quad [\![p\mathbb{1} - S]\!]\, n_\Sigma = \sigma\kappa n_\Sigma, &\quad \text{on } \Sigma(t),\\
v_\perp = 0, \quad \lambda v_{||} + (S n_{\partial\Omega})_{||} = 0, &\quad \text{on } \partial\Omega,\\
V_\Sigma = v\cdot n_\Sigma, &\quad \text{on } \Sigma(t),\\
V_\Gamma = v\cdot n_\Gamma, \quad \theta = f(V_\Gamma), &\quad \text{on } \Gamma(t),
\end{aligned}
\tag{8}
$$

where we require that

$$\eta \geq 0,\ \sigma \geq 0,\ \lambda \geq 0,\ V_\Gamma(f(V_\Gamma) - \theta_0) \geq 0.$$

[1]Note: The mathematical model (8) is one of the most commonly applied models for dynamic wetting in the literature. However, there are many more modeling approaches which aim at a regularization of the singularity and a prediction of the dynamics of wetting. For a survey of the field, we refer to the references [GBQ04; Bla06; Shi08; Bon+09; SA13; MC22]

Outline

A numerical benchmark for dynamic wetting simulations

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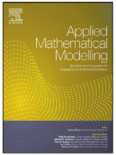
journal homepage: www.elsevier.com/locate/apm



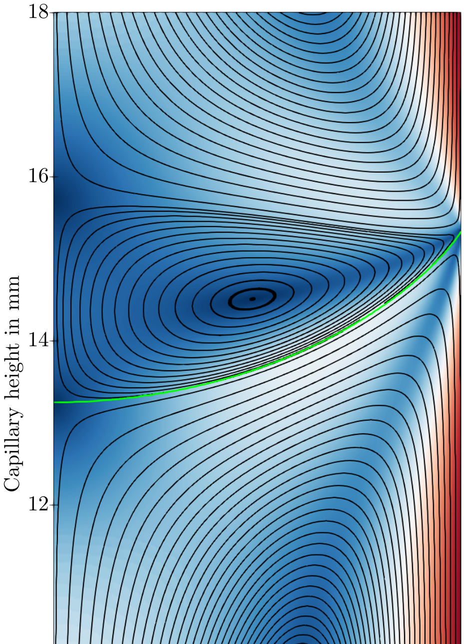
A comparative study of transient capillary rise using direct numerical simulations

D. Gründing[a], M. Smuda[b], T. Antritter[c], M. Fricke[a], D. Rettenmaier[d], F. Kummer[b], P. Stephan[c], H. Marschall[a], D. Bothe[a,*]

[a] *Institute for Mathematical Modeling and Analysis, Technische Universität Darmstadt, Germany*
[b] *Institute for Fluid Dynamics, Technische Universität Darmstadt, Germany*
[c] *Institute for Technical Thermodynamics, Technische Universität Darmstadt, Germany*
[d] *Institute for Fluid Mechanics and Aerodynamics, Technische Universität Darmstadt, Germany*

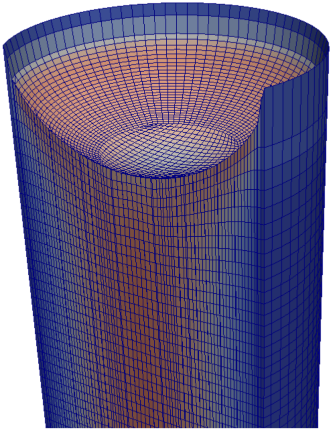
- Gründing et al.: *A comparative study of transient capillary rise using direct numerical simulations* [Grü+20a]

A numerical benchmark for dynamic wetting simulations



- **Observation:** There is a lack of accurate **reference** solutions.
- **Goal:** Establish a **numerical benchmark** for an instationary dynamic wetting problem.
- **Mathematical model:** Sharp interface two-phase Navier Stokes equations (8) with fixed contact angle and constant slip length.
- We provide an **extensive dataset** [Grü+20b] validated with **four different** numerical methods
  - OpenFoam ALE Interface Tracking
  - Geometrical Volume-of-Fluid (FS3D)
  - Algebraic Volume-of-Fluid InterFoam
  - Extended discontinuous Galerkin (BoSSS)
- Recent validation with **IsoAdvector**: Check out our recent preprint arXiv:2302.02629.

