FINITE ELEMENT METHODS FOR SURFACE DIFFUSION AND APPLICATIONS TO STRESSED EPITAXIAL FILMS

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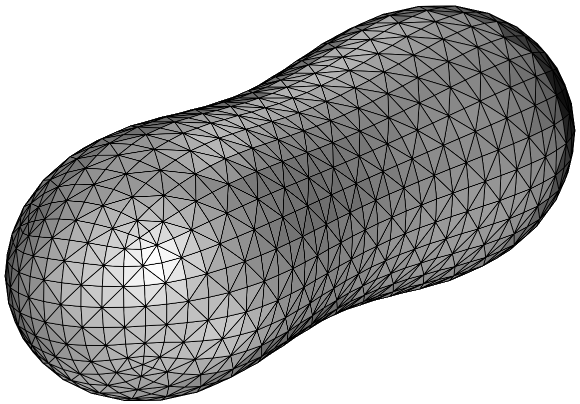
Outline

1. Problem Description and Challenges

2. FEM for Surface Diffusion

   - Time Discretization
   - Variational Formulation
   - Space Discretization
   - Mesh regularization and adaptivity
   - Simulations
   - Graphs: Formulation, Estimates and Simulations



3. Stressed Epitaxial Films

   - Coupling: 1st Approach
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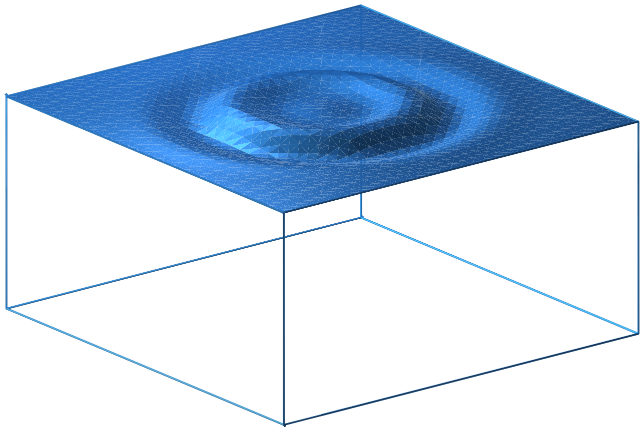
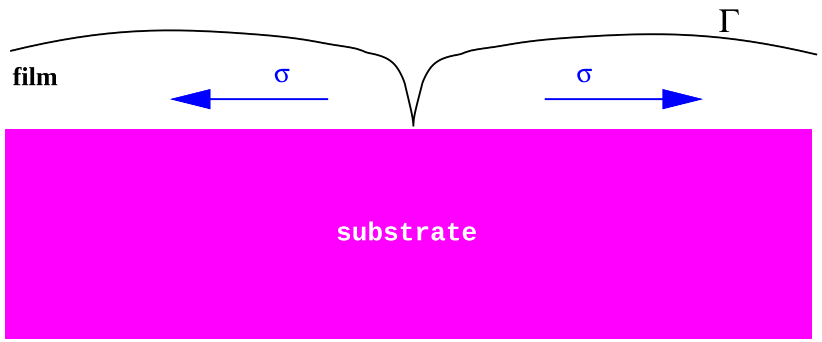
   - Simulations
   - Related Issues and Open Problems



1. Problem Description

Physical problem: morphological changes in epitaxial thin films



Missfit between crystalline structures

$\Rightarrow$ (linear) elasticity in bulk plus surface diffusion on free boundary

$\Rightarrow$ large deformations of $\Gamma(t)$ = morphological instabilities

$\Rightarrow$ **crack formation and fracture**

Simplest Model

Dynamics of free surface $\Gamma(t)$ $\rightsquigarrow$ $V = -\Delta_\Gamma\big(\kappa - \varepsilon\big)$

$V =$ normal velocity

$\Delta_\Gamma =$ surface Laplacian

$\kappa =$ mean curvature

$\varepsilon =$ elastic energy density

- **First step:** Understand the purely geometric PDE

$$V = -\Delta_\Gamma \kappa \qquad (\varepsilon = 0 \text{ or given}) \qquad \rightsquigarrow \qquad \text{Surface diffusion}$$

Related work: U.F. Mayer; Falk et al.; Deckelnick/Dziuk/Elliott; Sethian; Smereka.

- **Second step:** Couple with elasticity ($\varepsilon =$ solution of a problem in the bulk)

Basic Properties for Closed Surfaces

- Volume conservation

$$\frac{d}{dt}|\Omega(t)| = \int_{\Gamma(t)} V = -\int_{\Gamma(t)} \Delta_\Gamma(\kappa+\varepsilon) = \int_{\Gamma(t)} \nabla_\Gamma(\kappa+\varepsilon)\cdot\nabla_\Gamma 1 = 0.$$

- Area decrease (for $\varepsilon = 0$)

$$\frac{d}{dt}|\Gamma(t)| = -\int_{\Gamma(t)} V\,\kappa = -\int_{\Gamma(t)} |\nabla_\Gamma \kappa|^2 \le 0.$$

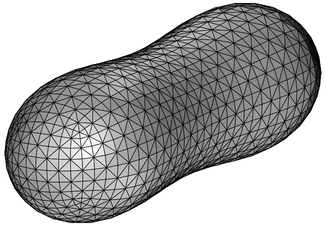
- A surface that starts as a graph may cease to be such in finite time.

- A closed embedded hypersurface may selfintersect in finite time.

