A Second Order Time Accurate SUSHI method for the Time-Fractional Diffusion Equation

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Aim of the presentation

The aim of this talk is to establish a second order time accurate finite volume scheme for a time fractional diffusion equation. The discretization in space is performed using SUSHI (Scheme Using Stabilization and Hybrid Interfaces) developed recently.

Plan of this presentation

Equation to be solved

Equation

We consider the following time fractional diffusion equation:

$$\partial_t^\alpha u(\boldsymbol{x},t) - \Delta u(\boldsymbol{x},t) = f(\boldsymbol{x},t), \;\; (\boldsymbol{x},t) \in \Omega \times (0,T), \tag{1}$$

where Ω an open polygonal bounded subset in $\mathbb{R}^d$. The operator ∂_t^α is the Caputo derivative:

$$\partial_t^\alpha u(\boldsymbol{x},t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial u(\boldsymbol{x},s)}{\partial s} ds, \quad 0 < \alpha < 1, \tag{2}$$

Initial condition

Initial condition is given by $u(\boldsymbol{x},0) = u^0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega$

Homogeneous Dirichlet boundary

$u(\boldsymbol{x},t) = 0, \;\; (\boldsymbol{x},t) \in \partial\Omega \times (0,T).$

What about time fractional diffusion equation?

Some physics

Fractional differential equations have been successfully used in the modeling of many different processes and systems. They are used, for instance, to describe anomalous transport in disordered semiconductors, penetration of light beam through a turbulent medium, transport of resonance radiation in plasma, blinking fluorescence of quantum dots, penetration and acceleration of cosmic ray in the Galaxy, and large-scale statistical Cosmography.

We refer to the monograph Uchaikin (Fractional Derivatives for Physicists and Engineers, Springer-Verlag Heidelberg, 2013) where we find many details.

References

References

1. Alikhanov, A.-A.: A new difference scheme for the fractional diffusion equation. J. Comput. Phys. 280, 424–438 (2015).

2. Eymard, R., Gallouët, T., Herbin, R.: Discretization of heterogeneous and anisotropic diffusion problems on general nonconforming meshes. IMA J. Numer. Anal. 30/4, 1009–1043 (2010).

3. Gao, G.-H., Sun, Z.-Z, Zhang, H.-W.: A new fractional numerical differentiation formula to approximate the Caputo fractional derivative and its applications. J. Comput. Phys. 259, 33–50 (2014)

4. Uchaikin, V.V.: Fractional Derivatives for Physicists and Engineers. Higher Education Press, Beijing and Springer-Verlag Heidelberg (2013).

Principles of the time discretization

Steps of Discretization in time

- First step: Definition of mesh points. We define $k = T/(M+1)$ and mesh points $t_n = nk$. We denote by ∂^1 and ∂^2 the discrete first time derivative and discrete second time derivative given respectively by

$$\partial^1 v^{j+1} = \frac{v^{j+1} - v^j}{k} \quad \text{and} \quad \partial^2 v^{j+1} = \partial^1(\partial^1 v^{j+1}) = \frac{v^{j+1} - 2v^j + v^{j-1}}{k^2}.$$

- Second step: Equation to be solved on the mesh points. Writing (1) with $t = t_{n+\sigma} = (n+\sigma)k = t_n + \sigma k$ with $0 < \sigma < 1$ will be chosen later:

$$\partial_t^\alpha u(t_{n+\sigma}) - \Delta u(t_{n+\sigma}) = f(t_{n+\sigma}). \qquad (3)$$

Principles of the time discretization (Suite)

Steps of Discretization in time (Suite)

- Third step: Principle idea of a second order approximation $\partial_t^\alpha u(t_{n+\sigma})$ (Idea of Alikhanov and Gao et al.). We write $\partial_t^\alpha u(t_{n+1})$ as

$$\frac{1}{\Gamma(1-\alpha)}\left(\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}(t_{n+\sigma}-s)^{-\alpha}u_s(s)ds+\int_{t_n}^{t_{n+\sigma}}(t_{n+\sigma}-s)^{-\alpha}u_s(s)\right)ds. \tag{4}$$

