Fractional Time-Stepping Techniques for Moving Contact Lines

Abner J. Salgado

Department of Mathematics
University of Maryland, College Park

Nonstandard Discretizations for Fluid Flows
November 25, 2010
Acknowledgments

Supported by NSF Grants CBET-0754983 and DMS-0807811
Outline

The Contact Line Paradox

The Generalized Navier Boundary Condition

Diffuse Interface Approach

Time Discretization

Numerical Experiments

Conclusions and Perspectives
Outline

The Contact Line Paradox

The Generalized Navier Boundary Condition

Diffuse Interface Approach

Time Discretization

Numerical Experiments

Conclusions and Perspectives
The Contact Line Paradox

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

\[
\begin{cases}
\rho_t + \nabla \cdot (\rho u) = 0, & \text{in } \Omega \times (0, T], \\
\rho(u_t + u \cdot \nabla u) - \nabla \cdot (2\eta \varepsilon(u)) + \nabla p = \rho f + \gamma Hn_{\Sigma} \delta_{\Sigma}, & \text{in } \Omega \times (0, T], \\
\nabla \cdot u = 0, & \text{in } \Omega \times (0, T], \\
\rho|_{t=0} = \rho_0, \quad u|_{t=0} = u_0, & \text{in } \Omega.
\end{cases}
\]

Where:

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

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

\[
\begin{aligned}
\rho_t + \nabla \cdot (\rho u) &= 0, \quad \text{in } \Omega \times (0, T], \\
\rho(u_t + u \cdot \nabla u) - \nabla \cdot (2\eta \varepsilon(u)) + \nabla p &= \rho f + \gamma H n_\Sigma \delta_\Sigma, \quad \text{in } \Omega \times (0, T], \\
\nabla \cdot u &= 0, \quad \text{in } \Omega \times (0, T], \\
\rho|_{t=0} &= \rho_0, \quad u|_{t=0} = u_0, \quad \text{in } \Omega.
\end{aligned}
\]

Where:

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

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

\[
\begin{align*}
\rho_t + \nabla \cdot (\rho u) &= 0, & \text{in } \Omega \times (0, T], \\
\rho(u_t + u \cdot \nabla u) - \nabla \cdot (2\eta \varepsilon(u)) + \nabla p &= \rho \mathbf{f} + \gamma H n_{\Sigma} \delta_{\Sigma}, & \text{in } \Omega \times (0, T], \\
\nabla \cdot u &= 0, & \text{in } \Omega \times (0, T], \\
\rho|_{t=0} &= \rho_0, \quad u|_{t=0} = u_0, & \text{in } \Omega.
\end{align*}
\]

Where:

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

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

\[
\begin{align*}
\rho_t + \nabla \cdot (\rho u) &= 0, & \text{in } \Omega \times (0, T], \\
\rho(u_t + u \cdot \nabla u) - \nabla \cdot (2\eta \varepsilon(u)) + \nabla p &= \rho f + \gamma H n_\Sigma \delta_\Sigma, & \text{in } \Omega \times (0, T], \\
\nabla \cdot u &= 0, & \text{in } \Omega \times (0, T], \\
\rho|_{t=0} = \rho_0, \quad u|_{t=0} = u_0, & \text{in } \Omega.
\end{align*}
\]

Where:

- $\Omega \subset \mathbb{R}^d \quad d = 2, 3$ is a fluid domain.
- $f$ is an external driving force density (gravity).
- $\gamma H n_\Sigma \delta_\Sigma$ is the surface tension at the interface $\Sigma$ between the fluids.
- $\rho > 0$—density, $u$—velocity, $p$—pressure.
The Contact Line Paradox

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

$$\begin{cases}
\rho_t + \nabla \cdot (\rho u) = 0, & \text{in } \Omega \times (0, T], \\
\rho(u_t + u \cdot \nabla u) - \nabla \cdot (2\eta \varepsilon(u)) + \nabla p = \rho f + \gamma Hn_\Sigma \delta_\Sigma, & \text{in } \Omega \times (0, T], \\
\nabla \cdot u = 0, & \text{in } \Omega \times (0, T], \\
\rho|_{t=0} = \rho_0, \quad u|_{t=0} = u_0, & \text{in } \Omega.
\end{cases}$$

