

# Numerical Approximation of Gradient Flows for Curve Networks and Surface Clusters

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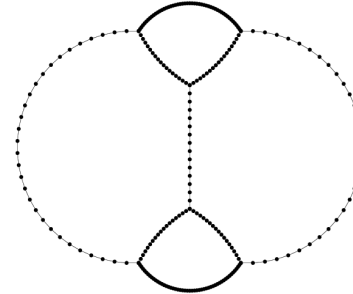
# Introduction

In this talk, we consider *Geometric Evolution Equations* for

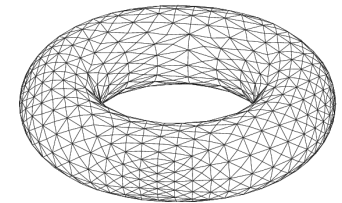
- Curves



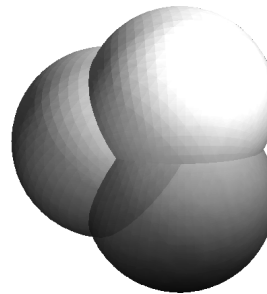
- Curve Networks



- Surfaces



- Surface Clusters



In each case, the flow will be given as a *Gradient Flow*, of second or fourth order, of the (weighted) surface area functional, e.g.

$$E(\Gamma) = |\Gamma| := \int_{\Gamma} 1 \, ds.$$

# Planar Curvature Flows

Evolving simple (embedded - no intersections) planar closed curve  $\Gamma(t)$ .

Let  $\vec{x}(\rho, t)$ ,  $\rho \in I := \mathbb{R}/\mathbb{Z}$  (periodic  $[0, 1]$ ), be a parameterization of  $\Gamma(t)$ .

Arclength  $s \Rightarrow$  unit tangent  $\vec{\tau} = \vec{x}_s = \frac{\vec{x}_\rho}{|\vec{x}_\rho|}$ .

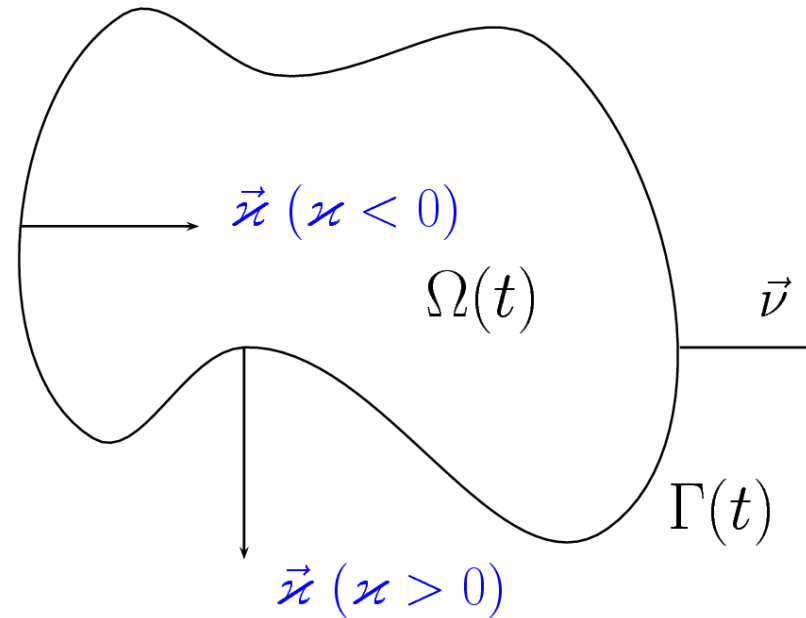
Curvature vector  $\vec{\kappa} = \vec{\tau}_s = \vec{x}_{ss} = \frac{1}{|\vec{x}_\rho|} \left( \frac{\vec{x}_\rho}{|\vec{x}_\rho|} \right)_\rho$ .

Unit normal  $\vec{\nu} \Rightarrow \vec{\kappa} \equiv \kappa \vec{\nu}$ , where  $\kappa$  is the curvature.

Let  $\Omega(t)$  be the region bounded by  $\Gamma(t)$ .

If  $\vec{\nu}$  is the outward normal, then  $\kappa$  is negative if  $\Omega(t)$  is locally convex.

## Planar Curvature Flows



For the evolution of  $\Gamma(t)$ , it suffices to prescribe its normal velocity

$$\mathcal{V} \equiv \vec{x}_t \cdot \vec{\nu}.$$

Note that tangential velocities just change the parameterization  $\vec{x}(\rho, t)$ .

Mean curvature flow:  $\mathcal{V} = \kappa$  (MC)

Surface diffusion:  $\mathcal{V} = -\kappa_{SS}$  (SD)

## Energy Decrease

These evolution equations have important applications in e.g. Materials Science, and they have the following properties.

$$\frac{d}{dt} |\Gamma(t)| = - \int_{\Gamma(t)} \mathcal{V} \kappa \, ds = \begin{cases} - \int_{\Gamma(t)} \kappa^2 \, ds \equiv -\|\mathcal{V}\|_{L^2(\Gamma(t))}^2 & \leq 0 & \text{(MC)}, \\ - \int_{\Gamma(t)} (\kappa_s)^2 \, ds \equiv -\|\mathcal{V}\|_{H^{-1}(\Gamma(t))}^2 & \leq 0 & \text{(SD)}. \end{cases}$$

(MC)  $\mathcal{V} = \kappa$  is the  $L^2$  gradient flow for the energy  $|\Gamma(t)|$ .  
(Curve-Shortening Flow).

(SD)  $\mathcal{V} = -\kappa_{ss}$  is the  $H^{-1}$  gradient flow for the energy  $|\Gamma(t)|$ .

$$\frac{d}{dt} |\Omega(t)| = \int_{\Gamma(t)} \mathcal{V} \, ds = \begin{cases} \int_{\Gamma(t)} \kappa \, ds & = -2\pi & \text{(MC)}, \\ - \int_{\Gamma(t)} \kappa_{ss} \, ds & = 0 & \text{(SD)}. \end{cases}$$

## Existing Parametric Approximations

There exist parametric finite element approximations of (MC) and (SD). They are based on the following formulations.

- Dziuk (91) (MC)  $\mathcal{V} \equiv \vec{x}_t \cdot \vec{\nu} = \kappa$

$$\vec{x}_t = \kappa \vec{\nu} \quad \text{and} \quad \vec{\kappa} = \kappa \vec{\nu} \equiv \vec{x}_{ss} \quad \Rightarrow \quad \vec{x}_t = \vec{x}_{ss} \equiv \frac{1}{|\vec{x}_\rho|} \left( \frac{\vec{x}_\rho}{|\vec{x}_\rho|} \right)_\rho.$$

- Dziuk, Kluwert, Schätzle (02) (SD)

$$\vec{x}_t = -\kappa_{ss} \vec{\nu} \equiv -\vec{\kappa}_{ss} - \frac{3}{2} (|\vec{\kappa}|^2 \vec{x}_s)_s + \frac{1}{2} |\vec{\kappa}|^2 \vec{\kappa}, \quad \vec{\kappa} = \vec{x}_{ss}.$$

- Bänsch, Morin, Nochetto (05) (SD)

$$\vec{x}_t = \vec{\mathcal{V}} = \mathcal{V} \vec{\nu}, \quad \mathcal{V} = -\kappa_{ss}, \quad \kappa = \vec{\kappa} \cdot \vec{\nu}, \quad \vec{\kappa} = \vec{x}_{ss}.$$

All these approaches have in common that they evolve the parameterization  $\vec{x}$  only in the *normal* direction.

This can lead to **coalescence** of mesh points in practice, and the need for remeshing.

## Parametric Finite Element Approximation for (MC)

Dziuk (91): a semi-implicit approximation using piecewise linear elements.

Let  $I \equiv \mathbb{R}/\mathbb{Z} = \cup_{j=1}^N J_j$ ,  $N \geq 3$ , partitioned into intervals  $J_j = [q_{j-1}, q_j]$ .

$\underline{V}^h := \{\vec{x} \in C(I, \mathbb{R}^2) : \vec{x}|_{J_j} \text{ is linear } \forall j = 1 \rightarrow N\} =: [V^h]^2 \subset H^1(I, \mathbb{R}^2)$

$0 = t_0 < t_1 < \dots < t_{M-1} < t_M = T$  partitioning of  $[0, T]$ ,  $\tau_m := t_{m+1} - t_m$ ,  $m = 0 \rightarrow M - 1$ .

$\vec{X}^m \in \underline{V}^h$  approximating  $\vec{x}(\cdot, t_m) \Rightarrow$  a polygonal approximation,  $\Gamma^m$ , to  $\Gamma(t_m)$ .

Find  $\vec{X}^{m+1} \in \underline{V}^h$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \vec{\eta} \right\rangle_m^h = - \langle \vec{X}_s^{m+1}, \vec{\eta}_s \rangle_m \equiv - \int_I \frac{\vec{X}_\rho^{m+1}}{|\vec{X}_\rho^m|} \cdot \frac{\vec{\eta}_\rho}{|\vec{X}_\rho^m|} |\vec{X}_\rho^m| \, d\rho \quad \forall \vec{\eta} \in \underline{V}^h;$$

where

$$\langle f, g \rangle_m := \int_{\Gamma^m} f \cdot g \, ds = \int_I f \cdot g |\vec{X}_\rho^m| \, d\rho$$

with  $\langle \cdot, \cdot \rangle_m^h$  the mass lumped inner product.

Linear tridiagonal periodic system for  $\{\vec{X}^{m+1}(q_j)\}_{j=0}^N$ .

Error analysis for semidiscrete approximation (continuous in time)

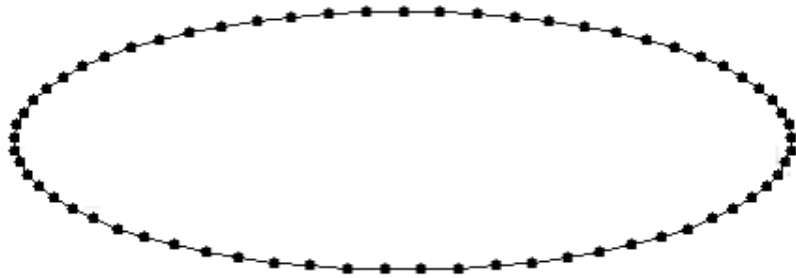
Dziuk (94).

# Coalescence

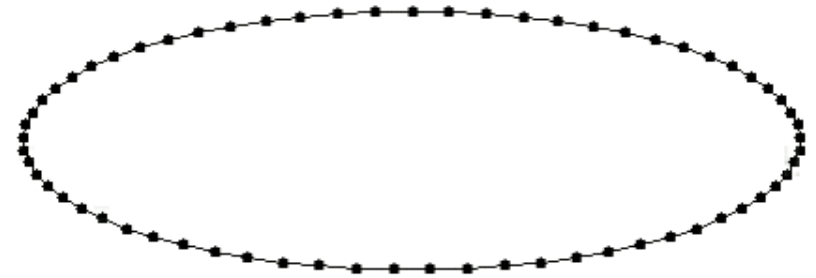
(SD)  $\vec{x}(\cdot, 0)$  is a 3 : 1 ellipse,

$$N = 64, \tau = 10^{-6}, T = 3 \times 10^{-4}.$$

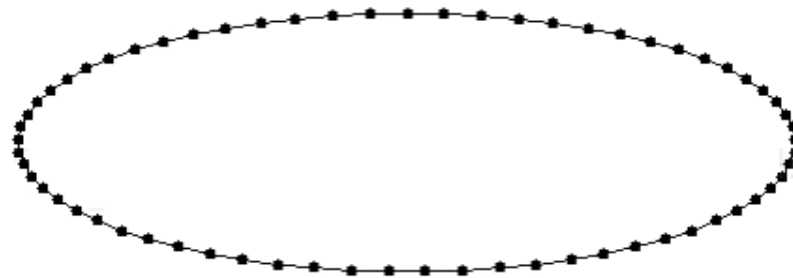
Recall (SD)  $\Rightarrow |\Gamma(t)|$  decreases, whilst  $|\Omega(t)| = |\Omega(0)|$ .



DKS



BMN



BGN

## New Formulation

We use the following formulation of (MC) and (SD).

$$\vec{x}_t \cdot \vec{\nu} = \begin{cases} \kappa \\ -\kappa_{SS} \end{cases}, \quad \kappa \vec{\nu} = \vec{x}_{SS}.$$

$$(MC) \quad \Rightarrow \quad (\vec{x}_t \cdot \vec{\nu}) \vec{\nu} = \vec{x}_{SS}.$$

As the tangential component  $\vec{x}_t \cdot \vec{\tau}$  of  $\vec{x}_t$  is not prescribed,  $\exists$  a whole family of solutions  $\vec{x}$ ; even though the evolution of  $\Gamma$  is uniquely determined.

Find  $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}^h \times V^h$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{\nu}^m \right\rangle_m^h - \begin{cases} \langle \kappa^{m+1}, \chi \rangle_m^h \\ \langle \kappa_s^{m+1}, \chi_s \rangle_m \end{cases} = 0 \quad \forall \chi \in V^h,$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_m^h + \langle \vec{X}_s^{m+1}, \vec{\eta}_s \rangle_m = 0 \quad \forall \vec{\eta} \in \underline{V}^h.$$

Linear system for  $\{\vec{X}^{m+1}(q_j), \kappa^{m+1}(q_j)\}_{j=0}^N$ .

(MC)  $\Rightarrow$  Find  $\vec{X}^{m+1} \in \underline{V}^h$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m} \cdot \vec{\omega}^m, \vec{\eta} \cdot \vec{\omega}^m \right\rangle_m^h + \langle \vec{X}_s^{m+1}, \vec{\eta}_s \rangle_m = 0 \quad \forall \vec{\eta} \in \underline{V}^h.$$

## Existence and Stability

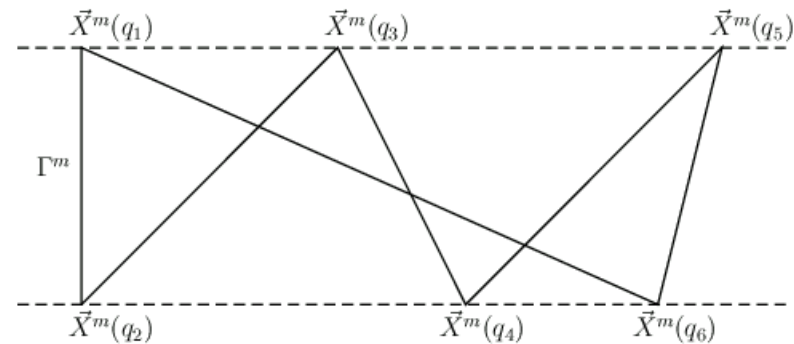
A very mild assumption on  $\vec{X}^m$  needed. Let  $\vec{\nu}_{j-\frac{1}{2}}^m := -\frac{[\vec{X}^m(q_j) - \vec{X}^m(q_{j-1})]^\perp}{|\vec{X}^m(q_j) - \vec{X}^m(q_{j-1})|}$ .

(A) Let  $|\vec{X}_\rho^m| > 0$  for a.a.  $\rho \in I$ . For  $j = 1 \rightarrow N$ , introduce the vertex normal (average of neighbouring edge unit normals weighted by edge length)

$$\begin{aligned} \vec{\omega}_j^m &:= \frac{|\vec{X}^m(q_j) - \vec{X}^m(q_{j-1})| \vec{\nu}_{j-\frac{1}{2}}^m + |\vec{X}^m(q_{j+1}) - \vec{X}^m(q_j)| \vec{\nu}_{j+\frac{1}{2}}^m}{|\vec{X}^m(q_j) - \vec{X}^m(q_{j-1})| + |\vec{X}^m(q_{j+1}) - \vec{X}^m(q_j)|} \\ &= -\frac{1}{\alpha} [\vec{X}^m(q_{j+1}) - \vec{X}^m(q_{j-1})]^\perp, \quad \text{where } \cdot^\perp \text{ is clockwise rotation by } \frac{\pi}{2}. \end{aligned}$$

Then we further assume that  $\dim \text{span}\{\vec{\omega}_j^m\}_{j=1}^N = 2$ .

Always true if no intersections.



A pathological example, (A) violated.

## THEOREM

Let (A) hold. Then  $\exists!$  solution  $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}^h \times V^h$ .  
Moreover, for  $k = 1 \rightarrow M$  it holds that

$$|\Gamma^k| + \sum_{m=0}^{k-1} \tau_m \begin{cases} \langle \kappa^{m+1}, \kappa^{m+1} \rangle_m^h \\ \langle \kappa_s^{m+1}, \kappa_s^{m+1} \rangle_m \end{cases} \leq |\Gamma^0|.$$

# Planar Equidistribution of Mesh Points

Continuous in time semidiscrete scheme:

$$\langle \vec{X}_t, \chi \vec{\nu}^h \rangle^h - \begin{cases} \langle \kappa, \chi \rangle^h \\ \langle \kappa_s, \chi_s \rangle \end{cases} = 0 \quad \forall \chi \in V^h,$$

$$\langle \kappa \vec{\nu}^h, \vec{\eta} \rangle^h + \langle \vec{X}_s, \vec{\eta}_s \rangle = 0 \quad \forall \vec{\eta} \in \underline{V}^h.$$

(a) **Area conservation** for (SD):  $0 = \langle \vec{X}_t, \vec{\nu}^h \rangle^h = \int_{\Gamma^h} \vec{X}_t \cdot \vec{\nu}^h \, ds = \frac{d}{dt} |\Omega^h(t)|.$

(b) **Equidistribution of mesh points** for  $\vec{X}(t)$ ,  
where  $\vec{X}(t)$  is not locally parallel, for any  $t > 0$ ;

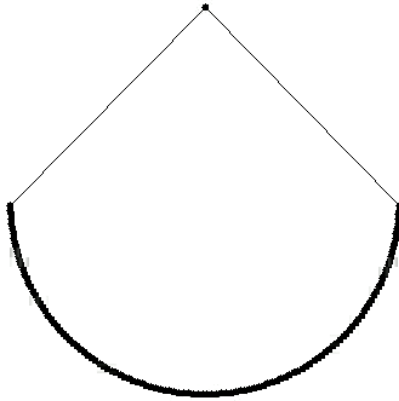
i.e. for  $j = 1 \rightarrow N$  and for any  $t > 0$

either  $|\vec{X}(q_j, t) - \vec{X}(q_{j-1}, t)| = |\vec{X}(q_{j+1}, t) - \vec{X}(q_j, t)|$

or  $[\vec{X}(q_j, t) - \vec{X}(q_{j-1}, t)] \parallel [\vec{X}(q_{j+1}, t) - \vec{X}(q_j, t)].$

## Planar Tangential Motion

Although (b) cannot be shown for the fully discrete scheme, (eventual) equidistribution is observed in practice.



(SD)

$$N = 128, \tau = 10^{-7}, T = 2 \times 10^{-5}.$$

There do exist schemes with tangential motion.

