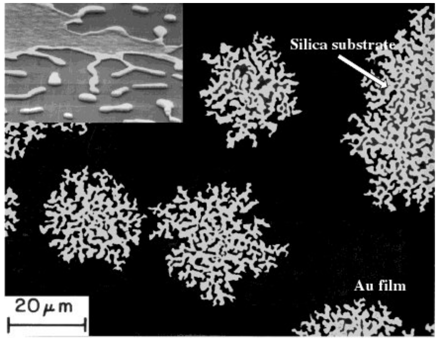
Energy-Stable Parametric Finite Element Methods (PFEM) for Geometric PDEs and Applications

Weizhu Bao



Department of Mathematics

National University of Singapore

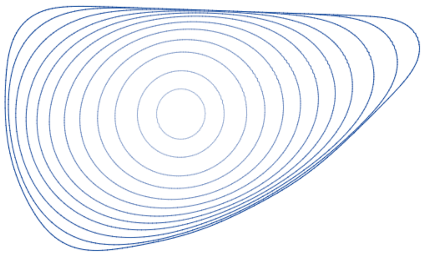
Email: matbaowz@nus.edu.sg

URL: http://blog.nus.edu.sg/matbwz/

Collaborators: Wei Jiang (Wuhan); H. Garcke (Regensburg, Germany); Yifei Li (PhD, NUS), R. Nuernberg (Trento, Italy); Yan Wang (CCNU), Quan Zhao (Regensburg)

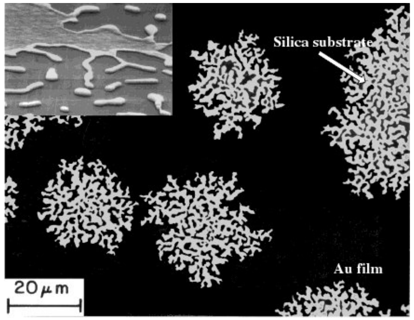
Outline

- Some geometric flows (PDEs)
  - Mean curvature (curve shortening) flow, surface diffusion, Willmore flow, ….
- PFEM for mean curvature flow
  - Variational formulation
  - Parametric finite element method (PFEM)
  - Enegy-stable & numerical results



curve-shortening flow

- Energy-stable/Structure-preserving PFEM
  - For surface diffusion
  - For anisotropic surface diffusion
  - For solid-state dewetting
- Conclusions

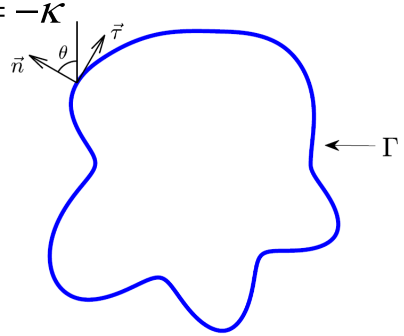


Solid-state dewetting

Mean Curvature Flow (MCF)

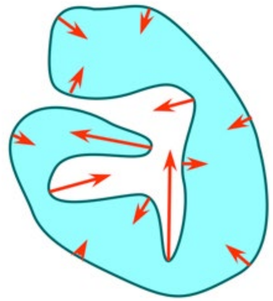
- Motion of curve/surface via mean curvature

$V_{\vec{n}} = -\kappa$



κ – curvature

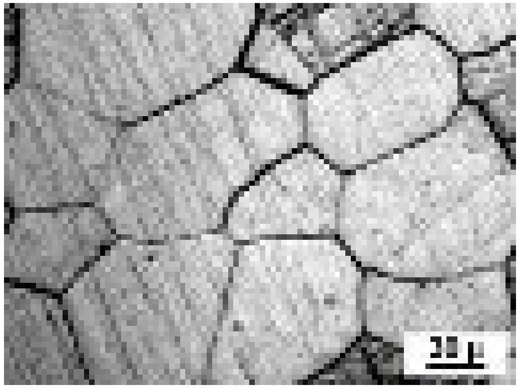
$\kappa = -(\partial_{ss}\vec{X}) \bullet \vec{n}$



In 3D:

$$V_{\vec{n}} = -H$$

- Typical applications
  - Grain boundary
  - Foam bubble/film
  - Liquid drop – surface tension
  - Computational graphics
  - Geometry, ...



grain boundary

soap bubble water

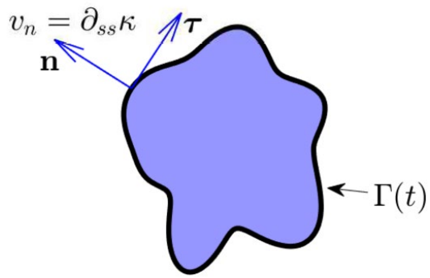
- Analytical solution for a circle/sphere in 2D/3D

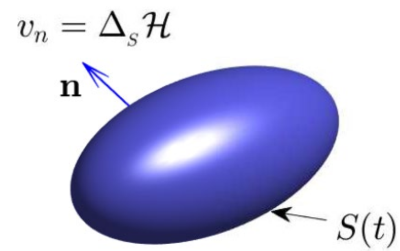
Surface Diffusion

- Motion of curve/surface via surface diffusion – W.W. Mullins, JAP 1957', ….

κ – curvature

$\kappa = -(\partial_{ss}\vec{X})\bullet\vec{n}$



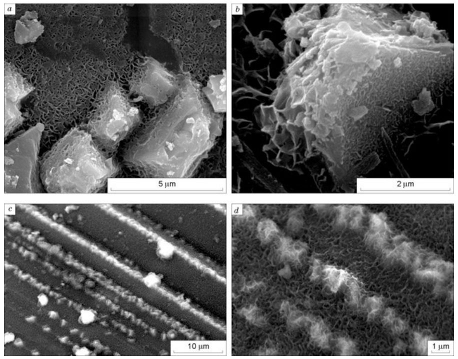


In 3D:

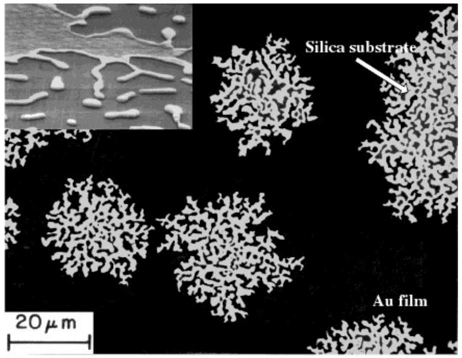
$V_{\vec{n}} = \Delta_S H$

$\vec{J} = \nabla_S H$

- Typical applications
  - Surface phase formation
  - Epitaxial growth
  - Heterogeneous catalysis
  - Solid-state dewetting



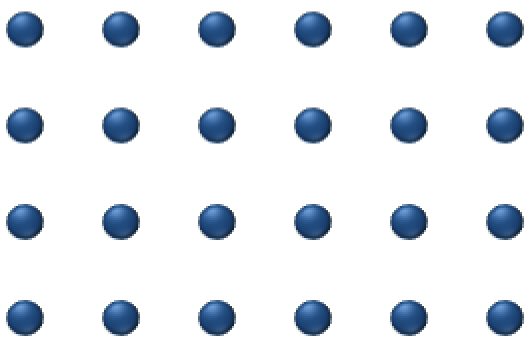
Formation on magnetite crystal



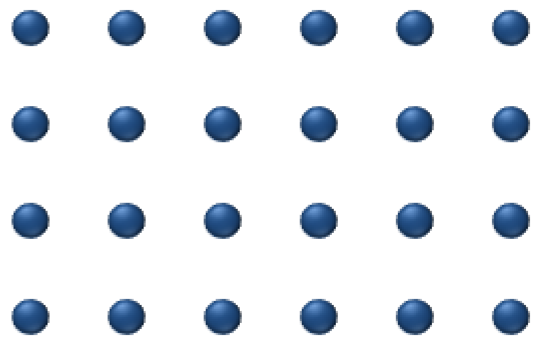
Dewetting on a flat substrate

- Steady state for a circle/sphere in 2D/3D

Surface Diffusion in Materials Sciences (Solids)

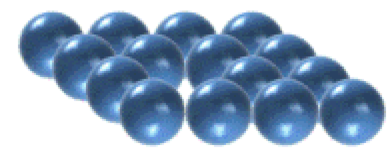


A single adatom diffusing across a square surface lattice

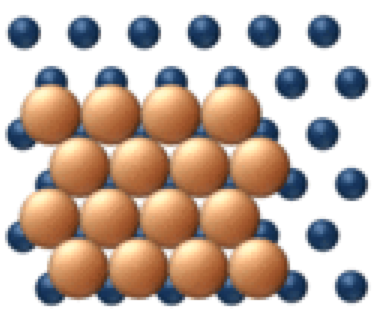


Six adatoms diffusing across a square surface lattice

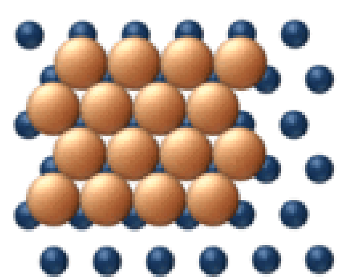
An atom exchange between adatom & surface atiom



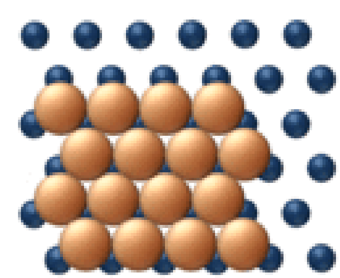
Surface diffusion via vacancy mechanism



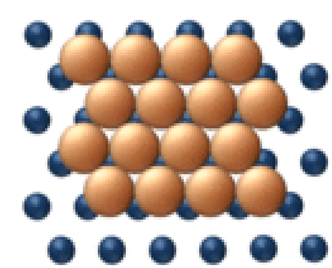
Dislocation



Glide



Reptation



Shear

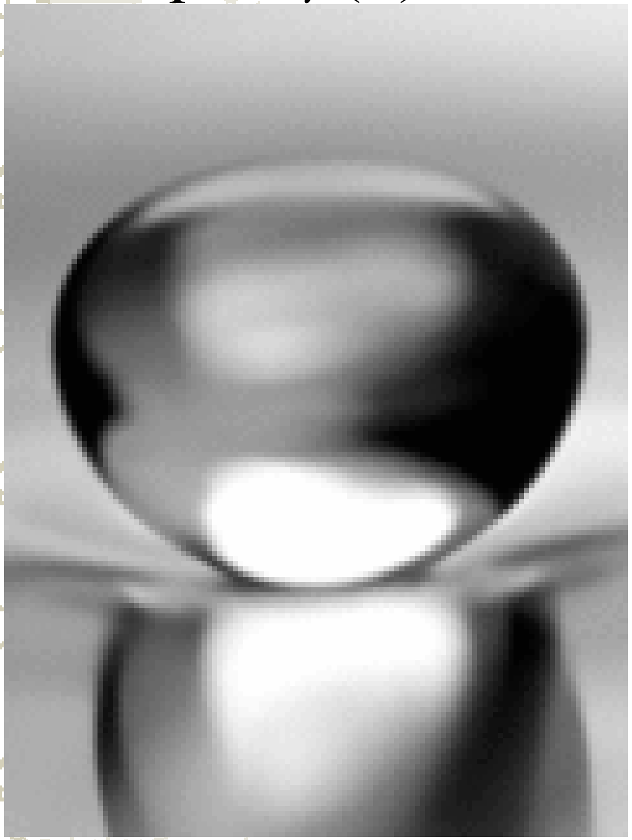
Isotropic/Anisotropic Surface Energy in Fluids/Solids

Isotropic: $\gamma(\theta) \equiv 1$

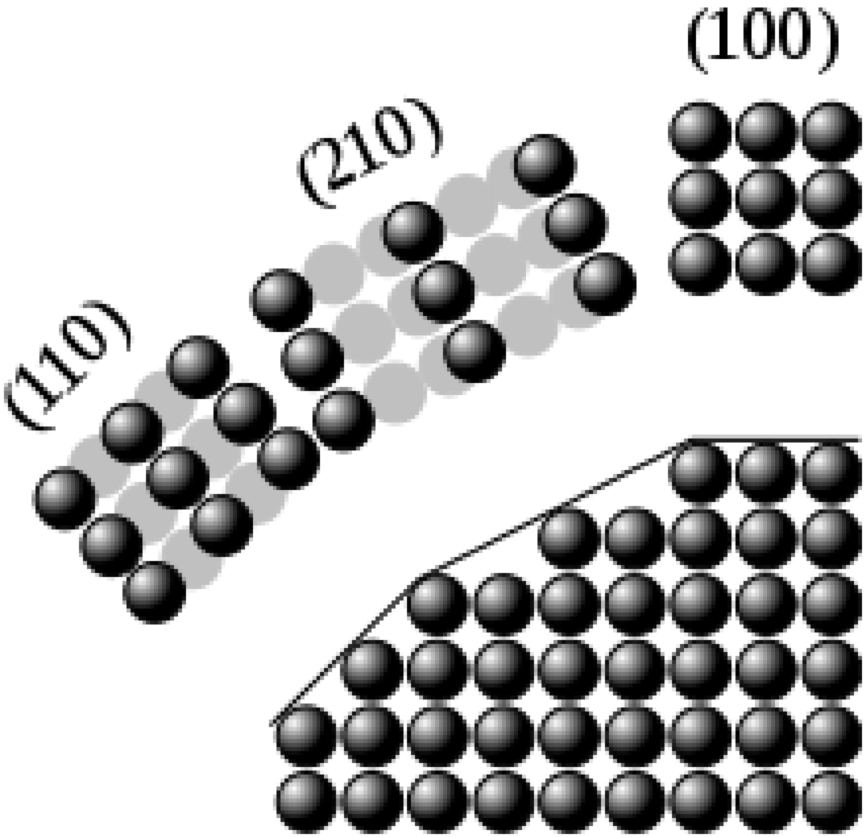
$\gamma(\theta)$ or $\gamma(\vec{n})$

$\gamma(\theta) = 1 + \beta\cos(m\theta),$

$\gamma(\theta) = |\sin\theta| + |\cos\theta|$



Drop of water bouncing on a water surface subject to vibrations → isotropic surface energy in fluids



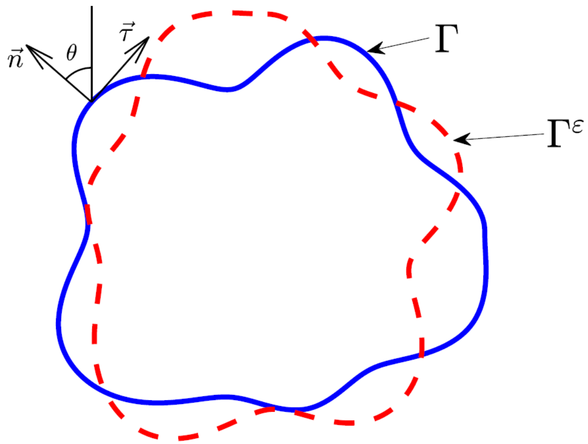
Dense crystallographic planes→ anisotropic surface energy in solids (materials science)

Thermodynamic Variation for Geometric Flows (PDEs)

$$\Gamma : \vec{X}(\bullet,t), \quad \Gamma^{\varepsilon} : \vec{X}(\bullet,t) + \varepsilon\phi\vec{n} \ \text{ with } \int_{\Gamma} \phi \, d\Gamma = 0$$

- Surface energy functional $\quad \kappa = -(\partial_{ss}\vec{X}) \bullet \vec{n} - \text{mean curvature}$

$$W(\Gamma) := \int_{\Gamma} F(\theta, \kappa, \ldots) \, d\Gamma \quad \text{or} \quad W(\Gamma) := \int_{\Gamma} F(\vec{n}, H, \ldots) \, d\Gamma$$



- Chemical potential

$$\mu := \frac{\delta W(\Gamma)}{\delta \Gamma} = \lim_{\varepsilon \to 0^+} \frac{W(\Gamma^{\varepsilon}) - W(\Gamma)}{\varepsilon}$$

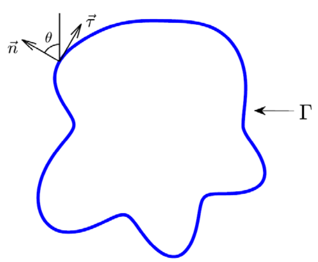
- L^2 – surface gradient flow:

$$\partial_t \vec{X} = -\mu \, \vec{n} \quad \text{or} \quad \partial_t \vec{X} = (-\mu + \lambda) \, \vec{n}$$

- H^{-1} – area conserved surface diffusion:

$$\partial_t \vec{X} = (\Delta_{\Gamma} \mu) \, \vec{n} \Leftarrow \partial_t \vec{X} = (\nabla_{\Gamma} \bullet \vec{J}) \, \vec{n} \ \text{ with } \vec{J} = \nabla_{\Gamma} \mu$$

Typical Geometric Flows in 2D



- Isotropic/anisotropic surface energy:

$$F(\theta,\kappa,\ldots)=\gamma(\theta) \Rightarrow \mu=(\gamma(\theta)+\gamma''(\theta))\kappa \overset{\gamma(\theta)\equiv 1}{\Rightarrow} \mu=\kappa=-(\partial_{ss}\vec{X})\bullet\vec{n}$$

