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

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International Conference on Mathematical Methods and Models in Biosciences and Young Scientist School, Balagoevgrad

June 14 – 19, 2015

fakultät für mathematik

1. **Introduction.**
2. **PDEs on evolving-in-time surface.**
3. **Numerical results.**
4. **Conclusion.**

Pattern forming model: (a)

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.

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Turing Pattern:

- **Animal coat: spots on leopard**

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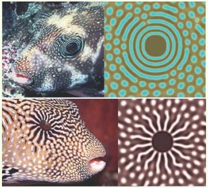
- **Animal coat: spots on leopard**
- **Sea fish: patterns around eyes**

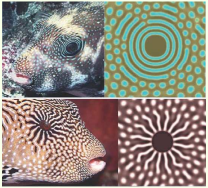


Pattern forming model: (a)

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.

Turing Pattern:

- **Animal coat: spots on leopard**
- **Sea fish: patterns around eyes**
- **Human beings: fingerprints**



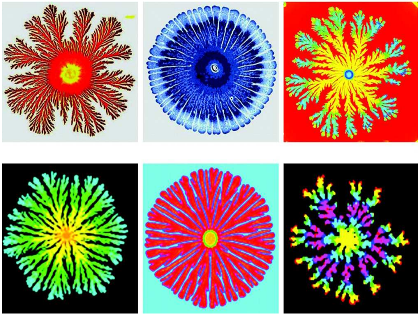
Pattern forming model: (b)

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:

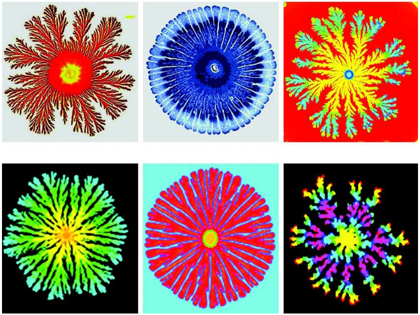
- **Colonial development of bacteria** (E. Ben-Jacob, J.R. Soc. Interface, 2006).

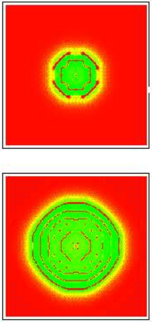


Pattern forming model: (b)

Chemotaxis Pattern:

- **Colonial development of bacteria** (E. Ben-Jacob, J.R. Soc. Interface, 2006).
- **Tumour growth** (M. Owen, Physica D, 2003).





$$\frac{\partial u_i}{\partial t} = \overbrace{D_i^u \Delta u_i}^{\text{diffusion}} + \nabla \cdot \overbrace{\left[\overbrace{\left(\sum_{k=1, k\neq i}^{n} \kappa_{i,k} u_i \nabla u_k \right)}^{\text{species-species}} - \overbrace{\left(\sum_{k=1}^{m} \chi_{i,k} u_i \nabla c_k \right)}^{\text{species-chemo}} \right]}^{\text{chemotaxis/advection}} + \underbrace{f_i(\mathbf{u}, \mathbf{c})}_{\text{kinetics}}, \text{ in } \Omega \times T,$$

$$\frac{\partial c_j}{\partial t} = \underbrace{D_j^c \Delta c_j}_{\text{diffusion}} - \underbrace{\sum_{k=1}^{m} \alpha_{k,j} c_k}_{\text{decay}} + \underbrace{\sum_{k=1}^{n} \beta_{k,j} u_k}_{\text{production}} + g_j(\mathbf{u}, \mathbf{c}), \text{ in } \Omega \times T$$

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

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

$$\frac{\partial^* \rho_l}{\partial t} + \nabla_{\Gamma(t)} \cdot (\mathbf{w}_l \rho_l) = D_l^\rho \Delta_{\Gamma(t)} \rho_l + s_l(\mathbf{u}, \mathbf{c}, \boldsymbol{\rho}), \text{ on } \Gamma(t)$$

