CG Method Comparison for a FEM IMEX Scheme

Math 693A Final Project Presentation

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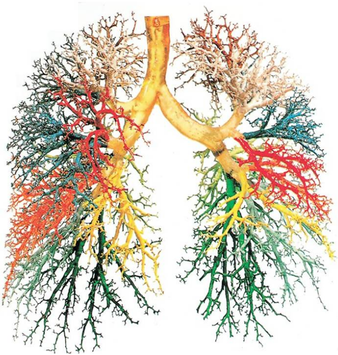
December 5, 2019



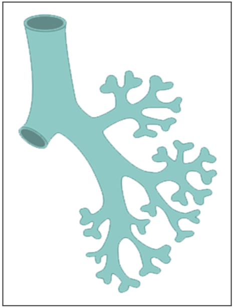
Motivation

Goal: Run implementations for my thesis in my pajamas

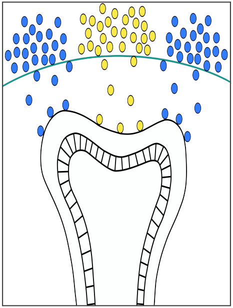
Problem: Takes several hours for a complete 10 second debug mode implementation on my laptop

Solution: Optimize time-stepping and linear solver process

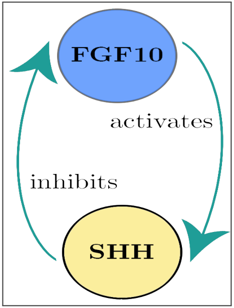
Thesis Background: Biology



Branching at the pseudoglandular stage



Gene proteins diffuse from lung surface



Feedback loop between FGF10 and SHH genes

Thesis Background: Theory

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

$$\dot{F} = \nabla_\Gamma^2 u + \gamma\left(\alpha - F + F^2 S\right)$$

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

Euler-Midpoint First/Second Order Method

First, time-step efficiently!

$$F^{(1)} = u_n + \Delta t\, f\left(u_n, v_n\right)$$
$$F^{(2)} = u_n + \Delta t\, f\left(u_n + \frac{1}{2}\Delta t F^{(1)}, v_n + \frac{1}{2}\Delta t G^{(1)}\right)$$

With

$$e_n = \left|F^{(2)} - F^{(1)}\right|, \qquad \tau = 10^{-3},$$
$$\chi = \left(\frac{\tau}{\text{norm}\left(e_n\right)}\right)^{1/4}, \qquad \Delta t_{n+1} = \chi \Delta t_n$$

Spatial Discretization

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

Multiply by test function, integrate:

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

Integrate Laplacian term by parts:

$$\int_\Omega \varphi_i \Delta_\Gamma F = \int_{\partial\Omega} \varphi_i \mathbf{n} \cdot \nabla F - \int_\Omega \nabla \varphi_i \cdot \nabla F$$

Discretize in space:

$$F \approx \sum_j \varphi_j f \quad \longrightarrow \quad \int_\Omega \varphi_i F \approx \sum_j (\varphi_i, \varphi_j f)$$

Linear System

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

$$\sum_j (\varphi_i, \varphi_j)\, \dot{f} + \sum_j (\nabla \varphi_i, \nabla \varphi_j)\, f =$$

$$\gamma \left[\alpha \sum_j (\varphi_i, 1) - \sum_j (\varphi_i, \varphi_j)\, f + \sum_j (\varphi_i, \varphi_j)\, f^2 s \right]$$

$$\mathbf{M} = \sum (\varphi_i, \varphi_j) \quad \mathbf{A} = \sum (\nabla \varphi_i, \nabla \varphi_j) \quad \mathbf{C} = \sum (\varphi_i, 1)$$

Time Discretization

$$\mathbf{M}\dot{f} + \mathbf{A}f = \gamma\left[\alpha\mathbf{C} - \mathbf{M}f + \mathbf{M}f^2 s\right]$$

IMEX scheme, first order backward Euler:

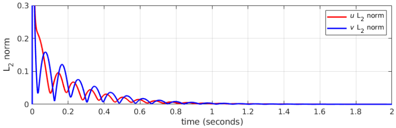
$$\frac{\mathbf{M}(f_{n+1} - f_n)}{\Delta t} + \mathbf{A}f_{n+1} = \gamma\left(\alpha\mathbf{C} - \mathbf{M}f_{n+1} + \mathbf{M}f_n^2 s_n\right)$$

Solve the linear system Ax=b:

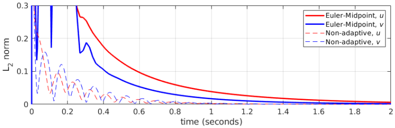
$$\left[(1 + \gamma\Delta t)\mathbf{M} + \Delta t\mathbf{A}\right] f_{n+1} = \gamma\Delta t\left(\alpha\mathbf{C} + \mathbf{M}f_n^2 s_n\right)$$

We solve the above linear system using the CG method, allowing no more than 10,000 iterations and requiring a convergence tolerance of 10^{-10}. I neglect a preconditioner.

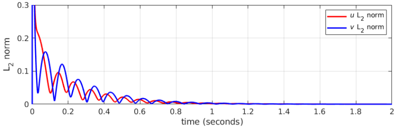
Comparison: Convergence (Release Mode)



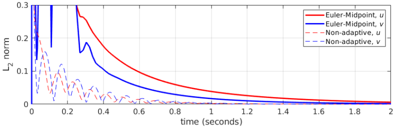
No adaptive time stepping, deal.ii's CG method: 76 seconds



Euler time stepping, deal.ii's CG method: 582 steps, 12 seconds



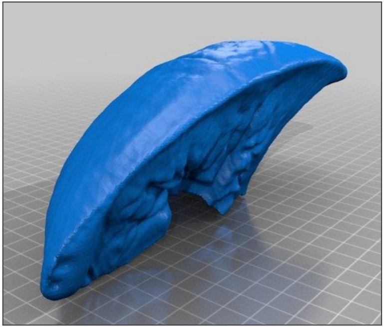
No adaptive time stepping, my CG method: 45 seconds (no error)



Euler time stepping, my CG method: 253 steps, 1 second! (error: 10^{-9})

Conclusions

Is the preconditioner useless for this problem?
Why does my method differ in time steps?
My CG method using Euler adaptive time steps is the most time efficient, with an acceptable error of 10^{-9} Next steps are:



3D model of left lung

- Use second order temporal discretization scheme for FEM
- Examine model on the mesh of a human lung
- Solve on growing domain of developing lung

Further Reading

- A. Madzvamuse, "Time-stepping schemes for moving grid finite elements applied to reaction-diffusion systems on fixed and growing domains," *Journal of Computational Physics*, vol. 214, no. 1, pp. 239–263, 2006.
- L. Murphy, C. Venkataraman, and A. Madzvamuse, "A Computational approach for Mode Isolation for Reaction-Diffusion Systems on Arbitraty Geometries," p. 26, 2016.
- M. Brake, "IMEX-a: An adaptive, fifth order implicit-explicit integration scheme," *Sandia Reports*, 2013.

Thank You!