- (Anisotropic) mean curvature flow – surface tension in fluids or grain boundary growth in solids:

$$\partial_t\vec{X}=-(\gamma(\theta)+\gamma''(\theta))\kappa\,\vec{n} \overset{\gamma(\theta)\equiv 1}{\Rightarrow} \partial_t\vec{X}=-\kappa\,\vec{n}$$

- Area conserved mean curvature flow – surface tension for liquid drop:

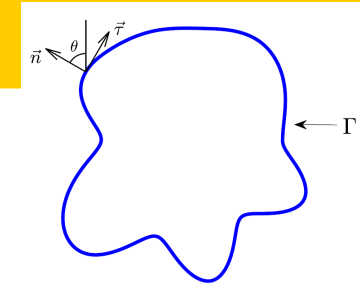
$$\partial_t\vec{X}=-(\gamma(\theta)+\gamma''(\theta))\kappa\,\vec{n}+\lambda_{\vec{X}}(t) \overset{\gamma(\theta)\equiv 1}{\Rightarrow} \partial_t\vec{X}=(-\kappa+\lambda)\,\vec{n}$$

- (Anisotropic) surface diffusion– in epitaxial growth or solid-state dewetting in solids:

$$\partial_t\vec{X}=(\partial_{ss}\mu)\,\vec{n} \overset{\gamma(\theta)\equiv 1}{\Rightarrow} \partial_t\vec{X}=(\partial_{ss}\kappa)\,\vec{n}$$

- Willmore flow – elastic bending energy in cell membrane in biology, …:

Mean Curvature Flow in 2D



- Two different parametrizations:
  - Arclength *s* parametrization – ``Lagrangeian'' coordinate

$$\partial_t \vec{X}(s,t) = -\kappa \vec{n}, \quad 0 \le s \le L(t), \quad \Leftrightarrow \partial_t \vec{X}(s,t) \bullet \vec{n} = -\kappa, \quad \partial_t \vec{X}(s,t) \bullet \vec{\tau} = 0$$

$$\kappa = -(\partial_{ss} \vec{X}) \bullet \vec{n}, \qquad \vec{X}(s,0) = \vec{X}_0(s), \quad 0 \le s \le L_0$$

  - Fixed spatial variable parametrization – ``Eulerian'' coordinate

$$s := s(\rho,t) = \int_0^\rho \left|\partial_\rho \vec{X}\right| d\rho \ \text{ or } \ \partial_\rho s = \left|\partial_\rho \vec{X}\right| \Leftrightarrow \partial_s \rho = 1/\left|\partial_\rho \vec{X}\right|$$

$$\Gamma(t): \quad \vec{X}(\rho,t) : [0,1] \times \mathbb{R}^+ \to \mathbb{R}^2 \qquad \Rightarrow \qquad 0 \le s \le L(t)$$

$$\begin{array}{c} \partial_t \vec{X}(s,t) = \partial_{ss} \vec{X} \\ \Downarrow \\ \partial_t \vec{X}(s,t) \bullet \vec{n} = -\kappa \end{array} \quad \Rightarrow \quad \partial_t \vec{X}(\rho,t) = \frac{1}{\left|\partial_\rho \vec{X}\right|} \partial_\rho \left(\frac{\partial_\rho \vec{X}}{\left|\partial_\rho \vec{X}\right|} \right), \quad \rho \in I = [0,1], \quad t > 0$$

$$\vec{X}(\rho,0) = \vec{X}_0(\rho) := \vec{X}_0(s/L_0), \quad 0 \le \rho \le 1$$

- PDE results — existence, uniqueness, shrinking to a point, pinch-off, … -- Hamilton, JDG 82'; Huisken, JDG, 84'; Gage & Hamilton, JDG 86'; Grayson, JDG, 87', …..

FEM for MCF

$$V := \{\psi \in H^1(I) \mid \psi(0)=\psi(1)\}$$

$$\partial_t \vec{X}(\rho,t) = \frac{1}{|\partial_\rho \vec{X}|}\partial_\rho\left(\frac{\partial_\rho \vec{X}}{|\partial_\rho \vec{X}|}\right)$$

$$\Downarrow$$

$$\partial_t \vec{X}(\rho,t)\bullet\vec{n} = -\kappa$$

- **Weak formulation** by multiplying $\vec{\phi}\,|\partial_\rho \vec{X}|$ – Dziuk, M3AS 94'

Take $\vec{X}(\rho,0)=\vec{X}_0(\rho)$, find $\vec{X}(\bullet,t)\in V\times V$ s.t.

$$\int_I \partial_t \vec{X}\bullet\vec{\phi}\,|\partial_\rho \vec{X}|\,d\rho + \int_I \frac{\partial_\rho \vec{X}\bullet\partial_\rho\vec{\phi}}{|\partial_\rho \vec{X}|}\,d\rho = 0, \quad \forall \vec{\phi}\in V\times V$$

$$V^h := V_1^h$$

- Finite element approximation (FEM)

$$V_k^h := \{\psi^h \in C^0(I)\cap V \mid \psi^h|_{[\rho_j,\rho_{j+1}]}\in P_k,\ 0\le j\le M-1\}$$

$0=\rho_0<\rho_1<\ldots<\rho_M=1$ being a partiton of $I=[0,1]$

  – Semi-discretization – Dziuk, M3AS 1994'
    - For piecewise linear element → linear convergence rate & preserving geometry quantity
  – Semi-implicit full discretization (mesh points on curve might clustered) – Li&Lubich, NM 19'; B. Li SINUM 2020', …

$$k\ge 3,\quad \tau = o(h^{2.5}),\quad h\le h_0$$

$$\left\|\vec{X}(\bullet,t_m=m\tau)-\vec{X}^m\right\|_{L^2(I)} \le C(\tau+h^k)$$

Take $\vec{X}^0(\rho) := P_h\vec{X}_0 \in V_k^h$, find $\vec{X}^{m+1}\in V_k^h\times V_k^h$ s.t.

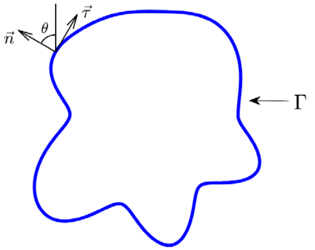
$$\int_I \frac{\vec{X}^{m+1}-\vec{X}^m}{\tau}\bullet\vec{\phi}^h\,|\partial_\rho \vec{X}^m|\,d\rho + \int_I \frac{\partial_\rho \vec{X}^{m+1}\bullet\partial_\rho\vec{\phi}^h}{|\partial_\rho \vec{X}^m|}\,d\rho = 0, \quad \forall \vec{\phi}^h\in V^h\times V^h$$

parametrization (global) → variation->discretization ---``Eulerian'' coordinate

Parametric Finite Element Method (PFEM)

variation (on manifold) ->discretization → parametrization (local) --- ``Lagrangeian'' coordinate

- A parametric variational formulation – Dziuk, Numer. Math. 91'
  - Same normal velocity as previous formulation
  - Different parametrization with introducing tangential velocity



$$\partial_t \vec{X}(\rho,t) - \Delta_\Gamma \vec{X} = 0 \Rightarrow \partial_t \vec{X}(\rho,t) \bullet \vec{n} = -\kappa$$

  - Weak formulation Take $\vec{X}(\rho,0) = \vec{X}_0(\rho)$, find $\Gamma(t): \vec{X}(\bullet,t) \in V \times V$ s.t.

s – arclength of $\Gamma(\mathrm{t}) \Rightarrow$ $$\int_{\Gamma(t)} \partial_t \vec{X} \bullet \vec{\phi}\, ds + \int_{\Gamma(t)} \partial_s \vec{X} \bullet \partial_s \vec{\phi}\, ds = 0, \quad \forall \vec{\phi} \in V \times V$$

- Semi-implicit PFEM (mesh points on curve might clustered) – Dziuk, Numer. Math. 1991'

Take $\Gamma^0 : \vec{X}^0(\rho) = P_h \vec{X}_0 \in V^h$ find $\Gamma^{\mathrm{m}+1} : \vec{X}^{m+1} \in V^h \times V^h$ s.t.

s – arclength of Γ^m

parametrize Γ^{m+1} vs s $\Rightarrow$ $$\int_{\Gamma^{\mathrm{m}}} \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau} \bullet \vec{\phi}^h\, ds + \int_{\Gamma^{\mathrm{m}}} \partial_s \vec{X}^{m+1} \bullet \partial_s \vec{\phi}^h\, ds = 0, \quad \forall \vec{\phi}^h \in V^h \times V^h$$

Energy-stable PFEM

$$K := \{\psi \in L^2(I) \mid \psi(0) = \psi(1)\}$$

$$\begin{matrix} \partial_t \vec{X}(\rho,t) = -\kappa \vec{n} \\ \kappa = -\partial_{ss}\vec{X}(s,t)\bullet\vec{n} \end{matrix} \Rightarrow \begin{matrix} \partial_t \vec{X}(\rho,t)\bullet\vec{n} + \kappa = 0 \\ \kappa\vec{n} + \partial_{ss}\vec{X}(\rho,t) = 0 \end{matrix}$$

- Weak formulation – Barrett, Garcke & Nurnberg, SISC 07', JCP 08',….

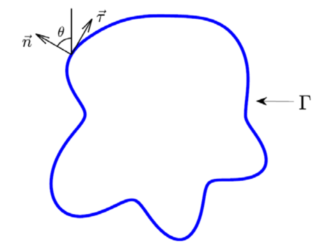
Find $\Gamma(t):\ \vec{X}(\bullet,t) \in V\times V \ \&\ \kappa(\bullet,t) \in K$ s.t. $V_{\vec{n}} = -\kappa$

Take $\vec{X}(\rho,0) = \vec{X}_0(\rho)$

s – arclength of $\Gamma(t)$ $\Rightarrow$

$$\int_{\Gamma(t)} \partial_t \vec{X}\bullet\vec{n}\psi\, ds + \int_{\Gamma(t)} \kappa\psi\, ds = 0, \quad \forall \psi \in K$$

$$\int_{\Gamma(t)} \kappa\vec{n}\bullet\vec{\phi}\, ds - \int_{\Gamma(t)} \partial_s\vec{X}\bullet\partial_s\vec{\phi}\, ds = 0, \quad \forall \vec{\phi} \in V\times V$$



- Semi-implicit PFEM:

Take $\Gamma^0 : \vec{X}^0(\rho) = I_h\vec{X}_0 \in V^h$ find $\Gamma^{m+1} : \vec{X}^{m+1} \in V^h\times V^h \ \&\ \kappa^{m+1} \in K^h$ s.t.

$\vec{n}^m = (\partial_s\vec{X}^m)^\perp$

s – arclength of Γ^m $\Rightarrow$

$$\int_{\Gamma^m} \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau}\bullet\vec{n}^m\psi^h\, ds + \int_{\Gamma^m} \kappa^{m+1}\psi^h\, ds = 0, \quad \forall \psi^h \in K^h$$

$$\int_{\Gamma^m} \kappa^{m+1}\vec{n}^m\bullet\vec{\phi}^h\, ds - \int_{\Gamma^m} \partial_s\vec{X}^{m+1}\bullet\partial_s\vec{\phi}^h\, ds = 0, \quad \forall \vec{\phi}^h \in V^h\times V^h$$

variation (on manifold)->discretization → parametrization (local) --- ``Lagrangeian'' coordinate

Energy-stable PFEM

- Unconditional energy stable – Barrett, Garcke & Nurnberg, JCP 08',….

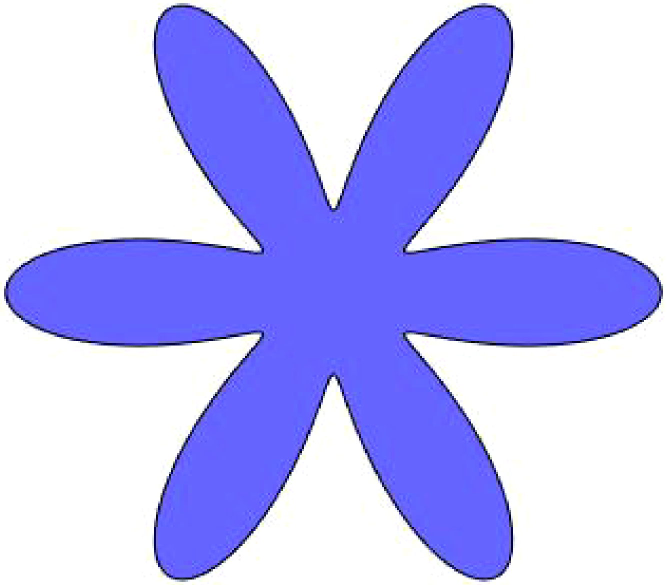
$$\left|\Gamma^{m+1}\right| + \tau\left\langle \kappa^{m+1}, \kappa^{m+1} \right\rangle_{\Gamma^m} \le \left|\Gamma^m\right|, \quad m = 0, 1, \cdots$$

- Asymptotic equal mesh distribution (AEMD)

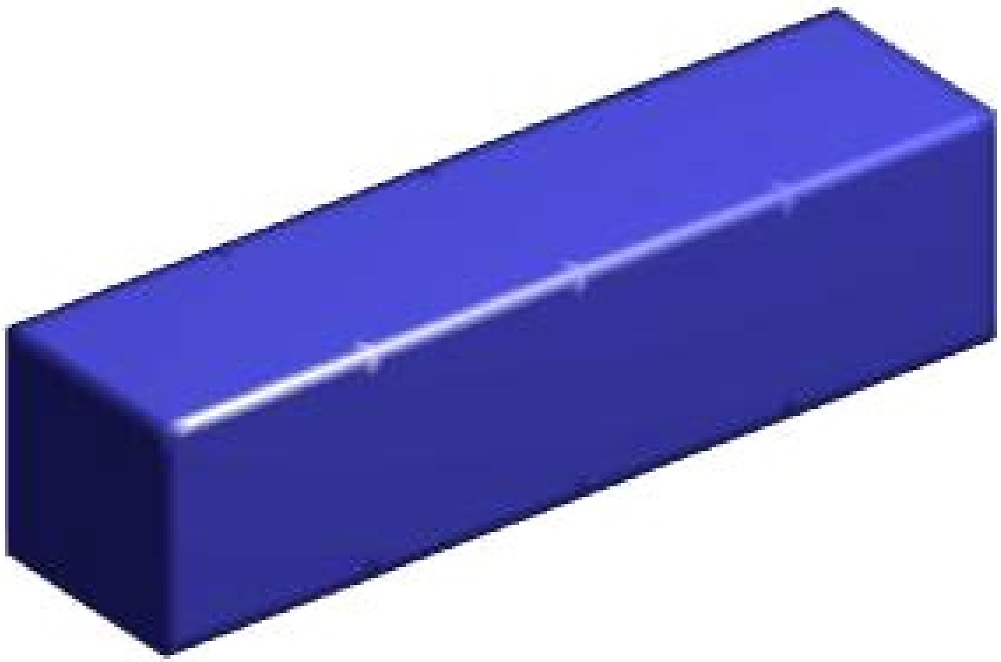
$$\frac{h_{\max}^m}{h_{\min}^m} := \frac{\max_{1\le j\le M} h_j^m}{\min_{1\le j\le M} h_j^m} \xrightarrow{m\gg 1} 1 \quad \text{with} \quad h_j^m := \left|\vec{X}^m(\rho_j) - \vec{X}^m(\rho_{j-1})\right|, \quad 1 \le j \le M$$

- Semi-Implicit
- Extension to anisotropic MCF & 3D: Yes
- Error estimates of PFEM ??????

Mean Curvature Flow (MCF) in 2D



Mean Curvature Flow (MCF) in 3D

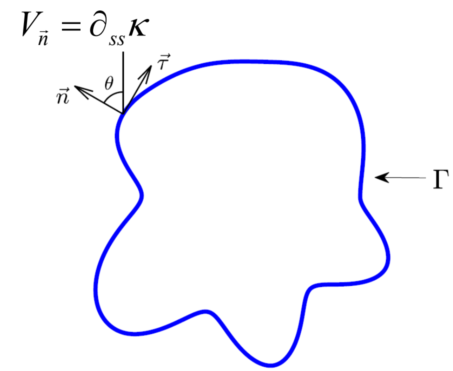


Surface Diffusion

$$\Gamma(t): \vec{X}(\bullet,t) = (x(\bullet,t), y(\bullet,t))^T$$

- Re-formulation – Barrett, Garcke & Nurnberg, SISC 08',….

$$\partial_t \vec{X}(\rho,t) = \partial_{ss}\kappa\vec{n} \qquad \partial_t \vec{X}(\rho,t)\bullet\vec{n} - \partial_{ss}\kappa = 0$$
$$\Rightarrow$$
$$\kappa = -\partial_{ss}\vec{X}(s,t)\bullet\vec{n} \qquad \kappa\vec{n} + \partial_{ss}\vec{X}(\rho,t) = 0$$



- Area conservation

$$A(t) = \int_{\Gamma(t)} y\partial_s x ds \Rightarrow A'(t) = 0, \quad t \ge 0 \Rightarrow A(t) \equiv A(0), \quad t \ge 0$$

- Energy dissipation

$$W(t) = \int_{\Gamma(t)} ds = L(t) \Rightarrow W'(t) \le 0, \quad t \ge 0$$

$$\Rightarrow W(t) \le W(t_1) \le W(0), \quad 0 \le t_1 \le t$$

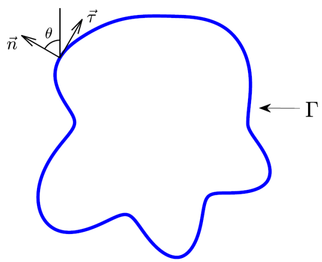
Energy-stable PFEM

$$V := \{\psi \in H^1(I) \mid \psi(0) = \psi(1)\}$$

$$\partial_t \vec{X}(\rho,t) \cdot \vec{n} - \partial_{ss}\kappa = 0$$
$$\kappa \vec{n} + \partial_{ss}\vec{X}(\rho,t) = 0$$

- **Weak formulation** – Barrett, Garcke & Nurnberg, SISC 08',….