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

$$
\frac{\partial^* \rho_l}{\partial t} + \nabla_{\Gamma(t)} \cdot (\mathbf{w}_l \rho_l) = D_l^\rho \Delta_{\Gamma(t)} \rho_l + s_l(\mathbf{u}, \mathbf{c}, \boldsymbol{\rho}), \ \text{on } \Gamma(t)
$$

introducing level set function ϕ

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

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

discretization

1. **standard θ −scheme for temporal discretization**
2. **hierarchical multilevel refinement of the spatial grid**
3. **conforming bilinear/trilinear finite elements**
4. **level set method to treat PDEs on surfaces**
5. **FCT/TVD techniques to overcome non-physical oscillations**

$$\frac{\partial^* \rho_l}{\partial t} + \nabla_{\Gamma(t)} \cdot (\mathbf{w}_l \rho_l) = D_l^{\rho} \Delta_{\Gamma(t)} \rho_l + s_l(\mathbf{u}, \mathbf{c}, \boldsymbol{\rho}), \text{ on } \Gamma(t) \times T$$

$$\frac{\partial^* \rho}{\partial t} = \frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla_{\Gamma} \cdot \mathbf{v}$$

$$\frac{\partial^* \rho_l}{\partial t} + \nabla_{\Gamma(t)} \cdot (\mathbf{w}_l \rho_l) = D_l^{\rho} \Delta_{\Gamma(t)} \rho_l + s_l(\mathbf{u}, \mathbf{c}, \boldsymbol{\rho}), \text{ on } \Gamma(t) \times T$$

$$\frac{\partial^* \rho}{\partial t} = \frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla_{\Gamma} \cdot \mathbf{v}$$

$\mathbf{w}$ velocity of chemo, $\mathbf{v}$ velocity of surface and the level-set function:

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

if ϕ is a signed distance, then $|\nabla \phi| = 1$.

Implicit, FEM, level-set based numerical scheme:

$$
\begin{aligned}
[\mathbf{M}(|\nabla\phi^{m+1}|) \quad &+ \quad \Delta t\,\mathbf{L}(D|\nabla\phi^{m+1}|) - \Delta t\,\mathbf{K}(\mathbf{w}^m|\nabla\phi^{m+1}|) \\
&- \quad \Delta t\,\mathbf{N}(\mathbf{v}^{m+1}|\nabla\phi^{m+1}|) + \Delta t\,\mathbf{R}(|\nabla\phi^{m+1}|)]\,P^{m+1} \\
&= \mathbf{M}(|\nabla\phi^m|)P^m + \Delta t\,s^m(|\nabla\phi^m|).
\end{aligned}
$$

Implicit, FEM, level-set based numerical scheme:

$$\begin{aligned}[\mathbf{M}(|\nabla\phi^{m+1}|) \quad + \quad & \Delta t\,\mathbf{L}(D|\nabla\phi^{m+1}|) - \Delta t\,\mathbf{K}(\mathbf{w}^m|\nabla\phi^{m+1}|) \\ - \quad & \Delta t\,\mathbf{N}(\mathbf{v}^{m+1}|\nabla\phi^{m+1}|) + \Delta t\,\mathbf{R}(|\nabla\phi^{m+1}|)]\,P^{m+1} \\ & = \mathbf{M}(|\nabla\phi^m|)P^m + \Delta t\,s^m(|\nabla\phi^m|).\end{aligned}$$

$$\mathbf{C}(\cdot) = \underbrace{\mathbf{K}(\mathbf{w}^m|\nabla\phi^{m+1}|)}_{\text{convection due to chemo}} + \underbrace{\mathbf{N}(\mathbf{v}^{m+1}|\nabla\phi^{m+1}|)}_{\text{surface convection}} - \underbrace{\mathbf{R}(|\nabla\phi^{m+1}|)}_{\text{normal to the boundary}}$$

Implicit, FEM, level-set based numerical scheme:

