

Numerical Modelling of Two-Phase Flows with moving Contact Lines

Erik Gros

erik.gros@epfl.ch

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Academic Background

- 02.2013 - B. Sc. Mechanical Engineering, RWTH
Thesis: FEM simulation of viscoelastic flow
- 10.2014 - M. Sc. Aeronautical Engineering, RWTH
Thesis: moving mesh implementation in FVM solver
- Since 03.2015 - Ph. D. student at LTCM, EPFL
 - Numerical simulation of two-phase flows
 - ALE, FEM, two-phase flow simulator
 - Contact lines, annular flow

Overview

- THERMAPOWER
- Two-Phase Flow Introduction
- Microchannel Simulation Results
- Contact Lines
- Conclusion & Further Work

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THERMAPOWER

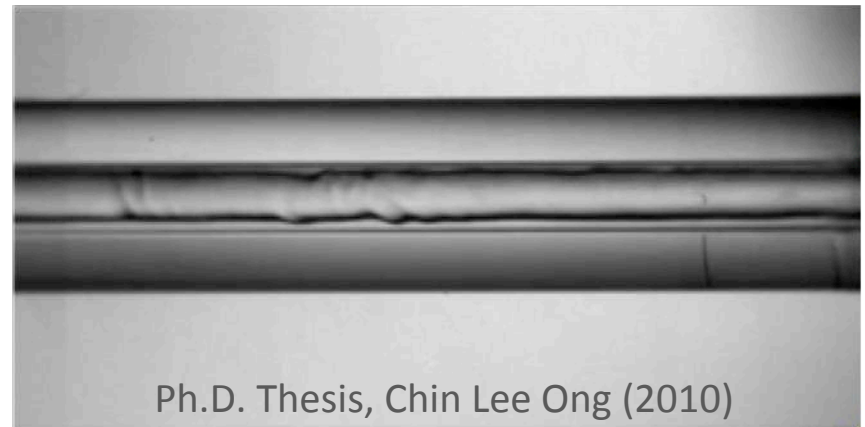
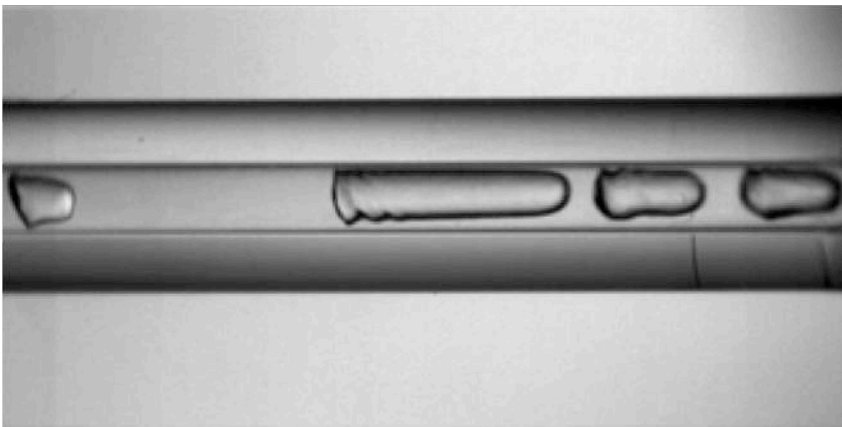
- Thermal Management of High Power Microsystems Using Multiphase Flows
- Funded by European Union
- Innovative cooling systems using two-phase flow for microelectronic devices
- Partner Universities:
 - University of Edinburgh, Shanghai Jiaotong, EPFL, University of Maryland, University of Nottingham and UERJ.

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Two-phase flow in microchannels

- Higher heat fluxes compared to single-phase cooling
- Small scales make it difficult to perform quantitative measurements
- Numerical simulation well suited
- Typical flow conditions slug or annular flow:



Ph.D. Thesis, Chin Lee Ong (2010)

Governing Equations

- One fluid formulation
- Incompressible Navier-Stokes equations:

$$\frac{D\vec{v}}{Dt} = \frac{\partial \vec{v}}{\partial t} + (\vec{v} - \vec{v}_{mesh}) \cdot \nabla \vec{v} = -\frac{\nabla p}{\rho} + \frac{\mu}{Re} \nabla \left(\nabla \vec{v} + (\nabla \vec{v})^T \right) + \frac{\vec{g}}{Fr^2} + \boxed{\frac{\sigma}{We} \kappa \vec{n} \delta} \text{ surface tension}$$

$$\nabla \cdot \vec{v} = 0$$

$$Re = \frac{\bar{\rho} \bar{v}_{\infty} \bar{L}}{\bar{\mu}}, \quad We = \frac{\bar{\rho} \bar{v}_{\infty}^2 \bar{L}}{\bar{\sigma}}, \quad Fr = \frac{\bar{v}_{\infty}}{\sqrt{\bar{g} \bar{L}}}$$