Find $\Gamma(t):\ \vec{X}(\bullet,t) \in V \times V \ \&\ \kappa(\bullet,t) \in V$ s.t.



Take $\vec{X}(\rho,0) = \vec{X}_0(\rho)$

s – arclength of $\Gamma(t)$ $\Rightarrow$

$$\int_{\Gamma(t)} \partial_t \vec{X} \bullet \vec{n} \psi \, ds + \int_{\Gamma(t)} \partial_s \kappa \, \partial_s \psi \, ds = 0, \quad \forall \psi \in V$$

$$\int_{\Gamma(t)} \kappa \vec{n} \bullet \vec{\phi} \, ds - \int_{\Gamma(t)} \partial_s \vec{X} \bullet \partial_s \vec{\phi} \, ds = 0, \quad \forall \vec{\phi} \in V \times V$$

- **Semi-implicit PFEM**: $V^h := \{\psi^h \in C^0(I) \cap V \mid \psi^h\big|_{[\rho_j,\rho_{j+1}]} \in P_1,\ 0 \le j \le M-1\}$

Take $\Gamma^0 : \vec{X}^0(\rho) = P_h \vec{X}_0 \in V^h$ find $\Gamma^{m+1} : \vec{X}^{m+1} \in V^h \times V^h \ \&\ \kappa^{m+1} \in V^h$ s.t.

$\vec{n}^m = (\partial_s \vec{X}^m)^\perp$

s – arclength of Γ^m $\Rightarrow$

$$\int_{\Gamma^m} \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau} \bullet \vec{n}^m \psi^h \, ds + \int_{\Gamma^m} \partial_s \kappa^{m+1} \, \partial_s \psi^h \, ds = 0, \quad \forall \psi^h \in V^h$$

$$\int_{\Gamma^m} \kappa^{m+1} \vec{n}^m \bullet \vec{\phi}^h \, ds - \int_{\Gamma^m} \partial_s \vec{X}^{m+1} \bullet \partial_s \vec{\phi}^h \, ds = 0, \quad \forall \vec{\phi}^h \in V^h \times V^h$$

Energy-stable PFEM

- Unconditional energy stable – Barrett, Garcke & Nurnberg, JCP 08',….

$$\left|\Gamma^{m+1}\right| \le \left|\Gamma^{m}\right| \le \ldots \le \left|\Gamma^{0}\right|, \quad m = 0, 1, \cdots$$

- Asymptotic equal mesh distribution (AEMD)

$$\frac{h^m_{\max}}{h^m_{\min}} := \frac{\max\limits_{1\le j\le M} h_j^m}{\min\limits_{1\le j\le M} h_j^m} \Longrightarrow 1, \quad m \gg 1 \quad \text{with} \quad h_j^m := \left|\vec{X}^m(\rho_j) - \vec{X}^m(\rho_{j-1})\right|, \quad 1 \le j \le M$$

- Semi-implicit
- Extension to anisotropic SDF & 3D: Yes
- Error estimates of PFEM ??????

Structure-preserving PFEM

$$V^h := \{\psi^h \in C^0(I) \cap V \mid \psi^h\big|_{[\rho_j,\rho_{j+1}]} \in P_1, 0 \le j \le M-1\}$$

- Structure-Preserving (SP-PFEM):

Take $\Gamma^0 : \vec{X}^0(\rho) = P_h \vec{X}_0 \in V^h$ find $\Gamma^{m+1} : \vec{X}^{m+1} \in V^h \times V^h \;\&\; \kappa^{m+1} \in V^h$ s.t.

$\vec{n}^m = (\partial_s \vec{X}^m)^\perp$

s – arclength of Γ^m

$$\Rightarrow \int_{\Gamma^m} \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau} \bullet \vec{n}^{m+\frac{1}{2}} \psi^h ds + \int_{\Gamma^m} \partial_s \kappa^{m+1} \partial_s \psi^h ds = 0, \quad \forall \psi^h \in V^h$$

$$\int_{\Gamma^m} \kappa^{m+1} \vec{n}^{m+\frac{1}{2}} \bullet \vec{\phi}^h ds - \int_{\Gamma^m} \partial_s \vec{X}^{m+1} \bullet \partial_s \vec{\phi}^h ds = 0, \quad \forall \vec{\phi}^h \in V^h \times V^h$$

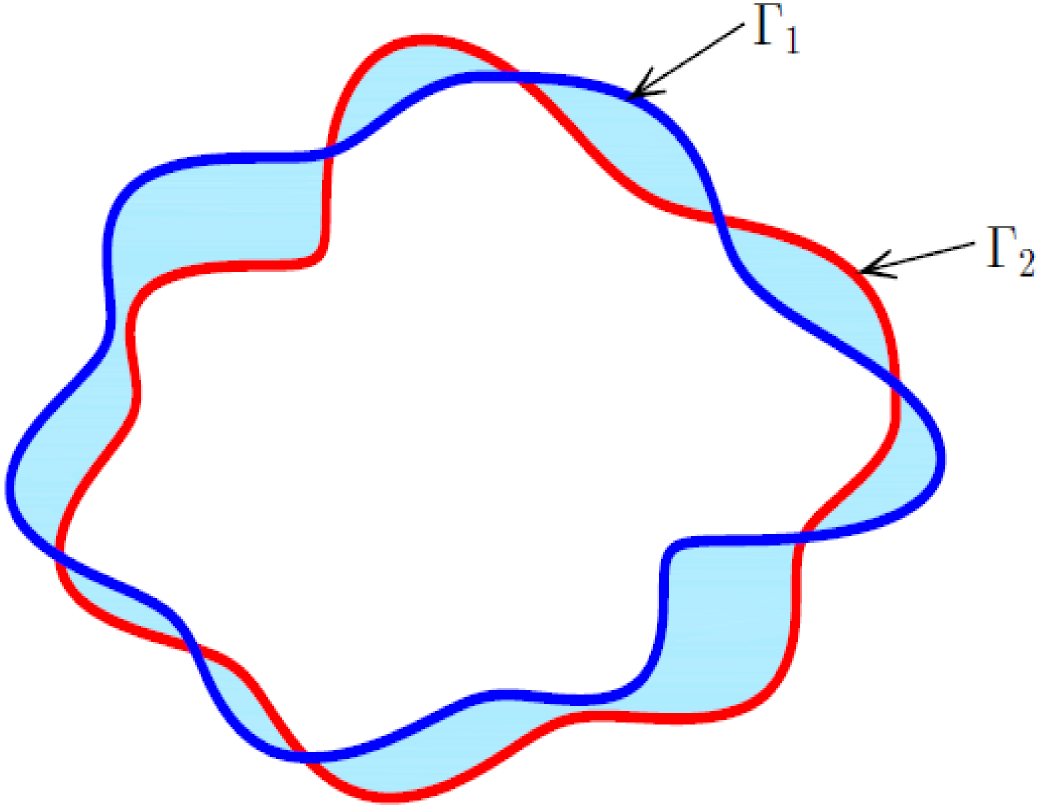
- Properties

$$\vec{n}^{m+\frac{1}{2}} = -\frac{1}{2}\left(\partial_s \vec{X}^m + \partial_s \vec{X}^{m+1}\right)^\perp = -\frac{1}{2}\left|\partial_\rho \vec{X}^m\right|^{-1}\left(\partial_\rho \vec{X}^m + \partial_\rho \vec{X}^{m+1}\right)^\perp$$

  - Area conservation
  - Energy dissipation -- unconditionally energy stable
  - Asymptotic equal mesh distribution (AEMD)

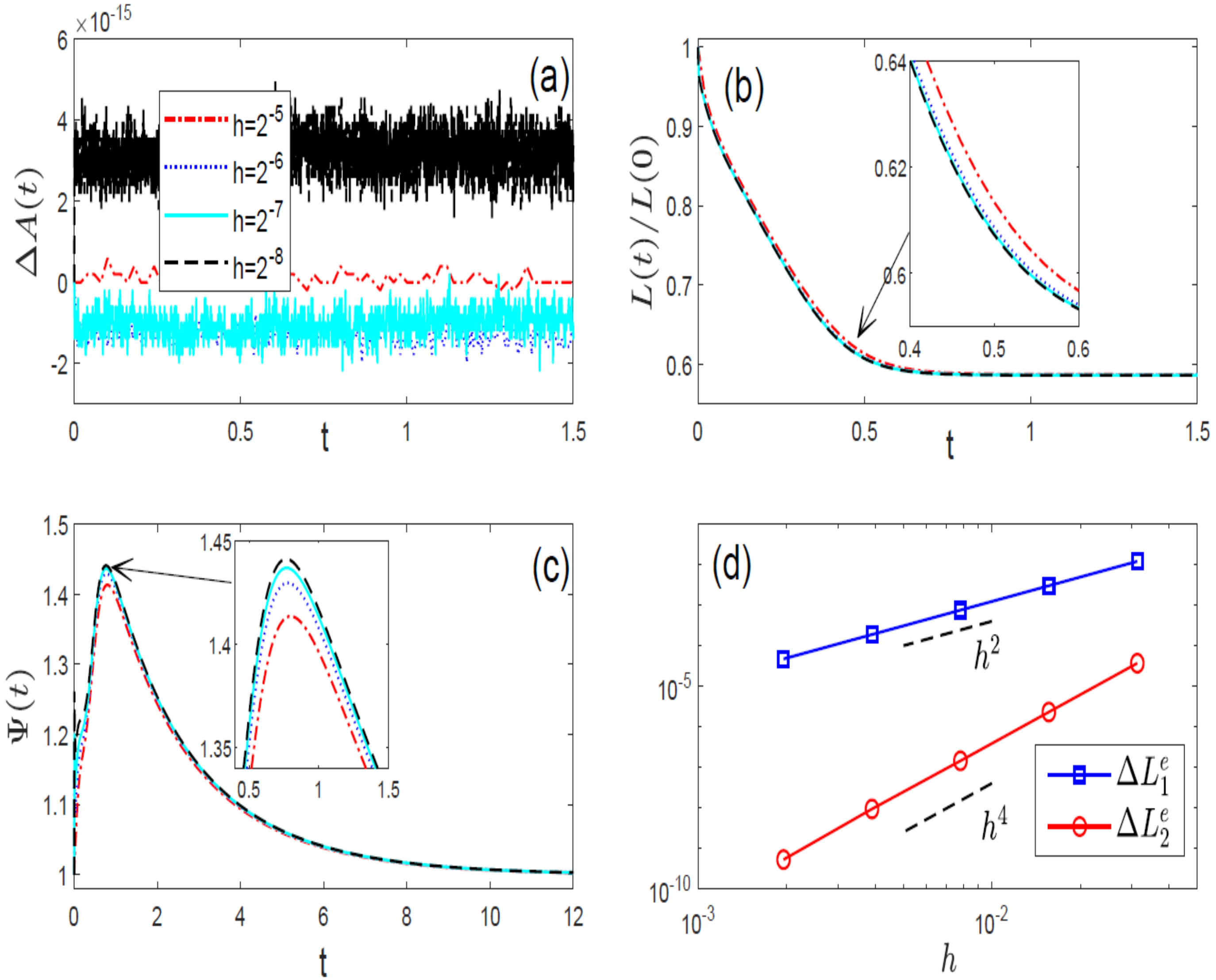
W. Bao and Q. Zhao, A structure-preserving parametric finite element method for surface diffusion, SIAM J. Numer. Anal., 59 (2021), 2775-2799.
W. Jiang & B. Li, A perimeter-decreasing and area-conserving algorithm for surface diffusion flow of curves, J. Comput. Phys. 443 (2021), 110531.

Manifold distance between two curves



$$\mathrm{M}(\Gamma_1,\, \Gamma_2) := \left|\, (\Omega_1 \backslash \Omega_2) \cup (\Omega_2 \backslash \Omega_1)\, \right| = |\Omega_1| + |\Omega_2| - 2|\Omega_1 \cap \Omega_2|,$$

Convergence of SP-PFEM



$$\Delta A(t)|_{t=t_m} := \frac{A^m - A^0}{A^0},$$

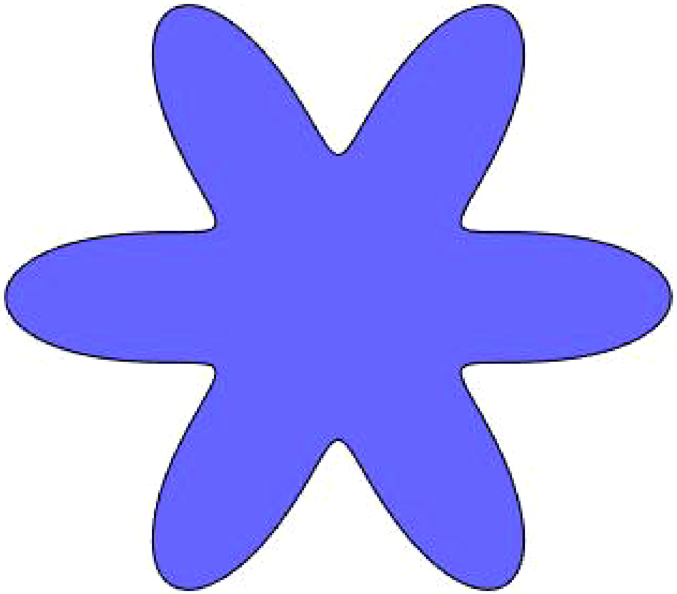
$$\Delta L_1^e := \lim_{m\to\infty}\left(L^m - 2\sqrt{A^0\pi}\right)$$

$$\Psi^m = \frac{\max_{1\le j\le N}\left|\mathbf{h}_j^m\right|}{\min_{1\le j\le N}\left|\mathbf{h}_j^m\right|}$$

