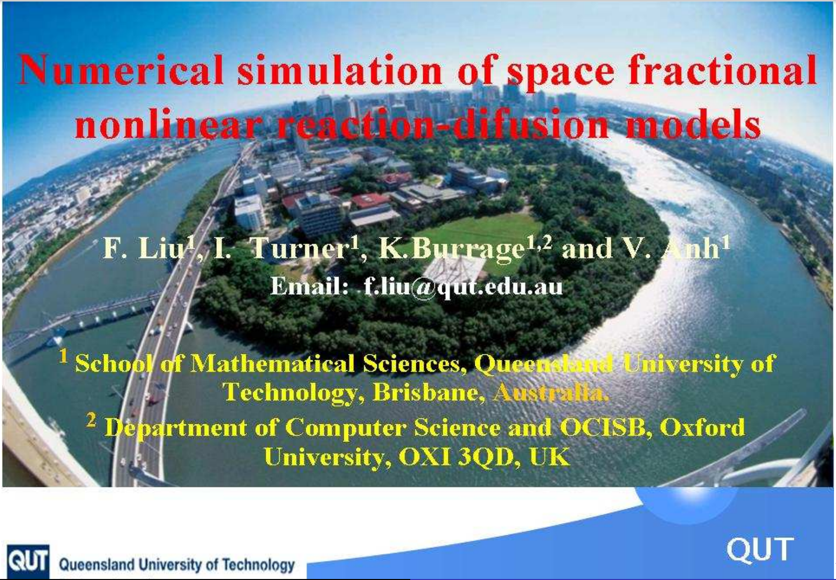

Numerical simulation of space fractional nonlinear reaction-difusion models
F. Liu[1], I. Turner[1], K.Burrage[1,2] and V. Anh[1]
Email: f.liu@qut.edu.au
[1] School of Mathematical Sciences, Queensland University of Technology, Brisbane, Australia.
[2] Department of Computer Science and OCISB, Oxford University, OXI 3QD, UK
QUT Queensland University of Technology
QUT

Outline

Introduction

- In 2000, the project "Modelling of saltwater intrusion into aquifers", which was supported by the ARC SPIRT grant.
- Fractional-order models provide an excellent instrument for describing the memory and hereditary properties of various processes. The fractional model is able to describe heavy-tailed motions more accurately.
- Space fractional diffusion equations with a nonlinear reaction term have been presented and used to model many problems in biology, chemistry, physics and engineering.
- However, there are still many issues to be resolved regarding numerical methods and error analysis to simulate fractional nonlinear reaction-diffusion models.

Introduction

- In 2000, the project "Modelling of saltwater intrusion into aquifers", which was supported by the ARC SPIRT grant.
- Fractional-order models provide an excellent instrument for describing the memory and hereditary properties of various processes. The fractional model is able to describe heavy-tailed motions more accurately.
- Space fractional diffusion equations with a nonlinear reaction term have been presented and used to model many problems in biology, chemistry, physics and engineering.
- However, there are still many issues to be resolved regarding numerical methods and error analysis to simulate fractional nonlinear reaction-diffusion models.

Introduction

- In 2000, the project "Modelling of saltwater intrusion into aquifers", which was supported by the ARC SPIRT grant.
- Fractional-order models provide an excellent instrument for describing the memory and hereditary properties of various processes. The fractional model is able to describe heavy-tailed motions more accurately.
- Space fractional diffusion equations with a nonlinear reaction term have been presented and used to model many problems in biology, chemistry, physics and engineering.
- However, there are still many issues to be resolved regarding numerical methods and error analysis to simulate fractional nonlinear reaction-diffusion models.

Introduction

- In 2000, the project "Modelling of saltwater intrusion into aquifers", which was supported by the ARC SPIRT grant.
- Fractional-order models provide an excellent instrument for describing the memory and hereditary properties of various processes. The fractional model is able to describe heavy-tailed motions more accurately.
- Space fractional diffusion equations with a nonlinear reaction term have been presented and used to model many problems in biology, chemistry, physics and engineering.
- However, there are still many issues to be resolved regarding numerical methods and error analysis to simulate fractional nonlinear reaction-diffusion models.

Introduction

Numerical simulation of the following three models:

- One-dimensional variable-order space fractional nonlinear reaction-diffusion model (1D-VOSFNRDM):

$$\frac{\partial u(x,t)}{\partial t} = K(x,t)R_{\alpha(x,t)}u(x,t) + f(u,x,t)$$

where

$$R_{\alpha(x,t)}u(x,t) = c_+(x,t)_a D_x^{\alpha(x,t)}u(x,t) + c_-(x,t)_x D_b^{\alpha(x,t)}u(x,t).$$

Introduction

- - $c_+(x,t) = 1, c_-(x,t) \equiv 0$: the variable-order left-handed Riemann-Liouville derivative;
  - $c_+(x,t) \equiv 0, c_-(x,t) = 1$: the variable-order right-handed Riemann-Liouville derivative;
  - $c_+(x,t) = c_-(x,t) = -\frac{1}{2\cos(\frac{\pi\alpha(x,t)}{2})}$: the variable-order Riesz fractional derivative

$$R_{\alpha(x,t)}u(x,t) = -\frac{1}{2\cos\frac{\pi\alpha(x,t)}{2}}\left[{}_aD_x^{\alpha(x,t)}u(x,t) + {}_xD_b^{\alpha(x,t)}u(x,t)\right].$$

- Two-dimensional Riesz space fractional nonlinear reaction-diffusion model (2D-RSFNRDM)

$$\frac{\partial u}{\partial t} = K_x\frac{\partial^\alpha u}{\partial |x|^\alpha} + K_y\frac{\partial^\alpha u}{\partial |y|^\alpha} + f(u,x,y,t)$$

and application to fractional FitzHugh-Nagumo monodomain model.

Introduction

- - $c_+(x,t) = 1, c_-(x,t) \equiv 0$: the variable-order left-handed Riemann-Liouville derivative;
  - $c_+(x,t) \equiv 0, c_-(x,t) = 1$: the variable-order right-handed Riemann-Liouville derivative;
  - $c_+(x,t) = c_-(x,t) = -\frac{1}{2\cos(\frac{\pi\alpha(x,t)}{2})}$: the variable-order Riesz fractional derivative

$$R_{\alpha(x,t)}u(x,t) = -\frac{1}{2\cos\frac{\pi\alpha(x,t)}{2}}\left[{}_aD_x^{\alpha(x,t)}u(x,t) + {}_xD_b^{\alpha(x,t)}u(x,t)\right].$$

- Two-dimensional Riesz space fractional nonlinear reaction-diffusion model (2D-RSFNRDM)

$$\frac{\partial u}{\partial t} = K_x\frac{\partial^\alpha u}{\partial|x|^\alpha} + K_y\frac{\partial^\alpha u}{\partial|y|^\alpha} + f(u,x,y,t)$$

  and application to fractional FitzHugh-Nagumo monodomain model.

Introduction

- Two-dimensional variable-order fractional nonlinear reaction-diffusion model with variable coefficients (2D-VOFNRDM-VC):

$$\begin{aligned}\frac{\partial u}{\partial t} &= \frac{\partial}{\partial x}\left(A(x,y)\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right) + \frac{\partial}{\partial y}\left(B(x,y)\frac{\partial^{\beta(x,y)}u}{\partial y^{\beta(x,y)}}\right) \\ &+ f(u,x,y,t),\end{aligned}$$

where $0 < \alpha(x,y), \beta(x,y) \leq 1$.

Numerical methods for 1-D VOFNRDM

- Recently, more and more researchers find that many dynamic processes appear to exhibit fractional order behavior that may vary with time or space.
- In various applications in science and engineering, in order to more accurately describe the evolution of a system, the concept of a variable-order operator has been developed.
- Different authors have used different definitions of variable order differential operators, each of these with a specific meaning to suit desired goals.

Numerical methods for 1-D VOFNRDM

- Recently, more and more researchers find that many dynamic processes appear to exhibit fractional order behavior that may vary with time or space.
- In various applications in science and engineering, in order to more accurately describe the evolution of a system, the concept of a variable-order operator has been developed.
- Different authors have used different definitions of variable order differential operators, each of these with a specific meaning to suit desired goals.

Numerical methods for 1-D VOFNRDM

- Recently, more and more researchers find that many dynamic processes appear to exhibit fractional order behavior that may vary with time or space.
- In various applications in science and engineering, in order to more accurately describe the evolution of a system, the concept of a variable-order operator has been developed.
- Different authors have used different definitions of variable order differential operators, each of these with a specific meaning to suit desired goals.

