Finite Volume method for Heat, Wave, and Time Fractional Heat Equations

Abdallah Bradji[1,2]

[1] Department of Mathematics, University of Annaba–Algeria

[2] EUR Visiting Professor in USPN-France

Email: abdallah.bradji@gmail.com

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Aim of the presentation

We investigate the approximation of the Heat, Wave, and Time Fractional Heat equations using either Finite Volume methods or the general framework of GDM (Gradient Discretization Method).

Plan of this presentation

1. Reminder on the previous course.
2. Finite Volumes methods (on Admissible and Non-Conforming meshes-SUSHI).
3. Finite Volume method for the Heat equation.
4. Finite Volume method for the Wave equation.
5. Overview on the recent framework of the GDM (Gradient Discretization Method)
6. GDM for **TFHE** (Time Fractional Heat equation).

Reminder on the previous course

Importance of the numerical methods for DEs and PDEs

DEs and PDEs represent real phenomenon.

Finite Difference method

It is based on the approximation of the derivatives which appear in (DE or PDE), over the mesh points, by convenient difference quotients (or divided differences).

Finite Element methods

They are based on a weak formulation for the problem under consideration.

Mixed Finite Element methods

They are based on the introduction of two variables: Velocity (called also Vector variable) and Pressure. We use often the so-called $\mathbb{RT}$ in the approximation.

Finite Volume methods

We integrate over Control Volumes and then we approximate.

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References on Finite Volume Methods and GDM

- J. Droniou, R. Eymard, T. Gallouët, C. Guichard, R. Herbin: The Gradient Discretisation Method. Mathématiques et Applications (Berlin) [Mathematics and Applications], 82. Springer, Cham, 2018.
- R. Eymard, T. Gallouët, R. Herbin: Finite volume methods. Handbook of numerical analysis, Vol. VII, 713–1020, Handb. Numer. Anal., VII, North-Holland, Amsterdam, 2000.
- R. Eymard, T. Gallouët, R. Herbin: Finite volume methods. Handbook of numerical analysis. hal-02100732 , version 2 (12-08-2019).
- R. Eymard, T. Gallouët, R. Herbin: Discretization of heterogeneous and anisotropic diffusion problems on general nonconforming meshes. SUSHI: A scheme using stabilization and hybrid interfaces. IMAJNA, 2010.

References on the Heat and Wave equations

- L. Evans: Partial Differential Equations. Graduate Studies in Mathematics, Volume 19, American Mathematical Society, 1998.
- Randall J. LeVeque: Finite Volume Methods for Hyperbolic Problems. Cambridge University Press, 2012.
- A. Quarteroni, A. Valli: Numerical Approximation of Partial Differential Equations. Springer Series in Computational Mathematics 23. Berlin: Springer, 2008.

Overview on Finite Volume Methods on Admissible Meshes: Principles

Fundamental highlight on the method

The finite volume method is a discretization method which is well suited for the numerical simulation of various types (elliptic, parabolic or hyperbolic, for instance) of conservation laws; it has been extensively used in several engineering fields, such as fluid mechanics, heat and mass transfer or petroleum engineering.

Main ingredients of the method

- We subdivide the domain into subsets called control volumes.
- Integration of the equation to be solved on each control volume.
- Integration by parts to transfer the integration on the control volumes to integration on the interfaces across the control volumes.
- When the control volumes satisfy a condition called transmissibility, the approximation of the integrals along the interfaces becomes easier.

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Finite Volume methods in several space dimensions 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.

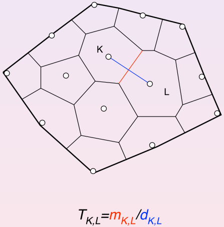

Figure: transmissivity between K and L: $\mathcal{T}_\sigma = \mathcal{T}_{K|L} = \frac{m_{K,L}}{d_{K,L}}$

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.

Finite Volume methods on admissible meshes

Model to be solved:

$$-\Delta u(\boldsymbol{x}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega \quad \text{and} \quad u(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \partial\Omega. \tag{1}$$

Principles of Finite Volume scheme:

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

Finite Volume methods on admissible meshes

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

$$-\sum_{\sigma \in \mathcal{E}_K} \frac{\mathrm{m}(\sigma)}{d_{K|L}} (u_L - u_K) = \int_K f(\boldsymbol{x}) d\boldsymbol{x}. \qquad (2)$$

Matrix Form

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

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

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*

$$\|e_{\mathcal{T}}\|_{1,\mathcal{T}} \leq Ch\|u\|_{2,\overline{\Omega}}, \tag{3}$$