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$$

use AFC, for a simplified scalar transport-like problem

Standard Galerkin

+ second order
− num. artifacts

$$M\partial u_t = C(u)u$$

Discrete Upwinding

+ fail safe
− first order

$$M^L\partial u_t = (C+D)(u)u = \widetilde{C}(u)u$$

AFC

+ mixed order
+ fail safe

$$M^L\partial u_t = \widetilde{C}(u)u + \underbrace{\widetilde{f}(u)}_{\text{antidiff. flux,}} \quad \widetilde{f} = \sum_{j\neq i} \underbrace{\alpha_{ij}}_{\text{flux limiter}} f_{ij}$$

solve

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

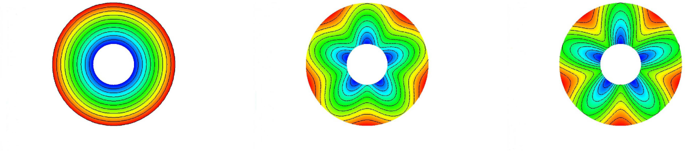
resp.,

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

where $\alpha = 0.2$ and

$$\phi(\mathbf{x}, t) = |\mathbf{x}| - (1.0 + b\,t\,\sin(5\gamma)),$$

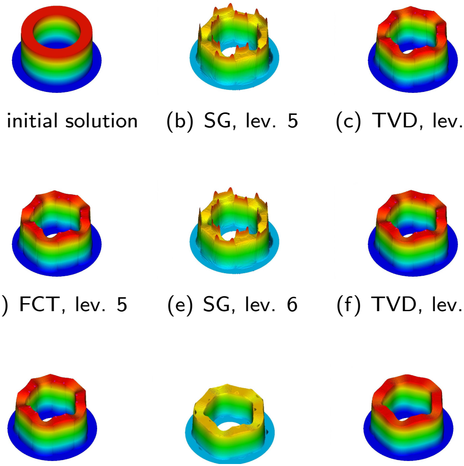
with $b = 10$ and $\gamma = atan2(x_2, x_1)$.



(q) ls $t = 0.00$ (r) ls, $t = 0.02$ (s) ls, $t = 0.05$

Figure : Evolution of the level set.

PDE on evolving Γ, 2D



(a) initial solution (b) SG, lev. 5 (c) TVD, lev. 5

(d) FCT, lev. 5 (e) SG, lev. 6 (f) TVD, lev. 6

(g) FCT, lev. 6 (h) SG, lev. 7 (i) FCT, lev. 7

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

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

and the advective velocity vector-field

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

are taken.

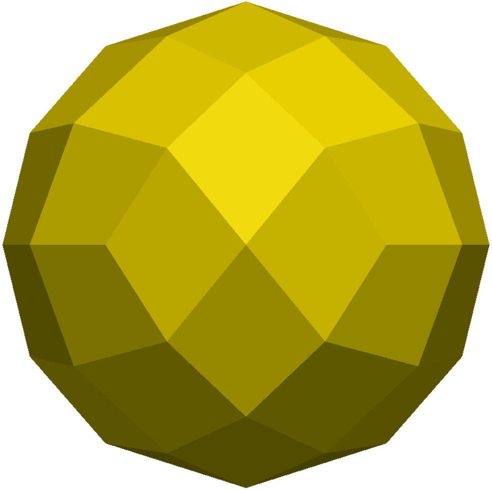


Figure : Γ, level 1.

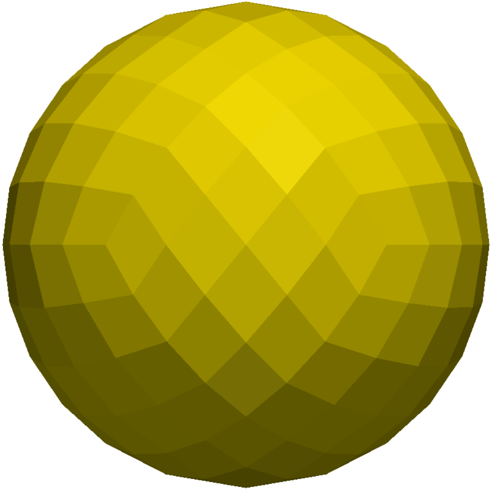


Figure : Γ, level 2.

Figure : Γ, level 3.