Note Dziuk scheme for (MC) based on

$$\vec{x}_t = \vec{x}_{ss} \equiv \frac{1}{|\vec{x}_\rho|} \left( \frac{\vec{x}_\rho}{|\vec{x}_\rho|} \right)_\rho \equiv \frac{1}{|\vec{x}_\rho|^2} (\vec{x}_{\rho\rho} - [\vec{x}_{\rho\rho} \cdot \vec{\tau}] \vec{\tau}) \quad \text{where} \quad \vec{\tau} := \frac{\vec{x}_\rho}{|\vec{x}_\rho|}$$

has no tangential motion, whereas the reparameterization  $|\vec{x}_\rho|^2 \vec{x}_t = \vec{x}_{\rho\rho}$  does. Error analysis for a semidiscrete approximation Deckelnick, Dziuk (95).

Strain (89) for (MC) uses formulation that intrinsically maintains  $|\vec{x}_\rho(\rho, t)| = |\Gamma(t)|$ . Extended by Hou, Lowengrub, Shelley (94) to e.g.  $|\vec{x}_\rho(\rho, t)| = \alpha(\rho) |\Gamma(t)|$ .

Mikula, Ševčovič (01) impose explicitly non-local tangential motion for the equidistribution of mesh points for (MC). See (05) for (SD).

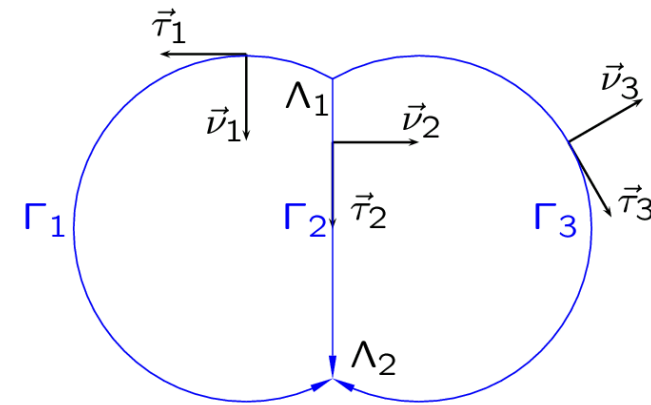
## Curve Networks

Geometric evolution equations for curve networks, e.g. three curves  $\Gamma := (\Gamma_1, \Gamma_2, \Gamma_3)$  meeting at two triple junction points  $\Lambda_1$  and  $\Lambda_2$ .

$$\text{On } \Gamma_i: \quad \mathcal{V}_i := (\vec{x}_i)_t \cdot \vec{\nu}_i = \begin{cases} \kappa_i & \text{(MC)} \\ -(\kappa_i)_{ss} & \text{(SD)} \end{cases}$$

$$\text{At } \Lambda_j: \quad \begin{aligned} \text{(a)} \quad & \vec{x}_1 = \vec{x}_2 = \vec{x}_3 \quad \text{(attachment)} \\ \text{(b)} \quad & \vec{\tau}_1 + \vec{\tau}_2 + \vec{\tau}_3 = \vec{0} \quad \text{(Young's Law)} \end{aligned}$$

$$\begin{aligned} + \text{ for (SD):} \quad \text{(c)} \quad & \kappa_1 + \kappa_2 + \kappa_3 = 0 \quad \text{(chem. pot. cont.)} \\ \text{(d)} \quad & (\kappa_1)_s = (\kappa_2)_s = (\kappa_3)_s \quad \text{(flux balance)} \end{aligned}$$



(MC) : • Evolution of phase boundaries in Materials Science, e.g. grain growth. See e.g. Bronsard, Reitich (93).  
 • Existing direct approaches  
 Bronsard, Wetton (95), Thaddey (99), Neubauer (02).

(SD) : • Formulation due to Garcke, Novick-Cohen (00).  
 • Models e.g. the evolution of soap bubbles.  
 • **No previous work on direct numerical approximation.**

## Energy Decrease

As before, these evolution equations arise as gradient flows for the total surface area. Let  $E(\Gamma) = |\Gamma| := \sum_{i=1}^3 \int_{\Gamma_i} 1 \, ds$ . Then

$$\frac{d}{dt} |\Gamma| = - \sum_{i=1}^3 \int_{\Gamma_i} \mathcal{V}_i \kappa_i \, ds = \begin{cases} - \sum_{i=1}^3 \int_{\Gamma_i} \kappa_i^2 \, ds \equiv -\|\mathcal{V}\|_{L^2(\Gamma)}^2 & \leq 0 & \text{(MC)}, \\ - \sum_{i=1}^3 \int_{\Gamma_i} ([\kappa_i]_s)^2 \, ds \equiv -\|\mathcal{V}\|_{H^{-1}(\Gamma)}^2 & \leq 0 & \text{(SD)}. \end{cases}$$

(MC)  $\mathcal{V}_i = \kappa_i$ ,  $i = 1 \rightarrow 3$ , and (a,b) is the  $L^2$  gradient flow for  $|\Gamma|$ .

(SD)  $\mathcal{V}_i = -(\kappa_i)_{ss}$ ,  $i = 1 \rightarrow 3$ , and (a-d) is the  $H^{-1}$  gradient flow.

For (SD), the enclosed areas are conserved. E.g. for the area  $a_{12}(t)$  of the phase enclosed by  $\Gamma_1$  and  $\Gamma_2$ , it holds that

$$\frac{d}{dt} a_{12}(t) = \int_{\Gamma_2} \mathcal{V}_2 \, ds - \int_{\Gamma_1} \mathcal{V}_1 \, ds = - \int_{\Gamma_2} (\kappa_2)_{ss} \, ds + \int_{\Gamma_1} (\kappa_1)_{ss} \, ds = 0,$$

## Variational Formulation of (SD) for Curve Networks

Let  $I := [0, 1]$  and set

$$\underline{V} := \{\vec{x} \equiv (\vec{x}_1, \vec{x}_2, \vec{x}_3) \in [C(I, \mathbb{R}^2)]^3 : \vec{x}_1 = \vec{x}_2 = \vec{x}_3 \text{ on } \partial I\}$$

$$\text{and } W := \{\chi \equiv (\chi_1, \chi_2, \chi_3) \in [C(I, \mathbb{R})]^3 : \chi_1 + \chi_2 + \chi_3 = 0 \text{ on } \partial I\}.$$

Using the following formulation of (SD)

$$(i) \quad (\vec{x}_i)_t \cdot \vec{\nu}_i = -(\kappa_i)_{ss}, \quad (ii) \quad \kappa_i \vec{\nu}_i = (\vec{x}_i)_{ss},$$

and multiplying (ii) with  $\vec{\eta} \in \underline{V} \cap [H^1(I, \mathbb{R}^2)]^3$  gives for the right hand side

$$\begin{aligned} \sum_{i=1}^3 \int_{\Gamma_i} (\vec{x}_i)_{ss} \cdot \vec{\eta}_i \, ds &= - \sum_{i=1}^3 \int_{\Gamma_i} (\vec{x}_i)_s \cdot (\vec{\eta}_i)_s \, ds + \sum_{i=1}^3 \int_{\partial\Gamma_i} (\vec{x}_i)_s \cdot \vec{\eta}_i \, ds \\ &= - \sum_{i=1}^3 \int_{\Gamma_i} (\vec{x}_i)_s \cdot (\vec{\eta}_i)_s \, ds + \sum_{j=1}^2 (-1)^j \vec{\eta}(\Lambda_j) \cdot \sum_{i=1}^3 (\vec{\tau}_i|_{\Lambda_j}). \end{aligned}$$

$\Rightarrow$  Weakly enforce  $\vec{\tau}_1 + \vec{\tau}_2 + \vec{\tau}_3 = \vec{0}$  at  $\Lambda_j$ , while  $\vec{x}_1 = \vec{x}_2 = \vec{x}_3$  holds via  $\vec{x} \in \underline{V}$ .

Similarly, testing (i) with  $\chi \in W \Rightarrow$  weak enforcing of  $(\kappa_1)_s = (\kappa_2)_s = (\kappa_3)_s$ .

## Parametric Finite Element Approximation

Introduce piecewise linears  $\underline{V}^h \subset \underline{V}$ ,  $W^h \subset W$  and  $W_{\mathcal{M}}^h \subset [C(I, \mathbb{R})]^3$ .

Find  $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}^h \times \begin{cases} W_{\mathcal{M}}^h \\ W^h \end{cases}$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{v}^m \right\rangle_m^h - \begin{cases} \langle \kappa^{m+1}, \chi \rangle_m^h \\ \langle \kappa_s^{m+1}, \chi_s \rangle_m \end{cases} = 0 \quad \forall \chi \in \begin{cases} W_{\mathcal{M}}^h \\ W^h \end{cases},$$

$$\langle \kappa^{m+1} \vec{v}^m, \vec{\eta} \rangle_m^h + \langle \vec{X}_s^{m+1}, \vec{\eta}_s \rangle_m = 0 \quad \forall \vec{\eta} \in \underline{V}^h;$$

where

$$\langle f, g \rangle_m := \int_{\Gamma^m} f \cdot g \, ds := \sum_{i=1}^3 \int_{\Gamma_i^m} f_i \cdot g_i \, ds$$

with  $\langle \cdot, \cdot \rangle_m^h$  the mass lumped inner product.

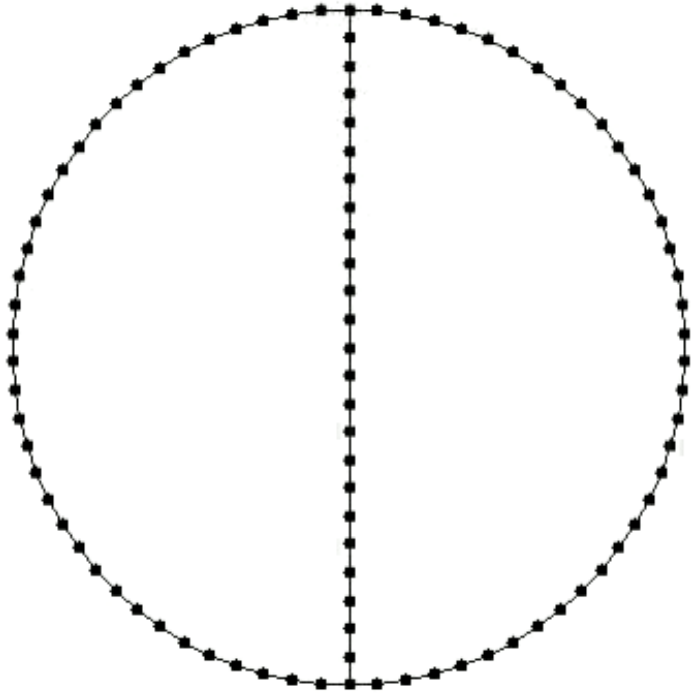
Linear system for  $\{\vec{X}^{m+1}, \kappa^{m+1}\}$ .

Existence, uniqueness and stability. Area conservation and equidistribution of mesh points (separate on each  $\Gamma_i^m$ ) as before.

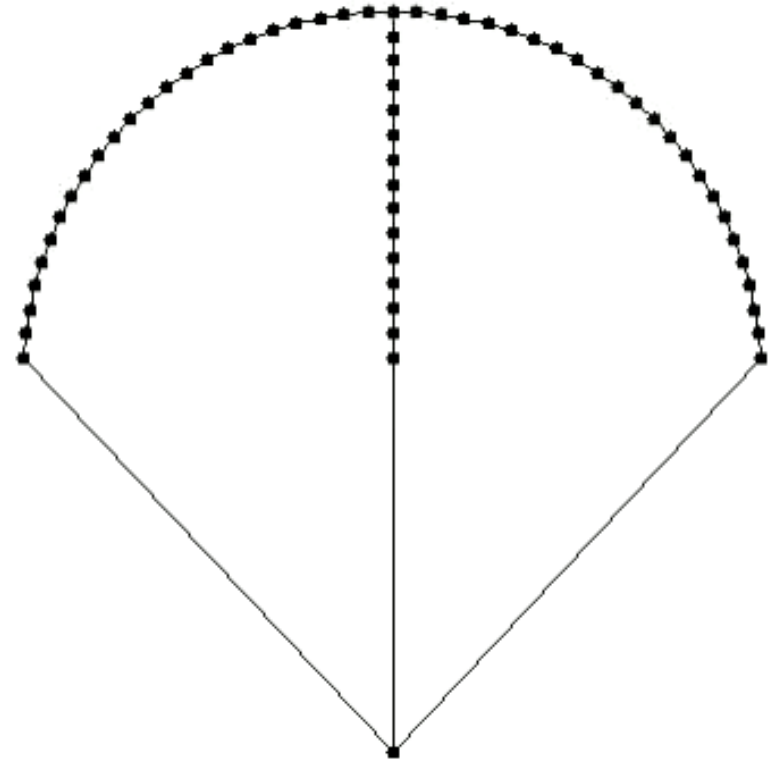
# Tangential Movement

Standard double bubble

$$N = 100, \tau = 10^{-3}, T = 0.2.$$



$$N = 64, \tau = 10^{-3}, T = 0.2.$$

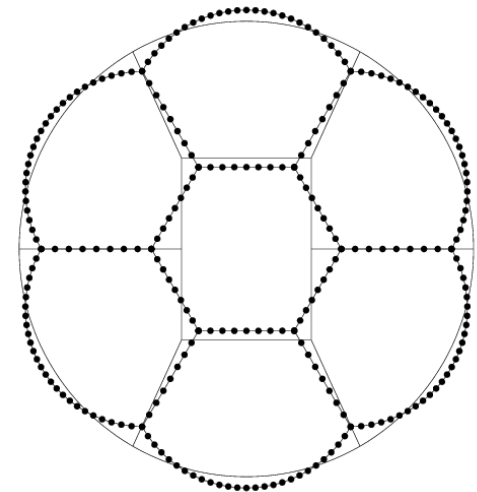
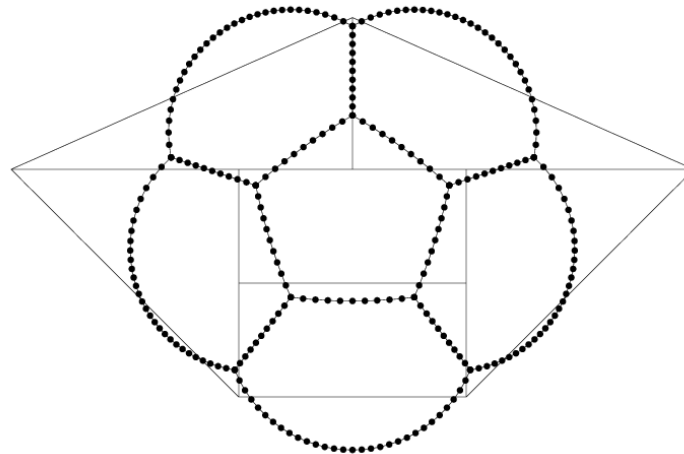
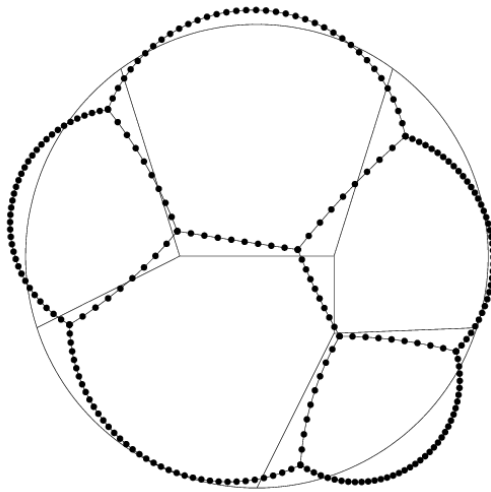
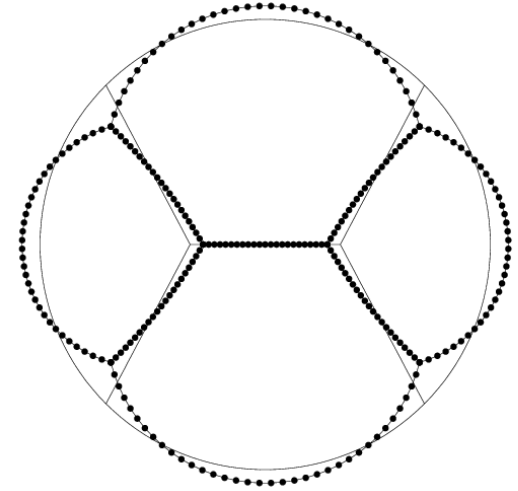
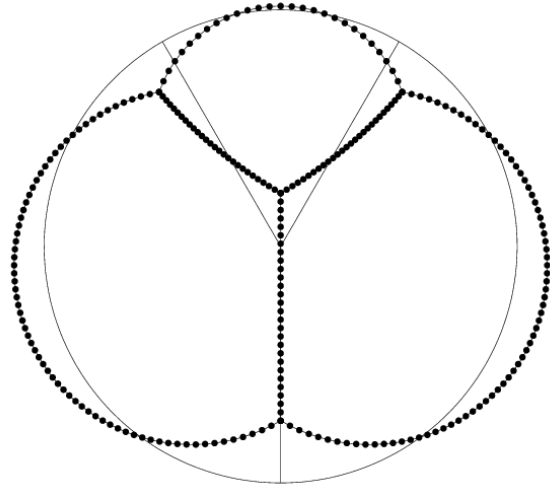
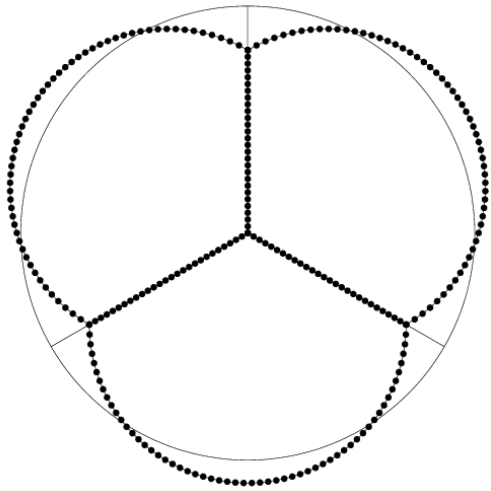


Surface diffusion:

Areas maintained, whilst the sum of the curve lengths decreases.

# Curve Networks

Surface diffusion on more complicated networks



## Curves in $\mathbb{R}^d$ , $d \geq 3$ , and Curves on Manifolds

Our scheme also easily generalises to curves in  $\mathbb{R}^d$ ,  $d \geq 3$ , and curves on manifolds.

E.g. let  $\mathcal{M} = \{\vec{z} \in \mathbb{R}^3 : F(\vec{z}) = 0\}$  be a 2-dimensional manifold  $\subset \mathbb{R}^3$ .

For a closed curve  $\Gamma$  on  $\mathcal{M}$  with a given parameterization  $\vec{x}(\rho, t) \in \mathcal{M}$ , mean curvature flow on the  $\mathcal{M}$ , also called geodesic curvature flow, is :

$$\vec{x}_t \cdot \vec{\nu}_{\mathcal{M}} = \kappa_{\mathcal{M}}, \quad \kappa_{\mathcal{M}} \vec{\nu}_{\mathcal{M}} + \kappa_F \vec{\nu}_F = \vec{x}_{ss},$$

where  $\vec{\nu}_F$  is the outward unit normal of  $\mathcal{M}$  and  $\vec{\nu}_{\mathcal{M}} := \vec{x}_s \times \vec{\nu}_F(\vec{x})$ .

