Sharp Interface Models for Solid-State Dewetting and Their Applications

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1. Introduction

2. Solid-state dewetting in 2D
   - Mathematical model
   - The parametric finite element method (PFEM)
   - Convergence test and numerical results

3. Extension to 3D case
   - Mathematical model
   - PFEM in 3D

4. Conclusion and future works
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Physical experiment I

Figure: Dewetting of Ni with different sizes (J. Ye and C.V. Thompson, 2011).
Figure: Dewetted patches that evolved from square ring patches with two different in-plane orientations. (a) Ni (110); (b) Ni (100) films. (J. Ye and C.V. Thompson, 2011)
Motivation

♠ Morphological characteristics

- Edge retraction, hole formation, pinch-off events, finger instability.

Applications

- Destroy micro-/nano-device performance.
- Used to produce sensors, optical and magnetic devices, catalysts for growth of carbon, semiconductor nanowires.
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♠ Morphological characteristics

- Edge retraction, hole formation, pinch-off events, finger instability.
- **Thin film geometry**: the size, orientation, location of holes.

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- Edge retraction, hole formation, pinch-off events, finger instability.
- Thin film geometry: the size, orientation, location of holes.
- Substrate topology: templated dewetting (W.L. Ling et al., 2004; A.L. Giermann et al., 2005, A. Sundar et al., 2012).
- Anisotropy: corner instability (D. Amram et al., 2012; R.V. Zucker et al., 2016), facet instability (J. Ye et al., 2011).

♣ Applications

- Destroy micro-/nano-device performance.
- Used to produce sensors, optical and magnetic devices, catalysts for growth of carbon, semiconductor nanowires.
Herring’s local Gibbs-Thomson equation in 3D (C. Herring, 1951)

\[
\mu = \Omega \left[ (\gamma + \frac{\partial^2 \gamma}{\partial n_x^2}) \kappa_x + (\gamma + \frac{\partial^2 \gamma}{\partial n_y^2}) \kappa_y \right],
\]

where \( \Omega \) is the atomic volume; \( \kappa_x, \kappa_y \) are the two principle curvatures, \( n_x, n_y \) are the two corresponding angles in the two principle directions.

Reduced to 2D

\[
\mu = \Omega (\gamma(\theta) + \gamma''(\theta)) \kappa,
\]

Extensions to 3D case are awkward and almost impossible, and numerical treatments not available.
\( \xi \)-vector formulation


\[
\xi(n) = \nabla \hat{\gamma}(p) \bigg|_{p=n}, \quad \hat{\gamma}(p) = |p| \gamma\left(\frac{p}{|p|}\right), \quad \forall p \in \mathbb{R}^3 \setminus \{0\}.
\]

$$\xi(n) = \nabla \hat{\gamma}(p) \Big|_{p=n}, \quad \hat{\gamma}(p) = |p| \gamma\left(\frac{p}{|p|}\right), \quad \forall p \in \mathbb{R}^3 \setminus \{0\}.$$ 

Mathematical construction of the equilibrium shape: $\xi$-plot.

$$\xi(n) = \gamma(\theta, \phi)n + \frac{\partial \gamma(\theta, \phi)}{\partial \theta} \tau_\theta + \frac{1}{\sin \theta} \frac{\partial \gamma(\theta, \phi)}{\partial \phi} \tau_\phi,$$

Surface diffusion flow (W.W. Mullins, 1957; J.W. Cahn and D.W. Hoffman, 1974.)

The normal velocity $v_n$ of the surface $S$ is given by

$$v_n = -\Omega_0 \nabla_s \cdot j, \quad j = -\frac{D_s \nu}{k_B T_e} \nabla_s \mu, \quad \mu = \Omega_0 \frac{\delta W}{\delta S} = \Omega_0 \nabla_s \cdot \xi.$$
Objectives

1. Derive sharp interface models via Cahn-Hoffman $\xi$-vector

2. Develop efficient parametric finite element methods (PFEM)

3. Explore the morphological characteristics
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Surface energy in 2D

Figure: A schematic illustration of solid thin film in 2D.

♠ Total surface energy

\[ W(\Gamma) = \int_{\Gamma_{FV}} \gamma_{FV} \, d\Gamma_{FV} + \int_{\Gamma_{FS}} \gamma_{FS} \, d\Gamma_{FS} + \int_{\Gamma_{VS}} \gamma_{VS} \, d\Gamma_{VS}. \]
First variation

- **Simplified energy**

$$W = \int_{\Gamma} \gamma(n) \, ds + \left( \gamma_{FS} - \gamma_{VS} \right) (x_c^r - x_c^l) + \gamma_{VS} (b-a),$$

Substrate energy

- **Perturbation, \( l = [0, 1] \)**

$$\Gamma^\varepsilon = X(\rho, \varepsilon) : l \times [0, \varepsilon_0] \to \mathbb{R}^2, \quad y(0, \varepsilon) = y(1, \varepsilon) = 0.$$

