A Computational Model for Anomalous Diffusion in Bio-Tissues using Fractional Calculus

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Introduction

Objectives

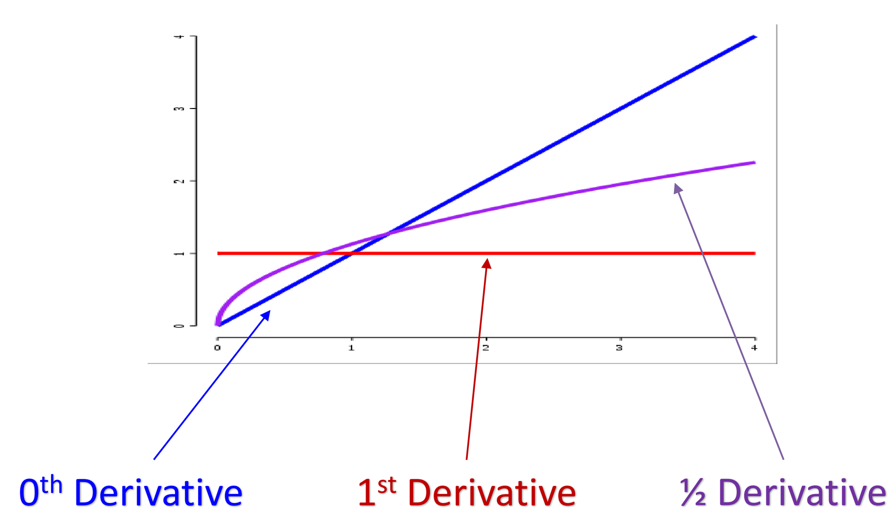
- Learn about fractional calculus.
- Become familiar with numerical methods for fractional partial differential equations, stochastic simulations, and sensitivity analysis.
- Capture the power law behavior characteristic of anomalous diffusion.
- Learn about diffusive processes from classical, 1D heat equation to multi-dimensional, time- and space-fractional heat diffusion.
- Investigate the nature of diffusive processes in the brain.

Fractional Calculus

Caputo fractional derivative

$$({}_0^C\mathcal{D}_t^\alpha T)(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{T'(x,s)}{(t-s)^\alpha}\, ds, \quad 0<\alpha<1$$

- Uses a power law kernel.
- The integral accounts for the history up to the beginning of the process.



- Fractional-order PDEs provide accurate modeling for anomalous diffusion [3].

One-Dimensional Heat Equation

Integer-Order Case

$$\rho C \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} K + \frac{I^2 R}{A_C \Delta x} - \frac{2h}{r}[T - T_{amb}] - \frac{2\sigma\epsilon}{r}[T^4 - T_{amb}^4]$$

Transient Term, Diffusion Term, Generation Term, Convection Term, Radiation Term

Forward-Euler finite difference in time:

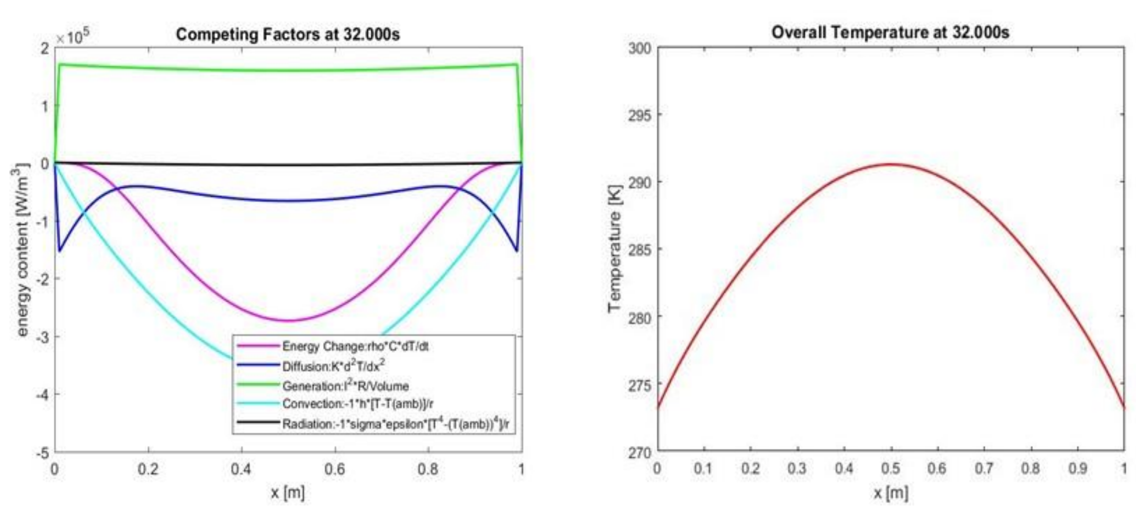
$$\frac{\partial T}{\partial t} = \frac{T_{x_j}^{t_{n+1}} - T_{x_j}^{t_n}}{\Delta t}$$