ALE Interface Tracking method



- We use the **Arbitrary-Lagrangian-Eulerian Interface Tracking** method in OpenFoam[a] originally developed by Željko Tuković and extended for dynamic wetting by Dirk Gründing [Grü20a].
- **Free surface** formulation
  (extension to two-phase flow ongoing, joint work with
  S. Raju, T. Maric, Z. Tuković).
- A **diffusion equation** is solved for the **mesh velocity** in the bulk to maintain a good mesh quality.
- The contact angle is **prescribed** during the advection step using the **control point algorithm** [TJ12].
- Extension to **"free contact angle"** evolution ongoing (joint work with S. Raju, T. Maric, Z. Tuković).
  $\Rightarrow$ Prerequisite for **force-based** wetting models.

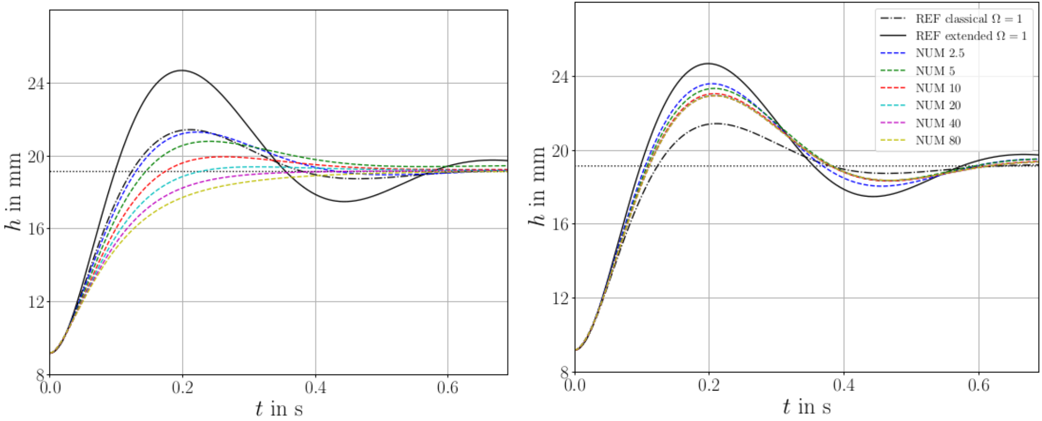
[a] See lecture notes by Željko Tuković for details.

No slip vs. Navier slip

- The **Navier slip** condition is used to regularize the moving contact line singularity

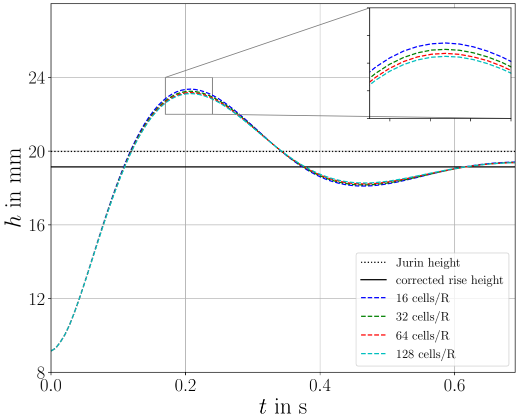
$$-\lambda v_{\|} = 2\eta (D n_{\partial\Omega})_{\|} \quad \text{at } \partial\Omega. \tag{9}$$

- **Note:** The slip length $L = \eta/\lambda$ must be **resolved** by the mesh.
  $\Rightarrow$ 3D simulations with a physical slip length $L \approx 1 \ldots 10\,\text{nm}$ are **infeasible**!
- We used a **very large slip length** ($1/50 \leq L/R \leq 1/5$) to obtain **mesh converged** solutions for numerical verification!

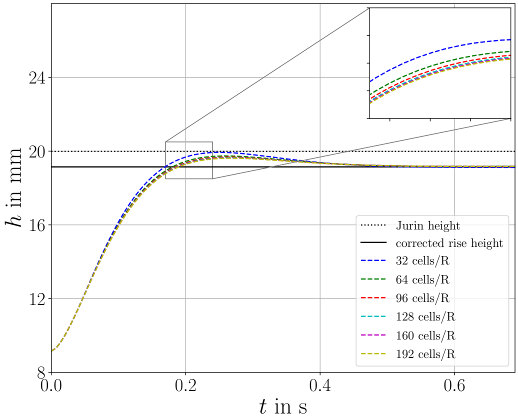


Influence of the slip length

- **Finding:** The slip length may change the character of the rise dynamics.

