

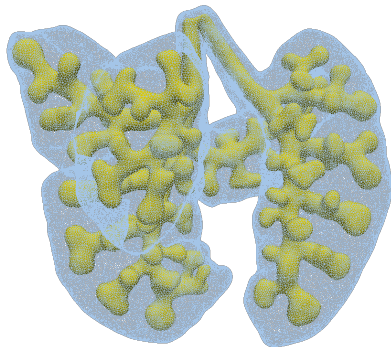
ANALYSIS TOOLS FOR THE FINITE ELEMENT METHOD

MATH 693B: ADVANCED COMPUTATIONAL PDE

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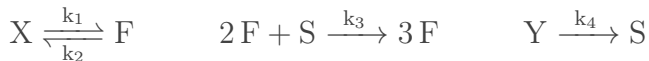
SAN DIEGO STATE UNIVERSITY
APPLIED MATHEMATICS

7 MAY 2020



REACTION-DIFFUSION MODELS

Auto-catalytic Reaction Model



+

Laplace-Beltrami Operator

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

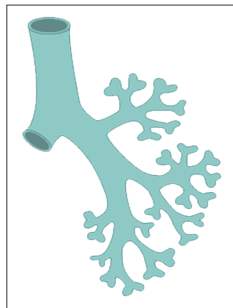
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Schnakenberg Equations on Surface

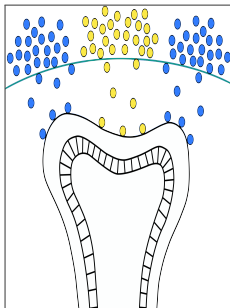
$$\dot{F} = \Delta_{\Gamma} F + \gamma (\alpha - F + F^2 S)$$

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

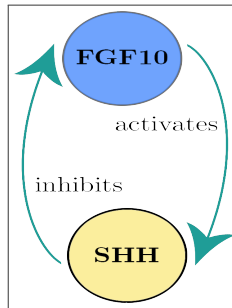
LUNG DEVELOPMENT



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].

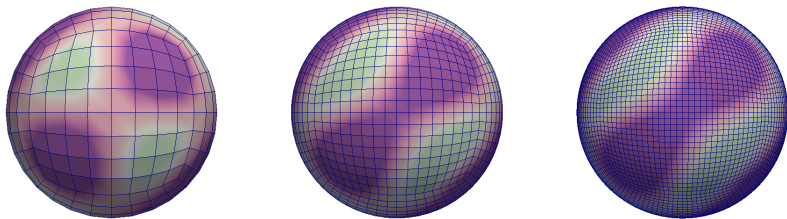


Figure: Sphere meshes with density refinements h_2 , h_3 , and h_4

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:

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

Simplify and substitute:

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

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

IMPLICIT-EXPLICIT TIME DISCRETIZATION

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

IMEX scheme,
first order
backward Euler:

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

Solve the linear
system $\mathbf{A}x=\mathbf{b}$:

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

Use the
updated u to
solve v :

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

CONSISTENCY

The FDM normally shows consistency by solving:

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

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

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

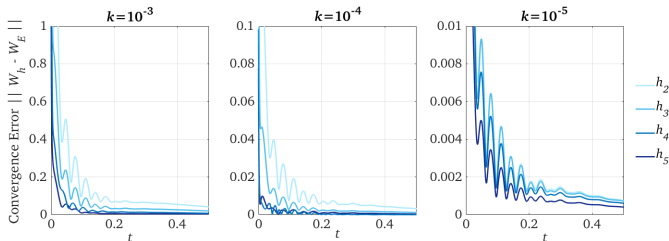
Which gives an order of accuracy (p_1, q_1) . Because we use the **Conjugate Gradient Method**, we can constrain the truncation error to an arbitrary amount. For this model, we used 10^{-20} .

CONVERGENCE

Because of computing limitations, we use the criteria:

$$\left| \|U_h\| - \|U_E\| \right| \leq \left| \|U_h - U_E\| \right| \approx |h^{q_1} + k^{q_2}| = h^{q_1} + k^{q_2}$$

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 p th-order convergence rate,

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

PATTERNS ON A SPHERE

This analysis continues with studying how changing the parameters α , β , δ , and γ influence the surface patterns.

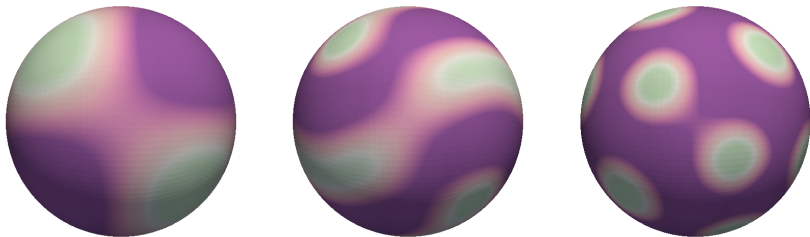
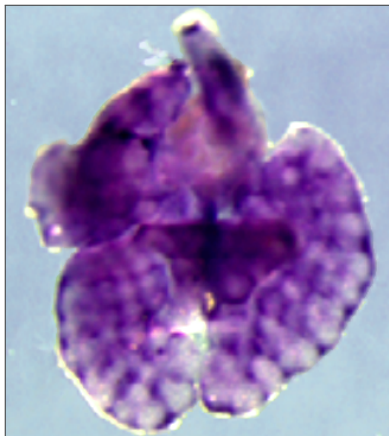
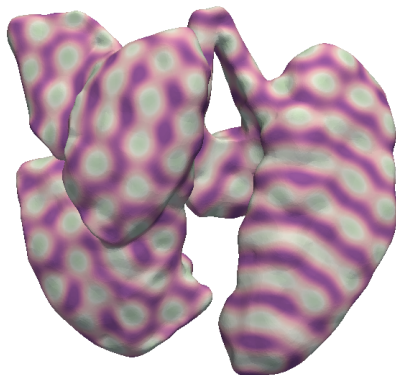


Figure: Some examples of modeling various parameters





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!