Where:

- $\Omega \subset \mathbb{R}^d$ $d = 2, 3$ is a fluid domain.
- $f$ is an external driving force density (gravity).
- $\gamma Hn_\Sigma \delta_\Sigma$ is the surface tension at the interface $\Sigma$ between the fluids.
- $\rho > 0$—density, $u$—velocity, $p$—pressure.
The Contact Line Paradox

What boundary conditions?

- The “container” is impermeable. Therefore:

  \[ u \cdot n \big|_\Gamma = 0, \]

  where \( \Gamma = \partial \Omega \) and \( n \) is the unit normal to \( \Gamma \).

- Impermeability implies that we do not need boundary conditions for the pressure and density.

- What about \( u \times n \)?

- The usual condition is no-slip:

  \[ u \big|_\Gamma = 0. \]
The Contact Line Paradox

What boundary conditions?

- The “container” is impermeable. Therefore:

\[ u \cdot n \big|_{\Gamma} = 0, \]

where \( \Gamma = \partial \Omega \) and \( n \) is the unit normal to \( \Gamma \).

- Impermeability implies that we do not need boundary conditions for the pressure and density.

- What about \( u \times n \)?

- The usual condition is no-slip:

\[ u \big|_{\Gamma} = 0. \]
The Contact Line Paradox

What boundary conditions?

- The “container” is impermeable. Therefore:

  \[ u \cdot n |_\Gamma = 0, \]

  where \( \Gamma = \partial \Omega \) and \( n \) is the unit normal to \( \Gamma \).

- Impermeability implies that we do not need boundary conditions for the pressure and density.

- What about \( u \times n \)?

- The usual condition is no-slip:

  \[ u |_\Gamma = 0. \]
The Contact Line Paradox

What boundary conditions?

▶ The “container” is impermeable. Therefore:

\[ u \cdot n \big|_{\Gamma} = 0, \]

where \( \Gamma = \partial \Omega \) and \( n \) is the unit normal to \( \Gamma \).

▶ Impermeability implies that we do not need boundary conditions for the pressure and density.

▶ What about \( u \times n \)?

▶ The usual condition is no-slip:

\[ u \big|_{\Gamma} = 0. \]
The Contact Line Paradox

- Sliding of a droplet
- Droplet relaxation
- Electrowetting on dielectric

- The no slip condition implies that there is no movement.
- Eppur si muove.
- This is the contact line paradox.
The no slip condition implies that there is no movement.

\textit{Eppur si muove.}

This is the contact line paradox.
The Contact Line Paradox

- Sliding of a droplet
- Droplet relaxation
- Electrowetting on dielectric

- The no slip condition implies that there is no movement.
- *Eppur si muove.*
- This is the contact line paradox.
Sliding of a droplet  Droplet relaxation  Electrowetting on dielectric

- The no slip condition implies that there is no movement.
- *Eppur si muove.*
- This is the contact line paradox.
Outline

The Contact Line Paradox

The Generalized Navier Boundary Condition

Diffuse Interface Approach

Time Discretization

Numerical Experiments

Conclusions and Perspectives
The Generalized Navier Boundary Condition

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

\[ \beta (u - U) \cdot \tau + 2\eta\varepsilon(u)n \cdot \tau = 0, \]

where \( U \) is the slip velocity and \( \tau \) is any vector tangent to \( \Gamma \).

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.
The Generalized Navier Boundary Condition

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

\[ \beta (u - U) \cdot \tau + 2 \eta \varepsilon(u)n \cdot \tau = 0, \]

where \(U\) is the slip velocity and \(\tau\) is any vector tangent to \(\Gamma\).