Numerical methods for 1-D VOFNDRM

- **Definition 1:** Variable-order Riemann-Liouville fractional derivatives [Zhuang and Liu et al. SIAM J NA, 2009]:

$$
{}_aD_x^{\alpha(x,t)}u(x,t) = \left[\frac{1}{\Gamma(m-\alpha(x,t))}\frac{\partial^m}{\partial\xi^m}\int_a^\xi(\xi-\eta)^{m-\alpha(x,t)-1}u(\eta,t)d\eta\right]_{\xi=x},
$$

$$
{}_xD_b^{\alpha(x,t)}u(x,t) = \left[\frac{(-1)^m}{\Gamma(m-\alpha(x,t))}\frac{\partial^m}{\partial\xi^m}\int_\xi^b(\eta-\xi)^{m-\alpha(x,t)-1}u(\eta,t)d\eta\right]_{\xi=x}.
$$

Definition 2: Variable-order Riesz fractional derivative [Zhuang and Liu et al. SIAM J NA, 2009]:

$$
\frac{\partial^{\alpha(x,t)}u(x,t)}{\partial|x|^{\alpha(x,t)}} = -\frac{1}{2\cos\frac{\pi\alpha(x,t)}{2}}\left[{}_aD_x^{\alpha(x,t)}u(x,t) + {}_xD_b^{\alpha(x,t)}u(x,t)\right].
$$

Numerical methods for 1-D VOFNDRM

- **Definition 1:** Variable-order Riemann-Liouville fractional derivatives [Zhuang and Liu et al. SIAM J NA, 2009]:

$$
{}_aD_x^{\alpha(x,t)}u(x,t) = \left[\frac{1}{\Gamma(m-\alpha(x,t))}\frac{\partial^m}{\partial \xi^m}\int_a^{\xi}(\xi-\eta)^{m-\alpha(x,t)-1}u(\eta,t)d\eta\right]_{\xi=x},
$$

$$
{}_xD_b^{\alpha(x,t)}u(x,t) = \left[\frac{(-1)^m}{\Gamma(m-\alpha(x,t))}\frac{\partial^m}{\partial \xi^m}\int_{\xi}^{b}(\eta-\xi)^{m-\alpha(x,t)-1}u(\eta,t)d\eta\right]_{\xi=x}.
$$

Definition 2: Variable-order Riesz fractional derivative [Zhuang and Liu et al. SIAM J NA, 2009]:

$$
\frac{\partial^{\alpha(x,t)}u(x,t)}{\partial|x|^{\alpha(x,t)}} = -\frac{1}{2\cos\frac{\pi\alpha(x,t)}{2}}\left[{}_aD_x^{\alpha(x,t)}u(x,t) + {}_xD_b^{\alpha(x,t)}u(x,t)\right].
$$

Numerical methods for 1-D VOFNDRM

Definition 3: Variable-order Grünwald-Letnikov fractional derivatives [Lin and Liu et al., Appl. Math. Comp., 2009]

$$
\begin{aligned}
&{}_a^G D_x^{\alpha(x,t)} u(x,t) \\
&= \lim_{h\to 0, nh = x-a} h^{-\alpha(x,t)} \sum_{j=0}^{n} (-1)^j \begin{pmatrix} \alpha(x,t) \\ j \end{pmatrix} u(x-jh,t), \\
&{}_x^G D_b^{\alpha(x,t)} u(x,t) \\
&= \lim_{h\to 0, nh = b-x} h^{-\alpha(x,t)} \sum_{j=0}^{n} (-1)^j \begin{pmatrix} \alpha(x,t) \\ j \end{pmatrix} u(x+jh,t).
\end{aligned}
$$

Numerical methods for 1D-VOSFNRDM

One-dimensional variable-order space fractional nonlinear reaction-diffusion model:

$$\frac{\partial u(x,t)}{\partial t} = K(x,t)R_{\alpha(x,t)}u(x,t) + f(u,x,t), \tag{1}$$

and the initial and boundary conditions

$$u(x,0) = \phi(x), \tag{2}$$

$$u(a,t) = 0, u(b,t) = 0, \tag{3}$$

where $1 < \underline{\alpha} \leq \alpha(x,t) \leq \overline{\alpha} \leq 2$; $0 < \underline{K} < K(x,t) < \bar{K}$; $f(u,x,t)$ is a source term which satisfies the Lipschitz condition, i.e.,

$$\forall u_1, u_2, \quad |f(u_1,x,t) - f(u_2,x,t)| \leq L|u_1 - u_2|.$$

Numerical methods for 1D-VOSFNRDM

- Baeumer et al. [Comput. & Math. with Appl., 2008] gave that $f : X \to X$ is globally Lipschitz continuous if for some $L > 0$, we have $\|f(u) - f(v)\| \le L\|u - v\|$ for all $u, v \in X$, and is locally Lipschitz continuous, if the latter holds for $\|u\|, \|v\| \le M$ with $L = L(M)$ for any $M > 0$.
- We assume that for all $k = 0, 1, 2, \cdots, N$, $\|u(x, t_k)\|, \|v(x, t_k)\| \le M_k$ with a constant $M_k > 0$, we have

$$\begin{aligned} & \|f(u(x,t_k) - f(v(x,t_k))\| \le L(M_k)\|u(x,t_k) - v(x,t_k)\| \\ = \; & L_k\|u(x,t_k) - v(x,t_k)\|, \;\; \forall \;\, (x,t) \in [a,b; t = t_k], \end{aligned}$$

where $L = L_{max} = \max_{0 \le k \le N} L_k$.

Numerical methods for 1D-VOSFNRDM

Lemma 1: Shift Grünwald formula:

$$
{}_{x}^{G}D_{a}^{\alpha_i^k} u_i^k = h^{-\alpha_{i+1}^k} \sum_{j=0}^{i+1} g_{\alpha_{i+1}^k}^{(j)} u_{i+1-j}^k + O(h),
$$

$$
{}_{x}^{G}D_{b}^{\alpha_i^k} u_i^k = h^{-\alpha_{i-1}^k} \sum_{j=0}^{m-i+1} g_{\alpha_{i-1}^k}^{(j)} u_{i-1+j}^k + O(h),
$$

where $g_{\alpha_i^k}^{(0)} = 1$, $g_{\alpha_i^k}^{(j)} = -\frac{\alpha_i^k - j + 1}{j} g_{\alpha_i^k}^{(j-1)}$ $(j = 1, 2, \cdots)$,
$\alpha_i^k = \alpha(x_i, t_k)$.

Remark 1: If the Standard Grünwald approximation for diffusion term is used, the numerical method is always unstable [Meerschaert et al., J. Comp. Appl. Math., 2004].

Numerical methods for 1D-VOSFNRDM

Lemma 1: Shift Grünwald formula:

$$ {}_{x}^{G}D_{a}^{\alpha_i^k} u_i^k = h^{-\alpha_{i+1}^k} \sum_{j=0}^{i+1} g_{\alpha_{i+1}^k}^{(j)} u_{i+1-j}^k + O(h), $$

$$ {}_{x}^{G}D_{b}^{\alpha_i^k} u_i^k = h^{-\alpha_{i-1}^k} \sum_{j=0}^{m-i+1} g_{\alpha_{i-1}^k}^{(j)} u_{i-1+j}^k + O(h), $$

where $g_{\alpha_i^k}^{(0)} = 1,\ g_{\alpha_i^k}^{(j)} = -\frac{\alpha_i^k - j + 1}{j} g_{\alpha_i^k}^{(j-1)}\ \ (j = 1, 2, \cdots),$
$\alpha_i^k = \alpha(x_i, t_k)$.

Remark 1: If the Standard Grünwald approximation for diffusion term is used, the numerical method is always unstable [Meerschaert et al., J. Comp. Appl. Math., 2004].

Numerical methods for 1D-VOSFNRDM

Fractional method of lines:

$$\frac{du_i(t)}{dt} = \frac{K_i(t)c_{+,i}(t)}{h^{\alpha_i(t)}} \sum_{j=0}^{i+1} g_i^{(j)}(t)u_{i-j+1}(t)$$

$$+ \quad \frac{K_i(t)c_{-,i}(t)}{h^{\alpha_i(t)}} \sum_{j=0}^{m-i+1} g_i^{(j)}(t)u_{i+j-1}(t) + f(u_i(t), x_i, t).$$

The system is thereby reduced from its partial differential equation to a system of ordinary differential equations, then integrated in time. In this work, we used DASSL as our solver. DASSL approximates the derivatives using the kth order backward difference, where k ranges from one to five. At every step it selects the order k and stepsize based on the behavior of the solution.

Numerical methods for 1D-VOSFNRDM

Explicit Euler approximation (EEA) with $|R_{i,k}^{(E)}| = O(\tau(\tau + h))$:

$$
\begin{aligned}
u_i^{k+1} &= u_i^k + r_{i,k}^{(1)} \sum_{j=0}^{i+1} g_{i+1,k}^{(j)} u_{i-j+1}^k \\
&+ r_{i,k}^{(2)} \sum_{j=0}^{m-i+1} g_{i-1,k}^{(j)} u_{i+j-1}^k + \tau f(u_i^k, x_i, t_k),
\end{aligned}
$$

where $r_{i,k}^{(1)} = K_i^k c_{+,i}^k \tau h^{-\alpha_{i+1}^k}$, $r_{i,k}^{(2)} = K_i^k c_{-,i}^k \tau h^{-\alpha_{i-1}^k}$.

