Analysis of a New Gradient Scheme Applied to a Distributed Order Diffusion Wave Problem

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On-Line Presentation

Dedicated to the memory of Professor Raytcho Lazarov

Few words to be said ...

Professor R. Lazarov:

- One of the pioneers of Finite Element and Mixed Finite Elements methods.
- One of the leaders in Fractional PDEs.
- Extraordinary leader in Numerical Analysis

Aim of the presentation

The aim of this talk is to establish a Gradient Discretization Scheme for a Distributed Order Wave Equation along with a convergence analysis.

Plan of this presentation

1. Some References
2. Equation to be solved
3. Introduction:
   - SUSHI as typical example of Gradient Discretization Method (GDM).
   - Definition of GDM and some numerical examples encompassed by GDM
4. Overview on the approximations of Distributed Caputo derivative.
5. Formulation of a GDM Scheme
6. Statement of the Convergence of the numerical scheme
7. Perspectives

Some references-Part I

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Some references-Part II

- R. Eymard, T. Gallouët, R. Herbin. Discretization of heterogeneous and anisotropic diffusion problems on general nonconforming meshes (SUSHI). IMA J. Numer. Anal. 30/4 (2010).
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Problem to be solved

Equation

We consider the following time fractional diffusion equation:

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

where $\Omega \subset \mathbb{R}^d$ is an open bounded domain of $\mathbb{R}^d$, $T > 0$, and f is a given function with:

Distributed Caputo derivative

$$\mathbb{D}_t^{\alpha} \varphi(t) = \int_1^2 \omega(\alpha) \partial_t^{\alpha} \varphi(t) d\alpha \tag{2}$$

with $\partial_t^{\alpha} \varphi(t) = \dfrac{1}{\Gamma(2-\alpha)} \displaystyle\int_0^t (t-s)^{1-\alpha} \varphi''(s) ds$ for $1 \le \alpha < 2$ with $\partial_t^2 \varphi(t) = \varphi''(t)$ and $\partial_t^1 \varphi(t) = \varphi'(t) - \varphi'(0)$.

Problem to be solved: Suite

Hypotheses on the weight function ω

$$\omega \in \mathcal{C}^2([1,2]) \quad \text{and} \quad \omega(\alpha) \geq 0, \quad \forall \alpha \in [1,2]. \tag{3}$$

and

$$\int_0^1 \omega(\alpha) d\alpha = c_0 > 0. \tag{4}$$

Initial and boundary conditions

Initial conditions

For two given functions defined on Ω

$$u(\boldsymbol{x},0) = u^0(\boldsymbol{x}) \quad \text{and} \quad u_t(\boldsymbol{x},0) = u^1(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega.$$

Homogeneous Dirichlet boundary

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

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.

Introduction: Finite Volume from Admissible meshes to Nonconforming meshes

Finite volume methods[1] are numerical methods approximating different types of Partial Differential Equations (PDEs). They are based on three principle ideas:

- Subdivision of the spatial domain into subsets called Control Volumes.
- Integration of the equation to be solved over the Control Volumes.
- Approximation of the derivatives appearing after integration.

[1] We mean here the "pure" finite volume methods and not finite volume-element methods

Introduction (suite): Finite Volume from Admissible meshes to Nonconforming meshes

Finite Volume methods passed by three steps:

First step

Finite Volume methods using Admissible meshes.

Second step

SUSHI method.

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Introduction (suite): Finite Volume methods on admissible meshes

Definition

Let $\mathcal{T}$ be an Admissible Mesh in the sense of Eymard et al. (Handbook, 2000).

$K \in \mathcal{T}$ are the control volumes and σ are the edges of the control volumes K.

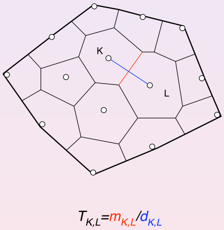

Figure: transmissivity between K and L: $\mathcal{T}_\sigma = \mathcal{T}_{K|L} = \dfrac{m_{K,L}}{d_{K,L}}$

Introduction (suite): Finite Volume methods on admissible meshes

Main properties of Admissible mesh:

1. Convexity of the Control Volumes.
2. The orthogonality property: the $(\boldsymbol{x}_K\boldsymbol{x}_L)$ is orthogonal to the common edge σ between the control volumes K and L.

