The surface finite element method for pattern formation on evolving biological surfaces

Jianggang Liu

School of Mathematics and Computational Science

Xiangtan University

June 12, 2018

Abstract

In this article we propose models and a numerical method for pattern formation on evolving curved surfaces. We formulate reaction-diffusion equations on evolving surfaces using the material transport formula, surface gradients and diffusive conservation laws. The evolution of the surface is defined by a material surface velocity. The numerical method is based on the evolving surface finite element method. The key idea is based on the approximation of S by a triangulated surface S_h consisting of a union of triangles with vertices on S. A finite element space of functions is then defined by taking the continuous functions on S_h which are linear affine on each simplex of the polygonal surface.

We assume that S is a C^2-hyper-surface which is the zero level set of a signed distance function $d(x)$ defined on an open subset $\mathcal{U} \subset \mathbb{R}^3$. $\boldsymbol{n}(x) = \nabla d(x)$ is then unit outward pointing normal on S. We define the tangential gradient of a function η by

$$\nabla_S v = \nabla v - (\nabla v \cdot \boldsymbol{n})\boldsymbol{n} \quad x \in S$$

where ∇ denotes the usual gradient in $\mathbb{R}^3$.
The Laplace-Beltrami operator on S is defined as the tangential divergence of the tangential gradient:

$$\Delta_S v = \nabla_S \cdot (\nabla_S v) = \Delta v - (\nabla v \cdot \boldsymbol{n})(\nabla \cdot \boldsymbol{n}) - \boldsymbol{n}^t \nabla^2 v \boldsymbol{n}$$

where $\nabla^2 v$ is the Hessian matrix of v.

Let S have a boundary ∂S whose intrinsic unit outer normal, tangential to S, is denoted by $\boldsymbol{\nu}$ Then, the formula for integration by parts on S is

$$\int_S \nabla_S v = -\int_S vH\boldsymbol{n} + \int_{\partial S} v\boldsymbol{\nu}$$

where H denotes the mean curvature of S with respect to $\boldsymbol{n}$, which is given by

$$H = -\nabla_S \cdot \boldsymbol{n}$$

Green's formula on the surface S is

$$\int_S \nabla_S u \cdot \nabla_S v = \int_{\partial S} u\nabla_S v \cdot \boldsymbol{\nu} - \int_S u\Delta_S v.$$

Let $S(t)$ be an evolving two-dimensional hypersurface in $\mathbb{R}^3$ bounding a time-dependent domain $\Omega(t)$. Let the velocity of material points on $S(t)$ be denoted by $\boldsymbol{v} := V\boldsymbol{n} + \boldsymbol{v}_T$ where $\boldsymbol{n}$ is the unit outward pointing normal to $\Omega(t)$, V is the normal velocity and $\boldsymbol{v}_T$ is a velocity field tangential to the surface. Let $\boldsymbol{u}$ be a vector of scalar concentration fields $\{u_i\}_{i=1}^m$, Let $\mathcal{R}(t)$ be an arbitrary material portion of $S(t)$ where each point moves with the material velocity.According to the mass balance conservation law:

$$\frac{d}{dt}\int_{\mathcal{R}(t)} u_i = -\int_{\partial\mathcal{R}(t)} \boldsymbol{q}_i \cdot \boldsymbol{\nu} + \int_{\mathcal{R}(t)} f_i(\boldsymbol{u}) \qquad (1)$$

where, for each component i, $\boldsymbol{q}_i$ and $f_i(\boldsymbol{u})$ are respectively, the surface flux through the boundary of $\mathcal{R}(t)$ and the net production rate within the surface.

The components of $\boldsymbol{q}$ normal to S do not contribute to the flux so we can assume $\boldsymbol{q}$ is a tangent vector. Using integration by parts it follows that

$$\int_{\partial\mathcal{R}(t)} \boldsymbol{q}\cdot\boldsymbol{n} = \int_{\mathcal{R}(t)} \nabla_S\cdot\boldsymbol{q} + \int_{\mathcal{R}(t)} \boldsymbol{q}\cdot\boldsymbol{n}H = \int_{\mathcal{R}(t)} \nabla_S\cdot\boldsymbol{q}$$

On the other hand, for the left-hand side of (1), we use the transport formula

$$\frac{d}{dt}\int_{\mathcal{R}(t)} \eta = \int_{\mathcal{R}(t)} \partial\bullet\eta + \eta\nabla_S\cdot\boldsymbol{v}$$

for any material region of the surface evolving with the material velocity $\boldsymbol{v}$ where

$$\partial\bullet\eta := \eta_t + \boldsymbol{v}\cdot\nabla\eta \qquad (2)$$

denotes the material derivative.

