A generalized MBO diffusion generated method for constrained harmonic maps

Braxton Osting

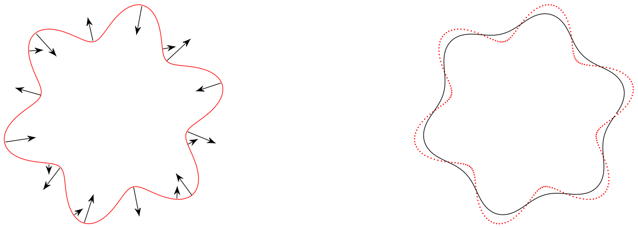
University of Utah

February 10, 2018

Inverse Problems and Machine Learning

Based on joint work with Dong Wang and Ryan Viertel

Motion by mean curvature



Mean curvature flow arises in a variety of physical applications

- Related to surface tension
- A model for the formation of grain boundaries in crystal growth

Some ideas for numerical computation:

- we could parameterize the surface and compute

$$H = -\frac{1}{2}\nabla \cdot \hat{n}$$

- If the surface is implicitly defined by the equation $F(x, y, z) = 0$, then mean curvature can be computed

$$H = -\frac{1}{2}\nabla \cdot \left(\frac{\nabla F}{|\nabla F|}\right)$$

MBO diffusion generated motion

In 1992, Merriman, Bence, and Osher (MBO) developed an iterative method for evolving an interface by mean curvature.

Repeat until convergence:

Step 1. Solve the Cauchy problem for the diffusion equation (heat equation)

$$u_t = \Delta u$$
$$u(x, t = 0) = \chi_D,$$

with initial condition given by the indicator function χ_D of a domain D until time τ to obtain the solution $u(x, \tau)$.

Step 2. Obtain a domain D_{new} by thresholding:

$$D_{\text{new}} = \left\{ x \in \mathbb{R}^d : u(x, \tau) \geq \frac{1}{2} \right\}.$$

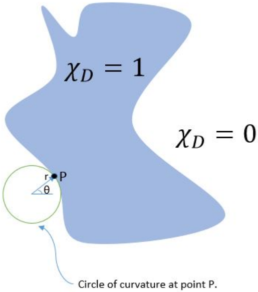
How to understand the MBO method?

From pictures, one can easily see:

- diffusion quickly blunts sharp points on the boundary and
- diffusion has little effect on the flatter parts of the boundary.

Formally, consider a point $P \in \partial D$. In local polar coordinates with the origin at P, the diffusion equation is given by

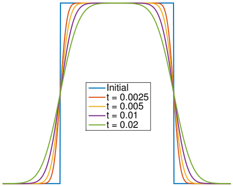
$$\frac{\partial u}{\partial t} = \frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}.$$



Considering local symmetry, we have

$$\begin{aligned}\frac{\partial u}{\partial t} &= \frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial r^2} \\ &= {\color{red}H}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial r^2}.\end{aligned}$$

The $\frac{1}{2}$ level set will move in the normal direction with velocity given by the mean curvature, H.



A variational point of view: Modica+Mortola, Allen+Cahn, Ginzburg+Landau

Define the energy

$$J_\varepsilon(u) = \int_\Omega \frac{1}{2}|\nabla u(x)|^2 + \frac{1}{\varepsilon^2} W(u(x))\, dx$$

where $W(u) = \frac{1}{4}\left(u^2 - 1\right)^2$ is a double well potential.

Theorem (Modica+ Mortola, 1977) A minimizing sequence (u_ε) converges (along a subsequence) to $\chi_D - \chi_{\Omega \setminus D}$ in L^1 for some $D \subset \Omega$. Furthermore,

$$\varepsilon J_\varepsilon(u_\varepsilon) \to \frac{2\sqrt{2}}{3}\mathcal{H}^{d-1}(\partial D) \qquad \text{as } \varepsilon \to 0.$$

Gradient flow. The L^2 gradient flow of J_ε gives the Allen-Cahn equation:

$$u_t = \Delta u - \frac{1}{\varepsilon^2} W'(u) \qquad \text{in } \Omega.$$

Operator/energy splitting. Repeat the following two steps until convergence:

- **Step 1.** Solve the diffusion equation until time τ with initial condition $u(x, t = 0) = \chi_D$

$$\partial_t u = \Delta u$$

- **Step 2.** Solve the (pointwise defined!) equation until time τ:

$$\phi_t = -W'(\phi)/\varepsilon^2, \quad \phi(x, 0) = u(x, \tau), \qquad \text{in } \Omega.$$

- **Step 2*.** Rescaling $\tilde{t} = \varepsilon^{-2} t$, we have as $\varepsilon \to 0$, $\varepsilon^{-2}\tau \to \infty$. So, Step 2 is equivalent to thresholding:

$$\phi(x, \infty) = \begin{cases} 1 & \text{if } \phi(x,0) > 1/2 \\ 0 & \text{if } \phi(x,0) < 1/2 \end{cases}.$$

Analysis, extensions, applications, connections, and computation

- Proof of convergence of the MBO method to mean curvature flow [Evans1993, Barles and Georgelin 1995, Chambolle and Novaga 2006, Laux and Swartz 2017, Swartz and Yip 2017].

- Multi-phase problems with arbitrary surface tensions [Esedoglu and Otto 2015, Laux and Otto 2016]

- Numerical algorithms [Ruuth 1996, Ruuth 1998]
- Adaptive methods based on NUFFT [Jiang et. al. 2017]

- Area or volume preserving interface motion [Ruuth 2003]
- Image processing [Esedoglu et al. 2006, Merkurjev et al. 2013, Wang et. al. 2017]
- Problems of anisotropic interface motion [Merriman et al. 2000, Ruuth et al. 2001, Bonnetier et al. 2010, Elsey et al. 2016]
- Diffusion generated motion using signed distance function [Esedoglu et al. 2009]
- High order geometric motion [Esedoglu 2008]
- Nonlocal threshold dynamics method [Caffarelli and Souganidis 2010]
- Wetting problem on solid surfaces [Xu et. al. 2017],
- Graph partitioning and data clustering [van Gennip et. al. 2013]
- Auction dynamics [Jacobs et. al. 2017]
- Centroidal Voronoi Tessellation [Du 1999]

Generalized energies

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with smooth boundary.
Let $T \subset \mathbb{R}^k$ be the "target set" and $f\colon \mathbb{R}^k \to \mathbb{R}_+$ be a smooth function such that $T = f^{-1}(0)$.
$\implies$ T is the set of global minimizers of f.
Roughly, we want $f(x) \approx \text{dist}^2(x, T)$.

Consider the generalized variational problem,

$$\inf_{u\colon \Omega \to T} E(u) \qquad \text{where} \quad E(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 \, dx$$

Relax the energy to obtain:

$$\min_{u \in H^1(\Omega;\mathbb{R}^k)} E_\varepsilon(u) \qquad \text{where} \quad E_\varepsilon(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 \; + \; \frac{1}{\varepsilon^2} f\left(u(x)\right) \, dx.$$

Examples.

k	T	f(x)	comment
1	$\{\pm 1\}$	$\frac{1}{4}(x^2 - 1)^2$	Allen-Cahn
2	$\mathbb{S}^1$	$\frac{1}{4}(\lvert x\rvert^2 - 1)^2$	Ginzburg-Landau
n^2	$O(n)$	$\frac{1}{4}\lVert x^t x - I_n\rVert_F^2$	orthogonal matrix valued fields
k	coordinate axes, Σ_k	$\frac{1}{4}\sum_{i\neq j} x_i^2 x_j^2$	Dirichlet partitions
k	$\mathbb{S}^{k-1}$	$\frac{1}{4}(\lvert x\rvert^2 - 1)^2$	
	$\mathbb{RP}^2$		Landau-de Gennes model for nematic liquid crystals
		$\vdots$	

A diffusion generated method for the Ginzburg-Landau model

$$E_\varepsilon(u) = \int_\Omega \frac{1}{2}|\nabla u(x)|^2 \; + \; \frac{1}{4\varepsilon^2}\left(|u(x)|^2 - 1\right)^2 \, dx.$$

k	T	f(x)	comment
2	$\mathbb{S}^1$	$\frac{1}{4}(\lvert x\rvert^2 - 1)^2$	Ginzburg-Landau

The nearest-point projection map, $\Pi_T : \mathbb{R}^2 \to T$, for $T = \mathbb{S}^1$ is given by

$$\Pi_T x = \frac{x}{|x|}.$$

- S. J. Ruuth, B. Merriman, J. Xin, and S. Osher, Diffusion-Generated Motion by Mean Curvature for Filaments, J. Nonlinear Sci. **11** (2001).