Find  $\{\vec{X}^{m+1}, \kappa_{\mathcal{M}}^{m+1}, \kappa_F^{m+1}\} \in \underline{V}^h \times V^h \times V^h$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{\omega}_{\mathcal{M}}^m \right\rangle_m^h - \langle \kappa_{\mathcal{M}}^{m+1}, \chi \rangle_m^h = 0 \quad \forall \chi \in V^h,$$

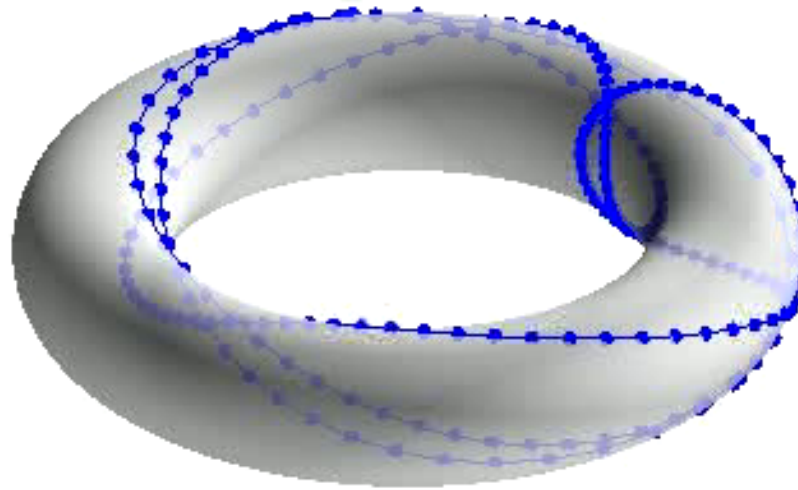
$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{\omega}_F^m \right\rangle_m^h = 0 \quad \forall \chi \in V^h,$$

$$\langle \kappa_{\mathcal{M}}^{m+1} \vec{\omega}_{\mathcal{M}}^m, \vec{\eta} \rangle_m^h + \langle \kappa_F^{m+1} \vec{\omega}_F^m, \vec{\eta} \rangle_m^h + \langle \vec{X}_s^{m+1}, \vec{\eta}_s \rangle_m = 0 \quad \forall \vec{\eta} \in \underline{V}^h.$$

Linear system. Existence, uniqueness, stability and equidistribution property.

## Numerical Result

Geodesic curvature flow on a torus of radii  $R = 4$  and  $r = 1$ .



$$|\Gamma(0)| = 86.3, \quad |\Gamma(T)| = 39.3. \quad (N = 200, \tau = 2 \times 10^{-3}, T = 250)$$

## Geometric Evolution Equations of Surfaces in $\mathbb{R}^3$

Let  $\{\Gamma(t)\}_t$  be a smooth family of compact orientable hypersurfaces without boundary in  $\mathbb{R}^3$ . Let  $\Omega(t)$  be the region bounded by  $\Gamma(t)$ .

Let  $\vec{x}(t) : \mathcal{M} \rightarrow \Gamma(t)$  be a parameterization of  $\Gamma(t)$ , where  $\mathcal{M} \subset \mathbb{R}^3$  is a suitable reference manifold.

Let  $\vec{\nu}(t) : \Gamma(t) \rightarrow \mathbb{R}^3$  be a unit normal to  $\Gamma(t)$ .

For the evolution of  $\Gamma$  it suffices to prescribe the normal velocity  $\mathcal{V} \equiv \vec{x}_t \cdot \vec{\nu}$ ,

$$\text{e.g.} \quad (\text{MC}) \quad \mathcal{V} = \kappa, \quad \text{or} \quad (\text{SD}) \quad \mathcal{V} = -\Delta_s \kappa.$$

Here  $\kappa$  is the “mean” curvature (sum of principal curvatures) of  $\Gamma$ , so that

$$\vec{\kappa} := \kappa \vec{\nu} = \Delta_s \vec{x} \quad (\vec{x}_{ss} \text{ for curves}),$$

and  $\Delta_s \equiv \nabla_s \cdot \nabla_s$  the Laplace–Beltrami operator (surface Laplacian) on  $\Gamma(t)$ .

Note that  $\kappa$  is positive if  $\Gamma$  is curved in the direction of  $\vec{\nu}$ .

$$(\text{MC}), (\text{SD}) \Rightarrow \frac{d}{dt} |\Gamma(t)| \leq 0, \quad (\text{SD}) \Rightarrow \frac{d}{dt} |\Omega(t)| = 0.$$

## Finite Elements on Surfaces

Following Dziuk (91), we now introduce piecewise linear finite elements on surfaces.

Let  $\Gamma \subset \mathbb{R}^d$  be a given smooth hypersurface.

Let  $\Gamma^h$  be a *polyhedral surface* approximating  $\Gamma$ , i.e. a union of non-degenerate  $(d-1)$ -dimensional simplices with no hanging vertices and with vertices on  $\Gamma$ .

This defines a  $(d-1)$ -dimensional triangulation  $\mathcal{T}^h$  in  $\mathbb{R}^d$  :

$$\Gamma^h = \bigcup_{\sigma \in \mathcal{T}^h} \bar{\sigma}$$

On this discrete surface, we define finite element spaces by

$$V^h(\Gamma^h) := \{\chi \in C(\Gamma^h, \mathbb{R}) : \chi|_{\sigma} \text{ is linear affine on each } \sigma \in \mathcal{T}^h\}$$

and

$$\underline{V}^h(\Gamma^h) := [V^h(\Gamma^h)]^d.$$

## Parametric Finite Element Approximation

Let  $0 = t_0 < t_1 < \dots < t_{M-1} < t_M = T$  be a partitioning of  $[0, T]$ ,  
 $\tau_m := t_{m+1} - t_m$ ,  $m = 0 \rightarrow M - 1$ .

For  $m = 0$ , choose a polyhedral surface  $\Gamma^0$  approximating the initial  $\Gamma(0)$ .

For  $m \geq 0$ , let  $\vec{X}^m \in \underline{V}^h(\Gamma^m)$  be the identity function on  $\Gamma^m$ .

$(\mathcal{P}^h)$  Find  $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}^h(\Gamma^m) \times V^h(\Gamma^m)$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{\nu}^m \right\rangle_m - \begin{cases} \langle \kappa^{m+1}, \chi \rangle_m^h \\ \langle \nabla_s \kappa^{m+1}, \nabla_s \chi \rangle_m \end{cases} = 0 \quad \forall \chi \in V^h(\Gamma^m),$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_m^h + \langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \rangle_m = 0 \quad \forall \vec{\eta} \in \underline{V}^h(\Gamma^m);$$

and set  $\Gamma^{m+1} := \vec{X}^{m+1}(\Gamma^m)$ .

Linear system for  $\{\vec{X}^{m+1}, \kappa^{m+1}\}$ .

Here

$$\langle f, g \rangle_m := \int_{\Gamma^m} f \cdot g \, ds$$

with  $\langle \cdot, \cdot \rangle_m^h$  the mass lumped inner product.

# Properties of the Scheme

## 1. Existence, Uniqueness

Under very mild assumptions on  $\Gamma^m$ , there exists a unique solution  $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}^h(\Gamma^m) \times V^h(\Gamma^m)$  to  $(\mathcal{P}^h)$ .

## 2. Stability

For all  $k = 1 \rightarrow M$  it holds that

$$|\Gamma^k| + \sum_{m=0}^{k-1} \tau_m \begin{cases} \langle \kappa^{m+1}, \kappa^{m+1} \rangle_m^h \\ \langle \nabla_s \kappa^{m+1}, \nabla_s \kappa^{m+1} \rangle_m \end{cases} \leq |\Gamma^0|.$$

## 3. Volume conservation

For (SD) for a continuous in time semidiscrete scheme.

## 4. Good distribution of mesh points

for a continuous in time semidiscrete scheme.

- For  $d = 2$ , equidistribution for  $\Gamma^h(t)$ , where  $\Gamma^h(t)$  not locally parallel.
- For  $d = 3$ ,  $\Gamma^h(t)$  are “conformal polyhedral surfaces”.

Both vertex normal definitions are in the same direction;  
i.e. weighted average of normals of neighbouring faces  $\parallel \Delta_s^h \vec{X}$ .

## Recall Existing Parametric Approximations for $d = 3$

There exist parametric finite element approximations of (MC) and (SD). They are based on the following formulations.

- Dziuk (91) (MC)

$$\vec{x}_t = \vec{\kappa} = \kappa \vec{\nu} \equiv \Delta_s \vec{x}.$$

- Bänsch, Morin, Nochetto (05) (SD)

$$\vec{x}_t = \vec{\nu} = \mathcal{V} \vec{\nu}, \quad \mathcal{V} = -\Delta_s \kappa, \quad \kappa = \vec{\kappa} \cdot \vec{\nu}, \quad \vec{\kappa} = \Delta_s \vec{x}.$$

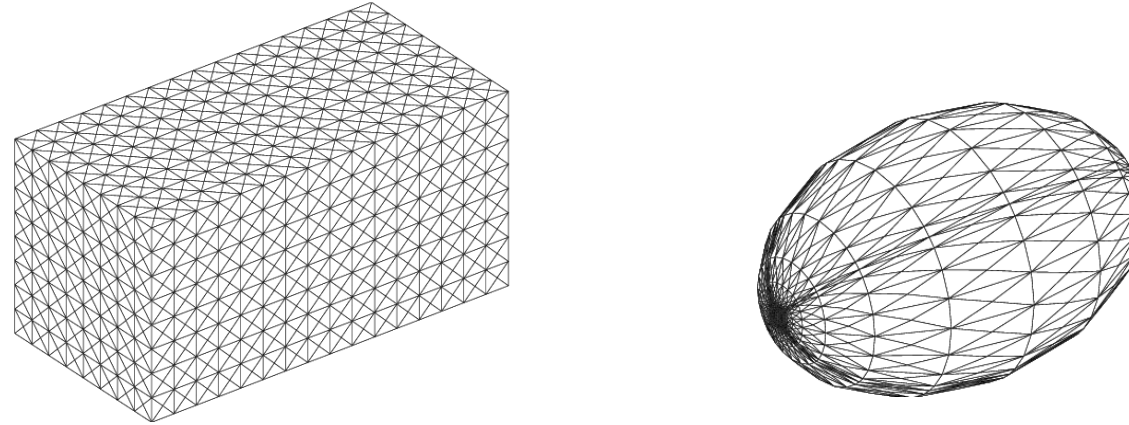
The two approaches have in common that they evolve the parameterization  $\vec{x}$  and its corresponding approximation  $\vec{X}$  only in the *normal* direction.

This can lead to **mesh distortions** in practice.

Can be overcome with a posteriori applied heuristic mesh smoothing steps, see e.g. Brakke (92). However, effect on normal velocity not clear.

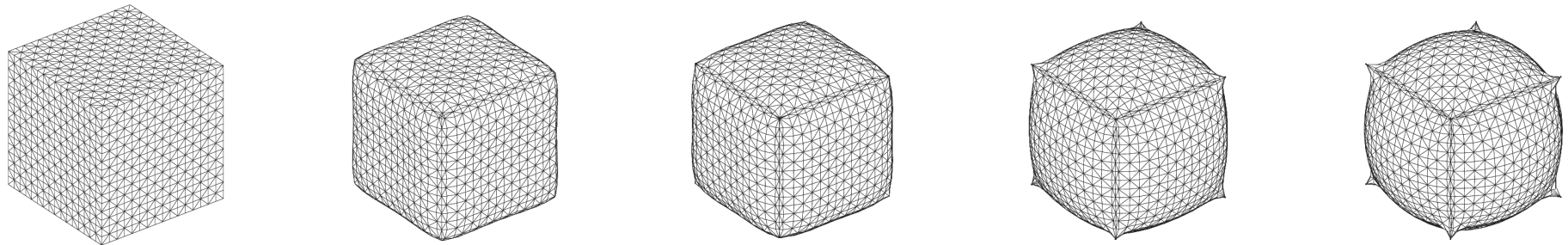
## Mesh Distortions

(MC) – Dziuk :



( $K = 1282$  vertices,  $J = 2560$  triangles,  $\tau = 10^{-3}$ ,  $T = 0.14$ )

(SD) – BMN :

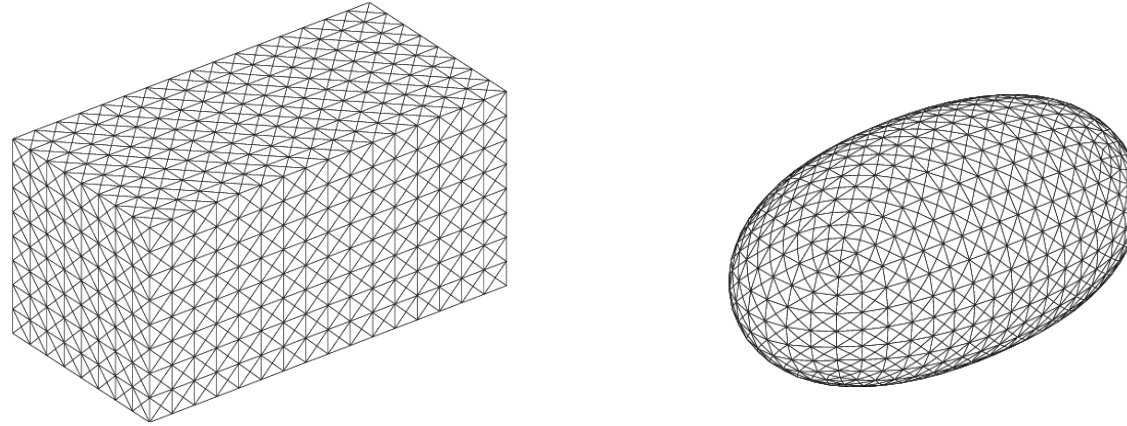


( $K = 1538$ ,  $J = 3072$ ,  $\tau = 10^{-4}$ ,  $T = 1.6 \times 10^{-3}$ )

Finite element toolbox ALBERTA Schmidt, Siebert (2005).

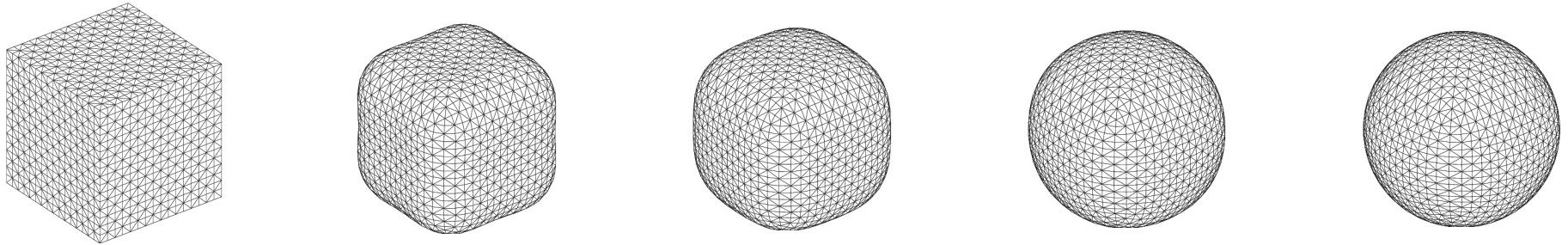
# Tangential Distribution of Mesh Points

(MC) – BGN :



( $K = 1282$  vertices,  $J = 2560$  triangles,  $\tau = 10^{-3}$ ,  $T = 0.14$ )

(SD) – BGN :

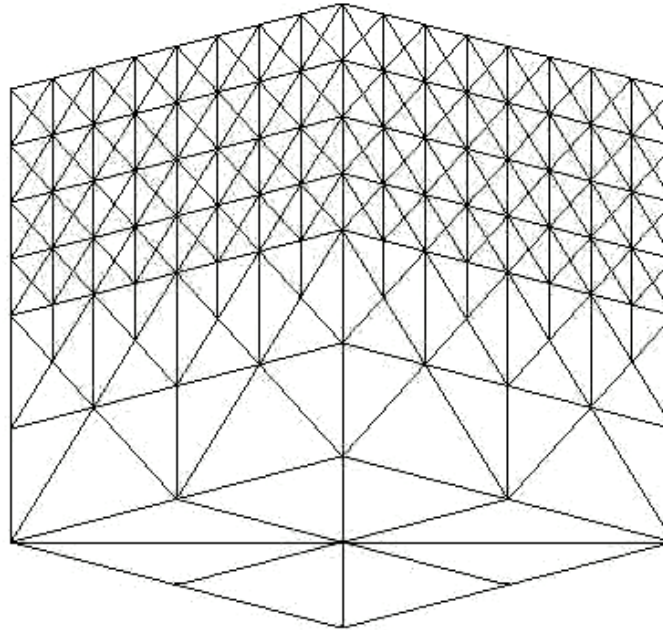


( $K = 1538$ ,  $J = 3072$ ,  $\tau = 10^{-4}$ ,  $T = 1.6 \times 10^{-3}$ )

## Tangential Distribution of Mesh Points

In general good meshes are obtained for  $d = 3$ :

(SD)



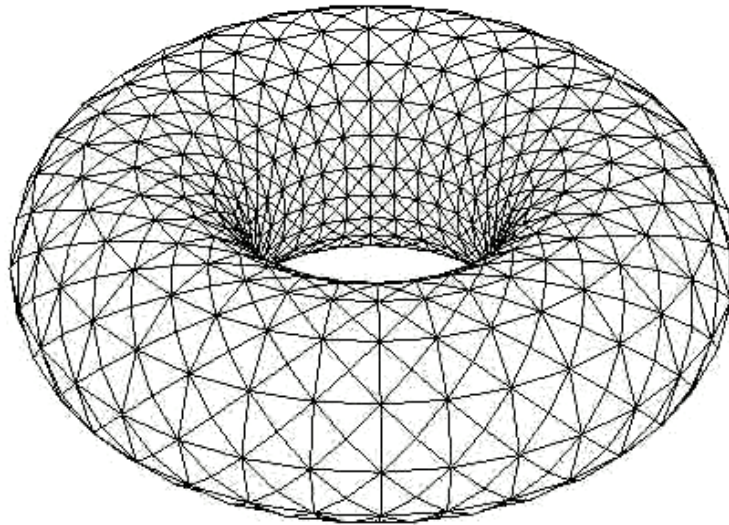
$$(K = 442, J = 880, \tau = 10^{-3}, T = 1)$$

No heuristical redistribution necessary.

Note: Ideas for curves from Strain (89), Hou, Lowengrub, Shelley (94) and Mikula, Ševčovič (01) **do not** generalize to surfaces in  $\mathbb{R}^3$ .

## Numerical Results

(MC) - torus with radii  $R = 2$  and  $r = 1$ .