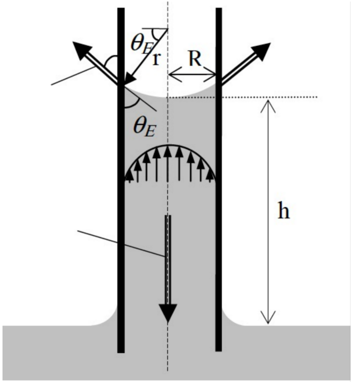


(a) $L = R/5$.



(b) $L = R/50$.

The classical model by Bosanquet



- **Classical model** due to Bosanquet (1923):

$$\boxed{2\pi R\sigma\cos\theta_0 = 8\pi\eta h\dot{h} + \frac{d}{dt}(\pi R^2 h\rho\dot{h}) + \pi R^2 h\rho g.} \qquad (10)$$

"Capillary force = Viscous resistance + inertia + gravity"

- **Simplifying assumptions:** Flat interface Σ (to compute M), Poiseuille flow profile (with no slip condition).

$$\text{Volume: } V = \pi R^2 h, \quad \text{Mass: } M = \rho V,$$

$$\text{Momentum: } P = M\dot{h}.$$

- Details of the flow near the contact line are **not** considered. $\rightarrow$ Dissipation close to the contact line and at the contact line are neglected!

Non-dimensional form

- Using the length and time scales

$$h_0 = \frac{2\sigma \cos\theta_0}{\rho g R} \quad \text{and} \quad t_{\text{ref}} = \sqrt{h_0/g}$$

in (10), one arrives at the non-dimensional form

$$\boxed{1 = (HH')' + \Omega\, HH' + H.} \qquad (11)$$

- Here $H(\tau) = h(\tau\, t_{\text{ref}})/h_0$ is the dimensionless rise height. The **dimensionless group**

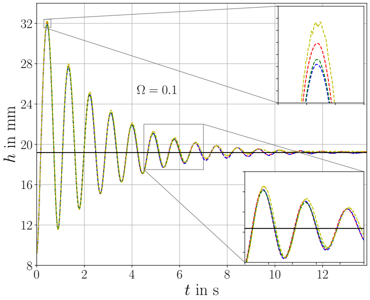
$$\boxed{\Omega = \sqrt{\frac{128\eta^2 \sigma \cos\theta_0}{R^5 \rho^3 g^2}} = \sqrt{128 \cos\theta_0}\, \frac{\text{Oh}}{\text{Bo}}.}$$

governs the behaviour of solutions of the ODE model (10).

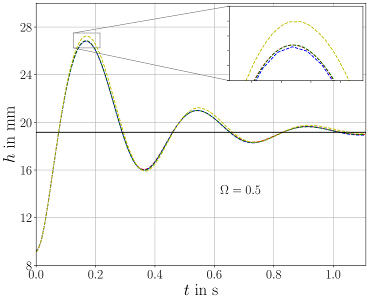
- Quéré showed that a **regime transition** for (11) occurs at