For each $j\in[\![1,N+1]\!]$, let $\Pi_{2,j}u$ be the quadratic interpolation defined on (t_{j-1},t_j) on the points t_{j-1},t_j,t_{j+1} of u. An explicit expansion for $\Pi_{2,j}u'$ yields:

$$\partial^1 u(t_{j+1})+\partial^2 u(t_{j+1})\left(s-t_{j+\frac{1}{2}}\right)=\partial^1 u(t_j)+\partial^2 u(t_{j+1})\left(s-t_{j-\frac{1}{2}}\right). \tag{5}$$

Principles of the time discretization (Suite)

Steps of Discretization in time (Suite)

- Fifth step: Computation of a second order approximation for $\partial_t^\alpha u(t_{n+\sigma})$. When approximating the terms of the sum (resp. the last term) using quadratic interpolations (resp. a linear interpolation) in (4) of $\partial_t^\alpha u(t_{n+\sigma})$, we have to compute the following integrals:
  1. First set of integrals:

$$\int_{t_{j-1}}^{t_j} \left(s - t_{j-\frac{1}{2}}\right)(t_{n+\sigma} - s)^{-\alpha} ds = \frac{k^{2-\alpha}}{1-\alpha} b_{n-j}^\sigma, \tag{6}$$

where

$$b_l^\sigma = \frac{1}{2-\alpha}\left((l+\sigma+1)^{2-\alpha} - (l+\sigma)^{2-\alpha}\right) - \frac{1}{2}\left((l+\sigma+1)^{1-\alpha} + (l+\sigma)^{1-\alpha}\right). \tag{7}$$

Principles of the time discretization (Suite)

Steps of Discretization in time (Suite)

- Fifth step: Computation of a second order approximation for $\partial_t^\alpha u(t_{n+\sigma})$ (Suite).
  2. Second set of integrals:

$$\int_{t_{j-1}}^{t_j} (t_{n+\sigma} - s)^{-\alpha} ds = \frac{k^{1-\alpha}}{1-\alpha} d_{n+\sigma-j,\alpha}, \tag{8}$$

with, for all $s > 0$, $d_{s,\alpha}$ is given by

$$d_{s,\alpha} = (s+1)^{1-\alpha} - s^{1-\alpha}. \tag{9}$$

3. Third set of integrals:

$$\int_{t_n}^{t_{n+\sigma}} (t_{n+\sigma} - s)^{-\alpha} ds = \frac{k^{1-\alpha}}{1-\alpha} \sigma^{1-\alpha}. \tag{10}$$

Formulation of a second order approximation for $\partial_t^\alpha u(t_{n+\sigma})$

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We then obtained approximation for the fractional derivative $\partial_t^\alpha u(t_{n+\sigma})$ using (4)–(10). This approximation is of order two if

$$\sigma = 1 - \frac{\alpha}{2}. \tag{11}$$

This approximation is given by

$$\begin{aligned} &\frac{1}{\Gamma(1-\alpha)}\left(\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}(t_{n+\sigma}-s)^{-\alpha}\left(\Pi_{2,j}u(s)\right)' ds + \frac{k^{1-\alpha}}{1-\alpha}\sigma^{1-\alpha}\partial^1 u(t_{n+1})\right)\\ = &\sum_{j=0}^{n} k\lambda_j^{n+1}\partial^1 u(t_{j+1}). \end{aligned} \tag{12}$$

Let us denote $\Lambda_{n+\sigma}u = \sum_{j=0}^{n} k\lambda_j^{n+1}\partial^1 u(t_{j+1})$.

Properties of the time approximation

Properties of the time approximation, cf. Alikhanov (2015)

Recall that

$$\Lambda_{n+\sigma}u = \sum_{j=0}^{n} k\lambda_j^{n+1}\partial^1 u(t_{j+1}) \approx \partial_t^\alpha u(t_{n+\sigma}). \qquad (13)$$

1. Properties of λ_j^{n+1}.

$$\sum_{j=0}^{n} k\lambda_j^{n+1} \le \frac{T^{1-\alpha}}{\Gamma(2-\alpha)}, \quad \sum_{j=0}^{n} k\lambda_j^{n+1} \le \frac{T^{1-\alpha}}{\Gamma(2-\alpha)}$$

and

$$\lambda_n^{n+1} > \lambda_{n-1}^{n+1} > \ldots > \lambda_0^{n+1} > \lambda_0 = \frac{1}{2T^\alpha\Gamma(1-\alpha)}.$$