Governing Equations

- One fluid formulation
- Incompressible Navier-Stokes equations:

inertia / viscous

$$Re = \frac{\bar{\rho} \bar{v}_{\infty} \bar{L}}{\bar{\mu}},$$

inertia / surface
tension

$$We = \frac{\bar{\rho} \bar{v}_{\infty}^2 \bar{L}}{\bar{\sigma}},$$

inertia / gravity

$$Fr = \frac{\bar{v}_{\infty}}{\sqrt{\bar{g} \bar{L}}}$$

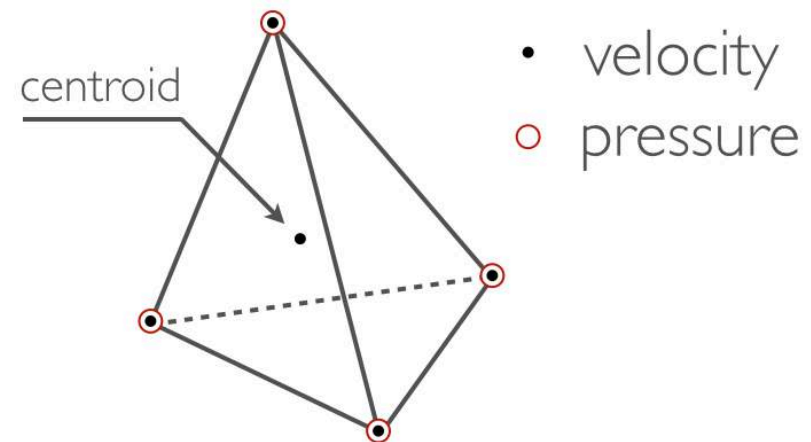
Discretization

- Time derivative: Semi Lagrangian method

$$\frac{D\phi(\vec{x}, t)}{Dt} \approx \frac{\phi(\vec{x}, t + \Delta t) - \phi(\vec{x} - \vec{v}^n \Delta t, t)}{\Delta t}$$

- Spatial derivatives:

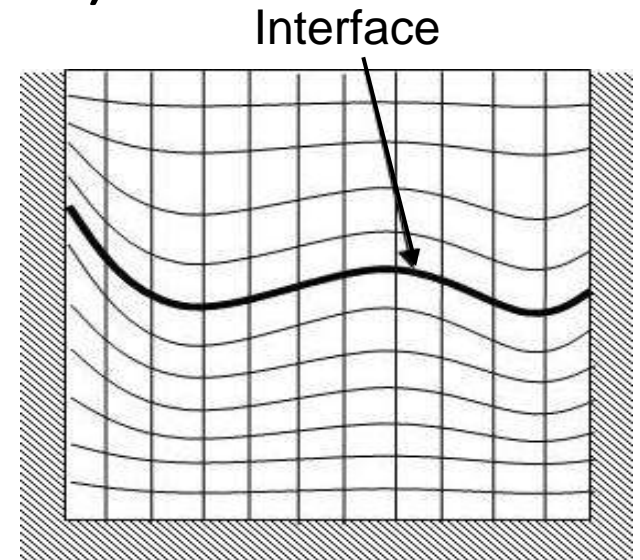
- Finite Element Method (FEM)
- LBB -> Mini Element
- Unstructured mesh
- 2d: triangular/ 3d: tetrahedral elements



Interface tracking

- Arbitrary Lagrangian Eulerian (ALE)

- Interface: Lagrangian
- Boundaries: Eulerian
- Inside: “arbitrary”
- Remeshing and smoothing operations to avoid mesh quality degradation



- + sharp interface, better resolution, no additional equations like VOF, Level-Set...
- expensive mesh operations, topology changes

