

A wide-angle photograph of the Prague skyline at sunset. The sky is filled with vibrant orange, pink, and purple clouds. In the foreground, the cobblestone bridge of the Charles Bridge is visible, flanked by large stone statues. The background features several historic buildings, including a prominent tower with a dark roof and a church with a green dome.

Dynamics of active droplet formation in reaction-driven Cahn-Hilliard models



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HUMBOLDT
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EMS Topical Activity Group Mixtures, Prague 2025
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Biological Motivation



- D. Zwicker, R. Seyboldt, C. A. Weber, A. A. Hyman, and F. Jülicher, Growth and division of active droplets provides a model for protocells. *Nature Phys.*, **3984** (2016).

Biological Motivation

A **protocell** is cell-like structure that models how the **first living cells might have formed**.

- **Droplets as early life models** as **chemical reaction** centers.
- **Protocell model**: active droplets could model early **protocells** with simple metabolic processes.

- H. Garcke, K.F. Lam, R. Nürnberg and **A.S.**, On a Cahn–Hilliard equation for the growth and division of chemically active droplets modeling protocells. *Work in progress*.
- H. Garcke, K.F. Lam, R. Nürnberg and **A.S.**, On a Mullins–Sekerka model for the growth of active droplets modeling protocells: Stability analysis and numerical computations. *Work in progress*.

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- J. Bauermann, G. Bartolucci, J. Boekhoven, C. A. Weber, and F. Jülicher, Formation of liquid shells in active droplet systems. *Phys. Review Research*, **5** (2023).
 - D. Zwicker, R. Seyboldt, C. A. Weber, A. A. Hyman, and F. Jülicher, Growth and division of active droplets provides a model for protocells. *Nature Phys.*, **3984** (2016).



Diffuse Interface Model (PF)

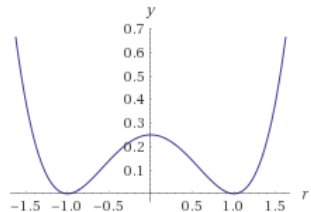
We consider the **diffuse interface model**

$$\begin{aligned}\partial_t \varphi &= \operatorname{div}(m(\varphi) \nabla \mu) + S_\varepsilon(\varphi) && \text{in } Q := \Omega \times (0, T), \\ \mu &= \beta(-\varepsilon \Delta \varphi + \tfrac{1}{\varepsilon} \psi'(\varphi)) && \text{in } Q, \\ m(\varphi) \partial_n \mu &= \partial_n \varphi = 0 && \text{on } \Gamma := \partial \Omega \times (0, T), \\ \varphi(0) &= \varphi_0 && \text{in } \Omega,\end{aligned}$$

with $\psi(r) = \frac{1}{4}(1 - r^2)^2$. The source term $S_\varepsilon \in C^1(\mathbb{R})$ is given by

$$S_\varepsilon(\varphi) = \begin{cases} S_+ - \frac{1}{\varepsilon} K_+(\varphi - 1) & \varphi \geq 1, \\ \text{cubic interpolation} & \varphi \in (-1, 1), \\ S_- - \frac{1}{\varepsilon} K_-(\varphi + 1) & \varphi \leq -1, \end{cases}$$

$S_+ < 0$, $S_- > 0$, and $K_\pm > 0$.



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- J. W. Cahn and J. E. Hilliard. Free energy of a nonuniform system. I. interfacial free energy. *J. Chem. Phys.*, **28**(2):258–267, 1958.
 - J. W. Cahn. On spinodal decomposition. *Acta metallurgica*, **9**(9):795–801, 1961.

Sharp Interface Model (SI)

We set: $\Omega^\pm = \Omega(t)^\pm := \{x \in \Omega : \varphi(x, t) = \pm 1\}$, $\Sigma(t) :=$ interface of the phases,

and $m_\pm := m(\pm 1)$. As $\varepsilon \rightarrow 0$, we find

$$-m_+ \Delta \mu = S_+ - \rho_+ \mu \quad \text{in } \Omega^+,$$

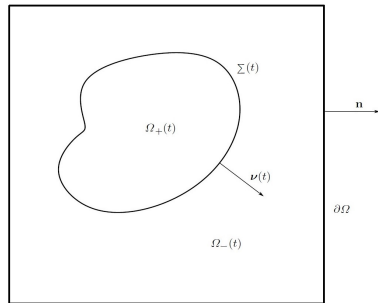
$$-m_- \Delta \mu = S_- - \rho_- \mu \quad \text{in } \Omega^-,$$

$$\mu = \frac{\gamma \beta \kappa}{2} \quad \text{on } \Sigma,$$

$$[\mu]_-^+ = 0 \quad \text{on } \Sigma,$$

$$-2\gamma = [m \nabla \mu]_-^+ \cdot \nu + \mathcal{S}_* \quad \text{on } \Sigma,$$

$$\partial_n \mu = 0 \quad \text{on } \partial \Omega,$$



$\rho_\pm = \frac{K_\pm}{\beta \psi''(\pm 1)}$, $\gamma \in \mathbb{R}$ depending on ψ , κ mean curvature of Σ , $\mathcal{S}_* \in \mathbb{R}$ depends on S .