Introduction (suite): Finite Volume methods on admissible meshes

Model to be solved:

$$-\Delta u(\boldsymbol{x}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega \quad \text{and} \quad u(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \partial\Omega. \tag{5}$$

Principles of Finite Volume scheme:

1. Integration on each control volume K :$-\int_K \Delta u(\boldsymbol{x}) d\boldsymbol{x} = \int_K f(\boldsymbol{x}) d\boldsymbol{x}$,
2. Integration by Parts gives :$-\int_{\partial K} \nabla u(\boldsymbol{x}) \cdot \mathbf{n}(\boldsymbol{x}) d\gamma(\boldsymbol{x}) = \int_K f(\boldsymbol{x}) d\boldsymbol{x}$
3. Summing on the lines of K: $-\sum_{\sigma \in \mathcal{E}_K} \int_\sigma \nabla u(\boldsymbol{x}) \cdot \mathbf{n}(\boldsymbol{x}) d\gamma(\boldsymbol{x}) = \int_K f(\boldsymbol{x}) d\boldsymbol{x}$

Introduction (suite): Finite Volume methods on admissible meshes

Approximate Finite Volume Solution $u_{\mathcal{T}} = (u_K)_K$

$$-\sum_{\sigma\in\mathcal{E}_K} \frac{\mathrm{m}(\sigma)}{d_{K|L}}(u_L - u_K) = \int_K f(\boldsymbol{x})d\boldsymbol{x}. \tag{6}$$

Matrix Form

$$\mathcal{A}^{\mathcal{T}} u_{\mathcal{T}} = f_{\mathcal{T}}.$$

Introduction (suite): Finite Volume methods on admissible meshes

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Introduction (suite): Finite Volume methods on admissible meshes

Theorem

Let $\mathcal{X}(\mathcal{T})$: functions which are constant on each control volume K. Let $e_{\mathcal{T}} \in \mathcal{X}(\mathcal{T})$ be defined by $e_K = u(\boldsymbol{x}_K) - u_K$ for any $K \in \mathcal{T}$. Assume that the exact solution u satisfies $u \in \mathcal{C}^2(\overline{\Omega})$. Then the following convergence results hold:

1. *H_0^1-error estimate*

$$\|e_{\mathcal{T}}\|_{1,\mathcal{T}} \leq Ch\|u\|_{2,\overline{\Omega}}, \tag{7}$$

where $\|\cdot\|_{1,\mathcal{T}}$ is the H_1^0-norm $\|e_{\mathcal{T}}\|_{1,\mathcal{T}}^2 = \displaystyle\sum_{\sigma=K|L\in\mathcal{E}} \frac{\mathrm{m}(\sigma)}{d_\sigma}(u_L - u_K)^2.$

2. *L^2-error estimate:*

$$\|e_{\mathcal{T}}\|_{L^2(\Omega)} \leq Ch\|u\|_{2,\overline{\Omega}}. \tag{8}$$

Introduction (suite): Finite Volume methods using nonconforming grids, SUSHI scheme

Definition (New mesh of Eymard et *al.*, IMAJNA 2010)

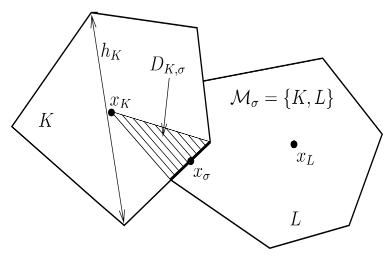

Figure: Notations for two neighbouring control volumes in $d = 2$

Introduction (suite): Finite Volume methods using nonconforming grids, 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.

Introduction (suite): Finite Volume methods using nonconforming grids, SUSHI scheme

Principles of discretization for Poisson's equation:

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

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

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.