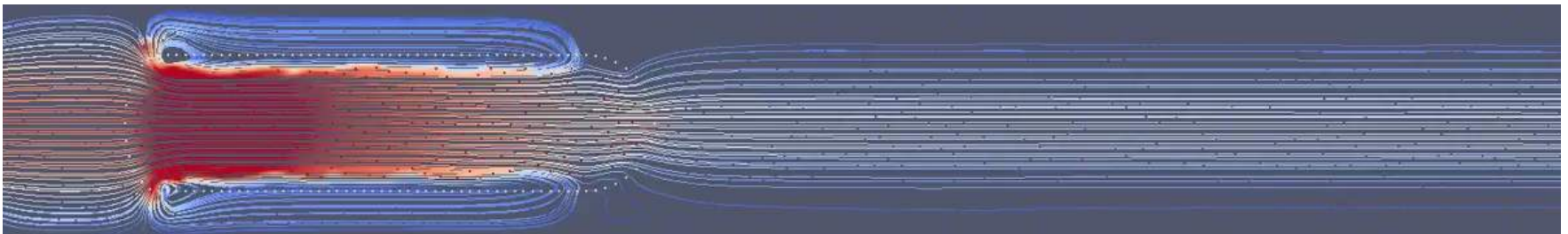
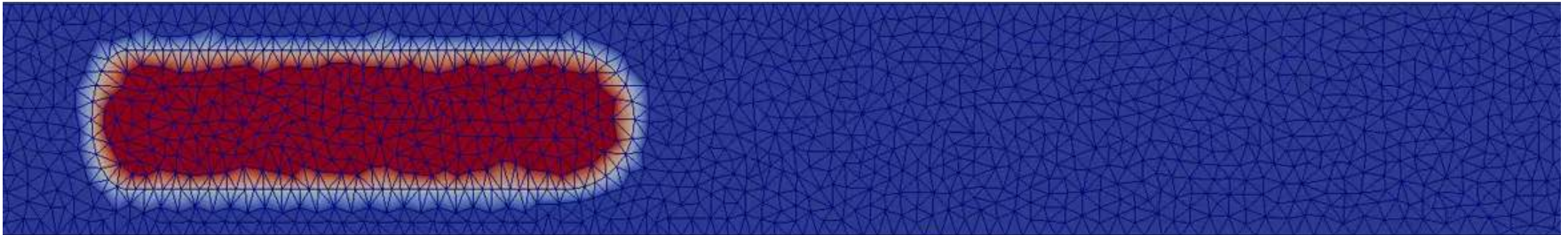
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- **Microchannel Simulation Results**
- Contact Lines
- Conclusion & Further Work