Theoretical results

Theorem (Well-posedness of the PF model)

For every $\varphi_0 \in H^1$, there exists a *unique weak solution* (φ, μ) :

$$\varphi \in H^1(0, T; (H^1)^*) \cap L^\infty(0, T; H^1) \cap L^2(0, T; H^2), \quad \mu \in L^2(0, T; H^1),$$

satisfying, for every $v \in H^1$ and almost every $t \in (0, T)$,

$$\begin{aligned} \langle \partial_t \varphi, v \rangle_{H^1} + \int_{\Omega} m(\varphi) \nabla \mu \cdot \nabla v &= \int_{\Omega} S_\varepsilon(\varphi) v, \\ \int_{\Omega} \mu v &= \beta \varepsilon \int_{\Omega} \nabla \varphi \cdot \nabla v + \frac{\beta}{\varepsilon} \int_{\Omega} \psi'(\varphi) v. \end{aligned}$$

Moreover, let $\{(\varphi_i, \mu_i)\}_i$, $i = 1, 2$, *two solutions* with initial data $\varphi_{0,i} \in H^1$, $i = 1, 2$ and $m \equiv 1$. Then, it holds that

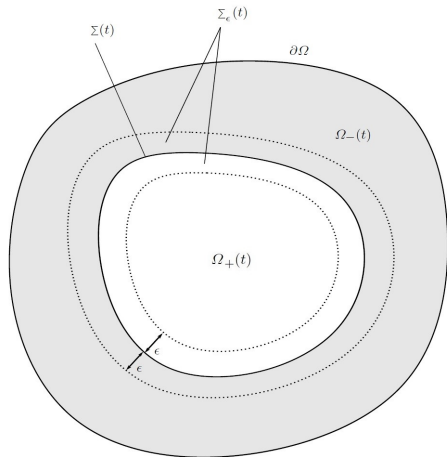
$$\begin{aligned} &\|(\varphi_1 - \varphi_2) - (\varphi_1 - \varphi_2)_\Omega\|_{L^\infty(0, T; (H^1)^*) \cap L^2(0, T; H^1)} + \|(\varphi_1)_\Omega - (\varphi_2)_\Omega\|_{L^\infty(0, T)} \\ &\leq K \left(\|(\varphi_{0,1} - (\varphi_{0,1})_\Omega) - (\varphi_{0,2} - (\varphi_{0,2})_\Omega)\|_* + |(\varphi_{0,1})_\Omega - (\varphi_{0,2})_\Omega| \right), \end{aligned}$$

for $K > 0$ just depending on structural data.

Schematic Idea of the Method

We introduce the **signed distance** function d to Σ_0 with $d > 0$ in Ω^+ and $d < 0$ in Ω^- , $\nabla d = \nu$ and set $z = \frac{d}{\varepsilon}$. We parametrize Σ_0 by arc-length as $g(t, s)$. In a tubular neighborhood of Σ_0 , a **smooth function** f is rewritten as:

$$f(x) = f(g(t, s) + \varepsilon z \nu(g(t, s))) =: F(t, s, z).$$

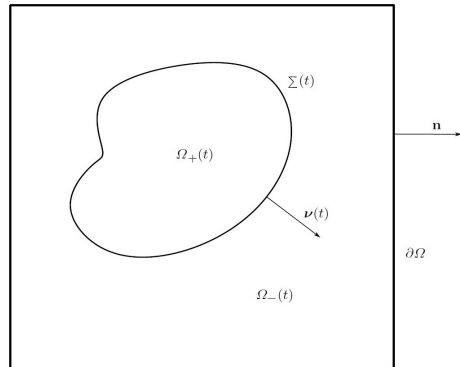


- $\partial_t f \approx -\frac{1}{\varepsilon} \nu \partial_z F$
- $\nabla_x f \approx \frac{1}{\varepsilon} \partial_z F \nu + \nabla_{\Sigma_0} F$
- $\Delta_x f \approx \frac{1}{\varepsilon^2} \partial_{zz} F - \frac{1}{\varepsilon} \kappa \partial_z F$

∇_{Σ_0} is the **surface gradient** on Σ_0 ,
 $\kappa = -\operatorname{div}_{\Sigma_0} \nu$ the **mean curvature**.

Sharp Interface Model (SI)

$$\begin{aligned}
 -m_+ \Delta \mu &= S_+ - \rho_+ \mu && \text{in } \Omega^+, \\
 -m_- \Delta \mu &= S_- - \rho_- \mu && \text{in } \Omega^-, \\
 \mu &= \frac{\gamma \beta \kappa}{2} && \text{on } \Sigma, \\
 [\mu]_-^+ &= 0 && \text{on } \Sigma, \\
 -2\mathcal{V} &= [m \nabla \mu]_-^+ \cdot \nu + \mathcal{S}_* && \text{on } \Sigma, \\
 \partial_n \mu &= 0 && \text{on } \partial \Omega,
 \end{aligned}$$



- $\rho_{\pm} = \frac{K_{\pm}}{\beta \psi''(\pm 1)}$;
- $\gamma \in \mathbb{R}$ depending on ψ ;

- κ is the mean curvature of Σ ;
- $\mathcal{S}_* \in \mathbb{R}$ depends on S .



Perturbation of Planar Solutions

Planar Solutions

We study the (SI) in:

$$\Omega = (0, \mathcal{L}) \times (0, \tilde{\mathcal{L}})^{d-1}, \quad \mathcal{L}, \tilde{\mathcal{L}} > 0,$$

and seek for a planar solution in

$$\Omega_+(t) = (0, q(t)) \times (0, \tilde{\mathcal{L}})^{d-1}, \quad \Omega_-(t) = (q(t), \mathcal{L}) \times (0, \tilde{\mathcal{L}})^{d-1},$$

where $q(t)$ encodes the location of the interface Σ_0 .