Combining the two equations results in

$$\int_{\mathcal{R}(t)} \partial \bullet u_i + u_i \nabla_S \cdot \boldsymbol{v} + \nabla_S \cdot \boldsymbol{q}_i = \int_{\mathcal{R}(t)} f_i(\boldsymbol{u})$$

Since $\mathcal{R}(t)$ is arbitrary for all time t, we conclude that

$$\partial \bullet u_i + u_i \nabla_S \cdot \boldsymbol{v} + \nabla_S \cdot \boldsymbol{q}_i = f_i(\boldsymbol{u}) \qquad (3)$$

For the constitutive law relating the flux to the concentrations, assuming no cross-diffusion between the chemical species, we set $\mathcal{D}$ to be a diffusivity tensor(a diagonal matrix diffusion coefficients)and assume that the chemical species diffuse according to Fick's law

$$\boldsymbol{q}_i = -\mathcal{D}_{ij} \nabla_S u_j \qquad (4)$$

where $\mathcal{D}_{ij} = d_i \delta_{ij}$, with δ_{ij} representing the usual Kronecker delta function.

Then (3) becomes

$$\partial \bullet u_i + u_i \nabla_S \cdot \boldsymbol{v} = \nabla_S (\mathcal{D}_{ij} \nabla_S u_j) + f_i(\boldsymbol{u}) \quad on \quad S(t)$$

In vector form, the system of reaction-diffusion equations on an evolving surface $S(t)$ takes the form

$$\partial \bullet \boldsymbol{u} + \boldsymbol{u} \nabla_S \cdot \boldsymbol{v} = D \Delta_S \boldsymbol{u} + \boldsymbol{f}(\boldsymbol{u}) \qquad (5)$$

where $D = diag(d_i)$. This system is supplemented with zero-flux boundary conditions if the boundary of $S(t)$ is non-empty and the initial conditions

$$\boldsymbol{u}(\cdot, 0) = \boldsymbol{u}_0(\cdot) \quad on \quad S(0) \qquad (6)$$

where the components of $\boldsymbol{u}_0(\cdot)$ are prescribed positive bounded functions.

3.1 Variational formulation

For an arbitray i

$$\partial \bullet u_i + u_i \nabla_S \cdot \boldsymbol{v} = d_i \Delta_S u_i + f_i(\boldsymbol{u}) \qquad (7)$$

Let $\varphi(\cdot, t) \in H^1(S(t))$ be a test function. Multiplying(7) by φ and integrating over $S(t)$ leads to

$$\begin{aligned}\int_{S(t)} f_i(\boldsymbol{u})\varphi &= \int_{S(t)} \partial \bullet u_i\varphi + u_i\varphi\nabla_S \cdot \boldsymbol{v} - d_i \int_{S(t)} \varphi\Delta_S u_i \\ &= \int_{S(t)} \partial \bullet u_i\varphi + u_i\varphi\nabla_S \cdot \boldsymbol{v} + d_i \int_{S(t)} \nabla_S u_i \cdot \nabla_S\varphi \\ &- \int_{\partial S(t)} \varphi\nabla_S u_i \cdot \boldsymbol{\nu}. \qquad (8)\end{aligned}$$

The last term vanishes if $\partial S(t) = \varnothing$ or $\partial S(t) \neq \varnothing$ but $\varphi = 0$ or $\nabla_S u_i \cdot \boldsymbol{\nu} = 0$ on $\partial S(t)$. Hence, assuming any of these conditions holds we have

$$\begin{aligned}\int_{S(t)} f_i(\boldsymbol{u})\varphi &= \int_{S(t)} \partial \bullet u_i\varphi + u_i\varphi\nabla_S \cdot \boldsymbol{v} + d_i \int_{S(t)} \nabla_S u_i \cdot \nabla_S\varphi \\ &= \int_{S(t)} \partial \bullet (u_i\varphi) - u_i\partial \bullet \varphi + u_i\varphi\nabla_S \cdot \boldsymbol{v} + d_i \int_{S(t)} \nabla_S u_i \cdot \nabla_S\varphi \\ &= \frac{d}{dt}\int_{S(t)} u_i\varphi - \int_{S(t)} u_i\partial \bullet \varphi + d_i \int_{S(t)} \nabla_S u_i \cdot \nabla_S\varphi \qquad (9)\end{aligned}$$

The variational form seeks to find $u_i \in H^1(S(t))$ satisfying

$$\begin{aligned}&\frac{d}{dt}\int_{S(t)} u_i\varphi - \int_{S(t)} u_i\partial \bullet \varphi + d_i \int_{S(t)} \nabla_S u_i \cdot \nabla_S\varphi \\ &= \int_{S(t)} f_i(\boldsymbol{u})\varphi, \quad \forall\varphi \in H^1(S(t)) \qquad (10)\end{aligned}$$