Introduction (suite): Finite Volume methods using nonconforming grids, SUSHI

Weak formulation for Poisson's equation: Find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega \nabla u(\boldsymbol{x}) \cdot \nabla v(\boldsymbol{x}) d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x}) v(\boldsymbol{x}) d\boldsymbol{x}, \quad \forall v \in H_0^1(\Omega). \tag{9}$$

SUSHI (Scheme Using stabilized Hybrid Interfaces) for Poisson's equation: Find $u_{\mathcal{D}} \in \mathcal{X}_{\mathcal{D},0}$ such that

$$\int_\Omega \nabla_{\mathcal{D}} u_{\mathcal{D}}(\boldsymbol{x}) \cdot \nabla_{\mathcal{D}} v(\boldsymbol{x}) d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x}) v(\boldsymbol{x}) d\boldsymbol{x}, \quad \forall v \in \mathcal{X}_{\mathcal{D},0}. \tag{10}$$

Introduction (suite): Finite Volume methods using nonconforming grids, SUSHI

Theorem

Assume that the exact solution u satisfies $u \in \mathcal{C}^2(\overline{\Omega})$. Then the following convergence result hold:

1. H_0^1*-error estimate*

$$\|\nabla u - \nabla_{\mathcal{D}} u_{\mathcal{D}}\|_{L^2(\Omega)^d} \leq Ch\|u\|_{2,\overline{\Omega}}. \tag{11}$$

2. L^2*-error estimate:*

$$\|u - \Pi_{\mathcal{M}} u_{\mathcal{D}}\|_{L^2(\Omega)} \leq Ch\|u\|_{2,\overline{\Omega}}. \tag{12}$$

Definition of GDM (Gradient Discretisation Method)

Definition

Let Ω be an open domain of $\mathbb{R}^d$, with $d \in \mathbb{N}^\star$. An approximate gradient discretization is given by $\mathcal{D} = (\mathcal{X}_{\mathcal{D},0}, \Pi_{\mathcal{D}}, \nabla_{\mathcal{D}})$, where

1. The set of discrete unknowns $\mathcal{X}_{\mathcal{D},0}$ is a finite dimensional vector space on $\mathbb{R}$.
2. The linear mapping $\Pi_{\mathcal{D}} : \mathcal{X}_{\mathcal{D},0} \to L^2(\Omega)$ is the reconstruction of the approximate function.
3. The gradient reconstruction $\nabla_{\mathcal{D}} : \mathcal{X}_{\mathcal{D},0} \to L^2(\Omega)^d$ is a linear mapping which reconstructs, from an element of $\mathcal{X}_{\mathcal{D},0}$, a "gradient" (vector-valued function) over Ω. The gradient reconstruction must be chosen such that $\|\nabla_{\mathcal{D}} \cdot \|_{L^2(\Omega)^d}$ is a norm on $\mathcal{X}_{\mathcal{D},0}$.

Parameters of GDM

Parameters of GDM

- **Coercivity** is measured via the constant $C_{\mathcal{D}}$ given by

$$C_{\mathcal{D}} = \max_{v \in \mathcal{X}_{\mathcal{D},0} \setminus \{0\}} \frac{\|\Pi_{\mathcal{D}} v\|_{L^2(\Omega)}}{\|\nabla_{\mathcal{D}} v\|_{L^2(\Omega)^d}}.$$

  This yields the Poincaré inequality $\|\Pi_{\mathcal{D}} v\|_{L^2(\Omega)} \leq C_{\mathcal{D}} \|\nabla_{\mathcal{D}} v\|_{L^2(\Omega)^d}$.

- **Strong Consistency**: For $\varphi \in H_0^1(\Omega)$, $S_{\mathcal{D}}(\varphi)$ is given by

$$S_{\mathcal{D}}(\varphi) = \min_{v \in \mathcal{X}_{\mathcal{D},0}} \left(\|\Pi_{\mathcal{D}} v - \varphi\|^2_{L^2(\Omega)} + \|\nabla_{\mathcal{D}} v - \nabla \varphi\|^2_{L^2(\Omega)^d} \right)^{\frac{1}{2}}.$$

