Fractional Time-Stepping Techniques for Moving Contact Lines

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Nonstandard Discretizations for Fluid Flows
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Acknowledgments

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The Contact Line Paradox

The Generalized Navier Boundary Condition

Diffuse Interface Approach

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The Contact Line Paradox

The motion of a viscous incompressible two-fluid system can be described by

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\begin{cases}
\rho_t + \nabla\cdot(\rho \mathrm{u}) = 0, & \text{in } \Omega \times (0, T], \\
\rho(\mathrm{u}_t + \mathrm{u}\cdot\nabla \mathrm{u}) - \nabla\cdot\left(2\eta\varepsilon(\mathrm{u})\right) + \nabla \mathrm{p} = \rho \mathbf{f} + \gamma H \mathbf{n}_\Sigma \delta_\Sigma, & \text{in } \Omega \times (0, T], \\
\nabla\cdot \mathrm{u} = 0, & \text{in } \Omega \times (0, T], \\
\rho\big|_{t=0} = \rho_0, \quad \mathrm{u}\big|_{t=0} = \mathrm{u}_0, & \text{in } \Omega.
\end{cases}
$$

Where:

- $\Omega \subset \mathbb{R}^d$ $d = 2, 3$ is a fluid domain.
- $\mathbf{f}$ is an external driving force density (gravity).
- $\gamma H \mathbf{n}_\Sigma \delta_\Sigma$ is the surface tension at the interface Σ between the fluids.
- $\rho > 0$–density, u–velocity, p–pressure.

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The Contact Line Paradox

What boundary conditions?

- The "container" is impermeable. Therefore:

$$u \cdot \mathbf{n}|_{\Gamma} = 0,$$

  where $\Gamma = \partial\Omega$ and $\mathbf{n}$ is the unit normal to Γ.

- Impermeability implies that we do not need boundary conditions for the pressure and density.
- What about $u \times \mathbf{n}$?
- The usual condition is no-slip:

$$u|_{\Gamma} = 0.$$

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The Contact Line Paradox

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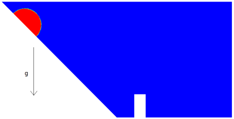
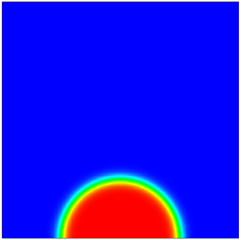
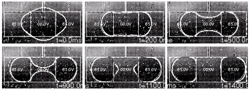


Droplet relaxation



Electrowetting on dielectric



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- *Eppur si muove.*
- This is the contact line paradox.

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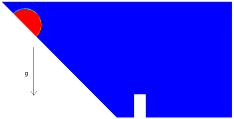

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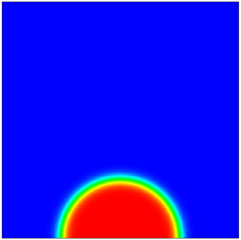

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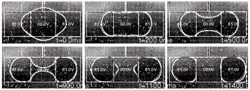

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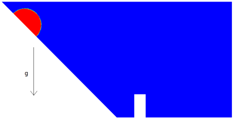

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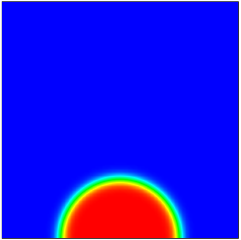

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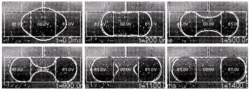

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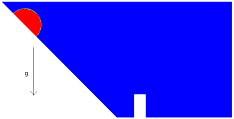

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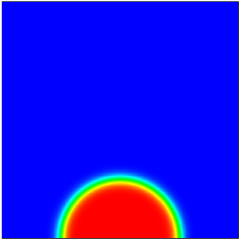

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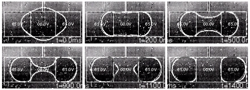

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The Generalized Navier Boundary Condition

- The no-slip condition can be understood as an approximation of the Navier boundary condition

$$\beta\left(\mathrm{u}-\mathbf{U}\right)\cdot\boldsymbol{\tau}+2\eta\varepsilon(\mathrm{u})\mathbf{n}\cdot\boldsymbol{\tau}=0,$$

where $\mathbf{U}$ is the slip velocity and $\boldsymbol{\tau}$ is any vector tangent to Γ.