Numerical methods for 1D-VOSFNRDM

Implicit Euler approximation (IEA) with $|R_{i,k}^{(l)}| = O(\tau(\tau+h))$:

$$\begin{aligned} u_i^{k+1} &= u_i^k + r_{i,k+1}^{(1)} \sum_{j=0}^{i+1} g_{i+1,k+1}^{(j)} u_{i-j+1}^{k+1} \\ &+ r_{i,k+1}^{(2)} \sum_{j=0}^{m-i+1} g_{i-1,k+1}^{(j)} u_{i+j-1}^{k+1} + \tau f(u_i^k, x_i, t_k). \end{aligned}$$

Stability and convergence

Lemma 2: The coefficients $g_{i,k}^{(j)}$ satisfy

$$(1)\quad g_{i,k}^{(0)} = 1,\ \ g_{i,k}^{(1)} = -\alpha_i^k < 0,\ \ g_{i,k}^{(j)} > 0,\ \ (j \neq 1),$$

$$(2)\quad \sum_{j=0}^{\infty} g_{i,k}^{(j)} = 0,\ \ (l = 1, 2, \ldots),\ \sum_{j=0}^{l} g_{i,k}^{(j)} < 0.$$

Lemma 3 [Discrete Gronwall Inequality]: Suppose that $\eta_0 = 0$, $f_k \geq 0$, $\eta_k \geq 0$, $\rho = 1 + C_0\tau$, $C_0 \geq 0$, and

$$\eta_{k+1} \leq \rho\eta_k + \tau f_k, \quad (k = 0, 1, 2, \cdots),$$

then

$$\eta_{k+1} \leq e^{C_0 t_k} \sum_{j=0}^{k} \tau f_j.$$

Stability and convergence

If $S_c = \overline{K}(c_1 + c_2)\overline{\alpha}\tau h^{-\underline{\alpha}} < 1$, using Lemma 2 and Lemma 3, we have

Theorem 1 [Stability of EEA]: If $S_c < 1$, then the Explicit Euler approximation defined by (4) is conditionally stable.

Theorem 2 [Convergence of EEA]: Suppose that the continuous problem (1)-(3) has a smooth solution $u(x,t) \in C_{x,t}^{1+\overline{\alpha},2}(\Omega)$. Let u_i^k be the numerical solution computed by use of EEA (4). If $S_c < 1$, then there is a positive constant C independent of i, k, h and τ such that

$$|u(x_i, t_k) - u_i^k| \leq C(\tau + h).$$

Stability and convergence

If $S_c = \overline{K}(c_1 + c_2)\overline{\alpha}\tau h^{-\underline{\alpha}} < 1$, using Lemma 2 and Lemma 3, we have

Theorem 1 [Stability of EEA]: If $S_c < 1$, then the Explicit Euler approximation defined by (4) is conditionally stable.

Theorem 2 [Convergence of EEA]: Suppose that the continuous problem (1)-(3) has a smooth solution $u(x, t) \in C_{x,t}^{1+\overline{\alpha},2}(\Omega)$. Let u_i^k be the numerical solution computed by use of EEA (4). If $S_c < 1$, then there is a positive constant C independent of i, k, h and τ such that

$$|u(x_i, t_k) - u_i^k| \leq C(\tau + h).$$

Stability and convergence

Using Lemma 2 and Lemma 3, we have

Theorem 3 [Stability of IEA]: The implicit Euler approximation defined by (4) is unconditionally stable.

Theorem 4 [Convergence of IEA]: Suppose that the continuous problem (1)-(3) has a smooth solution $u(x,t) \in C_{x,t}^{1+\overline{\alpha},2}(\Omega)$. Let u_i^k be the numerical solution computed by use of IEA (4). Then there is a positive constant C independent of i, k, h and τ such that

$$|u(x_i,t_k) - u_i^k| \leq C(\tau + h).$$

Stability and convergence

Using Lemma 2 and Lemma 3, we have

Theorem 3 [Stability of IEA]: The implicit Euler approximation defined by (4) is unconditionally stable.

Theorem 4 [Convergence of IEA]: Suppose that the continuous problem (1)-(3) has a smooth solution $u(x,t) \in C^{1+\overline{\alpha},2}_{x,t}(\Omega)$. Let u_i^k be the numerical solution computed by use of IEA (4). Then there is a positive constant C independent of i, k, h and τ such that

$$|u(x_i,t_k) - u_i^k| \leq C(\tau + h).$$

Extrapolation method for 1D-VOSFNRDM

The IEA is convergent at the rate $O(\tau + h)$. In order to improve the order of convergence, we propose an extrapolation method (EM):

- Apply the IEA on a (coarse) grid of size $\Delta t = \tau$, $\Delta x = h$;
- Apply the IEA on a finer grid of size $\Delta t = \tau/2$, $\Delta x = h/2$;
- The extrapolated solution:

$$u(x,t) \approx 2u_{2i}^{2k}(h/2, \tau/2) - u_i^k(h,\tau), \quad (i = 1, 2, \cdots, m-1),$$

where $t = t_k, x = x_i$ on the coarse grid, while $t = t_{2k}$, $x = x_{2i}$ on the fine grid. $u_i^k(h,\tau)$ and $u_{2i}^{2k}(h/2, \tau/2)$ are the numerical solutions on the coarse grid and the fine grid, respectively. Thus, the extrapolation method may be used to obtain a solution with convergence order $O(\tau^2 + h^2)$

Numerical examples

Example 1: Variable-order fractional nonlinear reaction-diffusion equation with $\alpha(x,t) = 1.5 + 0.5e^{-(xt)^2-1}$. Then

$$\frac{\partial u(x,t)}{\partial t} = R^{\alpha(x,t)}u(x,t) + f(u,x,t), \tag{4}$$

where

$f(u,x,t) = \frac{1}{80}(t+1)^{-1}u - \left(\frac{\Gamma(3)x^{2-\alpha(x,t)}(t+1)}{20\Gamma(3-\alpha(x,t))} - \frac{\Gamma(4)x^{3-\alpha(x,t)}(t+1)}{160\Gamma(4-\alpha(x,t))}\right)$,

$\varphi(x) = \frac{x^2(8-x)}{80}$, $a = 0$, $b = 8$, $T = 1$. We take $c_+ = 1$, $c_- = 0$.

The exact solution of the above equation is

$$u(x,t) = \frac{x^2(8-x)(t+1)}{80}.$$

Numerical examples

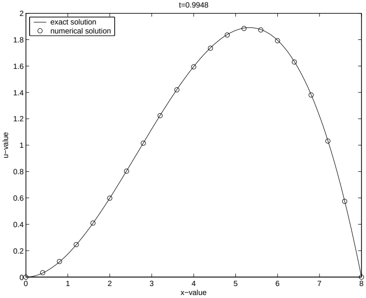


Figure: 1. A comparison of the numerical and the exact solutions in Example 1.

From Figure 1, it can be seen that the numerical solution is in excellent agreement with the exact solution.

Numerical examples

Example 2: We consider a variable-order fractional reaction-diffusion equation using Fisher's growth equation and a Riesz fractional derivative of variable order $\alpha(x,t) = 1.5 + 0.5e^{-(xt)^2-1}$. In this case,

$$\frac{\partial u(x,t)}{\partial t} = 0.1_x R^{\alpha(x,t)} u(x,t) + 0.25u(x,t)(1 - u(x,t)), \qquad (5)$$

where $c_+(x,t) = c_-(x,t) = -\frac{1}{2\cos(\frac{\pi\alpha(x,t)}{2})}$, $x \in [-80, 80]$, $t \in [0, 25]$ and a smooth step-like initial function $u(x,0) = \varphi(x)$ which takes the constant value $u = 0.8$ around the origin and rapidly decays to 0 away from the origin.

Numerical examples

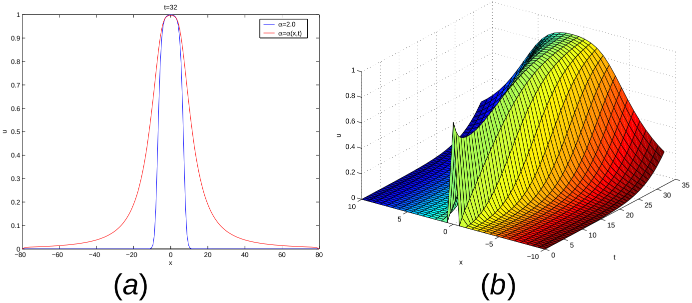


Figure: 2(a) Solutions of the fractional Fisher equation with $\alpha = 2.0$ and $\alpha = \alpha(x,t) < 2$, which shows heavier tails in the fractional case; (b) The numerical solution of (5) with the fractional case in different times.

Motivation for research

- Computation of electrical wave propagation in the heart is one of the most important recent applications of mathematical modeling in biology [Bueno-Orovio, Kay and Kevin, J. Copm. Phys., 2013].
- Mathematical models of cardiac electrophysiology consist of a system of partial differential equations (PDEs), coupled nonlinearly to a system of ordinary differential equations (ODEs).
- On some assumptions, the system of partial differential equations can be reduced to a monodomain model.