- **Dual Consistency**: For $\varphi \in H_{\mathrm{div}}(\Omega)$, $W_{\mathcal{D}}(\varphi)$ is given by

$$\max_{u \in \mathcal{X}_{\mathcal{D},0} \setminus \{0\}} \frac{1}{\|\nabla_{\mathcal{D}} u\|_{L^2(\Omega)^d}} \left| \int_\Omega \left(\nabla_{\mathcal{D}} u(\boldsymbol{x}) \cdot \varphi(\boldsymbol{x}) + \Pi_{\mathcal{D}} u(\boldsymbol{x}) \mathrm{div} \varphi(\boldsymbol{x}) \right) d\boldsymbol{x} \right|.$$

Some examples of GDM

Examples

1. SUSHI.
2. Conforming and Non-Conforming FEMs (Finite Element Methods).
3. Conforming and Non-Conforming MFEMs (Mixed Finite Element Methods)

Principles of the time- discretization

Step 1: Discretize the integral (2).

The integral (2) can be discretized, for instance, using the Mid-Point rule on the uniform mesh with constant step size $\rho = 1/q$, where $q \in \mathbb{N} \setminus \{0\}$:

$$\int_1^2 \omega(\alpha)\psi(\alpha)d\alpha = \frac{1}{q}\sum_{i=0}^{q-1}\omega(\alpha_i)\psi(\alpha_i) + \mathbb{T}_2(\psi), \tag{13}$$

where α_i are the mid points of the interval $(\xi_i, \xi_{i+1}) = (1 + \frac{i}{q}, 1 + \frac{i+1}{q})$ and

$$|\mathbb{T}_2(\psi)| \leq \frac{\rho^2}{24}\|\psi''\|_{\mathcal{C}([1,2])}. \tag{14}$$

By replacing ψ with $\partial_t^\alpha \varphi(t)$ in (13), we get

$$\mathbb{D}_t^\alpha \varphi(t) \approx \frac{1}{q}\sum_{i=0}^{q-1}\omega(\alpha_i)\partial_t^{\alpha_i}\varphi(t).$$

Principles of the time- discretization

Step 2: Approximation of the fractional Caputo derivatives.

The following approximation for $(\partial_t^{\alpha_i}\varphi)^{n+\frac{1}{2}}$ (which stems from a Crank-Nicolson type method) is given in B. [2000], for $t_{n+\frac{1}{2}} = (t_n + t_{n+1})/2$:

$$\begin{aligned}(\partial_t^{\alpha_i}\varphi)\left(t_{n+\frac{1}{2}}\right) &= \lambda_n^{n+1,\beta_i}\partial^1\varphi(t_{n+1}) + \sum_{j=0}^{n-1}(\lambda_j^{n+1,\beta_i} - \lambda_{j+1}^{n+1,\beta_i})\partial^1\varphi(t_{j+1}) \\ &- \lambda_0^{n+1,\beta_i}\varphi_t(0) + \mathbb{T}_3^{n+1,\alpha_i}(\varphi),\end{aligned} \tag{15}$$

where $\beta_i = \alpha_i - 1$ and for some positive constant C independent, in addition to the parameters of discretizations, of α_i

$$|\mathbb{T}_3^{n+1,\alpha_i}(\varphi)| \le Ck^{3-\alpha_i}\|\varphi\|_{\mathcal{C}^3([0,T])}. \tag{16}$$

Principles of the time- discretization

Step 3: Full approximation for the distributed order operator (2).

Thanks to the two previous steps, we have the following approximation for the distributed order operator [2]:

$$\begin{aligned}
\mathbb{D}_t^{\alpha}\varphi(t_{n+\frac{1}{2}}) &= P_n^{q,n+1}\partial^1\varphi(t_{n+1}) + \sum_{j=0}^{n-1}(P_j^{q,n+1} - P_{j+1}^{q,n+1})\partial^1\varphi(t_{j+1}) \\
&- P_0^{q,n+1}\varphi_t(0) + \mathbb{T}_4^{n+1}(\varphi),
\end{aligned} \tag{17}$$

where (recall that $\beta_i = \alpha_i - 1$)

$$P_j^{q,n+1} = \frac{1}{q}\sum_{i=0}^{q-1}\omega(\alpha_i)\lambda_j^{n+1,\beta_i}, \tag{18}$$

with λ_j^{n+1,β_i} are the coefficients of L1-formula associated to the Caputo derivative of order $\beta_i \in (0,1)$.