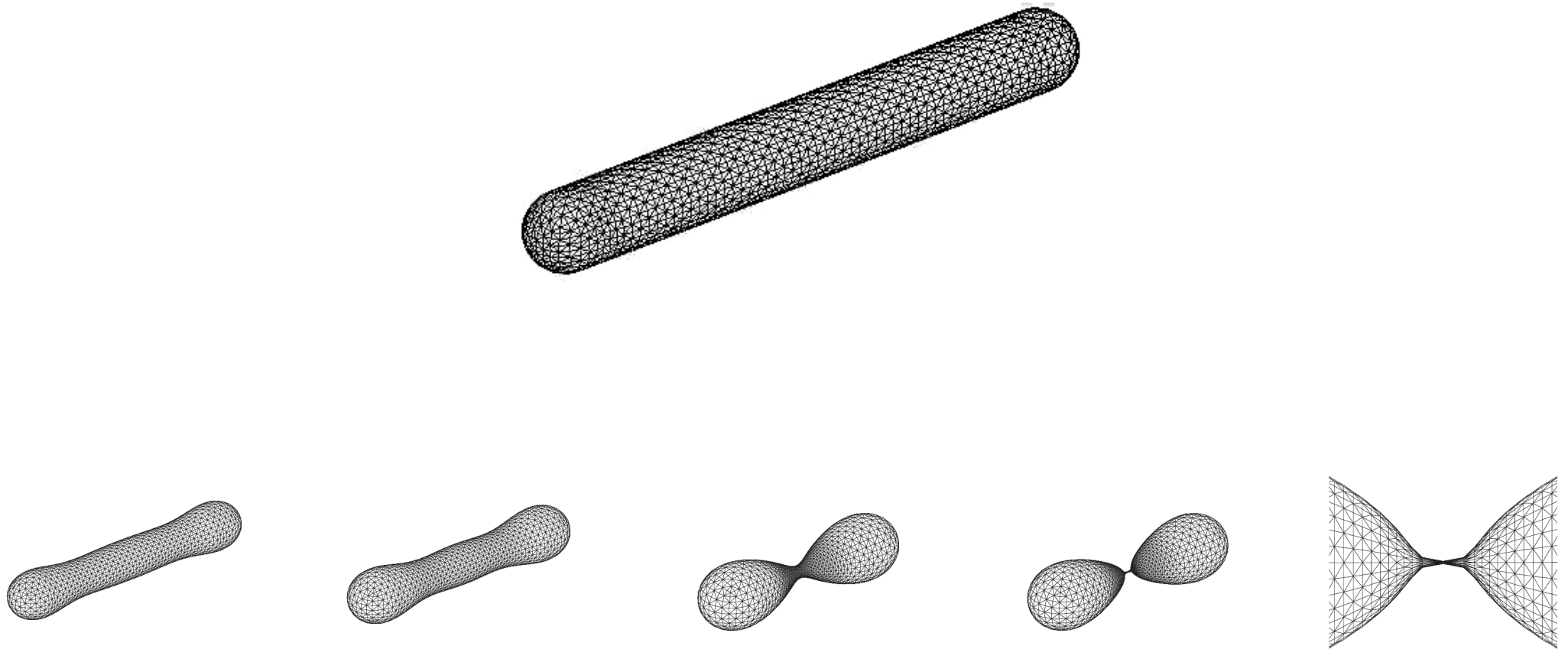


$(K = 1024, J = 2048, \tau = 10^{-3}, T = 0.538)$

## Numerical Results

(SD) leading to pinch-off

Rounded cylinder  $8 \times 1 \times 1$ .



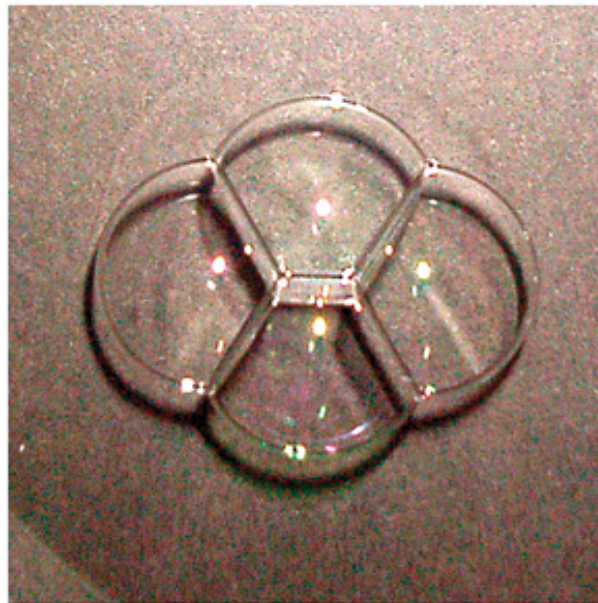
$\vec{X}(t)$  for  $t = 0.05, 0.1, 0.24, 0.2431$ . Volume loss = -0.03%.

( $K = 2178, J = 4352, \tau = 10^{-4}$ )

## Extension of Curve Networks to $\mathbb{R}^3$ : Surface Clusters

Generalisation of curve networks in the plane with triple junction points (where 3 curves meet) to

Surface clusters in  $\mathbb{R}^3$  with triple junction lines (where 3 surfaces meet) and quadruple junction points (where 4 TJLs meet).



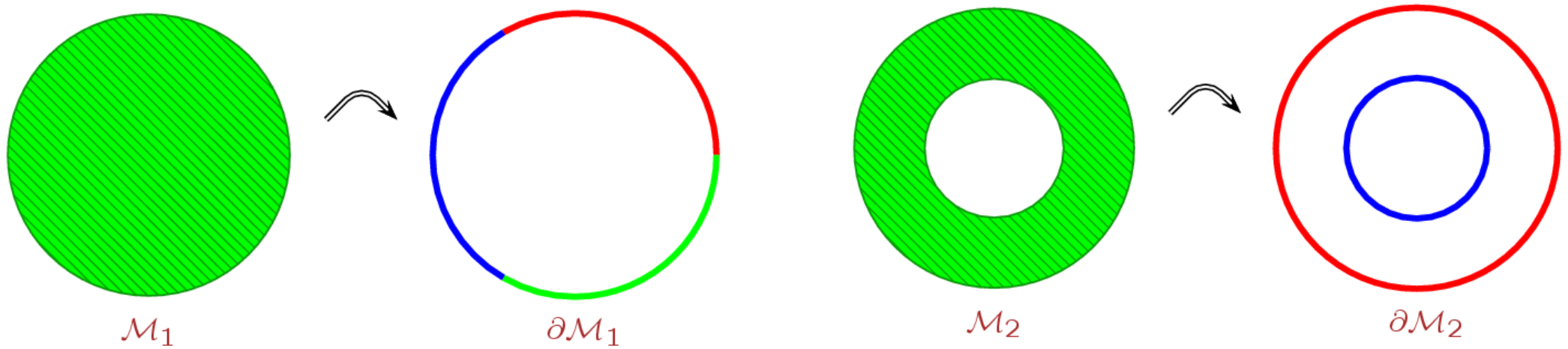
Once again the conditions on these triple junction lines will be naturally imposed in our formulation. Conditions on QJs implied by TJL conditions.

See Garcke, Novick-Cohen (00) and Bronsard, Garcke, Stoth (98).

## Surface Clusters

Geometric evolution equations for surface clusters. Let  $\Gamma := (\Gamma_1, \dots, \Gamma_{I_S})$  be a cluster of surface patches meeting at  $I_T$  triple junction lines  $\mathcal{T}_1, \dots, \mathcal{T}_{I_T}$ .

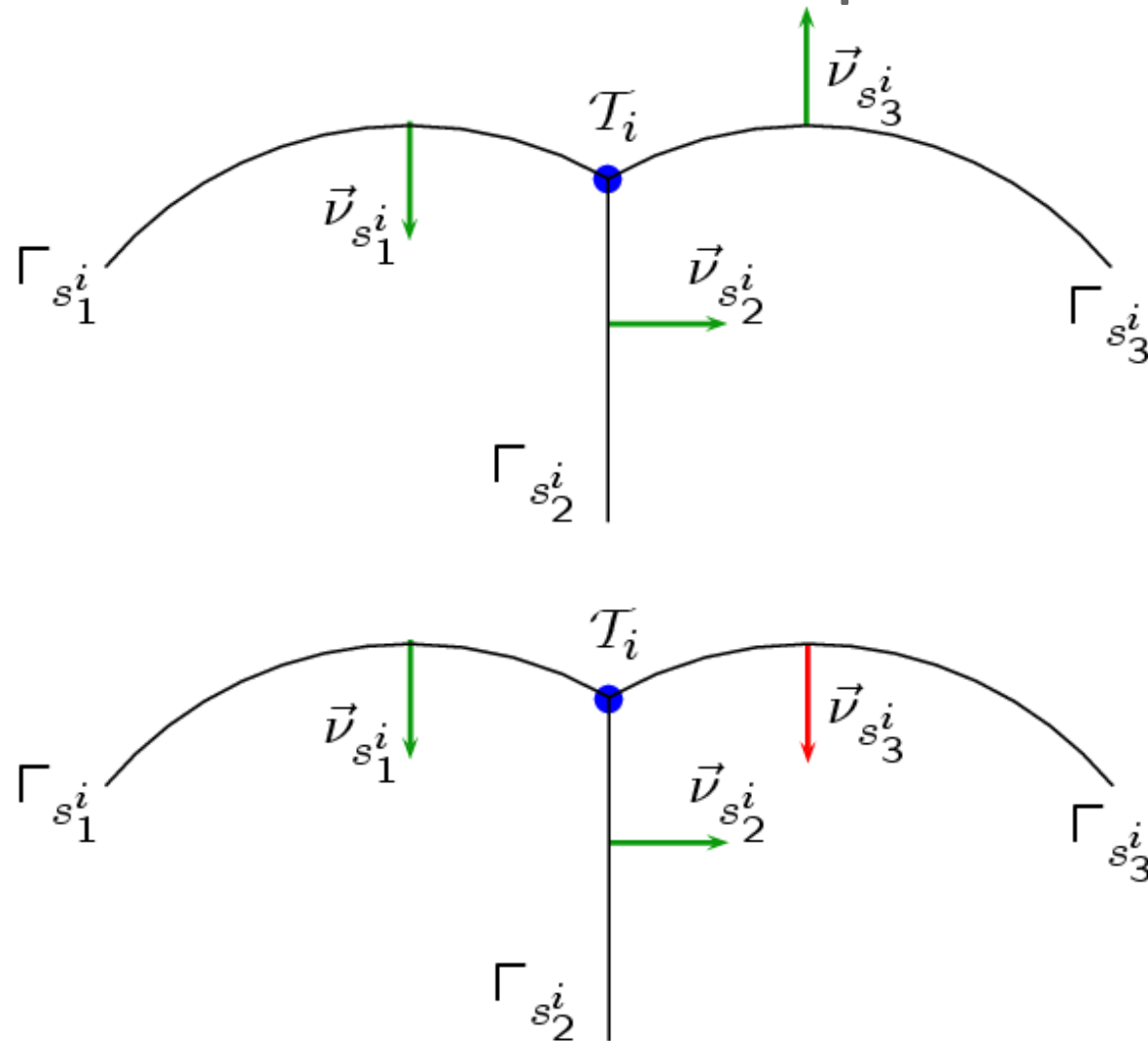
Let  $\mathcal{M} := (\mathcal{M}_1, \dots, \mathcal{M}_{I_S})$  be a collection of reference manifolds with boundaries  $\partial\mathcal{M}_i$  partitioned into  $\partial\mathcal{M}_i = \bigcup_{j=1}^{I_{P_i}} \partial_j\mathcal{M}_i$ ,  $i = 1 \rightarrow I_S$ .



Then the triple junction lines  $\mathcal{T}_i$ ,  $i = 1 \rightarrow I_T$ , are given by sets  $\{(s_j^i, p_j^i, o_j^i) : j = 1 \rightarrow 3\} \in \{(s, p, o) : s \in \{1, \dots, I_S\}, p \in \{1, \dots, I_{P_s}\}, o \in \{-1, 1\}\}^3$ .

Here  $o_j^i \in \{-1, 1\}$  denotes the choice of local normal for the surface  $\Gamma_{s_j^i}$  meeting at triple junction  $\mathcal{T}_i$ , in order align the orientation of the three normals.

## Local Orientation of Normals at Triple Junction Lines



Sketch of the local orientation of  $(\Gamma_{s_1^i}, \Gamma_{s_2^i}, \Gamma_{s_3^i})$  at the triple junction line  $\mathcal{T}_i$  (**blue**). Depicted is a plane that is perpendicular to  $\mathcal{T}_i$ . In the example above,  $o^i := (o_1^i, o_2^i, o_3^i)$  can be chosen as  $o^i = \pm(1, 1, 1)$ . However, in the example below we require  $o^i = \pm(1, 1, -1)$ .

## Geometric Evolution Equations

Let  $\vec{x}(t) := (\vec{x}_1, \dots, \vec{x}_{I_S})(t) : \mathcal{M} \rightarrow \Gamma(t)$  be a parameterization of  $\Gamma(t)$ .

On  $\Gamma_i$ : 
$$\mathcal{V}_i := (\vec{x}_i)_t \cdot \vec{\nu}_i = \begin{cases} \varkappa_i & \text{(MC)} \\ -\Delta_s \varkappa_i & \text{(SD)} \end{cases}, \quad i = 1 \rightarrow I_S.$$

In addition, the following triple junction line conditions have to hold for  $i = 1 \rightarrow I_T$ .

(a) 
$$\mathcal{T}_i(t) := \vec{x}_{s_1}^i (\partial_{p_1}^i \mathcal{M}_{s_1}^i) = \vec{x}_{s_2}^i (\partial_{p_2}^i \mathcal{M}_{s_2}^i) = \vec{x}_{s_3}^i (\partial_{p_3}^i \mathcal{M}_{s_3}^i), \quad \text{(attachment)}$$

(b) 
$$\sum_{j=1}^3 o_j^i \vec{\nu}_{s_j}^i = \vec{0} \quad \text{on } \mathcal{T}_i, \quad \text{(force balance)}$$

(c) 
$$o_1^i \vec{\mu}_{s_1}^i \cdot \nabla_s \varkappa_{s_1}^i = o_2^i \vec{\mu}_{s_2}^i \cdot \nabla_s \varkappa_{s_2}^i = o_3^i \vec{\mu}_{s_3}^i \cdot \nabla_s \varkappa_{s_3}^i \quad \text{on } \mathcal{T}_i, \quad \text{(flux balance)}$$

(d) 
$$\sum_{j=1}^3 o_j^i \varkappa_{s_j}^i = 0 \quad \text{on } \mathcal{T}_i, \quad \text{(chem. pot. cont.)}$$

Here  $\vec{\mu}_i$  denotes the intrinsic unit normal to  $\partial\Gamma_i$ , that lies within the tangent plane of  $\Gamma_i$ .

$$E(\Gamma) = |\Gamma| := \sum_{i=1}^{I_S} \int_{\Gamma_i} 1 \, ds \quad \Rightarrow \quad \frac{d}{dt} |\Gamma(t)| \leq 0 \quad \text{(MC) \& (a,b), (SD) \& (a-d)}$$

## Weak Formulation

Given the triple junction lines defined by  $\{(s_j^i, p_j^i, o_j^i) : j = 1 \rightarrow 3\}$ , set

$$\underline{V} := \{\vec{\chi} \equiv (\vec{\chi}_1, \dots, \vec{\chi}_{I_S}) \in \prod_{i=1}^{I_S} H^1(\mathcal{M}_i, \mathbb{R}^3) : \vec{\chi}_{s_1^i} = \vec{\chi}_{s_2^i} = \vec{\chi}_{s_3^i} \text{ on } \mathcal{T}_i, i = 1 \rightarrow I_T\}$$

and  $W := \{\chi \equiv (\chi_1, \dots, \chi_{I_S}) \in \underbrace{\prod_{i=1}^{I_S} H^1(\mathcal{M}_i, \mathbb{R})}_{=: W_0} : \sum_{j=1}^3 o_j^i \chi_{s_j^i} = 0 \text{ on } \mathcal{T}_i, i = 1 \rightarrow I_T\}.$

Find  $\vec{x} \in \underline{V}$  and  $\varkappa \in \begin{cases} W_0 \\ W \end{cases}$  such that

$$\begin{aligned} \langle \vec{x}_t, \eta \vec{\nu} \rangle - \begin{cases} \langle \varkappa, \eta \rangle \\ \langle \nabla_s \varkappa, \nabla_s \eta \rangle \end{cases} &= 0 & \forall \eta \in \begin{cases} W_0 \\ W \end{cases}, \\ \langle \varkappa \vec{\nu}, \vec{x} \rangle + \langle \nabla_s \vec{x}, \nabla_s \vec{x} \rangle &= 0 & \forall \vec{x} \in \underline{V}, \end{aligned}$$

where

$$\langle \eta, \chi \rangle := \sum_{i=1}^{I_S} \int_{\Gamma_i} \eta_i \cdot \chi_i \, ds.$$

(a,d) enforced via trial spaces, (c,d) enforced weakly via test spaces.

## Parametric Finite Element Approximation

Introduce piecewise linears  $\underline{V}^h \subset \underline{V}$ ,  $W^h \subset W$  and  $W_0^h \subset W_0$ .

Find  $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}^h \times \begin{cases} W_0^h \\ W^h \end{cases}$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{\nu}^m \right\rangle_m^h - \begin{cases} \langle \kappa^{m+1}, \chi \rangle_m^h \\ \langle \nabla_s \kappa^{m+1}, \nabla_s \chi \rangle_m \end{cases} = 0 \quad \forall \chi \in \begin{cases} W_0^h \\ W^h \end{cases},$$

$$\langle \kappa^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_m^h + \langle \nabla_s \vec{X}^{m+1}, \nabla_s \vec{\eta} \rangle_m = 0 \quad \forall \vec{\eta} \in \underline{V}^h;$$

where

$$\langle f, g \rangle_m := \int_{\Gamma^m} f \cdot g \, ds := \sum_{i=1}^{I_S} \int_{\Gamma_i^m} f_i \cdot g_i \, ds$$

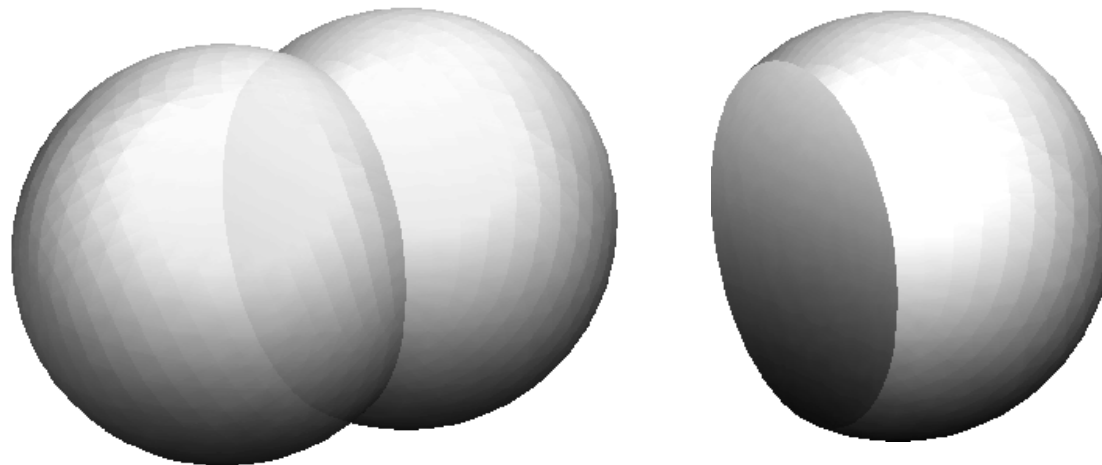
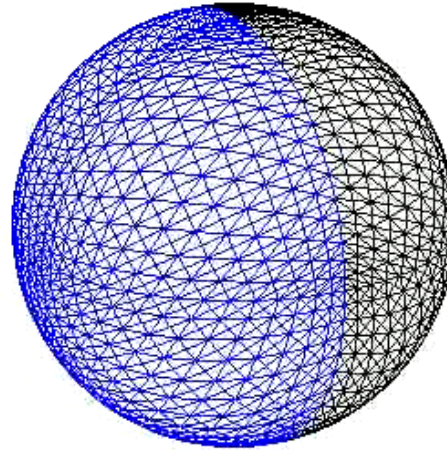
with  $\langle \cdot, \cdot \rangle_m^h$  the mass lumped inner product.

