A new numerical approach for simulation of pattern formation models on stationary and growing surfaces

Mahdieh Sattari
Jukka Tuomela

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BIOMAT Consortium
International Institute for Interdisciplinary Sciences

Outline

- Motivation
- Schnakenberg model
- Triangulation and implementation
- Examples on growing manifolds
- Role of eigenfunction in pattern evolution
- Conclusion

Motivation

Pattern formation on a evolving biological surface modelled by reaction-diffusion equation.

Schnakenberg Model

Let M be two dimensional manifold and $u : M \to \mathbb{R}^2$. The model is given by

$$\partial_t u_1 - d_1 \Delta_M u_1 = \gamma(a - u_1 + u_1^2 u_2) = \gamma f_1(u)$$
$$\partial_t u_2 - d_2 \Delta_M u_2 = \gamma(b - u_1^2 u_2) = \gamma f_2(u)$$

where d_j, a, b and γ are some positive constants.

Schnakenberg Model

The stationary problem

$$-d_1\Delta_M u_1 = \gamma(a - u_1 + u_1^2 u_2)$$
$$-d_2\Delta_M u_2 = \gamma(b - u_1^2 u_2)$$

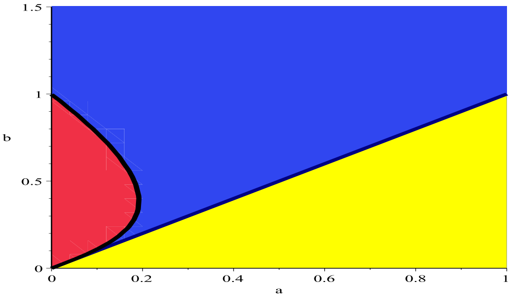
The constant (positive) solution is

$$u = \left(a + b, \frac{b}{(a+b)^2}\right)$$

Schnakenberg Model

To get diffusion-driven instability, choose a and b such that

$$(a+b)^3 + a - b > 0 \quad \text{and} \quad a < b$$



and diffusion parameters such that

$$\sqrt{\frac{d_2}{d_1}} > \frac{(a+b)\big(a+b+\sqrt{2b(a+b)}\big)}{b-a}$$

In particular $d_2 > d_1$.

Variational formulation

To solve model on the sphere S^2 with metric g, let V_h be some finite dimensional subspace of $H^1(S^2)$ and let

$$V_h = \mathsf{span}\big(\psi_1, \ldots, \psi_m\big)$$

The approximate solution $u = (u_1, u_2)$ can be written as

$$u_j(x,t) = \sum_{i=1}^{m} c_i^j(t)\psi_i(x)$$

Variational formulation

Find (u_1, u_2) such that

$$\partial_t \int_{S^2} u_1 \psi_j \omega_{S^2} + d_1 \int_{S^2} g(\mathsf{grad}(u_1), \mathsf{grad}(\psi_j))\omega_{S^2} = \gamma \int_{S^2} f_1(u)\psi_j \omega_{S^2}$$
$$\partial_t \int_{S^2} u_2 \psi_j \omega_{S^2} + d_2 \int_{S^2} g(\mathsf{grad}(u_2), \mathsf{grad}(\psi_j))\omega_{S^2} = \gamma \int_{S^2} f_2(u)\psi_j \omega_{S^2}$$

where ω_{S^2} is the area form.

Discretization

Let δt be the time step and $c_i^{j,n} = c_i^j(n\delta t)$ and

$$u_j^n = \sum_{i=1}^{m} c_i^{j,n}\psi_i \approx u_j(x, n\delta t)$$

using implicit Euler method for time discretization

$$\big((1+\delta t\,\gamma)M^{n+1} + \delta t\, d_1 R^{n+1} - \delta t\,\gamma\,\tilde{M}^n\big)c^{1,n+1} = M^n c^{1,n} + \delta t\,\gamma\, a F^{n+1}$$

$$\big(M^{n+1} + \delta t\, d_2 R^{n+1} + \delta t\,\gamma\,\hat{M}^n\big)c^{2,n+1} = M^n c^{2,n} + \delta t\,\gamma\, b F^{n+1}$$

