A generalized MBO diffusion generated motion for constrained harmonic maps

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Workshop on Modeling and Simulation of Interface-related Problems
IMS, NUS, Singapore, May. 3, 2018
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

\[ H = -\frac{1}{2} \nabla \cdot \left( \frac{\nabla F}{|\nabla F|} \right) \]
In 1989, 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 \( \chi_D \) of a domain \( D \) until time \( \tau \) to obtain the solution \( u(x, \tau) \).

**Step 2.** Obtain a domain \( D_{\text{new}} \) 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?

Intuitively, 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, 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

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

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

\[ J_\varepsilon(u) = \int_\Omega \frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} W(u) \, du \]

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

**Theorem** (Modica+ Mortola, 1977) A minimizing sequence \((u_\varepsilon)\) converges (along a subsequence) to \( \chi_D \) in \( L^1 \) for some \( D \subset \Omega \). Furthermore,

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

**Gradient flow.** The \( L^2 \) gradient flow of \( J_\varepsilon \) gives the Allen-Cahn equation:

\[ u_t = \Delta u - \frac{1}{\varepsilon^2} W'(u) \quad \text{in } \Omega. \]
A variational point of view:

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

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

  $\partial_t u = \Delta u$

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

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

- **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:

  $\tilde{\phi}(x, \infty) = \begin{cases} 1 & \text{if } \phi(x, 0) > 1/2 \\ 0 & \text{if } \phi(x, 0) < 1/2 \end{cases}.$
Analysis, extensions, applications, connections, and computation

- Multi-phase problems with arbitrary surface tensions [Esedoglu and Otto 2015, Laux and Otto 2016]
- Area or volume preserving interface motion [Ruuth and Weston 2003]
- Diffusion generated motion using signed distance function [Esedoglu et al. 2009]
- High order geometric motion [Esedoglu et al. 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 et al. 1999]
- Quad meshing [Viertel and Osting 2017]
Generalized energies

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with smooth boundary.

Let $T \subset \mathbb{R}^k$ be "target set" and $f : \mathbb{R}^k \rightarrow \mathbb{R}^+$ be a smooth function such that $T = f^{-1}(0)$.

$T$ is the set of global minimizers of $f$. Roughly, we want $f(x) \approx \text{dist}^2(x; T)$.

Consider a generalized variational problem,

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

Relax the energy to obtain:

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

Examples.

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<td>$\frac{1}{4} (x^2 - 1)^2$</td>
<td>Allen-Cahn</td>
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<td>Orthogonal matrix valued fields</td>
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<td>$\mathbb{R}P^2$</td>
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Orthogonal matrix valued fields

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

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

**Relaxation:**

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

The penalty term can be written:

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

**Gradient Flow.** The gradient flow of $E_\varepsilon$ is

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

**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 motion for $O_n$ valued fields.

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

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**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 $\tau$ with initial value given by $A_i(x)$:

$$\partial_t u = \Delta u, \quad u(x, t = 0) = A_i(x).$$

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

$$A_{i+1}(x) = \Pi_T u(x, \tau).$$
Computational Example I: flat torus, $n = 2$

Closed line defect  \quad \text{vol. const. closed line defect}

Parallel lines defect  \quad \text{parallel lines defect}

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

$x$ is yellow  \quad \iff \quad \det(A(x)) = 1  \quad \iff \quad A(x) \in SO(n)

$x$ is blue  \quad \iff \quad \det(A(x)) = -1  \quad \iff \quad A(x) \in SO^-(n)$
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 functional for MBO iterates

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

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

$$K_n = \text{conv } O_n = \{ A \in M_n : \|A\|_2 \leq 1 \}.$$
Lemma. The functional $E^\tau$ has the following elementary properties.

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

(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

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

**Lemma.** If $e^{A_s \tau} = U\Sigma V^t$, 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 $A^* = UV^t \in L^\infty(\Omega, O_n)$.

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).** [Osting + W., 2017] The functional $E^\tau$ is non-increasing on the iterates $\{A_s\}_{s=1}^\infty$, i.e., $E^\tau(A_{s+1}) \leq E^\tau(A_s)$. 
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 $A: \tilde{\Omega} \to O_n$, 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

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

Theorem (Convergence for $n = 1$.) [Osting + W., 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 $n \geq 2$.) [Osting + W., 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 $A_0: \tilde{\Omega} \rightarrow O_n$, there exists a partition $\tilde{\Omega} = \tilde{\Omega}_+ \sqcup \tilde{\Omega}_-$ 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. $\text{dist}(SO(n), SO^-(n)) = 2$. 
Volume constrained problem

Definitions:

- $D_n$: A diagonal matrix with diagonal entries 1 everywhere except in the $n$–th position, where it is $-1$.