Central finite-difference in space:

$$\frac{\partial^2 T}{\partial x^2} = \frac{\left[T_{x_j-1}^{t_n} - 2T_{x_j}^{t_n} + T_{x_j+1}^{t_n}\right]}{\Delta x^2}$$

- Generation and convection have the largest impact on the transient term

Influence of the terms and solution for temperature



Time-Fractional Case

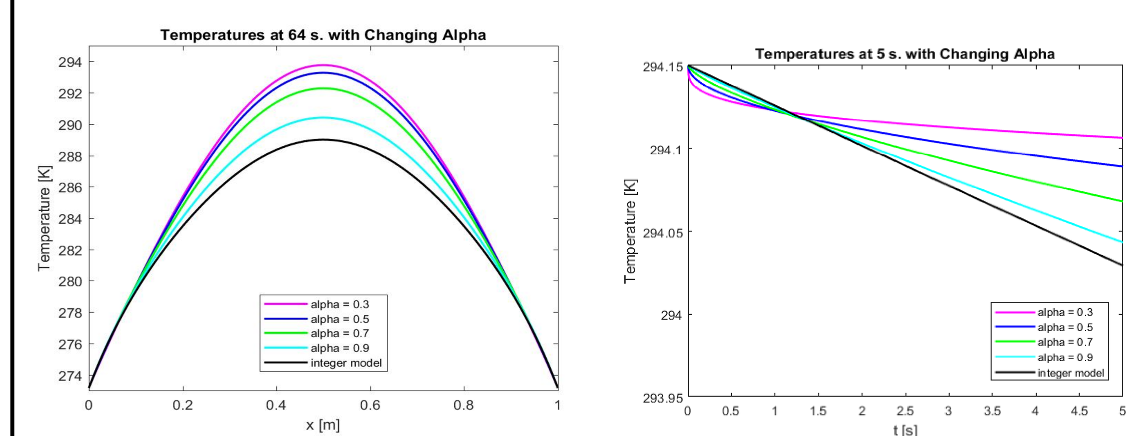
$$\rho C\, {}_0^C\mathcal{D}_t^\alpha (T_{x_j}^{t_n}) = K \frac{\partial^2 T}{\partial x^2} + f(x,t)$$

Finite-difference scheme for the Caputo derivative:

$$ {}_0^C\mathcal{D}_t^\alpha (T_{i,j}^n) = \frac{T_{i,j}^{n+1} - T_{i,j}^n + H^\alpha}{\Gamma(2-\alpha)\Delta t^\alpha}$$

- As α → 1, the fractional order recovers the integer order.
- H^α represents the history.

Effects of varying fractional-order in the solution



Observe that lower values of α result in a slower relaxation rate, and thus a higher overall temperature at a given time step.

We initially observe a period of "super-diffusivity" until around 1.3s, in which the lower values of α result in a higher rate of diffusion.

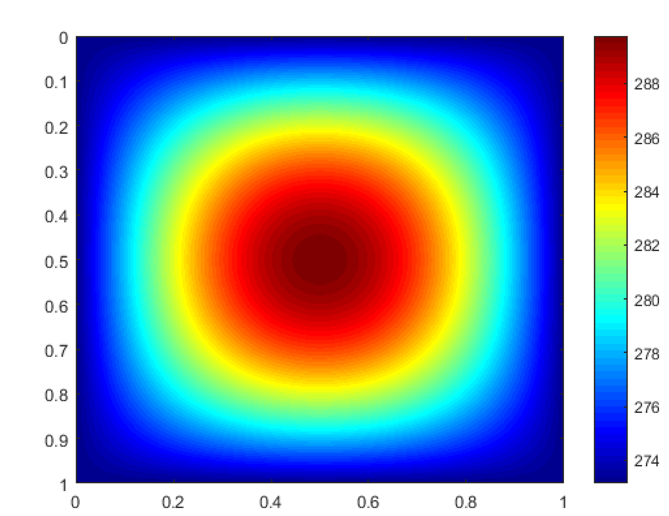
Two-Dimensional Heat Equation

Time-fractional, 2D Case

$$ {}_0^C\mathcal{D}_t^\alpha (T_{i,j}^n) = D\frac{\partial^2 T}{\partial x^2} + D\frac{\partial^2 T}{\partial y^2} + f(x,y,t)$$