- **Introduce a deformation vector field**:

$$V(\rho, \varepsilon) = \frac{\partial X(\rho, \varepsilon)}{\partial \varepsilon}, \quad \forall \varepsilon \in [0, \varepsilon_0],$$

- **For any functional \( F(\Gamma) \), define its first variation with respect to any smooth deformation vector field \( V \) as**

$$\delta F(\Gamma; V) = \lim_{\varepsilon \to 0} \frac{F(\Gamma^\varepsilon) - F(\gamma)}{\varepsilon}.$$
The first variation of the free energy functional in solid-state dewetting problems with respect to any smooth deformation field $V$ is given as:

$$
\delta W(\Gamma; V) = - \int_{\Gamma} \left[ (\partial_s \xi)^\perp \cdot n \right] (V_0 \cdot n) \, ds + \left[ (\xi_2 - \sigma) (V_0 \cdot e_1) \right] \bigg|_{s=0}^{s=L},
$$

where $\perp$ represents the clockwise rotation of a vector by 90 degrees, $\xi = (\xi_1, \xi_2)$ is the Cahn-Hoffman vector, $\sigma = \gamma_{VS} - \gamma_{FS}$, and $e_1 = (1, 0)$ represents the unit vector along the $x$-coordinate (or the substrate line).
Variation with respect to $\Gamma$, $x_l^c$ and $x_r^c$

\[
\frac{\delta W}{\delta \Gamma} = -\left(\partial_s \xi\right)^\perp \cdot n, \quad \frac{\delta W}{\delta x_l^c} = -\left(\xi_2 \bigg|_{s=0} - \sigma\right), \quad \frac{\delta W}{\delta x_r^c} = \xi_2 \bigg|_{s=L} - \sigma.
\]
Dynamics

♠ Variation with respect to $\Gamma$, $x^l_c$ and $x^r_c$

$$\frac{\delta W}{\delta \Gamma} = -(\partial_s \xi)^\perp \cdot n,$$

$$\frac{\delta W}{\delta x^l_c} = - (\xi_2|_{s=0} - \sigma),$$

$$\frac{\delta W}{\delta x^r_c} = \xi_2|_{s=L} - \sigma.$$ 

◇ Normal velocity for the curve: surface diffusion flow

- Chemical potential: Gibbs-Thomson relation

$$\mu = \Omega_0 \frac{\delta W}{\delta \Gamma},$$

- Fick’s law

$$j = -\frac{D_s \nu}{k_B T_e} \partial_s \mu \tau, \quad v_n = -\Omega_0 (\partial_s j) \cdot \tau = \frac{D_s \nu \Omega_0^2}{k_B T_e} \partial_{ss} \left[ \frac{\delta W}{\delta \Gamma} \right].$$

◇ Relaxed contact angle condition: energy gradient flow

$$\frac{dx^l_c(t)}{dt} = -\eta \frac{\delta W}{\delta x^l_c},$$

$$\frac{dx^r_c(t)}{dt} = -\eta \frac{\delta W}{\delta x^r_c}.$$
The dimensionless model in 2D

\[
\begin{aligned}
\partial_t X &= \partial_{ss} \mu \ n, \quad 0 < s < L(t), \quad t > 0, \\
\mu &= - (\partial_s \xi)^\perp \cdot n, \quad \xi = \nabla \hat{\gamma} (p) \bigg|_{p=n};
\end{aligned}
\]

with boundary conditions

(i) contact point condition

\[ y(0, t) = 0, \quad y(L, t) = 0, \quad t \geq 0; \]

(ii) relaxed contact angle condition

\[
\frac{dx^l_c}{dt} = \eta (\xi^2 \big|_{s=0} - \sigma), \quad \frac{dx^r_c}{dt} = -\eta (\xi^2 \big|_{s=L} - \sigma), \quad t \geq 0;
\]

(iii) zero-mass flux condition

\[ \partial_s \mu(0, t) = 0, \quad \partial_s \mu(L, t) = 0, \quad t \geq 0. \]
The sharp interface model

♠ Mass conservation

\[ A(t) \equiv A(0) = \int_{\Gamma(0)} y_0(s) \partial_s x_0(s) \, ds, \quad t \geq 0, \]

♠ Energy dissipation

\[ \frac{d}{dt} W(t) = -\int_{\Gamma(t)} (\partial_s \mu)^2 \, ds - \frac{1}{\eta} \left[ \left( \frac{dx^l_c}{dt} \right)^2 + \left( \frac{dx^r_c}{dt} \right)^2 \right] \leq 0. \]
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Variational formulation

- parameterize the curves as
  \[ \Gamma(t) = X(\rho, t) : I \times [0, T] \to \mathbb{R}^2, \]
  where the time-independent spatial variable \( \rho \in I \), and \( I \) denotes a fixed reference spatial domain, say \( I := [0, 1] \).