- 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.
The Generalized Navier Boundary Condition

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

\[ \beta (u - U) \cdot \tau + 2 \eta \varepsilon (u) n \cdot \tau = 0, \]

where \( U \) is the slip velocity and \( \tau \) is any vector tangent to \( \Gamma \).

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

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

where

- $\gamma$ is the surface tension coefficient.
- $\Sigma$ is the interface between the two fluids. $\partial \Sigma = \Sigma \cap \Gamma$ is the contact line.
- $\theta_d$ is the static contact angle (at equilibrium), $\theta_d$ is the current (dynamic) contact angle.
- $t = n \times E_{\Sigma}$, with $E_{\Sigma}$ the tangent vector to $\Sigma$. 

The Generalized Navier Boundary Condition
The Generalized Navier Boundary Condition

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

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

where

- \( \gamma \) is the surface tension coefficient.
- \( \Sigma \) is the interface between the two fluids. \( \partial \Sigma = \Sigma \cap \Gamma \) is the contact line.
- \( \theta_s \) is the static contact angle (at equilibrium), \( \theta_d \) is the current (dynamic) contact angle.
- \( t = n \times t_{\partial \Sigma} \), with \( t_{\partial \Sigma} \) the tangent vector to \( \Sigma \).
The Generalized Navier Boundary Condition

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

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

where

- \( \gamma \) is the surface tension coefficient.
- \( \Sigma \) is the interface between the two fluids. \( \partial \Sigma = \Sigma \cap \Gamma \) is the contact line.
- \( \theta_s \) is the static contact angle (at equilibrium), \( \theta_d \) is the current (dynamic) contact angle.
- \( t = n \times t_{\partial \Sigma} \), with \( t_{\partial \Sigma} \) the tangent vector to \( \Sigma \).
Qian et al. (2003-2006) have proposed the so-called generalized Navier boundary condition

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

where

- $\gamma$ is the surface tension coefficient.
- $\Sigma$ is the interface between the two fluids. $\partial \Sigma = \Sigma \cap \Gamma$ is the contact line.
- $\theta_s$ is the static contact angle (at equilibrium), $\theta_d$ is the current (dynamic) contact angle.
- $t = n \times t_{\partial \Sigma}$, with $t_{\partial \Sigma}$ the tangent vector to $\Sigma$. 
The Generalized Navier Boundary Condition

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

$$\beta (u - U) \cdot \tau + 2 \eta \varepsilon(u) n \cdot \tau + \gamma (\cos\theta_d - \cos\theta_s) t \cdot \tau \delta \partial \Sigma = 0,$$

where

- $\gamma$ is the surface tension coefficient.
- $\Sigma$ is the interface between the two fluids. $\partial \Sigma = \Sigma \cap \Gamma$ is the contact line.
- $\theta_s$ is the static contact angle (at equilibrium), $\theta_d$ is the current (dynamic) contact angle.
- $t = n \times t_{\partial \Sigma}$, with $t_{\partial \Sigma}$ the tangent vector to $\Sigma$. 
Outline

The Contact Line Paradox

The Generalized Navier Boundary Condition

Diffuse Interface Approach

Time Discretization

Numerical Experiments

Conclusions and Perspectives
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.
- \( \gamma_{fs} \) is the interfacial free energy per unit area at the fluid-solid interface,

\[
\gamma_{fs}(\phi) = \sigma \cos(\theta_s) \sin\left( \frac{\phi}{2} \right) + \sigma_{wi} 1_{i=1,2},
\]

- \( \sigma \) is the fluid-fluid and \( \sigma_{wi}, i=1,2 \) is the fluid-wall interfacial tension, resp.
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.
- \( \gamma_{fs} \) is the interfacial free energy per unit area at the fluid-solid interface,

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

\( \sigma \) is the fluid-fluid and \( \sigma_{wi}, \ i = 1, 2 \) is the fluid-wall interfacial tension, resp.
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.
- \( \gamma_{fs} \) is the interfacial free energy per unit area at the fluid-solid interface,