We set $x = (z, \hat{x})$ with $z \in \mathbb{R}$ and $\hat{x} \in \mathbb{R}^{d-1}$. As $\nu = (-1, 0)^\top$ we get $\mathcal{V} = -\dot{q}$ and make the ansatz

$$\mu_{\pm}(t, (z, \hat{x})) = \hat{\mu}_{\pm}(t, z), \quad z \in (0, \mathcal{L}), \hat{x} \in (0, \tilde{\mathcal{L}})^{d-1}.$$

Original System

$$-m_+ \Delta \mu = S_+ - \rho_+ \mu \quad \text{in } \Omega^+,$$

$$-m_- \Delta \mu = S_- - \rho_- \mu \quad \text{in } \Omega^-,$$

$$\mu = \frac{\gamma \beta \kappa}{2} \quad \text{on } \Sigma,$$

$$[\mu]_-^+ = 0 \quad \text{on } \Sigma,$$

$$-2\mathcal{V} = [m \nabla \mu]_-^+ \cdot \nu + S_I \quad \text{on } \Sigma,$$

$$\partial_n \mu = 0 \quad \text{on } \partial\Omega,$$

Planar Scenario

$$-m_+ \mu_+'' = S_+ - \rho_+ \mu_+ \quad \text{for } z \in (0, q(t)),$$

$$-m_- \mu_-'' = S_- - \rho_- \mu_- \quad \text{for } z \in (q(t), \mathcal{L}),$$

$$\mu_+'(t, 0) = 0,$$

$$\mu_-'(t, \mathcal{L}) = 0,$$

$$2\dot{q} = -[m \mu']_-^+ + S_I.$$

We obtain as solutions

$$\mu_+(t, z) = d_+ \left(1 - \frac{\cosh(\Lambda_+ z)}{\cosh(\Lambda_+ q(t))} \right), \quad \mu_-(t, z) = d_- \left(1 - \frac{\cosh(\Lambda_- (\mathcal{L} - z))}{\cosh(\Lambda_- (\mathcal{L} - q(t)))} \right),$$

where $d_{\pm} := \frac{S_{\pm}}{\rho_{\pm}} = \beta \frac{S_{\pm} \psi''(\pm 1)}{K_{\pm}}$, and $\Lambda_{\pm} := \sqrt{\frac{\rho_{\pm}}{m_{\pm}}}$. The evolution equation $2\dot{q} = -[m\mu']_{-}^{+} + S_I$ for the interface position becomes

$$\dot{q} = \frac{1}{2} (d_+ m_+ \Lambda_+ \tanh(\Lambda_+ q) + d_- m_- \Lambda_- \tanh(\Lambda_- (\mathcal{L} - q)) + S_I) =: \mathcal{H}(q).$$

We notice that

$$\mathcal{H}(0) = \frac{1}{2} (d_- m_- \Lambda_- \tanh(\Lambda_- \mathcal{L}) + S_I), \quad \mathcal{H}(\mathcal{L}) = \frac{1}{2} (d_+ m_+ \Lambda_+ \tanh(\Lambda_+ \mathcal{L}) + S_I).$$

Claim:

The existence of a root q^* of $\mathcal{H}$ can be guaranteed.

For instance: $S_+ = -1$, all other parameters equal to 1 $\Rightarrow q^* = \frac{\mathcal{L}}{2}$.

General case: after fixing parameters, one can adjust L in S_I to ensure the existence of a root.



Linear Stability of Planar Solutions

Goal: Analyse stability of planar solutions $\mu_{\pm}^*$ around position q^* .

We consider a perturbed interface $w := q^* + \epsilon Y$, with $Y = Y(t, \hat{x})$. We make the ansatz

$$\mu_{\pm}(t, x) = \mu_{\pm}^*(z) + \epsilon u_{\pm}(t, x),$$

and demand that those solve the **FBP**

$$\begin{aligned} -m_+ \Delta(\mu_+^* + \epsilon u_+) &= S_+ - \rho_+(\mu_+^* + \epsilon u_+) && \text{in } \{z < w\}, \\ -m_- \Delta(\mu_-^* + \epsilon u_-) &= S_- - \rho_-(\mu_-^* + \epsilon u_-) && \text{in } \{z > w\}, \\ \mu_+^* + \epsilon u_+ &= \mu_-^* + \epsilon u_- && \text{on } \{z = w\}, \\ 2(\mu_{\pm}^* + \epsilon u_{\pm}) &= \gamma \beta \kappa && \text{on } \{z = w\}, \\ -2\mathcal{V} &= [m \nabla(\mu^* + \epsilon u)]_{-}^{\pm} \cdot \nu + S_I && \text{on } \{z = w\}, \\ (\mu_+^* + \epsilon u_+)'(t, 0) &= 0, \quad (\mu_-^* + \epsilon u_-)'(t, \mathcal{L}) = 0. \end{aligned}$$

Linearizing the above equations around $\{z = q^*\}$, produces

$$\begin{aligned}
 -m_+ \Delta u_+ &= -\rho_+ u_+ && \text{in } \{z < q^*\}, \\
 -m_- \Delta u_- &= -\rho_- u_- && \text{in } \{z > q^*\}, \\
 (\mu_+^*)'|_{z=q^*} Y + u_+ &= (\mu_-^*)'|_{z=q^*} Y + u_- && \text{on } \{z = q^*\}, \\
 2((\mu_\pm^*)'|_{z=q^*} Y + u_\pm) &= -\gamma\beta \Delta_{\hat{x}} Y && \text{on } \{z = q^*\}, \\
 2\dot{Y} &= -m_+((\mu_+^*)''|_{z=q^*} Y + u'_+) + m_-((\mu_-^*)''|_{z=q^*} Y + u'_-) && \text{on } \{z = q^*\}, \\
 (u_+)'(t, 0) &= 0, \quad (u_-)'(t, \mathcal{L}) = 0.
 \end{aligned}$$

Ansatz: $u_\pm(x) = v_\pm(z)W(\hat{x})$ and choose W as an eigenfunction of the $\Delta_{\hat{x}}$ -operator with Neumann boundary conditions such that for $\hat{\ell} = (\ell_2, \dots, \ell_d) \in \mathbb{N}_0^{d-1}$,

$$\begin{cases} \Delta_{\hat{x}} W = \frac{\zeta_{\hat{\ell},d}}{(\tilde{\mathcal{L}})^2} W & \text{in } (0, \tilde{\mathcal{L}})^{d-1}, \\ \partial_n W = 0 & \text{on } \partial(0, \tilde{\mathcal{L}})^{d-1}. \end{cases}$$