Numerical Challenges

- Definition of curvature κ for a discrete surface
- Definition of $\Delta_\Gamma \kappa$: surface laplacian of a discrete variable
- 4th order problem
- Lack of maximum principle
- Volume conservation
- Area decrease
- Stability
- Error Analysis

2. General (closed) Surfaces



Issue: How to deal with $V = -\Delta_\Gamma \kappa$

Basic identity for Γ given: $\vec{\kappa} := \kappa \vec{\nu} = \Delta_\Gamma \vec{X}$

KEY IDEA: write the problem in the scalar and vector quantities

$$\vec{\kappa}, \quad \kappa, \quad V, \quad \vec{V} \qquad \Rightarrow \qquad \kappa = \vec{\kappa} \cdot \vec{\nu}, \quad \vec{V} = V \vec{\nu}$$

$$\Rightarrow \quad \boxed{\begin{aligned} \vec{\kappa} &= \Delta_\Gamma \vec{X} \\ \kappa &= \vec{\kappa} \cdot \vec{\nu} \\ V &= -\Delta_\Gamma \kappa \\ \vec{V} &= V \vec{\nu} \end{aligned}} \quad \text{(Mixed Method)}$$

Time Discretization: Semi-Implicit

Given Γ^n, describe Γ^{n+1} as the image of a mapping defined on Γ^n:

$$\Gamma^n \longrightarrow \Gamma^{n+1}, \qquad \vec{X} \longrightarrow \vec{X} + \tau \vec{V}^{\,n+1}$$

Semi-Implicit Discretization:

- Compute Δ_Γ and $\vec{\nu}$ on Γ^n $\qquad \Longrightarrow \qquad$ Take Γ^n as a fixed domain
- Take $\vec{X}$ implicitly in the curvature equation:

$$\kappa^{n+1} := \Delta_\Gamma \vec{X}^{\,n+1} = \Delta_\Gamma(\vec{X}^{\,n} + \tau \vec{V}^{\,n+1})$$

Time Discretization: Semi-Implicit

$$\vec{\kappa} = \Delta_\Gamma \vec{X}$$
$$\kappa = \vec{\kappa} \cdot \vec{\nu}$$
$$V = -\Delta_\Gamma \kappa$$
$$\vec{V} = V \vec{\nu}$$

$$\Rightarrow$$

$$\vec{\kappa}^{\,n+1} = \Delta_{\Gamma^n}(\vec{X}^{\,n} + \tau \vec{V}^{\,n+1})$$
$$\kappa^{n+1} = \vec{\kappa}^{\,n+1} \cdot \vec{\nu}^{\,n}$$
$$V^{n+1} = -\Delta_{\Gamma^n} \kappa^{n+1}$$
$$\vec{V}^{\,n+1} = V^{n+1} \vec{\nu}^{\,n}$$

$$\vec{\kappa}^{\,n+1} - \tau \Delta_{\Gamma^n} \vec{V}^{\,n+1} = \Delta_{\Gamma^n} \vec{X}^{\,n}$$
$$\kappa^{n+1} - \vec{\kappa}^{\,n+1} \cdot \vec{\nu}^{\,n} = 0$$
$$V^{n+1} + \Delta_{\Gamma^n} \kappa^{n+1} = 0$$
$$\vec{V}^{\,n+1} - V^{n+1} \vec{\nu}^{\,n} = 0$$

Variational Formulation

$$\Gamma := \Gamma^n, \qquad \mathcal{V}(\Gamma) := H^1(\Gamma), \qquad \vec{\mathcal{V}}(\Gamma) := \mathcal{V}(\Gamma)^d,$$

Seek $\boxed{\vec{V}^{n+1}, \vec{\kappa}^{n+1} \in \vec{\mathcal{V}}(\Gamma), \quad V^{n+1}, \kappa^{n+1} \in \mathcal{V}(\Gamma)}$ s.t.

$$\Big\langle \vec{\kappa}^{\,n+1}, \vec{\phi} \Big\rangle + \tau \Big\langle \nabla_\Gamma \vec{V}^{\,n+1}, \nabla_\Gamma \vec{\phi} \Big\rangle = - \Big\langle \nabla_\Gamma \vec{X}^{\,n}, \nabla_\Gamma \vec{\phi} \Big\rangle \qquad \forall \vec{\phi} \in \vec{\mathcal{V}}(\Gamma)$$

$$\big\langle \kappa^{\,n+1}, \phi \big\rangle - \big\langle \vec{\kappa}^{\,n+1} \cdot \vec{\nu}, \phi \big\rangle = 0 \qquad \forall \phi \in \mathcal{V}(\Gamma)$$

$$\big\langle V^{\,n+1}, \phi \big\rangle - \big\langle \nabla_\Gamma \kappa^{\,n+1}, \nabla_\Gamma \phi \big\rangle = 0 \qquad \forall \phi \in \mathcal{V}(\Gamma)$$

$$\Big\langle \vec{V}^{\,n+1}, \vec{\phi} \Big\rangle - \Big\langle V^{\,n+1}, \vec{\nu} \cdot \vec{\phi} \Big\rangle = 0 \qquad \forall \vec{\phi} \in \vec{\mathcal{V}}(\Gamma)$$

$$\big\langle V^{n+1}, 1 \big\rangle = \int_{\Gamma^n} V^{n+1} = 0 \qquad \Longrightarrow$$ discrete volume conservation

Finite Element Discretization

$$\Gamma = \Gamma_h^n, \qquad \mathcal{V}_h(\Gamma) \subseteq \mathcal{V}(\Gamma), \qquad \vec{\mathcal{V}}_h(\Gamma) \subseteq \vec{\mathcal{V}}(\Gamma).$$