Diffusion generated method. For $i = 1, 2, \ldots$,

- **Step 1.** Solve the diffusion equation until time τ

$$\partial_t u = \Delta u$$
$$u(x, t = 0) = \phi_i$$

- **Step 2.** Point-wise, apply the nearest-point projection map:

$$\phi_{i+1}(x) = \Pi_T u(x, \tau).$$

Application: Quad meshing, joint work with Ryan Viertel (U. Utah)

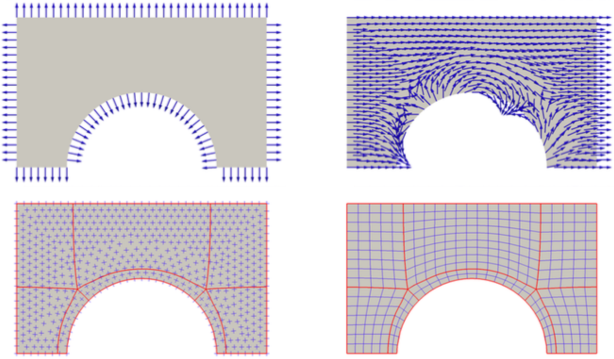
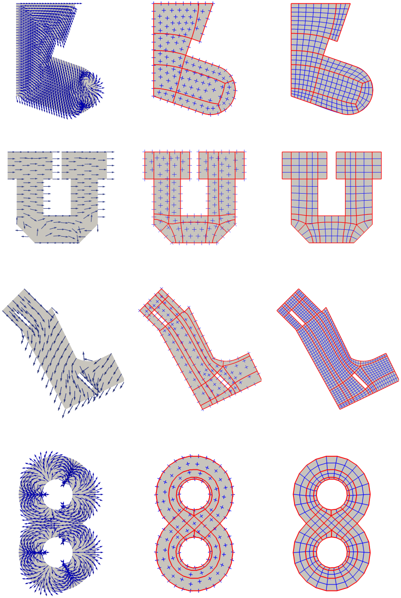
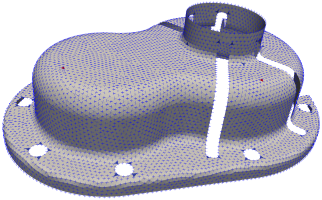


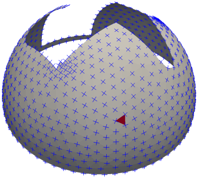
FIG. 2. **Overview of the cross field based meshing methods. (top left)** *The domain is shown with outward pointing normals.* **(top right)** *A 4-aligned boundary condition is assigned (see Definition 3.12) and a representation vector field is found by approximately minimizing the Ginzburg-Landau energy.* **(bottom left)** *The representation field is mapped to a smooth cross field and separatrices of the cross field are traced to partition the domain into a quad layout.* **(bottom right)** *A regular mesh is mapped into each region.*

Theorem [Viertel + O. (2017)] If no separatrix of u converges to a limit cycle, then the separatrices of U, along with ∂D partition D into a 4 sided partition.

Examples of quad meshes







Orthogonal matrix valued fields
— joint work with Dong Wang (U. Utah)

Let $O_n \subset M_n = \mathbb{R}^{n\times n}$ be the group of orthogonal matrices.

$$\inf_{A\colon \Omega\to O_n} E(A), \qquad \text{where } E(A) := \frac{1}{2}\int_\Omega \|\nabla A\|_F^2 \, dx.$$

Relaxation:

$$\min_{A\in H^1(\Omega,M_n)} E_\varepsilon(A), \qquad \text{where } E_\varepsilon(A) := \int_\Omega \frac{1}{2}\|\nabla A\|_F^2 + \frac{1}{4\varepsilon^2}\|A^tA - I_n\|_F^2 \, dx.$$

The penalty term can be written:

$$\frac{1}{4\varepsilon^2}\|A^tA - I_n\|_F^2 = \frac{1}{\varepsilon^2}\sum_{i=1}^n W(\sigma_i(A)), \qquad \text{where } W(x) = \frac{1}{4}\left(x^2-1\right)^2.$$

Gradient Flow. The gradient flow of E_ε is

$$\partial_t A = -\nabla_A E_\varepsilon(A) = \Delta A - \varepsilon^{-2}A(A^tA - I_n).$$

Special cases.