Principles of the discretization (suite)

Discretization in space

We use GDM

Formulation of scheme

Formulation of scheme

For any $n \in [\![0, N]\!]$, find $u_{\mathcal{D}}^{n+1} \in \mathcal{X}_{\mathcal{D},0}$ such that, for all $v \in \mathcal{X}_{\mathcal{D},0}$

$$\left(P_n^{q,n+1} \partial^1 \Pi_{\mathcal{D}} u_{\mathcal{D}}^{n+1} + \sum_{j=0}^{n-1} (P_j^{q,n+1} - P_{j+1}^{q,n+1}) \partial^1 \Pi_{\mathcal{D}} u_{\mathcal{D}}^{j+1}, \Pi_{\mathcal{D}} v \right)_{\mathbb{L}^2(\Omega)}$$

$$+ \quad \left(\nabla_{\mathcal{D}} u_{\mathcal{D}}^{n+\frac{1}{2}}, \nabla_{\mathcal{D}} v \right)_{L^2(\Omega)^d} = \left(f^{n+\frac{1}{2}} + P_0^{q,n+1} u^1, \Pi_{\mathcal{D}} v \right)_{\mathbb{L}^2(\Omega)}, \tag{19}$$

where, for all $v \in \mathcal{X}_{\mathcal{D},0}$

$$\left(\nabla_{\mathcal{D}} u_{\mathcal{D}}^0, \nabla_{\mathcal{D}} v \right)_{L^2(\Omega)^d} = - \left(\Delta u^0, \Pi_{\mathcal{D}} v \right)_{L^2(\Omega)}. \tag{20}$$

Convergence result

Theorem

(An $L^\infty(H_0^1)$—error estimate) For smooth solution u and weight function ω Then, there exists a unique solution $(u_{\mathcal{D}}^n)_{n=0}^{N+1} \in \mathcal{X}_{\mathcal{D},0}^{N+2}$ for the GS [19]–[20] and the following following $L^\infty(H_0^1)$–error estimate holds:

$$\max_{n=0}^{N+1} \|\nabla_{\mathcal{D}} u_{\mathcal{D}}^n - \nabla u(t_n)\|_{L^2(\Omega)^d} \leq C\left(\mathbb{E}_{\mathcal{D}}^k(u) + k^{1+\rho/2} + \rho^2\right), \tag{21}$$

where for any function $u \in \mathcal{C}([0,T];\ H^2(\Omega))$, we denote by

$$\mathbb{E}_{\mathcal{D}}^k(u) = \max_{j\in\{0,1\}} \max_{n\in[\![j,N+1]\!]} \mathbb{E}_{\mathcal{D}}(\partial^j u(t_n)) \tag{22}$$

and, for any $\overline{u} \in H^2(\Omega)$,

$$\mathbb{E}_{\mathcal{D}}(\overline{u}) = \max\left(C_{\mathcal{D}} W_{\mathcal{D}}(\nabla\overline{u}) + (C_{\mathcal{D}}+1)S_{\mathcal{D}}(\overline{u}), W_{\mathcal{D}}(\nabla\overline{u}(t_n)) + 2S_{\mathcal{D}}(\overline{u}(t_n))\right).$$

Conclusion and Perspectives

We established a fully discrete GS in which the discretization of the distributed order operator is given by Mid Point rule combined with the known $L1$-formula. The GS also uses a Crank–Nicolson type method. We proved an unconditional new $L^\infty(H^1)$–error estimate. The analysis allows also to prove an unconditional stability.

First perspective

Use $L2-1_\sigma$ and L2-formulas as high order approximations for the Caputo derivative.

Second perspective

Use of other high order numerical quadratures like the Sympson's method.

Third perspective

Use of Graded mesh in time, to deal with non-smooth exact solution, instead of Uniform mesh .

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