The Cahn–Hilliard Equation with Dynamic Boundary Conditions

Hao Wu

School of Mathematical Sciences
Fudan University

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Outline

Cahn–Hilliard Equation

- Dynamics of Mixtures

  – Phase separation, Formation of microstructure ...

- Cahn & Hilliard 1958: a basic building-block equation

$$\begin{cases} \phi_t = \nabla \cdot (M(\phi)\nabla\mu), \\ \mu = -\epsilon^2\Delta\phi + F'(\phi), \end{cases} \qquad \text{in } \Omega \times (0, T).$$

  – Spinodal decomposition, Nucleation and growth, Coarsening

- Extensions

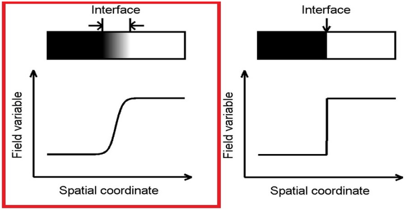
  – Image impainting, Ecology, Tumor growth, Fluid dynamics, Topology optimization ...

Mathematical Models

- Description of morphology changes $\longrightarrow$ dynamics of **interfaces**

(1) Sharp interface model
– Regard interface as a free boundary with zero thickness evolving in time

(2) Diffuse interface model
– Consider an interfacial layer of small width $\epsilon \in (0, 1)$: using a **smooth order parameter** ϕ (phase field) to distinguish two phases



Cahn–Hilliard Equation

$$\begin{cases} \phi_t = \nabla \cdot (M(\phi)\nabla \mu), \\ \mu = -\epsilon^2 \Delta \phi + F'(\phi), \end{cases} \qquad \text{in } \Omega \times (0,T).$$

- $\Omega \subset \mathbb{R}^d$, $\Gamma = \partial\Omega$, $\mathbf{n}$ outer unit normal vector on Γ
- ϕ: a **conserved** order parameter $\in [-1,1]$
- μ: chemical potential
- F: potential function with double-well structure (singular/regular)

$$F(\phi) = \frac{\theta}{2}\left[(1+\phi)\log(1+\phi) + (1-\phi)\log(1-\phi)\right] - \frac{\theta_c}{2}\phi^2, \quad \theta_c > \theta > 0$$

$$F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$$

- M: mobility

$$M(\phi) = 1, \quad M(\phi) = (1-\phi^2)^m \quad \ldots$$

Cahn–Hilliard Equation

- Boundary conditions / Initial condition

$$\begin{cases} M\nabla\mu\cdot\mathbf{n} = \partial_{\mathbf{n}}\phi = 0, & \text{on } \Gamma\times(0,T), \\ \phi|_{t=0} = \phi_0, & \text{in } \Omega. \end{cases}$$

- Mass conservation

$$\int_\Omega \phi(t)dx = \int_\Omega \phi_0 dx, \quad \forall t \geq 0.$$

- Energy dissipation

Basic energy law $\frac{d}{dt}E(\phi(t)) + \int_\Omega M|\nabla\mu(t)|^2 dx = 0, \quad \forall t \geq 0,$

with free energy $E(\phi) = \int_\Omega \left(\frac{\epsilon^2}{2}|\nabla\phi|^2 + F(\phi)\right) dx.$

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Structure

(1) 1st and 2nd Fick's law of diffusion

$$\frac{\partial \phi}{\partial t} + \mathrm{div}\mathbf{J} = 0, \qquad \mathbf{J} = -M\nabla \mu$$

(2) When M is a positive constant $\rightarrow$ **Gradient flow** in $(\dot{H}^1)'$:

$$\left\langle \frac{\partial \phi}{\partial t}, \xi \right\rangle_{(\dot{H}^1)'} = -M \int_\Omega \mu \xi dx = -M \frac{\delta E}{\delta \phi}(\phi)[\xi], \quad \forall \xi \in \dot{H}^1(\Omega)$$

$\star$ M be non-constant:

Gradient flow with respect to a Wasserstein-like transport metric (Lisini, Matthes & Savaré, JDE 2012)

Cahn–Hilliard Equation

- **Well-posedness**

  Elliott & Zheng SM 1986, Yin JX 1992, Caffarelli & Müler 1995, Debussche & Dettori 1995, Elliott & Garcke 1996 ...

- **Long-time behavior** $t \to +\infty$

  Rybka & Hoffmann 1998, Miranville & Zelik 2004, Abels & Wilke 2007 ...

- **Sharp-interface limit** $\epsilon \to 0^+$

  Pego 1989, Cahn, Elliott & Novick-Cohen 1996,

  Alikakos, Bates & Chen XF 1994, Chen XF 1996 ...

Boundary effects

- **Phase separation**

  – Effective short-range interactions between the binary mixture and the solid wall

  Fischer et al 1997 PRL ...

- **Wetting phenomena**

  – Moving Contact Line problem of two phase flows

  Jacqmin 2000 JFM, Qian, Wang & Sheng 2006 JFM,
  W.-Q Ren & W.-N. E 2007 Phys. Fluids ...