- For $n = 1$, we recover Allen-Cahn equation.
- For $n = 2$, if the initial condition is taken to be in $SO(2) \cong S^1$, we recover the complex Ginzburg-Landau equation.

Diffusion generated method for O_n valued fields

$$E_\varepsilon(A) := \int_\Omega \frac{1}{2}\|\nabla A\|_F^2 + \frac{1}{4\varepsilon^2}\|A^t A - I_n\|_F^2 \, dx.$$

k	T	f(x)	comment
n^2	$O(n)$	$\frac{1}{4}\|x^t x - I_n\|_F^2$	orthogonal matrix valued fields

Lemma. The nearest-point projection map, $\Pi_T : \mathbb{R}^{n\times n} \to T$, for $T = O_n$ is given by

$$\Pi_T A = A(A^t A)^{-\frac{1}{2}} = UV^t,$$

where A has the singular value decomposition, $A = U\Sigma V^t$.

Diffusion generated method. For $i = 1, 2, \ldots,$

- **Step 1.** Solve the diffusion equation until time τ

$$\partial_t u = \Delta u$$
$$u(x, t = 0) = \phi_i$$

- **Step 2.** Point-wise, apply the nearest-point projection map:

$$\phi_{i+1}(x) = \Pi_T u(x, \tau).$$

Computational Example I: flat torus, $n = 2$

closed line defect

vol. const. closed line defect

parallel lines defect

parallel lines defect

$$O(n) = SO(n) \cup SO^{-}(n),\ \ SO(2) \cong S^1$$

$$\begin{array}{lllll} x \text{ is yellow} & \iff & \det(A(x)) = 1 & \iff & A(x) \in SO(n) \\ x \text{ is blue} & \iff & \det(A(x)) = -1 & \iff & A(x) \in SO^{-}(n). \end{array}$$

$$\operatorname{ind}(\gamma) := \frac{1}{2\pi}\left[\arg v(\gamma(1)) - \arg v(\gamma(0))\right]$$

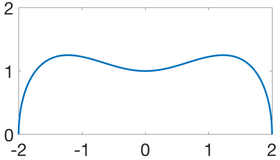
Computational Example II: sphere, $n = 3$

shrinking on sphere

vol. const. on sphere

Computational Example III: peanut, $n = 3$

$$x(t,\theta) = (3t - t^3),$$
$$y(t,\theta) = \frac{1}{2}\sqrt{(1+x^2)(4-x^2)}\cos(\theta),$$
$$z(t,\theta) = \frac{1}{2}\sqrt{(1+x^2)(4-x^2)}\sin(\theta)$$



peanut with closed geodesic

Lyapunov function for MBO iterates

Let Ω be a closed surface.
Motivated by (Esedoglu + Otto, 2015), we define the functional $E^\tau : H^1(\Omega, M_n) \to \mathbb{R}$, given by

$$E^\tau(A) := \frac{1}{\tau}\int_\Omega n - \langle A, e^{\Delta\tau}A\rangle_F \, dx$$

Here, $e^{\tau\Delta}A$ denotes the solution to the heat equation at time τ with initial condition at time $t = 0$ given by $A = A(x)$.

Denoting the spectral norm by $\|A\|_2 = \sigma_{\max}(A)$, the convex hull of O_n is

$$K_n = \text{conv } O_n = \{A \in M_n \colon \|A\|_2 \le 1\}.$$

Lemma. The functional E^τ has the following elementary properties.

(i) For $A \in L^2(\Omega, O_n)$, $\quad E^\tau(A) = E(A) + O(\tau)$.

(ii) $E^\tau(A)$ is concave.