$$\Omega_c = 2.$$

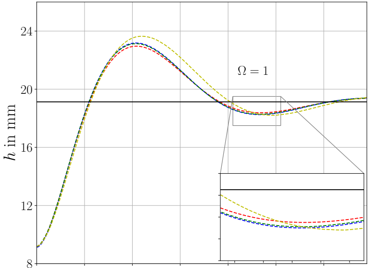
Variation of the parameter Ω in the DNS

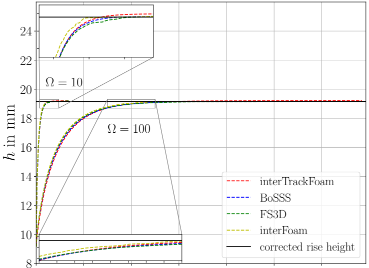


(a) $\Omega = 0.1$



(b) $\Omega = 0.5$





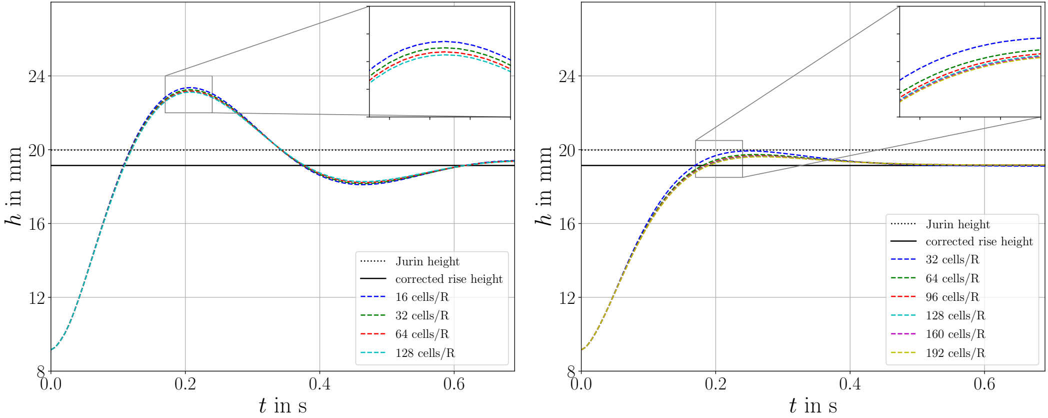
Outline

Guiding research question

- Can we derive a **generalization** of Quere's critical condition?

$$\Omega = \sqrt{\frac{128\eta^2\sigma\cos\theta_0}{R^5\rho^3 g^2}} < 2$$

- The parameter Ω does **not involve** the friction λ (hence the slip length)!



(a) $L = R/5$.　(b) $L = R/50$.

Capillary rise with dynamic contact angle effect

- **Dynamic contact angle model:** The Molecular Kinetic Theory yields (as Ca $\to$ 0)

$$\sigma\,(\cos\theta_0 - \cos\theta) = \zeta\, V_\Gamma \tag{12}$$

with a friction coefficient $\zeta \geq 0$. This leads to a quadratic form for the dissipation

$$\sigma \int_{\Gamma(t)} (\cos\theta - \cos\theta_0)\, V_\Gamma\, dl = -\zeta \int_{\Gamma(t)} V_\Gamma^2\, dl \leq 0.$$

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- The resulting model reads as (see Martic et al., Langmuir, 2002 [Mar+02])

$$\frac{2}{R}\sigma\cos\theta_{eq} = \frac{8\eta}{R^2}h\dot{h} + \rho\frac{d}{dt}(h\dot{h}) + \rho g h + \frac{2}{R}\zeta\dot{h}. \tag{13}$$

$\Rightarrow$ Dissipation **at the contact line** is added to the classical model.

- The new term $\propto \dot{h}$ has a different **mathematical structure**.

$\Rightarrow$ A **second non-dimensional parameter** is introduced into the problem.

Capillary rise with dynamic contact angle effect

- Experimental data by Quéré [Qué97] (open circles) are well described.
- **Best fit for the friction:** $\zeta = 80\,\text{mPa}\cdot\text{s}$.
- **Regime transition** is observed: (a) $\zeta = 80\,\text{mPa}\cdot\text{s}$, (b) $\zeta = 0$.

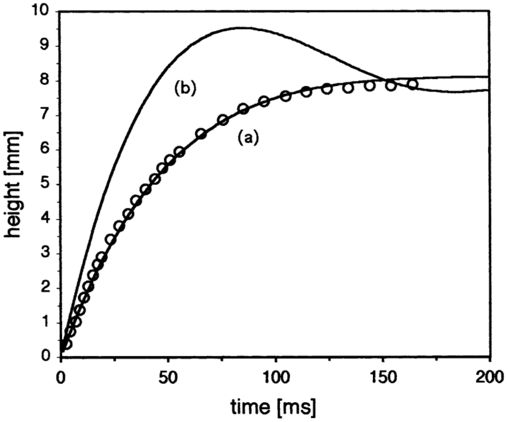


Figure: Results for ethanol from (Martic et al.,2003).

Critical condition for "Martic type" models

- We study models of the general form

$$(HH')' + \Omega\, HH' + \beta H' + H = 1. \tag{14}$$

- The parameter β may originate from different physical mechanisms. For example, in Martic's model, we have

$$\beta = \frac{\zeta}{\sqrt{\sigma \rho R \cos\theta_0}}.$$

- We show[2] that the generalization of the critical condition reads as

$$\boxed{\Omega + \beta < 2.} \tag{15}$$

- Hence, the oscillatory regime is **shifted** towards smaller values of Ω for positive β.