- Usually $\beta \gg 1$, which is why the no-slip condition is considered.
- At the contact line, it is important to consider the uncompensated Young stress, i.e., the extra stress due to the difference between the current contact angle and the contact angle at equilibrium.

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The Generalized Navier Boundary Condition

Qian et al. (2003-2006) have proposed the so-called generalized Navier boundary condition

$$\beta\,(\mathrm{u} - \mathbf{U})\cdot\boldsymbol{\tau} + 2\eta\varepsilon(\mathrm{u})\mathbf{n}\cdot\boldsymbol{\tau} + \gamma\,(\cos\theta_d - \cos\theta_s)\,\mathbf{t}\cdot\boldsymbol{\tau}\delta_{\partial\Sigma} = 0,$$

where

- γ is the surface tension coefficient.
- Σ is the interface between the two fluids. $\partial\Sigma = \Sigma \cap \Gamma$ is the contact line.
- θ_s is the static contact angle (at equilibrium), θ_d is the current (dynamic) contact angle.
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Diffuse Interface Approach

- Using a diffuse interface approach, it is possible to derive the generalized Navier boundary condition from variational principles (Qian et al. 2006).
- The free energy of the system is expressed by

$$\mathcal{F} = \int_\Omega \left[\frac{\lambda}{2} |\nabla \phi|^2 + F(\phi) \right] + \int_\Gamma \gamma_{fs}(\phi),$$

  where:

  - F is the double well Ginzburg-Landau potential.
  - γ_{fs} is the interfacial free energy per unit area at the fluid-solid interface,

$$\gamma_{fs}(\phi) = \frac{\sigma}{2} \cos(\theta_s) \sin\left(\frac{\pi\phi}{2}\right) + \frac{\sigma_{w1} + \sigma_{w2}}{2}.$$

  σ is the fluid-fluid and σ_{wi}, $i = 1, 2$ is the fluid-wall interfacial tension, resp.

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One arrives at a Cahn Hilliard Navier Stokes system with the generalized Navier boundary condition

$$\begin{cases} \phi_t + \mathrm{u}\cdot\nabla\phi = \gamma\Delta\mu, \quad \mu = F'(\phi) - \Delta\phi, & \text{in } \Omega, \\ \partial_{\mathbf{n}}\mu = 0, \quad \phi_t + \mathrm{u}_{\boldsymbol{\tau}}\partial_{\boldsymbol{\tau}}\phi = -(\lambda\partial_{\mathbf{n}}\phi + \gamma'_{fs}(\phi)), & \text{on } \Gamma, \end{cases}$$

where:

- ϕ–phase variable.
- μ–chemical potential.
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The velocity and pressure satisfy

$$\begin{cases} \rho(\mathrm{u}_t + \mathrm{u}\cdot\nabla \mathrm{u}) - \nabla\cdot(2\eta\varepsilon(\mathrm{u})) + \nabla \mathrm{p} = \rho\mathbf{f} + \lambda\mu\nabla\phi, & \text{in } \Omega, \\ \nabla\cdot\mathrm{u} = 0, & \text{in } \Omega, \\ \mathrm{u}_{\mathbf{n}} = 0, & \text{on } \Gamma, \\ \beta(\phi)\mathrm{u}_{\boldsymbol{\tau}} + 2\eta\varepsilon(\mathrm{u})_{\mathbf{n}\boldsymbol{\tau}} = \left(\lambda\partial_{\mathbf{n}}\phi + \gamma'_{fs}(\phi)\right)\partial_{\boldsymbol{\tau}}\phi, & \text{on } \Gamma. \end{cases}$$

where $\rho = \rho(\phi)$ and $\eta = \eta(\phi)$. Usually

$$\rho(\phi) = \frac{\rho_1 - \rho_2}{2}\phi + \frac{\rho_1 + \rho_2}{2} \quad \eta(\phi) = \frac{\eta_1 - \eta_2}{2}\phi + \frac{\eta_1 + \eta_2}{2}$$