Discretization

where

$$M_{ij}^n = \int_{S^2} \psi_i \psi_j \omega_{S^2}^n \qquad R_{ij}^n = \int_{S^2} g(\mathsf{grad}(\psi_i), \mathsf{grad}(\psi_j))\omega_{S^2}^n$$

$$E_{ijk\ell}^n = \int_{S^2} \psi_i \psi_j \psi_k \psi_\ell \omega_{S^2}^n \qquad F_i^n = \int_{S^2} \psi_i \omega_{S^2}^n$$

$$\tilde{M}_{ij}^n = \sum_{k,\ell} E_{ijk\ell}^{n+1} c_k^{1,n} c_\ell^{2,n} \qquad \hat{M}_{ij}^n = \sum_{k,\ell} E_{ijk\ell}^{n+1} c_k^{1,n} c_\ell^{1,n}$$

Domain composition

The sphere S^2 is covered with 6 patches D_j

$$D_1 = (-1,1) \times (-1,1) \qquad \varphi_1(z) = \gamma_1^{-\frac{1}{2}} \begin{pmatrix} z_1 \\ z_2 \\ 1 \end{pmatrix}$$

$$D_2 = (1,3) \times (-1,1) \qquad \varphi_2(z) = \gamma_2^{-\frac{1}{2}} \begin{pmatrix} 1 \\ z_2 \\ 2 - z_1 \end{pmatrix}$$

$$D_3 = (-1,1) \times (1,3) \qquad \varphi_3(z) = \gamma_3^{-\frac{1}{2}} \begin{pmatrix} z_1 \\ 1 \\ 2 - z_2 \end{pmatrix}$$

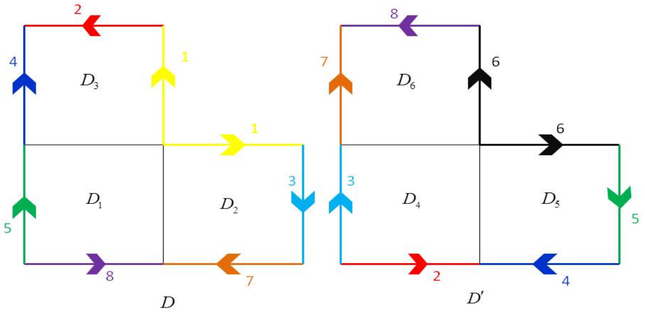
$$D_{j+3} = D_j \qquad \varphi_{j+3} = -\varphi_j$$

where

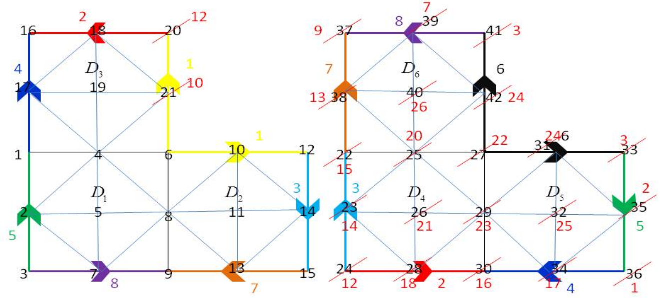
$$\gamma_1 = 1 + |z|^2 \quad , \quad \gamma_2 = 1 + (z_1 - 2)^2 + z_2^2 \quad , \quad \gamma_3 = 1 + z_1^2 + (z_2 - 2)^2$$

Hence $\varphi_j : D_j \to S^2$

Identification



Identification

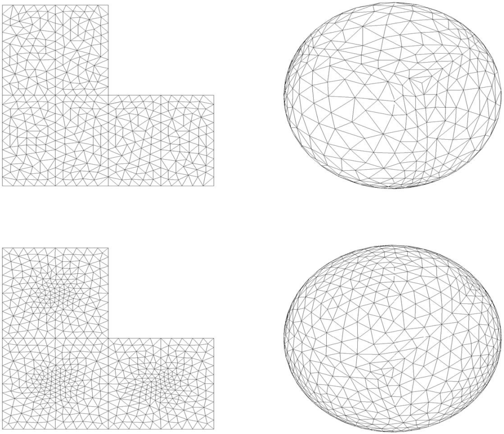


A:	1	2	3	4	. . .	19	10	12	15	14	. . .	26	3	24
	1	2	3	4	. . .	19	20	21	22	23	. . .	40	41	42

Triangulation

Using Riemannian metric $G_j = d\varphi_j^T d\varphi_j$ in triangulation

Triangulation



Changing manifold

The growing manifold is topologically the sphere S^2 with changing Riemannian metric.
To produce the growing manifold, define $\beta : S^2 \to \mathbb{R}^3$ and $\hat{\varphi}_j = \beta \circ \varphi_j$ then the Riemannian metric is

$$\hat{G}_j = d\hat{\varphi}_j^T d\hat{\varphi}_j = d\varphi_j^T d\beta^T d\beta d\varphi_j$$