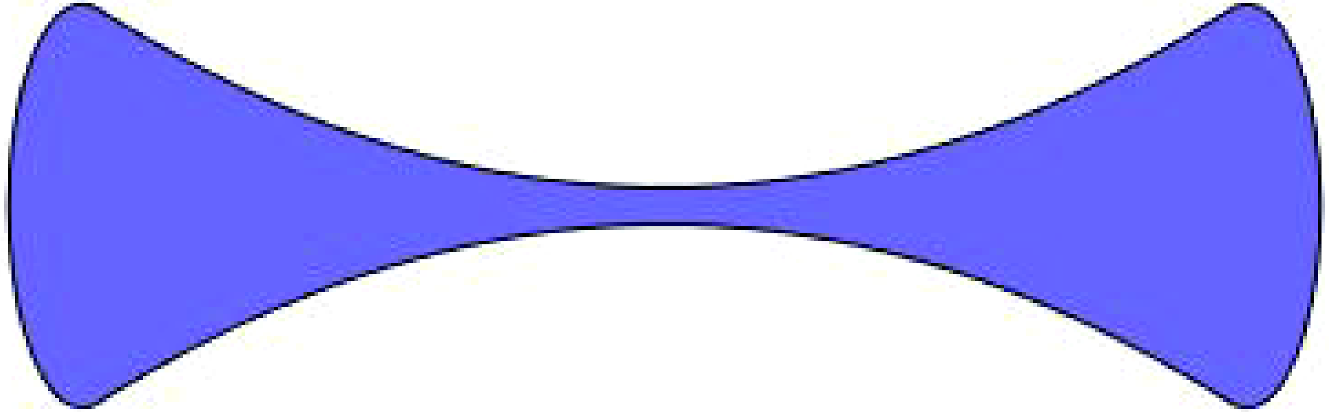
$$\Psi(t)|_{t=t_m} = \Psi^m,$$

$$\Delta L_2^e := \Delta L_1^e - \frac{\sqrt{A^0\pi}\pi^2}{3}h^2$$

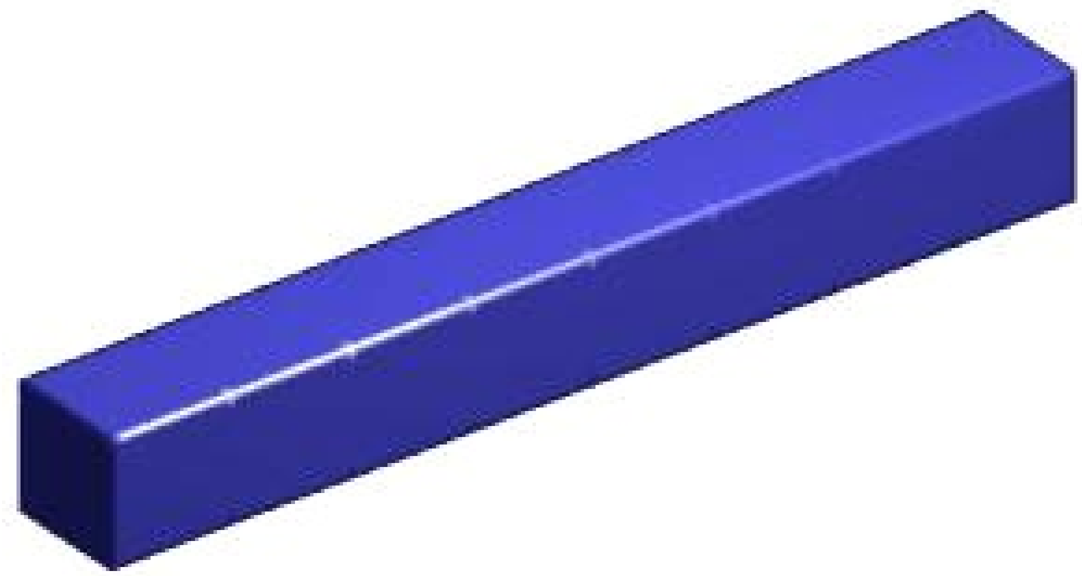
Surface Diffusion in 2D



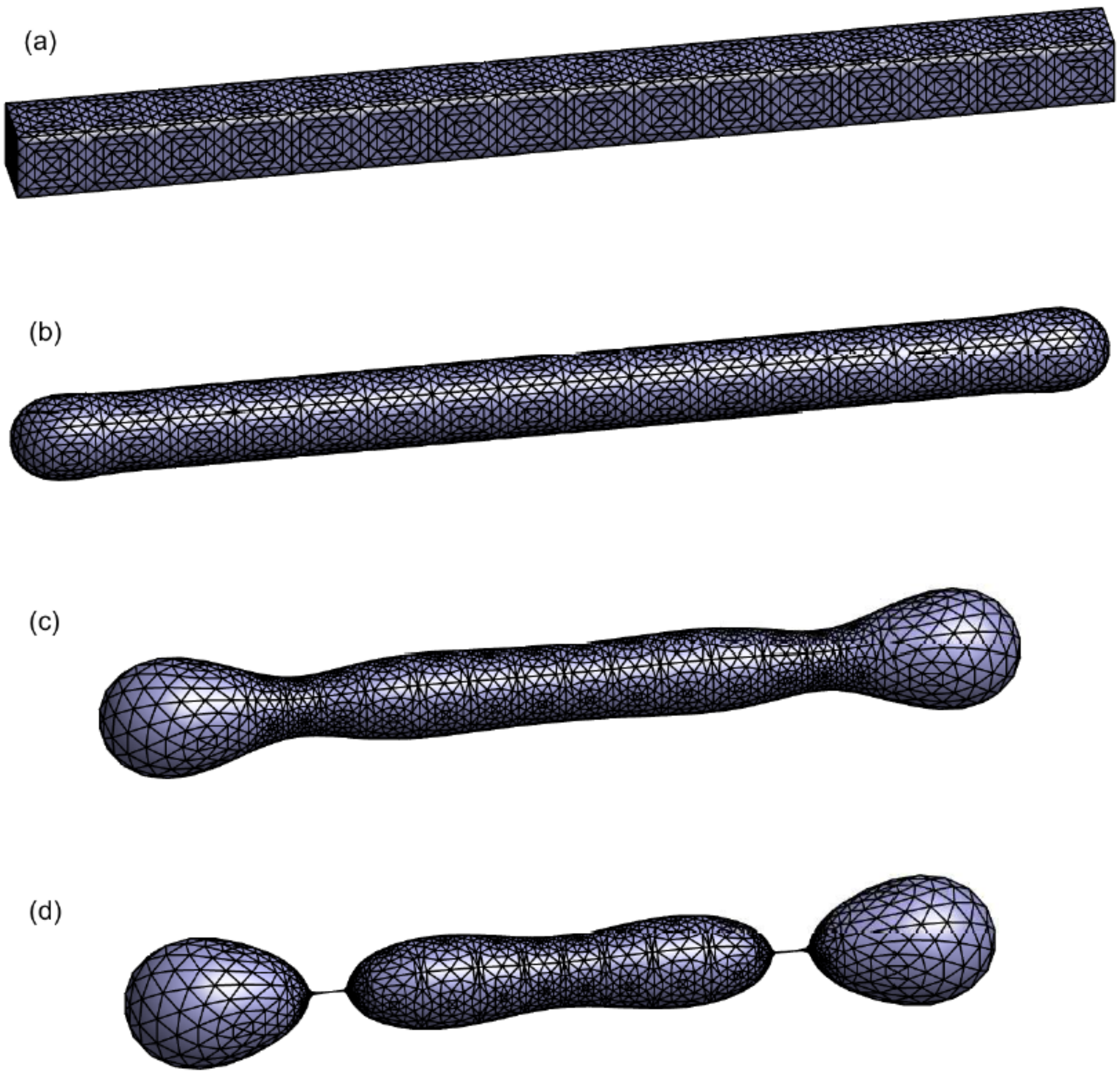
Surface Diffusion in 2D

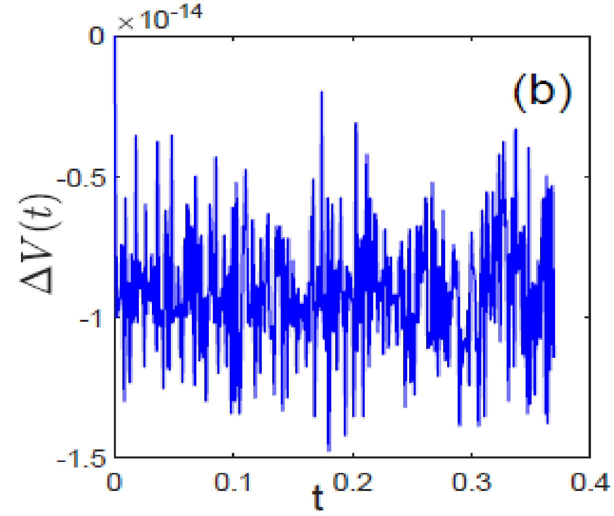


Surface Diffusion in 3D



Surface Diffusion in 3D

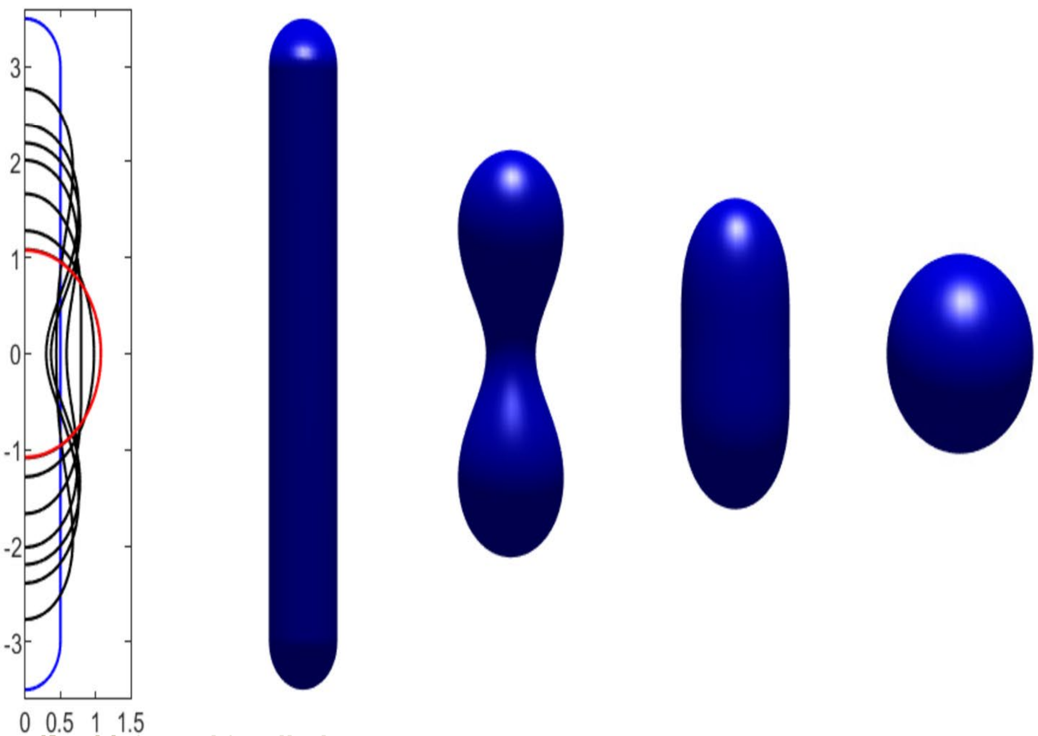


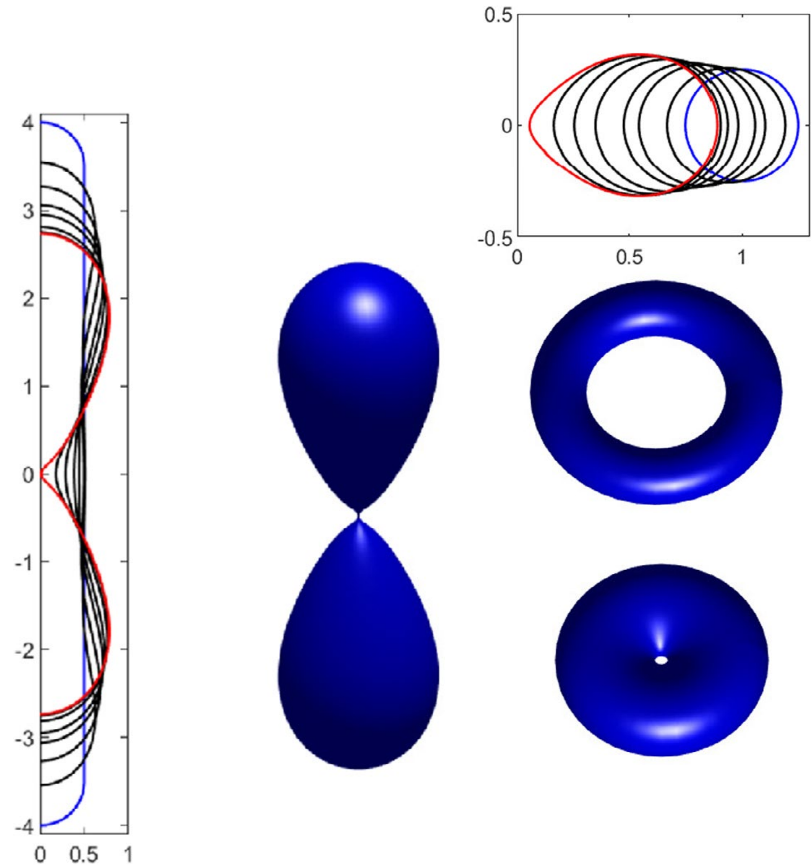


Extension to Axisymmetric Geometric flows

$$\mathcal{V}_n = -\Delta_s \mathcal{H} \qquad \text{on } \mathcal{S}(t),$$

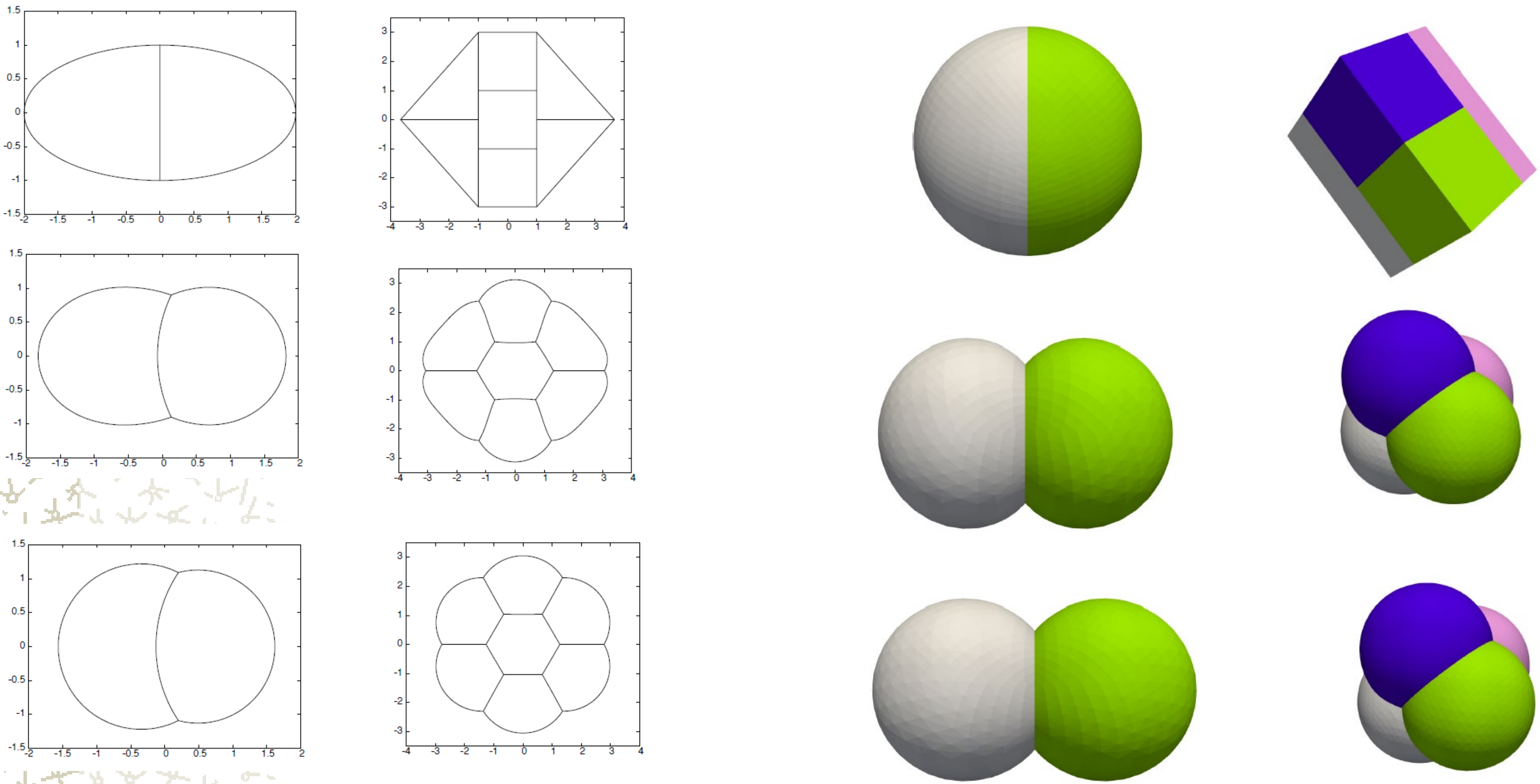
$$\mathcal{V}_n = -\Delta_s \mathcal{Y}, \qquad \left(-\frac{1}{\xi}\Delta_s + \frac{1}{\alpha}\right)\mathcal{Y} = \mathcal{H} \quad \text{on } \mathcal{S}(t),$$





W. Bao, H. Garcke, R. Nurnberg and Q. Zhao, Volume-preserving parametric finite element methods for axisymmetric geometric evolution equations, J. Comput. Phys., Vol. 460 (2022), 111180.

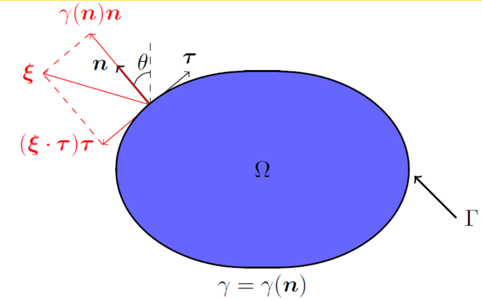
Extension to Surface Diffusion for Curve Networks and Surface Clusters



W. Bao, H. Garcke, R. Nurnberg and Q. Zhao, A structure-preserving finite element approximation of surface diffusion for curve networks and surface clusters, arXiv: 2202.06775.