Properties of the time approximation (Suite)

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2. Stability result. For all $\left(\beta^j\right)_{j=0}^{N+1} \in \mathbb{R}^{N+2}$, for any $n \in [\![0, N+1]\!]$:

$$\left(\sigma\beta^{n+1} + (1-\sigma)\beta^n\right)\sum_{j=0}^{n}\lambda_j^{n+1}(\beta^{j+1}-\beta^j) \geq \frac{1}{2}\sum_{j=0}^{n}\lambda_j^{n+1}\left((\beta^{j+1})^2 - (\beta^j)^2\right).$$

3. Consistency result. For any $\varphi \in \mathcal{C}^3\left([0,T]\right)$:

$$|\partial^\alpha\varphi(t_{n+\sigma}) - \Lambda_{n+\sigma}\varphi| \leq Ck^{3-\alpha}\left|\varphi^{(3)}\right|_{\mathcal{C}([0,T])}. \tag{14}$$

Formulation of a suitable approximation for $\partial_t^\alpha u(t_{n+\sigma}) - \Delta u(t_{n+\sigma}) = f(t_{n+\sigma})$

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- First fact. As justified before

$$\partial^\alpha u(t_{n+\sigma}) = \sum_{j=0}^{n} k\lambda_j^{n+1}\partial^1 u(t_{j+1}) + \mathcal{O}(k^{3-\alpha}). \tag{15}$$

- Second fact. Using a Taylor expansion yields

$$\Delta u(t_{n+\sigma}) = \sigma\Delta u(t_{n+1}) + (1-\sigma)\Delta u(t_n) + \mathcal{O}(k^2). \tag{16}$$

From (15) and (16), we deduce that

$$\sum_{j=0}^{n} k\lambda_j^{n+1}\partial^1 u(t_{j+1}) - \sigma\Delta u(t_{n+1}) + (1-\sigma)\Delta u(t_n) = f(t_{n+\sigma}) + \mathcal{O}(k^2). \tag{17}$$

Discretization in space

Discretization in space

We use SUSHI scheme

Main properties of this new mesh:

1. (mesh defined at any space dimension): $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$
2. (orthogonality property is not required): the orthogonality property is not required in this new mesh. But, additional discrete unknowns are required.
3. (convexity): the classical admissible mesh should satisfy that the control volumes are convex, whereas the convexity property is not required in this new mesh.

Discretization in space

1. Discrete unknowns: the space of solution as well as the space of test functions are in

$$\mathcal{X}_{\mathcal{D},0} = \{ \left((v_K)_{K \in \mathcal{M}} \,,\, (v_\sigma)_{\sigma \in \mathcal{E}} \right) ,\;\; v_K, v_\sigma \in \mathbb{R},\;\; v_\sigma = 0,\, \forall \sigma \in \mathcal{E}_{\mathrm{ext}} \}$$

2. Discretization of the gradient: the discretization of ∇ can be performed using a stabilized discrete gradient denoted by $\nabla_{\mathcal{D}}$, see Eymard et *al.* (IMAJNA, 2010):
   1. The discrete gradient $\nabla_{\mathcal{D}}$ is stable
   2. The discrete gradient $\nabla_{\mathcal{D}}$ is consistent.

Formulation of scheme

The finite volume scheme can then be defined as:

- Discretization of initial condition: Find $u_{\mathcal{D}}^0 \in \mathcal{X}_{\mathcal{D},0}$ such that

$$\left(\nabla_{\mathcal{D}} u_{\mathcal{D}}^0, \nabla_{\mathcal{D}}\, v\right)_{(\mathbb{L}^2(\Omega))^d} = -\left(\Delta u^0, \Pi_{\mathcal{M}}\, v\right)_{\mathbb{L}^2(\Omega)}, \quad \forall\, v \in \mathcal{X}_{\mathcal{D},0}, \tag{18}$$