Seek $\boxed{\vec{V}^{\,n+1}, \vec{\kappa}^{\,n+1} \in \vec{\mathcal{V}}_h(\Gamma), \quad V^{\,n+1}, \kappa^{\,n+1} \in \mathcal{V}_h(\Gamma)}$ s.t.

$$\begin{aligned}
\left\langle \vec{\kappa}^{\,n+1}, \vec{\phi}_h \right\rangle + \tau \left\langle \nabla_\Gamma \vec{V}^{\,n+1}, \nabla_\Gamma \vec{\phi}_h \right\rangle &= -\left\langle \nabla_\Gamma \vec{X}^n, \nabla_\Gamma \vec{\phi}_h \right\rangle & \forall \vec{\phi}_h \in \vec{\mathcal{V}}_h(\Gamma) \\
\left\langle \kappa^{\,n+1}, \phi_h \right\rangle - \left\langle \vec{\kappa}^{\,n+1} \cdot \vec{\nu}, \phi_h \right\rangle &= 0 & \forall \phi_h \in \mathcal{V}_h(\Gamma) \\
\left\langle V^{\,n+1}, \phi_h \right\rangle - \left\langle \nabla_\Gamma \kappa^{\,n+1}, \nabla_\Gamma \phi_h \right\rangle &= 0 & \forall \phi_h \in \mathcal{V}_h(\Gamma) \\
\left\langle \vec{V}^{\,n+1}, \vec{\phi}_h \right\rangle - \left\langle V^{\,n+1}, \vec{\nu} \cdot \vec{\phi}_h \right\rangle &= 0 & \forall \vec{\phi}_h \in \vec{\mathcal{V}}_h(\Gamma)
\end{aligned}$$

- $\left\langle V^{n+1}, 1 \right\rangle = \int_{\Gamma^n} V^{n+1} = 0 \qquad \Longrightarrow$ discrete volume conservation
- $|\Gamma^{n+1}| + \tau_n \int_{\Gamma^n} |\nabla_S \kappa^{n+1}|^2 \leq |\Gamma^n| \qquad \Longrightarrow$ area decrease + stability

Nodal Representation and Schur Complement

$$\begin{bmatrix} \tau\vec{A} & 0 & \vec{M} & 0 \\ 0 & -A & 0 & M \\ \vec{M} & 0 & 0 & -\vec{N} \\ 0 & M & -\vec{N}^T & 0 \end{bmatrix} \begin{bmatrix} \vec{\mathbf{V}} \\ \mathbf{K} \\ \vec{\mathbf{K}} \\ \mathbf{V} \end{bmatrix} = \begin{bmatrix} -\vec{A}\vec{\mathbf{X}}^n \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

Schur complement for $\mathbf{V}$:

$$Q\Big(\tau\vec{N}^T\vec{M}^{-1}\vec{A}\vec{M}^{-1}\vec{N} + MSM\Big)Q\mathbf{V} = -Q\vec{N}^T\vec{M}^{-1}\vec{A}\mathbf{X}^n$$

S is the inverse of $A_{|\ker(A)^\perp}$: $\qquad AS = I = SA \qquad$ on $\ker(A)^\perp$

Q is the $L^2(\Gamma)$ projection onto $\mathcal{X}_h(\Gamma) = \{\phi \in \mathcal{V}_h(\Gamma) : \int_\Gamma \phi = 0\}$

The system is symmetric and positive definite $\quad\Rightarrow\quad$ Solvability

(Basic) Final Procedure

1. Let $\mathfrak{T}$ be the initial triangulation of Γ with nodes $\vec{\mathbf{X}}$.

2. Build the matrices A, $\vec{A}$, M, $\vec{M}$, $\vec{N}$.

3. Solve for $\mathbf{V}$ the system

$$Q\Big(\tau \vec{N}^T \vec{M}^{-1} \vec{A} \vec{M}^{-1} \vec{N} + MSM\Big) Q\mathbf{V} = -Q\vec{N}^T \vec{M}^{-1} \vec{A}\mathbf{X}.$$

