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Numerical Study of Mass Variation in Time-Fractional Diffusion Equation with Nonlinear terms

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Abstract

In this study, we analyze the discrete mass variation in the time-fractional Allen-Cahn equation. The classical Allen-Cahn equation is solved by the convex splitting method. We compute the discrete total mass at each time step using midpoint method. Then we observe that (1) the total mass is conservative without nonlinear terms on periodic boundary condition and (2) the variation of total mass decay to zero with nonlinear term. For the fractional case without nonlinear terms. (1) The variation of total mass tend to zero as α tend to 1 and (2) when α close to zero the variation of total mass dose not converge to 0.

Keywords: Fractional Calculus, Time-fractional Allen-Cahn Equation, Fractional Finite Difference.

Problem Description

Denote the function

$$w_\alpha(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)},$$

where $\Gamma(\cdot)$ is the gamma function and α is any positive real number. And the integration is

$$\int_0^t w_\alpha(s)ds = \int_0^t \frac{s^{\alpha-1}}{\Gamma(\alpha)}ds = \frac{t^{(1+\alpha)-1}}{\Gamma(1+\alpha)} = w_{1+\alpha}(t)$$

Caputo Derivative

Given f is n-differentiable on $[0,t]$, the Caputo fractional derivative with order $\alpha \in [n-1, n)$, $n \in \mathbb{N}$, denoted by ${}_CD_t^\alpha$ is defined as

$${}_CD_t^\alpha f(t) = \left(I^{(n-\alpha)} f^{(n)}\right)(t) = \int_0^t w_{n-\alpha}(t-s) f^{(n)}(s)ds.$$

L1 Scheme[1]

For approximated the Caputo derivative with $0 < \alpha < 1$, L1 scheme treats the first derivative $f'(s)$ by the piecewise linear interpolation such as Lagrange interpolation.

$${}_C\bar{D}_t^\alpha u_N = \Delta t^{-\alpha} \sum_{k=1}^{N} q_k \nabla u_{N-k+1}$$

where $q_k = \int_{k-1}^k w_{1-\alpha}(s)ds = k^{1-\alpha} - (k-1)^{1-\alpha}$ and $\nabla u_{N-k+1} = u^{N-k+1} - u^{N-k}$.

q_k	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
$\alpha=0.1$	1.0398	0.9005	0.8545	0.8259	0.8053	0.7892
$\alpha=0.5$	1.1284	0.4674	0.3586	0.3023	0.2664	0.2408
$\alpha=0.9$	1.0511	0.0754	0.0466	0.0342	0.0272	0.0227

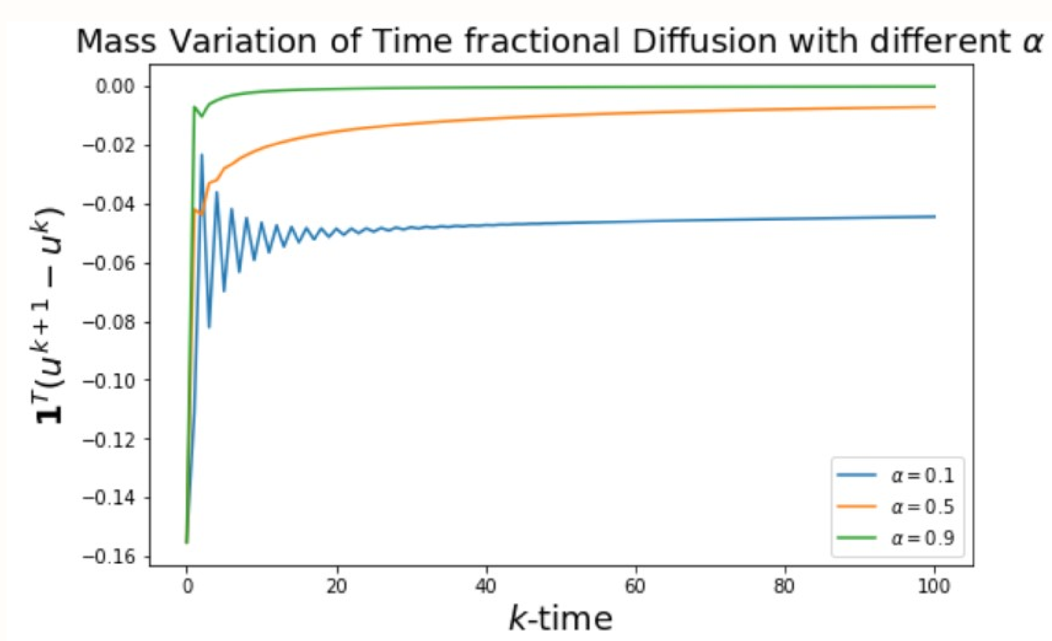
Table 1: The first 6-th coefficients of L1 scheme in difference α with rounded.