Linear system for  $\{\vec{X}^{m+1}, \kappa^{m+1}\}$ .

Existence, uniqueness and stability. Volume conservation and good mesh properties as before.

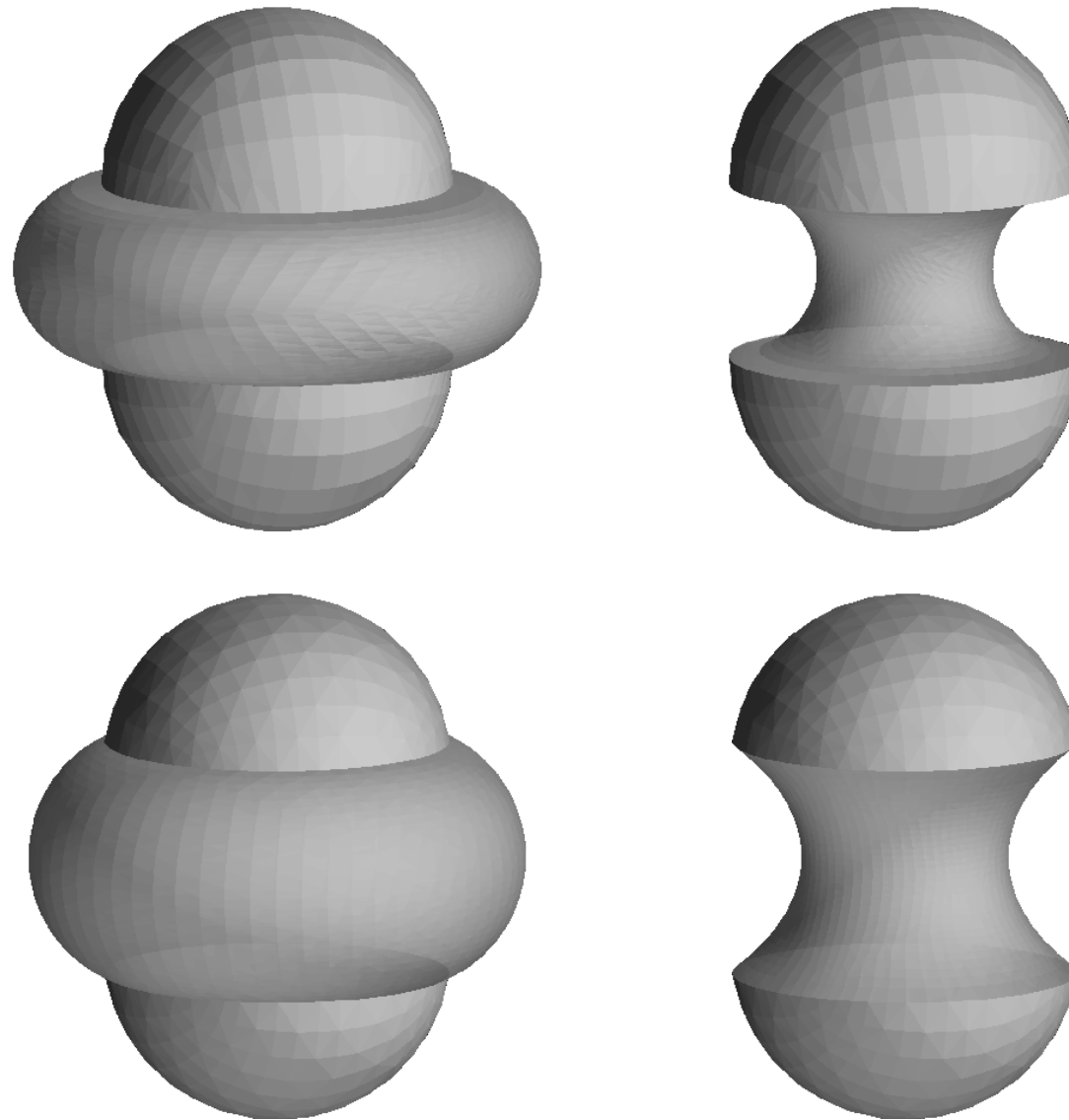
# Numerical Results

(SD)



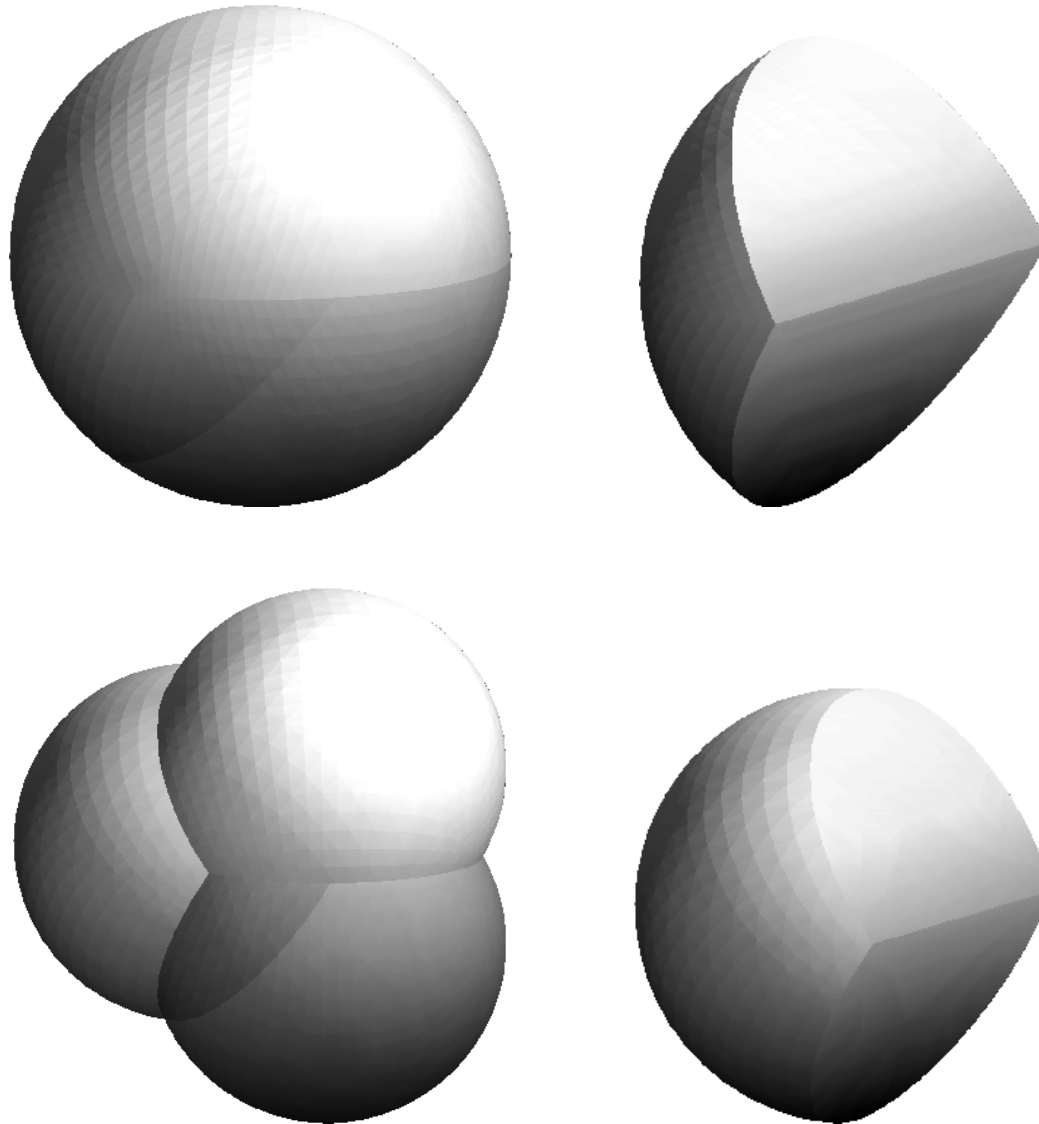
( $K = 3267$ ,  $J = 6240$ ,  $\tau = 10^{-3}$  and  $T = 1$ )

## Numerical Results



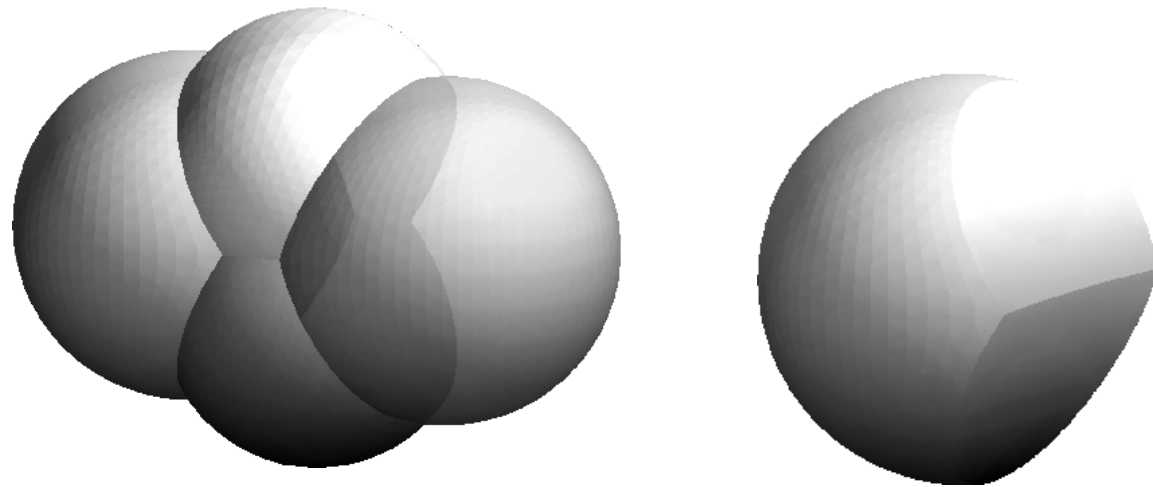
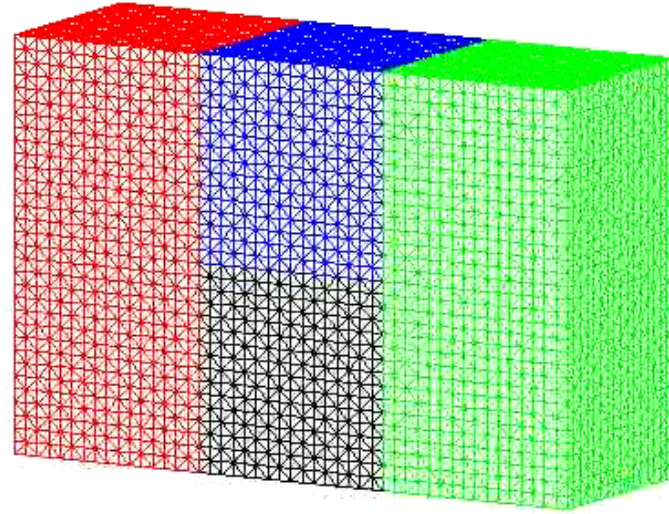
(SD) Two volumes (dumbbell and torus) with 4 surfaces.  
Plot of  $\Gamma^0$  and  $\Gamma^M$ . On the right,  $\Gamma_i^m$ ,  $i = 1, 2, 4$ ,  $m = 0, M$ .  
( $K = 4802$ ,  $J = 9216$ ,  $\tau = 10^{-3}$  and  $T = 1$ )

## Numerical Results



(SD) Triple bubble.  $\Gamma^0$  is partitioned unit ball into 3 equal segments.  
Plot of  $\Gamma^0$  and  $\Gamma^M$ . On the right,  $\Gamma_i^m$ ,  $i = 1, 4, 5$ ,  $m = 0, M$ .  
( $K = 6534$ ,  $J = 12288$ ,  $\tau = 10^{-4}$  and  $T = 1$ )

## Numerical Results



$(K = 7305, J = 13824, \tau = 10^{-4}$  and  $T = 0.5)$

## Anisotropic Surface Energy

All of the presented schemes naturally generalize to an anisotropic surface energy

$$|\Gamma|_\gamma := \int_\Gamma \gamma(\vec{\nu}) \, ds$$

where  $\gamma : \mathbb{R}^d \setminus \{\vec{0}\} \rightarrow \mathbb{R}_{>0}$  is a given anisotropy function, which we will assume is absolutely homogeneous of degree one, i.e.

$$\gamma(\lambda \vec{p}) = |\lambda| \gamma(\vec{p}) \quad \forall \vec{p} \in \mathbb{R}^d \setminus \{\vec{0}\}, \quad \forall \lambda \in \mathbb{R} \setminus \{0\}.$$

In order to obtain unconditionally stable approximations, we restrict ourselves to the following class of anisotropies:

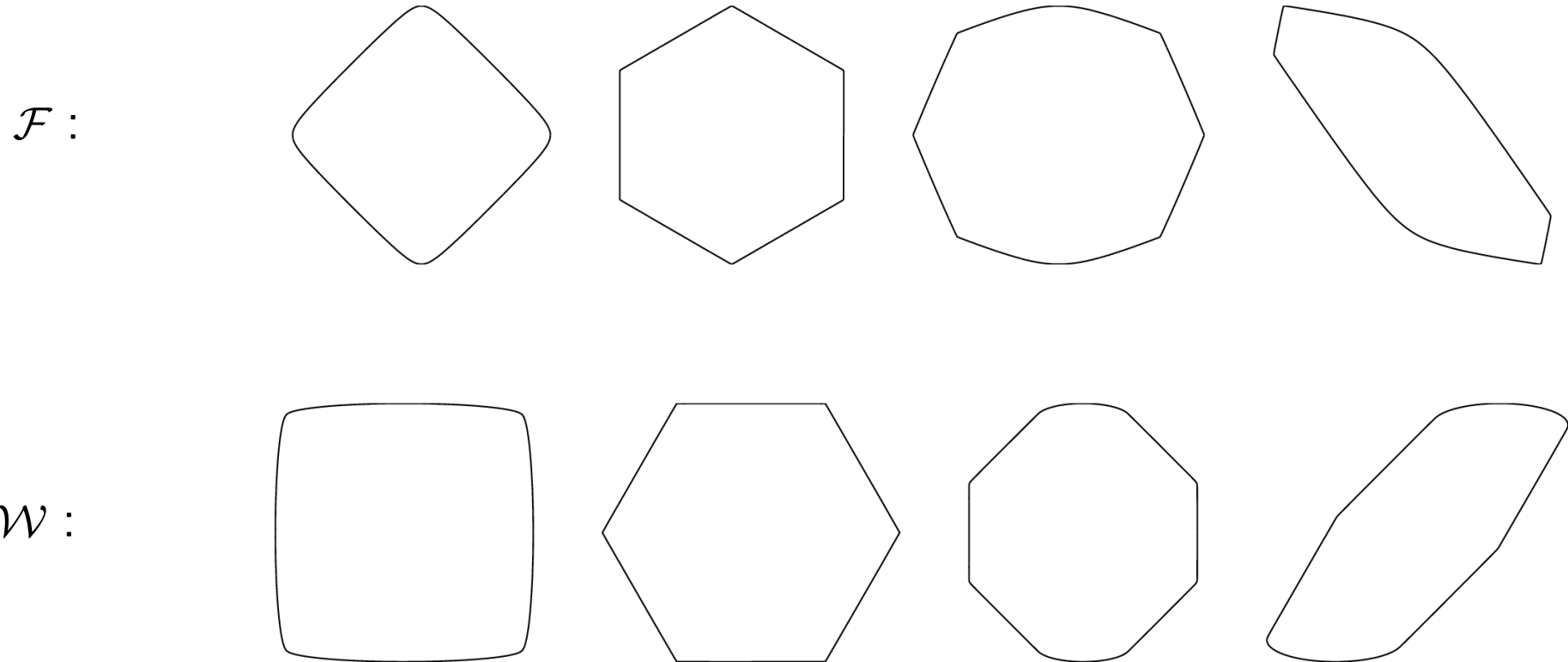
$$\gamma(\vec{p}) = \left( \sum_{\ell=1}^L [\gamma_\ell(\vec{p})]^r \right)^{\frac{1}{r}}, \quad \gamma_\ell(\vec{p}) := \sqrt{\vec{p} \cdot G_\ell \vec{p}}, \quad r \in [1, \infty),$$

where  $G_\ell \in \mathbb{R}^{d \times d}$ ,  $\ell = 1 \rightarrow L$ , are symmetric and positive definite.

## Example Anisotropies, $d = 2$

Frank diagram:  $\mathcal{F} := \{\vec{p} \in \mathbb{R}^d : \gamma(\vec{p}) \leq 1\}$

Wulff shape:  $\mathcal{W} := \{\vec{q} \in \mathbb{R}^d : \gamma^*(\vec{q}) \leq 1\}$ , where  $\gamma^*(\vec{q}) = \sup_{\vec{p} \in \mathbb{R}^d \setminus \{\vec{0}\}} \frac{\vec{p} \cdot \vec{q}}{\gamma(\vec{p})}$ .

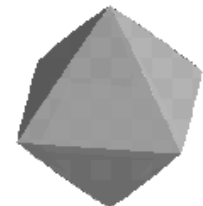
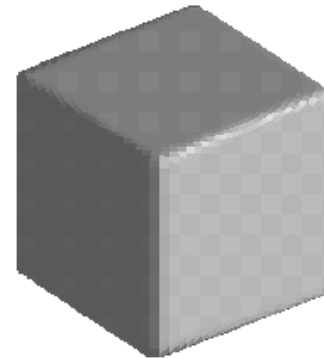
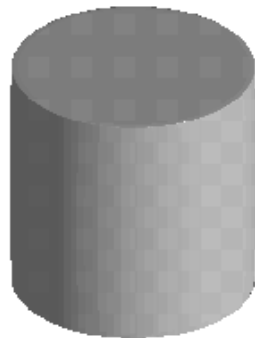
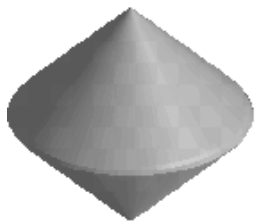
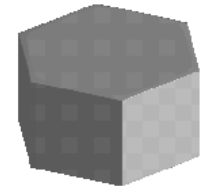
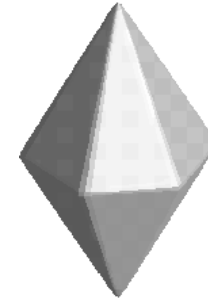
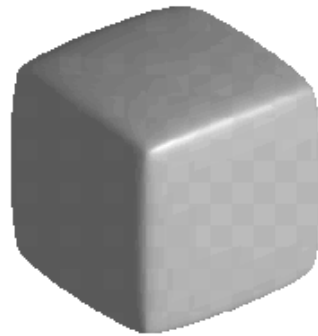


A wide class of anisotropies can be modelled by this choice.

Including regularized crystalline surface energies.

