Numerical framework for pattern-forming models on evolving-in-time surfaces

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1. Introduction.
2. PDEs on evolving-in-time surface.
4. Conclusion.
**Turing Pattern:** Alan Turing (1952) proposed that under certain conditions, chemicals can react and diffuse in such a way that they can produce steady state patterns.
Pattern forming model: (a)

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**Turing Pattern:**
- Animal coat: spots on leopard
- Sea fish: patterns around eyes
- Human beings: fingerprints
Chemotaxis describes an oriented movement towards or away from regions of higher concentrations of chemical agents and plays a vitally important role in the evolution of many living organisms.
Pattern forming model: (b)

Chemotaxis Pattern:
- **Colonial development of bacteria** (E. Ben-Jacob, J.R. Soc. Interface, 2006).
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Generalized system

\[
\begin{align*}
\frac{\partial u_i}{\partial t} &= \text{diffusion} \left( D_i^u \Delta u_i + \nabla \cdot \left( \sum_{k=1, k \neq i}^{n} \kappa_{i,k} u_i \nabla u_k \right) \right) - \text{chemotaxis/advection} \left( \sum_{k=1}^{m} \chi_{i,k} u_i \nabla c_k \right) + f_i(u, c), \quad \text{in } \Omega \times T, \\
\frac{\partial c_j}{\partial t} &= \text{diffusion} \left( D_j^c \Delta c_j \right) - \sum_{k=1}^{m} \alpha_{k,j} c_k + \sum_{k=1}^{n} \beta_{k,j} u_k + g_j(u, c), \quad \text{in } \Omega \times T
\end{align*}
\]
\[
\frac{\partial u_i}{\partial t} = D_i^u \Delta u_i + \nabla \cdot \left[ \left( \sum_{k=1, k \neq i}^n \kappa_{i,k} u_i \nabla u_k \right) - \left( \sum_{k=1}^m \chi_{i,k} u_i \nabla c_k \right) \right] + f_i(u, c, \rho), \quad \text{in } \Omega \times T,
\]

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\]

\[
\frac{\partial^* \rho_l}{\partial t} + \nabla \Gamma(t) \cdot (w_l \rho_l) = D_l^\rho \Delta \Gamma(t) \rho_l + s_l(u, c, \rho), \quad \text{on } \Gamma(t)
\]
Generalized system $+ \Gamma(t)$

\[
\frac{\partial u_i}{\partial t} = D_i^u \Delta u_i + \nabla \cdot \left[ \left( \sum_{k=1, \, k \neq i}^{n} \kappa_{i,k} u_i \nabla u_k \right) - \left( \sum_{k=1}^{m} \chi_{i,k} u_i \nabla c_k \right) \right] \\
+ f_i(u, c, \rho), \text{ in } \Omega \times T,
\]

\[
\frac{\partial c_j}{\partial t} = D_j^c \Delta c_j - \sum_{k=1}^{m} \alpha_{k,j} c_k + \sum_{k=1}^{n} \beta_{k,j} u_k + g_j(u, c, \rho), \text{ in } \Omega \times T
\]

\[
\frac{\partial^* \rho_l}{\partial t} + \nabla \Gamma(t) \cdot (w_l \rho_l) = D^\rho_l \Delta \Gamma(t) \rho_l + s_l(u, c, \rho), \text{ on } \Gamma(t)
\]

Introducing level set function $\phi$

where $\Gamma(t) = \{ x \in \Omega | \phi(t, x) = 0 \}$. 
Numerical challenges

- Treatment of time-dependent solutions.
- Nonphysical oscillations due to chemotaxis/surface convection.
- Catch patterns, depending on initial guess and domain.
- Treatment of equations, which are defined on (evolving in time) surfaces.
Numerical setup

discretization

- standard $\theta$ -scheme for temporal discretization
- hierarchical multilevel refinement of the spatial grid
- conforming bilinear/trilinear finite elements
- level set method to treat PDEs on surfaces
- FCT/TVD techniques to overcome non-physical oscillations
Numerical setup:

\[
\frac{\partial^* \rho_l}{\partial t} + \nabla \Gamma(t) \cdot (w_l \rho_l) = D^\rho_l \Delta \Gamma(t) \rho_l + s_l(u, c, \rho), \quad \text{on} \quad \Gamma(t) \times T
\]