Anisotropic Surface Diffusion

$$\Gamma(t): \vec{X}(\bullet,t) = (x(\bullet,t), y(\bullet,t))^T$$



- Mathematical model

$$\partial_t \vec{X}(\rho,t) = \partial_{ss}\mu\vec{n}$$

$$\mu = \left[\tilde{\gamma}(\theta) + \tilde{\gamma}''(\theta)\right]\kappa \Rightarrow \begin{array}{l} \vec{n}\bullet\partial_t \vec{X}(\rho,t) - \partial_{ss}\mu = 0 \\ \mu\vec{n} + \left[\tilde{\gamma}(\theta) + \tilde{\gamma}''(\theta)\right]\partial_{ss}\vec{X}(\rho,t) = 0 \end{array}$$

$$\kappa = -\partial_{ss}\vec{X}(s,t)\bullet\vec{n}$$

- Area conservation $\tilde{\gamma}(\theta) = \gamma(-\sin\theta, \cos\theta) = 1 + \beta\cos(k(\theta-\theta_0)), \quad \theta\in[-\pi,\pi]$

$$A(t) = \int_{\Gamma(t)} y\partial_s x ds \Rightarrow A'(t) = 0, \quad t\geq 0 \Rightarrow A(t)\equiv A(0), \quad t\geq 0$$

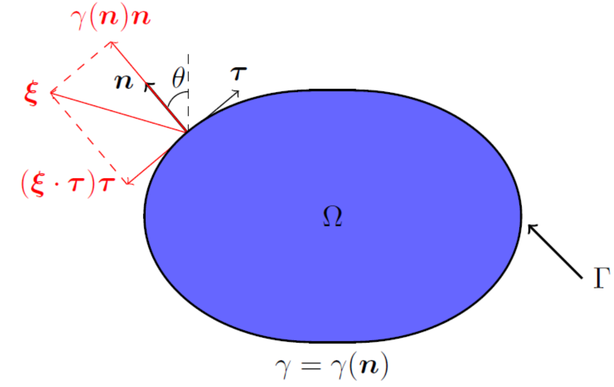
- Energy dissipation

$$W(t) = \int_{\Gamma(t)} \tilde{\gamma}(\theta)ds = L(t) \Rightarrow W'(t)\leq 0, \quad t\geq 0 \Rightarrow W(t)\leq W(t_1)\leq W(0), \quad 0\leq t_1\leq t$$

Anisotropic Surface Diffusion (ASD)

- Cahn-Hoffman ξ-vector:

$$\boldsymbol{\xi} := \boldsymbol{\xi}(\boldsymbol{n}) = \nabla\gamma(\boldsymbol{p})\big|_{\boldsymbol{p}=\boldsymbol{n}} = \gamma(\boldsymbol{n})\boldsymbol{n} + (\boldsymbol{\xi}\cdot\boldsymbol{\tau})\boldsymbol{\tau}, \qquad \forall \boldsymbol{n} \in \mathbb{S}^1,$$



  – with

$$\gamma(\boldsymbol{p}) := |\boldsymbol{p}|\gamma\left(\frac{\boldsymbol{p}}{|\boldsymbol{p}|}\right), \qquad \forall \boldsymbol{p} = (p_1, p_2)^T \in \mathbb{R}^2_* := \mathbb{R}^2 \setminus \{\mathbf{0}\},$$

- Geometric PDE for ASD

$$\begin{cases} \partial_t \boldsymbol{X} = \partial_{ss}\mu\, \boldsymbol{n}, & 0 < s < L(t), \quad t > 0, \\ \mu = -\boldsymbol{n}\cdot\partial_s\boldsymbol{\xi}^{\perp}, & \boldsymbol{\xi} = \nabla\gamma(\boldsymbol{p})\big|_{\boldsymbol{p}=\boldsymbol{n}}, \end{cases} \qquad \begin{cases} \boldsymbol{n}\cdot\partial_t \boldsymbol{X} = \partial_{ss}\mu, & 0 < s < L(t), \quad t > 0, \\ \mu\,\boldsymbol{n} = -\partial_s\boldsymbol{\xi}^{\perp}, & \boldsymbol{\xi} = \nabla\gamma(\boldsymbol{p})\big|_{\boldsymbol{p}=\boldsymbol{n}}. \end{cases}$$

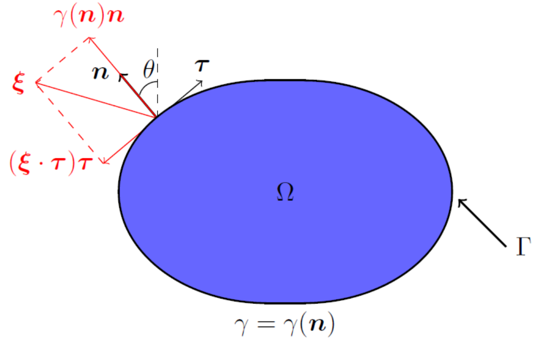
- A symmetric surface energy matrix

$$Z_k(\boldsymbol{n}) = \gamma(\boldsymbol{n})I_2 - \boldsymbol{n}\boldsymbol{\xi}(\boldsymbol{n})^T - \boldsymbol{\xi}(\boldsymbol{n})\boldsymbol{n}^T + k(\boldsymbol{n})\boldsymbol{n}\boldsymbol{n}^T, \qquad \forall \boldsymbol{n} \in \mathbb{S}^1, \qquad \begin{cases} \boldsymbol{n}\cdot\partial_t\boldsymbol{X} = \partial_{ss}\mu, \\ \mu\,\boldsymbol{n} = -\partial_s(Z_k(\boldsymbol{n})\partial_s\boldsymbol{X}). \end{cases}$$

W. Bao, W. Jiang and Y. Li, A symmetrized parametric finite element method for anisotropic surface diffusion of closed curves, arXiv: 2112.00508.
Y. Li and W. Bao, An energy-stable parametric finite element method for anisotropic surface diffusion, J. Comput. Phys., Vol. 446 (2021), article 110658.

Structure-Preserving PFEM for ASD

- A new symmetric variational formulation



$$\Big(\boldsymbol{n}\cdot\partial_t\boldsymbol{X},\varphi\Big)_{\Gamma(t)}+\Big(\partial_s\mu,\partial_s\varphi\Big)_{\Gamma(t)}=0,\qquad\forall\varphi\in H^1(\mathbb{T}),$$

$$\Big(\mu,\boldsymbol{n}\cdot\boldsymbol{\omega}\Big)_{\Gamma(t)}-\Big(Z_k(\boldsymbol{n})\partial_s\boldsymbol{X},\partial_s\boldsymbol{\omega}\Big)_{\Gamma(t)}=0,\quad\forall\boldsymbol{\omega}\in[H^1(\mathbb{T})]^2.$$

- Structure-Preserving PFEM

$$\Big(\frac{\boldsymbol{X}^{m+1}-\boldsymbol{X}^m}{\tau}\cdot\boldsymbol{n}^{m+\frac{1}{2}},\varphi^h\Big)^h_{\Gamma^m}+\Big(\partial_s\mu^{m+1},\partial_s\varphi^h\Big)^h_{\Gamma^m}=0,\ \forall\varphi^h\in\mathbb{K}^h,$$

$$\Big(\mu^{m+1},\boldsymbol{n}^{m+\frac{1}{2}}\cdot\boldsymbol{\omega}^h\Big)^h_{\Gamma^m}-\Big(Z_k(\boldsymbol{n}^m)\partial_s\boldsymbol{X}^{m+1},\partial_s\boldsymbol{\omega}^h\Big)^h_{\Gamma^m}=0,\ \forall\boldsymbol{\omega}^h\in[\mathbb{K}^h]^2,$$

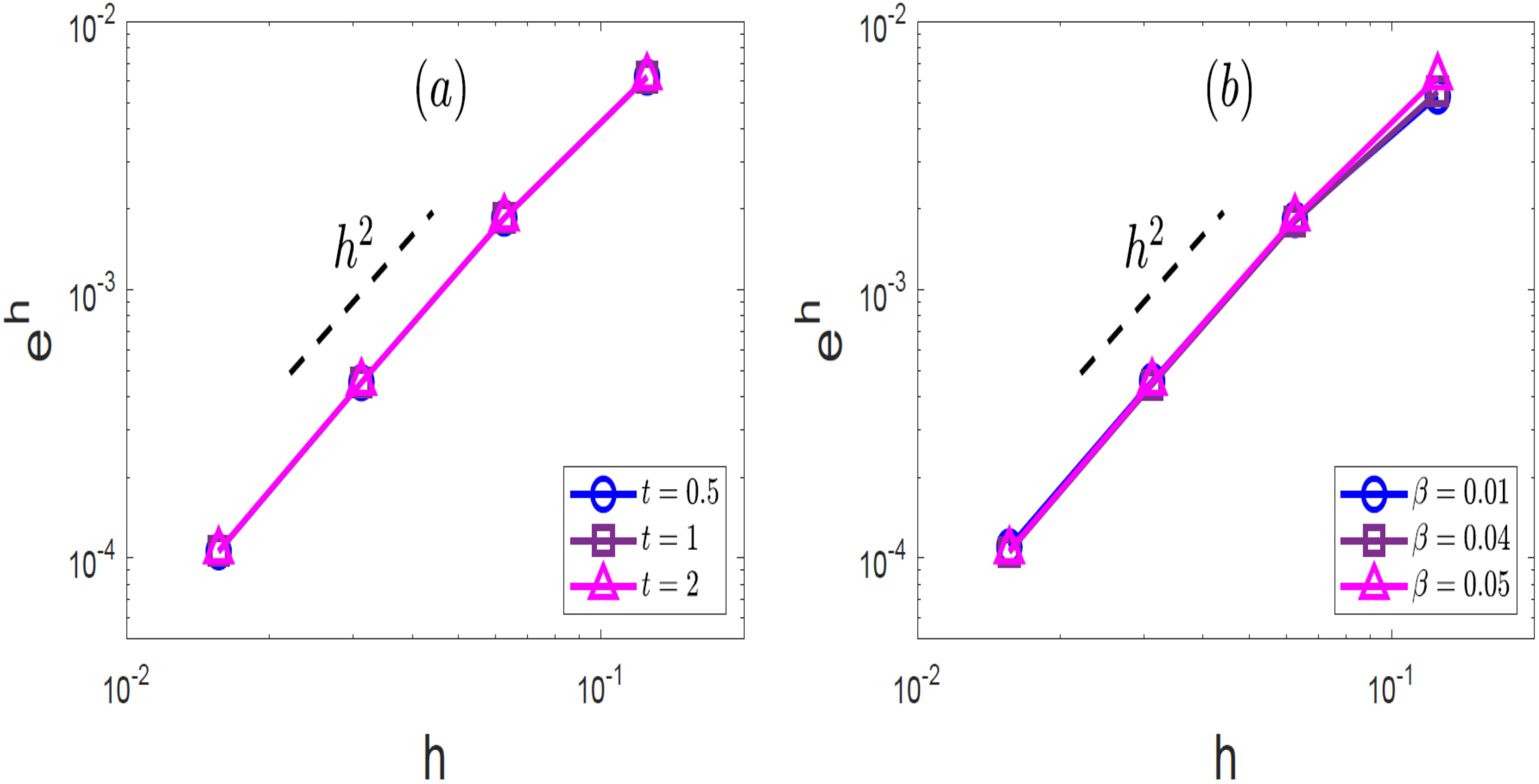
$$\boldsymbol{n}^{m+\frac{1}{2}}:=-\frac{1}{2}\left(\partial_s\boldsymbol{X}^m+\partial_s\boldsymbol{X}^{m+1}\right)^\perp=-\frac{1}{2}\frac{1}{|\partial_\rho\boldsymbol{X}^m|}\left(\partial_\rho\boldsymbol{X}^m+\partial_\rho\boldsymbol{X}^{m+1}\right)^\perp,$$

$$Z_k(\boldsymbol{n}^m)=\gamma(\boldsymbol{n}^m)I_2-\boldsymbol{n}^m\boldsymbol{\xi}(\boldsymbol{n}^m)^T-\boldsymbol{\xi}(\boldsymbol{n}^m)(\boldsymbol{n}^m)^T+k(\boldsymbol{n}^m)\,\boldsymbol{n}^m(\boldsymbol{n}^m)^T$$

- Properties: mass conservation, asymptotic quasi-equal mesh distribution, energy dissipation if $\gamma(-\boldsymbol{n})=\gamma(\boldsymbol{n}),\quad\forall\boldsymbol{n}\in\mathbb{S}^1,\qquad\gamma(\boldsymbol{p})\in C^2(\mathbb{R}^2\setminus\{\boldsymbol{0}\}),$

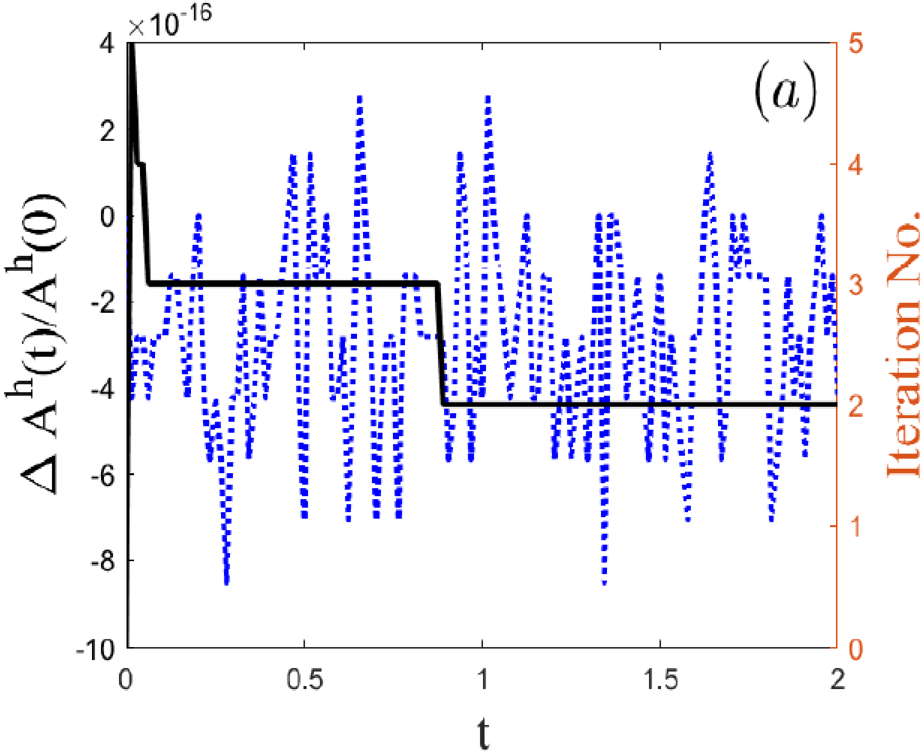
W. Bao, W. Jiang and Y. Li, A symmetrized parametric finite element method for anisotropic surface diffusion of closed curves, arXiv: 2112.00508.
W. Bao and Y. Li, A symmetrized parametric finite element method for anisotropic surface diffusion II. Three dimensions, arXiv: 2206.01883.