3.2 Evolving surface finite element method

We approximate $S(t)$ by $S_h(t)$, a triangulated surface whose vertices lie on $S(t)$, *i, e.* $S_h(t) = \mathcal{T}_h(t) = \bigcup_k T_k(t)$, where each $T_k(t)$ is a triangle. The diameter of the largest triangle in the initial surface is denoted by h. We choose the vertices of the triangulation to evolve with the material velocity so that

$$\dot{X}_j(t) = \boldsymbol{v}(X_j(t), t) \qquad (11)$$

and it is easy to see that $X_j(t)$ lies on $S(t)$ if $\boldsymbol{v}$ is the exact material velocity. We assume $S_h(t)$ is smooth in time. For each t we define a finite element space

$$S_h(t) = \left\{ \phi \in C^0(S_h(t)) : \phi\Big|_{T_k} \text{ is linear affine for each } T_k \in \mathcal{T}_k(t) \right\}.$$

For each $t \in [0, T]$ we denote by $\left\{\chi_j(\cdot, t)_{j=1}^N\right\}$ the moving nodal basis functions and by $X_j(t)$, $j = 1, \cdots, N$ the nodes. These functions will satisfy

$$\chi_j(\cdot, t) \in C^0(S_h(t)), \quad \chi_j(X_i(t), t) = \delta_{ij}, \quad \chi_j(\cdot, t)\Big|_{T_k} \; is \quad linear \quad affine$$

and on $T_k \in \mathcal{T}_h(t)$

$$\chi_j\Big|_e = \lambda_k, \quad for \quad each \quad e \in \mathcal{T}_h(t)$$

where $k = k(T_k, j)$ and $(\lambda_1, \lambda_2, \lambda_3)$ are the barycentric coordinates. On $S_h(t)$ we define the discrete material velocity

$$\boldsymbol{v}_h = \sum_{j=1}^{N} \dot{X}_j(t)\chi_j \qquad (12)$$

and the discrete material derivative

$$\partial_h \bullet \phi = \phi_t + v_h \cdot \nabla\phi \qquad (13)$$

We seek approximations $U_i(\cdot, t) \in S_h(t)$ to u_i. Since $\left\{\chi_j(\cdot, t)_{j=1}^N\right\}$ is the basis of $S_h(t)$ we know for each $U_i(\cdot, t) \in S_h(t)$ and each $t \in [0, T]$ that there exist unique $\boldsymbol{\alpha}_i = \left\{\alpha_i^1(t), \ldots, \alpha_i^N(t)\right\}$ satisfying

$$U_i(\cdot, t) = \sum_{j=1}^{N} \alpha_i^j(t)\chi_j(\cdot, t).$$

Substituting $U_i(\cdot, t)$, $S_h(t)$ and $\phi \in S_h(t)$ for u_i, $S_(t)$ and φ in (10) we obtain

$$\frac{d}{dt}\int_{S_h(t)} \sum_{j=1}^{N} \alpha_i^j(t)\chi_j\phi - \int_{S_h(t)} \sum_{j=1}^{N} \alpha_i^j(t)\chi_j\partial_h \bullet \phi$$

$$+ d_i \int_{S_h(t)} \sum_{j=1}^{N} \alpha_i^j(t)\nabla_{S_h(t)}\chi_j \cdot \nabla_{S_h(t)}\phi = \int_{S_h(t)} f_i\phi, \qquad (14)$$

for all $\phi \in S_h(t)$ and taking $\phi = \chi_k, k = 1, \cdots, N$ and using the transport property of the basis functions we obtain

$$\frac{d}{dt}(\mathcal{M}(t)\boldsymbol{\alpha}_i) + d_i\mathcal{S}(t)\boldsymbol{\alpha}_i = \boldsymbol{F}_i(t) \qquad (15)$$

where $\mathcal{M}(t)$ is the evolving mass matrix

$$\mathcal{M}(t)_{jk} = \int_{S_h(t)} \chi_j \chi_k$$

$\mathcal{S}(t)$ is the evolving stiffness matrix

$$\mathcal{S}(t)_{jk} = \int_{S_h(t)} \nabla_{S_h}\chi_j \cdot \nabla_{S_h}\chi_k$$

and $\boldsymbol{F}_i$ is the right hand side $\boldsymbol{F}_{ij} = \int_{S_h(t)} f_i(\boldsymbol{U})\phi_j$