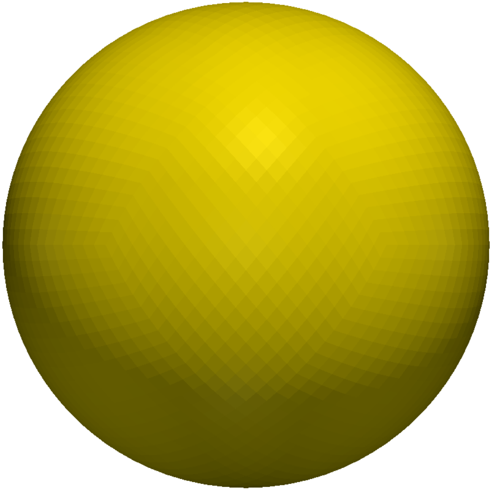


Figure : Γ, level 4.

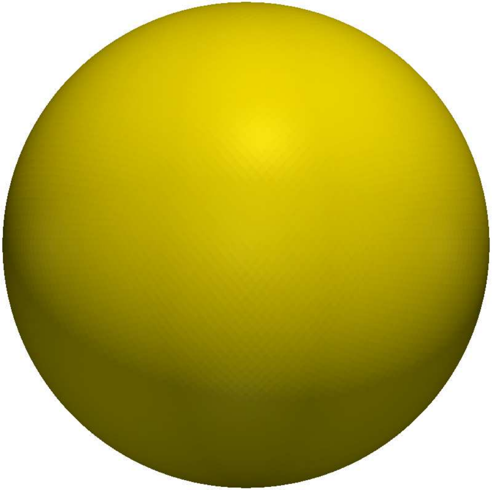


Figure : Γ, level 5.

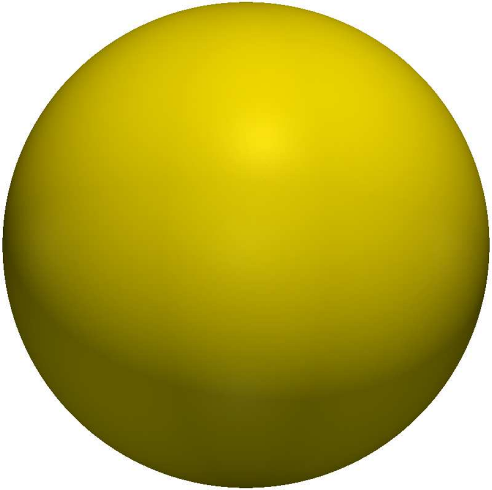
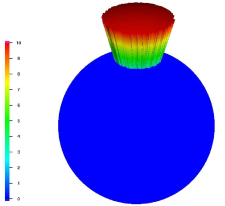
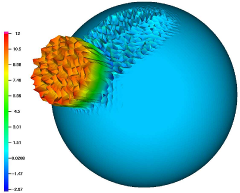


Figure : Γ, level 6, 835 618 d.o.f. and 786 432 cells.

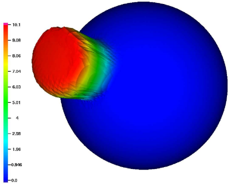
Stationary surface Γ, 3D



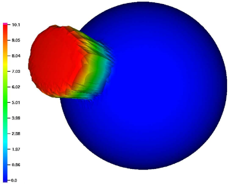
(a) initial solution



(b) pure Galerkin method



(c) TVD



(d) FCT

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

Schnakenberg model:

$$\begin{aligned}\frac{\partial \rho_1}{\partial t} &= \Delta_\Gamma \rho_1 + \gamma(a - \rho_1 + \rho_1^2 \rho_2)\,,\\ \frac{\partial \rho_2}{\partial t} &= D\Delta_\Gamma \rho_2 + \gamma(b - \rho_1^2 \rho_2)\,.\end{aligned}$$

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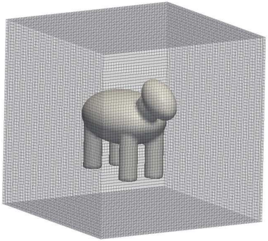
$$\begin{aligned} \frac{\partial \rho_1}{\partial t} &= \Delta_\Gamma \rho_1 + \gamma(a - \rho_1 + \rho_1^2 \rho_2)\,, \\ \frac{\partial \rho_2}{\partial t} &= D\Delta_\Gamma \rho_2 + \gamma(b - \rho_1^2 \rho_2)\,. \end{aligned}$$