- **Near the Boundary: Different Dynamics Driven by Surface Energy**

  $\Longrightarrow$ Different types of Boundary Conditions

Dynamic Boundary Condition A

- Fischer et al 1997

Total energy $$\mathcal{E}(\phi) = \underbrace{\int_\Omega \left(\frac{1}{2}|\nabla\phi|^2 + F(\phi)\right) dx}_{\text{bulk energy}} + \underbrace{\int_\Gamma \left(\frac{\kappa}{2}|\nabla_\Gamma\phi|^2 + G(\phi)\right) dS}_{\text{surface energy}}$$

with $\epsilon = 1$, $\kappa \geq 0$.

Boundary conditions $$\begin{cases} \partial_{\mathbf{n}}\mu = 0, \\ \phi_t - \kappa\Delta_\Gamma\phi + G'(\phi) + \partial_{\mathbf{n}}\phi = 0. \end{cases}$$

$\Longrightarrow$

Mass conservation $$\int_\Omega \phi(t)dx = \int_\Omega \phi_0 dx, \quad \forall\, t \geq 0,$$

Energy dissipation $$\frac{d}{dt}\mathcal{E}(\phi(t)) + \int_\Omega |\nabla\mu(t)|^2 dx + \int_\Gamma |\phi_t(t)|^2 dS = 0, \quad \forall\, t \geq 0.$$

Derivation

$$\frac{d}{dt}\mathcal{E}(\phi(t)) = \int_\Omega \nabla\phi\cdot\nabla\phi_t + F'(\phi)\phi_t dx + \int_\Gamma \kappa\nabla_\Gamma\phi\cdot\nabla_\Gamma\phi_t + G'(\phi)\phi_t dS$$
$$= \int_\Omega \underbrace{\big[-\Delta\phi + F'(\phi)\big]}_{=\mu}\phi_t dx + \int_\Gamma \big[-\kappa\Delta_\Gamma\phi + G'(\phi) + \partial_{\mathbf{n}}\phi\big]\phi_t dS$$

- In Ω: CHE $\phi_t = \Delta\mu$ with **no-flux** BC $\partial_{\mathbf{n}}\mu = 0$
- On Γ: **Choose** an Allen–Cahn type relaxation

$$\phi_t = -\big[-\kappa\Delta_\Gamma\phi + G'(\phi) + \partial_{\mathbf{n}}\phi\big]$$

$\sim$ A variational BC that leads to non-increasing of $\mathcal{E}$

$\sim$ Dynamic contact angle on Γ

$\sim$ A sufficient condition for energy dissipation, not uniquely determined

Analysis Results

- **Well-posedness and Long-time behavior**

  Racke & Zheng 2003,
  Wu & Zheng 2004, Chill et al 2006,
  Miranville & Zelik 2005, 2010,
  Prüss, Racke & Zheng 2006, Prüss & Wilke 2006,
  Gal & Grasselli 2007, 2008, 2013,
  Gilardi, Miranville & Schimperna 2009, 2010,
  Chen, Wang & Xu 2014,
  Colli, Gilardi & Sprekels 2017, 2018 ...

- **Sharp interface limit**

  Chen, Wang & Xu 2014,
  Wang & Wang 2007, Xu, Di & Yu 2018

Dynamic Boundary Condition B

- Goldstein, Miranville & Schimperna 2011 Phy. D

Γ is a **non-permeable wall**: $$\begin{cases} \partial_t(\phi|_\Gamma) - \alpha\Delta_\Gamma(\mu|_\Gamma) + \partial_{\mathbf{n}}\mu = 0, \\ \mu|_\Gamma = -\kappa\Delta_\Gamma\phi|_\Gamma + G'(\phi|_\Gamma) + \partial_{\mathbf{n}}\phi. \end{cases}$$

- **Total mass conservation** in Ω + on Γ[1]

$$\int_\Omega \phi(t)dx + \int_\Gamma \phi|_\Gamma(t)dS = \int_\Omega \phi_0 dx + \int_\Gamma \phi_0|_\Gamma dS, \quad \forall\, t \geq 0,$$

- **Energy dissipation**

$$\frac{d}{dt}\mathcal{E}(\phi(t)) + \int_\Omega |\nabla\mu(t)|^2 dx + \underbrace{\alpha\int_\Gamma |\nabla_\Gamma(\mu|_\Gamma(t))|^2 dS}_{\text{Relaxation of CH type}} = 0, \quad \forall\, t \geq 0.$$

[1] Bulk-surface measure space $(\overline{\Omega}, d\sigma) = (\Omega, dx) \oplus (\Gamma, dS)$

Related Case: Wentzell Boundary Condition

- Gal 2006 MMAS

Γ is a **permeable wall**:
$$\begin{cases} (\Delta\mu)|_\Gamma + c\mu|_\Gamma + \partial_{\mathbf{n}}\mu = 0, \\ \mu|_\Gamma = -\kappa\Delta_\Gamma\phi|_\Gamma + G'(\phi|_\Gamma) + \partial_{\mathbf{n}}\phi. \end{cases}$$

- **Total mass conservation** (when $c = 0$)

$$\int_\Omega \phi(t)dx + \int_\Gamma \phi(t)|_\Gamma dS = \int_\Omega \phi_0 dx + \int_\Gamma \phi_0|_\Gamma dS, \quad \forall\, t \geq 0,$$

- **Energy dissipation**

$$\frac{d}{dt}\mathcal{E}(\phi(t)) + \int_\Omega |\nabla\mu(t)|^2 dx + c\int_\Gamma |\mu|_\Gamma(t)|^2 dS = 0, \quad \forall\, t \geq 0.$$

Summary

- Dynamic BC-A, Dynamic BC-B, Wentzell BC:

  All based on physical considerations (**Mass** + **Energy**),

  Not uniquely determined.