- $T^+(A) = \begin{cases} 
UV^t, & \text{if } \det A > 0, \\
UD_nV^t, & \text{if } \det A < 0.
\end{cases}$

- $T^-(A) = \begin{cases} 
UD_nV^t, & \text{if } \det A > 0, \\
UV^t, & \text{if } \det A < 0.
\end{cases}$

- $\Delta E(x) = \langle T^+(A(\tau, x)) - T^-(A(\tau, x)), A(\tau, x) \rangle_F$,

- $\Omega^\lambda_+ = \{x: \Delta E(x) \geq \lambda\}, \quad \Omega^\lambda_- = \Omega \setminus \Omega^\lambda_+$. 
Volume constrained problem

Similar as that in [Ruuth+Weston, 2003], we treat the volume of $\Omega_+^\lambda$ as a function of $\lambda$ and identify the value $\lambda$ such that $f(\lambda) = V$.

For the matrix case, the following lemma leads us to the optimal choice:

**Lemma.** Assume $\lambda_0$ satisfies $f(\lambda_0) = V$. Then,

$$B^* = \begin{cases} T^+(A(\tau, x)) & \text{if } \Delta E(x) \geq \lambda_0 \\ T^-(A(\tau, x)) & \text{if } \Delta E(x) < \lambda_0 \end{cases}$$

attains the minimum in

$$\min_{B \in L_\infty(\Omega, O_n)} L^T_A(B)$$

s.t. \(\text{vol}\{x : B(x) \in SO(n)\} = V\).

**Theorem (Stability).** [Osting+W., 2017] For any $\tau > 0$, the functional $E^\tau$, is non-increasing on the volume-preserving iterates $\{A_s\}_{s=1}^\infty$, i.e., $E^\tau(A_{s+1}) \leq E^\tau(A_s)$. 

Dirichlet partitions

Let $U \subset \mathbb{R}^d$ be either an open bounded domain with Lipschitz boundary. **Dirichlet k-partition:** A collection of $k$ disjoint open sets, $U_1, U_2, \ldots, U_k \subseteq U$, attains

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

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

- $\lambda_1(U)$ is the first Dirichlet eigenvalue of the Laplacian, $-\Delta$.
- Monotonicity of eigenvalues $\Rightarrow \overline{U} = \bigcup_{\ell=1}^{k} \overline{U_\ell}$. 
A mapping formulation of Dirichlet partitions [Cafferelli and Lin 2007]

Consider vector valued functions \( u = (u_1, u_2, \ldots, u_k) \), that takes values in the singular space, \( \Sigma_k \), given by the coordinate axes,

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

The Dirichlet partition problem for \( U \) is equivalent to the mapping problem

\[
\min \left\{ E(u) : u = (u_1, \ldots, u_k) \in H^1_0(U; \Sigma_k), \int_U u^2_\ell(x) \, dx = 1 \quad \forall \ell \in [k] \right\},
\]

where \( E(u) := \sum_{\ell=1}^k \int_U |\nabla u_\ell|^2 \, dx \) is the Dirichlet energy of \( u \) and \( H^1_0(U; \Sigma_k) = \{ u \in H^1_0(U, \mathbb{R}^k) : u \in \Sigma_k \text{ a.e.} \} \).

Refer to minimizers \( u \) as ground states, and WLOG take \( u > 0 \) and quasi-continuous.

\[
u \text{ is a ground state} \quad \iff \quad U = \coprod U_\ell \text{ with } U_\ell = u_\ell^{-1}((0, \infty)) \text{ for } \ell \in [k] \text{ is a Dirichlet partition.}\]
Diffusion generated method for computing Dirichlet partitions

\[ E_\varepsilon (u) := \int_\Omega \frac{1}{2} \| \nabla u \|^2_F + \frac{1}{4\varepsilon^2} \sum_{i \neq j} u_i^2(x) u_j^2(x) \, dx. \]

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

The nearest-point projection map, \( \Pi_T : \mathbb{R}^k \to T \), 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 \( i = 1, 2, \ldots \),

\[ \text{Step 1.} \text{ Solve the diffusion equation until time } \tau \]

\[ \partial_t \phi = \Delta \phi, \quad \phi(x, t = 0) = u_i(x). \]

\[ \text{Step 2.} \text{ Point-wise, apply the nearest-point projection map:} \]

\[ \tilde{u}_{i+1}(x) = \Pi_T \phi(x, \tau). \]

\[ \text{Step 3.} \text{ Normalize:} \]

\[ u_{i+1}(x) = \frac{\tilde{u}_{i+1}(x)}{\| \tilde{u}_{i+1} \|_{L^2(\Omega)}}. \]
Results for 2D flat tori, $k = 3 - 9, 11, 12, 15, 16, \text{ and } 20$. 
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
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 multi-phase problem as was accomplished for $n = 1$ in [Esedoglu+Otto, 2015].

For $O(n)$ valued fields with $n = 2$, 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: dwang@math.utah.edu
