Analysis Tools for the Finite Element Method

Math 693B: Advanced Computational PDE

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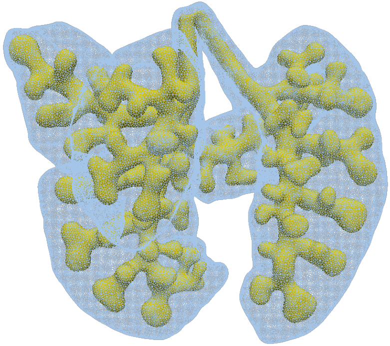


REACTION-DIFFUSION MODELS

Auto-catalytic Reaction Model

$$\mathrm{X} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathrm{F} \qquad 2\,\mathrm{F} + \mathrm{S} \xrightarrow{k_3} 3\,\mathrm{F} \qquad \mathrm{Y} \xrightarrow{k_4} \mathrm{S}$$

+

Laplace-Beltrami Operator

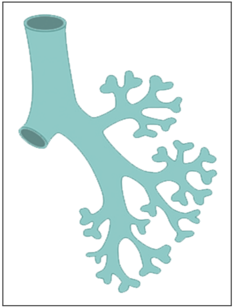
$$\Delta_\Gamma u = \nabla_\Gamma \cdot \nabla_\Gamma u \quad \text{with} \quad \nabla_\Gamma u = \nabla u - (\nabla u \cdot \vec{n})\vec{n}$$

=

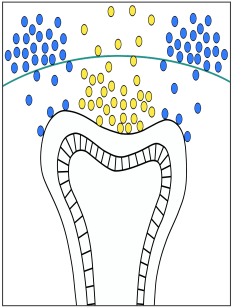
Schnakenberg Equations on Surface

$$\dot{F} = \Delta_\Gamma F + \gamma\left(\alpha - F + F^2 S\right)$$
$$\dot{S} = \delta \Delta_\Gamma S + \gamma\left(\beta - F^2 S\right)$$

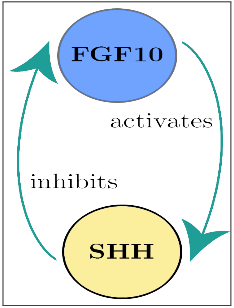
Lung Development



Branching at the pseudoglandular stage



Gene proteins diffuse from lung surface



Feedback loop between FGF10 and SHH genes

Sphere Study Validation

The problem is considered *well posed*: existence, uniqueness, and continuity in initial data effects. The system is guaranteed to be well posed, since it is parabolic, has at least 2 boundary conditions and the spatial derivative is of the second degree [1].

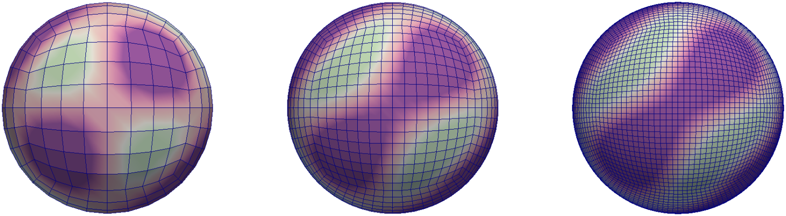


Figure: Sphere meshes with density refinements h_2, h_3, and h_4

The Finite Element Method

Multiply by test function φ, integrate, and apply Green's Theorem:

$$\int_\Gamma \varphi \frac{\partial u}{\partial t} + \int_\Gamma \nabla_\Gamma \varphi \cdot \nabla_\Gamma u = \gamma \int_\Gamma \varphi f(u,v)$$

Discretize the domain and the solution:

$$\sum_j \int_K \varphi_i \cdot \vartheta_j \left[\frac{\partial U_j}{\partial t}\right] + \sum_j \int_K \nabla_K \varphi_i \cdot \nabla_K \vartheta_j \left[U_j\right] \quad = \gamma \sum_j \int_K \varphi_i f_K(U_j, V_j)$$

Simplify and substitute:

$$\mathbf{M} = (\varphi_i, \varphi_j) \qquad \mathbf{L} = (\nabla\varphi_i, \nabla\varphi_j) \qquad \mathbf{A} = (\varphi_i, \mathbf{a}) \qquad \mathbf{B} = (\varphi_i, \mathbf{b})$$

$$\mathbf{M} \cdot \frac{d}{dt}[U_j] + \mathbf{L} \cdot U_j = \gamma(\mathbf{A} - \mathbf{M} \cdot U_j + \mathbf{M} \cdot U_j^2 V_j)$$

Implicit-Explicit Time Discretization

$$\mathbf{M}\dot{U} + \mathbf{L}U = \gamma\left[\mathbf{A} - \mathbf{M}U + \mathbf{M}U^2V\right]$$

IMEX scheme, first order backward Euler:

$$\frac{\mathbf{M}(U_{n+1} - U_n)}{k} + \mathbf{L}U_{n+1} = \gamma\left(\mathbf{A} - \mathbf{M}U_{n+1} + \mathbf{M}U_n^2V_n\right)$$

Solve the linear system Ax=b:

$$\left[\,(1+\gamma k)\mathbf{M} + k\mathbf{L}\,\right]U_{n+1} = \gamma k\left(\,\mathbf{A} + \mathbf{M}U_n^2V_n\right)$$