- Hidden physics? Other possible choice of BC ?

Outline

1. Kinematics

Assume

- Continuity equation in the bulk

$$\phi_t + \nabla \cdot (\phi \mathbf{u}) = 0, \quad (x,t) \in \Omega \times (0,T),$$

$$\text{no-flux b.c.} \quad \mathbf{u} \cdot \mathbf{n} = 0, \quad (x,t) \in \Gamma \times (0,T).$$

- Continuity equation on the boundary

$$\phi_t + \nabla_\Gamma \cdot (\phi \mathbf{v}) = 0, \quad (x,t) \in \Gamma \times (0,T),$$

$\mathbf{u}, \mathbf{v}$: microscopic effective velocity (due to diffusion) in Ω and on Γ.

$\Longrightarrow$ **Mass Conservation** in Ω and on Γ,

$$\frac{d}{dt}\int_\Omega \phi(t)dx = \frac{d}{dt}\int_\Gamma \phi(t)dS = 0.$$

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$$\frac{d}{dt}\int_\Omega \phi(t)dx = \frac{d}{dt}\int_\Gamma \phi(t)dS = 0.$$

2. Energy Dissipation

Assume

- **Basic Energy Law**

$$\frac{d}{dt}E^{total}(t) = -\mathcal{D}^{total}(t) \leq 0$$

* Free Energy (neglecting macroscopic kinetic energy)

$$E^{total}(t) = E^{bulk}(t) + E^{surf}(t),$$

$$E^{bulk}(t) = \int_\Omega W_b(\phi, \nabla\phi)dx, \quad E^{surf}(t) = \int_\Gamma W_s(\phi, \nabla_\Gamma\phi)dS$$

* Energy Dissipation

$$\mathcal{D}^{total}(t) = \mathcal{D}^{bulk}(t) + \mathcal{D}^{surf}(t),$$

$$\mathcal{D}^{bulk}(t) = \int_\Omega \frac{\phi^2}{M_b}|\mathbf{u}|^2dx, \quad \mathcal{D}^{surf}(t) = \int_\Gamma \frac{\phi^2}{M_s}|\mathbf{v}|^2dS$$

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* Energy Dissipation

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3. Force Balance

Aim: **Uniquely determine** the velocities $\mathbf{u}$, $\mathbf{v}$ and form a closed PDE system

Method: An Energetic Variational Approach

- Bulk flow map $x(X,t) : \Omega_0^X \to \Omega_t^x$

$$\begin{cases} \dfrac{d}{dt}x(X,t) = \mathbf{w}(x(X,t),t), & t > 0, \\ x(X,0) = X. \end{cases}$$

- Similarly, define a surface flow map $x_s(X_s,t)$ [2]
- Bulk/surface action functionals

$$\mathcal{A}^{bulk}(x(X,t)) = -\int_0^T \int_{\Omega_t^x} W_b(\phi, \nabla_x \phi) dx dt,$$

$$\mathcal{A}^{surf}(x_s(X_s,t)) = -\int_0^T \int_{\Gamma_t^x} W_s(\phi, \nabla_\Gamma^x \phi) dS_x dt.$$

[2]Koba, Giga & Liu 2017 QAM

Least Action Principle

- Total action $\mathcal{A}^{total} = \mathcal{A}^{bulk} + \mathcal{A}^{surf}$

$$\delta_{(x,x_s)}\mathcal{A}^{total} = -\int_0^T\int_{\Omega_t^x}(\phi\nabla_x\mu)\cdot y\,dxdt - \int_0^T\int_{\Gamma_t^x}\left[\phi\nabla_\Gamma^x\left(\mu_s + \frac{\partial W_b}{\partial\nabla_x\phi}\cdot\mathbf{n}\right)\right]\cdot y_s\,dS_xdt.$$

with $\mu = -\nabla_x\cdot\frac{\partial W_b}{\partial\nabla_x\phi} + \frac{\partial W_b}{\partial\phi}, \quad \mu_s = -\nabla_\Gamma^x\cdot\frac{\partial W_s}{\partial\nabla_\Gamma^x\phi} + \frac{\partial W_s}{\partial\phi}.$

- $\delta_x\mathcal{A} = (F_{inertial} + F_{con})\cdot\delta x \Longrightarrow$ **Conservative forces**[3]

$$F_{con}^{bulk} = -\phi\nabla_x\mu, \quad F_{con}^{surf} = -\phi\nabla_\Gamma^x\left(\mu_s + \frac{\partial W_b}{\partial\nabla_x\phi}\cdot\mathbf{n}\right).$$