- \( L^2 \) inner product
  \[
  \langle u, v \rangle_\Gamma := \int_{\Gamma(t)} u(s)v(s) \, ds = \int_I u(s(\rho, t))v(s(\rho, t))|\partial_\rho X| \, d\rho.
  \]

- Functional space
  \[
  H^1_{a, b}(I) = \{ u \in H^1(I) : u(0) = a, u(1) = b \}.
  \]
Variational formulation

- Re-formulate the PDEs

\[
\frac{\partial}{\partial t} X = \partial_{ss} \mu \cdot n \quad \Rightarrow \quad \frac{\partial}{\partial t} X \cdot n = \partial_{ss} \mu.
\]

\[
\mu = -\left(\partial_s \xi\right)^\perp \cdot n \quad \Rightarrow \quad \mu \cdot n = -\left(\partial_s \xi\right)^\perp.
\]

Find \( X \in H_{a,b}(I) \times H^1_0(I), \quad \mu \in H^1(I) \) with \( a = x^l_c(t) \leq x^r_c(t) = b \),

\[
\left\langle \frac{\partial}{\partial t} X, \varphi n \right\rangle_{\Gamma} + \left\langle \partial_s \mu, \partial_s \varphi \right\rangle_{\Gamma} = 0, \quad \forall \varphi \in H^1(I),
\]

\[
\left\langle \mu n, \omega \right\rangle_{\Gamma} - \left\langle \xi^\perp, \partial_s \omega \right\rangle_{\Gamma} = 0, \quad \forall \omega \in H^1_0(I) \times H^1_0(I),
\]
Semi-implicit PFEM

- **Finite element spaces**

  \[ V^h := \{ u \in C(I) : u \mid_{I_j} \in P_1, \quad \forall j = 1, 2, \ldots, N \} \subseteq H^1(I), \]

  \[ V_{a,b}^h := \{ u \in V^h : u(0) = a, \ u(1) = b \} \subseteq H^1_{a,b}(I). \]

- **Inner product**

  \[ \langle u, v \rangle^h = \frac{1}{2} \sum_{j=1}^{N} \left| X^m(\rho_j) - X^m(\rho_{j-1}) \right| \left[ (u \cdot v)(\rho_j^-) + (u \cdot v)(\rho_{j-1}^+) \right]. \]

Find \( X^{m+1} \in V_{a,b}^h \times V_0^h, \quad \mu \in V^h \) such that

\[ \langle \frac{X^{m+1} - X^m}{t_{m+1} - t_m}, \varphi_h n^m \rangle^h_{\Gamma_m} + \langle \partial_s \mu^{m+1}, \partial_s \varphi_h \rangle^h_{\Gamma_m} = 0, \quad \forall \varphi_h \in V^h, \]

\[ \langle \mu^{m+1} n^m, \omega_h \rangle^h_{\Gamma_m} - \langle [\xi^{m+\frac{1}{2}}]_\perp, \partial_s \omega_h \rangle^h_{\Gamma_m} = 0, \quad \forall \omega_h \in V_0^h \times V_0^h, \]
Properties

◊ Linearization of $\xi$

$$\xi^{m+\frac{1}{2}} = \begin{cases} 
\gamma(\theta^m)n^{m+1} - \gamma'(\theta^m)\tau^{m+1}, & \text{if } \gamma = \gamma(\theta), \\
\gamma(n^m)n^{m+1} + (\xi^m \cdot \tau^m)\tau^{m+1}, & \text{if } \gamma = \gamma(n). 
\end{cases}$$

◊ Anisotropy Riemannian metric form (K. Deckelnick et al. (2005), J.W. Barrett et al. (2007))

$$\gamma(n) = \sum_{l=0}^{L} \sqrt{G_l n \cdot n}, \quad \xi(n) = \sum_{l=0}^{L} \left[\sqrt{G_l n \cdot n}\right]^{-1} G_k n,$$

where $G_l$, $l = 0, \cdots, L$, is a symmetric positive definite matrix. In this special case, the numerical approximation term $\xi^{m+\frac{1}{2}}$ can be defined as:

$$\xi^{m+\frac{1}{2}} = \sum_{k=0}^{L} \left[\sqrt{G_l n^m \cdot n^m}\right]^{-1} G_l n^{m+1}.$$
Properties

\[ a = x_c^l(t_{m+1}) \leq x_c^r(t_{m+1}) = b \text{ are updated via Euler forward scheme} \]

\[
\begin{align*}
\frac{x_c^l(t_{m+1}) - x_c^l(t_m)}{\tau_m} &= \eta \left[ \xi_2^m \bigg|_{\rho=0} - \sigma \right], \\
\frac{x_c^r(t_{m+1}) - x_c^r(t_m)}{\tau_m} &= -\eta \left[ \xi_2^m \bigg|_{\rho=1} - \sigma \right].
\end{align*}
\]
Properties

\( a = x_c^l(t_{m+1}) \leq x_c^r(t_{m+1}) = b \) are updated via Euler forward scheme

\[
\frac{x_c^l(t_{m+1}) - x_c^l(t_m)}{\tau_m} = \eta \left[ \xi_2^m \right]_{\rho=0} - \sigma,
\]

\[
\frac{x_c^r(t_{m+1}) - x_c^r(t_m)}{\tau_m} = -\eta \left[ \xi_2^m \right]_{\rho=1} - \sigma.
\]