## Example Anisotropies, $d = 3$

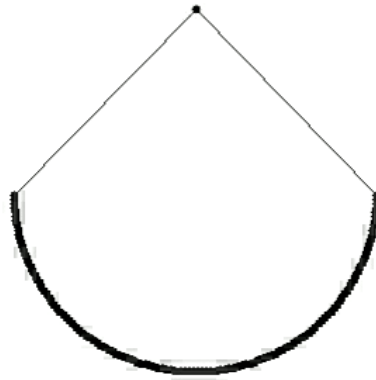
Examples of Frank diagrams  $\mathcal{F}$  and associated Wulff shapes  $\mathcal{W}$ :



# Tangential Movement

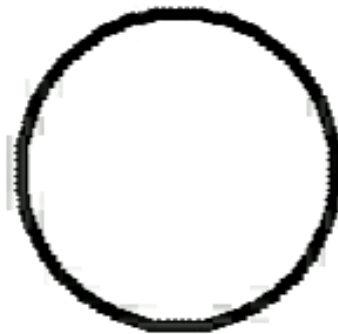
(SD<sub>γ</sub>)  $\gamma(\vec{p}) = \sqrt{p_1^2 + 0.1 p_2^2} \Rightarrow$  Wulff shape is  $\sqrt{10} : 1$  ellipse

$N = 128, \tau = 10^{-3}, T = 1.$



(SD<sub>γ</sub>)  $\gamma(\vec{p}) = \sqrt{p_1^2 + 0.01 p_2^2} \Rightarrow$  Wulff shape is 10 : 1 ellipse

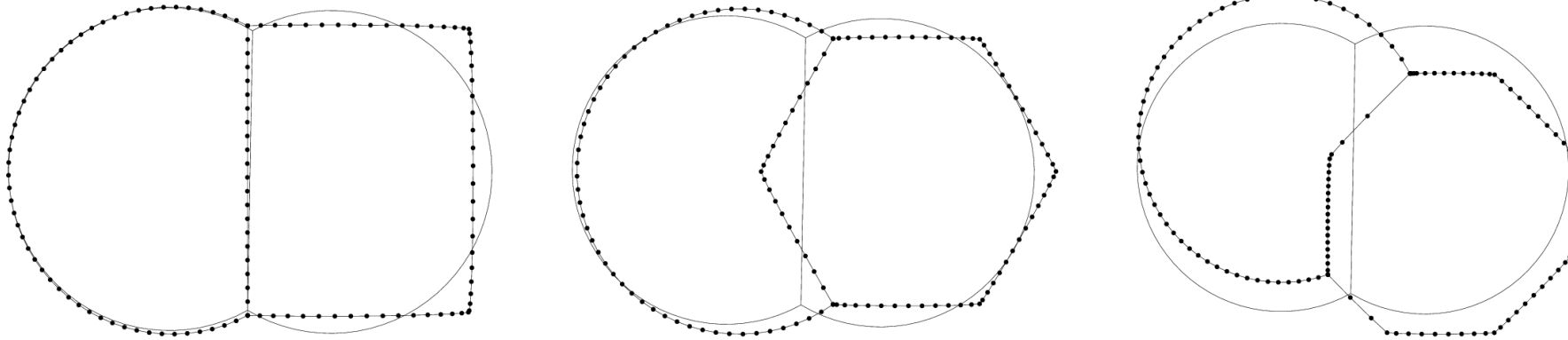
$N = 128, \tau = 10^{-3}, T = 1.$



# Anisotropic Planar Double Bubbles

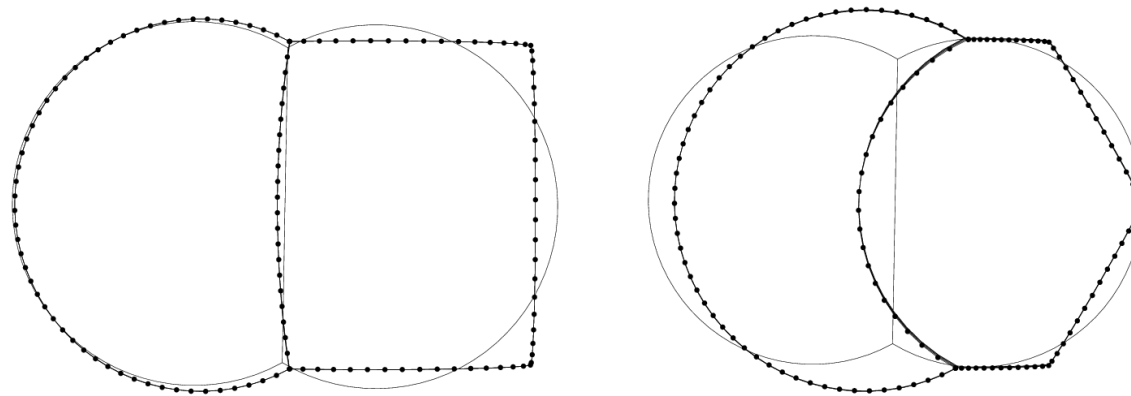
E.g.  $(SD_\gamma)$  :  $\gamma_1(\vec{p}) = |\vec{p}|$ ,  $\gamma_i(\vec{p}) = \gamma_0(\vec{p})$ ,  $i = 2 \rightarrow 3$ .

$$\varepsilon_\ell^2 \equiv 0.001$$



$\gamma_1(\vec{p}) = \gamma_2(\vec{p}) = |\vec{p}|$ ,  $\gamma_3(\vec{p}) = \gamma_0(\vec{p})$ .

$$\varepsilon_\ell^2 \equiv 0.001$$

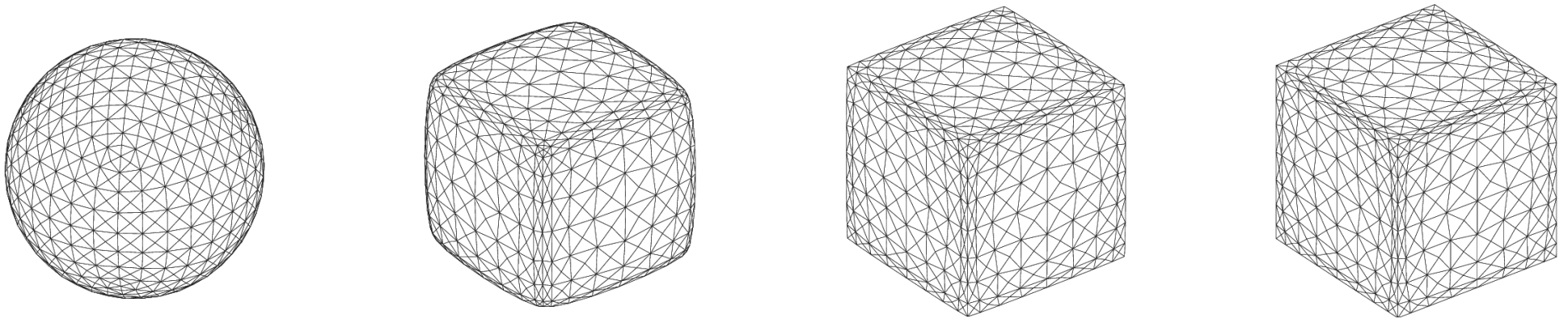


## Numerical Results

(SD $_{\gamma}$ ) - Cubic Wulff Shape,

i.e.  $\gamma(\vec{p}) = \sum_{i=1}^d \sqrt{\varepsilon^2 |\vec{p}|^2 + p_i^2 (1 - \varepsilon^2)}$  is a regularized  $l^1$ -norm.

( $r = 1$ ,  $L = 3$ ,  $G_1 = \text{diag}(1, \varepsilon^2, \varepsilon^2)$ ,  $G_2 = \text{diag}(\varepsilon^2, 1, \varepsilon^2)$ ,  $G_3 = \text{diag}(\varepsilon^2, \varepsilon^2, 1)$ )



A plot of  $\vec{X}(0.5)$  for  $\varepsilon = 10^{-k}$ ,  $k = 0 \rightarrow 3$ .

( $K = 770$ ,  $J = 1536$ ,  $\tau = 10^{-3}$ )

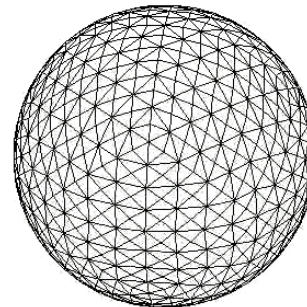
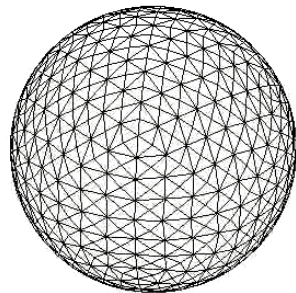
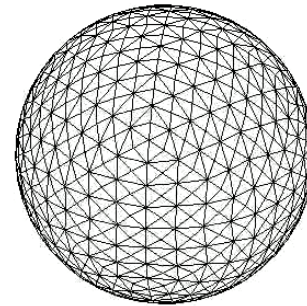
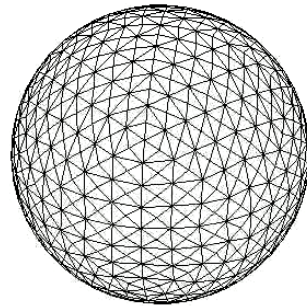
## Numerical Results

$(SD_\gamma)$  - Cube ( $r = 1, L = 3$ ),

Hexagonal Prism ( $r = 1, L = 4$ ),

Octahedron ( $r = 30, L = 3$ ),

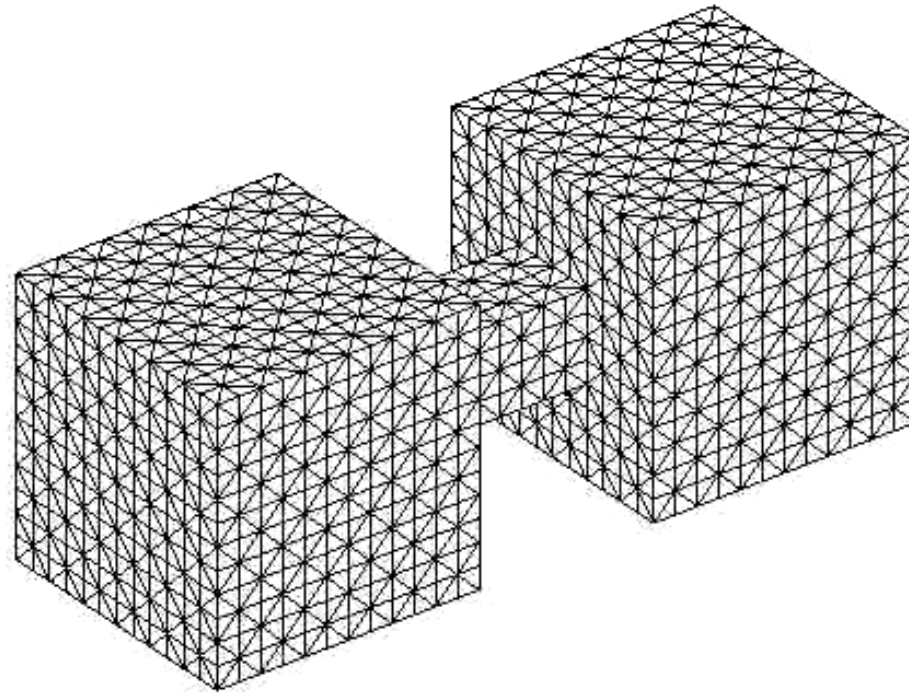
Cylinder Wulff Shape ( $r = 1, L = 2$ ).



$(\varepsilon = 10^{-2}, K = 770, J = 1536, \tau = 10^{-4}, T = 0.1, 0.25, 0.02, 0.25)$

## Numerical Results

$(MC_\gamma)$  - Cubic Wulff Shape ( $r = 1$ ,  $L = 3$ ,  $\varepsilon = 10^{-2}$ )

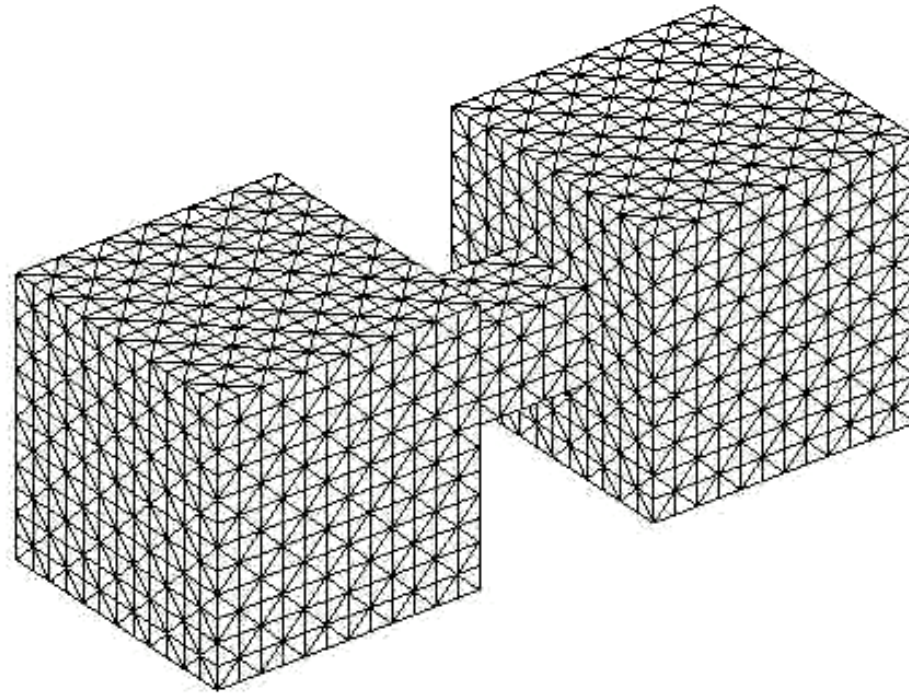


Dumbbell

$(K = 1826, J = 3648, \tau = 10^{-4}$  and  $T = 0.18)$

## Numerical Results

$(SD_\gamma)$  - Cubic Wulff Shape ( $r = 1$ ,  $L = 3$ ,  $\varepsilon = 10^{-2}$ )

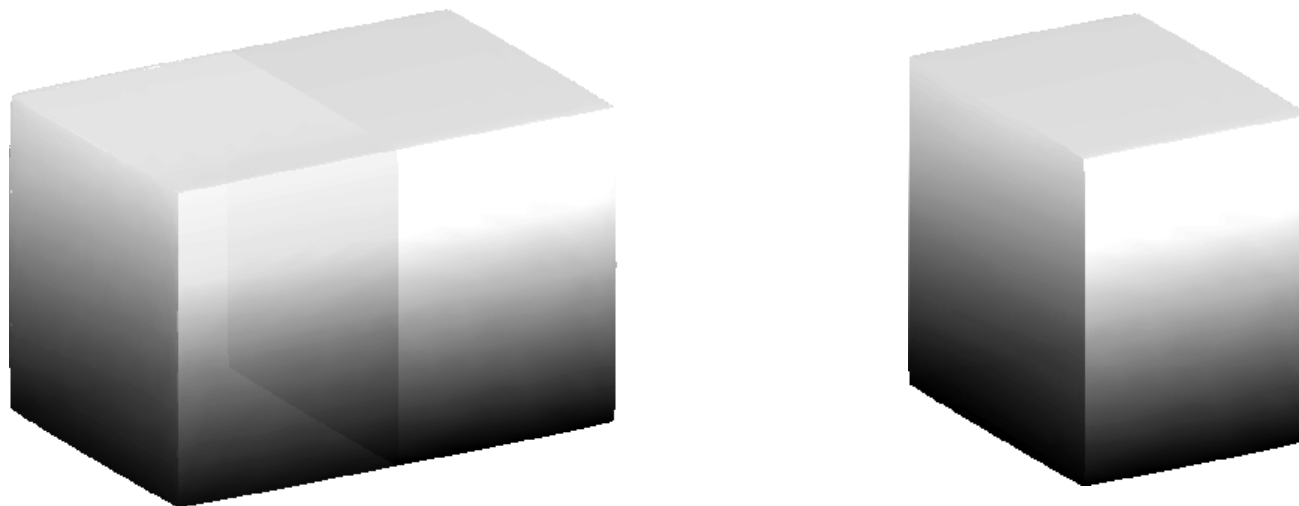
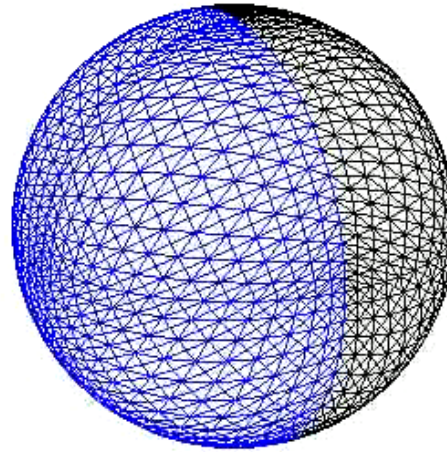


Dumbbell

$(K = 1826, J = 3648, \tau = 10^{-4}$  and  $T = 3.5)$

## Numerical Results

$(SD_\gamma)$  - Cubic Wulff Shape ( $r = 1$ ,  $L = 3$ ,  $\varepsilon = 10^{-1}$ )



( $K = 3267$ ,  $J = 6240$ ,  $\tau = 10^{-3}$  and  $T = 1$ )

## References

1. J. W. Barrett, H. Garcke, and R. Nürnberg, *A parametric finite element method for fourth order geometric evolution equations*, [J. Comput. Phys.](#), **222** (2007), pp. 441–467.
2. —, *On the variational approximation of combined second and fourth order geometric evolution equations*, [SIAM J. Sci. Comput.](#), **29** (2007), pp. 1006–1041.
3. —, *Numerical approximation of anisotropic geometric evolution equations in the plane*, [IMA J. Numer. Anal.](#), **28** (2008), pp. 292–330.
4. —, *Numerical approximation of gradient flows for closed curves in  $\mathbb{R}^d$* , 2008. Preprint No. 13/2008, University Regensburg, Germany.
5. —, *On the parametric finite element approximation of evolving hypersurfaces in  $\mathbb{R}^3$* , [J. Comput. Phys.](#), **227** (2008), pp. 4281–4307.
6. —, *A variational formulation of anisotropic geometric evolution equations in higher dimensions*, [Numer. Math.](#), **109** (2008), pp. 1–44.
7. —, *Parametric approximation of three dimensional surface clusters*, 2008 (in preparation).