Motivation for research

- Computation of electrical wave propagation in the heart is one of the most important recent applications of mathematical modeling in biology [Bueno-Orovio, Kay and Kevin, J. Copm. Phys., 2013].
- Mathematical models of cardiac electrophysiology consist of a system of partial differential equations (PDEs), coupled nonlinearly to a system of ordinary differential equations (ODEs).
- On some assumptions, the system of partial differential equations can be reduced to a monodomain model.

Motivation for research

- Computation of electrical wave propagation in the heart is one of the most important recent applications of mathematical modeling in biology [Bueno-Orovio, Kay and Kevin, J. Copm. Phys., 2013].
- Mathematical models of cardiac electrophysiology consist of a system of partial differential equations (PDEs), coupled nonlinearly to a system of ordinary differential equations (ODEs).
- On some assumptions, the system of partial differential equations can be reduced to a monodomain model.

Motivation for research

- A dimensionless FitzHugh-Nagumo monodomain model in $2D$ is given:

$$\begin{aligned} \frac{\partial v}{\partial t} &= \nabla \cdot (K \nabla v) + I_{ion}(v, w), \\ \frac{\partial w}{\partial t} &= av - bw + c, \end{aligned}$$

  v normalized transmembrane potential; w recovery variable;
  K diffusion tensor; $I_{ion}(v, w)$ ionic current;
  It is known that this model has traveling wave solutions with an appropriate choice of parameters: K, a, b and c.

- We propose a fundamental rethink of the fractional FitzHugh-Nagumo monodomain model (FFHNMM) in which we capture the spatial heterogeneities in the extracellular domain through the use of fractional derivatives.

Motivation for research

- A dimensionless FitzHugh-Nagumo monodomain model in $2D$ is given:

$$\begin{aligned} \frac{\partial v}{\partial t} &= \nabla \cdot (K \nabla v) + I_{ion}(v, w), \\ \frac{\partial w}{\partial t} &= av - bw + c, \end{aligned}$$

  v normalized transmembrane potential; w recovery variable;
  K diffusion tensor; $I_{ion}(v, w)$ ionic current;
  It is known that this model has traveling wave solutions with an appropriate choice of parameters: K, a, b and c.

- We propose a fundamental rethink of the fractional FitzHugh-Nagumo monodomain model (FFHNMM) in which we capture the spatial heterogeneities in the extracellular domain through the use of fractional derivatives.

Motivation for research

Using fractional $Fick's$ law and the isotropic setting, this leads to the two-dimensional fractional FitzHugh-Nagumo monodomain model [Bueno-Orovio, Kay and Kevin, J. Copm. Phys., 2013]:

$$\frac{\partial v}{\partial t} = K\mathbf{R}^{\alpha} v + I_{ion}(v, w),$$

with Eq. (6)

or

$$\frac{\partial v}{\partial t} = K_x \frac{\partial^{\alpha} v}{\partial |x|^{\alpha}} + K_y \frac{\partial^{\alpha} v}{\partial |y|^{\alpha}} + I_{ion}(v, w),$$

with Eq. (6), where $1 < \alpha \leq 2$, $\mathbf{R}^{\alpha} = (R_x^{\alpha}, R_y^{\alpha}) = (\frac{\partial^{\alpha}}{\partial |x|^{\alpha}}, \frac{\partial^{\alpha}}{\partial |y|^{\alpha}})$ is a sequential Riesz fractional order operator in space.

Motivation for research

Using fractional $Fick's$ law and the isotropic setting, this leads to the two-dimensional fractional FitzHugh-Nagumo monodomain model [Bueno-Orovio, Kay and Kevin, J. Copm. Phys., 2013]:

$$\frac{\partial v}{\partial t} = K\mathbf{R}^{\alpha} v + I_{ion}(v, w),$$

with Eq. (6)
or

$$\frac{\partial v}{\partial t} = K_x \frac{\partial^{\alpha} v}{\partial |x|^{\alpha}} + K_y \frac{\partial^{\alpha} v}{\partial |y|^{\alpha}} + I_{ion}(v, w),$$

with Eq. (6), where $1 < \alpha \leq 2$, $\mathbf{R}^{\alpha} = (R_x^{\alpha}, R_y^{\alpha}) = (\frac{\partial^{\alpha}}{\partial |x|^{\alpha}}, \frac{\partial^{\alpha}}{\partial |y|^{\alpha}})$ is a sequential Riesz fractional order operator in space.

Motivation for research

The space Riesz fractional operators $\frac{\partial^\alpha}{\partial|x|^\alpha}$ and $\frac{\partial^\alpha}{\partial|y|^\alpha}$ on a finite domain $[0, L_x] \times [0, L_y]$ are defined as

$$\frac{\partial^\alpha v}{\partial|x|^\alpha} = -\frac{1}{2\cos(\frac{\pi\alpha}{2})}\left(\frac{\partial^\alpha v}{\partial x^\alpha} + \frac{\partial^\alpha v}{\partial(-x)^\alpha}\right),$$

and

$$\begin{aligned}
\frac{\partial^\alpha v(x,y,t)}{\partial x^\alpha} &= \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_0^x \frac{v(\xi,y,t)d_\xi}{(x-\xi)^{\alpha-1}},\\
\frac{\partial^\alpha v(x,y,t)}{\partial(-x)^\alpha} &= \frac{(-1)^2}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_x^{L_x} \frac{v(\xi,y,t)d_\xi}{(\xi-x)^{\alpha-1}}.
\end{aligned}$$

Similarly, we can define the space Riesz fractional derivative $\frac{\partial^\alpha u}{\partial|y|^\alpha}$ of order α $(1 < \alpha \leq 2)$ with respect to y.

Motivation for research

The space Riesz fractional operators $\frac{\partial^\alpha}{\partial|x|^\alpha}$ and $\frac{\partial^\alpha}{\partial|y|^\alpha}$ on a finite domain $[0, L_x] \times [0, L_y]$ are defined as

$$\frac{\partial^\alpha v}{\partial|x|^\alpha} = -\frac{1}{2\cos(\frac{\pi\alpha}{2})}\left(\frac{\partial^\alpha v}{\partial x^\alpha} + \frac{\partial^\alpha v}{\partial(-x)^\alpha}\right),$$

and

$$\begin{aligned}
\frac{\partial^\alpha v(x,y,t)}{\partial x^\alpha} &= \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_0^x \frac{v(\xi,y,t)d_\xi}{(x-\xi)^{\alpha-1}}, \\
\frac{\partial^\alpha v(x,y,t)}{\partial(-x)^\alpha} &= \frac{(-1)^2}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_x^{L_x} \frac{v(\xi,y,t)d_\xi}{(\xi-x)^{\alpha-1}}.
\end{aligned}$$

Similarly, we can define the space Riesz fractional derivative $\frac{\partial^\alpha u}{\partial|y|^\alpha}$ of order α $(1 < \alpha \leq 2)$ with respect to y.

Motivation for research

- We re-emphasise that the fractional monodomain equation is solved by operator splitting in which we first solve the partial differential equation for v and then the ODE for w at each time step.
- The 2D-FFHNMM is decoupled, which is equivalent to solving a two-dimensional fractional Riesz space nonlinear reaction-diffusion model (2D-FRSNRDM)

$$\frac{\partial u}{\partial t} = K_x \frac{\partial^\alpha u}{\partial |x|^\alpha} + K_y \frac{\partial^\alpha u}{\partial |y|^\alpha} + f(u, x, y, t) \tag{6}$$

coupled with an ODE.
- It is difficult to solve fractional Riesz space nonlinear reaction-diffusion model, and analyze the stability and convergence of the numerical method.

Motivation for research

- We re-emphasise that the fractional monodomain equation is solved by operator splitting in which we first solve the partial differential equation for v and then the ODE for w at each time step.
- The 2D-FFHNMM is decoupled, which is equivalent to solving a two-dimensional fractional Riesz space nonlinear reaction-diffusion model (2D-FRSNRDM)

$$\frac{\partial u}{\partial t} = K_x \frac{\partial^\alpha u}{\partial |x|^\alpha} + K_y \frac{\partial^\alpha u}{\partial |y|^\alpha} + f(u, x, y, t) \tag{6}$$

coupled with an ODE.
- It is difficult to solve fractional Riesz space nonlinear reaction-diffusion model, and analyze the stability and convergence of the numerical method.

Motivation for research

- We re-emphasise that the fractional monodomain equation is solved by operator splitting in which we first solve the partial differential equation for v and then the ODE for w at each time step.
- The 2D-FFHNMM is decoupled, which is equivalent to solving a two-dimensional fractional Riesz space nonlinear reaction-diffusion model (2D-FRSNRDM)

$$\frac{\partial u}{\partial t} = K_x \frac{\partial^\alpha u}{\partial |x|^\alpha} + K_y \frac{\partial^\alpha u}{\partial |y|^\alpha} + f(u, x, y, t) \tag{6}$$

  coupled with an ODE.
- It is difficult to solve fractional Riesz space nonlinear reaction-diffusion model, and analyze the stability and convergence of the numerical method.