Diffuse Interface Approach

Theorem

Assume $\mathbf{f} \equiv 0$. *The Cahn Hilliard Navier Stokes system with generalized Navier boundary condition has the following energy law:*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_\Omega \left(\frac{1}{2}|\sigma \mathsf{u}|^2 + \frac{\lambda}{2}|\nabla\phi|^2 + F(\phi)\right) + \int_\Gamma \gamma_{fs}(\phi)\right] + \int_\Omega \left(\eta|\varepsilon(\mathsf{u})|^2 + \lambda\gamma|\nabla\mu|^2\right) + \int_\Gamma \left(\beta(\phi)|\mathsf{u}_{\boldsymbol{\tau}}|^2 + L(\phi)^2\right) = 0,$$

where

$$L(\phi) = \lambda\partial_{\mathbf{n}}\phi + \gamma_{fs}'(\phi).$$

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The Cahn Hilliard equation is a fourth order system. ⇒ Operator splitting.

- Kim, Kang and Lowengrub, *Conservative multigrid method for Cahn Hilliard fluids* JCP 2004.
- Kay and Welford, *Efficient numerical solution of Cahn Hilliard Navier Stokes fluids in 2D*, SIAM J. Sci. Comput. 2007.
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$$\Delta\Phi = \Psi$$

instead of

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- Guermond, Salgado *Error analysis of a fractional time-stepping technique for incompressible flows with variable density.* Submitted 2009.
- Guermond, Salgado *A fractional step method based on a pressure Poisson equation for incompressible flows with variable density.* JCP 2009.
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Nonstandard boundary conditions.

- Several works deal with "moving contact lines" by adding an *ad hoc* term to the contact line that *does the trick.*
- Only one reference deals with this boundary condition: Gerbeau-Lelièvre *Generalized Navier Boundary Condition and Geometric Conservation Law for surface tension.* CMAME 2009 (ALE approach).

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Nonstandard boundary conditions.

- Several works deal with "moving contact lines" by adding an *ad hoc* term to the contact line that *does the trick.*
- Only one reference deals with this boundary condition: Gerbeau-Lelièvre *Generalized Navier Boundary Condition and Geometric Conservation Law for surface tension.* CMAME 2009 (ALE approach).

Time Discretization

- Cahn Hilliard: Find (ϕ^{k+1}, μ^{k+1}) that solve

$$\begin{cases} \frac{\phi^{k+1}-\phi^k}{\Delta t} + u^{k+1} \cdot \nabla \phi^{k+1} = \gamma \Delta \mu^{k+1}, & \text{in } \Omega \\ \mu^{k+1} = F'(\phi^k) + A\left(\phi^{k+1} - \phi^k\right) - \Delta \phi^{k+1}, & \text{in } \Omega \\ \frac{\phi^{k+1}-\phi^k}{\Delta t} + u_{\boldsymbol{\tau}}^{k+1} \partial_{\boldsymbol{\tau}} \phi^{k+1} = -L(\phi^{k+1}, \phi^k), & \text{on } \Gamma, \\ \partial_{\mathbf{n}} \mu^{k+1} = 0, & \text{on } \Gamma, \end{cases}$$

where

$$L(\phi^{k+1}, \phi^k) = \lambda \partial_{\mathbf{n}} \phi^{k+1} + \gamma'_{fs}(\phi^k) + B\left(\phi^{k+1} - \phi^k\right).$$

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Time Discretization

- Auxiliary Variables: Define

$$\rho^{k+1} = \frac{\rho_1 - \rho_2}{2}\phi^{k+1} + \frac{\rho_1 + \rho_2}{2}, \quad \rho^\star = \frac{1}{2}\left(\rho^{k+1} + \rho^k\right),$$
$$p^\sharp = 2p^k - p^{k-1}.$$

- Velocity: Find u^{k+1} that solves:

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Time Discretization

Theorem

The scheme is stable provided that

$$A \geq \frac{1}{2} \sup_{x \in \mathbb{R}} |F''(x)|, \quad B \geq \frac{1}{2} \sup_{x \in \mathbb{R}} |\gamma_{fs}''(x)|.$$

- The Ginzburg-Landau potential F can be modified so that the condition on A can be easily satisfied.
- The interface free energy γ_{fs} is smooth and bounded.
- The the phase field and velocity steps are coupled through terms of the form $u^{k+1}\nabla\phi^{k+1}$. In practice, these terms can be treated semi-implicitly, i.e., $u^k\nabla\phi^{k+1}$.