A possible **eigenfunction** is

$$W(x_2, \dots, x_d) = \cos\left(\frac{\pi}{\tilde{\mathcal{L}}} \ell_2 x_2\right) \times \dots \times \cos\left(\frac{\pi}{\tilde{\mathcal{L}}} \ell_d x_d\right), \quad \zeta_{\hat{\ell},d} = -\pi^2(\ell_2^2 + \dots + \ell_d^2).$$

With this ansatz for $u_{\pm}$ we find that

$$-m_{\pm}(v_{\pm}''W + v_{\pm}\Delta_{\hat{x}}W) = -\rho_{\pm}v_{\pm}W$$

and this yields

$$v_{\pm}'' = \left(\Lambda_{\pm}^2 - \frac{\zeta_{\hat{\ell},d}}{(\tilde{\mathcal{L}})^2}\right)v_{\pm} = (\Gamma_{\pm}^{\hat{\ell}})^2 v_{\pm}, \quad \Lambda_{\pm}^2 = \frac{\rho_{\pm}}{m_{\pm}} \quad \text{and} \quad \Gamma_{\pm}^{\hat{\ell}} = \sqrt{\Lambda_{\pm}^2 - \frac{\zeta_{\hat{\ell},d}}{(\tilde{\mathcal{L}})^2}}.$$

We set

$$v_{+}(z) = a_{+} \cosh(\Gamma_{+}^{\hat{\ell}} z), \quad v_{-}(z) = a_{-} \cosh(\Gamma_{-}^{\hat{\ell}} (\mathcal{L} - z)),$$

for some unknowns $a_{+}(t)$ and $a_{-}(t)$ to be determined and choose $Y = W$. Imposing the boundary conditions, we obtain

$$a_{+}(q^{*}) = \frac{1}{\cosh(\Gamma_{+}^{\hat{\ell}} q^{*})} \left(d_{+} \Lambda_{+} \tanh(\Lambda_{+} q^{*}) - \frac{\gamma \beta}{2} \frac{\zeta_{\hat{\ell},d}}{(\tilde{\mathcal{L}})^2} \right),$$

$$a_{-}(q^{*}) = -\frac{1}{\cosh(\Gamma_{-}^{\hat{\ell}} (\mathcal{L} - q^{*}))} \left(d_{-} \Lambda_{-} \tanh(\Lambda_{-} (\mathcal{L} - q^{*})) + \frac{\gamma \beta}{2} \frac{\zeta_{\hat{\ell},d}}{(\tilde{\mathcal{L}})^2} \right).$$

Meanwhile, we have

$$2\dot{Y} = (S_+ - S_- - m_+ a_+(q^*) \Gamma_+^{\hat{\ell}} \sinh(\Gamma_+^{\hat{\ell}} q^*) - m_- a_-(q^*) \Gamma_-^{\hat{\ell}} \sinh(\Gamma_-^{\hat{\ell}} (\mathcal{L} - q^*))) Y =: \alpha Y$$

with **amplification** factor α .

We consider parameters s.t. $\alpha > 0 \Rightarrow$ **instabilities** from interface perturbations.

We fix $\hat{\ell} = (\ell_2, \dots, \ell_d)$, and take

$$S_+ = -1, \quad S_- = m_{\pm} = \rho_{\pm} = 1, \quad d_+ = -1, \quad d_- = 1, \quad \Lambda_{\pm} = 1,$$

so that the stationary state is $q^* = \frac{\mathcal{L}}{2}$. Moreover $\Gamma_{\pm}^{\hat{\ell}}, a_+(q^*)$ and $a_-(q^*)$ are **explicit** and

$$\alpha = -2 + \sqrt{1 + \frac{|\hat{\ell}|^2 \pi^2}{\tilde{\mathcal{L}}^2}} \tanh \left(\frac{\mathcal{L}}{2} \sqrt{1 + \frac{|\hat{\ell}|^2 \pi^2}{\tilde{\mathcal{L}}^2}} \right) \left(2 \tanh \left(\frac{\mathcal{L}}{2} \right) - \gamma \beta \frac{|\hat{\ell}|^2 \pi^2}{\tilde{\mathcal{L}}^2} \right).$$

Perturbation of Planar Solutions - Conclusion

From $2\dot{Y} = \alpha Y$ we draw the following conclusions:

- $\hat{\ell} = \hat{0}$: translational perturbations $w = q^* + \epsilon$, we see that the amplification factor becomes negative. Thus:

$$\hat{\ell} = \hat{0} \Rightarrow \text{stability with respect to translational perturbations}$$

- $|\hat{\ell}| > 0$: perturbations of the form $w = q^* + \epsilon \cos(\pi \ell_2 x_2 / \tilde{\mathcal{L}}) + \dots + \epsilon \cos(\pi \ell_d x_d / \tilde{\mathcal{L}})$. We see that α is positive when $\beta < \beta_{\text{crit}}(\hat{\ell})$, where

$$\beta_{\text{crit}}(\hat{\ell}) = \frac{2}{\gamma} \frac{\tilde{\mathcal{L}}^2}{|\hat{\ell}|^2 \pi^2} \left(\tanh\left(\frac{\mathcal{L}}{2}\right) - \frac{1}{\sqrt{1 + |\hat{\ell}|^2 \pi^2 / \tilde{\mathcal{L}}^2} \tanh\left(\frac{\mathcal{L}}{2} \sqrt{1 + |\hat{\ell}|^2 \pi^2 / \tilde{\mathcal{L}}^2}\right)} \right).$$