## Anisotropic Surface Energy

$$|\Gamma|_\gamma := \int_\Gamma \gamma(\vec{\nu}) \, ds$$

where  $\gamma : \mathbb{R}^d \setminus \{\vec{0}\} \rightarrow \mathbb{R}_{>0}$  is a given anisotropy function, which we will assume is absolutely homogeneous of degree one, i.e.

$$\gamma(\lambda \vec{p}) = |\lambda| \gamma(\vec{p}) \quad \forall \vec{p} \in \mathbb{R}^d \setminus \{\vec{0}\}, \quad \forall \lambda \in \mathbb{R} \setminus \{0\}.$$

Let  $\Gamma(\varepsilon) := \{\vec{z} + \varepsilon \vec{g}(\vec{z}) : \vec{z} \in \Gamma\}$ . First variation of this energy yields

$$\frac{d}{d\varepsilon} |\Gamma(\varepsilon)|_\gamma \Big|_{\varepsilon=0} = - \int_\Gamma \vec{\kappa}_\gamma \cdot \vec{g} \, ds;$$

where

Weighted mean curvature vector:  $\vec{\kappa}_\gamma := \kappa_\gamma \vec{\nu},$

Weighted mean curvature:  $\kappa_\gamma := -\nabla_s \cdot \vec{\nu}_\gamma,$

Cahn–Hoffmann vector:  $\vec{\nu}_\gamma := \gamma'(\vec{\nu}) \quad \text{Cahn, Hoffmann (74).}$

In the isotropic case,  $\gamma(\vec{p}) = |\vec{p}|$ , we have that

$$|\Gamma|_\gamma \equiv |\Gamma|, \quad \vec{\nu}_\gamma \equiv \vec{\nu}, \quad \kappa_\gamma \equiv \kappa \quad \text{and} \quad \vec{\kappa}_\gamma \equiv \vec{\kappa}.$$

## Anisotropic Energy Decrease

This leads to the geometric evolution equations

$$\text{Anisotropic mean curvature flow:} \quad \mathcal{V} = \beta(\vec{\nu}) \kappa_\gamma \quad (\text{MC}_\gamma),$$

$$\text{Anisotropic surface diffusion:} \quad \mathcal{V} = -\nabla_s \cdot (\beta(\vec{\nu}) \nabla_s \kappa_\gamma) \quad (\text{SD}_\gamma);$$

where  $\beta : S^{d-1} \rightarrow \mathbb{R}_{>0}$  is an anisotropic mobility.

Similarly to the isotropic case,  $\gamma(\vec{p}) = |\vec{p}|$ , we have that

$$\frac{d}{dt} |\Gamma(t)|_\gamma = - \int_{\Gamma(t)} \mathcal{V} \kappa_\gamma \, ds = \begin{cases} - \int_{\Gamma(t)} \beta(\vec{\nu}) \kappa_\gamma^2 \, ds & \leq 0 & (\text{MC}_\gamma), \\ - \int_{\Gamma(t)} \beta(\vec{\nu}) (\nabla_s \kappa_\gamma)^2 \, ds & \leq 0 & (\text{SD}_\gamma). \end{cases}$$

Let  $\Omega(t)$  be bounded region with boundary  $\Gamma(t)$ ,  $\vec{\nu}$  outward unit normal  $\Rightarrow$

$$\frac{d}{dt} |\Omega(t)| = \int_{\Gamma(t)} \mathcal{V} \, ds = - \int_{\Gamma(t)} \nabla_s \cdot (\beta(\vec{\nu}) \nabla_s \kappa_\gamma) \, ds = 0 \quad (\text{SD}_\gamma).$$

$\vec{x} : \mathcal{M} \rightarrow \mathbb{R}^d$  a parameterization of  $\Gamma$ , anisotropic analogue of  $\kappa \vec{\nu} = \Delta_s \vec{x}$  is

$$\begin{aligned} \kappa_\gamma \vec{\nu} &= -\nabla_s \cdot (\vec{\nu} [\gamma'(\vec{\nu})]^T) + \nabla_s \cdot (\gamma(\vec{\nu}) \nabla_s \vec{x}) - \gamma(\vec{\nu}) \Delta_s \vec{x} \\ &\equiv [\gamma'(\vec{\nu})]_s^\perp \quad (\text{if } d = 2, \text{ i.e. a curve, and } \vec{\nu} = -\vec{x}_s^\perp). \end{aligned}$$

## Existing Parametric Approaches

There exist parametric finite element approximations for  $(MC_\gamma)$  and  $(SD_\gamma)$ .

- Dziuk (99)  $(MC_\gamma)$   $d = 2$ , i.e. curves in  $\mathbb{R}^2$   $\vec{\nu} = -\vec{x}_s^\perp$

$$\int_\Gamma [\beta(\vec{\nu})]^{-1} \vec{x}_t \cdot \vec{\varphi} \, ds + \int_\Gamma \gamma'(\vec{x}_s^\perp) \cdot \vec{\varphi}_s^\perp \, ds = 0.$$

Stability and error bounds for semidiscrete scheme, for an admissible class of anisotropies.

See also Pozzi (07) for an extension to curves in  $\mathbb{R}^d$ ,  $d \geq 2$ .

- Clarenz, Dziuk, Rumpf (03)  $(MC_\gamma)$   $\beta(\vec{\nu}) \equiv 1$  and  $d = 3$ , i.e. surfaces in  $\mathbb{R}^3$

$$\int_\Gamma \vec{x}_t \cdot \vec{\varphi} \, ds + \int_\Gamma \gamma(\vec{\nu}) \nabla_s \vec{x} \cdot \nabla_s \vec{\varphi} \, ds = \int_\Gamma [\vec{\nu} [\gamma'(\vec{\nu})]^T] \cdot \nabla_s \vec{\varphi} \, ds$$

- Haußer, Voigt (06)  $(SD_\gamma)$   $\beta(\vec{\nu}) \equiv 1$  and  $d = 3$

$$\vec{x}_t = \vec{\mathcal{V}} = \nu \vec{\nu}, \quad \nu = -\Delta_s \kappa_\gamma, \quad \kappa_\gamma = \vec{x}_{\gamma\gamma} \cdot \vec{\nu},$$

$$\int_\Gamma \vec{x}_{\gamma\gamma} \cdot \vec{\varphi} \, ds + \int_\Gamma \gamma(\vec{\nu}) \nabla_s \vec{x} \cdot \nabla_s \vec{\varphi} \, ds = \int_\Gamma [\vec{\nu} [\gamma'(\vec{\nu})]^T] \cdot \nabla_s \vec{\varphi} \, ds$$

There exist **no stability results** for the corresponding fully discrete approximations. All of these approaches have zero tangential velocity.

## Anisotropic Surface Energy

The desired stability property leads us to the following class of anisotropies.

$$\gamma(\vec{p}) = \sum_{\ell=1}^L \gamma_{\ell}(\vec{p}) = \sum_{\ell=1}^L \sqrt{\vec{p} \cdot G_{\ell} \vec{p}} \quad \text{in the case } d = 2,$$

where  $G_{\ell} \in \mathbb{R}^{2 \times 2}$ ,  $\ell = 1 \rightarrow L$ , are symmetric and positive definite.

Example:  $\gamma(\vec{p}) = \left[ \sum_{i=1}^2 \alpha_i^2 p_i^2 \right]^{\frac{1}{2}}$  and the regularized  $l^1$ -norm

$$\gamma(\vec{p}) = \sum_{i=1}^2 \sqrt{\varepsilon^2 |\vec{p}|^2 + p_i^2}, \quad \varepsilon > 0.$$

In the latter case

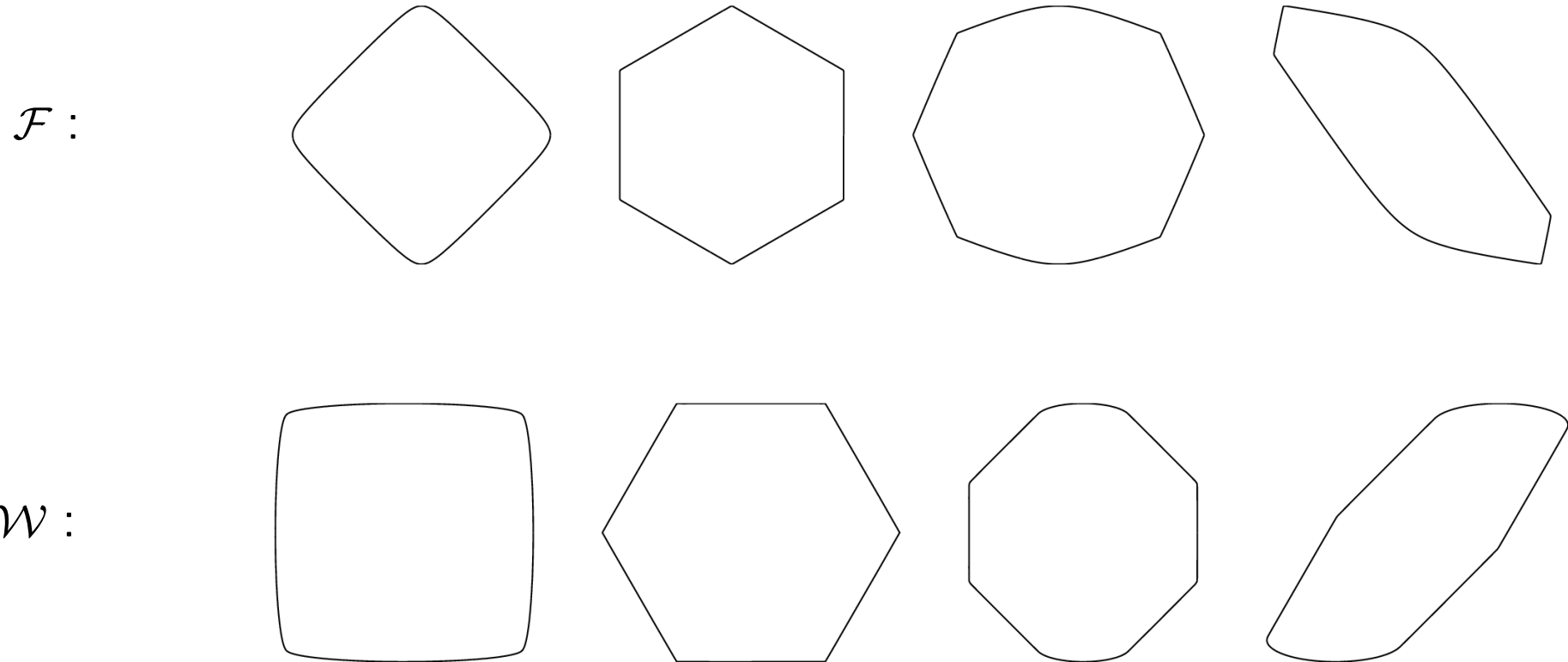
$$G_1 = \begin{pmatrix} 1 + \varepsilon^2 & 0 \\ 0 & \varepsilon^2 \end{pmatrix} \quad \text{and} \quad G_2 = \begin{pmatrix} \varepsilon^2 & 0 \\ 0 & 1 + \varepsilon^2 \end{pmatrix}.$$

Note that  $\gamma'(\vec{p}) = \sum_{\ell=1}^L [\gamma_{\ell}(\vec{p})]^{-1} G_{\ell} \vec{p}$ .

## Visualization of Anisotropy

Frank diagram:  $\mathcal{F} := \{\vec{p} \in \mathbb{R}^d : \gamma(\vec{p}) \leq 1\}$

Wulff shape:  $\mathcal{W} := \{\vec{q} \in \mathbb{R}^d : \gamma^*(\vec{q}) \leq 1\}$ , where  $\gamma^*(\vec{q}) = \sup_{\vec{p} \in \mathbb{R}^d \setminus \{\vec{0}\}} \frac{\vec{p} \cdot \vec{q}}{\gamma(\vec{p})}$ .



A wide class of anisotropies can be modelled by this choice.

Including regularized crystalline surface energies.

# Parametric Finite Element Approximation

Recall

$$\int_{\Gamma} \vec{x}_t \cdot \vec{\nu} \varphi \, ds = \begin{cases} \int_{\Gamma} \beta(\vec{\nu}) \kappa_{\gamma} \varphi \, ds \\ \int_{\Gamma} \beta(\vec{\nu}) \nabla_s \kappa_{\gamma} \cdot \nabla_s \varphi \, ds \end{cases}, \quad \int_{\Gamma} \kappa_{\gamma} \vec{\nu} \cdot \vec{\varphi} \, ds + \int_{\Gamma} \gamma'(\vec{x}_s^{\perp}) \cdot \vec{\varphi}_s^{\perp} \, ds = 0.$$

$(\mathcal{P}_{\gamma}^h)$  Find  $\{\vec{X}^{m+1}, \kappa_{\gamma}^{m+1}\} \in \underline{V}^h \times V^h$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{\nu}^m \right\rangle_m^h - \begin{cases} \langle \beta(\vec{\nu}^m) \kappa_{\gamma}^{m+1}, \chi \rangle_m^h \\ \langle \beta(\vec{\nu}^m) \nabla_s \kappa_{\gamma}^{m+1}, \nabla_s \chi \rangle_m \end{cases} = 0 \quad \forall \chi \in V^h,$$

$$\langle \kappa_{\gamma}^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_m^h + \sum_{\ell=1}^L \langle [\gamma_{\ell}(\vec{\nu}^m)]^{-1} G_{\ell} [\vec{X}_s^{m+1}]^{\perp}, \vec{\eta}_s^{\perp} \rangle_m = 0 \quad \forall \vec{\eta} \in \underline{V}^h,$$

where

$$\langle f, g \rangle_m := \int_{\Gamma^m} f \cdot g \, ds = \int_I f \cdot g |\vec{X}_{\rho}^m| \, d\rho.$$

Linear system for  $\{\vec{X}^{m+1}, \kappa_{\gamma}^{m+1}\}$ .

Note that for  $\gamma(\vec{p}) = |\vec{p}|$  and  $\beta \equiv 1$  the scheme  $(\mathcal{P}_{\gamma}^h)$  collapses to the isotropic scheme discussed earlier.

## THEOREM

Let  $(\mathcal{A})$  hold. Then  $\exists!$  solution  $\{\vec{X}^{m+1}, \kappa_\gamma^{m+1}\} \in \underline{V}^h \times V^h$ . Moreover, for  $k = 1 \rightarrow M$  it holds that

$$|\Gamma^k|_\gamma + \sum_{m=0}^{k-1} \tau_m \begin{cases} \langle \beta(\vec{\nu}^m) \kappa_\gamma^{m+1}, \kappa_\gamma^{m+1} \rangle_m^h \\ \langle \beta(\vec{\nu}^m) \nabla_s \kappa_\gamma^{m+1}, \nabla_s \kappa_\gamma^{m+1} \rangle_m \end{cases} \leq |\Gamma^0|_\gamma.$$

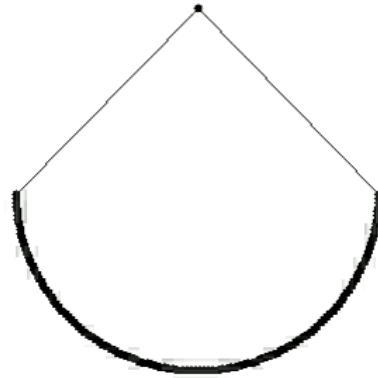
Continuous in time semidiscrete scheme  $\{\vec{X}(t), \kappa_\gamma(t)\}$ :

- (a) **Area conservation** for  $(SD_\gamma)$ :  $0 = \langle \vec{X}_t, \vec{\nu}^h \rangle^h = \int_{\Gamma^h} \vec{X}_t \cdot \vec{\nu}^h \, ds = \frac{d}{dt} |\Omega^h(t)|$
- (b) **Equidistribution of mesh points** for  $\vec{X}(t)$ , where  $\vec{X}(t)$  not locally parallel, for any  $t > 0$ , with respect to a non-trivial weighting function.

## Tangential Movement

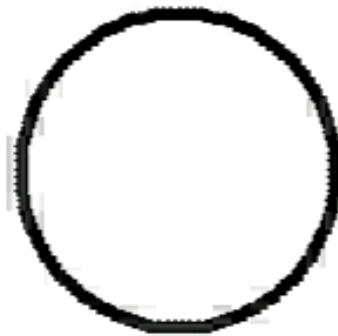
$$(SD_\gamma) \quad \gamma(\vec{p}) = \sqrt{p_1^2 + 0.1 p_2^2} \quad \Rightarrow \quad \text{Wulff shape is } \sqrt{10} : 1 \text{ ellipse}$$

$$N = 128, \tau = 10^{-3}, T = 1.$$



$$(SD_\gamma) \quad \gamma(\vec{p}) = \sqrt{p_1^2 + 0.01 p_2^2} \quad \Rightarrow \quad \text{Wulff shape is } 10 : 1 \text{ ellipse}$$

$$N = 128, \tau = 10^{-3}, T = 1.$$



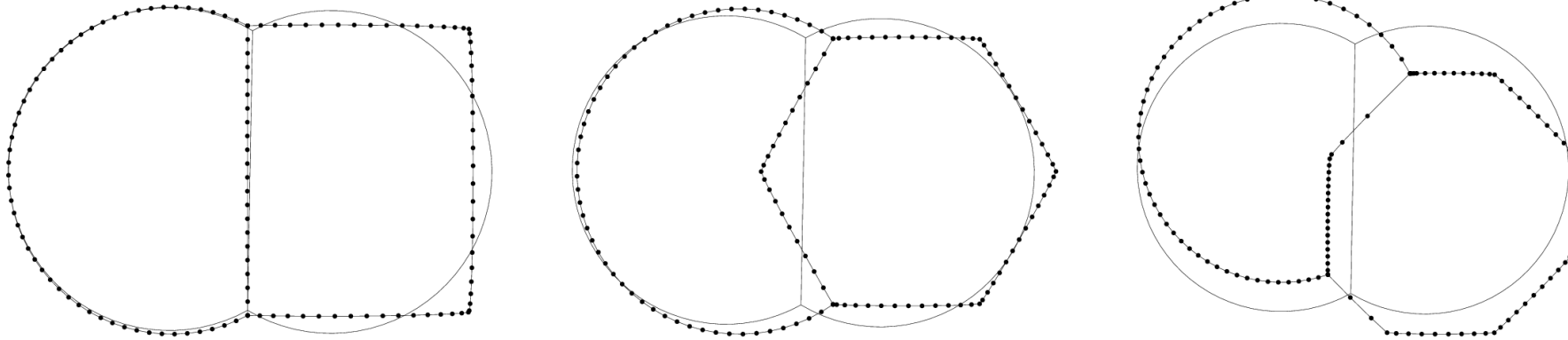
All the previous algorithms for curves (e.g networks,  $\mathbb{R}^d$ , geodesic flows) can be generalised to the anisotropic case.

Linear system. Existence, uniqueness, stability and equidistribution.