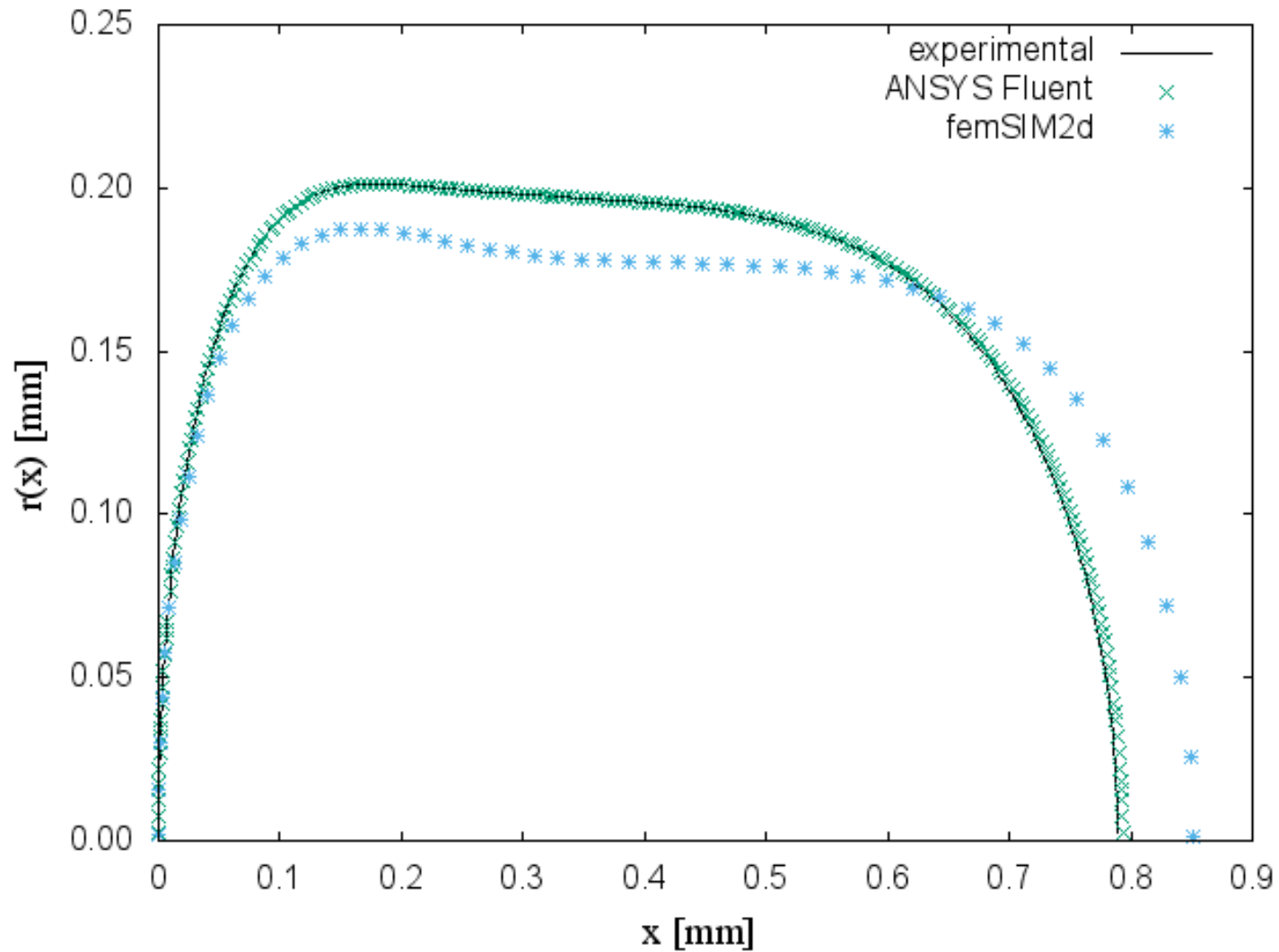
Microchannel Simulation

- Single elongated air bubble in glycerol solution:

$$Re = 0.0128552, \quad We = 0.00127691, \quad \frac{\rho_{in}}{\rho_{out}} = 9.632 \cdot 10^{-4}, \quad \frac{\mu_{in}}{\mu_{out}} = 3.455 \cdot 10^{-5}$$



Microchannel Simulation

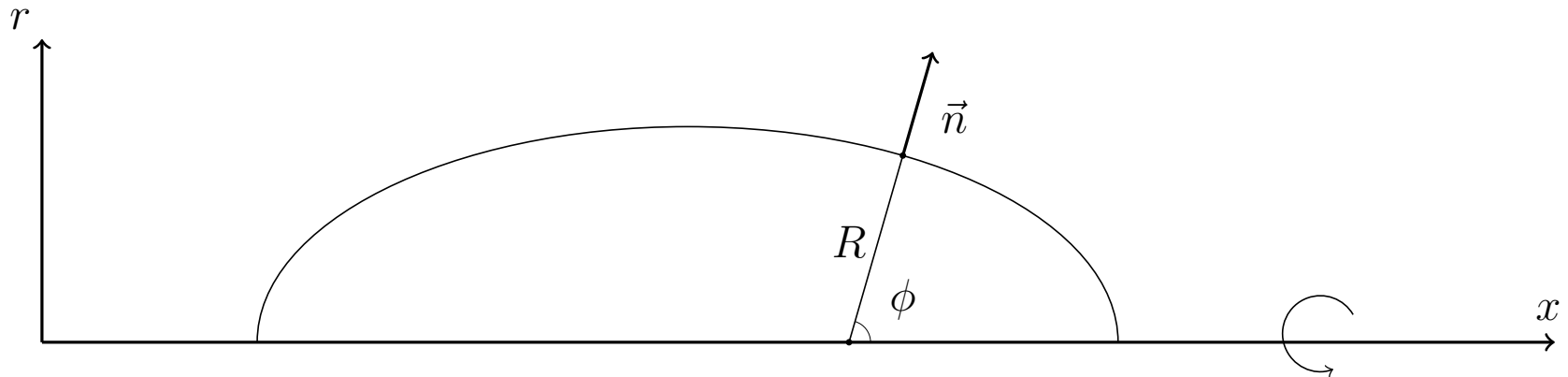


Axisymmetric Formulation

$$\rho \frac{Dv_x}{Dt} = -\frac{\partial p}{\partial x} + \mu \Delta v_x \quad \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} = 0$$