\[
\frac{\partial^* \rho}{\partial t} = \frac{\partial \rho}{\partial t} + v \cdot \nabla \rho + \rho \nabla \Gamma \cdot v
\]
Numerical setup: level set

\[
\begin{align*}
\frac{\partial^* \rho_l}{\partial t} + \nabla \Gamma(t) \cdot (w_l \rho_l) &= D_l^\rho \Delta \Gamma(t) \rho_l + s_l(u, c, \rho), \quad \text{on } \Gamma(t) \times T \\
\frac{\partial^* \rho}{\partial t} &= \frac{\partial \rho}{\partial t} + v \cdot \nabla \rho + \rho \nabla \Gamma \cdot v
\end{align*}
\]

\(w\) velocity of chemo, \(v\) velocity of surface and the level-set function:

\[
\phi(x) = \begin{cases} 
< 0 & \text{if } x \text{ is inside } \Gamma \\
0 & \text{if } x \in \Gamma \\
> 0 & \text{if } x \text{ is outside } \Gamma
\end{cases}
\]

if \(\phi\) is a signed distance, then \(|\nabla \phi| = 1|\).
Implicit, FEM, level-set based numerical scheme:

\[
[M(\vert \nabla \phi^m \vert)] + \Delta t \left[ L(D(\vert \nabla \phi^m \vert)) - K(w^m) \right] - \Delta t \left[ N(v^{m+1}) + R(\vert \nabla \phi^m \vert) \right] P^{m+1}
\]

\[
= M(\vert \nabla \phi^m \vert) P^m + \Delta t s^m(\vert \nabla \phi^m \vert).
\]
Equation on surfaces (Discrete)

Implicit, FEM, level-set based numerical scheme:

\[
[M(|\nabla \phi^{m+1}|)] + \Delta t \ L(D|\nabla \phi^{m+1}|) - \Delta t \ K(w^m|\nabla \phi^{m+1}|) \\
- \Delta t \ N(v^{m+1}|\nabla \phi^{m+1}|) + \Delta t \ R(|\nabla \phi^{m+1}|) P^{m+1} \\
= M(|\nabla \phi^m|)P^m + \Delta t s^m(|\nabla \phi^m|).
\]

\[
C(\cdot) = \underbrace{K(w^m|\nabla \phi^{m+1}|)}_{\text{convection due to chemo}} + \underbrace{N(v^{m+1}|\nabla \phi^{m+1}|)}_{\text{surface convection}} - \underbrace{R(|\nabla \phi^{m+1}|)}_{\text{normal to the boundary}}
\]
Implicit, FEM, level-set based numerical scheme:

\[
[M(\vert \nabla \phi^{m+1} \vert)] + \Delta t L(D\vert \nabla \phi^{m+1} \vert) - \Delta t K(w^m|\nabla \phi^{m+1}|)
\]

\[
- \Delta t N(v^{m+1}|\nabla \phi^{m+1}|) + \Delta t R(|\nabla \phi^{m+1}|) P^{m+1}
\]

\[
= M(|\nabla \phi^m|) P^m + \Delta t s^m(|\nabla \phi^m|).
\]

\[
C(\cdot) = K(w^m|\nabla \phi^{m+1}|) + N(v^{m+1}|\nabla \phi^{m+1}|) - R(|\nabla \phi^{m+1}|)
\]

- convection due to chemo
- surface convection
- normal to the boundary

use AFC, for a simplified scalar transport-like problem
AFC technique

- **Standard Galerkin**
  + second order
  - num. artifacts

- **Discrete Upwinding**
  + fail safe
  - first order

- **AFC**
  + mixed order
  + fail safe

\[ M \partial u_t = C(u)u \]

\[ M^L \partial u_t = (C + D)(u)u = \tilde{C}(u)u \]

\[ M^L \partial u_t = \tilde{C}(u)u + \tilde{f}(u) \quad \tilde{f} = \sum_{j \neq i} \alpha_{ij} f_{ij} \]