(iii) We have

$$\min_{A \in L^2(\Omega, O_n)} E^\tau(A) = \min_{A \in L^2(\Omega, K_n)} E^\tau(A).$$

(iv) $E^\tau(A)$ is Fréchet differentiable with derivative $L^\tau_A : L^\infty(\Omega, M_n) \to \mathbb{R}$ at A in the direction B given by

$$L^\tau_A(B) = -\frac{2}{\tau}\int_\Omega \langle e^{\Delta\tau}A, B\rangle_F \, dx.$$

Stability

The *sequential linear programming* approach to minimizing $E^\tau(A)$ subject to $A \in L^\infty(\Omega, K_n)$ is to consider a sequence of functions $\{A_s\}_{s=0}^\infty$ which satisfies

$$A_{s+1} = \arg \min_{A \in L^\infty(\Omega, K_n)} L^\tau_{A_s}(A), \qquad A_0 \in L^\infty(\Omega, O_n) \text{ given.}$$

Lemma. If $e^{\Delta\tau} A_s = U \Sigma V^t$, the solution to the linear optimization problem,

$$\min_{A \in L^\infty(\Omega, K_n)} L^\tau_{A_s}(A).$$

is attained by the function $A^\star = UV^t \in L^\infty(\Omega, O_n)$.

Thus, $A_s \in L^\infty(\Omega, O_n)$ for all $s \geq 0$ and these are precisely the iterations generated by the generalized MBO diffusion generated motion!

Theorem (Stability). [O. + Wang, 2017] The functional E^τ is non-increasing on the iterates $\{A_s\}_{s=1}^\infty$, *i.e.*, $E^\tau(A_{s+1}) \leq E^\tau(A_s)$.

Proof. By the concavity of E^τ and linearity of $L^\tau_{A_s}$,

$$E^\tau(A_{s+1}) - E^\tau(A_s) \leq L^\tau_{A_s}(A_{s+1} - A_s) = L^\tau_{A_s}(A_{s+1}) - L^\tau_{A_s}(A_s).$$

Since $A_s \in L^\infty(\Omega, K_n)$, $L^\tau_{A_s}(A_{s+1}) \leq L^\tau_{A_s}(A_s)$ which implies $E^\tau(A_{s+1}) \leq E^\tau(A_s)$. □

Convergence

We consider a discrete grid $\tilde{\Omega} = \{x_i\}_{i=1}^{|\tilde{\Omega}|} \subset \Omega$ and a standard finite difference approximation of the Laplacian, $\tilde{\Delta}$, on $\tilde{\Omega}$. For $A\colon \tilde{\Omega} \to O_n$, define the discrete functional

$$\tilde{E}^\tau(A) = \frac{1}{\tau} \sum_{x_i \in \tilde{\Omega}} 1 - \langle A_i, (e^{\tilde{\Delta}\tau} A)_i \rangle_F$$

and its linearization by

$$\tilde{L}_A^\tau(B) = -\frac{2}{\tau} \sum_{x_i \in \tilde{\Omega}} \langle B_i, (e^{\tilde{\Delta}\tau} A)_i \rangle_F.$$

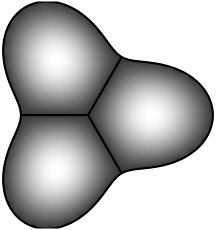
Theorem (Convergence for $n = 1$.) [O. + Wang, 2017]
Let $n = 1$. Non-stationary iterations of the generalized MBO diffusion generated motion strictly decrease the value of $\tilde{E}^\tau$ and since the state space is finite, $\{\pm 1\}^{|\tilde{\Omega}|}$, the algorithm converges in a finite number of iterations. Furthermore, for $m := e^{-\|\tilde{\Delta}\|\tau}$, each iteration reduces the value of J by at least $2m$, so the total number of iterations is less than $\tilde{E}^\tau(A_0)/2m$.