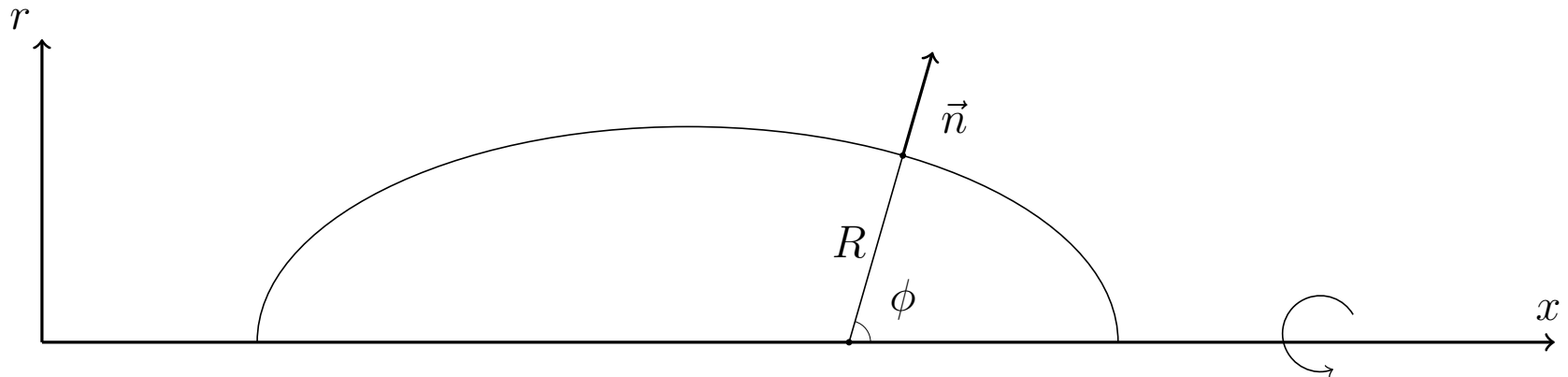
$$\rho \frac{Dv_r}{Dt} = -\frac{\partial p}{\partial r} + \mu \left(\Delta v_r - \frac{v_r}{r^2} \right)$$

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r}$$



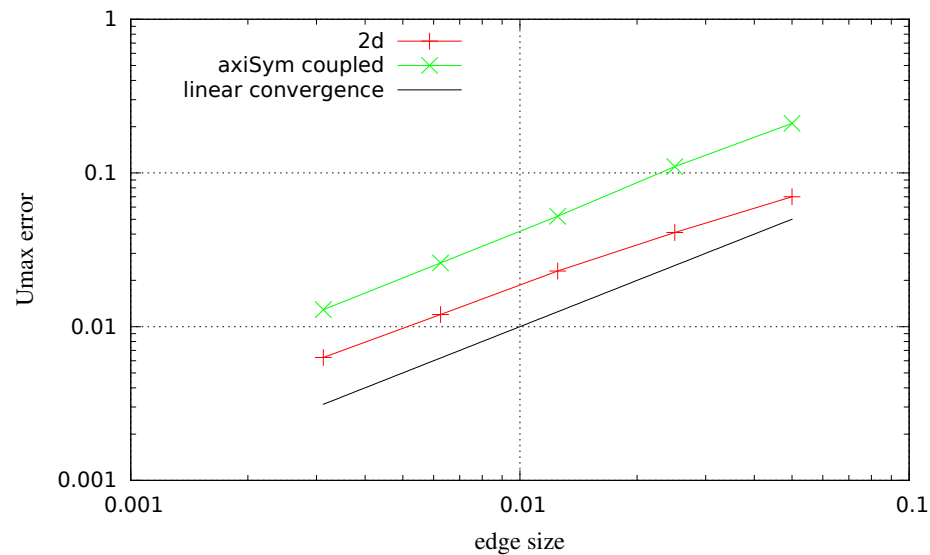
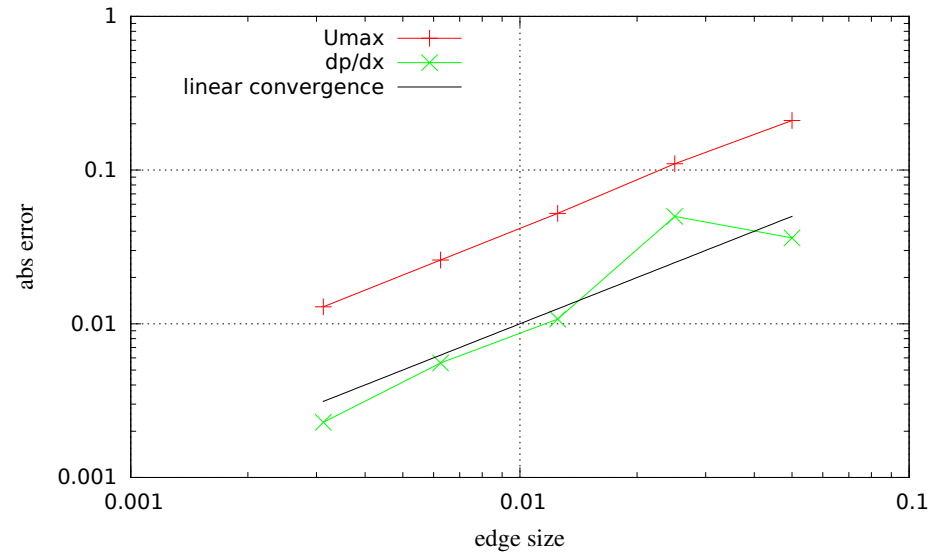
Axisymmetric Formulation