- **Linear system**: sparse matrix, \( \Delta t = O((\Delta s)^2) \).
- **Well-posedness**.
- Good preservation of mesh quality for isotropic case, Re-meshing is needed for strongly anisotropic case.
Stabilized scheme

For $m \geq 0$, find $\Gamma^{m+1} = X^{m+1} \in \mathcal{V}_{a,b}^h \times \mathcal{V}_0^h$ with the $x$-coordinate positions of the moving contact points $a := x^l_c(t_{m+1}) \leq b := x^r_c(t_{m+1})$ and $\mu^{m+1} \in \mathcal{V}^h$ such that

$$\left\langle \mu^{m+1} n^m, \omega_h \right\rangle_{\Gamma_m}^h - \left\langle (\xi^m) \perp , \partial_s \omega_h \right\rangle_{\Gamma_m}^h$$

$$-\lambda \left\langle \gamma(n^m) \partial_s (X^{m+1} - X^m), \partial_s \omega_h \right\rangle_{\Gamma_m}^h = 0, \quad \forall \omega_h \in \mathcal{V}_0^h \times \mathcal{V}_0^h,$$
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Convergence test I

\[ e_{h, \tau}(t) = \| X_{h, \tau} - X_{h, \tau}^{\frac{\tau}{2/4}} \|_{L^\infty} = \max_{0 \leq j \leq N} \min_{\rho \in [0,1]} | X_{h, \tau}(\rho_j, t) - X_{h, \tau}^{\frac{\tau}{2/4}}(\rho, t) |, \]

**Table:** Convergence rates (closed curve; isotropic case)

<table>
<thead>
<tr>
<th>( e_{h, \tau}(t) )</th>
<th>( h = h_0 )</th>
<th>( h_0/2 )</th>
<th>( h_0/2^2 )</th>
<th>( h_0/2^3 )</th>
<th>( h_0/2^4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau = \tau_0 )</td>
<td>( \tau_0/2 )</td>
<td>( \tau_0/2^2 )</td>
<td>( \tau_0/2^4 )</td>
<td>( \tau_0/2^6 )</td>
<td>( \tau_0/2^8 )</td>
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<tr>
<td>( e_{h, \tau}(t = 0.5) )</td>
<td>4.58E-3</td>
<td>1.09E-3</td>
<td>2.63E-4</td>
<td>6.40E-5</td>
<td>1.58E-5</td>
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<tr>
<td>order</td>
<td>–</td>
<td>2.07</td>
<td>2.05</td>
<td>2.04</td>
<td>2.02</td>
</tr>
<tr>
<td>( e_{h, \tau}(t = 2.0) )</td>
<td>3.61E-3</td>
<td>9.43E-4</td>
<td>2.45E-4</td>
<td>6.31E-5</td>
<td>1.61E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.94</td>
<td>1.95</td>
<td>1.96</td>
<td>1.97</td>
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<td>( e_{h, \tau}(t = 5.0) )</td>
<td>3.63E-3</td>
<td>9.47E-4</td>
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<td>6.33E-5</td>
<td>1.62E-5</td>
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<tr>
<td>order</td>
<td>–</td>
<td>1.94</td>
<td>1.95</td>
<td>1.96</td>
<td>1.97</td>
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</tbody>
</table>
### Table: Convergence rates (closed curve; anisotropic case)

<table>
<thead>
<tr>
<th>( e_{h,\tau}(t) )</th>
<th>( h = h_0 ) ( \tau = \tau_0 )</th>
<th>( h_0/2 ) ( \tau_0/2^2 )</th>
<th>( h_0/2^2 ) ( \tau_0/2^4 )</th>
<th>( h_0/2^3 ) ( \tau_0/2^6 )</th>
<th>( h_0/2^4 ) ( \tau_0/2^8 )</th>
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<td>( e_{h,\tau}(t = 0.5) )</td>
<td>1.24E-2</td>
<td>2.25E-3</td>
<td>6.71E-4</td>
<td>2.48E-4</td>
<td>7.10E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>2.46</td>
<td>1.74</td>
<td>1.44</td>
<td>1.80</td>
</tr>
<tr>
<td>( e_{h,\tau}(t = 2.0) )</td>
<td>4.86E-3</td>
<td>1.44E-3</td>
<td>4.57E-4</td>
<td>1.37E-4</td>
<td>3.71E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.76</td>
<td>1.66</td>
<td>1.74</td>
<td>1.89</td>
</tr>
<tr>
<td>( e_{h,\tau}(t = 5.0) )</td>
<td>4.88E-3</td>
<td>1.44E-3</td>
<td>4.58E-4</td>
<td>1.37E-5</td>
<td>3.74E-5</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.76</td>
<td>1.66</td>
<td>1.74</td>
<td>1.89</td>
</tr>
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</table>
### Convergence test III