L1 scheme is nonlocal, in others world, for computing u^k it needs previous u^i information $i = 0, 1, \ldots, k-1$.

Mass Variation of the Time-Fractional Diffusion without nonlinear term

$${}_CD_t^\alpha u = \epsilon^2 \Delta u.$$

Figure 1: 1D time-fractional diffusion. Initial $u_0 = \cos(x)$ on $x \in [-5, 5]$ with mesh points 64, time step $\Delta t = 0.01$, $\epsilon = 0.1$



Allen-Cahn Equation

Consider the Ginzburg–Landau free energy

$$E[u] = \int_\Omega \frac{\epsilon^2}{2}|\nabla u|^2 + W(u)dx$$

where $W(u) = \dfrac{(1-u^2)^2}{4}$ is the double-well potential.

$$\begin{aligned}\frac{\partial u}{\partial t} &= -\frac{\delta E}{\delta u} \\ &= \epsilon^2 \Delta u + W'(u)\end{aligned}$$

For the time-fractional,

$${}_CD_t^\alpha u = \epsilon^2 \Delta u + W'(u)$$

Convex Splitting Method

$$\begin{aligned}E[u] &= E_c[u] - E_e[u] \\ &= \int_\Omega \frac{\epsilon^2}{2} + |\nabla u|^2 + W_c(u)dx - \int_\Omega W_e(u)dx\end{aligned}$$

where $W_c(u) = \dfrac{u^4+1}{4}$ and $W_e(u) = \dfrac{u^2}{2}$

The contractive part $E_c[u]$ and expansive part $E_e[u]$ are convex. And $E_c[u]$ is handled implicitly, $E_e[u]$ is handled explicitly.

Then the classical Allen-Cahn finite difference scheme is

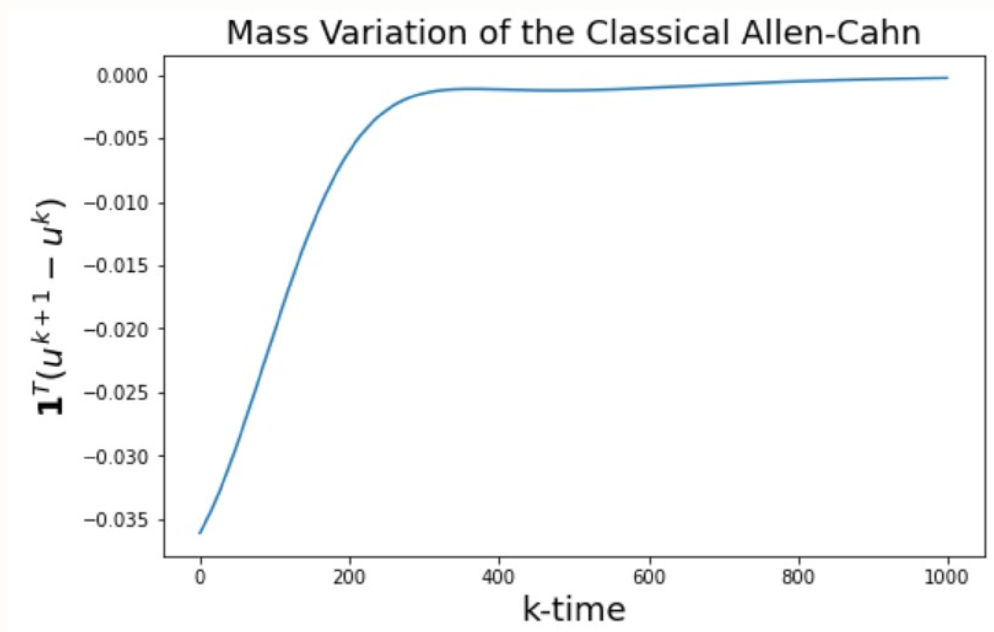
$$u^k = K^{-1}[(3 + \frac{1}{\Delta t})u^{k-1} - (u^{k-1})^3] \qquad (1)$$

where $K = \left(2 + \dfrac{1}{\Delta t}\right)\mathbb{I} - \epsilon^2 L$, L is the discrete laplacian operator and $\mathbb{I}$ is identity matrix.