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The Contact Line Paradox

The Generalized Navier Boundary Condition

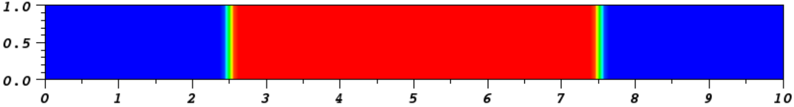
Diffuse Interface Approach

Time Discretization

Numerical Experiments

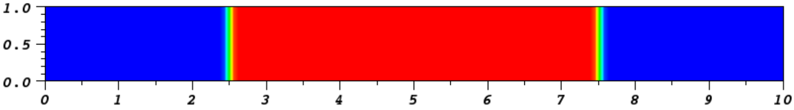
Conclusions and Perspectives

Numerical Experiments. “Couette Flow” (Symmetric)



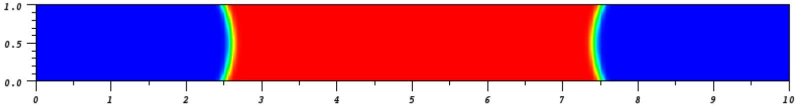
- $\rho_1 = 1 \ \rho_2 = 100.$
- $\eta_1 = \eta_2 = 10^{-2}.$
- $\beta_1 = \beta_2 = 1.5$
- $\gamma = 0.02.$
- $\lambda = 0.001.$
- $\theta_s = \pi/2.$
- $V = 0.25.$

Numerical Experiments. "Couette Flow" (Asymmetric)



- $\rho_1 = 1$ $\rho_2 = 100$.
- $\eta_1 = \eta_2 = 10^{-2}$.
- $\beta_1 = 1.5$, $\beta_2 = 0.591$
- $\gamma = 0.02$.
- $\lambda = 0.001$.
- θ_s is such that $\cos\theta_s \approx 0.38$.
- $V = 0.25$.

Numerical Experiments. Couette Flow (Curved Interfaces)



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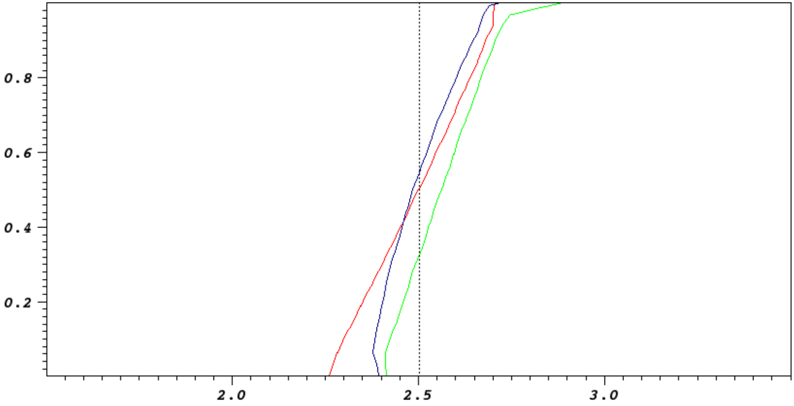
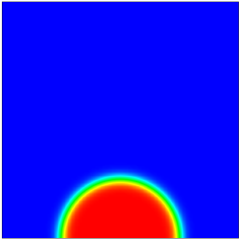
Numerical Experiments. Couette Flow (Comparison)

Comparison between the steady-state profiles for the symmetric, asymmetric and curved cases.



— Symmetric — Asymmetric — Curved

Droplet Relaxation



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- $\beta_1 = 1.5, \ \beta_2 = 0.591$
- $\gamma = 0.02.$
- $\lambda = 0.001.$
- $\theta_s = \pi/4.$

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Future Work

- Contact line pinning. ▸ Pictures
- Efficient solvers for the Cahn Hilliard part.
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Thank you!