#### Table: Convergence rates (open curve; anisotropic case)

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<tr>
<th>$e_{h,\tau}(t)$</th>
<th>$h = h_0$</th>
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<td>$\tau_0/2^2$</td>
<td>$\tau_0/2^4$</td>
<td>$\tau_0/2^6$</td>
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<td>2.82E-2</td>
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<tr>
<td>order</td>
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<td>0.99</td>
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<td>1.00</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 2.0)$</td>
<td>2.71E-2</td>
<td>1.37E-2</td>
<td>6.78E-3</td>
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</tr>
<tr>
<td>order</td>
<td>–</td>
<td>0.98</td>
<td>1.02</td>
<td>0.99</td>
</tr>
<tr>
<td>$e_{h,\tau}(t = 5.0)$</td>
<td>2.32E-2</td>
<td>1.12E-3</td>
<td>5.80E-3</td>
<td>2.92E-3</td>
</tr>
<tr>
<td>order</td>
<td>–</td>
<td>1.00</td>
<td>1.00</td>
<td>0.99</td>
</tr>
</tbody>
</table>
Small island film (5 × 1)

- \( m \)-fold anisotropy

\[
\gamma(\theta) = 1 + 0.06 \cos(4\theta), \quad \sigma = \cos(3\pi/4)
\]
Define the mesh distribution function $\psi(t)$ as

$$
\psi(t_m) = \frac{\max_{1 \leq j \leq N} |h_j^m|}{\min_{1 \leq j \leq N} |h_j^m|},
\Gamma^m = \bigcup_{j=1}^{N} h_j^m
$$

**Figure:** (a) The temporal evolution of the normalized total free energy and the normalized total area/mass; (b) the temporal evolution of the mesh distribution function $\psi(t)$. 

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Small island: application of the stabilised scheme

\[ \gamma(\theta) = 1 + \beta |\cos \frac{k\theta}{2}|, \quad \gamma(\theta) = 1 + \beta \sqrt{\delta^2 + \cos^2 \frac{k\theta}{2}}. \]

\[ k = 5, \beta = 0.19, \delta = 0.1, \lambda = 20. \]

Figure: Several snapshots in the evolution of a small, initially rectangular islands film towards its equilibrium shape (a) \( t = 0 \); (b) \( t = 0.1 \); (c) \( t = 0.6 \); (d) \( t = 7.5 \).
Riemannian metric

\[
\gamma(n) = \sum_{l=0}^{L} \sqrt{R(-\phi_l)D(\delta_l)R(\phi_l)n \cdot n}, \quad D(\delta_l) = \begin{pmatrix} 1 & 0 \\ 0 & \delta_l^2 \end{pmatrix},
\]

\[L = 1, \ \phi_0 = \pi/4, \ \phi_1 = 3\pi/4, \ \delta_0 = \delta_1 = 0.1, \ \sigma = \cos(5\pi/6)\]
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A sharp interface model

\[ \gamma_{FV} = \gamma(n) \]

Figure: A schematic illustrate of solid-state dewetting on a substrate in 3D

♦ The total surface energy

\[ W = W_{int} + W_{sub} = \int \int_{S} \gamma(n) \, dS + (\gamma_{FS} - \gamma_{VS})A(\Gamma), \]

Substrate energy
Speed method

♠ Transformation $T_\varepsilon$
A domain $D \in \mathbb{R}^3$ with boundary $\partial D$ piecewise $C^k$ for a given integer $k \geq 0$, define the one to one transformation as

$$T_\varepsilon : \bar{D} \rightarrow \bar{D}, \quad \varepsilon \in [0, \varepsilon_0),$$

♠ The speed vector field
Let $x(X, \varepsilon) = T_\varepsilon(X)$, the speed vector field $V(x, \varepsilon)$

$$V(x, \varepsilon) = \frac{\partial x}{\partial \varepsilon}(T_\varepsilon^{-1}(x), \varepsilon).$$

♠ Remarks
- $T_\varepsilon$ is uniquely determined by $V$, vice versa.
- Assumption: $V \in C(C^k(\bar{D}, \bar{D}); [0, \varepsilon_0)), \ V_0 = V(X, 0)$.
- Surface $S \subset \bar{D}, \ S_\varepsilon = T_\varepsilon(S)$.  

Zhao Quan (NUS) Solid-State Dewetting
Theorem

Suppose $S \in \mathbb{R}^3$ is an open surface with smooth boundary $\Gamma \subset S_{sub}$ ($xOy$ plane), $T_\varepsilon$ is a transformation on $S$ such that $T_\varepsilon \Gamma \subset S_{sub}$. Let $W(S) = \int\int_S \gamma(n) \, dS + (\gamma_{FS} - \gamma_{VS})A(\Gamma)$, then we have

$$
\delta W(S; V) = \int\int_S (\nabla_S \cdot \xi)(V_0 \cdot n) \, dS + \int_{\Gamma}(c^\gamma_\Gamma \cdot n_\Gamma + \gamma_{FS} - \gamma_{VS})(n_\Gamma \cdot V_0) \, d\Gamma.
$$

- $V$ is the vector field associated with $T_\varepsilon$.
- $\xi(n)$ is the Cahn-Hoffman vector defined as
  $$
  \xi(n) = \nabla \hat{\gamma}(p) \bigg|_{p=n}, \text{ with } \hat{\gamma}(p) = |p|\gamma\left(\frac{p}{|p|}\right), \forall p \in \mathbb{R}^3 \setminus \{0\}.
  $$
- $c^\gamma_\Gamma = (\xi \cdot n)c_\Gamma - (\xi \cdot c_\Gamma)n$. 