4. Solve for $\vec{\mathbf{V}}$ the system: $\qquad \vec{M}\vec{\mathbf{V}} = \vec{N}\mathbf{V}$.

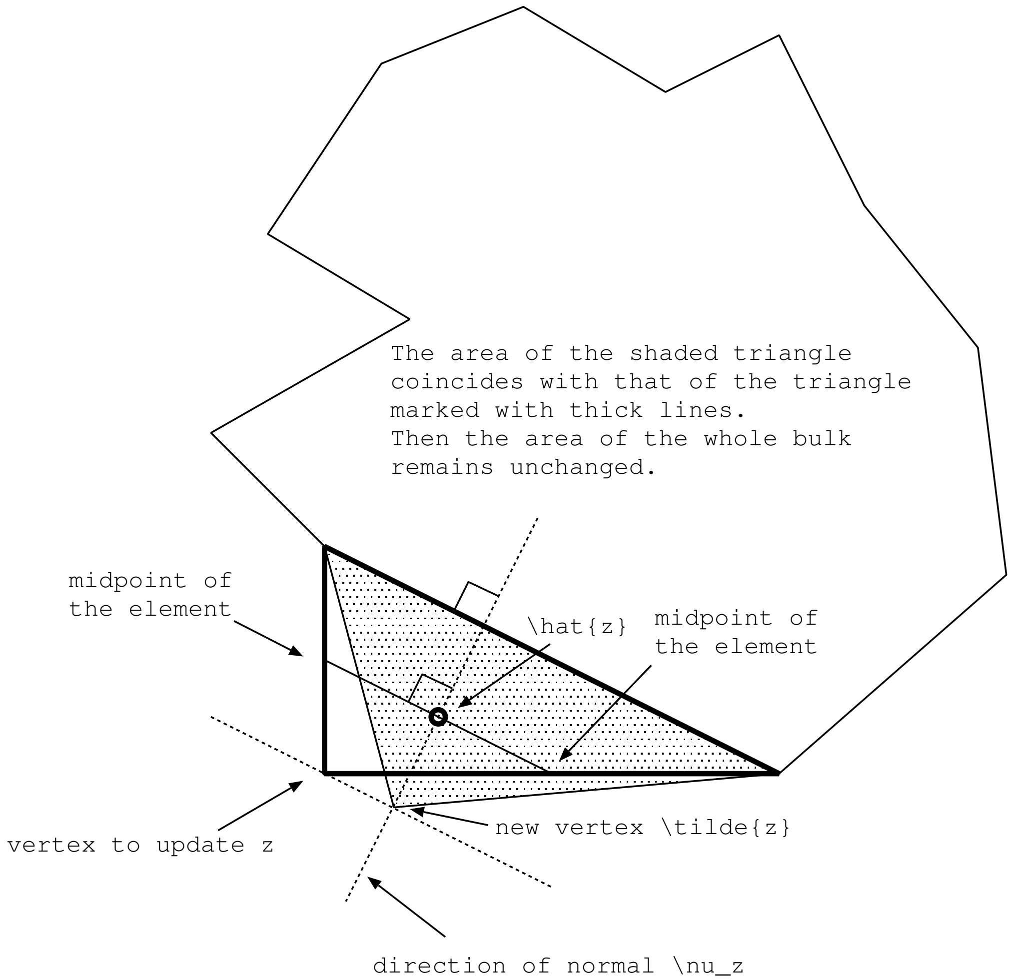
5. Update $\vec{\mathbf{X}} \leftarrow \vec{\mathbf{X}} + \tau \vec{\mathbf{V}}$.

6. Go to step 2.

Mesh Regularization

Regularization sweep

1. For each node z of the mesh do the following:
   (a) Compute a *normal* $\vec{\nu}_z$ to the node z.
   (b) Compute a weighted average $\hat{z}$ of all the vertices that belong to the star centered at z.
   (c) Consider the line that passes through $\hat{z}$ in the direction of the normal $\vec{\nu}_z$. Replace the node z by the only point belonging to this line that keeps the volume enclosed by the surface unchanged.



Timestep Control

Two goals:

1. Prevent large timesteps for which the position change of a node, is larger than the element size (to avoid crossing).

2. Allow large timesteps when the normal velocity does not exhibit large variations.

$$\text{Relative position change } = \tau|\vec{V}(z_0) - \vec{V}(z)| \approx \tau h_T |\nabla_\Gamma \vec{V}| \approx \epsilon_t h_T$$

$$\text{Compute} \quad \rho = \frac{\epsilon_t}{\max|\nabla_\Gamma V|} \quad \text{and try to use} \quad \tau \approx \rho$$

Goal: Have an accurate representation of Γ in the sense that the density of nodes should correlate with the local variation (regularity) of Γ.

We achieve this by enforcing

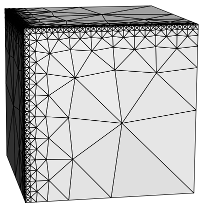
$$h_S |\angle(\vec{\nu}_1, \vec{\nu}_2)| \approx \alpha$$

on every side S of the mesh.

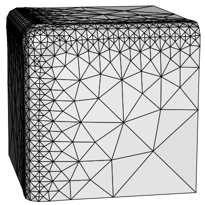
Angle Width Control

Split those elements with an angle wider than a certain α_{max}.