[3] $F_{inertial} = 0$ since kinetic energy is neglected

Onsager's Maximum Dissipation Principle

- The Rayleigh dissipation function

$$\mathcal{R} = \frac{1}{2}\mathcal{D} \geq 0$$

- Variation with respective to $\mathbf{u}$ (the velocity)

$$\delta_{\mathbf{u}}\mathcal{R} = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \mathcal{R}(\mathbf{u}+\varepsilon\mathbf{v}) \Longrightarrow \text{ weak form of } \; -F_{diss}$$

- For present case

$$\delta_{(\mathbf{u},\mathbf{v})}\left(\frac{1}{2}\mathcal{D}^{total}\right) = \int_{\Omega_t^x} \frac{\phi^2}{M_b}\mathbf{u}\cdot\tilde{\mathbf{u}}dx + \int_{\Gamma_t^x} \frac{\phi^2}{M_s}\mathbf{v}\cdot\tilde{\mathbf{v}}dS,$$

$\Longrightarrow$ **Dissipative forces**

$$F_{diss}^{bulk} = -\frac{\phi^2}{M_b}\mathbf{u}, \quad F_{diss}^{surf} = -\frac{\phi^2}{M_s}\mathbf{v}.$$

Force Balance

- Netwon's force balance law

$$F_{inertial} + F_{conv} + F_{diss} = 0$$

- Phrasing the evolution equations for a dissipative system within a Hamiltonian principle formalism (in "strong" form): [4]

$$\delta_x \mathcal{A} - \delta_{\mathbf{u}} \mathcal{R} = 0$$

$\sim$ extended Euler–Lagrange equations

$$F_{con} + F_{diss} = 0 \quad \Longrightarrow \begin{cases} \phi \nabla_x \mu + \dfrac{\phi^2}{M_b} \mathbf{u} = 0, & \text{in } \Omega, \\ \phi \nabla_\Gamma^x \left(\mu_s + \dfrac{\partial W_b}{\partial \nabla_x \phi} \cdot \mathbf{n} \right) + \dfrac{\phi^2}{M_s} \mathbf{v} = 0, & \text{on } \Gamma. \end{cases}$$

[4] Sonnet & Virga, Springer 2012

Resulting PDE System

C. Liu and H. Wu 2019 ARMA

$$
\begin{cases}
\phi_t = \nabla \cdot (M_b \nabla \mu), & \text{in } \Omega \times (0,T), \\
\mu = -\nabla \cdot \dfrac{\partial W_b}{\partial \nabla \phi} + \dfrac{\partial W_b}{\partial \phi}, & \text{in } \Omega \times (0,T), \\
\partial_{\mathbf{n}} \mu = 0, & \text{on } \Gamma \times (0,T), \\
\phi_t = \nabla_\Gamma \cdot \left[M_s \nabla_\Gamma \left(\mu_s + \dfrac{\partial W_b}{\partial \nabla \phi} \cdot \mathbf{n} \right) \right], & \text{on } \Gamma \times (0,T), \\
\mu_s = -\nabla_\Gamma \cdot \dfrac{\partial W_s}{\partial \nabla_\Gamma \phi} + \dfrac{\partial W_s}{\partial \phi}, & \text{on } \Gamma \times (0,T), \\
\phi|_{t=0} = \phi_0(x), & \text{in } \Omega.
\end{cases}
$$

- **Mass Conservation** + **Energy Dissipation** + **Force Balance**
- Different physical considerations can be easily included by choosing free energies W_b, W_s and mobilities M_b, M_s
- Consistent with the surface-layer scaling process (Qian, Qiu & Sheng 2008)

Outline

IBVP of the Cahn–Hilliard Equation with NEW DBC

For simplicity, choose $M_b = M_s = 1$,

$$W_b(\phi, \nabla\phi) = \frac{1}{2}|\nabla\phi|^2 + F(\phi), \quad W_s(\phi, \nabla_\Gamma\phi) = \frac{\kappa}{2}|\nabla_\Gamma\phi|^2 + \frac{1}{2}\phi^2 + G(\phi).$$

Introduce boundary variable

$\psi = \phi|_\Gamma$ $\sim$ a bulk-to-boundary transmission condition

Consider a coupled system for (ϕ, ψ)

$$(P)\begin{cases} \phi_t = \Delta\mu, \quad \text{with } \mu = -\Delta\phi + F'(\phi), & \text{in } (0,T)\times\Omega, \\ \partial_{\mathbf{n}}\mu = 0, & \text{on } (0,T)\times\Gamma, \\ \phi|_\Gamma = \psi, & \text{on } (0,T)\times\Gamma, \\ \psi_t = \Delta_\Gamma\mu_\Gamma, \quad \text{with } \mu_\Gamma = -\kappa\Delta_\Gamma\psi + \psi + G'(\psi) + \partial_{\mathbf{n}}\phi, & \text{on } (0,T)\times\Gamma, \\ \phi|_{t=0} = \phi_0(x), & \text{in } \Omega, \\ \psi|_{t=0} = \psi_0(x) := \phi_0(x)|_\Gamma, & \text{on } \Gamma. \end{cases}$$