- Discretization of the time factional diffusion equation. For any $n \in [\![0, N]\!]$, find $u_{\mathcal{D}}^{n+1} \in \mathcal{X}_{\mathcal{D},0}$ such that, for all $v \in \mathcal{X}_{\mathcal{D},0}$

$$\sum_{j=0}^{n} \lambda_j^{n+1} \left(\Pi_{\mathcal{M}}(u_{\mathcal{D}}^{j+1} - u_{\mathcal{D}}^j), \Pi_{\mathcal{M}} v\right)_{\mathbb{L}^2(\Omega)} + \left(\nabla_{\mathcal{D}} u_{\mathcal{D}}^{n+\sigma}, \nabla_{\mathcal{D}} v\right)_{\mathbb{L}^2(\Omega)} = \left(f(t_{n+\sigma}), \Pi_{\mathcal{M}} v\right)_{\mathbb{L}^2(\Omega)}, \tag{19}$$

where $v^{n+\sigma}$ denotes the two-point barycentric element given by

$$v^{n+\sigma} = \sigma v^{n+1} + (1-\sigma) v^n. \tag{20}$$

Convergence result

Theorem (An error estimate for the gradient)

- $\mathbb{L}^\infty(\mathbb{L}^2)$*–estimate. For all* $n \in [\![0, N+1]\!]$

$$\|u(t_n) - \Pi_{\mathcal{M}} u_{\mathcal{D}}^n\|_{\mathbb{L}^2(\Omega)} \le C(k^2 + h_{\mathcal{D}})\|u\|_{\mathcal{C}^3\left([0,T];\, \mathcal{C}^2(\overline{\Omega})\right)}. \tag{21}$$

- $\mathbb{L}^\infty(H_0^1)$*–estimate. For all* $n \in [\![0, N]\!]$

$$\left(\lambda_n^{n+1}\right)^{-\frac{1}{2}} \|\nabla u^{n+\sigma} - \nabla_{\mathcal{D}} u_{\mathcal{D}}^{n+\sigma}\|_{\mathbb{L}^2(\Omega)} \le C(k^2 + h_{\mathcal{D}})\|u\|_{\mathcal{C}^3\left([0,T];\, \mathcal{C}^2(\overline{\Omega})\right)}. \tag{22}$$

Idea on the proof

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1. Comparison with an auxiliary scheme: for any $n \in [\![0, N+1]\!]$, find $\bar{u}_{\mathcal{D}}^n \in \mathcal{X}_{\mathcal{D},0}$ such that

$$\left(\nabla_{\mathcal{D}}\bar{u}_{\mathcal{D}}^n, \nabla_{\mathcal{D}}v\right)_{\left(\mathbb{L}^2(\Omega)\right)^d} = -\left(\Delta u(t_n), \Pi_{\mathcal{M}}\, v\right)_{\mathbb{L}^2(\Omega)}, \quad \forall v \in \mathcal{X}_{\mathcal{D},0}. \tag{23}$$

2. A discrete *a priori estimate*
3. Other technical details can be found in Proceedings NMA2018.

A remark on the convergence rate for the gradient approximation

A remark on the convergence rate for the gradient approximation

1. Convergence order in $\mathbb{L}^\infty(\mathbb{L}^2)$ is optimal, i.e. $k^2 + h_{\mathcal{D}}$.
2. Convergence order in $\mathbb{L}^\infty(H_0^1)$ seems NOT optimal. Indeed, using (22) and the fact that $\lambda_n^{n+1} = \mathcal{O}(k^{-\alpha})$

$$\|\nabla u^{n+\sigma} - \nabla_{\mathcal{D}} u_{\mathcal{D}}^{n+\sigma}\|_{\mathbb{L}^2(\Omega)} = \mathcal{O}\left(k^{-\frac{\alpha}{2}}(k^2 + h_{\mathcal{D}})\right). \tag{24}$$

Which is a conditional convergence.

Conclusion

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We established a second order time accurate finite volume scheme for a time fractional diffusion equation in any space dimension.

Perspectives

First perspective

We work on a new *a priori estimate* which serves to derive optimal error estimate in $\mathbb{L}^\infty(H_0^1)$, see estimate (24).

Second perspective

Writing the present results in a general setting where σ is depending on n.

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Writing the present results in a general setting where σ is depending on n.