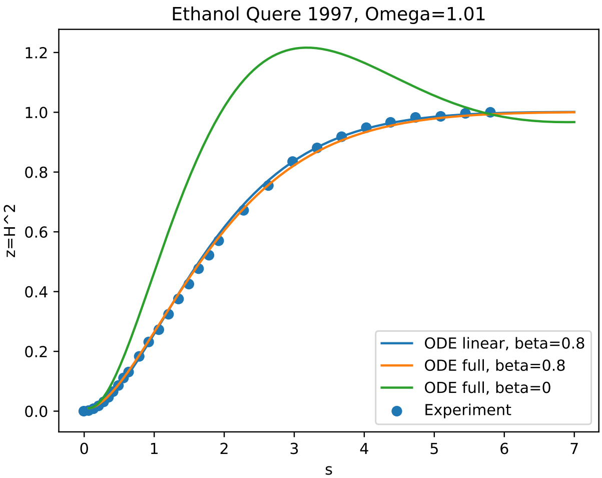
[2] This part is joint work with El Assad Ouro-Koura (B. Sc.). His Bachelor Thesis on the topic has the title "Zur mathematischen Modellierung des kapillaren Anstiegs: Dissipative Mechanismen und nicht-lineare Oszillationen", TU Darmstadt (2023).

Comparison with experimental data (I)

- Using the fit from Martic et al. for the data for ethanol by Quere, we have

$$\beta = \frac{\zeta}{\sqrt{\sigma \rho R \cos\theta_0}} \approx \frac{80\,\mathrm{mPa}\cdot\mathrm{s}}{107\,\mathrm{mPa}\cdot\mathrm{s}} \approx 0.75, \quad \Omega \approx 1.01.$$

- We expect **oscillations** since $\Omega + \beta \approx 1.8 < 2$ (!).



Comparison with experimental data (II)

- In fact, the **analytical theory** gives more information than just the critical damping.
- From a linearization of the problem, we obtain[3]

$$H(s)^2 \approx 1 + A \exp\left(-\frac{\Omega+\beta}{2} s\right) \cos(\omega s + \phi), \tag{16}$$

  where $\omega = \sqrt{1 - (\Omega+\beta)^2/4}$.
- Note that the dimensionless time-period of oscillation

$$S = \frac{2\pi}{\sqrt{1-(\Omega+\beta)^2/4}} \to \infty \quad \text{as} \quad \Omega + \beta \to 2$$

  goes to infinity as the critical damping is approached. The **exponential decay part** will dominate in this case.
- In the present example, we have

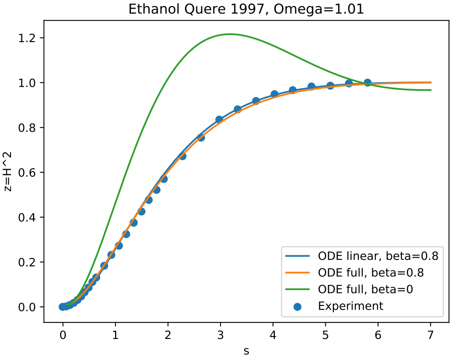
$$S = \frac{2\pi}{\sqrt{1-1.8^2/4}} \approx 14.4.$$

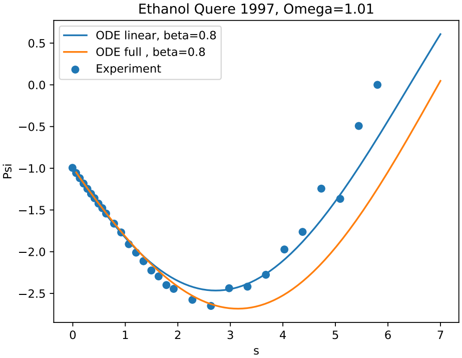
[3] For more details, please take a look at our publication [Fri+23].