Mathematical Difficulties

- **Higher-order, multi-scale coupling** between bulk and boundary

⋆ $\kappa > 0$: a surface Cahn-Hilliard equation

$$\psi_t = \Delta_\Gamma(-\kappa\Delta_\Gamma\psi + \psi + G'(\psi)) + \underbrace{\Delta_\Gamma(\partial_{\mathbf{n}}\phi)}_{\text{coupling from bulk}}$$

⋆ $\kappa = 0$ (e.g., the MCL problem): may be ill-posed

$$\psi_t = \underbrace{[1 + G''(\psi)]\Delta_\Gamma\psi}_{\text{backwards diffusion ??}} + G'''(\psi)|\nabla_\Gamma\psi|^2 + \underbrace{\Delta_\Gamma(\partial_{\mathbf{n}}\phi)}_{\text{higher order}}$$

- **Key issue**: A parabolic Dirichlet-to-Neumann operator via CHE

$$\phi|_\Gamma = \psi \quad \Longrightarrow \quad \partial_{\mathbf{n}}\phi$$

Outline

Notations

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$: a bounded domain with smooth boundary Γ.
- Function spaces

$$\mathcal{H} = L^2(\Omega) \times L^2(\Gamma),$$

$$\mathcal{V}^s = \{(\phi, \psi) \in H^s(\Omega) \times H^s(\Gamma) : \ \psi = \phi|_\Gamma\}, \quad \forall\, s > \frac{1}{2},$$

$$V^s = \{(\phi, \psi) \in H^s(\Omega) \times H^{s-\frac{1}{2}}(\Gamma) : \ \psi = \phi|_\Gamma\}, \quad \forall\, s > \frac{1}{2}.$$

Set

$$\mathbb{V}^s_\kappa := \mathcal{V}^s \ \text{ if } \kappa > 0, \qquad \mathbb{V}^s_\kappa := V^s \ \text{ if } \kappa = 0.$$

$$\mathbb{V}^s_{\kappa,m} = \{(\phi, \psi) \in \mathbb{V}^s_\kappa \ : \ \langle \phi \rangle_\Omega = m_1, \ \langle \psi \rangle_\Gamma = m_2\}, \quad m = (m_1, m_2) \in \mathbb{R}^2.$$

In particular, $\mathbb{V}^s_{\kappa,0} = \mathbb{V}^s_{\kappa,(0,0)}$

Assumptions

(A1) **Regular potentials**:

$$F, G \in C^4(\mathbb{R}).$$

(A2) **Dissipative conditions**:

$\exists$ nonnegative constants independent of $y \in \mathbb{R}$

$$F(y) \geq -C_F, \quad F''(y) \geq -\widetilde{C}_F, \quad G(y) \geq -C_G, \quad G''(y) \geq -\widetilde{C}_G, \quad \forall\, y \in \mathbb{R}.$$

(A3) **Growth conditions**:

$\exists$ positive constants independent of $y \in \mathbb{R}$

$$|F''(y)| \leq \widehat{C}_F(1 + |y|^p), \quad |G''(y)| \leq \widehat{C}_G(1 + |y|^q), \quad \forall\, y \in \mathbb{R},$$

$\kappa > 0$: $p, q \in [0, +\infty)$ arbitrary if $d = 2$; $p = 2$ and q arbitrary if $d = 3$;

$\kappa = 0$: p arbitrary if $d = 2$ and $p = 2$ if $d = 3$; $q = 0$ for $d = 2, 3$.

Weak Solutions

Definition

Let $\kappa > 0$. For $T \in (0, +\infty)$ and $(\phi_0, \psi_0) \in \mathcal{V}^1$, a pair (ϕ, ψ) is called a **weak solution** to problem (P) on $[0, T]$, if

$$
\begin{aligned}
&(\phi, \psi) \in C([0,T]; \mathcal{V}^1) \cap L^2(0,T; \mathcal{V}^3),\\
&\mu \in L^2(0,T; H^1(\Omega)), \quad \mu_\Gamma \in L^2(0,T; H^1(\Gamma)),\\
&\phi_t \in L^2(0,T; (H^1(\Omega))^*), \quad \psi_t \in L^2(0,T; (H^1(\Gamma))^*),\\
&\langle \phi_t(t), \zeta \rangle_{(H^1(\Omega))^*, H^1(\Omega)} + \int_\Omega \nabla \mu(t) \cdot \nabla \zeta dx = 0,\\
&\langle \psi_t(t), \eta \rangle_{(H^1(\Gamma))^*, H^1(\Gamma)} + \int_\Gamma \nabla_\Gamma \mu_\Gamma \cdot \nabla_\Gamma \eta dS = 0,
\end{aligned}
$$

for every $\zeta \in H^1(\Omega)$ and $\eta \in H^1(\Gamma)$ and a.e. $t \in (0, T)$, with

$$
\begin{aligned}
&\mu = -\Delta \phi + F'(\phi), && \text{a.e. in } (0,T) \times \Omega,\\
&\mu_\Gamma = -\kappa \Delta_\Gamma \psi + \psi + G'(\psi) + \partial_{\mathbf{n}} \phi, && \text{a.e. on } (0,T) \times \Gamma.
\end{aligned}
$$

Main Result I

Theorem (Liu & Wu 2019 ARMA)

*Suppose that $\kappa > 0$ and (**A1**)–(**A3**) are satisfied.*

(1) *For any $(\phi_0, \psi_0) \in \mathcal{V}^1$, problem (P) admits a unique global weak solution.*

(2) *For $t > 0$, the weak solution becomes a strong one and*

$$\|\phi(t)\|_{H^3(\Omega)} + \|\psi(t)\|_{H^3(\Gamma)} \leq C \left(\frac{1+t}{t} \right)^{\frac{1}{2}},$$

where C depends on $E(\phi_0, \psi_0)$, Ω, Γ, κ and other coefficients.