$$\begin{aligned}\rho \frac{Dv_x}{Dt} &= -\frac{\partial p}{\partial x} + \mu \Delta v_x & \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} &= 0 \\ \rho \frac{Dv_r}{Dt} &= -\frac{\partial p}{\partial r} + \mu \left(\Delta v_r - \frac{v_r}{r^2} \right) & \Delta &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r}\end{aligned}$$



$$\kappa_{axi} = \kappa_{2d} + \frac{1}{R} = \kappa_{2d} + \frac{\sin(\phi)}{r}$$

Convergence with Mesh Refinement

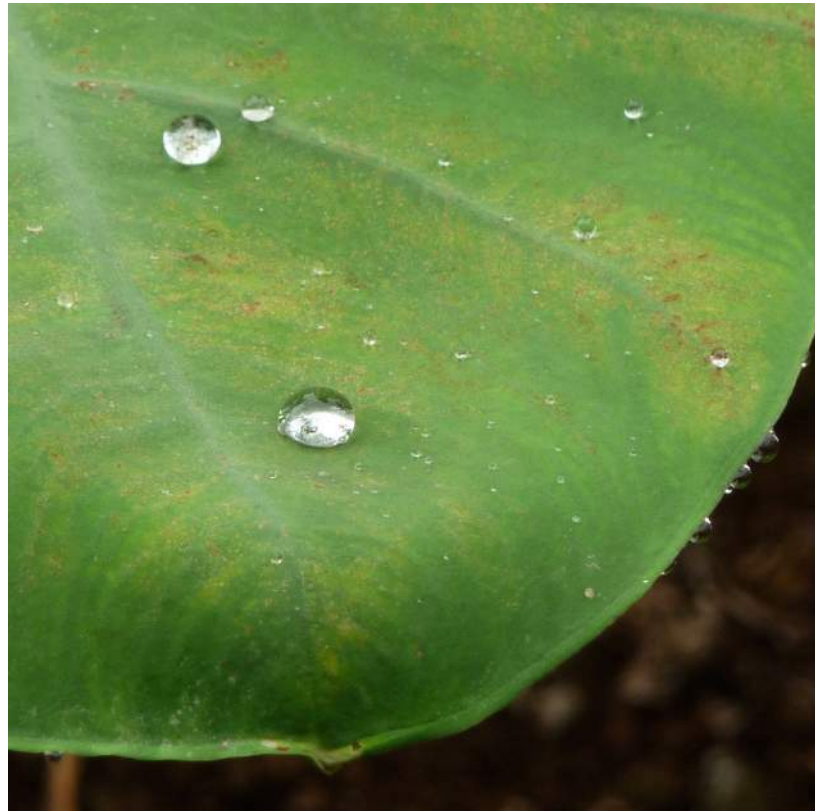


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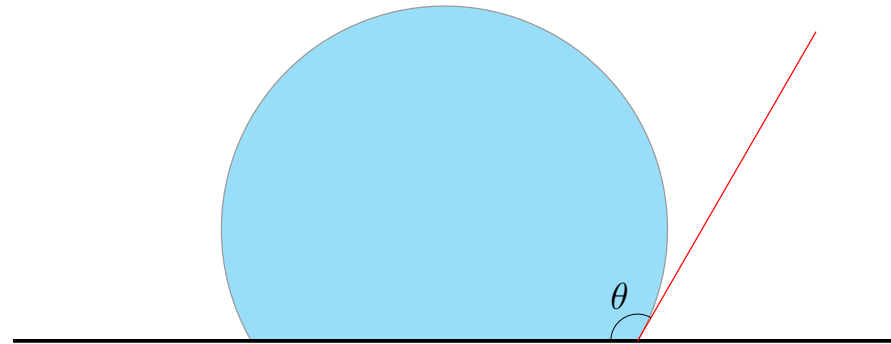
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Contact Line