Comparison with experimental data (III)

- **Idea:** We can visualize the **oscillatory part** of the solution (16) by factoring out the exponential decay. I.e. we plot the function

$$\Psi(s) := \exp\left(\frac{\Omega+\beta}{2}\,s\right)\left(H(s)^2-1\right).$$



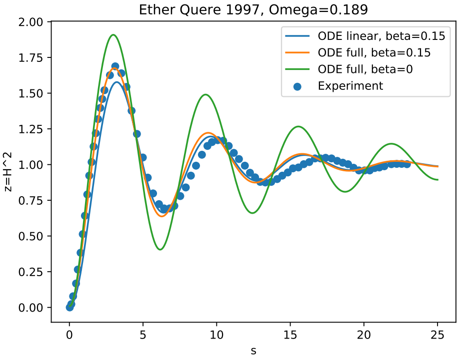


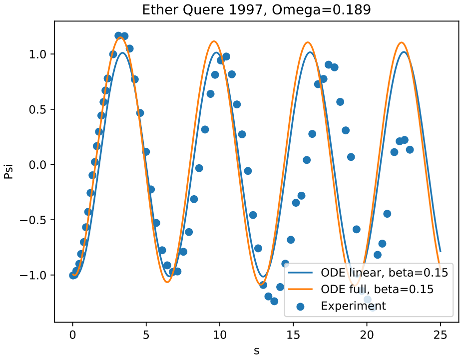
- Indeed, the oscillation is **confirmed** from the experimental data.

Comparison with experimental data (IV)

- The model is also able to describe the strong oscillations of **ether** in [Qué97] quite well. In this case, the system is far from critical damping.

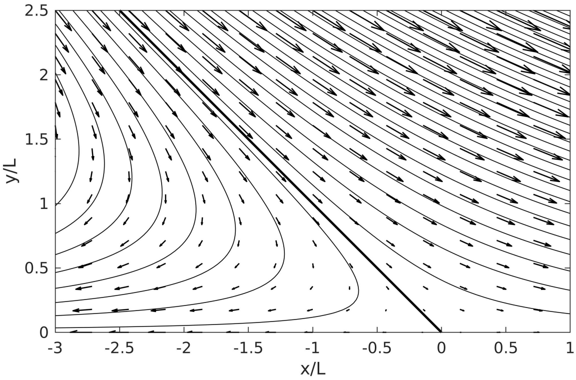
$$\Omega \approx 0.19, \quad \beta \approx 0.15 \quad \Rightarrow \Omega + \beta \approx 0.34 < 2.$$





Including dissipation near the contact line: The model by Gründing

- D. Gründing: *An enhanced model for the capillary rise problem*, International Journal of Multiphase Flow (2020) [Grü20b]
- **Major contribution:** Modeling of viscous dissipation in the **contact line vicinity**.
  $\Rightarrow$ Effect of the **slip length** on the dissipation can be modeled.
- Known **asymptotic solutions** are used ($\Delta^2\psi = 0$, stream function ψ).



Including dissipation near the contact line: The model by Gründing

- The model in two spatial dimensions reads as (for $L = \eta/\lambda \ll R$)

$$\boxed{\rho\frac{\mathrm{d}}{\mathrm{d}t}(h\dot{h}) = -\frac{3\eta}{R^2}\dot{h}h - \frac{\eta\bar{h}}{RL}\dot{h} + \frac{\sigma\cos\theta_0}{R} - \rho g h + \frac{6}{5}\rho\dot{h}^2.} \tag{17}$$

- Wedge dissipation term $\propto -\dot{h}/L$. $\Rightarrow$ **Formal equivalence** to Martic's model (up to some minor details).
- Observation: **Ill-posedness** of the original continuum problem as $L \to 0$ is recovered.
- Results about critical condition in Martic's model **carry over**.

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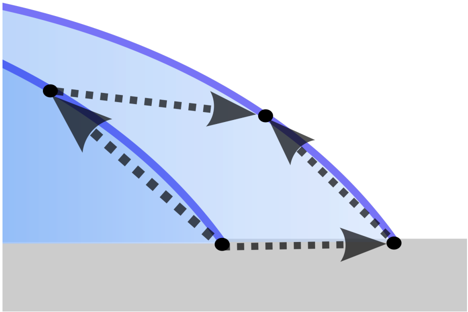
A fundamental question

How to distinguish the models? Are the models predictive?

Outline

Kinematics of moving contact lines in a nutshell



Assume that we are provided with

- a (sufficiently regular) **velocity field** $v = v(t, x)$ satisfying

$$v_\perp = 0 \quad \text{at } \partial\Omega$$

- and an **initial interface** $\Sigma(t_0) \subset \mathbb{R}^n$.