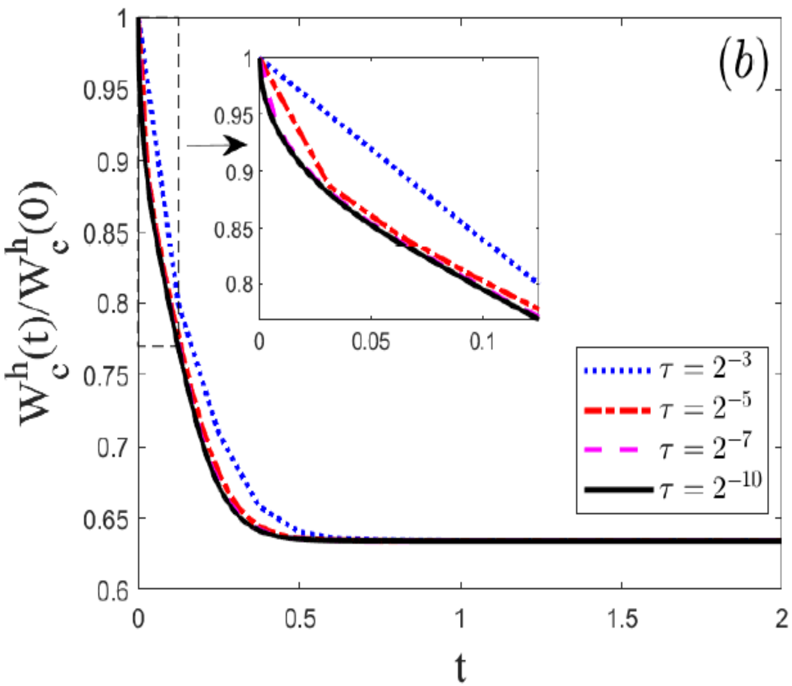
Convergence rate



$$\gamma(\vec{n}) = 1 + \beta n_1^4$$

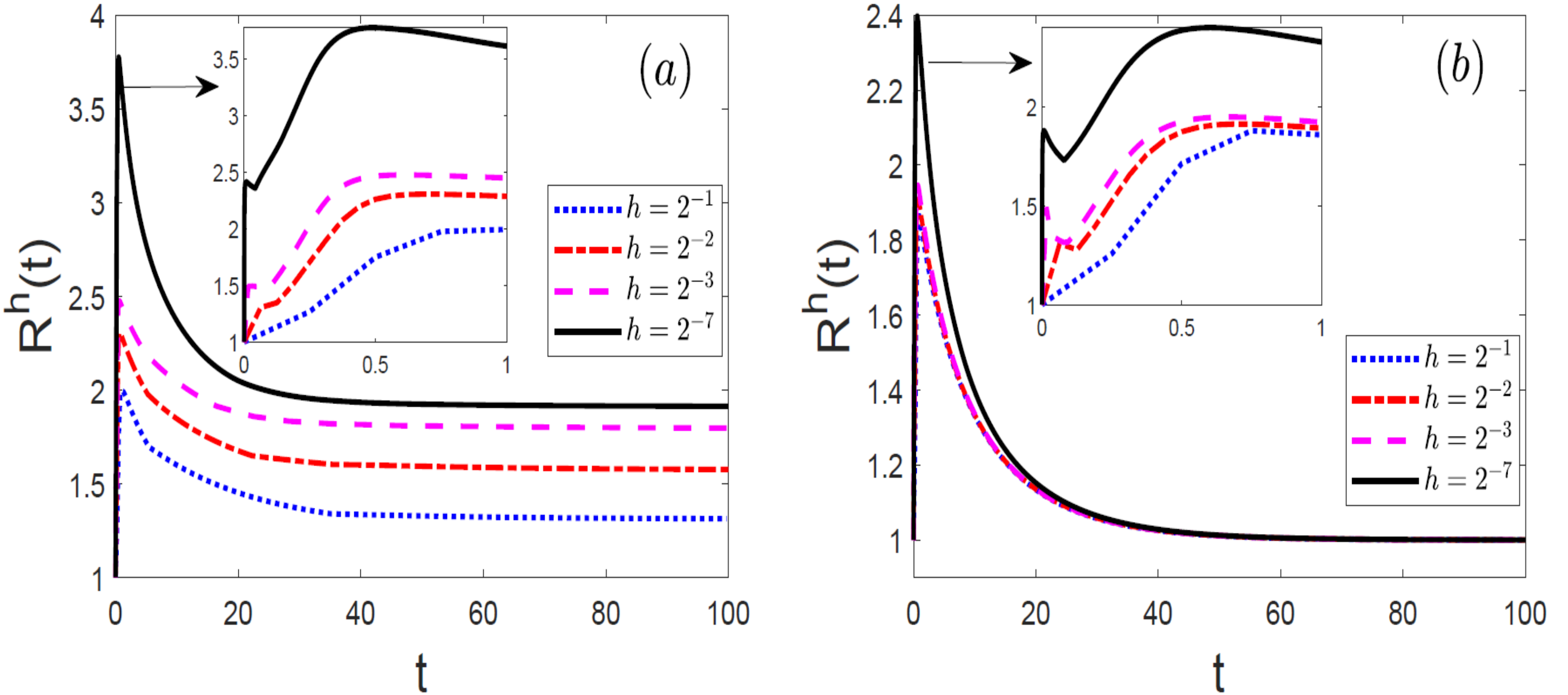
Area conservation& Energy Dissipation





$$\gamma\left(\vec{n}\right)=1+0.05n_1^2$$

Mesh ratio



$\gamma(\vec{n}) = 1 + 0.05 n_1^4$

$\gamma(\vec{n}) \equiv 1$

Anisotropic Surface Diffusion

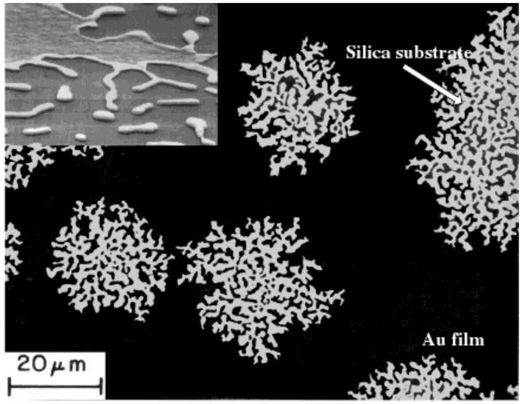
$$\gamma(\vec{n}) = 1 + 0.06 n_1^4$$

Anisotropic Surface Diffusion

$$\gamma(\vec{n}) = |n_1| + |n_2| \Rightarrow \gamma_\varepsilon(\vec{n}) = \sqrt{\left(1-\varepsilon^2\right)n_1^2 + \varepsilon^2} + \sqrt{\left(1-\varepsilon^2\right)n_2^2 + \varepsilon^2}$$

Solid-State Dewetting (SSD)

- Solid-state dewetting
  - Is driven by capillarity effects
  - Occurs through surface diffusion controlled mass transport
  - Belongs to capillarity-controlled interface/surface evolution
  - Surface diffusion + contact line migration

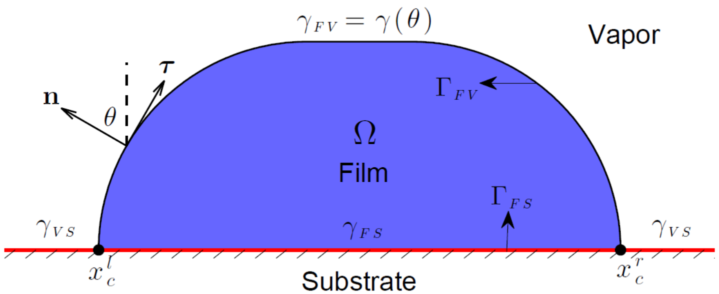


- Applications of dewetting of thin films
  - Play an improtant role in micorelectronics processing
  - A common method to produce nanoparticles
  - Catalyst for the growth of carbon nanotubes & semiconductor nanowires
- Recent experiments -- [1]
  - Geometric complexity, capillarity-driven instabilities, faceting
  - Crystalline anisotropy, corner-induced instabilities, pinch-off, ….
- Wetting/dewetting in fluids: TZ Qian, XP Wang&P Sheng; W. Ren&W E, ...

[1] J. Ye & C.V. Thompson, Acta Mater. 23 (2011), 1567; 59 (2011), 582; Appl. Phys. Lett. 97 (2010), 071904

Sharp Interface Model for Solid-State Dewetting

$\Gamma: \quad \vec{X}(s,t) = (x(s,t), y(s,t))^T \qquad s$ -- arclength



θ_c^r --Dynamical contact angle

θ_i----Isotropic Young contace angle

- **The Model** (Wang, Jiang, Bao, Srolovitz, PRB 15')

$$\partial_t \vec{X}(s,t) = V_n \vec{n}, \qquad \text{with} \qquad V_n = B\partial_{ss}\mu$$

$$\mu = (\tilde{\gamma}(\theta) + \tilde{\gamma}''(\theta))\kappa$$

- **Boundary conditions**
  - Contact point condition (BC1): $y(x_c^r, t) = 0$
  - Relaxed contact angle condition (BC2): $\frac{dx_c^r(t)}{dt} = -\eta \frac{\delta W}{\delta x_c^r} = -\eta f(\theta_c^r),$
  - Zero-mass flux condition (BC3): $\partial_s \mu(x_c^r, t) = 0$

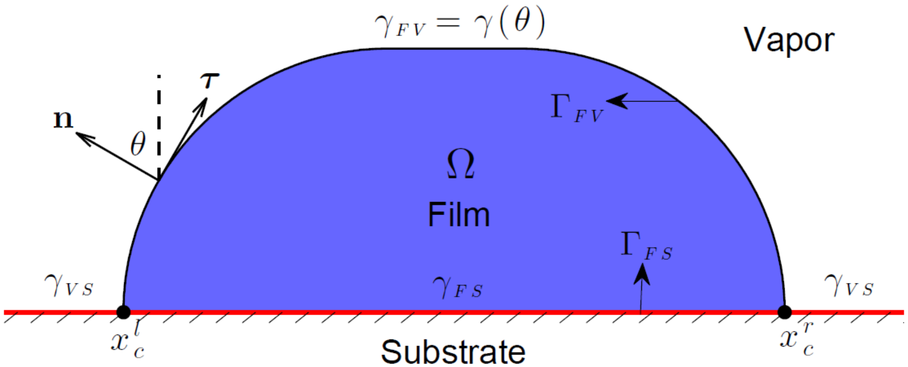
- **Anisotropic Young equation** $\eta \to \infty$

$$\tilde{\gamma}(\theta)\cos\theta - \tilde{\gamma}'(\theta)\sin\theta - \gamma_0 \cos\theta_i = 0 \quad \overset{\gamma(\theta)\equiv\gamma_0}{\Longrightarrow} \quad \cos\theta = \cos\theta_i$$

Y. Wang, W. Jiang, W. Bao & D. J. Srolovitz, Sharp interface model for solid-state dewetting problems with weakly anisotropic surface energy, Phys. Rev. B, Vol. 91 (2015), article 045303.

W. Bao, W. Jiang, D. J. Srolovitz & Y. Wang, Stable equilibria of anisotropic particles on substrates: a generalized Winterbottom construction, SIAM J. Appl. Math., Vol. 77 (2017), pp. 2093-2118

Area Conservation & Energy Dissipation



- Area (Mass) conservation

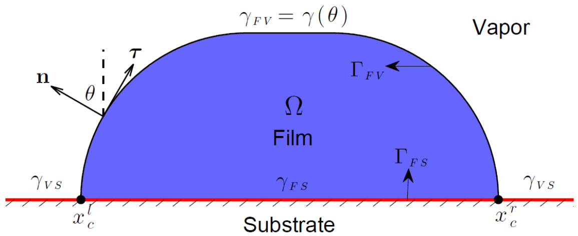
$$A(t) = \int_{\Gamma(t)} y\partial_s x ds \Rightarrow A'(t) = 0, \quad t \geq 0 \Rightarrow A(t) \equiv A(0), \quad t \geq 0$$

- Energy dissipation

$$W(t) = \int_{\Gamma(t)} \gamma_{FV}(\theta) ds + (\gamma_{FS} - \gamma_{VS})(x_c^r - x_c^l) \Rightarrow W'(t) \leq 0, \quad t \geq 0$$

$$\Rightarrow W(t) \leq W(t_1) \leq W(0), \quad 0 \leq t_1 \leq t$$

Energy-stable PFEM



- Isotropic case $\gamma(\theta) = 1$
  - Re-formulation

$$\partial_t \vec{X}(s,t) = \partial_{ss}\kappa\vec{n} \qquad \Rightarrow \qquad (\partial_t \vec{X}(s,t))\bullet\vec{n} = \partial_{ss}\kappa$$

$$\kappa = -(\partial_{ss}\vec{X}(s,t))\bullet\vec{n} \qquad\qquad \kappa\vec{n} = -\partial_{ss}\vec{X}(s,t)$$

  - Re-write the relaxed contact BC $y(x_c^r,t) = 0,\ \partial_s \mu(x_c^r,t) = 0$

$$\partial_s x(s,t)\Big|_{s=0} = \sigma + \frac{1}{\eta}\frac{dx_c^l(t)}{dt}, \qquad \partial_s x(s,t)\Big|_{s=L(t)} = \sigma - \frac{1}{\eta}\frac{dx_c^r(t)}{dt}.$$

W. Bao, W. Jiang, Y. Wang & Q. Zhao, A parametric finite element method for solid-state dewetting problems with anisotropic surface energies, J. Comput. Phys., Vol. 330 (2017), pp. 380-400.
Q. Zhao, W. Jiang & W. Bao, An energy-stable parametric finite element method for simulating solid-state dewetting, IMA J. Numer. Anal., Vol. 41 (2021), pp. 2026-2055.

Energy-stable PFEM

- A variational formulation

$$\vec{X}(\rho,t) \in X := H^1(\mathrm{I}) \times H_0^1(I), \quad \kappa \in H^1(I) \quad \text{s.t.}$$

$$\left(\mathbf{n}\cdot\partial_t\mathbf{X},\ \psi\right)_{\Gamma(t)} + \left(\partial_s\kappa,\ \partial_s\psi\right)_{\Gamma(t)} = 0, \qquad \forall\psi \in H^1(\mathbf{I}),$$

$$\left(\kappa,\mathbf{n}\cdot\boldsymbol{\omega}\right)_{\Gamma(t)} - \left(\partial_s\mathbf{X},\ \partial_s\boldsymbol{\omega}\right)_{\Gamma(t)} - \frac{1}{\eta}\left[\frac{dx_c^l(t)}{dt}\omega_1(0) + \frac{dx_c^r(t)}{dt}\omega_1(1)\right]$$

$$+\ \sigma\left[\omega_1(1) - \omega_1(0)\right] = 0, \quad \forall\boldsymbol{\omega} = (\omega_1,\ \omega_2)^T \in \mathbb{X};$$

$$x_c^l(t) = x(\rho = 0, t) \text{ and } x_c^r(t) = x(\rho = 1, t)$$

Q. Zhao, W. Jiang & W. Bao, An energy-stable parametric finite element method for simulating solid-state dewetting, IMA J. Numer. Anal., Vol. 41 (2021), pp. 2026-2055.

Energy-stable PFEM

$$K^h \subset H^1(I), \quad K_0^h \subset H_0^1(I), \quad X^h = K^h \times K_0^h$$

- PFEM by finding $\vec{X}^{m+1} \in X^h, \quad \kappa^{m+1} \in K^h$ s.t.

$$\left(\frac{\mathbf{X}^{m+1}-\mathbf{X}^m}{\tau}\cdot \mathbf{n}^m,\ \psi^h\right)_{\Gamma^m}^h + \left(\partial_s \kappa^{m+1},\ \partial_s \psi^h\right)_{\Gamma^m} = 0, \qquad \forall \psi^h \in \mathbb{K}^h,$$

$$\Leftarrow \quad \vec{n}^m = (\partial_s \vec{X}^m)^\perp, \quad s-\text{arclength of } \Gamma^m$$

$$\left(\kappa^{m+1}, \mathbf{n}^m \cdot \boldsymbol{\omega}^h\right)_{\Gamma^m}^h - \left(\partial_s \mathbf{X}^{m+1},\ \partial_s \boldsymbol{\omega}^h\right)_{\Gamma^m} + \sigma\left[\omega_1^h(1) - \omega_1^h(0)\right]$$

$$-\frac{1}{\eta\,\tau}\left[\omega_1^h(0)(x_l^{m+1}-x_l^m) + \omega_1^h(1)(x_r^{m+1}-x_r^m)\right] = 0, \quad \forall \boldsymbol{\omega}^h = (\omega_1^h,\ \omega_2^h)^T \in \mathbb{X}^h;$$

$$x_l^{m+1} = x^{m+1}(\rho=0) \text{ and } x_r^{m+1} = x^{m+1}(\rho=1)$$

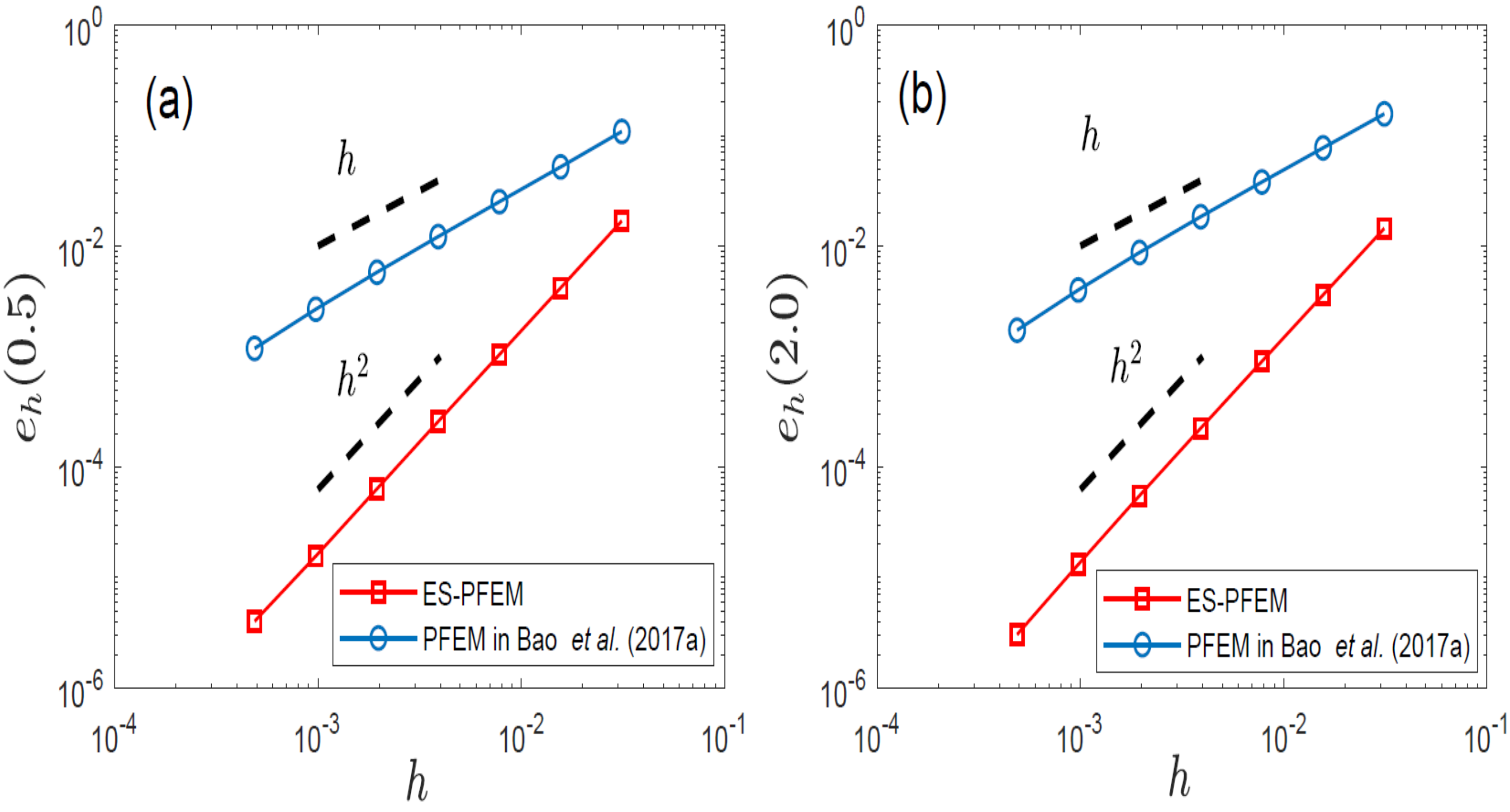
- Properties: Well-posedness, Energy dissipation & unconditionally stable, Asymptotic mesh equal distribution, semi-implicit, extension to 3D, …

Q. Zhao, W. Jiang & W. Bao, An energy-stable parametric finite element method for simulating solid-state dewetting, IMA J. Numer. Anal., Vol. 41 (2021), pp. 2026-2055.