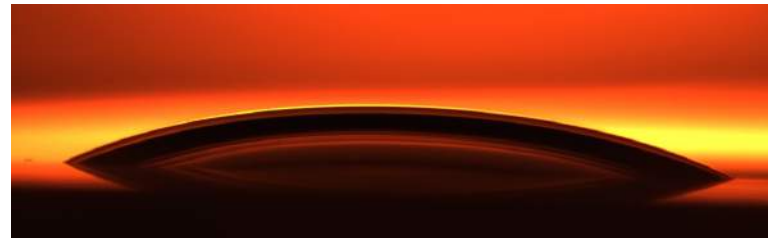
- Region of interaction of three different materials



Contact angle



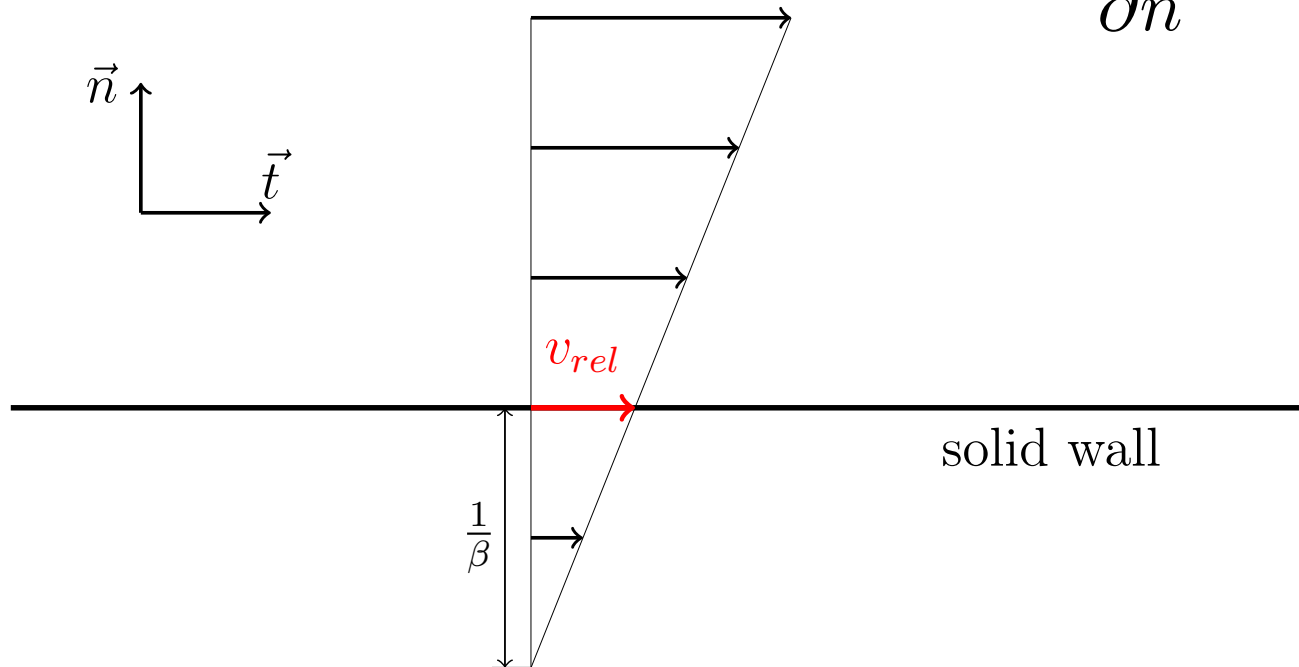
- Young's equation: $\sigma_{gs} = \sigma_{ls} + \sigma_{lg} \cos(\theta)$



Moving Contact Lines

- The moving contact line problem
- Navier-Slip b.c.

$$\tau \propto \frac{\partial v_t}{\partial n} = \beta v_{rel}$$



Moving Contact Lines

- The moving contact line problem
- Navier-Slip b.c.

$$\vec{n} \cdot \vec{v}_{rel} = 0$$

$$\vec{t} \cdot \boldsymbol{\sigma}(\vec{v}, p) \vec{n} = \beta \vec{t} \cdot \vec{v}_{rel}$$