Idea of proof

- Galerkin scheme ??

  – three Laplace operators (Neumann Laplace operator, Laplace-Beltrami operator, Wentzell Laplace operator)

- Abstract framework ?? (e.g., L^p maximal regularity theory [5])

  – Lopatinskii–Shapiro condition not fulfilled for the linear problem

- **Idea**

  Solve a regularized system (via the fixed point argument)

  + derive uniform estimates

  + pass to the limit

[5] Denk, Prüss & Zacher 2008

Regularization: The Viscous CHE

For any given $\alpha \in (0,1]$, consider

$$\begin{cases} \phi_t^\alpha = \Delta\mu^\alpha, \quad \text{with } \mu^\alpha = -\Delta\phi^\alpha + \alpha\phi_t^\alpha + F'(\phi^\alpha), & \text{in } (0,T)\times\Omega, \\ \partial_{\mathbf{n}}\mu^\alpha = 0, & \text{on } (0,T)\times\Gamma, \\ \phi^\alpha|_\Gamma = \psi^\alpha, & \text{on } (0,T)\times\Gamma, \\ \psi_t^\alpha = \Delta_\Gamma\mu_\Gamma^\alpha, & \text{on } (0,T)\times\Gamma, \\ \quad \text{with } \mu_\Gamma^\alpha = -\kappa\Delta_\Gamma\psi^\alpha + \psi^\alpha + \alpha\psi_t^\alpha + G'(\psi^\alpha) + \partial_{\mathbf{n}}\phi^\alpha, & \text{on } (0,T)\times\Gamma, \\ \phi^\alpha|_{t=0} = \phi_0(x), & \text{in } \Omega, \\ \psi^\alpha|_{t=0} = \psi_0(x) := \phi_0(x)|_\Gamma, & \text{on } \Gamma. \end{cases}$$

- **First Advantage**: better regularity for time derivatives $(\phi_t^\alpha, \psi_t^\alpha)$

$$\frac{d}{dt}E(\phi^\alpha,\psi^\alpha) + \|\nabla\mu^\alpha\|_{L^2(\Omega)}^2 + \|\nabla_\Gamma\mu_\Gamma^\alpha\|_{L^2(\Gamma)}^2 + \alpha\|(\phi_t^\alpha,\psi_t^\alpha)\|_{L^2(\Omega)\times L^2(\Gamma)}^2 = 0.$$

Local Well-posedness of VCHE

Lemma

*Let $\alpha \in (0,1]$ and $\kappa > 0$. Suppose that (**A1**) is satisfied.*
*For any $(\phi_0, \psi_0) \in \mathcal{V}^2$, there exists $T_\alpha > 0$ such that the regularized problem admits **a unique local strong solution** $(\phi^\alpha, \psi^\alpha)$ on $[0, T_\alpha]$ satisfying*

$$
\begin{aligned}
&(\phi^\alpha, \psi^\alpha) \in C([0, T_\alpha]; \mathcal{V}^2) \cap L^2(0, T_\alpha; \mathcal{V}^3) \\
&(\phi^\alpha_t, \psi^\alpha_t) \in L^\infty(0, T_\alpha; L^2(\Omega) \times L^2(\Gamma)) \cap L^2(0, T_\alpha; \mathcal{V}^1), \\
&\mu^\alpha \in L^2(0, T_\alpha; H^2(\Omega)), \quad \mu^\alpha_\Gamma \in L^2(0, T_\alpha; H^2(\Gamma)).
\end{aligned}
$$

- **Proof**: Contraction mapping theorem
- **Key issue**: Solve the linearized problem

The Linear Problem

$$
\begin{cases}
\phi_t - \Delta\widetilde{\mu} = 0, & \text{in } (0,T)\times\Omega,\\
\quad \text{with } \widetilde{\mu} = -\Delta\phi + \alpha\phi_t + h_1, & \text{in } (0,T)\times\Omega,\\
\partial_{\mathbf{n}}\widetilde{\mu} = 0, & \text{on } (0,T)\times\Gamma,\\
\phi|_\Gamma = \psi, & \text{on } (0,T)\times\Gamma,\\
\psi_t - \Delta_\Gamma\widetilde{\mu}_\Gamma = 0, & \text{on } (0,T)\times\Gamma,\\
\quad \text{with } \widetilde{\mu}_\Gamma = -\kappa\Delta_\Gamma\psi + \psi + \alpha\psi_t + \partial_{\mathbf{n}}\phi + h_2, & \text{on } (0,T)\times\Gamma,\\
\phi|_{t=0} = \phi_0(x), & \text{in } \Omega,\\
\psi|_{t=0} = \psi_0(x) := \phi_0(x)|_\Gamma, & \text{on } \Gamma.
\end{cases}
$$

Idea:

(1) **Decoupling** between bulk and boundary evolution

(2) **Second Advantage** of $\alpha > 0$ and $\kappa > 0$:
$\Longrightarrow$ solve 2nd order parabolic equations **instead of** 4th order equations.