Theorem (Convergence for $n \geq 2$.) [O. + Wang, 2017]
Let $n \geq 2$. The non-stationary iterations of the generalized MBO diffusion generated motion strictly decrease the value of $\tilde{E}^\tau$. For a given initial condition $A_0\colon \tilde{\Omega} \to O_n$, there exists a partition $\tilde{\Omega} = \tilde{\Omega}_+ \amalg \tilde{\Omega}_-$ and an $S \in \mathbb{N}$ such that for $s \geq S$,

$$\det A_s(x_i) = \begin{cases} +1 & x_i \in \tilde{\Omega}_+ \\ -1 & x_i \in \tilde{\Omega}_- \end{cases}.$$

Lemma. $\operatorname{dist}\big(SO(n),\ SO^-(n)\big) = 2.$

Dirichlet partitions



3-partition of $U \subset \mathbb{R}^2$

Let $U \subseteq \mathbb{R}^d$ with $d \geq 2$ be an open bounded domain with Lipschitz boundary.

We say a collection of k disjoint open sets, $U_1, \ldots, U_k \subseteq U$ is a *Dirichlet k-partition of U* or simply a *Dirichlet partition* if it attains

$$\inf_{\substack{U_\ell \subset U \\ U_\ell \cap U_m = \emptyset}} \sum_{\ell=1}^{k} \lambda_1(U_\ell) \qquad \text{where} \quad \lambda_1(U) := \min_{\substack{u \in H_0^1(U) \\ \|u\|_{L^2(U)}=1}} E(u).$$

$E(u) := \int_U |\nabla u|^2 \, dx$ is the Dirichlet energy and $\|u\|_{L^2(U)} := \left(\int_U u^2(x) \, dx \right)^{\frac{1}{2}}$.

$\implies \lambda_1(U)$ is the first Dirichlet eigenvalue of the Laplacian, $-\Delta$.

Monotonicity of eigenvalues $\implies \overline{U} = \cup_{\ell=1}^{k} \overline{U_\ell}$.

A mapping formulation of Dirichlet partitions [Cafferelli and Lin (2007)]

Consider vector valued functions $\mathbf{u} = (u_1, u_2, \ldots, u_k)$, that take values in the singular space, Σ_k, given by the coordinate axes,

$$\Sigma_k := \left\{ x \in \mathbb{R}^k \colon \ \sum_{i \neq j}^k x_i^2 x_j^2 = 0 \right\}.$$

The Dirichlet partition problem for U is equivalent to the mapping problem

$$\min \left\{ \mathbf{E}(\mathbf{u}) \colon \mathbf{u} \in H_0^1(U; \Sigma_k), \int_U u_\ell^2(x)\, dx = 1 \text{ for all } \ell \in [k] \right\},$$

where $\mathbf{E}(\mathbf{u}) = \sum_{\ell=1}^k \int_U |\nabla u_\ell|^2 \, dx$ is the (weighted) Dirichlet energy and $H_0^1(U; \Sigma_k) = \{\mathbf{u} \in H_0^1(U; \mathbb{R}^k) \colon \mathbf{u}(x) \in \Sigma_k \text{ a.e.}\}$.

We refer to minimizers $\mathbf{u}$ as *ground states* and WLOG take $\mathbf{u} \geq 0$ and quasi-continuous.

$$\mathbf{u} \text{ is a ground state}$$
$$\Longleftrightarrow$$
$$U = \amalg_\ell U_\ell \text{ with } U_\ell = u_\ell^{-1}\big((0,\infty)\big) \text{ for } \ell \in [k] \text{ is a Dirichlet partition.}$$

Reformulation used to prove regularity results, such as $C^{1,\alpha}$-smoothness of the partition interfaces away from a set of codimension two.

Using the $TL^2(\Omega)$ framework developed by N. Garcia Trillos and D. Slepčev, together with Todd Reeb, we proved the consistency of Dirichlet partitions [O.+Reeb (2017)].