An implicit numerical method for 2D-RSFNRDM

Using the shifted *Grünwald – Letnikov* schemes, the 2D-RSFNRDM can be cast into the following implicit numerical method with shifted *Grünwald – Letnikov* schemes, then a modified iterative technique is used for solving the implicit numerical approximation:

$$\frac{u_{i,j}^{n}-u_{i,j}^{n-1}}{\tau} = -\frac{K_x c_\alpha}{(h_x)^\alpha}\left[\sum_{k=0}^{i+1} g_\alpha^{(k)} u_{i-k+1,j}^{n} + \sum_{k=0}^{m_1-i+1} g_\alpha^{(k)} u_{i+k-1,j}^{n}\right] - \frac{K_y c_\alpha}{(h_y)^\alpha}\left[\sum_{k=0}^{j+1} g_\alpha^{(k)} u_{i,j-k+1}^{n} + \sum_{k=0}^{m_2-j+1} g_\alpha^{(k)} u_{i,j+k-1}^{n}\right] + f_{i,j}^{n-1} \quad (7)$$

where $c_\alpha = \frac{1}{2\cos(\frac{\pi\alpha}{2})}$, $f_{i,j}^{n-1} = f(u_{i,j}^{n-1}, x_i, y_j, t_{n-1})$.

An implicit numerical method for 2D-RSFNRDM

Remark 2: We say that $f : X \to X$ is globally Lipschitz continuous if for some $L > 0$, we have $\|f(u) - f(v)\| \leq L\,\|u - v\|$ for all $u, v \in X$, and is locally Lipschitz continuous, if the latter holds for $\|u\|, \|v\| \leq M_k$ with $L_k = L(M_k)$ at $t = t_k$ for any $M_k > 0$.

Theorem 5. The implicit numerical method (7) with shifted $Grünwald - Letnikov$ schemes is unconditionally stable.

Theorem 6. The implicit numerical method (7) with shifted $Grünwald - Letnikov$ schemes is consistent to the 2D-RSFNRDM (6) with convergence order $O(\tau + h_x + h_y)$.

An implicit numerical method for 2D-RSFNRDM

Remark 2: We say that $f : X \to X$ is globally Lipschitz continuous if for some $L > 0$, we have $\|f(u) - f(v)\| \leq L\,\|u - v\|$ for all $u, v \in X$, and is locally Lipschitz continuous, if the latter holds for $\|u\|, \|v\| \leq M_k$ with $L_k = L(M_k)$ at $t = t_k$ for any $M_k > 0$.

Theorem 5. The implicit numerical method (7) with shifted $Grünwald - Letnikov$ schemes is unconditionally stable.

Theorem 6. The implicit numerical method (7) with shifted $Grünwald - Letnikov$ schemes is consistent to the 2D-RSFNRDM (6) with convergence order $O(\tau + h_x + h_y)$.

An implicit numerical method for 2D-RSFNRDM

Remark 2: We say that $f : X \to X$ is globally Lipschitz continuous if for some $L > 0$, we have $\|f(u) - f(v)\| \leq L \|u - v\|$ for all $u, v \in X$, and is locally Lipschitz continuous, if the latter holds for $\|u\|, \|v\| \leq M_k$ with $L_k = L(M_k)$ at $t = t_k$ for any $M_k > 0$.

Theorem 5. The implicit numerical method (7) with shifted $Grünwald - Letnikov$ schemes is unconditionally stable.

Theorem 6. The implicit numerical method (7) with shifted $Grünwald - Letnikov$ schemes is consistent to the 2D-RSFNRDM (6) with convergence order $O(\tau + h_x + h_y)$.

An alternating direction implicit method for 2D-RSFNRDM

- Our aim is to divide the calculation into two steps with reduced calculation. In the first step, we solve the problem in the x-direction, in the second step, we solve the problem in the y-direction.
- Define the following fractional partial difference operator:

$$\delta_x u_{i,j}^n = -K_x c_\alpha \left[\frac{1}{(h_x)^\alpha} \sum_{k=0}^{i+1} g_\alpha^{(k)} u_{i-k+1,j}^n + \frac{1}{(h_x)^\alpha} \sum_{k=0}^{m_1-i+1} g_\alpha^{(k)} u_{i+k-1,j}^n \right],$$

with similar definition for δ_y.
- With these operator definitions, the implicit numerical method for the 2D-RSFNRDM with zero Dirichlet boundary conditions may be written in the following operator form:

$$(1 - \tau\delta_x - \tau\delta_y) u_{i,j}^n = u_{i,j}^{n-1} + \tau f(u_{i,j}^{n-1}, x_i, y_j, t_{n-1}). \quad (8)$$

An alternating direction implicit method for 2D-RSFNRDM

- Our aim is to divide the calculation into two steps with reduced calculation. In the first step, we solve the problem in the x-direction, in the second step, we solve the problem in the y-direction.
- Define the following fractional partial difference operator:

$$\delta_x u_{i,j}^n = -K_x c_\alpha \left[\frac{1}{(h_x)^\alpha} \sum_{k=0}^{i+1} g_\alpha^{(k)} u_{i-k+1,j}^n + \frac{1}{(h_x)^\alpha} \sum_{k=0}^{m_1-i+1} g_\alpha^{(k)} u_{i+k-1,j}^n \right],$$

  with similar definition for δ_y.
- With these operator definitions, the implicit numerical method for the 2D-RSFNRDM with zero Dirichlet boundary conditions may be written in the following operator form:

$$(1 - \tau\delta_x - \tau\delta_y) u_{i,j}^n = u_{i,j}^{n-1} + \tau f(u_{i,j}^{n-1}, x_i, y_j, t_{n-1}). \qquad (8)$$

An alternating direction implicit method for 2D-RSFNRDM

- Our aim is to divide the calculation into two steps with reduced calculation. In the first step, we solve the problem in the x-direction, in the second step, we solve the problem in the y-direction.
- Define the following fractional partial difference operator:

$$\delta_x u_{i,j}^n = -K_x c_\alpha \left[\frac{1}{(h_x)^\alpha} \sum_{k=0}^{i+1} g_\alpha^{(k)} u_{i-k+1,j}^n + \frac{1}{(h_x)^\alpha} \sum_{k=0}^{m_1-i+1} g_\alpha^{(k)} u_{i+k-1,j}^n \right],$$

  with similar definition for δ_y.
- With these operator definitions, the implicit numerical method for the 2D-RSFNRDM with zero Dirichlet boundary conditions may be written in the following operator form:

$$(1 - \tau\delta_x - \tau\delta_y) u_{i,j}^n = u_{i,j}^{n-1} + \tau f(u_{i,j}^{n-1}, x_i, y_j, t_{n-1}). \qquad (8)$$

An alternating direction implicit method for 2D-RSFNRDM

- Eq. (8) is written in the following directional separation product form

$$(1-\tau\delta_x)(1-\tau\delta_y)u_{i,j}^n = u_{i,j}^{n-1} + \tau f(u_{i,j}^{n-1}, x_i, y_j, t_{n-1}), \quad (9)$$

  which introduces an additional perturbation error equal to $(\tau)^2(\delta_x\delta_y)u_{i,j}^n$.

- The additional perturbation error is not large compared to the approximation errors for the other terms in (8), and hence (9) is consistent with convergence order $O(\tau + h_x + h_y)$.

An alternating direction implicit method for 2D-RSFNRDM

- Eq. (8) is written in the following directional separation product form

$$(1-\tau\delta_x)(1-\tau\delta_y)u_{i,j}^n = u_{i,j}^{n-1} + \tau f(u_{i,j}^{n-1}, x_i, y_j, t_{n-1}), \quad (9)$$

which introduces an additional perturbation error equal to $(\tau)^2(\delta_x\delta_y)u_{i,j}^n$.

- The additional perturbation error is not large compared to the approximation errors for the other terms in (8), and hence (9) is consistent with convergence order $O(\tau + h_x + h_y)$.

An alternating direction implicit method for 2D-RSFNRDM

Alternating direction implicit method (ADIM) can now be solved by the following iterative scheme. At time $t = t_n$:

- (1) First, solve the problem in the x-direction (for each fixed y_j) to obtain an intermediate solution $u^*_{i,j}$ in the form

$$(1 - \tau\delta_x))u^*_{i,j} = u^{n-1}_{i,j} + \tau f(u^{n-1}_{i,j}, x_i, y_j, t_{n-1});$$

- (2) Then solve in the y-direction (for each fixed x_i)

$$(1 - \tau\delta_y))u^n_{i,j} = u^*_{i,j}.$$

An alternating direction implicit method for 2D-RSFNRDM

Alternating direction implicit method (ADIM) can now be solved by the following iterative scheme. At time $t = t_n$:

- (1) First, solve the problem in the x-direction (for each fixed y_j) to obtain an intermediate solution $u^*_{i,j}$ in the form

$$(1 - \tau\delta_x))u^*_{i,j} = u^{n-1}_{i,j} + \tau f(u^{n-1}_{i,j}, x_i, y_j, t_{n-1});$$

- (2) Then solve in the y-direction (for each fixed x_i)

$$(1 - \tau\delta_y))u^n_{i,j} = u^*_{i,j}.$$

An alternating direction implicit method for 2D-RSFNRDM

Theorem 7. The alternating direction implicit method (9) for 2D-RSFNRDM (6) is unconditionally stable.