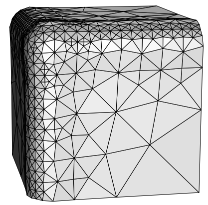
(Natural) Boundary Conditions



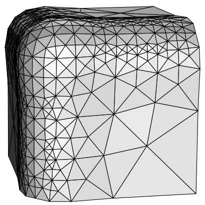
$t = 0$



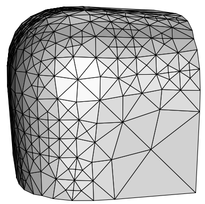
$t = 0.113 \times 10^{-5}$



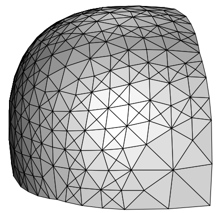
$t = 0.932 \times 10^{-5}$



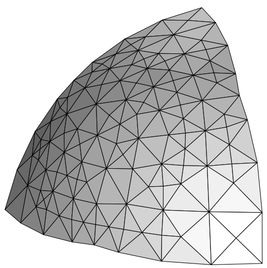
$t = 0.4300 \times 10^{-4}$



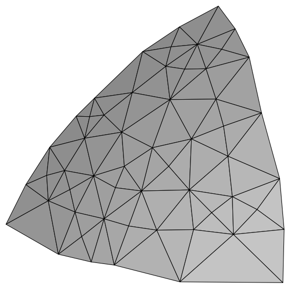
$t = 0.35039 \times 10^{-3}$



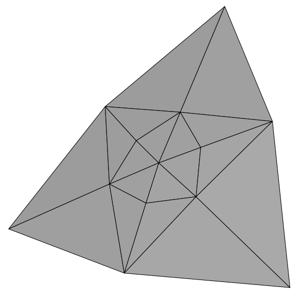
$t = 0.31211 \times 10^{-2}$



$t = 0.02545$



$t = 0.07545$

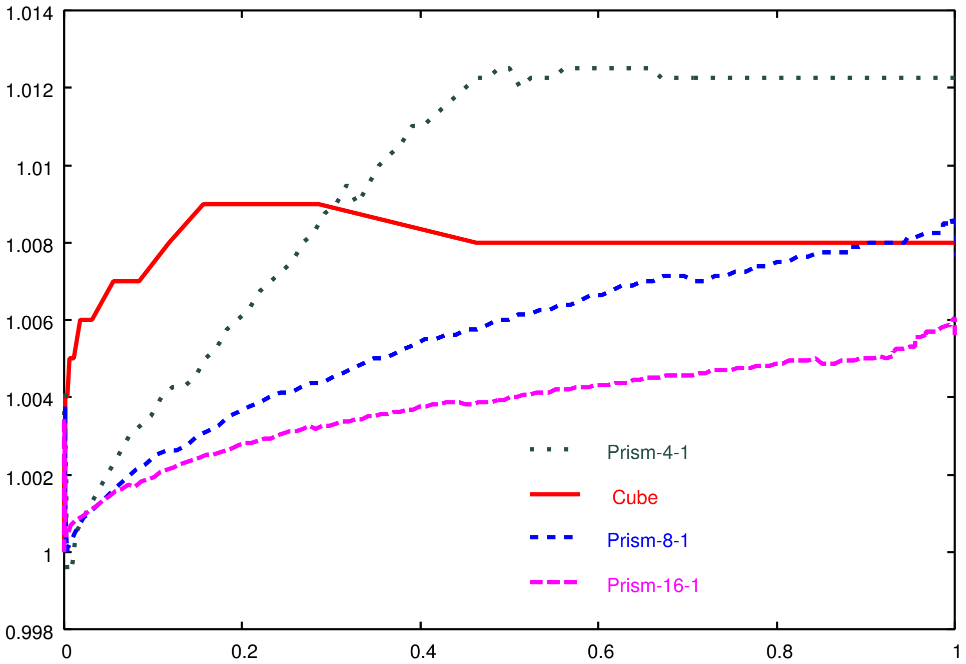


$t = 0.12545$

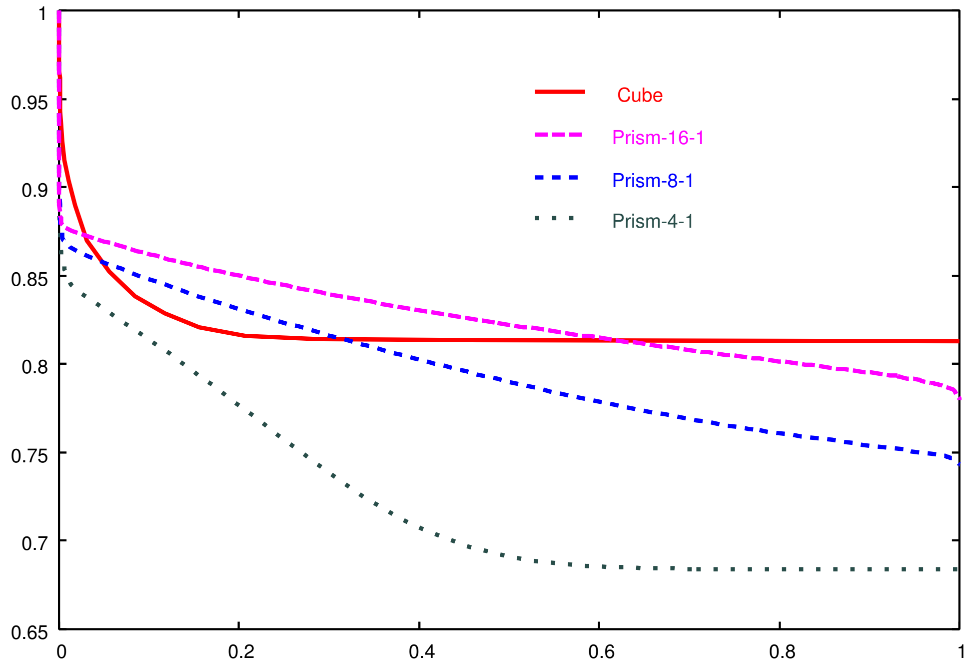
Features of Final Procedure

- Consistent approximation, no smoothing of normals etc. needed
- Only C^0 regularity for the finite element spaces
- Arbitrary polynomial degree for the finite element spaces
- Nearly volume conservative (exact volume conservation in the graph case)
- Area decrease / stability
- Time/Space Adaptation and volume conservative Mesh Regularization
- Simulations using **ALBERT** with P^1 elements (A. Schmidt and K. Siebert) and **GEOMVIEW** (Geomety Center-Minneapolis)

Volume Conservation and Area Decrease



Volume



Area

Relative volume and surface area with respect to the initial values vs. time. The computations were performed with the full adaptive algorithm.