Diffusion generated method for computing Dirichlet partitions — joint work with Dong Wang (U. Utah)

k	T	f(x)	comment
k	coordinate axes, Σ_k	$\frac{1}{4}\sum_{i\neq j} x_i^2 x_j^2$	Dirichlet partitions

Relaxed energy: $E_\varepsilon(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 \ + \ \frac{1}{4\varepsilon^2}\sum_{i\neq j} u_i^2(x) u_j^2(x)\ dx$
Relaxed problem:

$$\min_{u\in H^1(\Omega;\mathbb{R}^k)} E_\varepsilon(u)$$
$$\text{s.t. } \|u_j\|_{L^2(\Omega)} = 1$$

The nearest-point projection map, $\Pi_T\colon \mathbb{R}^k \to T$, for $T = \Sigma_k$ is given by

$$(\Pi_T x)_i = \begin{cases} x_i & x_i = \max_j x_j \\ 0 & \text{otherwise} \end{cases}.$$

Diffusion generated method. For $i = 1, 2, \ldots,$

- **Step 1.** Solve the diffusion equation until time τ

$$\partial_t u = \Delta u$$
$$u(x, t = 0) = \phi_i$$

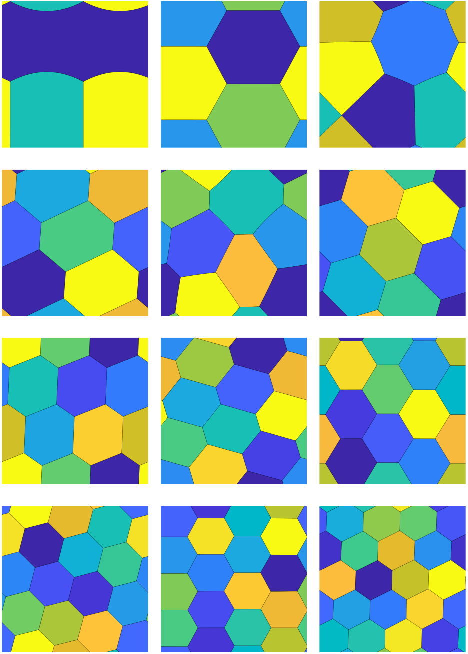
- **Step 2.** Point-wise, apply the nearest-point projection map:

$$\tilde{\phi}(x) = \Pi_T u(x, \tau).$$

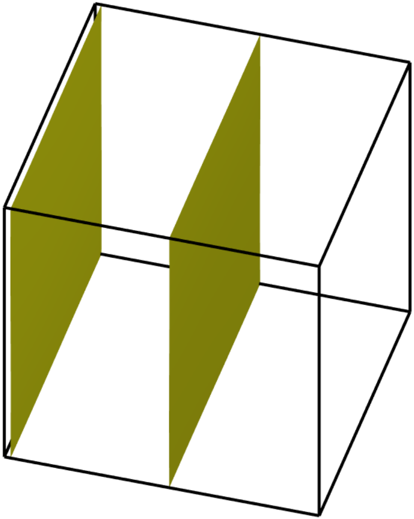
- **Step 3.** Normalize:

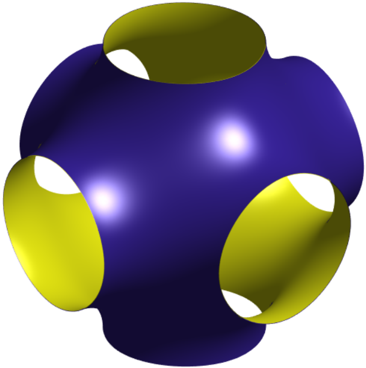
$$\phi_{i+1}(x) = \frac{\tilde{\phi}(x)}{\|\tilde{\phi}\|_{L^2(\Omega)}}.$$