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**Dynamics**

♠ **Variation**

\[
\frac{\delta W}{\delta S} = \nabla_S \cdot \xi.
\]

\[
\frac{\delta W}{\delta \Gamma} = c^\gamma \cdot n_\Gamma + \gamma_{FS} - \gamma_{VS}.
\]

♠ **Surface diffusion flow**

The normal velocity \( v_n \) of the surface \( S \)

\[
v_n = \frac{D_s \nu \Omega_0}{k_B T_e} \nabla^2_S \mu, \quad \mu = \Omega_0 \frac{\delta W}{\delta S} = \Omega_0 \nabla_S \cdot \xi.
\]

♠ **Relaxed contact angle conditions**

The normal velocity \( v_c \) of the \( \Gamma \)

\[
v_c = -\eta \frac{\delta W}{\delta \Gamma} = -\eta \left[ c_\Gamma^\gamma \cdot n_\Gamma + \gamma_{FS} - \gamma_{VS} \right].
\]
A dimensionless sharp interface model

\[
\begin{aligned}
\frac{\partial_t \mathbf{X}}{} &= \nabla_s^2 \mu \mathbf{n}, \quad t > 0, \\
\mu &= \nabla_s \cdot \mathbf{\xi}, \quad \mathbf{\xi} = \nabla (\hat{\gamma}(\mathbf{p})) \bigg|_{\mathbf{p}=\mathbf{n}}; \\
\end{aligned}
\]

with boundary conditions
(1) contact line condition

\[ \Gamma \subset S_{\text{sub}}, \quad t \geq 0; \]

(2) relaxed contact angle condition

\[
\frac{\partial_t \mathbf{X}}{\Gamma} = -\eta \left[ \mathbf{c}_\Gamma \cdot \mathbf{n}_\Gamma - \sigma \right] \mathbf{n}_\Gamma, \quad t \geq 0,
\]

where \( \sigma = \frac{\gamma_{VS} - \gamma_{FS}}{\gamma_0}, \mathbf{c}_\Gamma = (\mathbf{\xi} \cdot \mathbf{n}) \mathbf{c}_\Gamma - (\mathbf{\xi} \cdot \mathbf{c}_\Gamma) \mathbf{n}. \)

(3) zero mass flux condition

\[
(\mathbf{c}_\Gamma \cdot \nabla_s \mu) \bigg|_{\Gamma} = 0, \quad t \geq 0.
\]
Mass conservation and energy dissipation

♠ Mass conservation

\[ M(t) \equiv M(0) = \iiint_{\Omega(0)} dx, \quad \forall t \geq 0. \]

♠ Energy dissipation

\[ \frac{d}{dt} W(t) = - \iint_{S(t)} |\nabla s \mu|^2 \, dS - \eta \int_{\Gamma(t)} (c^\gamma \cdot n_{\Gamma} - \sigma)^2 \, d\Gamma \leq 0. \]
Outline

1. Introduction

2. Solid-state dewetting in 2D
   - Mathematical model
   - The parametric finite element method (PFEM)
   - Convergence test and numerical results

3. Extension to 3D case
   - Mathematical model
   - PFEM in 3D

4. Conclusion and future works
PFEM: Isotropic model

\[
\begin{cases}
\partial_t X = \nabla^2_S \mu \; n, & t \geq 0; \\
\mu = \mathcal{H} = -\nabla^2_S X \cdot n;
\end{cases}
\]

with boundary conditions

(1) contact line condition

\[ \Gamma \subset S_{sub}, \quad t \geq 0; \]

(2) relaxed contact angle condition

\[ \partial_t \mathbf{X}_\Gamma = -\eta \left[ \mathbf{c}_\Gamma \cdot \mathbf{n}_\Gamma - \sigma \right] \mathbf{n}_\Gamma, \quad t \geq 0; \]

(3) zero-mass flux condition

\[ (\mathbf{c} \cdot \nabla_S \mu)|_\Gamma = 0, \quad t \geq 0. \]
PFEM: Variational formulation

Find \( S(t) = X(\cdot, t) \in W_\Gamma(U), \mu \in H^1(S) \) such that

\[
\langle \partial_t X \cdot n, \phi \rangle_S + \langle \nabla_s \mu, \nabla_s \phi \rangle_S = 0, \quad \forall \phi \in H^1(S),
\]

\[
\langle \mu, n \cdot g \rangle_S - \langle \nabla_s X, \nabla_s g \rangle_S = 0, \quad \forall g \in (H^1_0(S))^3.
\]

- **Functional space**

\[
W_\Gamma(U) := \{ X \in (H^1(U))^3, \quad X|_{\partial U} = \Gamma \},
\]

with \( \Gamma = \Gamma(t) \) is determined by the relaxed contact angle condition.