antidiff. flux, flux limiter
solve

\[
\frac{\partial^* \rho}{\partial t} + \alpha \rho = D \Delta_{\Gamma(t)} \rho \quad \text{on} \quad \Gamma(t),
\]

resp.,

\[
\frac{\partial \rho}{\partial t} + v \cdot \nabla \rho + \rho \nabla_{\Gamma} \cdot v + \alpha \rho = D \Delta_{\Gamma(t)} \rho \quad \text{on} \quad \Gamma(t),
\]

where \( \alpha = 0.2 \) and

\[
\phi(x, t) = |x| - (1.0 + b t \sin(5 \gamma)),
\]

with \( b = 10 \) and \( \gamma = \text{atan2}(x_2, x_1) \).
PDE on evolving $\Gamma$, 2D

Figure: Evolution of the level set.
Figure: Comparision of SG, TVD and FCT.
Solve

$$\partial_t \rho + \mathbf{v} \cdot \nabla_{\Gamma} \rho = 0$$

where $\Gamma = \{ \mathbf{x} : |\mathbf{x}| = 1 \}$. The following initial condition

$$\rho(\mathbf{x}, t) = \begin{cases} 10 & \text{if } |\mathbf{x} - (0, 0, 1)^T| \leq 0.3, \\ 0 & \text{else}. \end{cases}$$

and the advective velocity vector-field

$$\mathbf{v} = \{x_1, 0, -x_3\}^T$$

are taken.
Mesh of sphere, Jens Acker.

Figure: $\Gamma$, level 1.
Mesh refinement 2

Figure: \( \Gamma, \) level 2.
Mesh refinement 3

Figure: $\Gamma$, level 3.
Figure : $\Gamma$, level 4.
Mesh refinement 5

Figure: \( \Gamma \), level 5.
Mesh refinement 6

Figure: $\Gamma$, level 6, 835 618 d.o.f. and 786 432 cells.
Stationary surface $\Gamma$, 3D

(a) initial solution

(b) pure Galerkin method

(c) TVD

(d) FCT

Figure: Numerical results for the transport problem, $\Delta t = 0.001$. 
Schnakenberg model:

\[
\frac{\partial \rho_1}{\partial t} = \Delta_\Gamma \rho_1 + \gamma (a - \rho_1 + \rho_1^2 \rho_2),
\]
\[
\frac{\partial \rho_2}{\partial t} = D \Delta_\Gamma \rho_2 + \gamma (b - \rho_1^2 \rho_2).
\]
Turing-type system on $\Gamma$

**Schnakenberg model:**

\[
\frac{\partial \rho_1}{\partial t} = \Delta_{\Gamma} \rho_1 + \gamma(a - \rho_1 + \rho_1^2 \rho_2),
\]
\[
\frac{\partial \rho_2}{\partial t} = D \Delta_{\Gamma} \rho_2 + \gamma(b - \rho_2^2 \rho_2).
\]

where $a = 1.0$, $b = 1.0$, and

\[\rho_1(x, t = 0) = 1.0 + \text{rand} \ast 10^{-2}, \quad \rho_2(x, t = 0) = 1.0 + \text{rand} \ast 10^{-2},\]
Turing-type system on $\Gamma$

(a) mesh

(b) initial condition
Turing-type system on $\Gamma$

(c) mesh

(d) $\rho_1$
The Koch-Meinhardt reaction-diffusion model

\[
\frac{\partial \rho_1}{\partial t} = \alpha_1 \rho_1 (1 - r_1 \rho_2^2) - \rho_2 (1 - r_2 \rho_1) + D^1 \Delta_{\Gamma(t)} \rho_1 ,
\]

\[
\frac{\partial \rho_2}{\partial t} = \beta_1 \rho_2 \left(1 + \frac{\alpha_1 r_1}{\beta_1} \rho_1 \rho_2\right) + \rho_1 (\gamma_1 - r_2 \rho_2) + D^2 \Delta_{\Gamma(t)} \rho_2 ,
\]

introducing level set function \( \phi \)
The Koch-Meinhardt reaction-diffusion model

\[
\frac{\partial \rho_1}{\partial t} = \alpha_1 \rho_1 (1 - r_1 \rho_2^2) - \rho_2 (1 - r_2 \rho_1) + D^{\rho_1} \Delta \Gamma(t) \rho_1 ,
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\[
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\]

introducing level set function \( \phi \)