Results for 2D flat tori, $k = 3$–$9, 11, 12, 15, 16$, and 20

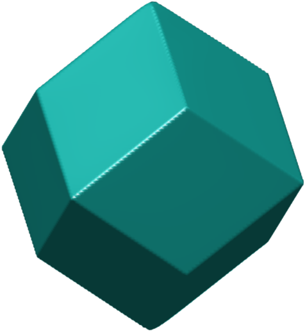


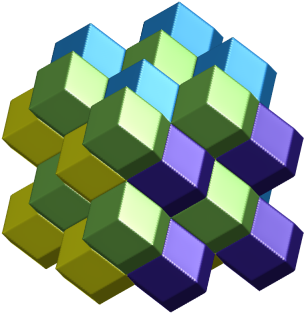
Results for 3D flat tori, $k = 2$



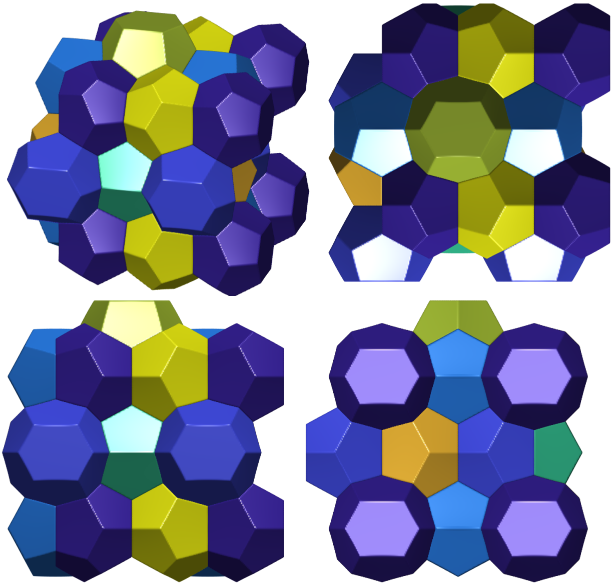


Results for 3D flat tori, $k = 4$, tessellation by rhombic dodecahedra

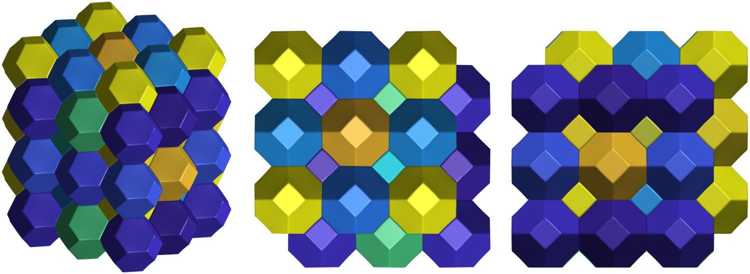




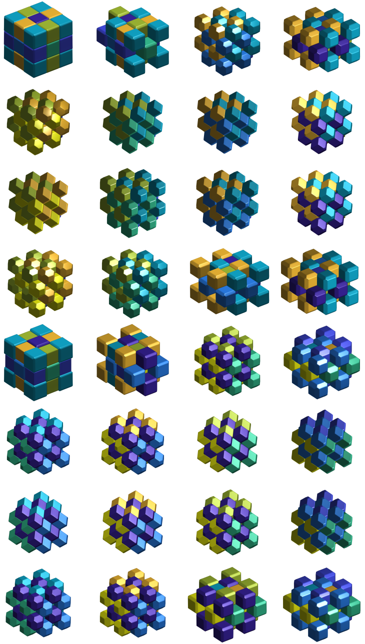
Results for 3D flat tori, $k = 8$, Weaire-Phelan structure



Results for 3D flat tori, $k = 12$, Kelvin's structure composed of truncated octahedra



Results for 4D flat tori, $k = 8$, 24-cell honeycomb



Discussion and future directions for generalized MBO methods

- We only considered a single matrix valued field that has two "phases" given by when the determinant is positive or negative. It would be very interesting to extend this work to the mutli-phase problem as was accomplished for $n = 1$ in [Esedoglu+Otto, 2015].
- For $O(n)$ valued fields with $n \geq 2$, the motion law for the interface is unknown.
- For $n = 2$ on a two-dimensional flat torus, further analysis regarding the winding number of the field is required. Is it possible to determine the final solution based on the winding number of the initial field?
- For problems with a non-trivial boundary condition, it not obvious how to adapt the Lyapunov functional.

Thanks! Questions? Email: osting@math.utah.edu

R. Viertel and B. Osting, An approach to quad meshing based on harmonic cross-valued maps and the Ginzburg-Landau theory, *submitted, arXiv:1708.02316* (2017).

B. Osting and D. Wang, A generalized MBO diffusion generated motion for orthogonal matrix valued fields, *submitted, arXiv:1711.01365* (2017).

D. Wang and B. Osting, A diffusion generated method for computing Dirichlet partitions, *submitted, arXiv:1802.02682* (2018).

Y. van Gennip, N. Guillen, B. Osting, and A. Bertozzi, Mean curvature, threshold dynamics, and phase field theory on finite graphs, *Milan J. Mathematics* **82** (2014).

Thanks to support by NSF DMS 16-19755.