Use the updated u to solve v:

$$\left[\,\mathbf{M} + k\delta\mathbf{A}\,\right]V_{n+1} = \gamma k\left(\,\mathbf{B} - \mathbf{M}U_{n+1}^2V_n\right)$$

CONSISTENCY

The FDM normally shows consistency by solving:

$$P\phi - P_{k,h}\phi \to 0 \quad \text{as} \quad k,\ h \to 0$$

For the linearized system used in the FEM, we show consistency using the truncation error:

$$\left\| \gamma k \left(\mathbf{A} + \mathbf{M} U_n^2 V_n \right) - \left[(1 + \gamma k)\mathbf{M} + k\mathbf{L} \right] U_{n+1} \right\| \lessapprox h^{p_1} + k^{p_2}$$

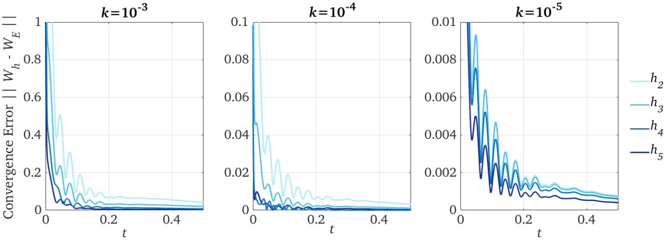
Which gives an order of accuracy (p_1, q_1). Because we use the **Conjugate Gradient Method**, we can constrain the truncation error to an arbitrary amount. For this model, we used 10^{-20}.

Convergence

Because of computing limitations, we use the criteria:

$$\Big|\, ||U_h|| - ||U_E|| \,\Big| \leq \Big|\, ||U_h - U_E|| \,\Big| \lessapprox |h^{q_1} + k^{q_2}| = h^{q_1} + k^{q_2}$$

with convergence rate (q_1, q_2). Errors were compared with a domain of the same density but with $k = 10^{-6}$.



All permutations converge, with the highest rate at (5, 5).

STABILITY

Theorem (Lax-Richtmyer [2])

Let U_h be the solution of a numerical method consistent with a well-posed time-dependent problem; in particular, assume that it is accurate of order $p > 0$. Then, if and only if the numerical method is stable, its solution converges with pth-order convergence rate,

$$\left|\left| U_h - U_E \right|\right| \lessapprox \sum_{m=0}^{n} k \cdot ||\{truncation\ error\}|| \lessapprox h^{p_1} + k^{p_2}, \quad t^n \in [0, T].$$

Patterns on a Sphere

This analysis continues with studying how changing the parameters $\alpha,\ \beta,\ \delta,$ and γ influence the surface patterns.

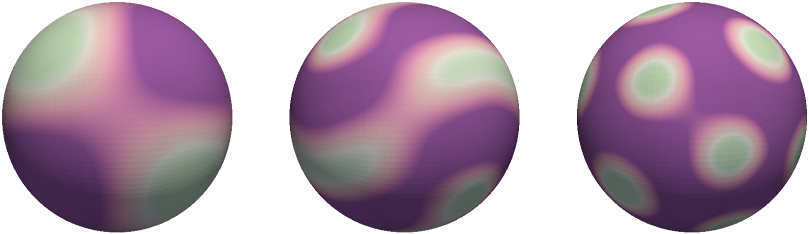
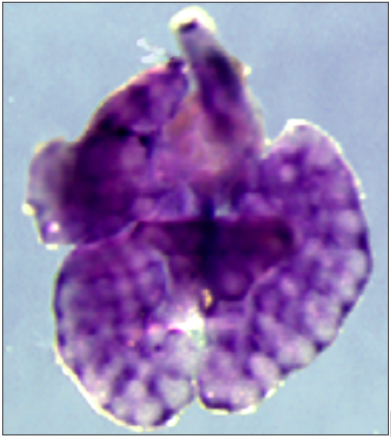
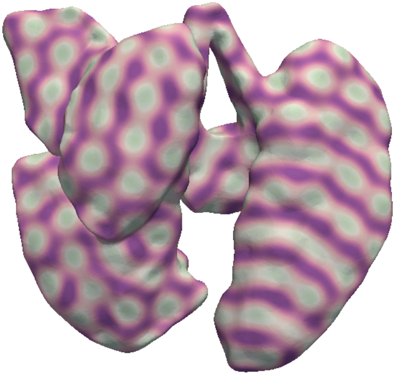


Figure: Some examples of modeling various parameters

FGF-10 Distribution on the Lung


[3]



Further Reading

- D. N. Arnold, "Stability, Consistency, and Convergence of Numerical Discretizations," *Encyclopedia of Applied and Computational Mathematics*, pp. 1358–1364, 2015.
- G. Dziuk and C. M. Elliott, "Finite element methods for surface PDEs," *Acta Numerica*, vol. 22, pp. 289–396, may 2013.
- T. Volckaert, A. Campbell, E. Dill, C. Li, P. Minoo, and S. De Langhe, "Localized Fgf10 expression is not required for lung branching morphogenesis but prevents differentiation of epithelial progenitors," *Development (Cambridge)*, vol. 140, no. 18, pp. 3731–3742, 2013.
- R. Barreira, C. M. Elliott, and A. Madzvamuse, "The surface finite element method for pattern formation on evolving biological surfaces," *Journal of Mathematical Biology*, vol. 63, pp. 1095–1119, dec 2011.

Thank You!