Growing sphere (Isotropic grow)

Let $\beta(x) = \rho(t)(x_1\,,\, x_2\,,\, x_3)$ where

$$\rho(t) = \frac{e^{rt}}{1 + \frac{1}{K}(e^{rt} - 1)}$$

Then $\hat{\varphi}_j = \rho(t)\varphi_j$ and the corresponding Riemannian metric is $\hat{G}_j = \rho(t)^2 G_j$

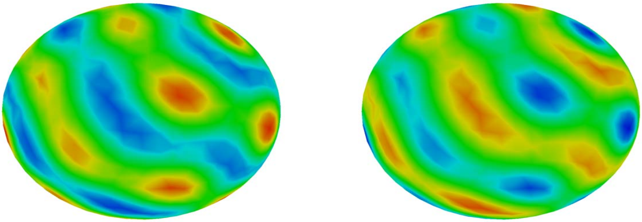
Growing sphere (Isotropic grow)

choosing parameters as follows

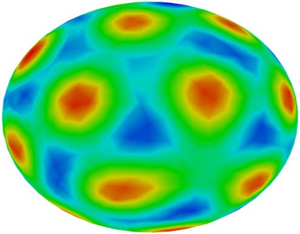
d_1	d_2	γ	a	b	K	r	δt
1	10	200	0.1	0.9	1.5	0.1	0.01

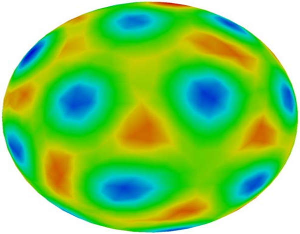
Growing sphere (Isotropic grow)

The concentrations u_1 and u_2 at $t = 5$



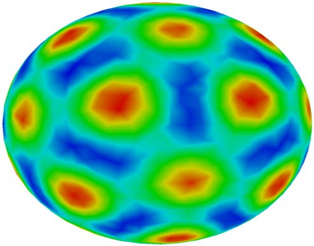
The concentrations u_1 and u_2 at $t = 10$

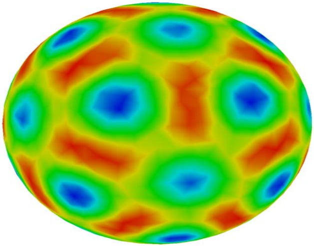




Growing sphere (Isotropic grow)

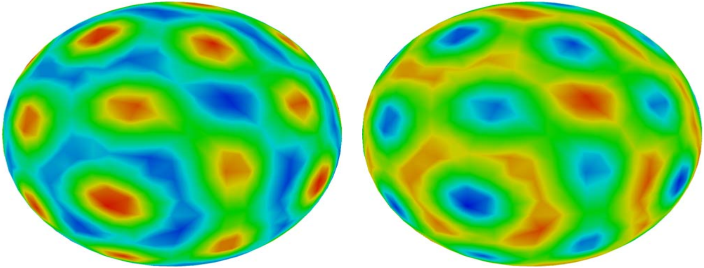
The concentrations u_1 and u_2 at $t = 20$





Growing sphere (Isotropic grow)

The concentrations u_1 and u_2 at $t = 50$



Evolving sphere (Anisotropic grow)

Define

$$\beta(x) = \big(lx_1\,,\, lx_2\,,\, (lx_3/h)^{1/2p}\big)$$

such that

$$\begin{cases} h(t) = \frac{l(t)}{q(t)^{2p}} \\ q(t) = \frac{q_0}{\beta+(1-\beta)e^{-rt}} \\ l(t) = l_0\big(1+\alpha(1-e^{-kt})\big) \end{cases}$$

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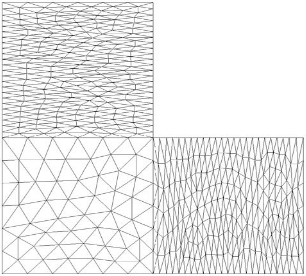
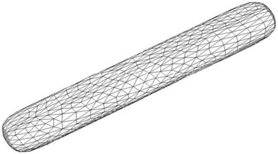
Choose parameters as

d_1	d_2	γ	a	b	q_0	l_0	α	β	r	k	p
1	100	500	0.1	0.9	0.5	0.1	0.8	0.3	0.5	0.5	5

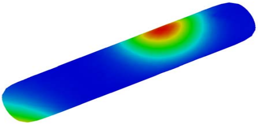
Evolving sphere (Anisotropic grow)