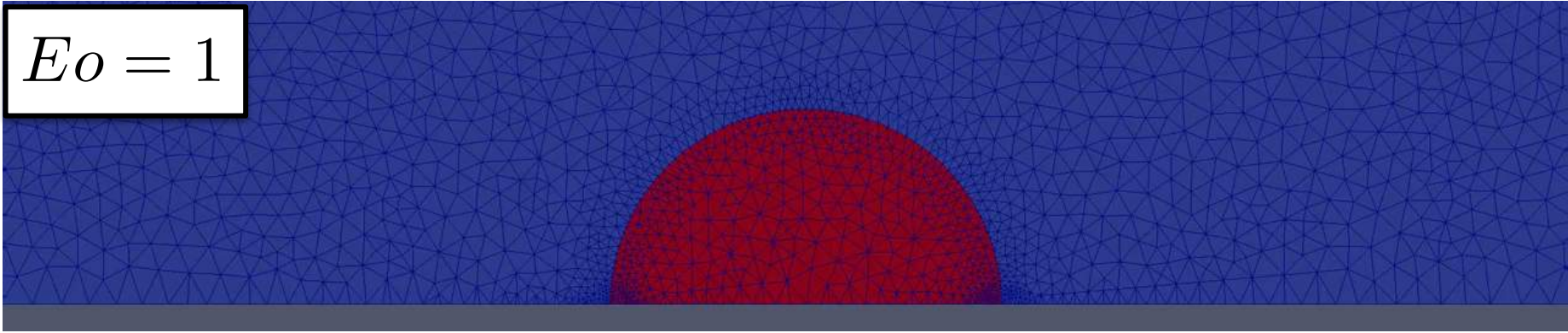
$$\vec{b} \cdot \boldsymbol{\sigma}(\vec{v}, p) \vec{n} = \beta \vec{b} \cdot \vec{v}_{rel}$$

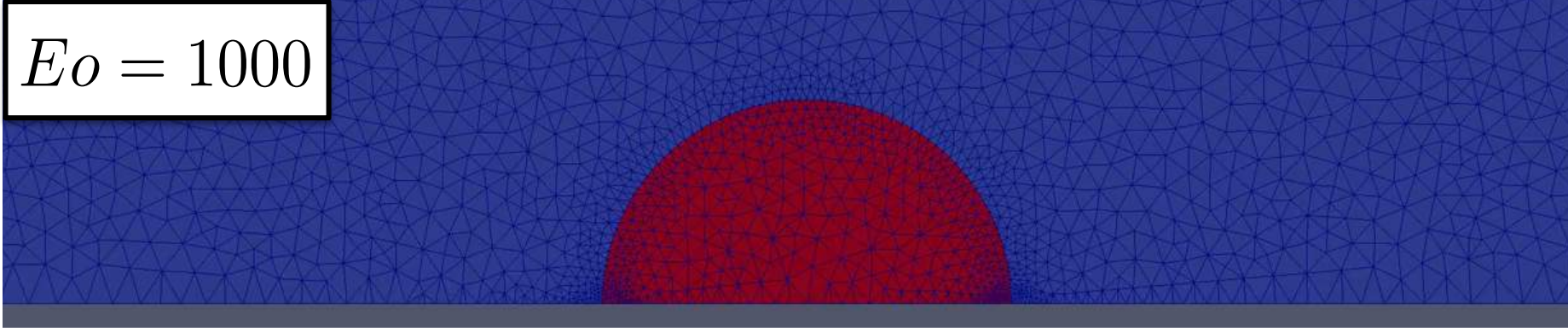
$$\vec{v}_{rel} = \vec{v} - \vec{v}_{wall}$$

Drop Spreading on a Surface

$$\theta = 50^\circ, \quad \frac{\rho_{in}}{\rho_{out}} = 100, \quad \frac{\mu_{in}}{\mu_{out}} = 1.111$$

$$Eo = \frac{We}{Fr^2}$$

$$Eo = 1$$
A numerical simulation showing a red drop spreading on a blue surface. The drop is in an intermediate state, partially flattened. The background is a fine triangular mesh. A thin grey line at the bottom represents the solid surface.

$$Eo = 1000$$
A numerical simulation showing a red drop spreading on a blue surface. Compared to the Eo = 1 case, this drop is significantly more flattened and spread out. The background is a fine triangular mesh. A thin grey line at the bottom represents the solid surface.

Drop Spreading on a Surface

- Height of the bubble at steady-state

➤ **$Eo \gg 1$:**

$$h_{\infty} = 2 \sqrt{\frac{\sigma}{\rho_l g}} \sin\left(\frac{\theta}{2}\right)$$

➤ **$Eo \ll 1$:** (no gravity \Rightarrow spherical cap)

$$h_{\infty} = R_0 (1 - \cos(\theta)) \sqrt{\frac{\pi}{2\theta - \sin(2\theta)}}$$

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Conclusion & Further Work

- For problems with rotational symmetry axisymmetric formulation is very efficient
- Moving contact lines: imposing static contact angle can already give meaningful results
- Next steps:
 - Navier-Slip boundary condition
 - Dynamic contact angle
 - Periodic boundary conditions
 - Annular flow simulation

Thank you for your attention!