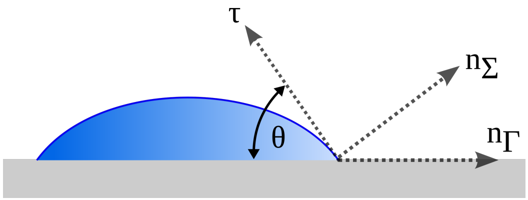
Then, we can **uniquely solve** for the evolution of the moving interface $\Sigma(t)$ using the characteristic equation

$$\begin{aligned} \dot{x}(t; t_0, x_0) &= v(t, x(t; t_0, x_0)), \\ x(t_0; t_0, x_0) &= x_0. \end{aligned} \tag{18}$$

Contact angle evolution equation

- **Important consequence:** The velocity field alone **determines** (by kinematics!) the evolution of the contact angle, provided that it is sufficiently **regular** and **tangential** to the solid boundary.
- In fact, we prove that (co-moving) **time-derivative of the contact angle** is given as

$$\boxed{\frac{D\theta}{Dt} = (\partial_\tau v) \cdot n_\Sigma.} \tag{19}$$



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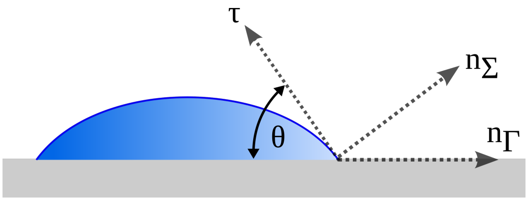


- **Finding:** The "standard model" (8) is **inconsistent** regarding the contact angle kinematics. ⇒ Only (at least weakly) **singular solutions** are possible.
- For more details, see our publications [FKB19] and [FMB20; FKB18; Fri21].

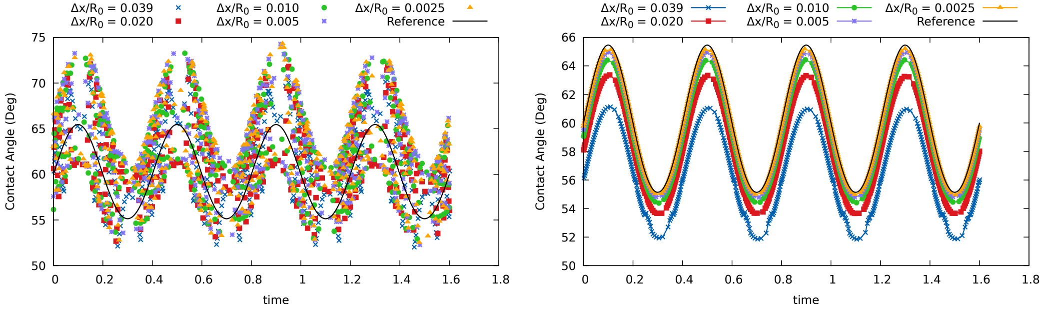
Contact line advection schemes

- **Goal:** Develop an interface advection scheme that is able to solve the advection problem (φ : phase indicator or level set)

$$\begin{aligned} \partial_t \varphi + v \cdot \nabla \varphi = 0, \quad t > 0,\ x \in \Omega, \\ \varphi(0, x) = \varphi_0(x), \quad x \in \Omega \end{aligned} \tag{20}$$

without prescribing a contact angle (provided that $v_\perp = 0$ at $\partial\Omega$).

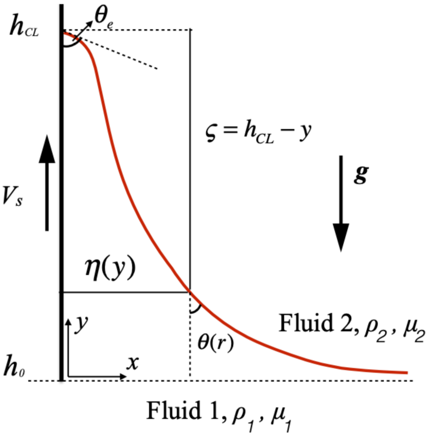
- **Key ingredient:** Second-order accurate interface reconstruction **at the boundary**, see our publications [FMB20] for GeoVOF and [FMB19] for Level Set.



(a) Boundary Youngs [FMB20].

(b) Boundary ELVIRA [FMB20].