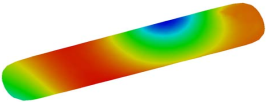




Evolving sphere (Anisotropic grow)

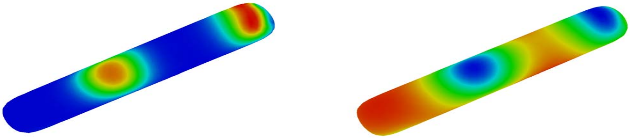
The concentrations u_1 and u_2 at $t = 0.1$ with $\delta t = 0.0005$





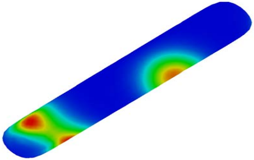
Evolving sphere (Anisotropic grow)

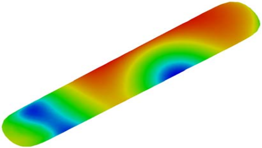
The concentrations u_1 and u_2 at $t = 1.6$ with $\delta t = 0.0005$



Evolving sphere (Anisotropic grow)

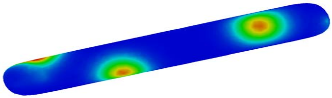
The concentrations u_1 and u_2 at $t = 1.68$ with $\delta t = 0.0005$

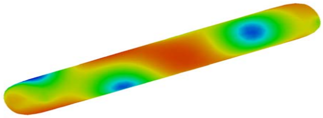




Evolving sphere (Anisotropic grow)

The concentrations u_1 and u_2 at $t = 2.75$ with $\delta t = 0.0005$





Eigenfunctions role in pattern formation

y_1 and y_2 are two positive roots of

$$p_0(y) = d_1 d_2 (a+b) y^2 + \Big((a+b)^3 d_1 + (a-b) d_2 \Big) y + (a+b)^3$$

Then we call $I = (y_1, y_2)$ critical interval.
Let λ be an eigenvalue of $-\Delta$ and v_λ be the corresponding eigenfunction.
If $\lambda/\gamma \in (y_1, y_2)$ then the linearized Schnackenberg problem has a solution of form $C v_\lambda e^{\mu\gamma t}$ where μ is the positive solution of

$$p_1(\mu, \lambda) = (a+b)\mu^2 + \Big((d_1+d_2)(a+b)\lambda + (a+b)^3 + a - b \Big) \mu + p_0(\lambda)$$

Choosing parameters as follows

d_1	d_2	a	b
1	10	0.1	0.9

The computed critical interval is $I = [0.2, 0.5]$.

Eigenfunction and pattern formation

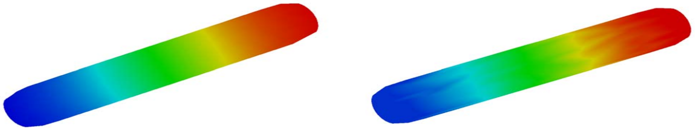
Let $t = 1.6$ be the ending time.

$\lambda_1 = 3.64$ and $\lambda_2 = 14.76$ are two first eigenvalues.

Set $\gamma = 15$ then just $\lambda_1/\gamma \in I = [0.2, 0.5]$.

Eigenfunction and pattern formation

The eigenfunction and concentration u_1



Changing the parameter as follows

d_1	d_2	a	b
1	20	0.2	1

The computed critical interval is $I = [0.169, 0.425]$.

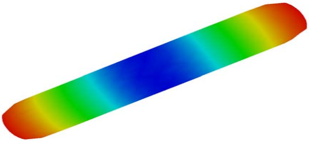
Eigenfunction and pattern formation

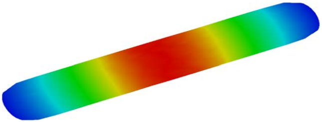
The ending time $t = 1.6$ and $\lambda_3 = 15.01$.

Set $\gamma = 72$ then $\lambda_3/\gamma \in I$.

Eigenfunction and pattern formation

The eigenfunction and concentration u_1





- Our approach can also readily be extended to more complicated surfaces.
- Since all computations are done in two dimensional domains there is no error related to the approximation of the surface in three dimensional space.
- In the case of restricting the parameters such that one eigenvalue of Laplace operator belongs to the critical interval, we are able to predict sort of pattern formation.
- The method benefits from simplicity in programming for different kinds of curved surfaces.

Question?

Thanks for your attention