Initial and Boundary Conditions

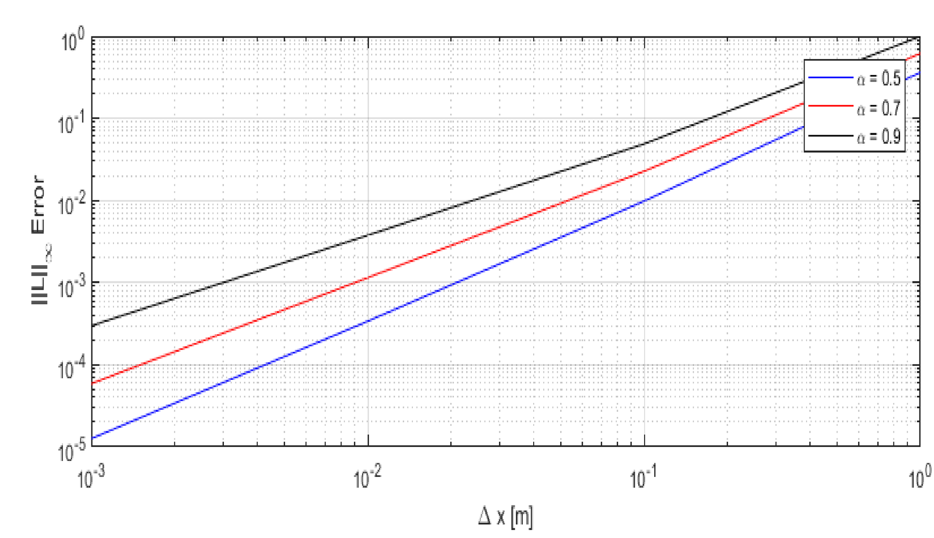
$$T(x,y,0) = 273.15 + 21\left(\sin\left(\frac{\pi x}{L_x}\right)\sin\left(\frac{\pi y}{L_y}\right)\right)$$



Convergence Analysis

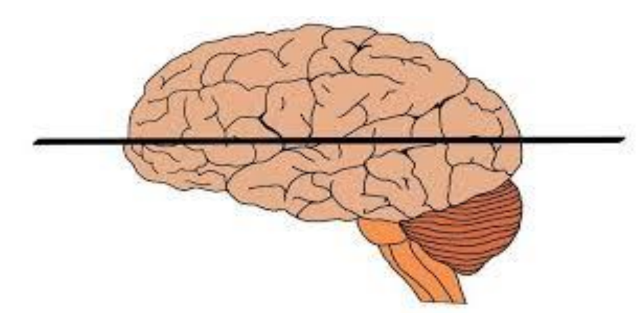
- A fabricated solution was used to test the accuracy of the discretization scheme:

$$T^\delta(x,y,t) = T_0 \sin\left(\frac{\pi x}{L_x}\right)\sin\left(\frac{\pi y}{L_y}\right)\left(\frac{t}{t_F}\right)^q$$

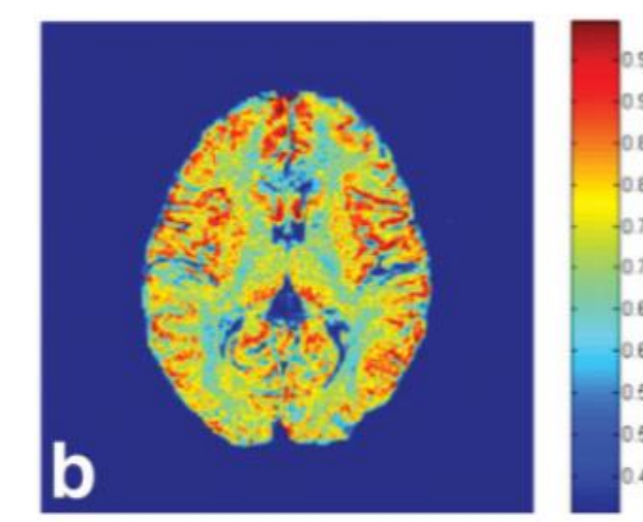


Future Work

- Discretize the time- and space-fractional two-dimensional heat equation to obtain a more accurate model of bio-tissues.



- Simulate diffusion within the brain, incorporating "hot spots" of activation.



- Generalize the two-dimensional model into a practical three-dimensional model.

References

[1] Magin, Richard L., et al. "Anomalous diffusion expressed through fractional order differential operators in the Bloch–Torrey equation." Journal of Magnetic Resonance 190.2 (2008): 255-270.

[2] Magin, Richard, Xu Feng, and Dumitru Baleanu. "Solving the fractional order Bloch equation." Concepts in magnetic resonance. Part A, Bridging education and research 34.1 (2009): 16.

[3] Zhou, Xiaohong Joe, et al. "Studies of anomalous diffusion in the human brain using fractional order calculus." Magnetic resonance in medicine 63.3 (2010): 562-569.

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