Solvability I

Let $\widetilde{h}_1 = h_1 - \langle h_1 \rangle_\Omega$ and $\widetilde{h}_2 = h_2 - \langle h_2 \rangle_\Gamma$.

$$\begin{cases} [\alpha + (A^0_\Omega)^{-1}]\phi_t = \Delta\phi - \frac{|\Gamma|}{|\Omega|}\langle \partial_{\mathbf{n}}\phi\rangle_\Gamma - \widetilde{h}_1, & \text{in } (0,T)\times\Omega, \\ \phi|_\Gamma = \psi, & \text{on } (0,T)\times\Gamma, \\ \phi|_{t=0} = \phi_0(x), & \text{in } \Omega, \\ [\alpha + (A^0_\Gamma)^{-1}]\psi_t = \kappa\Delta_\Gamma\psi - \psi + \langle\psi\rangle_\Gamma - \partial_{\mathbf{n}}\phi + \langle\partial_{\mathbf{n}}\phi\rangle_\Gamma - \widetilde{h}_2, & \text{on } (0,T)\times\Gamma, \\ \psi|_{t=0} = \psi_0(x) := \phi_0(x)|_\Gamma, & \text{on } \Gamma. \end{cases}$$

Step 1. Set

$$\rho(t) = e^{-\kappa\Delta_\Gamma}\psi_0, \quad t \geq 0.$$

Given ψ, solve the auxiliary system and denote the solution by $\varphi = \mathfrak{T}(\psi - \rho)$

$$\begin{cases} [\alpha + (A^0_\Omega)^{-1}]\varphi_t = \Delta\varphi - \frac{|\Gamma|}{|\Omega|}\langle \partial_{\mathbf{n}}\varphi\rangle_\Gamma, & \text{in } \Omega\times(0,T), \\ \varphi|_\Gamma = \psi - \rho, & \text{on } \Gamma\times(0,T), \\ \varphi|_{t=0} = 0, & \text{in } \Omega. \end{cases}$$

Solvability II

Step 2. Set

$$\phi = u + \mathfrak{T}(\psi - \rho).$$

For new unknown variables (u, ψ):

$$\begin{cases} [\alpha + (A^0_\Omega)^{-1}]u_t = \Delta u - \dfrac{|\Gamma|}{|\Omega|}\langle \partial_{\mathbf{n}} u\rangle_\Gamma - \widetilde{h}_1, & \text{in } \Omega \times (0,T), \\ u|_\Gamma = \rho, & \text{on } \Gamma \times (0,T), \\ u|_{t=0} = \phi_0(x), & \text{in } \Omega, \\ [\alpha + (A^0_\Gamma)^{-1}]\psi_t = \kappa \Delta_\Gamma \psi - \psi + \langle \psi \rangle_\Gamma - \partial_{\mathbf{n}}(\mathfrak{T}(\psi - \rho)) & \\ \qquad + \langle \partial_{\mathbf{n}}(\mathfrak{T}(\psi - \rho))\rangle_\Gamma - \widehat{h}_2, & \text{on } \Gamma \times (0,T), \\ \text{with } \widehat{h}_2 = \partial_{\mathbf{n}} u - \langle \partial_{\mathbf{n}} u\rangle_\Gamma + \widetilde{h}_2, & \text{on } \Gamma \times (0,T), \\ \psi|_{t=0} = \psi_0(x) := \phi_0(x)|_\Gamma, & \text{on } \Gamma. \end{cases}$$

A decoupled system for (u, ψ) ! !

Solvability III

Step 3. Solve u first, and then solve ψ that satisfies

$$\alpha\psi_t - \kappa\Delta_\Gamma\psi + \psi = \mathfrak{K}\psi - \alpha[\alpha + (A_\Gamma^0)^{-1}]^{-1}\widehat{h}_2, \qquad \text{on } \Gamma \times (0,T),$$

$$\begin{aligned}\mathfrak{K}\psi = & -[\alpha + (A_\Gamma^0)^{-1}]^{-1}(A_\Gamma^0)^{-1}\big(\kappa\Delta_\Gamma\psi - \psi + \langle\psi\rangle_\Gamma - \partial_{\mathbf{n}}(\mathfrak{T}(\psi-\rho)) + \langle\partial_{\mathbf{n}}(\mathfrak{T}(\psi-\rho))\rangle_\Gamma\big) \\ & + \langle\psi\rangle_\Gamma - \partial_{\mathbf{n}}(\mathfrak{T}(\psi-\rho)) + \langle\partial_{\mathbf{n}}(\mathfrak{T}(\psi-\rho))\rangle_\Gamma .\end{aligned}$$