Mass Variation of Classical Allen Cahn Euqation

$$\mathbf{1}^T(u^k - u^{k-1}) = \frac{\Delta t}{2\Delta t + 1}\mathbf{1}^T\left[u^{k-1} - (u^{k-1})^3\right]$$

Figure 2: 1D Classical Allen-Cahn equation. Initial $u_0 = \cos(x)$ on $x \in [-5, 5]$ with mesh points 64, time step $\Delta t = 0.01$, $\epsilon = 0.1$



Time-Fractional Allen-Cahn Equation Scheme

The linear convex splitting scheme is

$$u^N = H^{-1}\left[(3+q_1)u^{N-1} - (u^{N-1})^3 - \sum_{k=2}^{N} q_k \nabla u_{N-k+1}\right]$$

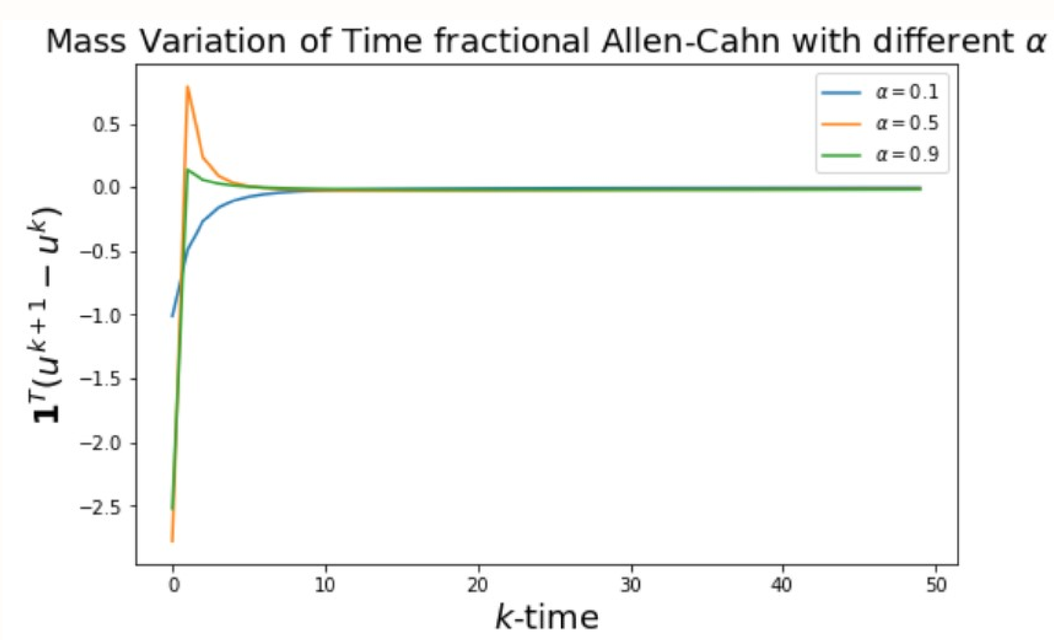
where $H = (q_1+3)\mathbb{I} - \epsilon^2 L$, L is the discrete laplacian operator and $\mathbb{I}$ is identity matrix.

Mass Variation of the Time-fractional Allen-Cahn Equation

For the L1 time-fractional Allen-Cahn scheme the variation of discrete mass is

$$\begin{aligned}\mathbf{1}^T(u^k - u^{k-1}) =& \frac{1}{q_1+2}\mathbf{1}^T\left[u^{k-1} - (u^{k-1})^3\right] \\ &- \mathbf{1}^T \sum_{i=2}^{k} \frac{q_i}{q_1+2}(u^{k-i+1} - u^{k-i})\end{aligned}$$

Figure 3: 1D time-fractional Allen-Cahn equation. Inital $u_0 = \cos(x)$ on $x \in [-5, 5]$ with mesh points 64, time step $\Delta t = 0.01$, $\epsilon = 0.1$



Summary and conclusions

We given the numerical simulation of time-fractional diffusion without nonlinear term, Classical and fractional Allen-Cahn equation. Compare Figure 2. and Figure 3. with the same initial value and step size, the total mass variation of the time-fractional Allen-Cahn changed rapidly in early time steps. And the total mass variation of the time-fractional diffusion without nonlinear term tend to zero except as α tend to 0.

References

[1] Oldham, Keith, and Jerome Spanier, The fractional calculus theory and applications of differentiation and integration to arbitrary order, *Elsevier, 1974.*