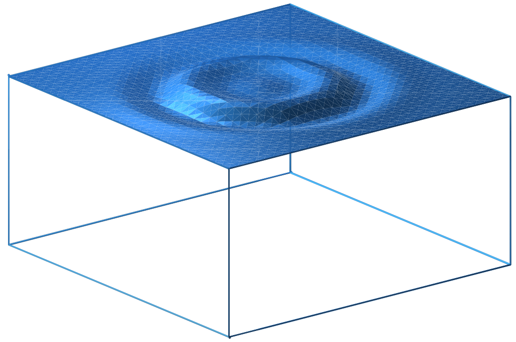
Graphs: Formulation

If $\Omega \subseteq \mathbb{R}^d \quad \Gamma(t) = \{(x, u(x,t)) | x \in \Omega\} \subset \mathbb{R}^d$, and $Q := \sqrt{1 + |\nabla u|^2}$, then

$$\nu = \frac{1}{Q}(-\nabla u, 1) \qquad \text{(outward unit normal)},$$

$$\kappa = \operatorname{div}\left(\frac{\nabla u}{Q}\right) \qquad \text{(mean curvature)},$$

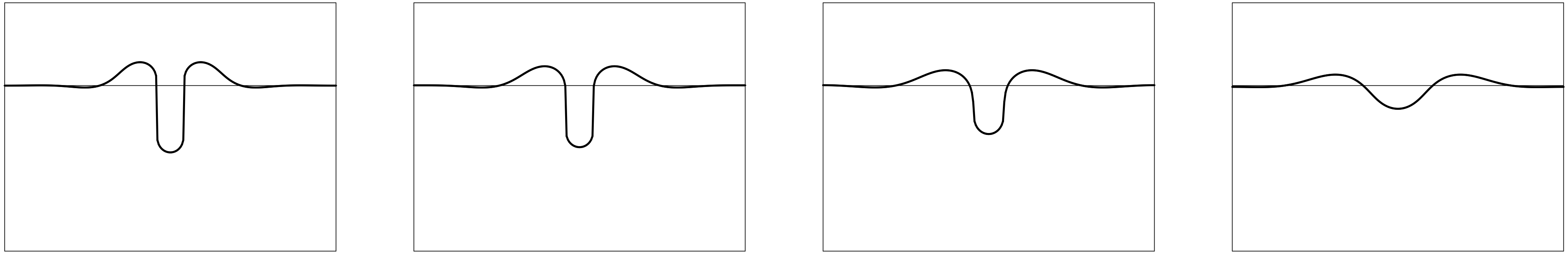
$$V = \frac{u_t}{Q}, \qquad \text{(normal velocity)}.$$



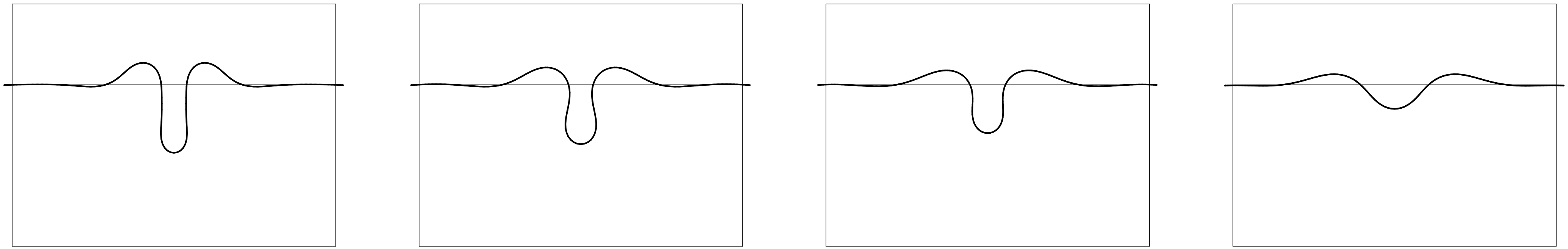
$$\boxed{V = -\Delta_\Gamma \kappa} \qquad \Rightarrow \qquad \boxed{\frac{u_t}{Q} = -\Delta_\Gamma \kappa, \quad \kappa = \nabla \cdot \left(\frac{\nabla u}{Q}\right)}$$

Anisotropic surface diffusion of graphs: Deckelnick, Dziuk, Elliott (2003)

Comparison between Graph and General Formulation AFTER MUSHROOM



$t = 4.8 \times 10^{-5}$ $t = 9.6 \times 10^{-5}$ $t = 19.2 \times 10^{-5}$ $t = 38.4 \times 10^{-5}$



$t = 4.8 \times 10^{-5}$ $t = 9.6 \times 10^{-5}$ $t = 19.2 \times 10^{-5}$ $t = 38.4 \times 10^{-5}$

$\Rightarrow$ Same time-scale and dynamics!

A Priori Error Estimate for the SPACE discretization

$$\sup_{s\in[0,T]}\left(\|e_u(s)\|^2+\int_{\Gamma_h(s)}|\nabla_\Gamma e_u(s)|^2\right)+\int_0^T\left(\|e_\kappa(s)\|^2+\int_{\Gamma_h(s)}|\nabla_\Gamma e_\kappa(s)|^2\right)ds\le C\,h^{2k}$$