Lemma

*Let $\alpha \in (0,1]$, $\kappa > 0$. Suppose that $(\phi_0,\psi_0) \in \mathcal{V}^2$ and $(h_1,h_2) \in L^2(0,T;H^1(\Omega)\times H^1(\Gamma)) \cap H^1(0,T;L^2(\Omega)\times L^2(\Gamma))$ for some $T \in (0,+\infty)$. The linear problem admits **a unique strong solution** (ϕ,ψ) on $[0,T]$ such that*

$$(\phi,\psi) \in C([0,T];\mathcal{V}^2) \cap L^2(0,T;\mathcal{V}^3),$$
$$(\phi_t,\psi_t) \in L^\infty(0,T;L^2(\Omega)\times L^2(\Gamma)) \cap L^2(0,T;\mathcal{V}^1).$$

Main Result I'

Theorem (Liu & Wu 2019 ARMA)

*Suppose that $\kappa = 0$, $T > 0$ and (**A1**)–(**A3**) are satisfied.*
If $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) satisfies

$$c_{\mathcal{R}} |\Gamma|^{\frac{1}{2}} |\Omega|^{-1} < 1,$$

where $c_{\mathcal{R}} > 0$ is a constant related to the inverse trace theorem.
Then for any $(\phi_0, \psi_0) \in \mathcal{V}^1$, problem (P) admits a unique global weak solution (ϕ, ψ) on $[0, T]$ with

$$(\phi, \psi) \in C([0, T]; V^1) \cap L^2(0, T; V^{\frac{5}{2}}).$$

- **Proof**: Derive uniform estimates w.r.t. κ and take limit $\kappa \to 0^+$

Remark A

- **Drawbacks**

  – vanishing boundary diffusion $\Longrightarrow$ loss of regularity

  – unnatural geometric constraint

$$c_{\mathcal{R}}|\Gamma|^{\frac{1}{2}}|\Omega|^{-1} < 1.$$

- **Technical difficulty**

  – uniform estimate on $\partial_{\mathbf{n}}\phi$ w.r.t κ (the parabolic DtN operator) to recover the **strong form**

$$\begin{aligned} &\mu = -\Delta\phi + F'(\phi), && \text{a.e. in } (0,T)\times\Omega,\\ &\mu_\Gamma = -\kappa\Delta_\Gamma\psi + \psi + G'(\psi) + \partial_{\mathbf{n}}\phi, && \text{a.e. on } (0,T)\times\Gamma. \end{aligned}$$

Remark A

An alternative choice [6]

- Consider a **weaker notion** of weak solutions

$$\int_0^T\int_\Omega \mu\eta dxdt + \int_0^T\int_\Gamma \mu_\Gamma\eta_\Gamma dSdt$$
$$= \int_0^T\int_\Omega \nabla\phi\cdot\nabla\eta dxdt + \int_0^T\int_\Omega F'(\phi)\eta dxdt$$
$$+ \int_0^T\int_\Gamma \kappa\nabla_\Gamma\psi\cdot\nabla_\Gamma\eta_\Gamma dSdt + \int_0^T\int_\Gamma (\psi + G'(\psi))\eta_\Gamma dSdt$$

for $(\eta,\eta_\Gamma)\in L^2(0,T;\mathbb{V}^1_\kappa)\cap(L^\infty((0,T)\times\Omega)\times L^\infty((0,T)\times\Gamma))$.

:-) No $\partial_{\mathbf{n}}\phi \Longrightarrow$ Drop the assumption $c_{\mathcal{R}}|\Gamma|^{\frac{1}{2}}|\Omega|^{-1}<1$ for $\kappa=0$.

[6] Garcke & Knopf 2020 SIMA

Remark A

- **Key observation**:

  Gradient flow structure

$$\langle (\phi_t, \psi_t), (\eta, \eta_\Gamma) \rangle_{(\mathbb{V}^1_{\kappa,0})'} = -\frac{\delta E}{\delta(\phi, \psi)}((\phi, \psi))[(\eta, \eta_\Gamma)],$$

  for all $(\eta, \eta_\Gamma) \in \mathbb{V}^1_{\kappa,0} \cap (L^\infty(\Omega) \times L^\infty(\Gamma))$.

$\Longrightarrow$ Existence of a global weak solution ($\kappa \geq 0$):

An implicit time discretization

+ Convergence of the time-discrete solution

Remark B

- Well-posedness for the case with singular potentials?
- $\kappa > 0$: Colli, Fukao & Wu 2020 Math. Nachr.

  Existence and Uniqueness of Weak/Strong Solutions for a general setting of singular potentials **including** the logarithmic potential
- **Proof**:

  Regularization: the Moreau–Yosida approximation for singular potentials + adding viscous terms in chemical potentials

  + solve a time-discretization scheme (by using general theory of the maximal monotone operator)

  + derive uniform estimates and pass to the limit

Extensions and Future Work

- **General bulk-boundary interactions**
  - Knopf and Lam, 2020 Nonlinearity
  - Knopf, Lam, Liu and Metzger, 2021 ESAIM Math. Model. Numer Anal.
  - Knopf and Signori, 2021 JDE.
- **Role of the boundary diffusion**
  - Asymptotics as $\kappa \to 0^+$
- **Physically relevant case**
  - Thermal effects
- **Coupling with fluids**
  - The MCL problem / Electrowetting

The End

Thank You !