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

\( \sigma \) is the fluid-fluid and \( \sigma_{wi}, \ i = 1, 2 \) is the fluid-wall interfacial tension, resp.
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

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

where:

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

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

\( \sigma \) is the fluid-fluid and \( \sigma_{wi}, \ i = 1, 2 \) is the fluid-wall interfacial tension, resp.
Diffuse Interface Approach

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

\[
\begin{cases}
\phi_t + u \cdot \nabla \phi = \gamma \Delta \mu, & \mu = F'(\phi) - \Delta \phi, \\
\partial_n \mu = 0, & \phi_t + u \tau \partial_\tau \phi = - (\lambda \partial_n \phi + \gamma'_{fs}(\phi)),
\end{cases}
\]

in \( \Omega \),
on \( \Gamma \),

where:

- \( \phi \)–phase variable.
- \( \mu \)–chemical potential.
- \( \gamma \)–mobility.
- \( \lambda \)–mixing energy density.
Diffuse Interface Approach

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

\[
\begin{align*}
\phi_t + u \cdot \nabla \phi &= \gamma \Delta \mu, \\
\mu &= F'(\phi) - \Delta \phi, \\
\partial_n \mu &= 0, \\
\phi_t + u_\tau \partial_\tau \phi &= -(\lambda \partial_n \phi + \gamma'_{fs}(\phi)),
\end{align*}
\]

in \( \Omega \), on \( \Gamma \),

where:

- \( \phi \)–phase variable.
- \( \mu \)–chemical potential.
- \( \gamma \)–mobility.
- \( \lambda \)–mixing energy density.
Diffuse Interface Approach

The velocity and pressure satisfy

\[
\begin{cases}
\rho(u_t + u \cdot \nabla u) - \nabla \cdot (2\eta \varepsilon(u)) + \nabla p = \rho f + \lambda \mu \nabla \phi, & \text{in } \Omega, \\
\nabla \cdot u = 0, & \text{in } \Omega, \\
u_n = 0, & \text{on } \Gamma, \\
\beta(\phi) u_\tau + 2\eta \varepsilon(u)_n = \left(\lambda \partial_n \phi + \gamma_{fs}'(\phi)\right) \partial_\tau \phi, & \text{on } \Gamma.
\end{cases}
\]

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

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

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

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

where

$$L(\phi) = \lambda \partial_n \phi + \gamma_{fs}'(\phi).$$
Outline

The Contact Line Paradox

The Generalized Navier Boundary Condition

Diffuse Interface Approach

Time Discretization

Numerical Experiments

Conclusions and Perspectives
Time Discretization. Difficulties

The Cahn Hilliard equation is a fourth order system. \( \Rightarrow \) Operator splitting.

Time Discretization. Difficulties

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


Time Discretization. Difficulties

Navier Stokes equations with variable density. ⇒ Fractional time-stepping based on penalization of the divergence. Solve

$$\Delta \phi = \psi$$

instead of

$$\nabla \cdot \left( \frac{1}{\rho^{k+1}} \nabla \phi \right) = \psi$$

Time Discretization. Difficulties

Navier Stokes equations with variable density. ⇨ Fractional time-stepping based on penalization of the divergence. Solve

$$\Delta \Phi = \Psi$$

instead of

$$\nabla \cdot \left( \frac{1}{\rho^{k+1}} \nabla \Phi \right) = \Psi$$

- Guermond, Salgado A fractional step method based on a pressure Poisson equation for incompressible flows with variable density. JCP 2009.
Time Discretization. Difficulties

Nonstandard boundary conditions.

- Several works deal with “moving contact lines” by adding an *ad hoc* term to the contact line that *does the trick*.

Nonstandard boundary conditions.

- Several works deal with “moving contact lines” by adding an *ad hoc* term to the contact line that *does the trick*.