Initial \( \Gamma(t) \) is

\[
\Gamma_r(t = 0) = \{ x | \phi(x, t = 0) = |x| - r \}. 
\]
PDEs coupled with evolution of $\Gamma(t)$

(e) mesh

(f) $\rho_1(x, t = 0)$
PDEs coupled with evolution of $\Gamma(t)$

(g) $\rho_1$ at $t = 0.2$

(h) level set $\phi$ at $t = 0.2$
PDEs coupled with evolution of $\Gamma(t)$

(i) $\rho_1$ at $t = 1.0$

(j) level set $\phi$ at $t = 1.0$
PDEs coupled with evolution of $\Gamma(t)$

(k) $\rho_1$ at $t = 2.0$

(l) level set $\phi$ at $t = 2.0$
Conclusions

- two different kinds of pattern forming models
- an AFC stabilized finite element solver of reaction-diffusion-convection equations in 2D and 3D domains
- solve PDEs on stationary and evolving-in-time surfaces
- positivity preserving schemes
- solve Turing Pattern on surfaces
Thank you


Applying integration by parts

\[ \int_{\Omega} D\nabla_{\Gamma\rho} \cdot \nabla_{\Gamma\varphi} |\nabla\phi| = - \int_{\Omega} \nabla_{\Gamma} \cdot D\nabla_{\Gamma\rho} \varphi |\nabla\phi| + \]

\[ + \int_{\Omega} \nabla_{\Gamma} \cdot (D\nabla_{\Gamma\rho} \varphi) |\nabla\phi| \text{ in } \Omega \]

together with the condition

\[ \int_{\Omega} \nabla_{\Gamma} \cdot (D\nabla_{\Gamma\rho} \varphi) |\nabla\phi| = \int_{\partial\Omega} D\nabla_{\Gamma\rho} \cdot n_{\Omega} \varphi |\nabla\phi| = 0 \]

(where \( n_{\Omega} \) is an outside normal to \( \partial\Omega \)) we get

\[ (|\nabla\phi|\Delta_{\Gamma\rho}, \varphi)_{L^2(\Omega)} = -(|\nabla\phi|\nabla_{\Gamma\rho}, \nabla_{\Gamma\varphi})_{L^2(\Omega)} = \]

\[ = -(|\nabla\phi| \left( I - \frac{\nabla\phi \otimes \nabla\phi}{|\nabla\phi|^2} \right) \nabla_{\Gamma\rho}, \nabla_{\Gamma\varphi})_{L^2(\Omega)} = \]

\[ P_{\Gamma} \]
Applying

\[ \int_{\Omega} \left| \nabla \phi \right| \nabla \Gamma \cdot (w \rho) \varphi = - \int_{\Omega} \left| \nabla \phi \right| w \rho \cdot \nabla \Gamma \varphi + \int_{\partial \Omega} \left| \nabla \phi \right| w \cdot n_{\partial \Omega} \rho \varphi, \]

and assuming

\[ \int_{\partial \Omega} \left| \nabla \phi \right| w \cdot n_{\partial \Omega} \rho \varphi = 0, \]

we get

\[ \int_{\Omega} \left| \nabla \phi \right| \nabla \Gamma \cdot (w \rho) \varphi = - \int_{\Omega} \left| \nabla \phi \right| w \rho \cdot \nabla \Gamma \varphi. \]
Treatment of the $\Gamma$-convection $\nabla_\Gamma \cdot (w\rho)$

Applying

$$\int_\Omega |\nabla \phi| \nabla_\Gamma \cdot (w\rho) \phi = - \int_\Omega |\nabla \phi| w \rho \cdot \nabla \phi + \int_{\partial \Omega} |\nabla \phi| w \cdot n_{\partial \Omega} \rho \phi,$$

and assuming

$$\int_{\partial \Omega} |\nabla \phi| w \cdot n_{\partial \Omega} \rho \phi = 0,$$

we get

$$\int_\Omega |\nabla \phi| \nabla_\Gamma \cdot (w\rho) \phi = - \int_\Omega |\nabla \phi| w \rho \cdot \nabla \phi.$$