As $|\hat{\ell}|^2 = (\ell_2)^2 + \dots + (\ell_d)^2$, we obtain that the possible perturbations lead to **amplification factors via sum of squares**. For $d = 2$ we obtain $|\hat{\ell}|^2 = 0, 1, 4, 9, \dots$ and for $d = 3$ we have $|\hat{\ell}|^2 = 0, 1, 2, 4, 5, 8, 9, 10, \dots$

$$|\hat{\ell}| > 0 \text{ and } \beta \text{ small} \Rightarrow \text{instabilities}$$



Numerical
results



Figure 3: ($\varepsilon = \frac{1}{32\pi}$, $\Omega = (0,1)^2$) Evolution for $\beta = 0.1$, $S_- = 8$, $S_+ = -8$. We show the solution at times $t = 0, 0.1, 1, 2, 10$.



Figure 14: ($\varepsilon = \frac{1}{32\pi}$, $\Omega = (0,2)^2$) Evolution for $\beta = 0.002$, $S_- = 0.25$, $S_+ = -4$. We show the solution at times $t = 0, 0.2, 1, 2, 5$.



Figure 15: ($\varepsilon = \frac{1}{32\pi}$, $\Omega = (0,1)^2$) Evolution for $\beta = 0.002$, $S_- = 0.25$, $S_+ = -4$. We show the solution at times $t = 0, 0.2, 1, 2, 5$.

Numerics - 2D



Figure 16: ($\varepsilon = \frac{1}{16\pi}$, $\Omega = (0, 2)^2$) Evolution for $\beta = 0.02$, $S_- = 1$, $S_+ = -4$. We show the solution at times $t = 0, 2, 4, 6, 8, 10$.



Figure 17: ($\varepsilon = \frac{1}{16\pi}$, $\Omega = (0, 4)^2$) Evolution for $\beta = 0.02$, $S_- = 1$, $S_+ = -4$. We show the solution at times $t = 0, 2, 4, 6, 8, 10$.

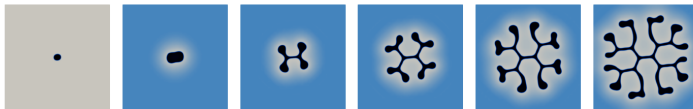


Figure 18: ($\varepsilon = \frac{1}{16\pi}$, $\Omega = (0, 8)^2$) Evolution for $\beta = 0.02$, $S_- = 1$, $S_+ = -4$. We show the solution at times $t = 0, 2, 4, 6, 8, 10$.

Numerics - 3D



Figure 45: $(\Omega = (-4, 4)^3)$ perturbed data with $r_0 = 0.65$, $m_- = 0.1$, $m_+ = 7$, $\beta = 0.1$, $S_- = 1.4$, $S_+ = -7$, $\rho_- = 0.065$, $\rho_+ = 0.1$, $L = -1$. Below the solution at times $t = 0.5, 1, 1.5, 2$.





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Conclusions:

We propose a **Cahn–Hilliard** model for **active droplets**, deriving a **sharp interface** model and performing stability analysis that identifies both stable and unstable solutions. **Numerical simulations** validate the theoretical findings.



Recap (continues)

Dynamics of active droplet formation in reaction-driven Cahn-Hilliard models

EMS Topical Activity Group Meetings, Prague 2025
A. Singer (Humboldt-Universität zu Berlin, 4-5 Jan 2025, 4-5 Jan 2025)

Slide 1

Biological Motivation

Slide 2

Biological Motivation

A **protocol** is cell-like structure that models how the **first living cells might have formed**:

- **Droplets as early life models as chemical reaction centers.**
- **Protocell model:** active droplets could model early **protocells** with simple metabolic processes.

• H. Garcke, K.F. Lam, R. Nürnberg and A.S., On a Cahn-Hilliard equation for the growth and division of chemically active droplets modeling protocells. *Work in progress.*

• H. Garcke, K.F. Lam, R. Nürnberg and A.S., On a Mullins-Sekerka model for the growth of active droplets modeling protocells: Stability analysis and numerical computations. *Work in progress.*

• D. Zwicker, R. Seyboldt, C. A. Vitale, A. A. Holmes, and F. Jülicher, Growth and division of active droplets provides a model for protocells. *Nature Phys.*, **2008** (2008).

Slide 3

Diffuse Interface Model (PF)

We consider the **diffuse interface model**

$$\begin{aligned} \Delta \varphi &= \Delta(\varphi(\nabla \varphi) + S, \varphi) & \text{in } Q := \Omega \times (0, T), \\ \mu &= \varphi(-\Delta \varphi + \frac{1}{2} \varphi^2) & \text{in } Q, \\ \varphi|_{\partial \Omega} &= \varphi_0 & \text{on } \partial \Omega \times (0, T), \\ \varphi(0) &= \varphi_0 & \text{in } \Omega, \end{aligned}$$

with $\varphi(t) = \frac{1}{2}(1 - \varphi^2)^2$. The source term $S \in C^2(\Omega)$ is given by

$$S, \varphi = \begin{cases} S_+ - \frac{1}{2}K_+(\varphi - 1) & \varphi \geq 1, \\ S_- - \frac{1}{2}K_-(\varphi + 1) & \varphi \leq -1, \\ S_+ - \frac{1}{2}K_+(\varphi + 1) & \varphi \leq -1, \\ S_- - \frac{1}{2}K_-(\varphi - 1) & \varphi \geq 1. \end{cases}$$

$S_+ \leq 0, S_- \geq 0$, and $K_+ \geq 0, K_- \geq 0$.

• J. W. Cahn and J. E. Hilliard, Free energy of a nonuniform system. I. interfacial free energy. *J. Chem. Phys.*, **28**(2), 258-267, 1958.