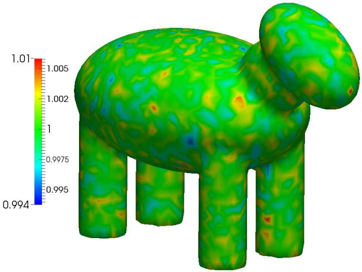
where $a = 1.0, \quad b = 1.0$, and

$$\rho_1(\mathbf{x}, t = 0) = 1.0 + \mathrm{rand} * 10^{-2}, \quad \rho_2(\mathbf{x}, t = 0) = 1.0 + \mathrm{rand} * 10^{-2},$$

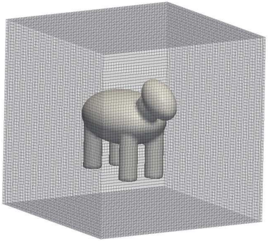
Turing-type system on Γ



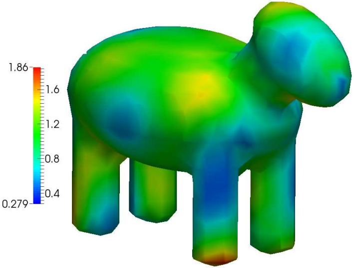
(a) mesh



(b) initial condition



(c) mesh



(d) ρ_1

The Koch-Meinhardt reaction-diffusion model

$$\begin{aligned}\frac{\partial \rho_1}{\partial t} &= \alpha_1 \rho_1 \left(1 - r_1 {\rho_2}^2\right) - \rho_2 \left(1 - r_2 \rho_1\right) + D^{\rho_1} \Delta_{\Gamma(t)} \rho_1 \,, \\ \frac{\partial \rho_2}{\partial t} &= \beta_1 \rho_2 \left(1 + \frac{\alpha_1 r_1}{\beta_1} \rho_1 \rho_2\right) + \rho_1 \left(\gamma_1 - r_2 \rho_2\right) + D^{\rho_2} \Delta_{\Gamma(t)} \rho_2 \,,\end{aligned}$$

introducing level set function ϕ

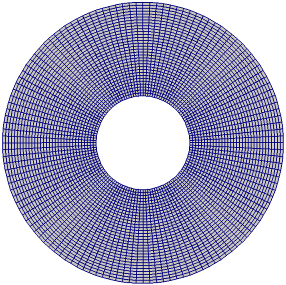
The Koch-Meinhardt reaction-diffusion model

$$
\begin{aligned}
\frac{\partial \rho_1}{\partial t} &= \alpha_1 \rho_1 \left(1 - r_1 {\rho_2}^2\right) - \rho_2 \left(1 - r_2 \rho_1\right) + D^{\rho_1} \Delta_{\Gamma(t)} \rho_1 \, , \\
\frac{\partial \rho_2}{\partial t} &= \beta_1 \rho_2 \left(1 + \frac{\alpha_1 r_1}{\beta_1} \rho_1 \rho_2\right) + \rho_1 \left(\gamma_1 - r_2 \rho_2\right) + D^{\rho_2} \Delta_{\Gamma(t)} \rho_2 \, ,
\end{aligned}
$$

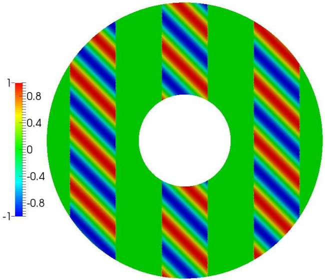
introducing level set function ϕ
Initial $\Gamma(t)$ is

$$
\Gamma_r(t=0) = \{\mathbf{x} \,|\, \phi(\mathbf{x}, t=0) = |\mathbf{x}| - r\}.
$$