Theorem 8. The alternating direction implicit method (9) is consistent to the 2D-RSFNRDM (6) with convergence order $O(\tau + h_x + h_y)$.

An alternating direction implicit method for 2D-RSFNRDM

Theorem 7. The alternating direction implicit method (9) for 2D-RSFNRDM (6) is unconditionally stable.

Theorem 8. The alternating direction implicit method (9) is consistent to the 2D-RSFNRDM (6) with convergence order $O(\tau + h_x + h_y)$.

Numerical results

Example 3. Consider the following two-dimensional fractional Riesz space nonlinear reaction-diffusion model:

$$\frac{\partial u}{\partial t} = K\left(\frac{\partial^\alpha u}{\partial |x|^\alpha} + \frac{\partial^\alpha u}{\partial |y|^\alpha}\right) + f(u, x, y, t), \tag{10}$$

with zero initial condition and zero Dirichlet boundary conditions.
The exact solution is $u(x, y, t) = t^{1+\alpha} x^2 (1-x)^2 y^2 (1-y)^2$.
Here $f(u, x, y, t)$ can be found by substituting directly into (10).

Numerical Results

$$
\begin{aligned}
f(u,x,y,t)) &= \frac{Kt^{\alpha}}{2cos(\alpha\pi/2)}((\frac{2}{\Gamma(3-\alpha)}[x^{2-\beta}+(1-x)^{2-\alpha}] \\
&- \frac{12}{\Gamma(4-\alpha)}[x^{3-\beta}+(1-x)^{3-\alpha}]+\frac{24}{\Gamma(5-\alpha)}[x^{4-\alpha} \\
&+ (1-x)^{4-\alpha}])y^2(1-y)^2+(\frac{2}{\Gamma(3-\alpha)}[y^{2-\alpha}+(1-y)^{2-\alpha}] \\
&- \frac{12}{\Gamma(4-\alpha)}[y^{3-\alpha}+(1-y)^{3-\alpha}] \\
&+ \frac{24}{\Gamma(5-\alpha)}[y^{4-\alpha}+(1-y)^{4-\alpha}])x^2(1-x)^2) \\
&+ \frac{\Gamma(\alpha+2)}{\Gamma(\alpha+1)}t^{\alpha}x^2(1-x)^2)y^2(1-y)^2.
\end{aligned}
$$

Numerical results

Table: 1. Maximum error for the implicit numerical method (7) with $\tau = 0.01$ as the grid size is reduced in Example 3 at time $T_{end} = 1.0$

$h_x = h_y = h$	$\|e_h^n\|_\infty$
1/8	7.700794e-005
1/16	1.110088e-005
1/32	8.611998e-006

From Table 1, it can be seen that the numerical solution using implicit numerical method (7) is in good agreement with the exact solution.

Numerical results

Table: 2. Comparison of CPU time (seconds) between ADIM and INM with temporal step $\tau = 1/100$ at time $t = 1.0$ using Gauss elimination, Jacobi iteration and Gauss-Seidel iteration

$h_x = h_y$	ADIM	INM		
		G-E	J	G-S
$\frac{1}{8}$	0.15	5.52	3.86	3.19
$\frac{1}{16}$	0.32	28.06	12.77	11.90
$\frac{1}{32}$	2.58	1356.33	63.05	59.34

From Table 2, it can be seen that the alternating direction implicit method is clearly the most efficient of the methods investigated here for solving large fractional-in-space linear systems.

Numerical results

Example 4. The two-dimensional fractional FitzHugh–Nagumo Monodomain Model given by (Bueno-Orovio et al., J. Comp. Phys., 2013):

$$\frac{\partial u}{\partial t} = K_x \frac{\partial^{\alpha_1} u}{\partial |x|^{\alpha_1}} + K_y \frac{\partial^{\alpha_2} u}{\partial |y|^{\alpha_2}} + u(1-u)(u-0.1) - v, \tag{11}$$

$$\frac{\partial v}{\partial t} = 0.01(0.5u - v), \tag{12}$$

with the initial conditions:

$$u(x,y,0) = \begin{cases} 1.0, & 0 < x \leq 1.25, 0 < y < 1.25, \\ 0.0, & 1.25 \leq x < 2.5, 0 < y < 1.25, \\ 0.0, & 0 < x \leq 1.25, 1.25 \leq y < 2.5, \\ 0.0, & 1.25 \leq x < 2.5, 1.25 \leq y < 2.5, \end{cases}$$

$$v(x,y,0) = \begin{cases} 0.0, & 0 < x \leq 1.25, 0 < y < 1.25, \\ 0.0, & 1.25 \leq x < 2.5, 0 < y < 1.25, \\ 0.1, & 0 < x \leq 1.25, 1.25 \leq y < 2.5, \\ 0.1, & 1.25 \leq x < 2.5, 1.25 \leq y < 2.5 \end{cases}$$

with zero Dirichlet boundary conditions.

Numerical results

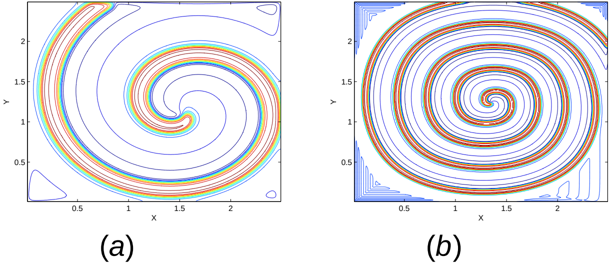
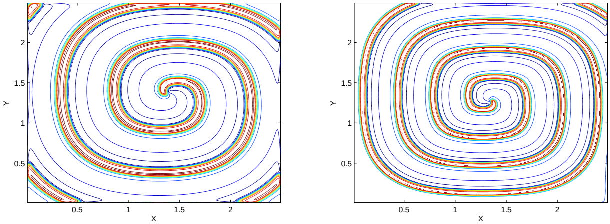


Figure: 3. Spiral waves in the Fitzhugh-Nagumo model with $\alpha_1 = \alpha_2 = 2$ at $t = 1000$. (a) $K_x = K_y = 10^{-4}$; (b) $K_x = K_y = 10^{-5}$.

Figure 3 shows the effect of the diffusion coefficients K_x and K_y.

Numerical results



(*a*) (*b*)

Figure: 4. Spiral waves in the Fitzhugh-Nagumo model with $K_x = K_y = 10^{-4}$ at $t = 1000$. (*a*) $\alpha_1 = \alpha_2 = 1.7$; (*b*) $\alpha_1 = \alpha_2 = 1.5$.

Figure 4 shows the effect of fractional power in the Riesz space fractional Fitzhugh-Nagumo model.

Numerical results

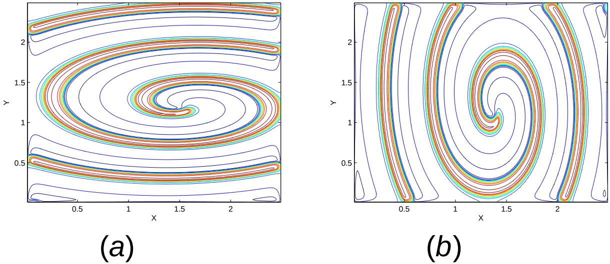


Figure: 5. Spiral waves in the Fitzhugh-Nagumo model with $\alpha_1 = \alpha_2 = 2$ at $t = 1000$. (*a*) $K_x = 10^{-4}$, $\frac{K_y}{K_x} = 0.25$; (*b*) $K_y = 10^{-4}$, $\frac{K_x}{K_y} = 0.25$.

Figure 5 shows the wave propagation for anisotropic diffusion ratios $K_x = 10^{-4}$, $\frac{K_y}{K_x} = 0.25 < 1$ and $K_y = 10^{-4}$, $\frac{K_x}{K_y} = 0.25 < 1$. The spiral wave now proceeds to follow an elliptical pattern.

Numerical results

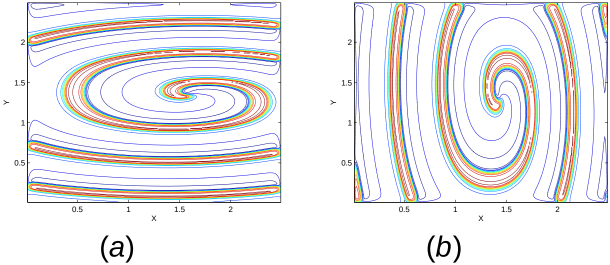


Figure: 6. Spiral waves in the Fitzhugh-Nagumo model with $K_x = K_y = 10^{-4}$ at $t = 1000$. (a) $\alpha_1 = 2$, $\frac{\alpha_2}{\alpha_1} = 0.825$; ($b$) $\alpha_2 = 2$, $\frac{\alpha_1}{\alpha_2} = 0.825$.