- **Inner product**

\[
\langle u, v \rangle_S = \int \int_S u \cdot v \, dS.
\]
PFEM: Temporal/spatial discretization

- **Temporal discretization:** \( 0 = t_0 < t_1 < t_2 < \cdots < t_M = T \).

- **Spatial discretization:**
  - \( S^m = \bigcup_{j=1}^{N} \tilde{D}_j^m \), with \( \{D_j\}_{j=1}^{N} \) are triangle with vertices \( \{q^m_k\}_{k=1}^{K} \).
  - \( \Gamma^m = \bigcup_{j=1}^{N_c} \tilde{h}_j^m \) with \( \{h\}_{j=1}^{N_c} \) are line segment with vertices \( \{p^m_k\}_{k=1}^{K_c} \).

- **Finite element space:**
  - P1 linear finite element

\[
\mathcal{V}^h(S^m) := \{ \phi \in C(S^m, \mathbb{R}) : \phi \big|_{D_j^m} \text{ is linear } \forall 1 \leq i \leq N \} \subset H^1(S^m).
\]

\[
\mathcal{W}^h_{\Gamma} = \{ g \in (\mathcal{V}(S^m))^3, g \big|_{\Gamma_m} = X_{\Gamma^h} \}, \quad \Gamma^h := X_{\Gamma^h} \in (\mathcal{V}^h(\Gamma^m))^3.
\]

- **Numerical integration:** mass lumped inner product

\[
\langle u, v \rangle_{S^m} = \frac{1}{3} \sum_{j=1}^{N} \sum_{k=1}^{3} u(q^m_{jk}) v(q^m_{jk}) | D_j^m |.
\]
PFEM: Semi-implicit PFEM:

Given $S^0 = \bigcup_{j=1}^{N} \bar{D}_j$ with $\Gamma^0 = \bigcup_{j=1}^{N_c} \bar{h}_j$, for $m = 0, 1, \ldots, M - 1$, find $S^{m+1} = X^{m+1} \in \mathcal{W}^h_{\Gamma_{m+1}}(S^m)$, $\mu^{m+1} \in \mathcal{V}^h(S^m)$ such that

$$
\left\langle \frac{X^{m+1} - X^m}{\tau_m} \cdot n^m, \phi_h \right\rangle_{S^m} + \left\langle \nabla_s \mu^{m+1}, \nabla_s \phi_h \right\rangle_{S^m} = 0, \quad \forall \phi_h \in \mathcal{V}^h(S^m),
$$

$$
\left\langle \mu^{m+1}, n^m \cdot g_h \right\rangle_{S^m} - \left\langle \nabla_s X^{m+1}, \nabla_s g_h \right\rangle_{S^m} = 0, \quad \forall g_h \in (\mathcal{V}_0^h(S^m))^3,
$$
PFEM: Update $\Gamma^{m+1}$

♦ Relaxed contact angle condition

$$\partial_t \mathbf{X}_r = -\eta \left[ \mathbf{c}_r \cdot \mathbf{n}_r - \sigma \right] \mathbf{n}_r$$

The boundary is given by a polygonal curve

1. update each edge of the curve $\Gamma^m$ via the discrete relaxed contact angle condition.
2. compute the intersection of the neighbour edges and obtain the new points for curve $\Gamma^{m+1}$. 

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Advantages

- Integration is valued on $S^m$, $n^m$ and $n_{rm}$ valued explicitly.
- Assume new surface $S^{m+1}$ is parametrized on surface $S^m$, $\nabla S$ is easy to valued (G. Dziuk, 1991).
- Forward Euler, linear system to solve, $\tau_m = O(h^2_X)$.
- Good mesh quality is preserved (J.W. Barrett, et al., 2008).

Disadvantages

- Re-meshing for the polygonal curve (W. Bao, et al., 2017)
- Regularization for the surface (E, Bansch, et al., 2008)
PFEM: Alternative way for contact line migration

Adding a small regularization term

\[ \partial_t X_\Gamma = \varepsilon^2 \partial_{ss} \kappa n_\Gamma - \eta \left[ c_\Gamma \cdot n_\Gamma - \sigma \right] n_\Gamma, \quad t \geq 0. \]

\[ \Gamma^{m+1} \text{ can be found by the following approximation:} \]

\[ \langle \frac{X_{\Gamma^{m+1}} - X_{\Gamma^m}}{\tau_m} \cdot n_{\Gamma^m}, \varphi_h \rangle_{\Gamma^m} + \varepsilon^2 \langle M_{\Gamma} \partial_s \kappa^{m+1}, \partial_s \varphi_h \rangle_{\Gamma^m} \]

\[ + \eta \langle c_{\Gamma^m} \cdot n_{\Gamma^m} - \sigma, \varphi_h \rangle_{\Gamma^m} = 0, \quad \forall \varphi_h \in \mathcal{V}^h(\Gamma^m), \]

\[ \langle \kappa^{m+1}, n_{\Gamma^m} \cdot \omega_h \rangle_{\Gamma^m} - \langle \partial_s X_{\Gamma^{m+1}}, \partial_s \omega_h \rangle_{\Gamma^m} = 0, \quad \forall \omega_h \in (\mathcal{V}^h(\Gamma^m))^3. \]

Mobility \( M_{\Gamma} = (c_{\Gamma^m} \cdot n_{\Gamma^m} - \sigma)^2 \).