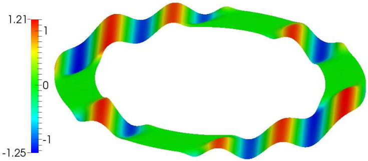
PDEs coupled with evolution of $\Gamma(t)$



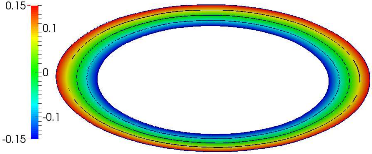
(e) mesh



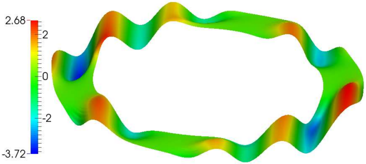
(f) $\rho_1(\mathbf{x}, t = 0)$



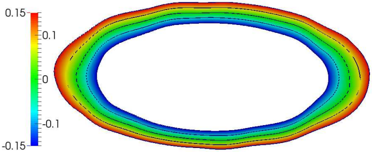
(g) ρ_1 at $t = 0.2$



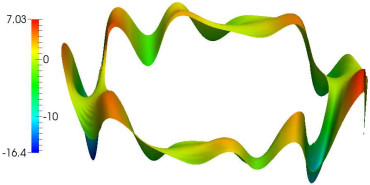
(h) level set ϕ at $t = 0.2$



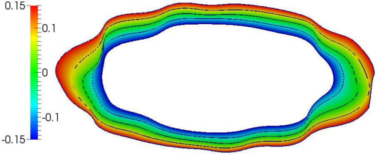
(i) ρ_1 at $t = 1.0$



(j) level set ϕ at $t = 1.0$



(k) ρ_1 at $t = 2.0$



(l) level set ϕ at $t = 2.0$

Conclusions

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

Thank you

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Applying integration by parts

$$\int_\Omega D\nabla_\Gamma\rho\cdot\nabla_\Gamma\varphi|\nabla\phi| \;=\; -\int_\Omega \nabla_\Gamma\cdot D\nabla_\Gamma\rho\varphi|\nabla\phi| + \\ + \int_\Omega \nabla_\Gamma\cdot(D\nabla_\Gamma\rho\varphi)|\nabla\phi| \quad \text{in} \quad \Omega$$

together with the condition

$$\int_\Omega \nabla_\Gamma\cdot(D\nabla_\Gamma\rho\varphi)|\nabla\phi| = \int_{\partial\Omega} D\nabla_\Gamma\rho\cdot\mathbf{n}_\Omega\varphi|\nabla\phi| = 0$$

(where $\mathbf{n}_\Omega$ is an outside normal to $\partial\Omega$) we get

$$(|\nabla\phi|\Delta_\Gamma\rho,\varphi)_{L_2(\Omega)} = -(|\nabla\phi|\nabla_\Gamma\rho,\nabla_\Gamma\varphi)_{L_2(\Omega)} =$$

$$= -(|\nabla\phi|\underbrace{\left(I-\frac{\nabla\phi\otimes\nabla\phi}{|\nabla\phi|^2}\right)}_{P_\Gamma}\nabla\rho,\nabla\varphi)_{L_2(\Omega)} =$$

Applying

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

and assuming

$$\int_{\partial\Omega}|\nabla\phi|\mathbf{w}\cdot\mathbf{n}_{\partial\Omega}\rho\varphi = 0,$$

we get

$$\int_\Omega |\nabla\phi|\nabla_\Gamma \cdot (\mathbf{w}\,\rho)\varphi = -\int_\Omega |\nabla\phi|\mathbf{w}\,\rho\cdot\nabla_\Gamma\varphi.$$

Applying

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

and assuming

$$\int_{\partial\Omega} |\nabla\phi| \mathbf{w} \cdot \mathbf{n}_{\partial\Omega} \rho\varphi = 0,$$

we get

$$\int_\Omega |\nabla\phi| \nabla_\Gamma \cdot (\mathbf{w}\,\rho)\varphi = -\int_\Omega |\nabla\phi| \mathbf{w}\,\rho \cdot \nabla_\Gamma \varphi.$$