The wave propagation for anisotropic fractional ratios $\alpha_1 = 2$, $\frac{\alpha_2}{\alpha_1} = 0.825 < 1$ and $\alpha_2 = 2$, $\frac{\alpha_1}{\alpha_2} = 0.825 < 1$ are shown in Figure 6, reflecting a distinct super-diffusion scale in each of spatial dimensions of the system.

Numerical method of 2D-VOFNRDM-VC

A two-dimensional variable-order fractional nonlinear reaction-diffusion model with variable coefficients (2D-VOFNRDM-VC):

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(A(x,y)\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right) + \frac{\partial}{\partial y}\left(B(x,y)\frac{\partial^{\beta(x,y)}u}{\partial y^{\beta(x,y)}}\right) + f(u,x,y,t). \tag{13}$$

subject to the initial condition

$$u(x,y,0) = \phi(x,y), \quad (x,y) \in \Omega, \tag{14}$$

and the Dirichlet boundary conditions

$$\begin{aligned} &u(a_1,y,t) = u(x,b_1,t) = 0, \\ &u(a_2,y,t) = \varphi_1(y,t), \;\; u(x,b_2,t) = \phi_2(x,t). \end{aligned}$$

Numerical method of 2D-VOFNRDM-VC

Eq. (13) can be written as follows:

$$\begin{aligned}\frac{\partial u}{\partial t} &= \frac{\partial A(x,y)}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right) + A(x,y)\frac{\partial}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right)\\ &+ \frac{\partial B(x,y)}{\partial y}\left(\frac{\partial^{\beta(x,y)}u}{\partial y^{\beta(x,y)}}\right) + B(x,y)\frac{\partial}{\partial y}\left(\frac{\partial^{\beta(x,y)}u}{\partial y^{\beta(x,y)}}\right) + f(u,x,y,t). \end{aligned} \quad (15)$$

Let $t_n = n(\Delta t)$, $\Delta x = (a_2 - a_1)/m_1$, $\Delta y = (b_2 - b_1)/m_2$, $x_i = a_1 + i(\Delta x)$, $y_j = b_1 + j(\Delta y)$, $A_{i,j} = A(x_i, y_j)$, $B_{i,j} = B(x_i, y_j)$, $\tilde{A}_{i,j} = \frac{\partial A(x_i,y_j)}{\partial x}$, $\tilde{B}_{i,j} = \frac{\partial B(x_i,y_j)}{\partial y}$, $\alpha_{i,j} = \alpha(x_i, y_j)$, $\beta_{i,j} = \beta(x_i, y_j)$, $u(x_i, y_j, t_n) = u^n_{i,j}$, $f^n_{i,j} = f(u^n_{i,j}, x_i, y_j, t_n)$.

Numerical method of 2D-VOFNRDM-VC

- We use the backward Euler difference scheme for the first order time derivative:

$$\frac{\partial u}{\partial t}\Big|_{(x_i,y_j,t_n)} \sim \frac{u_{i,j}^n - u_{i,j}^{n-1}}{\Delta t} + O(\Delta t).$$

- For the advection term in the x-direction:

$$\frac{\partial A(x,y)}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right)\Big|_{(x_i,y_j,t_n)} = \frac{\tilde{A}_{i,j}}{(\Delta x)^{\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n + O(\Delta x).$$

- For the diffusion term in the x-direction:

$$A(x,y)\frac{\partial}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right)\Big|_{(x_i,y_j,t_n)}$$

$$= \frac{A_{i,j}}{\Delta x}\Big[\frac{1}{(\Delta x)^{\alpha_{i+1,j}}}\sum_{k=0}^{i} g_{\alpha_{i+1,j}}^{(k)} u_{i+1-k,j}^n - \frac{1}{(\Delta x)^{\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n\Big] + O(\Delta x).$$

Numerical method of 2D-VOFNRDM-VC

- We use the backward Euler difference scheme for the first order time derivative:

$$\frac{\partial u}{\partial t}\Big|_{(x_i,y_j,t_n)} \sim \frac{u_{i,j}^{n} - u_{i,j}^{n-1}}{\Delta t} + O(\Delta t).$$

- For the advection term in the x-direction:

$$\frac{\partial A(x,y)}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right)\Big|_{(x_i,y_j,t_n)} = \frac{\tilde{A}_{i,j}}{(\Delta x)^{\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^{n} + O(\Delta x).$$

- For the diffusion term in the x-direction:

$$A(x,y)\frac{\partial}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right)\Big|_{(x_i,y_j,t_n)}$$

$$= \frac{A_{i,j}}{\Delta x}\Big[\frac{1}{(\Delta x)^{\alpha_{i+1,j}}}\sum_{k=0}^{i} g_{\alpha_{i+1,j}}^{(k)} u_{i+1-k,j}^{n} - \frac{1}{(\Delta x)^{\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^{n}\Big] + O(\Delta x).$$

Numerical method of 2D-VOFNRDM-VC

- We use the backward Euler difference scheme for the first order time derivative:

$$\frac{\partial u}{\partial t}\Big|_{(x_i,y_j,t_n)} \sim \frac{u_{i,j}^n - u_{i,j}^{n-1}}{\Delta t} + O(\Delta t).$$

- For the advection term in the x-direction:

$$\frac{\partial A(x,y)}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right)\Big|_{(x_i,y_j,t_n)} = \frac{\tilde{A}_{i,j}}{(\Delta x)^{\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n + O(\Delta x).$$

- For the diffusion term in the x-direction:

$$A(x,y)\frac{\partial}{\partial x}\left(\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right)\Big|_{(x_i,y_j,t_n)}$$

$$= \frac{A_{i,j}}{\Delta x}\Big[\frac{1}{(\Delta x)^{\alpha_{i+1,j}}}\sum_{k=0}^{i} g_{\alpha_{i+1,j}}^{(k)} u_{i+1-k,j}^n - \frac{1}{(\Delta x)^{\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n\Big] + O(\Delta x).$$

Numerical method of 2D-VOFNRDM-VC

- Similar results hold in the y-direction. Here

$$g_{\alpha_{i,j}}^{(k)} = (-1)^k \begin{pmatrix} \alpha_{i,j} \\ k \end{pmatrix} = (-1)^k \frac{\Gamma(\alpha_{i,j}+1)}{\Gamma(\alpha_{i,j}-k+1)\Gamma(k+1)}.$$

- The implicit numerical method for 2D-VOFNRDM-VC with convergence order $O(\Delta t + \Delta x + \Delta y)$:

$$\begin{aligned}
&\frac{u_{i,j}^n - u_{i,j}^{n-1}}{\Delta t} \\
= \; & \frac{\tilde{A}_{i,j}}{(\Delta x)^{\alpha_{i,j}}} \sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n - \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i,j}}} \sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n \\
+ \; & \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i+1,j}}} \sum_{k=0}^{i} g_{\alpha_{i+1,j}}^{(k)} u_{i+1-k,j}^n + \frac{\tilde{B}_{i,j}}{(\Delta y)^{\beta_{i,j}}} \sum_{k=0}^{j-1} g_{\beta_{i,j}}^{(k)} u_{i,j-k}^n \\
- \; & \frac{B_{i,j}}{(\Delta y)^{1+\beta_{i,j}}} \sum_{k=0}^{j-1} g_{\beta_{i,j}}^{(k)} u_{i,j-k}^n + \frac{B_{i,j}}{(\Delta y)^{1+\beta_{i,j+1}}} \sum_{k=0}^{j} g_{\beta_{i,j+1}}^{(k)} u_{i,j+1-k}^n + f_{i,j}^n.
\end{aligned}$$

Numerical method of 2D-VOFNRDM-VC

- Similar results hold in the y-direction. Here

$$g_{\alpha_{i,j}}^{(k)} = (-1)^k \begin{pmatrix} \alpha_{i,j} \\ k \end{pmatrix} = (-1)^k \frac{\Gamma(\alpha_{i,j}+1)}{\Gamma(\alpha_{i,j}-k+1)\Gamma(k+1)}.$$

- The implicit numerical method for 2D-VOFNRDM-VC with convergence order $O(\Delta t + \Delta x + \Delta y)$:

$$\begin{aligned}
&\frac{u_{i,j}^n - u_{i,j}^{n-1}}{\Delta t} \\
= \quad & \frac{\tilde{A}_{i,j}}{(\Delta x)^{\alpha_{i,j}}} \sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n - \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i,j}}} \sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n \\
+ \quad & \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i+1,j}}} \sum_{k=0}^{i} g_{\alpha_{i+1,j}}^{(k)} u_{i+1-k,j}^n + \frac{\tilde{B}_{i,j}}{(\Delta y)^{\beta_{i,j}}} \sum_{k=0}^{j-1} g_{\beta_{i,j}}^{(k)} u_{i,j-k}^n \\
- \quad & \frac{B_{i,j}}{(\Delta y)^{1+\beta_{i,j}}} \sum_{k=0}^{j-1} g_{\beta_{i,j}}^{(k)} u_{i,j-k}^n + \frac{B_{i,j}}{(\Delta y)^{1+\beta_{i,j+1}}} \sum_{k=0}^{j} g_{\beta_{i,j+1}}^{(k)} u_{i,j+1-k}^n + f_{i,j}^n.
\end{aligned}$$