• J. W. Cahn, On spinodal decomposition. *Acta Metallurgica*, **9**(9), 930-951, 1961.

Slide 4

Sharp Interface Model (SI)

We set: $\Omega^t = \Omega(t)^+ := \{x \in \Omega : \varphi(x, t) = 1\}$, $\Sigma(t) := \text{interface of the phases}$, and $m_\Sigma := m_\Sigma(t)$. As $t \rightarrow 0$, we find

$$\begin{aligned} -m_\Sigma \Delta \varphi &= S_+ - \mu, \mu & \text{in } \Omega^+, \\ -m_\Sigma \Delta \varphi &= S_- - \mu, \mu & \text{in } \Omega^-, \\ \mu &= \frac{1}{2} & \text{on } \Sigma, \\ |\dot{\varphi}|^2 &= 0 & \text{on } \Sigma, \\ -2\Gamma = |\nabla \varphi|^2|_{\Sigma} : \nu + S_+ & & \text{on } \Sigma, \\ \dot{\varphi}|_{\Sigma} &= 0 & \text{on } \partial \Omega, \end{aligned}$$

$\mu = \frac{1}{2} \frac{\Delta \varphi}{|\nabla \varphi|^2}$, $\gamma \in \mathbb{R}$ depending on φ , κ mean curvature of Σ , $S_\pm \in \mathbb{R}$ depends on S .

• W. W. Mullins and R. F. Sekerka, *J. Appl. Phys.*, **47**, *J. Appl. Phys.*, **47**, *J. Chem. Phys.*, **47**.

Slide 5

Theoretical results

Slide 6

Theorem (Well-posedness of the PF model)

For every $\varphi_0 \in H^1$, there exists a unique weak solution (φ, μ) :

$$\varphi \in L^2(0, T; (H^1)^2) \cap L^\infty(0, T; H^1), \quad \mu \in L^2(0, T; H^1),$$

satisfying, for every $v \in H^1$ and almost every $t \in (0, T)$,

$$\frac{d}{dt} \int_\Omega \varphi v + \int_\Omega m_\Sigma \nabla \varphi \cdot \nabla v = \int_\Omega S v,$$

Moreover, let $(\varphi_0, \mu_0) \in H^1 \times L^2$, $\varphi_0 \in H^1$, $\mu_0 \in L^2$ and $\mu_0 \geq 0$. Then, it holds that

$$\begin{aligned} \|\varphi_0 - \mu_0\| - \|\varphi_0 - \mu_0\|_{H^1} &\leq \|\varphi_0 - \mu_0\|_{H^1} + \|\varphi_0 - \mu_0\|_{H^1} \\ &\leq K(\|\varphi_0 - \mu_0\|_{H^1} - \|\varphi_0 - \mu_0\|_{H^1}) + \|\varphi_0 - \mu_0\|_{H^1} \end{aligned}$$

for $K > 0$ just depending on structural data.

Slide 7

Schematic Idea of the Method

We introduce the **signed distance function** d of Σ_0 with $d > 0$ in Ω^+ and $d < 0$ in Ω^- , $\nabla d \cdot \nu = \kappa$ and $\kappa \in \mathbb{R}$. We parameterize Σ_0 by arc-length as $g(t, s)$. In a tubular neighborhood of Σ_0 a **smooth function** f is written as

$$f(x) = f(g(t, s) + \kappa g(t, s)) = f(t, s, \kappa)$$

$\nabla_x f \approx -\frac{1}{2} \nabla \Sigma_0 f$
 $\nabla_x f \approx \frac{1}{2} \nabla \Sigma_0 f + \nabla_{\Sigma_0} f$
 $\Delta_x f \approx \frac{1}{2} \Delta \Sigma_0 f - \frac{1}{2} \kappa \Delta \Sigma_0 f$

∇_x is the surface gradient on Σ_0 , $\kappa = -\text{div}_{\Sigma_0} \nu$ the mean curvature.

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Sharp Interface Model (SI)

$$\begin{aligned} -m_\Sigma \Delta \varphi &= S_+ - \mu, \mu & \text{in } \Omega^+, \\ -m_\Sigma \Delta \varphi &= S_- - \mu, \mu & \text{in } \Omega^-, \\ \mu &= \frac{1}{2} & \text{on } \Sigma, \\ |\dot{\varphi}|^2 &= 0 & \text{on } \Sigma, \\ -2\Gamma = |\nabla \varphi|^2|_{\Sigma} : \nu + S_+ & & \text{on } \Sigma, \\ \dot{\varphi}|_{\Sigma} &= 0 & \text{on } \partial \Omega, \end{aligned}$$

* $\mu = \frac{1}{2} \frac{\Delta \varphi}{|\nabla \varphi|^2}$, $\gamma \in \mathbb{R}$ depending on φ , κ is the mean curvature of Σ , $S_\pm \in \mathbb{R}$ depends on S .

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Perturbation of Planar Solutions

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Planar Solutions

We study the (SI):

$$\Omega = \{x \in \mathbb{R}^2 : |x| \leq R\}, \quad R > 0,$$

and seek for a planar solution in

$$\Omega = \{x \in \mathbb{R}^2 : |x| \leq R\}, \quad \Omega = \{x \in \mathbb{R}^2 : |x| \leq R\},$$

where $g(t)$ encodes the location of the interface Σ_0 . We set $v = (v, \mu)$ and $v \in C^1(\mathbb{R}^2)$. As $v = (-1, 0)$ we get $v = -q$ and make the ansatz

$$\mu(x, t) = \mu(x, t), \quad x \in \mathbb{R}^2, t \in [0, \infty).$$

Original System

$$\begin{aligned} -m_\Sigma \Delta \varphi &= S_+ - \mu, \mu & \text{in } \Omega^+, \\ -m_\Sigma \Delta \varphi &= S_- - \mu, \mu & \text{in } \Omega^-, \\ \mu &= \frac{1}{2} & \text{on } \Sigma, \\ |\dot{\varphi}|^2 &= 0 & \text{on } \Sigma, \\ -2\Gamma = |\nabla \varphi|^2|_{\Sigma} : \nu + S_+ & & \text{on } \Sigma, \\ \dot{\varphi}|_{\Sigma} &= 0 & \text{on } \partial \Omega. \end{aligned}$$