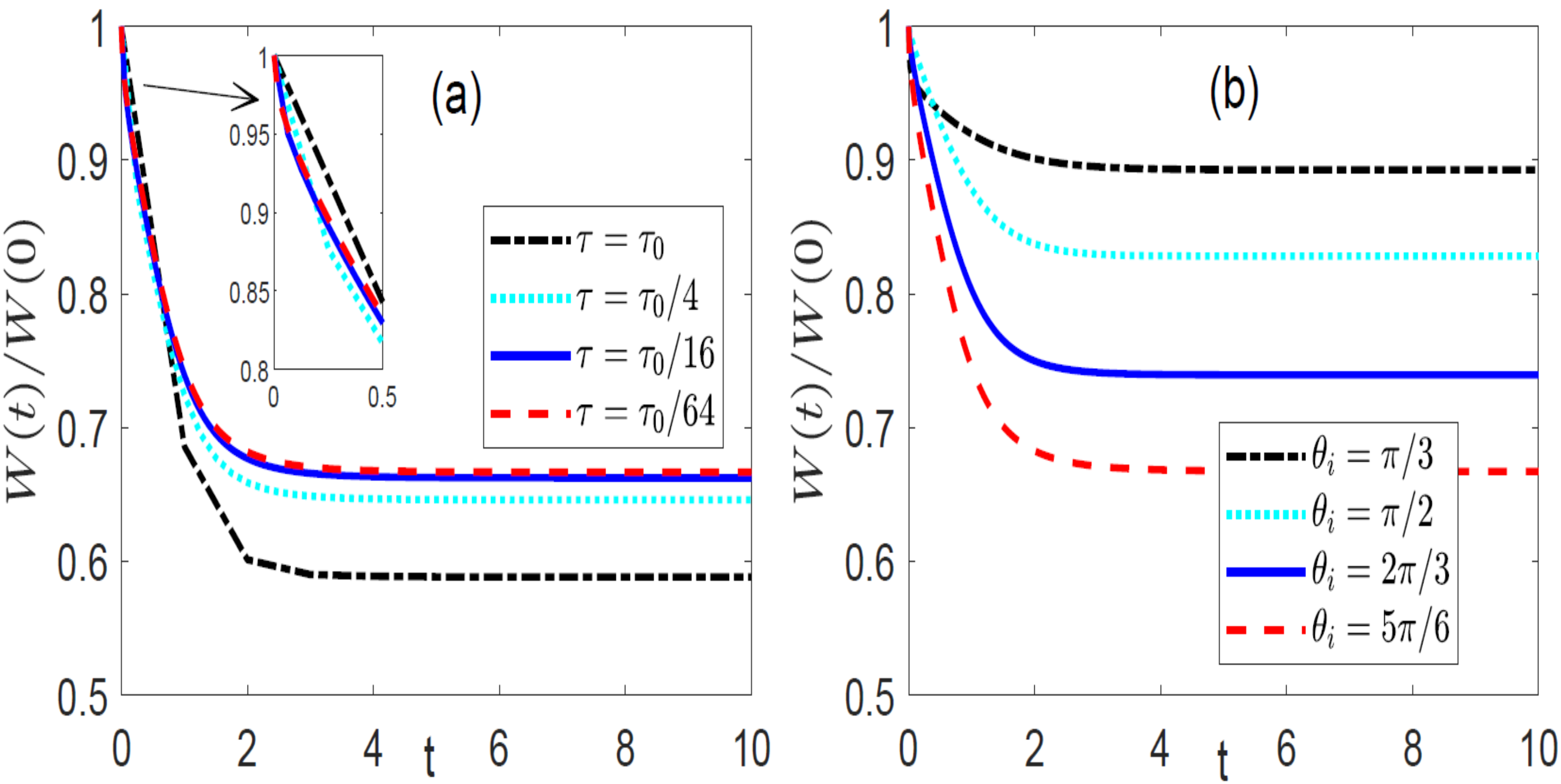
Q. Zhao, W. Jiang & W. Bao, A parametric finite element method for solid-state dewetting problems in three dimensions, SIAM J. Sci. Comput., Vol. 42 (2020), B327-B352.

W. Bao & Q. Zhao, An energy-stable parametric finite element method for simulating solid-state dewetting problems in three dimensions, J. Comput. Math., arXiv: 2012.11404.

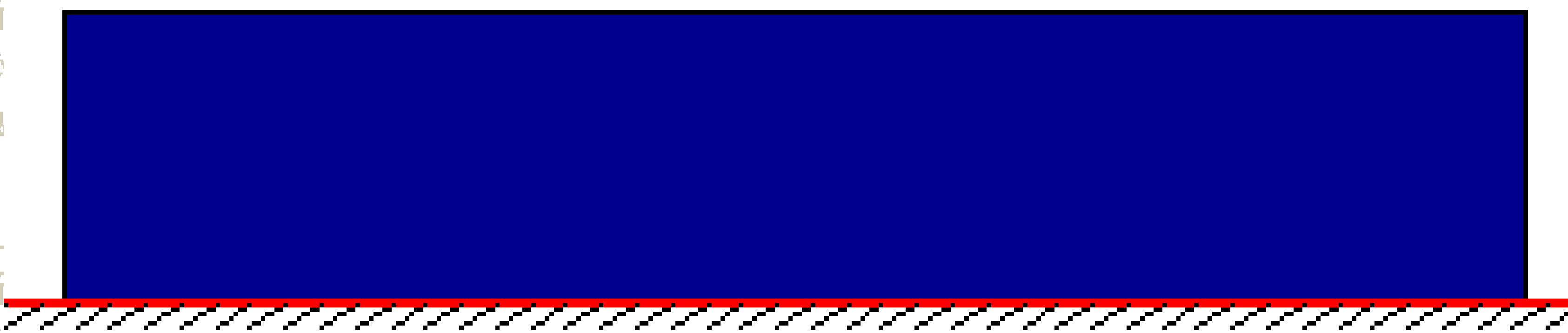
Energy-stable PFEM



Energy-stable PFEM

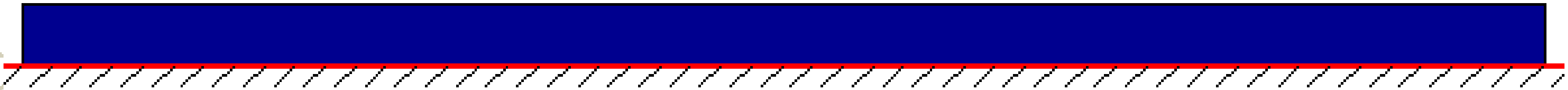


$$L = 5, \beta = 0, \sigma = \cos(3\pi/4)$$



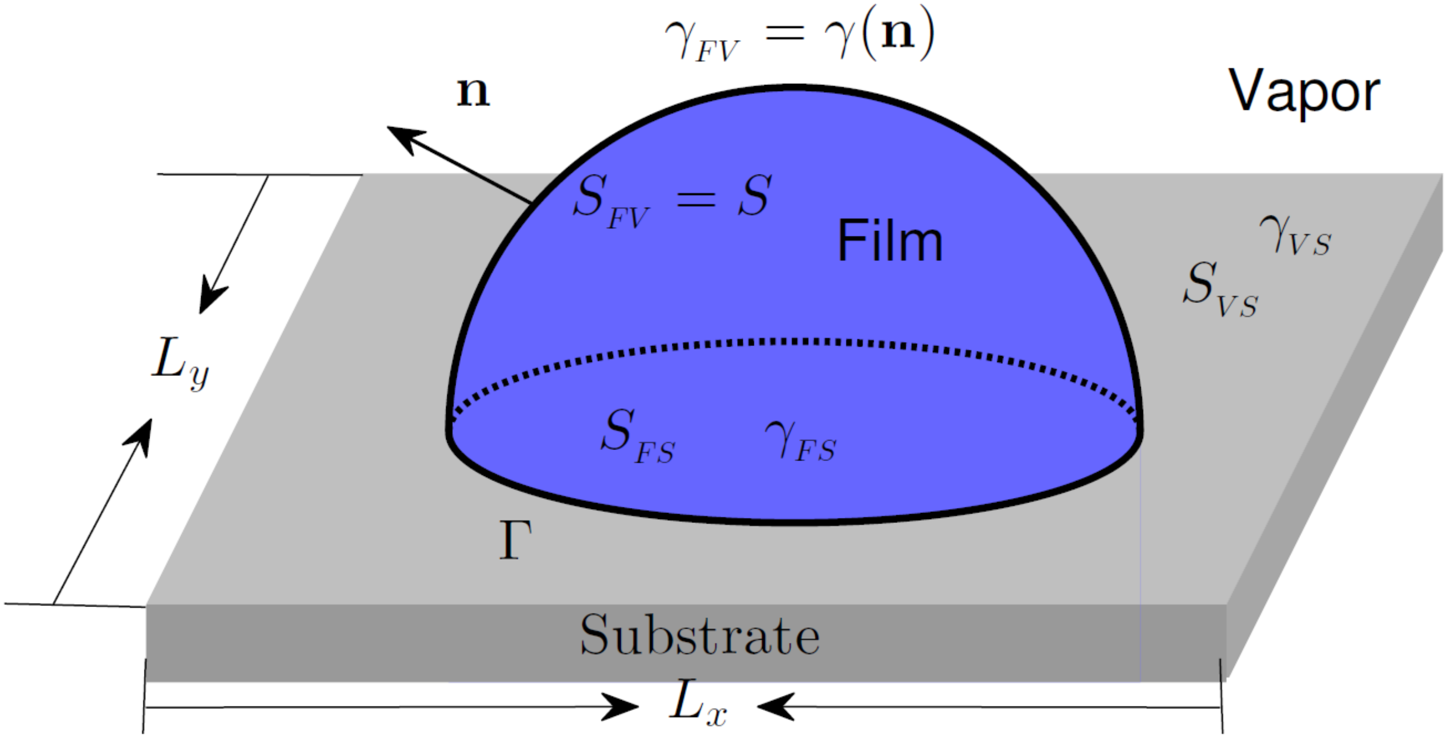
Isotropic surface energy and short

$$L = 60, m = 4, \beta = 0.06, \sigma = \cos(5\pi/6)$$



Weakly anisotropic surface energy & long for pinch-off

Solid-State Dewetting in 3D



- Total interfacial energy

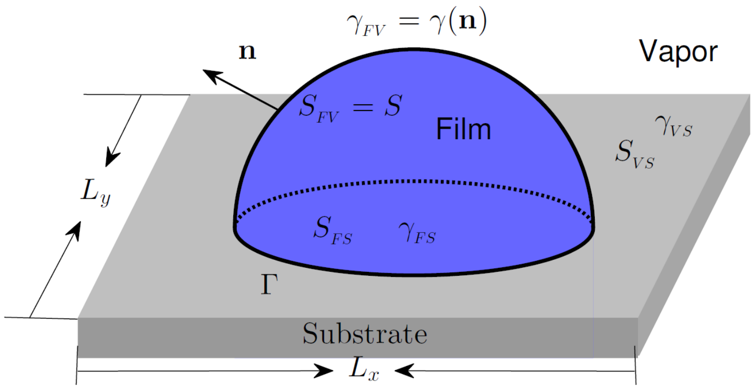
$$W = W_I + W_S = \iint_S \gamma(\mathbf{n})\, dS + (\gamma_{FS} - \gamma_{VS})A(\Gamma),$$

Sharp Interface Model for SSD in 3D

- Main ideas -- thermodynamic variation, shape derivatives & Cahn-Hoffman \xi-vector
- The sharp interface model

$$\partial_t \mathbf{X} = \Delta_S \mu\, \mathbf{n}, \qquad t > 0,$$

$$\mu = \nabla_S \cdot \boldsymbol{\xi}, \qquad \boldsymbol{\xi} = \nabla \hat{\gamma}(\mathbf{n}),$$



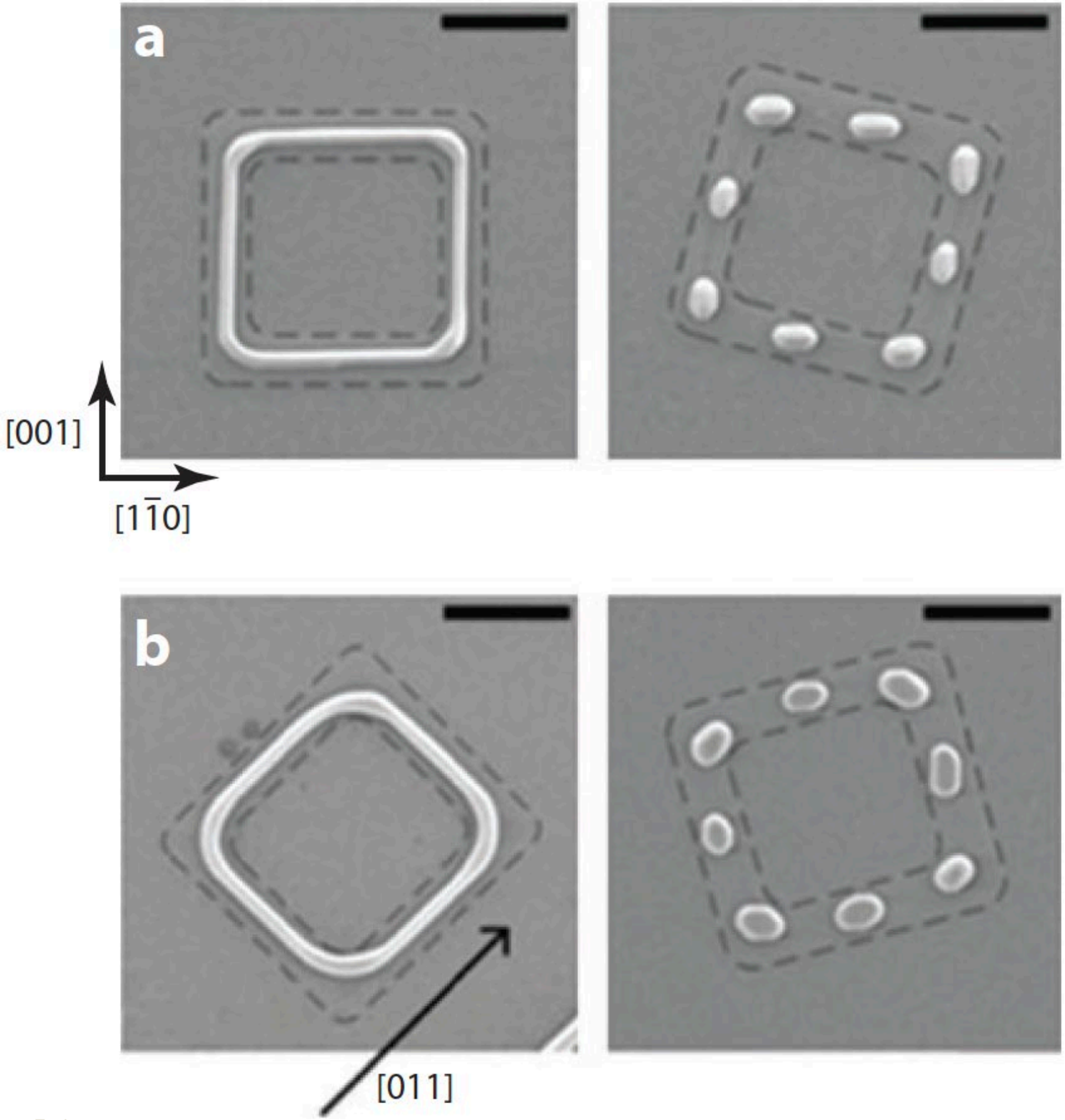
  - Contact line condition $\Gamma \subset S_{sub}$
  - Relaxed contact angle condition $\partial_t \mathbf{X}_\Gamma = -\eta \left[\mathbf{c}_\Gamma^\gamma \cdot \mathbf{n}_\Gamma - \sigma \right] \mathbf{n}_\Gamma$
  - Zero-flux condition $\left(\mathbf{c}_\Gamma \cdot \nabla_S \mu \right)\Big|_\Gamma = 0,$