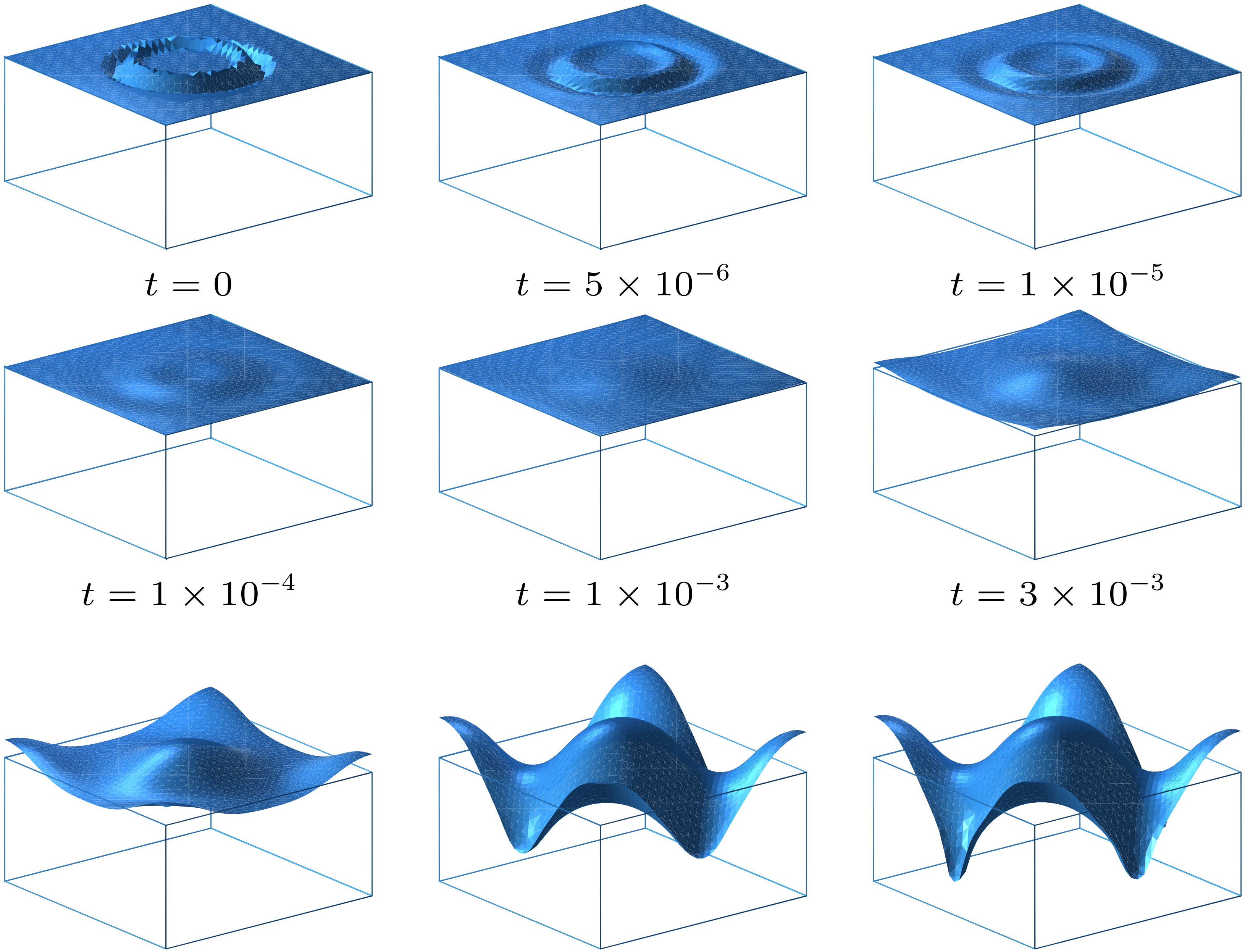
with $\quad e_u=u-u_h,\quad e_\kappa=\kappa-\kappa_h,\quad k=$ polynomial degree $\ge 1,\quad \tau=h^2.$

linears

h	err$_{\nu,0}$	EOC	err$_{u,1}$	EOC	err$_{\kappa,1}$	EOC	err$_{u,0}$	EOC	err$_{\kappa,0}$	EOC
1/2	0.5597		0.6051		18.4		0.0835		2.2214	
1/4	0.2470	1.18	0.2782	1.12	7.67	1.26	0.0254	1.71	0.4073	2.45
1/8	0.1240	0.99	0.1365	1.03	4.61	0.73	0.0082	1.63	0.1466	1.47
1/16	0.0611	1.02	0.0669	1.03	2.38	0.96	0.0022	1.93	0.0392	1.90
1/32	0.0304	1.01	0.0332	1.01	1.19	1.00	0.0005	1.98	0.0099	1.99

quadratics

h	err$_{\nu,0}$	EOC	err$_{u,1}$	EOC	err$_{\kappa,0}$	EOC	err$_{u,0}$	EOC	err$_{\kappa,0}$	EOC
1/2	0.1271		0.1376		7.38		0.0101		0.3277	
1/4	0.0419	1.60	0.0487	1.50	2.47	1.58	0.0040	1.35	0.0797	2.04
1/8	0.0102	2.03	0.0122	1.99	0.71	1.80	0.0009	2.19	0.0152	2.39
1/16	0.0025	2.01	0.0030	2.00	0.17	2.07	0.0002	2.11	0.0032	2.24



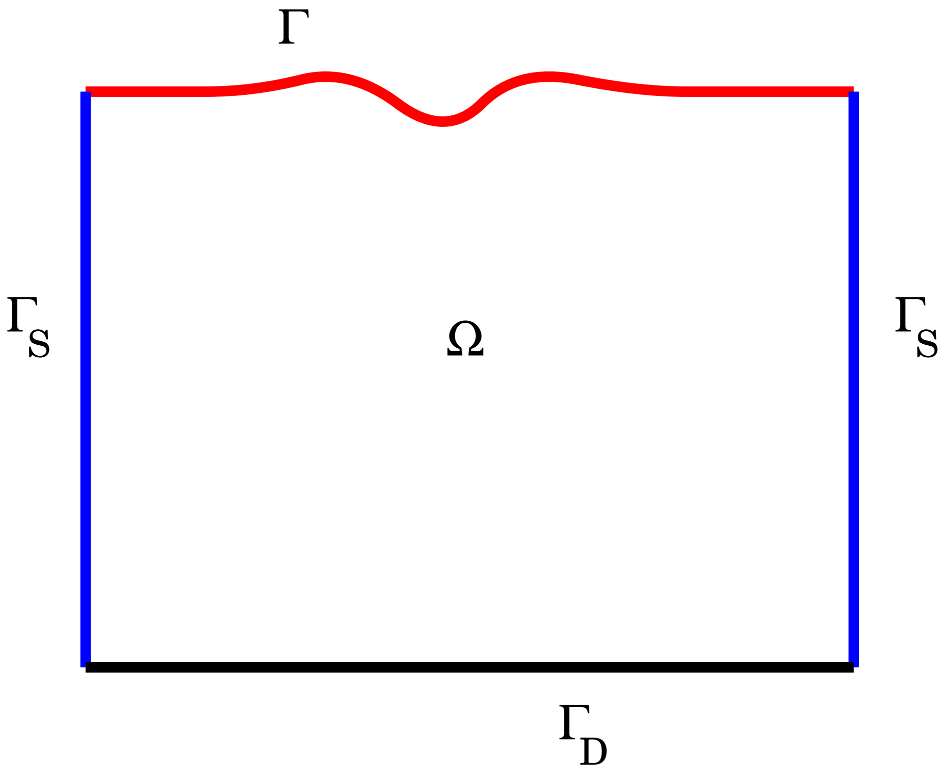
$t = 0$ $\quad$ $t = 5 \times 10^{-6}$ $\quad$ $t = 1 \times 10^{-5}$