Planar Scenario

$$\begin{aligned} -m_\Sigma \Delta \varphi &= S_+ - \mu, \mu & \text{for } x \in [0, d(t)], \\ -m_\Sigma \Delta \varphi &= S_- - \mu, \mu & \text{for } x \in [d(t), R], \\ \mu &= \frac{1}{2} & \text{on } \Sigma, \\ |\dot{\varphi}|^2 &= 0 & \text{on } \Sigma, \\ -2\Gamma = |\nabla \varphi|^2|_{\Sigma} : \nu + S_+ & & \text{on } \Sigma, \\ \dot{\varphi}|_{\Sigma} &= 0 & \text{on } \partial \Omega. \end{aligned}$$

$2\Gamma = -|\nabla \varphi|^2|_{\Sigma} = S_+$

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We obtain an solution:

$$\mu_+(t, x) = d_+ \left(1 - \frac{\cosh(x-d_+)}{\cosh(d_+)}\right), \quad \mu_-(t, x) = d_- \left(1 - \frac{\cosh(x-d_-)}{\cosh(d_-)}\right),$$

where $d_\pm = \frac{1}{2} \pm \frac{1}{2} \frac{S_\pm}{\kappa}$ and $A_\pm = \sqrt{\frac{2}{\kappa}}$. The evolution equation $2\Gamma = -|\nabla \varphi|^2 = S_+$ for the interface position becomes

$$\dot{d} = \frac{1}{2} d_+ m_\Sigma \tanh(A_+ d_+) + d_+ m_\Sigma \tanh(A_+ (L - d_+)) = 3(d_+)$$

We notice that

$$3(d_+) = \frac{1}{2} d_+ m_\Sigma \tanh(A_+ d_+) + S_+, \quad 3(d_-) = \frac{1}{2} d_- m_\Sigma \tanh(A_- d_-) + S_-.$$

Claim:
 The existence of a root q^* of $\mathcal{H}$ can be guaranteed.

For instance: $S_\pm = -1$, all other parameters equal to 1 $\Rightarrow q^* = \frac{1}{2}$.

General case: after fixing parameters, one can adjust L in $S_\pm$ to ensure the existence of a root.

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Recap (continues)

Linear Stability of Planar Solutions

Goal: Analyze stability of planar solutions p^* around position q^*

We consider a perturbed interface $W = q^* + \epsilon Y$, with $Y = Y(x, z)$. We make the ansatz

$$p(x, z) = p^*(z) + \epsilon p_1(z, t),$$

and demand that those solve the FBP

$$\begin{aligned} -m_1 \Delta p_1 + \epsilon p_1 &= S_1 - p_1 (p_1^* + \epsilon p_1) & \text{in } \{z < w\}, \\ -m_2 \Delta p_1 + \epsilon p_1 &= S_2 - p_1 (p_1^* + \epsilon p_1) & \text{in } \{z > w\}, \\ p_1^* + \epsilon p_1 &= p^* + \epsilon p_1 & \text{on } \{z = w\}, \\ 2(p_1^* + \epsilon p_1) &= \gamma \kappa & \text{on } \{z = w\}, \\ -2\epsilon \gamma \kappa [p_1^* + \epsilon p_1] &= \epsilon \kappa & \text{on } \{z = w\}, \\ (p_1^* + \epsilon p_1)(x, 0) &= 0, \quad (p_1^* + \epsilon p_1)(x, L) = 0. \end{aligned}$$

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Linearizing the above equations around $\{z = q^*\}$, produces

$$\begin{aligned} -m_1 \Delta p_1 &= -p_1 p_1^* & \text{in } \{z < q^*\}, \\ -m_2 \Delta p_1 &= -p_1 p_1^* & \text{in } \{z > q^*\}, \\ (p_1^*)' [p_1^* + \epsilon p_1] &= (p_1^*)' [p_1^* + \epsilon p_1] & \text{on } \{z = q^*\}, \\ 2(p_1^*)' [p_1^* + \epsilon p_1] &= -\gamma \kappa \Delta Y & \text{on } \{z = q^*\}, \\ 2\epsilon \gamma \kappa [p_1^* + \epsilon p_1] &= -\gamma \kappa \Delta Y & \text{on } \{z = q^*\}, \\ 2\epsilon \gamma \kappa [p_1^* + \epsilon p_1] &= -\gamma \kappa \Delta Y & \text{on } \{z = q^*\}, \\ (p_1^*)'(x, 0) &= 0, \quad (p_1^*)'(x, L) = 0. \end{aligned}$$

Ansatz: $w(x) = w(z)W(x)$ and choose W as an eigenfunction of the Δ -operator with Neumann boundary conditions such that for $\tilde{z} \in \{0, \dots, L\} \in \mathbb{N}^{L-1}$,

$$\begin{cases} \Delta W = -\frac{\lambda}{L^2} W & \text{in } (0, L)^{d-1}, \\ \partial_\nu W = 0 & \text{on } \partial(0, L)^{d-1}. \end{cases}$$

A possible eigenfunction is

$$W(x_1, \dots, x_{d-1}) = \cos\left(\frac{\tilde{z}}{L} x_1\right) \times \dots \times \cos\left(\frac{\tilde{z}}{L} x_{d-1}\right), \quad \tilde{z}_d = -x_1^2 + \dots + x_{d-1}^2.$$