**Cahn Hilliard:** Find \((\phi^{k+1}, \mu^{k+1})\) that solve

\[
\begin{align*}
\frac{\phi^{k+1} - \phi^k}{\Delta t} + u^{k+1} \cdot \nabla \phi^{k+1} &= \gamma \Delta \mu^{k+1}, & \text{in } \Omega \\
\mu^{k+1} &= F'(\phi^k) + A (\phi^{k+1} - \phi^k) - \Delta \phi^{k+1}, & \text{in } \Omega \\
\frac{\phi^{k+1} - \phi^k}{\Delta t} + u^{k+1}_\tau \partial_\tau \phi^{k+1} &= -L(\phi^{k+1}, \phi^k), & \text{on } \Gamma, \\
\partial_n \mu^{k+1} &= 0, & \text{on } \Gamma,
\end{align*}
\]

where

\[
L(\phi^{k+1}, \phi^k) = \lambda \partial_n \phi^{k+1} + \gamma'_{fs}(\phi^k) + B \left(\phi^{k+1} - \phi^k\right).
\]
Cahn Hilliard: Find \((\phi^{k+1}, \mu^{k+1})\) that solve

\[
egin{aligned}
\frac{\phi^{k+1} - \phi^k}{\Delta t} + u^{k+1} \cdot \nabla \phi^{k+1} &= \gamma \Delta \mu^{k+1}, \quad \text{in } \Omega \\
\mu^{k+1} &= F'(\phi^k) + A(\phi^{k+1} - \phi^k) - \Delta \phi^{k+1}, \quad \text{in } \Omega \\
\frac{\phi^{k+1} - \phi^k}{\Delta t} + u^{k+1}_\tau \partial_\tau \phi^{k+1} &= -L(\phi^{k+1}, \phi^k), \quad \text{on } \Gamma, \\
\partial_n \mu^{k+1} &= 0, \quad \text{on } \Gamma,
\end{aligned}
\]

where

\[
L(\phi^{k+1}, \phi^k) = \lambda \partial_n \phi^{k+1} + \gamma'_fs(\phi^k) + B(\phi^{k+1} - \phi^k).
\]
Time Discretization

- **Auxiliary Variables:** Define

\[
\rho_{k+1} = \frac{\rho_1 - \rho_2}{2} \phi_{k+1} + \frac{\rho_1 + \rho_2}{2}, \quad \rho^* = \frac{1}{2} \left( \rho_{k+1} + \rho_k \right),
\]

\[
p^\# = 2p^k - p^{k-1}.
\]

- **Velocity:** Find \( u^{k+1} \) that solves:

\[
\begin{cases}
\frac{\rho^* u^{k+1} - \rho^k u^k}{\Delta t} + \rho^k u^k \cdot \nabla u^{k+1} + \frac{1}{2} \nabla \cdot (\rho^k u^k) u^{k+1} \\
- \nabla \cdot (2\eta \varepsilon (u^{k+1})) + \nabla p^\# = \rho^k f^{k+1} + \lambda \mu^{k+1} \nabla \phi^{k+1}, & \text{in } \Omega, \\
u^{k+1}_n = 0, & \text{on } \Gamma, \\
\beta(\phi^k)u^{k+1}_\tau + \eta \varepsilon (u^{k+1})_{n\tau} = L(\phi^{k+1}, \phi^k)\partial_\tau \phi^{k+1}, & \text{on } \Gamma.
\end{cases}
\]
Time Discretization

- **Auxiliary Variables**: Define

\[
\rho^{k+1} = \frac{\rho_1 - \rho_2}{2} \phi^{k+1} + \frac{\rho_1 + \rho_2}{2}, \quad \rho^* = \frac{1}{2} \left( \rho^{k+1} + \rho^k \right),
\]

\[
p^\# = 2p^k - p^{k-1}.
\]