$t = 1 \times 10^{-4}$ $\quad$ $t = 1 \times 10^{-3}$ $\quad$ $t = 3 \times 10^{-3}$

$t = 5 \times 10^{-3}$ $\quad$ $t = 7 \times 10^{-3}$ $\quad$ $t = 7.1 \times 10^{-3}$

3. Stressed Epitaxial Films

Dynamics of free surface $\Gamma(t)$ $\rightsquigarrow$ $V = -\Delta_\Gamma(\kappa - \varepsilon)$



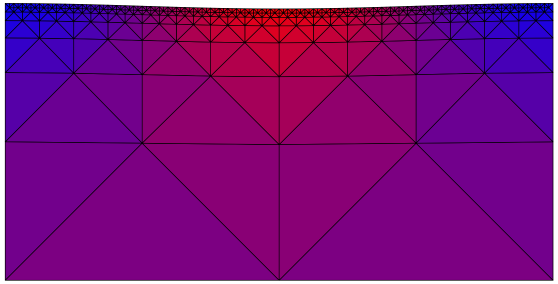
where $\varepsilon = |\nabla u|^2$, and

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \\ u = x & \text{on } \Gamma_D \\ u = x + \text{periodic} & \text{on } \Gamma_S \\ \nabla u \cdot \nu = 0 & \text{on } \Gamma \end{cases}$$

ε is *destabilizing* $\rightsquigarrow$ we take it *explicit* in the equation for the velocity.

Coupling: 1st version

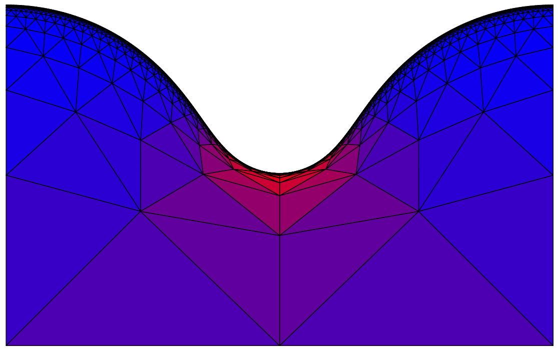
- Start with an initial mesh of the bulk, such that part of its boundary is the free surface



- Solve the equation in the bulk, and obtain ε
- Update the surface by surface diffusion

. . . after many timesteps

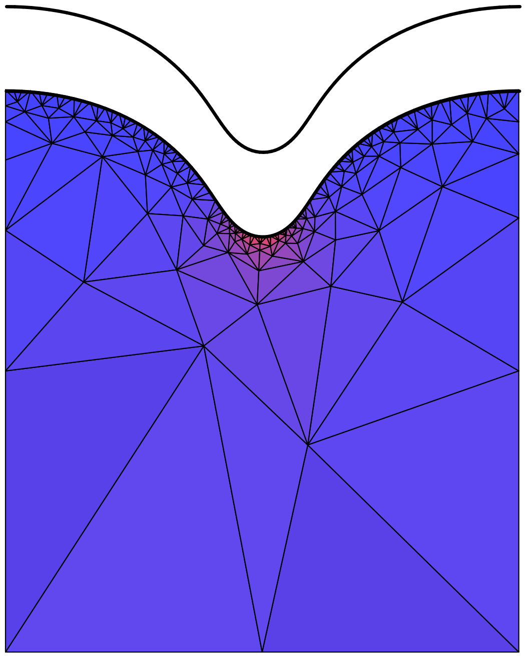
- Adjust the mesh to the new boundary



- Repeat

Large deformations and topological changes $\rightsquigarrow$ **remeshing** will be necessary

Coupling: 2nd version



- Start with a given (discrete) surface
- Generate a bulk mesh (TRIANGLE by Jonathan R. Shewchuk, Berkeley)
- Solve the equation in the bulk, and obtain ε
- Update the surface by surface diffusion
- Repeat

This method seems to work very well!!

Related Issues and Open Questions

- Error analysis for surface diffusion (without coupling)
  - graphs:
    * optimal **a priori** error estimates for a space semidiscretization: Bänsch, Morin, Nochetto
    * extension to ful discretization with anisotropy Deckelnik, Dziuk, Elliott
    * **a posteriori** error estimates: nothing done
  - parametric surfaces: nothing done

- More open problems:
  - coupled problem: nothing done
  - mesh smoothing
  - balance of accuracy between bulk and surface
  - 3d version of the coupled problem