For simplicity we restrict the description to the two components system $\boldsymbol{u} = (u, w)$ with kinetics given by

$$\boldsymbol{f}(\boldsymbol{u}) = (f_1, f_2)^T = \big(\gamma(a - u + u^2 w), \gamma(b - u^2 w)\big)^T$$

and $d_1 = 1, d_2 = d$. We discretise in time using a uniform time step τ. We represent by (U^n, W^n) the solution at time $n\tau$. Let $U^0, W^0 \in S_h(0)$ be given. For $n = 0, \cdots, n_T$, solve the nonlinear system

$$\begin{cases} \dfrac{1}{\tau}\displaystyle\int_{S_h^{n+1}} U^{n+1}\chi_j^{n+1} + \int_{S_h^{n+1}} \nabla_{S_h^n} U^{n+1} \cdot \nabla_{S_h^n}\chi_j^{n+1} \\ = \dfrac{1}{\tau}\displaystyle\int_{S_h^n} U^n\chi_j^n + \int_{S_h^{n+1}} f_1(U^{n+1}, W^{n+1})\chi_j^{n+1} \\ \dfrac{1}{\tau}\displaystyle\int_{S_h^{n+1}} W^{n+1}\chi_j^{n+1} + d\int_{S_h^{n+1}} \nabla_{S_h^n} W^{n+1} \cdot \nabla_{S_h^n}\chi_j^{n+1} \\ = \dfrac{1}{\tau}\displaystyle\int_{S_h^n} W^n\chi_j^n + \int_{S_h^{n+1}} f_2(U^{n+1}, W^{n+1})\chi_j^{n+1} \end{cases}$$

For all $j = 1, \cdots, N$. To linearise $f_1(U^{n+1}, W^{n+1})$ we assume slow deformation of the evolving surface which allows us to write $(U^{n+1})^2 \approx U^n U^{n+1}$ (Madzvamuse 2006).
Using this linearisation, we can derive the following fully discrete algorithm:
Let $U^0, W^0 \in S_h(0)$ be given. For $n = 0, \cdots, n_T$, solve the linear system

$$\begin{cases} (\frac{1}{\tau} + \gamma) \int_{S_h^{n+1}} U^{n+1} \chi_j^{n+1} + \int_{S_h^{n+1}} \nabla_{S_h^n} U^{n+1} \cdot \nabla_{S_h^n} \chi_j^{n+1} \\ - \gamma \int_{S_h^{n+1}} U^n W^n U^{n+1} \chi_j^{n+1} = \frac{1}{\tau} \int_{S_h^n} U^n \chi_j^n + \gamma a \int_{S_h^n} \chi_j^n \\ \frac{1}{\tau} \int_{S_h^{n+1}} W^{n+1} \chi_j^{n+1} + d \int_{S_h^{n+1}} \nabla_{S_h^n} W^{n+1} \cdot \nabla_{S_h^n} \chi_j^{n+1} \\ + \gamma \int_{S_h^{n+1}} (U^{n+1})^2 W^{n+1} \chi_j^{n+1} = \frac{1}{\tau} \int_{S_h^n} W^n \chi_j^n + \gamma b \int_{S_h^n} \chi_j^n \end{cases}$$

For all $j = 1, \cdots, N$. Using a matrix representation we have

$$\begin{cases} \left(\left(\frac{1}{\tau} + \gamma\right) \mathcal{M}^{n+1} + \mathcal{S}^{n+1} - \gamma \mathcal{M}_1^{n+1}\right) \boldsymbol{U}^{n+1} = \frac{1}{\tau} \mathcal{M}^n \boldsymbol{U}^n + \boldsymbol{F}_1^n \\ \left(\frac{1}{\tau} \mathcal{M}^{n+1} + d\mathcal{S}^{n+1} + \gamma \mathcal{M}_2^{n+1}\right) \boldsymbol{W}^{n+1} = \frac{1}{\tau} \mathcal{M}^n \boldsymbol{W}^n + \boldsymbol{F}_2^n \end{cases}$$

with

$$\mathcal{M}_{ij}^n = \int_{S_h^n} \chi_i^n \chi_j^n, \quad \mathcal{M}_{1ij}^n = \int_{S_h^n} U^n W^n \chi_i^n \chi_j^n, \quad \mathcal{M}_{2ij}^n = \int_{S_h^n} (U^{n+1})^2 \chi_i^n \chi_j^n,$$

$$\mathcal{S}_{ij}^n = \int_{S_h^n} \nabla_{S_h^n} \chi_i^n \cdot \nabla_{S_h^n} \chi_j^n, \quad \boldsymbol{F}_{1i}^n = \gamma a \int_{S_h^n} \chi_i^n, \quad \boldsymbol{F}_{2i}^n = \gamma b \int_{S_h^n} \chi_i^n$$