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With this ansatz for w_1 we find that

$$-m_1 (\epsilon^2 W + \epsilon_1 \Delta W) = -p_1 p_1 W$$

and this yields

$$v_1^* = \left(\lambda_1^2 - \frac{\lambda}{L^2}\right) w_1 = \left(\lambda_1^2 - \frac{\lambda}{L^2}\right) w_1, \quad \lambda_1^2 = \frac{\lambda}{L^2} \text{ and } \lambda_1^2 = \sqrt{\lambda_1^2 - \frac{\lambda}{L^2}}.$$

We set

$$v_1(x) = a_1 \cosh(\lambda_1^2 x), \quad v_2(x) = a_2 \cosh(\lambda_2^2 (L - x)),$$

for some unknown a_1, λ_1 and a_2, λ_2 to be determined and choose $Y = W$. Imposing the boundary conditions, we obtain

$$\begin{aligned} a_1(\lambda_1^2) &= \frac{1}{\cosh(\lambda_1^2 L)} \left(d_1 A_1 \tanh(\lambda_1^2 L) - \frac{\lambda}{L^2} \right), \\ a_2(\lambda_2^2) &= \frac{1}{\cosh(\lambda_2^2 L)} \left(d_2 A_2 \tanh(\lambda_2^2 L) - \frac{\lambda}{L^2} \right). \end{aligned}$$

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Perturbation of Planar Solutions - Conclusion

From $2Y = \epsilon Y$ we draw the following conclusions:

- $\tilde{z} = 0$: translational perturbations $w = q^* + \epsilon$, we see that the amplification factor becomes negative. Thus:

$$\tilde{z} = 0 \Rightarrow \text{stability with respect to translational perturbations}$$

- $|\tilde{z}| > 0$: perturbations of the form $w = q^* + \epsilon \cos(\tilde{z} p_1^*/2) + \dots + \epsilon \cos(\tilde{z} p_{d-1}^*/2)$. We see that w is positive when $\tilde{z} < \tilde{z}_{\text{crit}}(\tilde{z})$, where

$$\tilde{z}_{\text{crit}}(\tilde{z}) = \frac{1}{2} \sqrt{\frac{2}{\lambda_1^2}} \left(\tanh\left(\frac{\tilde{z}}{L}\right) - \frac{1}{\sqrt{1 + \lambda_1^2 L^2}} \tanh\left(\frac{\tilde{z}}{L}\right) \right).$$

As $\tilde{z}^2 = (\tilde{z}_1^2 + \dots + \tilde{z}_{d-1}^2)$, we obtain that the possible perturbations lead to amplification factors via sum of squares. For $d = 2$ we obtain $\tilde{z}^2 = 0, 1, 4, 9, \dots$ and for $d = 3$ we have $\tilde{z}^2 = 0, 1, 2, 4, 5, 8, 9, 10, \dots$

$$\tilde{z} > 0 \text{ and } |\tilde{z}| \leq \tilde{z}_{\text{crit}} \Rightarrow \text{instabilities}$$

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Numerical results

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Numerics - 2D



Figure 18: $\tilde{z} = \frac{1}{2} \sqrt{\frac{2}{\lambda_1^2}}$, $\tilde{z} = 0.5$. Evolution for $\tilde{z} = 0.5$, $\lambda_1 = 1$, $\lambda_2 = -1$. We show the evolution of the droplet for $t = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$.



Figure 19: $\tilde{z} = \frac{1}{2} \sqrt{\frac{2}{\lambda_1^2}}$, $\tilde{z} = 0.5$. Evolution for $\tilde{z} = 0.5$, $\lambda_1 = 1$, $\lambda_2 = -1$. We show the evolution of the droplet for $t = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$.



Figure 20: $\tilde{z} = \frac{1}{2} \sqrt{\frac{2}{\lambda_1^2}}$, $\tilde{z} = 0.5$. Evolution for $\tilde{z} = 0.5$, $\lambda_1 = 1$, $\lambda_2 = -1$. We show the evolution of the droplet for $t = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$.

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Numerics - 2D



Figure 21: $\tilde{z} = \frac{1}{2} \sqrt{\frac{2}{\lambda_1^2}}$, $\tilde{z} = 0.5$. Evolution for $\tilde{z} = 0.5$, $\lambda_1 = 1$, $\lambda_2 = -1$. We show the evolution of the droplet for $t = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$.

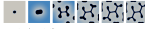


Figure 22: $\tilde{z} = \frac{1}{2} \sqrt{\frac{2}{\lambda_1^2}}$, $\tilde{z} = 0.5$. Evolution for $\tilde{z} = 0.5$, $\lambda_1 = 1$, $\lambda_2 = -1$. We show the evolution of the droplet for $t = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$.



Figure 23: $\tilde{z} = \frac{1}{2} \sqrt{\frac{2}{\lambda_1^2}}$, $\tilde{z} = 0.5$. Evolution for $\tilde{z} = 0.5$, $\lambda_1 = 1$, $\lambda_2 = -1$. We show the evolution of the droplet for $t = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$.

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Numerics - 3D



Figure 24: $\tilde{z} = (-4, 4)^T$ perturbed data with $\lambda_1 = 0.05$, $\lambda_2 = 0.1$, $\lambda_3 = 0.1$, $\lambda_4 = 1.4$, $\lambda_5 = -1.7$, $\lambda_6 = 0.005$, $\lambda_7 = 0.1$, $\lambda_8 = -1$. Below the solution at times $t = 0.5, 1, 1.5, 2$.



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Conclusions:

We propose a Cahn-Hilliard model for active droplets, deriving a sharp interface model and performing stability analysis that identifies both stable and unstable solutions. Numerical simulations validate the theoretical findings.

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