Numerical method of 2D-VOFNRDM-VC

- Define the following fractional partial difference operators:

$$\delta_x u_{i,j}^n = \frac{\tilde{A}_{i,j}}{(\Delta x)^{\alpha_{i,j}}} \sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n + \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i+1,j}}} \sum_{k=0}^{i} g_{\alpha_{i+1,j}}^{(k)} u_{i+1-k,j}^n - \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i,j}}} \sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n,$$

  and similarly for δ_y.
- With these operator definitions, the implicit Euler method may be written in the operator form

$$(1 - \Delta t \delta_x - \Delta t \delta_y) u_{i,j}^n = u_{i,j}^{n-1} + \Delta t\, f_{i,j}^n,$$

Numerical method of 2D-VOFNRDM-VC

- Define the following fractional partial difference operators:

$$\begin{aligned}\delta_x u_{i,j}^n &= \frac{\tilde{A}_{i,j}}{(\Delta x)^{\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n + \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i+1,j}}}\sum_{k=0}^{i} g_{\alpha_{i+1,j}}^{(k)} u_{i+1-k,j}^n \\ &- \frac{A_{i,j}}{(\Delta x)^{1+\alpha_{i,j}}}\sum_{k=0}^{i-1} g_{\alpha_{i,j}}^{(k)} u_{i-k,j}^n,\end{aligned}$$

  and similarly for δ_y.
- With these operator definitions, the implicit Euler method may be written in the operator form

$$(1-\Delta t\delta_x-\Delta t\delta_y)u_{i,j}^n = u_{i,j}^{n-1}+\Delta t\, f_{i,j}^n,$$

Numerical method of 2D-VOFNRDM-VC

- For the ADI method, the operator form is written in a directional separation product form

$$(1-\Delta t\delta_x)(1-\Delta t\delta_y)u_{i,j}^n = u_{i,j}^{n-1} + \Delta t \; f_{i,j}^n, \qquad (16)$$

  which introduces an additional perturbation error equal to $(\Delta t)^2(\delta_x\delta_y)u_{i,j}^n$.
- We can conclude the additional perturbation error is not larger compared to the approximation errors, and Equation (16) (which is called as ADI-Euler method) is consistent with order $O(\Delta t + \Delta x + \Delta y)$.

Numerical method of 2D-VOFNRDM-VC

- For the ADI method, the operator form is written in a directional separation product form

$$(1-\Delta t\delta_x)(1-\Delta t\delta_y)u_{i,j}^n = u_{i,j}^{n-1} + \Delta t \; f_{i,j}^n, \qquad (16)$$

which introduces an additional perturbation error equal to $(\Delta t)^2(\delta_x\delta_y)u_{i,j}^n$.

- We can conclude the additional perturbation error is not larger compared to the approximation errors, and Equation (16) (which is called as ADI-Euler method) is consistent with order $O(\Delta t + \Delta x + \Delta y)$.

Numerical method of 2D-VOFNRDM-VC

The ADI-Euler method defined by (16) can now be solved by the following iterative scheme. At time t_n:

- (1) first, solve the problem in the x-direction(for each fixed y_j) to obtain an intermediate solution $u_{i,j}^*$ form

$$(1 - \Delta t\delta_x)\, u_{i,j}^* = u_{i,j}^{n-1} + \Delta t\, f_{i,j}^n, \tag{17}$$

- (2) then solve in the y-direction (for each fixed x_i)

$$(1 - \Delta t\delta_y)\, u_{i,j}^n = u_{i,j}^*. \tag{18}$$

Prior to carrying out step one of solving (17), the boundary conditions for the intermediate solution $u_{i,j}^*$ should be set from Equation (18) (which incorporates the values of $u_{i,j}^n$ at the boundary), otherwise the order of convergence will be adversely affected.

Numerical method of 2D-VOFNRDM-VC

The ADI-Euler method defined by (16) can now be solved by the following iterative scheme. At time t_n:

- (1) first, solve the problem in the x-direction(for each fixed y_j) to obtain an intermediate solution $u^*_{i,j}$ form

$$(1 - \Delta t \delta_x)\, u^*_{i,j} = u^{n-1}_{i,j} + \Delta t\ f^n_{i,j}, \tag{17}$$

- (2) then solve in the y-direction (for each fixed x_i)

$$(1 - \Delta t \delta_y)\, u^n_{i,j} = u^*_{i,j}. \tag{18}$$

Prior to carrying out step one of solving (17), the boundary conditions for the intermediate solution $u^*_{i,j}$ should be set from Equation (18) (which incorporates the values of $u^n_{i,j}$ at the boundary), otherwise the order of convergence will be adversely affected.

Numerical method of 2D-VOFNRDM-VC

Example 5: Consider the following 2D-VOFNRDM-VC:

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \frac{\partial}{\partial x}\left(\frac{\Gamma(3-\alpha(x,y))}{2}\frac{\partial^{\alpha(x,y)}u}{\partial x^{\alpha(x,y)}}\right) \\
&+ \frac{\partial}{\partial y}\left(\frac{\Gamma(4-\beta(x,y))}{6}\frac{\partial^{\beta(x,y)}u}{\partial y^{\beta(x,y)}}\right) \\
&- u - ux^{-\alpha(x,y)}\left(-0.4y\ln x + \frac{2-\alpha(x,y)}{x}\right) \\
&- uy^{-\beta(x,y)}\left(-0.6x\ln y + \frac{3-\beta(x,y)}{y}\right), \\
& u(x,y,0) = x^2y^3, \\
& u(0,y,t) = u(x,0,t) = 0,\ \ u(1,y,t) = y^3e^{-t},\ \ u(x,1,t) = x^2e^{-t},
\end{aligned}$$

where $\alpha(x,y) = 0.5 + 0.4xy$, $\beta(x,y) = 0.3 + 0.6xy$.

The exact solution of the above problem is given by $u(x,y,t) = x^2y^3e^{-t}$.

Numerical method of 2D-VOFNRDM-VC

Table: 3. Maximum error behavior for the ADI-Euler method as the grid size is reduced for Example 5 at time $T_{end} = 1$.

$\Delta t = \Delta x = \Delta y = h$	$\|e_h^n\|_\infty$	G_h
$1/20$	0.0047979	
$1/40$	0.0024968	0.9423
$1/80$	0.0012724	0.9725
$1/160$	0.00064223	0.9864

From Table 3, it can be seen that the ADI-Euler method is also unconditionally stable and convergent.

Conclusions

- In this talk, some numerical methods to approximate three fractional nonlinear reaction-diffusion models and application to fractional FitzHugh-Nagumo Monodomain Model were described and demonstrated.
- Although the nonlinear source term is not globally Lipschitz continuous, the solution of the discrete numerical method still yields bounds on the solution of the continuous problem and the solution of the numerical method converges to the unique solution of the continuous problem as the time and space steps tend to zero.

Conclusions

- In this talk, some numerical methods to approximate three fractional nonlinear reaction-diffusion models and application to fractional FitzHugh-Nagumo Monodomain Model were described and demonstrated.
- Although the nonlinear source term is not globally Lipschitz continuous, the solution of the discrete numerical method still yields bounds on the solution of the continuous problem and the solution of the numerical method converges to the unique solution of the continuous problem as the time and space steps tend to zero.

Conclusions

- These numerical methods and analysis techniques provide computationally efficient tools for simulating the behavior of solutions of the complex fractional nonlinear reaction diffusion models.
- The numerical results demonstrate the effectiveness of this approach and suggest that such models can have very different dynamics to the standard models and represent a powerful modeling approach for understanding the many aspects of electrophysiological dynamics in heterogeneous cardiac tissue and other areas as well.
- We hope to study the consequences of these new approaches to cardiac electrophysiology in future work.

Conclusions

- These numerical methods and analysis techniques provide computationally efficient tools for simulating the behavior of solutions of the complex fractional nonlinear reaction diffusion models.
- The numerical results demonstrate the effectiveness of this approach and suggest that such models can have very different dynamics to the standard models and represent a powerful modeling approach for understanding the many aspects of electrophysiological dynamics in heterogeneous cardiac tissue and other areas as well.
- We hope to study the consequences of these new approaches to cardiac electrophysiology in future work.

Conclusions

- These numerical methods and analysis techniques provide computationally efficient tools for simulating the behavior of solutions of the complex fractional nonlinear reaction diffusion models.
- The numerical results demonstrate the effectiveness of this approach and suggest that such models can have very different dynamics to the standard models and represent a powerful modeling approach for understanding the many aspects of electrophysiological dynamics in heterogeneous cardiac tissue and other areas as well.
- We hope to study the consequences of these new approaches to cardiac electrophysiology in future work.


Thank you !
QUT Queensland University of Technology
QUT