# Anisotropic Double Bubbles

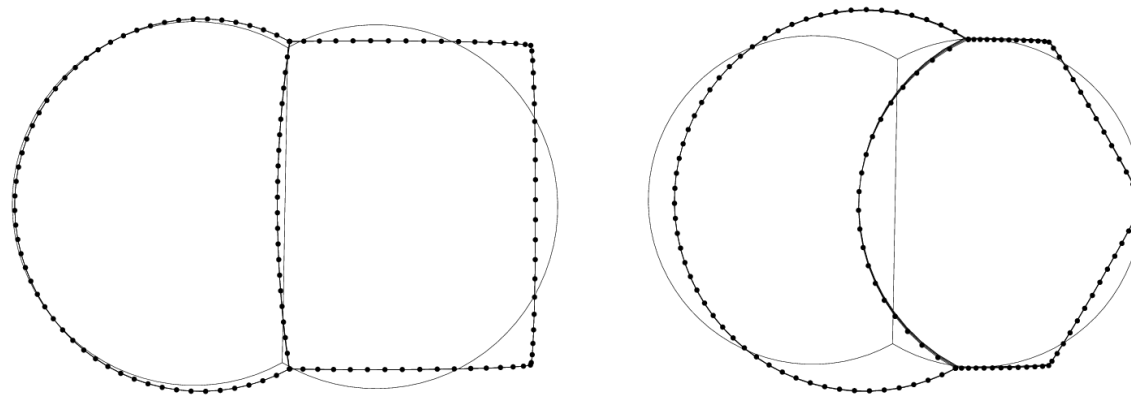
E.g.  $(SD_\gamma)$  :  $\gamma_1(\vec{p}) = |\vec{p}|$ ,  $\gamma_i(\vec{p}) = \gamma_0(\vec{p})$ ,  $i = 2 \rightarrow 3$ .

$$\varepsilon_\ell^2 \equiv 0.001$$



$\gamma_1(\vec{p}) = \gamma_2(\vec{p}) = |\vec{p}|$ ,  $\gamma_3(\vec{p}) = \gamma_0(\vec{p})$ .

$$\varepsilon_\ell^2 \equiv 0.001$$



## Anisotropic Surface Energies for $d = 3$

Introduce a symmetric anisotropic version of  $\varkappa \vec{\nu} = \Delta_s \vec{x}$ , as opposed to

$$\varkappa_\gamma \vec{\nu} = -\nabla_s \cdot (\vec{\nu} [\gamma'(\vec{\nu})]^T) + \nabla_s \cdot (\gamma(\vec{\nu}) \nabla_s \vec{x}) - \gamma(\vec{\nu}) \Delta_s \vec{x}.$$

For

$$\gamma(\vec{p}) = \left( \sum_{\ell=1}^L [\gamma_\ell(\vec{p})]^r \right)^{\frac{1}{r}}, \quad \gamma_\ell(\vec{p}) := \sqrt{\vec{p} \cdot G_\ell \vec{p}}, \quad r \in [1, \infty),$$

where  $G_\ell \in \mathbb{R}^{3 \times 3}$ ,  $\ell = 1 \rightarrow L$ , are symmetric and positive definite, we obtain the identity

$$\varkappa_\gamma \vec{\nu} = \sum_{\ell=1}^L \gamma_\ell(\vec{\nu}) \tilde{G}_\ell \nabla_s^{\tilde{G}_\ell} \cdot \left[ \left[ \frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})} \right]^{r-1} \nabla_s^{\tilde{G}_\ell} \vec{x} \right].$$

Here

$$\tilde{G}_\ell := [\det G_\ell]^{\frac{1}{2}} G_\ell^{-1}, \quad \ell = 1 \rightarrow L,$$

and  $\nabla_s^{\tilde{G}_\ell}$ ,  $\nabla_s^{\tilde{G}_\ell}$  are anisotropic surface gradient and divergence operators induced by the inner product

$$(\vec{u}, \vec{v})_{\tilde{G}_\ell} := \vec{u} \cdot \tilde{G}_\ell \vec{v} \quad \forall \vec{u}, \vec{v} \in \mathbb{R}^3.$$

# Parametric Finite Element Approximation

Based on the identity

$$\kappa_\gamma \vec{\nu} = \sum_{\ell=1}^L \gamma_\ell(\vec{\nu}) \tilde{G}_\ell \nabla_s^{\tilde{G}_\ell} \cdot \left[ \left[ \frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})} \right]^{r-1} \nabla_s^{\tilde{G}_\ell} \vec{x} \right],$$

we obtain

( $\mathcal{P}_\gamma^h$ ) Find  $\{\vec{X}^{m+1}, \kappa_\gamma^{m+1}\} \in \underline{V}^h(\Gamma^m) \times V^h(\Gamma^m)$  such that

$$\left\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi \vec{\nu}^m \right\rangle_m^h - \begin{cases} \langle \kappa_\gamma^{m+1}, \chi \rangle_m^h \\ \langle \nabla_s \kappa_\gamma^{m+1}, \nabla_s \chi \rangle_m \end{cases} = 0 \quad \forall \chi \in V^h(\Gamma^m),$$

$$\langle \kappa_\gamma^{m+1} \vec{\nu}^m, \vec{\eta} \rangle_m^h + \sum_{\ell=1}^L \int_{\Gamma^m} \left[ \frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})} \right]^{r-1} (\nabla_s^{\tilde{G}_\ell} \vec{X}^{m+1}, \nabla_s^{\tilde{G}_\ell} \vec{\eta})_{\tilde{G}_\ell} \gamma_\ell(\vec{\nu}^m) ds = 0$$

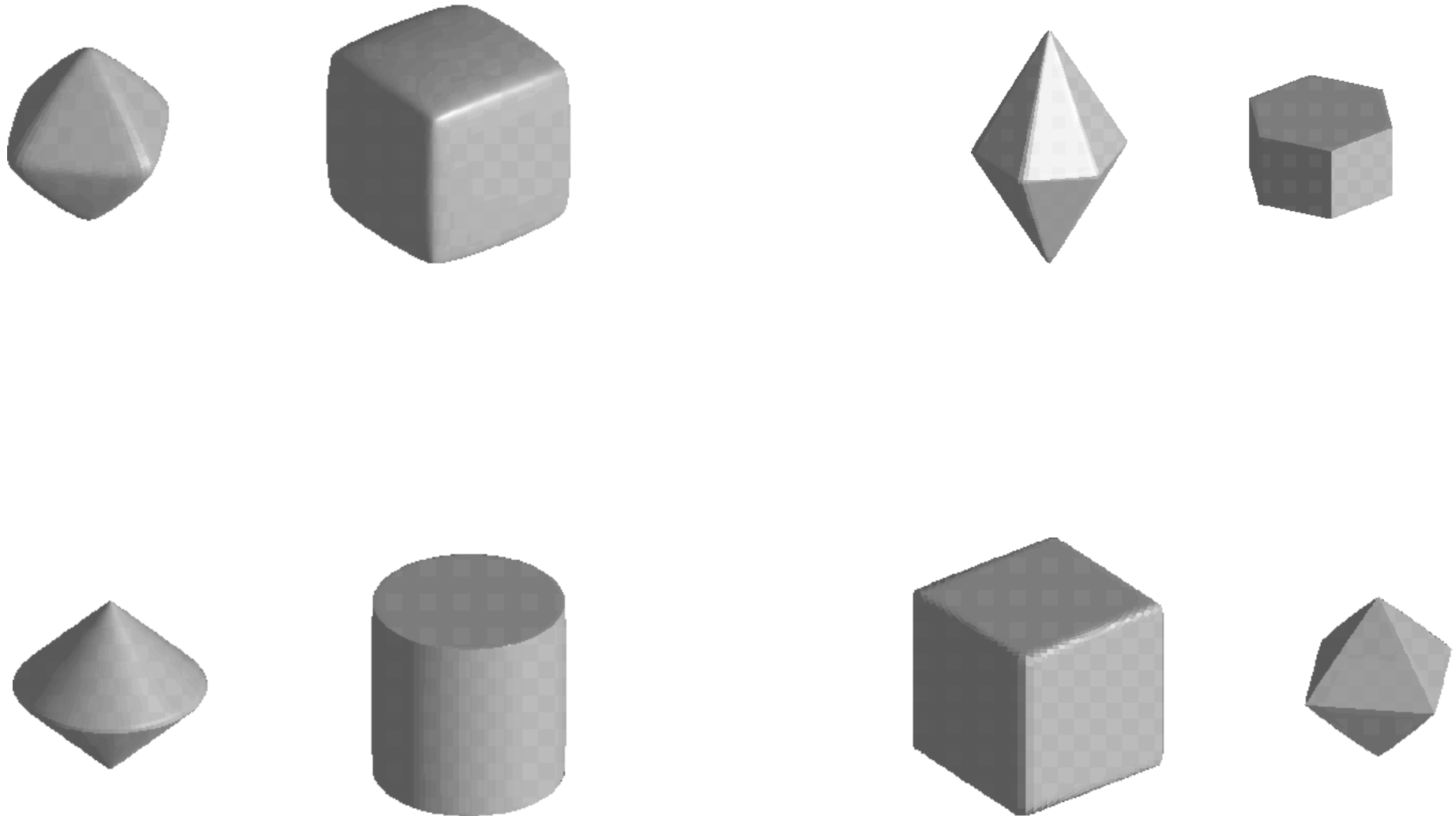
$$\forall \vec{\eta} \in \underline{V}^h(\Gamma^m).$$

$r = 1$ : Linear system. Existence, uniqueness and stability.

$r > 1$ : Nonlinear system. Stability.

# Wulff Shapes $d = 3$

Examples of Frank diagrams  $\mathcal{F}$  and associated Wulff shapes  $\mathcal{W}$ :

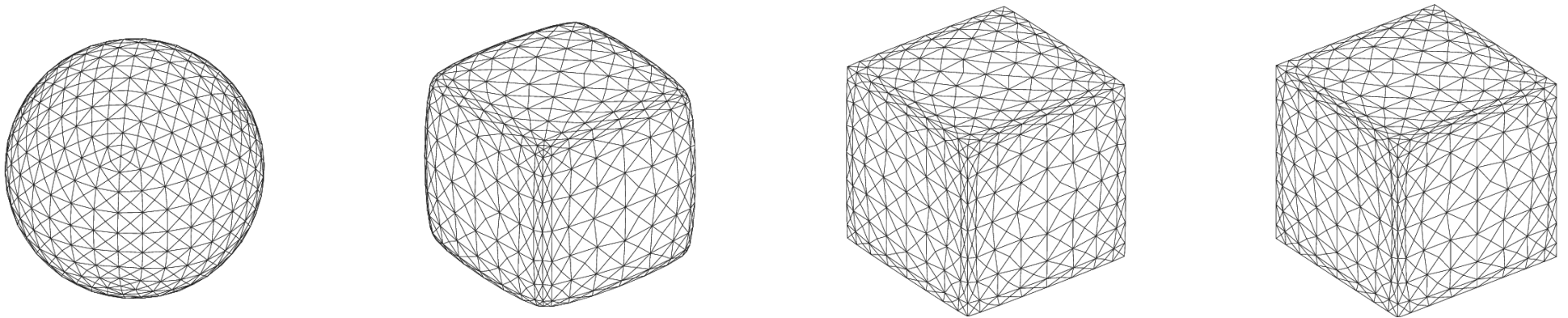


## Numerical Results

(SD $_{\gamma}$ ) - Cubic Wulff Shape,

i.e.  $\gamma(\vec{p}) = \sum_{i=1}^d \sqrt{\varepsilon^2 |\vec{p}|^2 + p_i^2 (1 - \varepsilon^2)}$  is a regularized  $l^1$ -norm.

( $r = 1$ ,  $L = 3$ ,  $G_1 = \text{diag}(1, \varepsilon^2, \varepsilon^2)$ ,  $G_2 = \text{diag}(\varepsilon^2, 1, \varepsilon^2)$ ,  $G_3 = \text{diag}(\varepsilon^2, \varepsilon^2, 1)$ )



A plot of  $\vec{X}(0.5)$  for  $\varepsilon = 10^{-k}$ ,  $k = 0 \rightarrow 3$ .

( $K = 770$ ,  $J = 1536$ ,  $\tau = 10^{-3}$ )

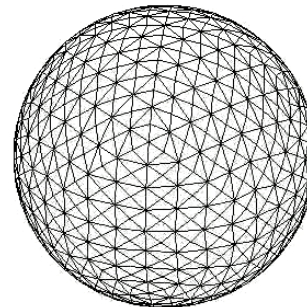
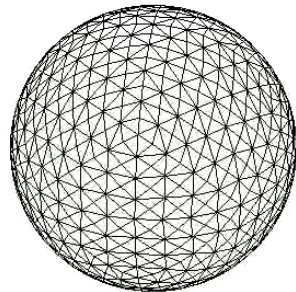
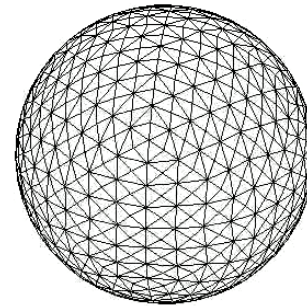
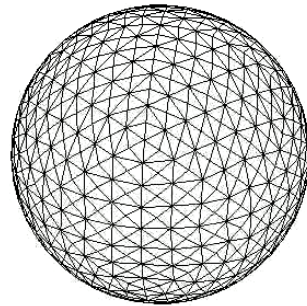
## Numerical Results

$(SD_\gamma)$  - Cube ( $r = 1, L = 3$ ),

Hexagonal Prism ( $r = 1, L = 4$ ),

Octahedron ( $r = 30, L = 3$ ),

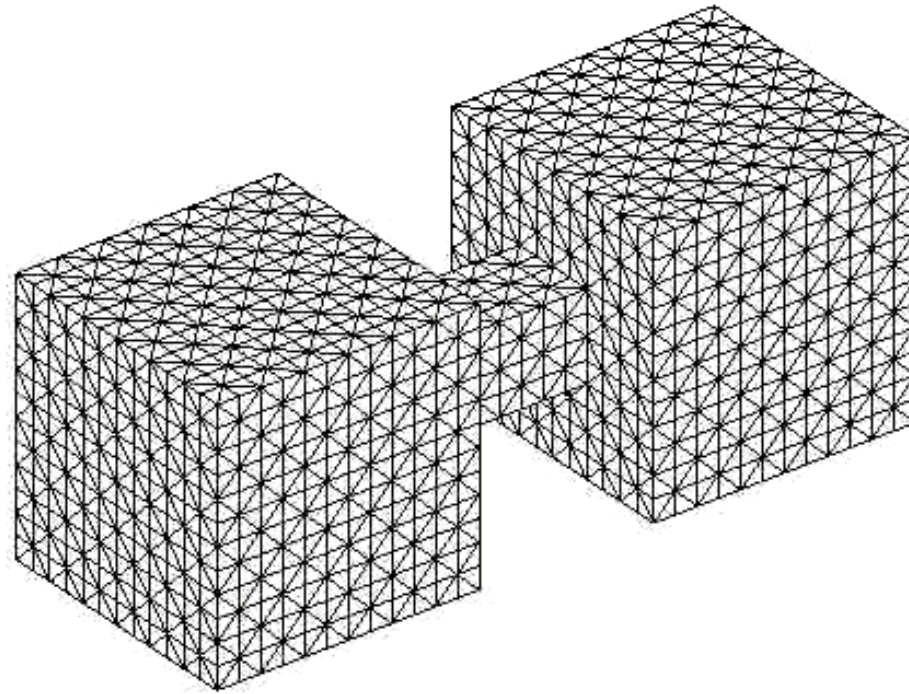
Cylinder Wulff Shape ( $r = 1, L = 2$ ).



$(\varepsilon = 10^{-2}, K = 770, J = 1536, \tau = 10^{-4}, T = 0.1, 0.25, 0.02, 0.25)$

## Numerical Results

$(MC_\gamma)$  - Cubic Wulff Shape ( $r = 1$ ,  $L = 3$ ,  $\varepsilon = 10^{-2}$ )

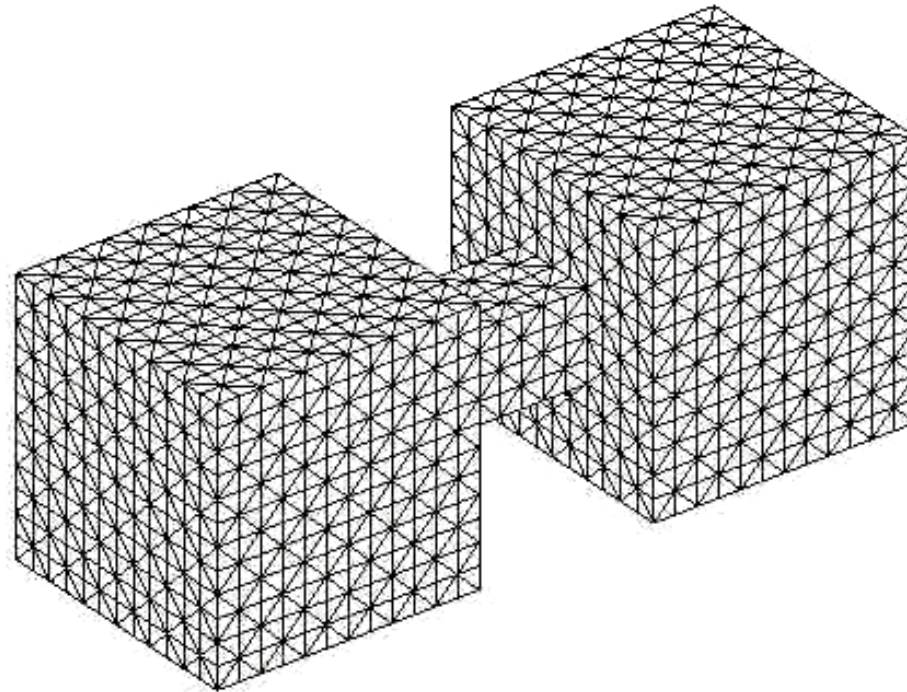


Dumbbell

$(K = 1826, J = 3648, \tau = 10^{-4}$  and  $T = 0.18)$

## Numerical Results

$(SD_\gamma)$  - Cubic Wulff Shape ( $r = 1$ ,  $L = 3$ ,  $\varepsilon = 10^{-2}$ )

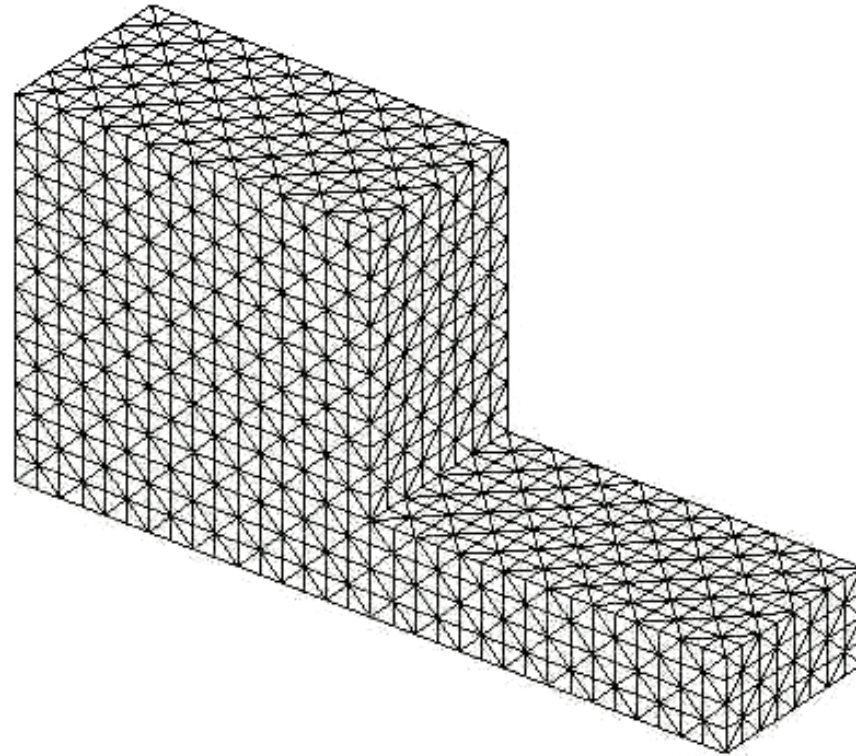


Dumbbell

$(K = 1826, J = 3648, \tau = 10^{-4}$  and  $T = 3.5)$

## Numerical Results

$(SD_\gamma)$  - Cubic Wulff Shape ( $r = 1$ ,  $L = 3$ ,  $\varepsilon = 10^{-2}$ )



Facet breaking

$(K = 1410, J = 2816, \tau = 10^{-3}, T = 5)$

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