- Parameter finite element (PFEM) method

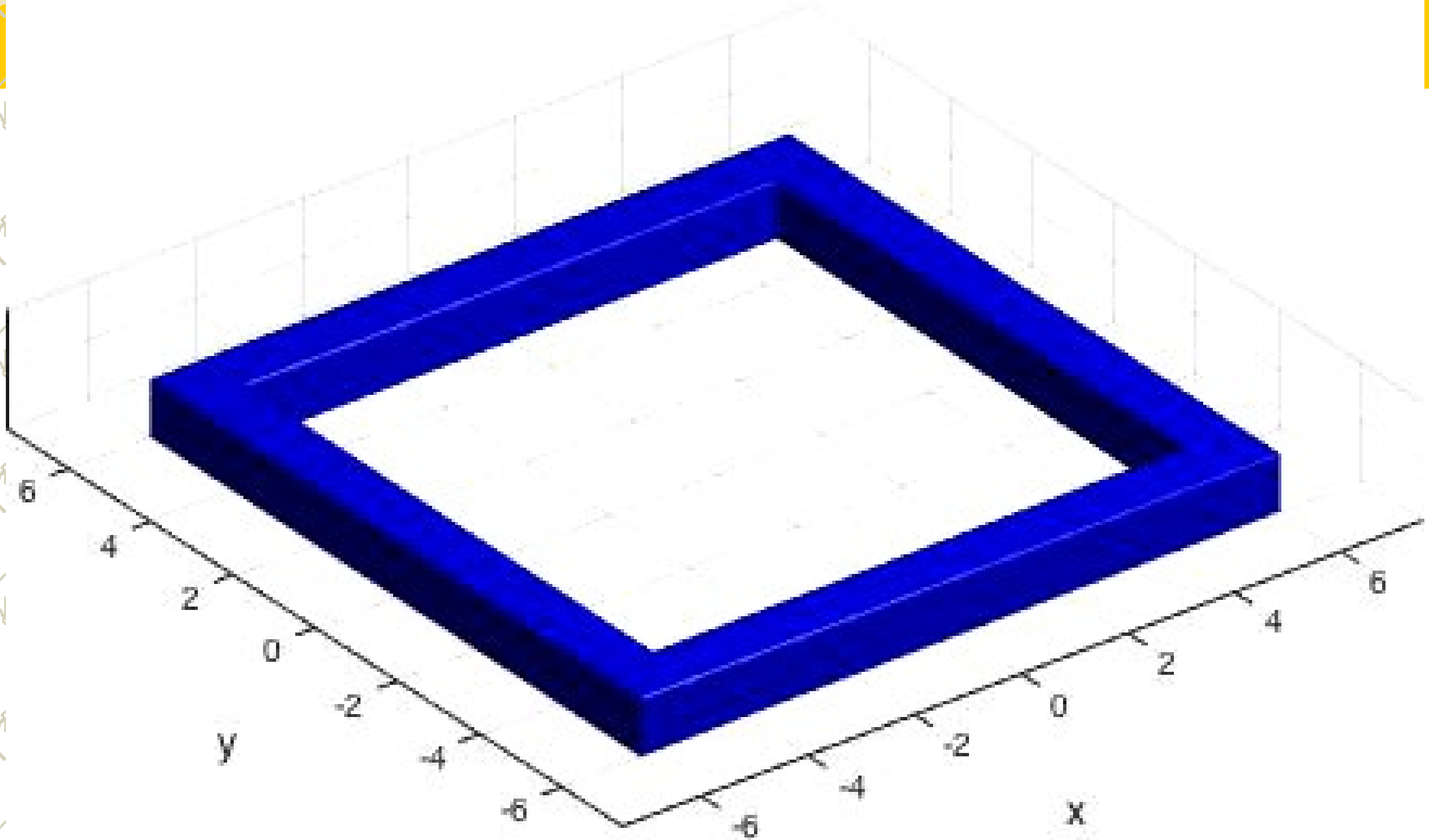
Q. Zhao, W. Jiang & W. Bao, A parametric finite element method for solid-state dewetting problems in three dimensions, SIAM J. Sci. Comput., Vol. 42 (2020), B327-B352.

W. Jiang, Q. Zhao & W. Bao, Sharp-interface model for simulating solid-state dewetting in three dimensions, SIAM J. Appl. Math., Vol. 80 (2020), 1654-1677

W. Bao & Q. Zhao, An energy-stable parametric finite element method for simulating solid-state dewetting problems in three dimensions, arXiv: 2012.11404.

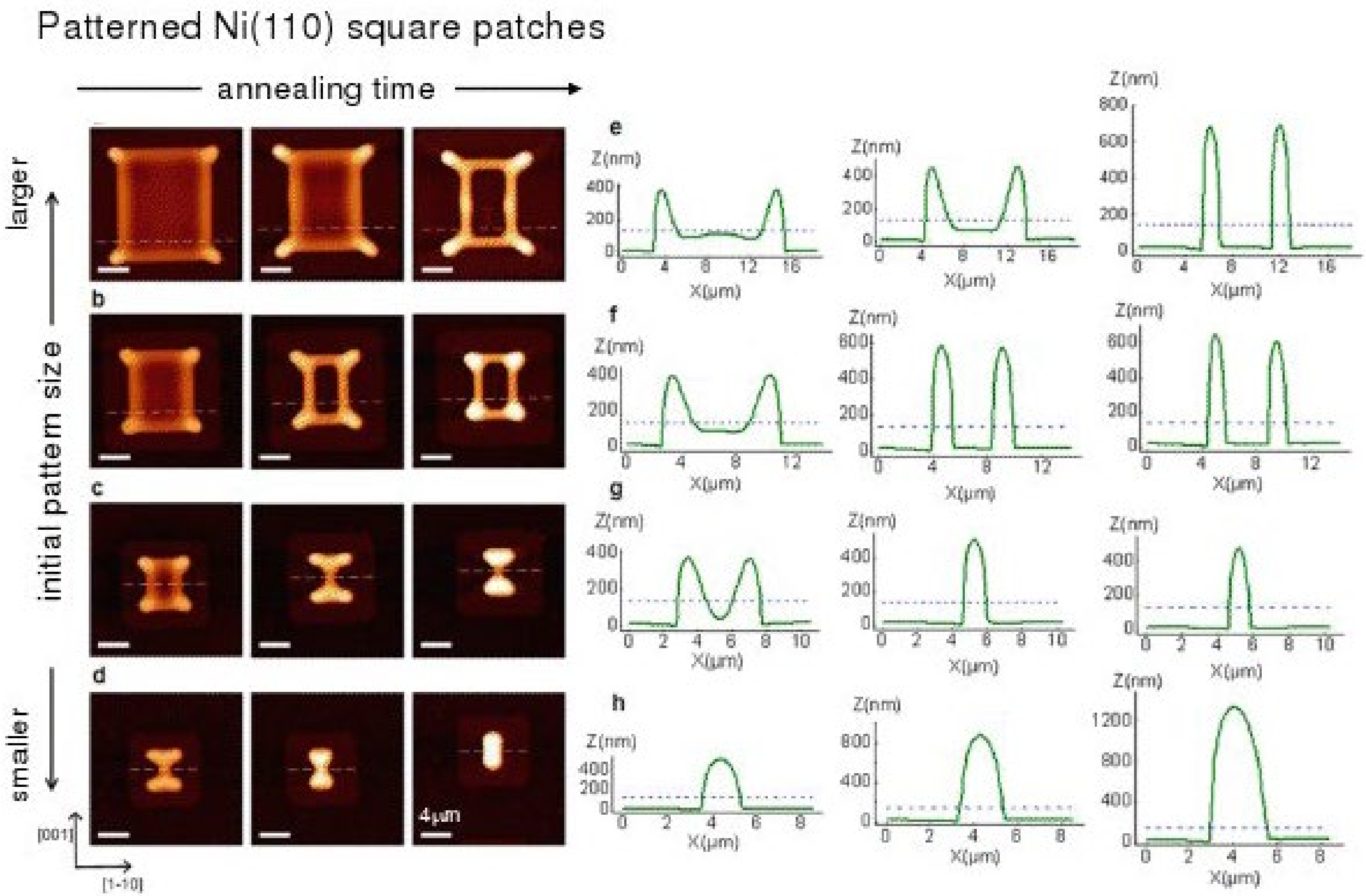


[1] J. Ye & C.V. Thompson, Acta Mater. 23 (2011), 1567; 59 (2011), 582; Appl. Phys. Lett. 97 (2010), 071904



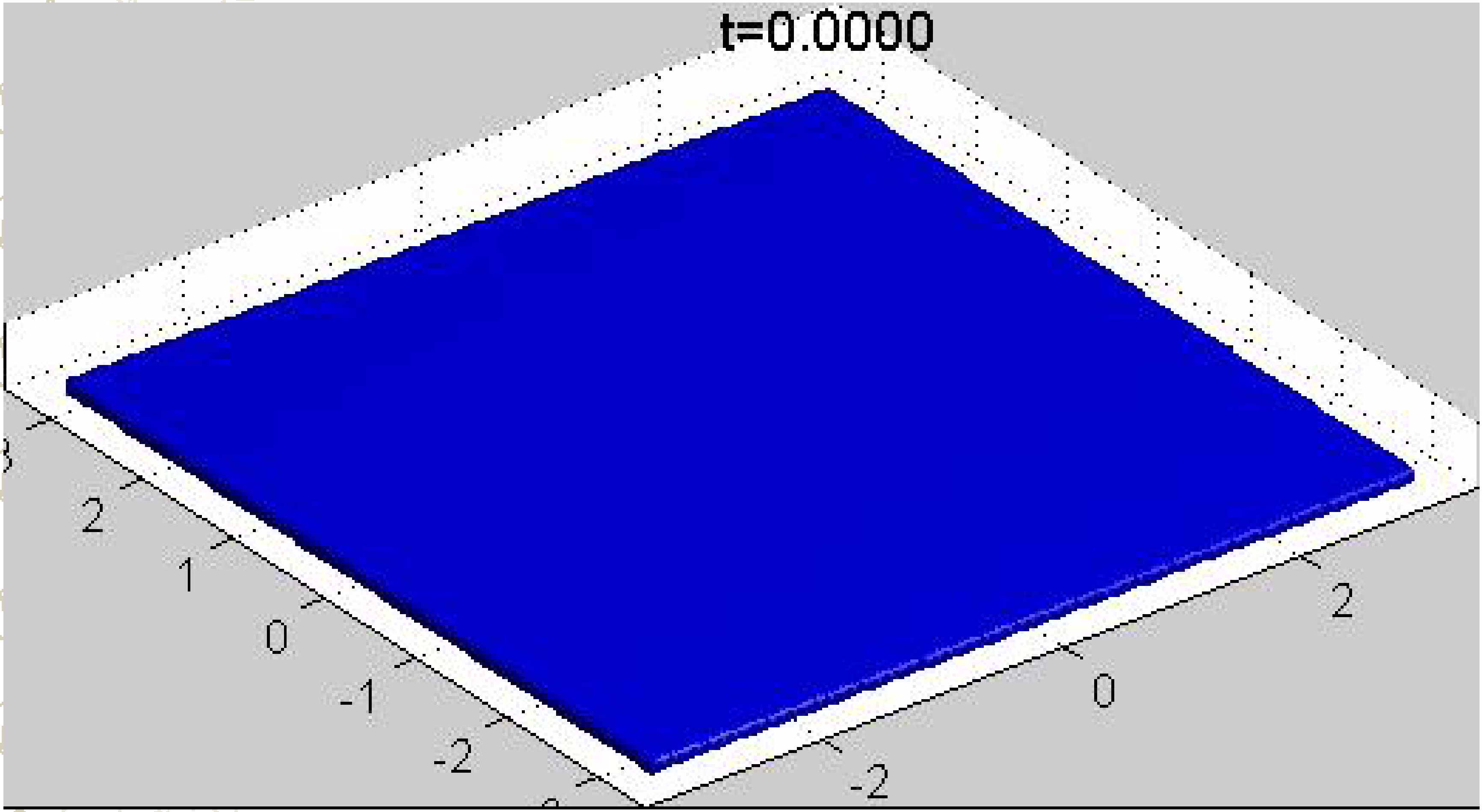
6
4
2
0
-2
-4
-6
y
-6
-4
-2
0
2
4
6
x

Dewetting Patterned Films

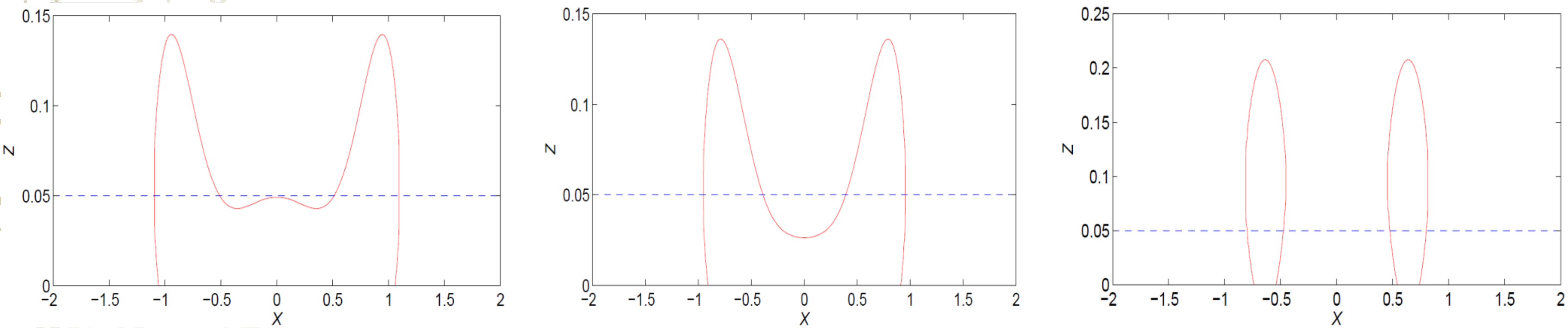


[1] J. Ye & C.V. Thompson, Phys. Rev. B, 82 (2010), 193408.

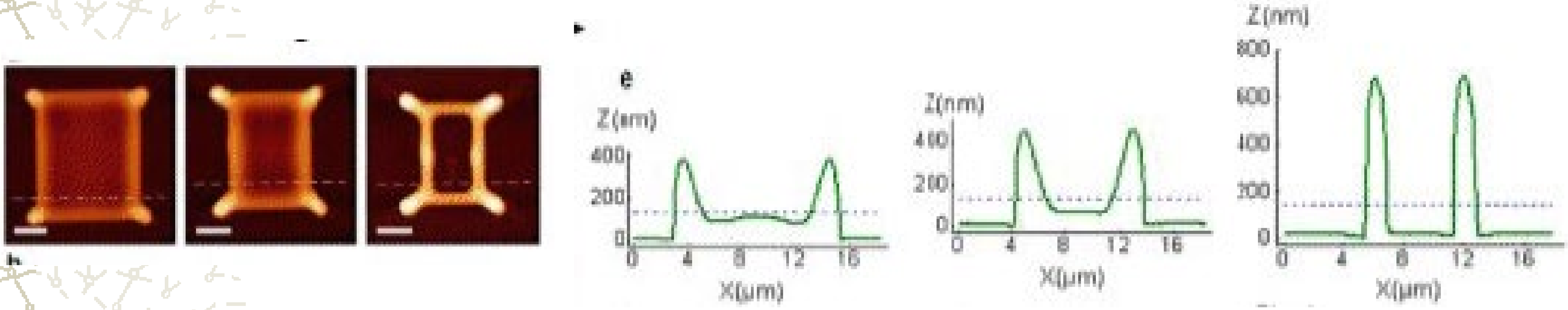
Solid-state dewetting in 3D via SIM



3D Results – Comparison with Experiment



Computational Results



Experimental Results

Conclusion & Future Works

- Conclusion
  - Review of different geometric flows (PDEs)
  - ES-PFEM for mean curvature flow (MCF)
  - ES-PFEM & SP-PFEM for surface diffusion
  - Extension to axisymmetric, surface clusters, anistropic surface diffustion
  - Applications of ES-PFEM for solid-state dewetting (SSD)
- Future works
  - Error estimates of ES-PFEM & SP-PFEM
  - Extension to other geometric flows
  - PDE results for solid-state dewetting
  - Compare with experiments quantitatively in SSD
  - Guide new experiments in SSD