- **Velocity**: Find \( u^{k+1} \) that solves:

\[
\begin{cases}
\quad \frac{\rho^* u^{k+1} - \rho^k u^k}{\Delta t} + \rho^k u^k \cdot \nabla u^{k+1} + \frac{1}{2} \nabla \cdot (\rho^k u^k) u^{k+1} \\
\quad - \nabla \cdot (2\eta \varepsilon(u^{k+1})) + \nabla p^\# = \rho^k f^{k+1} + \lambda \mu^{k+1} \nabla \phi^{k+1}, & \text{in } \Omega, \\
\quad u_n^{k+1} = 0, & \text{on } \Gamma, \\
\quad \beta(\phi^k) u_{\tau}^{k+1} + \eta \varepsilon(u^{k+1})_{n\tau} = L(\phi^{k+1}, \phi^k) \partial_{\tau} \phi^{k+1}, & \text{on } \Gamma.
\end{cases}
\]
Time Discretization

- **Pressure:** Find $p^{k+1}$ that solves:

$$
\Delta \left( p^{k+1} - p^k \right) = \frac{\rho}{\Delta t} \nabla \cdot u^{k+1}, \quad \partial_n \left( p^{k+1} - p^k \right) = 0.
$$

where

$$
\rho = \min\{\rho_1, \rho_2\}.
$$
Pressure: Find $p^{k+1}$ that solves:

$$\Delta \left( p^{k+1} - p^k \right) = \frac{\varrho}{\Delta t} \nabla \cdot u^{k+1}, \quad \partial_n \left( p^{k+1} - p^k \right) = 0.$$ 

where

$$\varrho = \min \{ \rho_1, \rho_2 \}.$$
Pressure: Find $p^{k+1}$ that solves:

$$\Delta \left( p^{k+1} - p^k \right) = \frac{\varrho}{\Delta t} \nabla \cdot u^{k+1}, \quad \partial_n \left( p^{k+1} - p^k \right) = 0,$$

where

$$\varrho = \min\{\rho_1, \rho_2\}. $$
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 $\gamma_{fs}$ is smooth and bounded.
- 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., $u^{k} \nabla \phi^{k+1}$.
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 \( \gamma_{fs} \) is smooth and bounded.
- 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., \( u^k \nabla \phi^{k+1} \).
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 \( \gamma_{fs} \) is smooth and bounded.

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., \( u^k \nabla \phi^{k+1} \).
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 \( \gamma_{fs} \) is smooth and bounded.
- 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., \( u^{k} \nabla \phi^{k+1} \).
Outline

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)

- \( \rho_1 = 1, \rho_2 = 100 \).
- \( \eta_1 = \eta_2 = 10^{-2} \).
- \( \beta_1 = 1.5, \beta_2 = 0.591 \).
- \( \gamma = 0.02 \).
- \( \lambda = 0.001 \).
- \( \theta_s \) is such that \( \cos \theta_s \approx 0.38 \).
- \( V = 0.25 \).
Numerical Experiments. Couette Flow (Curved Interfaces)

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

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

- $\rho_1 = 1$, $\rho_2 = 100$.
- $\eta_1 = \eta_2 = 10^{-2}$.
- $\beta_1 = 1.5$, $\beta_2 = 0.591$.
- $\gamma = 0.02$.
- $\lambda = 0.001$.
- $\theta_s = \pi/4$. 
Outline

The Contact Line Paradox

The Generalized Navier Boundary Condition

Diffuse Interface Approach

Time Discretization

Numerical Experiments

Conclusions and Perspectives
Conclusions

- The generalized Navier boundary condition is one possible solution to the contact line paradox.
- The Cahn Hilliard Navier Stokes system with generalized Navier boundary condition has an energy law.
- Unconditionally stable time-discrete scheme.
Conclusions

- The generalized Navier boundary condition is one possible solution to the contact line paradox.
- The Cahn Hilliard Navier Stokes system with generalized Navier boundary condition has an energy law.
- Unconditionally stable time-discrete scheme.
Conclusions

- The generalized Navier boundary condition is one possible solution to the contact line paradox.
- The Cahn Hilliard Navier Stokes system with generalized Navier boundary condition has an energy law.
- Unconditionally stable time-discrete scheme.
Future Work

- Contact line pinning.
Future Work

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