Advantages

- help smoothen the corner of the initial contact line
- have good properties with respect to distribution of the mesh points.
Pinch off of long island film \((1 \times 12 \times 1, \sigma = \cos 3\pi/4)\)
Pinch off of long island \((1 \times 16 \times 1, \sigma = \cos 3\pi/4)\)
Large square island \((3.2 \times 3.2 \times 0.1, \sigma = \cos \frac{5\pi}{6})\)
Large square \((6.4 \times 6.4 \times 0.1, \sigma = \cos 5\pi/6)\)

Figure: Temporal evolution of an initial \(6.4 \times 6.4 \times 0.1\) cuboid until its pinch off at time \(t = 0, 0.005, 0.01, 0.032\) with \(\sigma = \cos(5\pi/6)\).
Square ring I - shrining instability
For square ring, $\sigma = \cos \frac{3\pi}{4}$ - Rayleigh instability
Variational formulation

♣ Isotropic case

\[ \int \int_S \mu \mathbf{n} \cdot \mathbf{g} \, dS - \int \int_S \nabla_S \mathbf{X} \cdot \nabla_S \mathbf{g} \, dS = 0, \quad \forall \mathbf{g} \in (H_0^1(S))^3. \]

♣ Anisotropic case

\[ \mu = \nabla_S \cdot \xi. \]

For \( \mathbf{g} \in (H_0^1(S))^3 \), a similar equation has been derived for anisotropic case (J.E. Taylor et al., 1992; K. Deckelnick et al., 2005; P. Pozzi et al., 2008;)

\[ \int \int_S \mu \mathbf{n} \cdot \mathbf{g} \, dS - \int \int_S \gamma(n) \nabla_S \mathbf{X} \cdot \nabla_S \mathbf{g} \, dS = \sum_{k,l=1}^{3} \int \int_S \xi_k n_l \nabla_S x_k \cdot \nabla_S g_l \, dS. \]
Variational formulation

♠ Given $S(0) = X(U, 0)$ with its boundary $\Gamma(0) = X(\partial U, 0)$, find $S = S(t) := X \in W_{\Gamma}(U), \mu \in H^1(S(t))$ such that

\[
\langle \partial_t X \cdot n, \phi \rangle_S + \langle \nabla_s \mu, \nabla_s \phi \rangle_S = 0, \quad \forall \phi \in H^1(S),
\]

\[
\langle \mu, n \cdot g \rangle_S - \langle \gamma(n) \nabla_s X, \nabla_s g \rangle_S = \sum_{l,k=1}^{3} \langle \xi_k \nabla_s X_k, n_l \nabla_s g_l \rangle_S, \quad \forall g \in (H_0^1(S))^3.
\]

♠ $\Gamma = \Gamma(t) := X_{\Gamma}(\partial U, t) \in (H^1(\partial U))^3, \kappa \in H^1(\Gamma)$ such that

\[
\langle \partial_t X_{\Gamma} \cdot n_{\Gamma}, \varphi \rangle_{\Gamma} + \varepsilon^2 \langle M_{\Gamma} \partial_s \kappa, \partial_s \varphi \rangle_{\Gamma} = -\eta \langle c_{\Gamma}^\gamma \cdot n_{\Gamma} - \sigma, \varphi \rangle_{\Gamma}, \quad \forall \varphi \in H^1(\Gamma),
\]

\[
\langle \kappa, n_{\Gamma} \cdot \omega \rangle_{\Gamma} - \langle \partial_s X_{\Gamma}, \partial_s \omega \rangle_{\Gamma} = 0, \quad \forall \omega \in (H^1(\Gamma))^3.
\]

Here $M_{\Gamma} = (c_{\Gamma}^\gamma \cdot n_{\Gamma} - \sigma)^2$. 
Cubic surface energy

\[ \gamma_c(n) = 1 + 0.25[n_1^4 + n_2^4 + n_3^4]. \]

**Figure:** The equilibrium shapes for (a) \( \gamma = \gamma_c(M_x(\frac{\pi}{6})n) \); (b) \( \gamma = \gamma_c(M_x(-\frac{\pi}{6})n) \); \( \sigma = \cos \frac{3\pi}{4} \).
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4 Conclusion and future works
Conclusion

- Developed sharp interface models via Cahn-Hoffman $\xi$-vector.
- Proposed parametric finite element methods.
- Presented numerical simulation examples.
Future works

- Extensions to the strongly anisotropic case, curved substrate.
- Efficient mesh generation and re-meshing, parallel computation.
- Mathematical theory about the well-posedness, equilibrium shape.
- The phase field approach.
- Compare with physical experiments, set up new numerical experiments.