Application: Generalized Navier Slip Condition (GNBC)



S. Afkhami, J. Buongiorno, A. Guion, Stéphane Popinet, Y. Saade, R. Scardovelli, S. Zaleski. Journal of Computational Physics, Elsevier, 2018

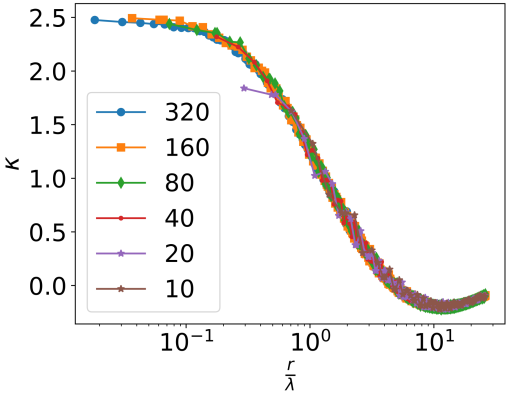
- **Application:** We implement the Generalized Navier Slip condition [QWS03; QWS06] in the Geometrical Volume-of-Fluid solver **Basilisk**.
- The contact angle is transported **kinematically** and an out-of-balance **Young stress** enters the velocity boundary condition

$$\lambda v_{\|} + (S n_{\partial\Omega})_{\|} = \sigma(\cos\theta_0 - \cos\theta) n_{\Gamma} f_{\varepsilon}(x).$$

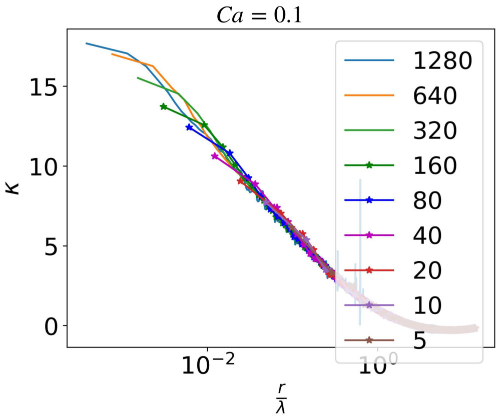
- Note: The contact angle is not prescribed, but an outcome of a local **balance of forces!**
- This is joint work with Y. Kulkarni, T. Fullana and S. Zaleski (Sorbonne University).

Regularization of the curvature singularity

- A **mesh convergent curvature at the moving contact line** is found with the new GNBC implementation using the kinematic contact angle transport.



(a) GNBC.

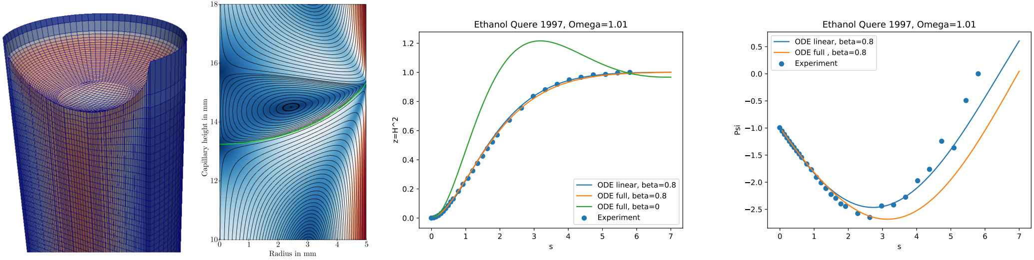


(b) Navier Slip.

Outline

Summary and Outlook

- Derivation of **complexity-reduced (ODE) models** guided by DNS.
- **Framework** for ODE models: Variational formulation using different **channels of dissipation** (to be modeled from DNS)[4].
- Mathematical analysis of ODE leads to new **physical insights**.
- Work in progress: **Calibration** of ODE models with DNS to make predictions **beyond** current DNS capabilities.
- **Long-term goal:** Subgrid-scale models for the moving contact line?



(a) DNS. (b) Local flow. (c) ODE model. (d) Oscillation.

[4]Please check out our publication [Fri+23] for more details.

Acknowledgements

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- The authors gratefully acknowledge the computing time provided to them on the **high-performance computer Lichtenberg** at the NHR Centers NHR4CES at TU Darmstadt. This is funded by the Federal Ministry of Education and Research, and the state governments participating on the basis of the resolutions of the GWK for national high performance computing at universities (www.nhr-verein.de/unsere-partner).

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