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

2. *L^2-error estimate:*

$$\|e_{\mathcal{T}}\|_{L^2(\Omega)} \leq Ch\|u\|_{2,\overline{\Omega}}. \tag{4}$$

Finite Volume methods on admissible meshes: three useful remarks

First remark: Conservativity of the numerical fluxes

It means that fluxes, that is the numerical flux is conserved from one discretization cell to its neighbour. This last feature makes the finite volume method quite attractive when modelling problems for which the flux is of importance, such as in fluid mechanics, semi-conductor device simulation, heat and mass transfer...
For the approximation given above

$$-\frac{\mathrm{m}(\sigma)}{d_{K|L}}(u(\boldsymbol{x}_L) - u(\boldsymbol{x}_K)) \approx -\int_\sigma \nabla u(\boldsymbol{x}) \cdot \mathbf{n}(\boldsymbol{x}) d\gamma(\boldsymbol{x})$$

If we denote by the numerical flux $F_{K,L} = -\dfrac{\mathrm{m}(\sigma)}{d_{K|L}}(u(\boldsymbol{x}_L) - u(\boldsymbol{x}_K))$, then the following **Conservativity** property holds

$$F_{K,L} = -F_{L,K}.$$

Finite Volume methods on admissible meshes: two useful remarks (Suite)

Second remark: Consistency of the approximation of the Flux

In contrast of Finite Difference Methods, in which we approximate directly the derivatives and quantities of the equation to be solved, in Finite Volume Methods we approximate these terms after integration. In the case of the Poisson's problem, we have to approximate the Flux which yields the **Consistency** of the approximation of the Flux.

Third remark: FVM is different from FDM and FEM

The Finite Volume Method is quite different from (but sometimes related to) the Finite Difference Method and the Finite Element Method, see details in Handbook (2010).

Finite Volume methods using nonconforming grids, SUSHI scheme

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

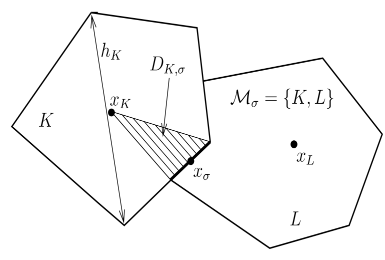

Figure: Notations for two neighbouring control volumes in $d = 2$

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.

Finite Volume methods using nonconforming grids, SUSHI scheme

Principles of discretization for the Poisson's problem:

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

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

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.

Finite Volume methods using nonconforming grids, SUSHI

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

$$\int_\Omega \nabla u(\boldsymbol{x}) \cdot \nabla v(\boldsymbol{x}) d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x}) v(\boldsymbol{x}) d\boldsymbol{x}, \quad \forall v \in H_0^1(\Omega). \tag{5}$$

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

$$\int_\Omega \nabla_\mathcal{D} u_\mathcal{D}(\boldsymbol{x}) \cdot \nabla_\mathcal{D} v(\boldsymbol{x}) d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x}) v(\boldsymbol{x}) d\boldsymbol{x}, \quad \forall v \in \mathcal{X}_{\mathcal{D},0}. \tag{6}$$

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*

$$\|\nabla u - \nabla_{\mathcal{D}} u_{\mathcal{D}}\|_{L^2(\Omega)^d} \leq Ch\|u\|_{2,\overline{\Omega}}. \tag{7}$$

2. L^2*-error estimate:*

$$\|u - \Pi_{\mathcal{M}} u_{\mathcal{D}}\|_{L^2(\Omega)} \leq Ch\|u\|_{2,\overline{\Omega}}. \tag{8}$$

FVM for the Heat equation: Problem to be solved

Heat equation

$$u_t(\boldsymbol{x},t) - \Delta u(\boldsymbol{x},t) = f(\boldsymbol{x},t), \quad (x,t) \in \Omega \times (0,T), \tag{9}$$

where $\Omega \subset \mathbb{R}^d$ is bounded ($d = 2$ or $d = 3$), $T > 0$, and f is a source term .

Initial condition

$$u(\boldsymbol{x},0) = u^0(x), \quad \boldsymbol{x} \in \Omega. \tag{10}$$

Homogeneous Dirichlet boundary conditions

$$u(\boldsymbol{x},t) = 0, \quad (\boldsymbol{x},t) \in \partial\Omega \times (0,T). \tag{11}$$

FVM for the Heat equation: What about Heat equation?

Heat equation-Classification of equations

Heat equation is a is the prototypical example of a parabolic partial differential equation.

Heat equation-Analysis

The well-posedness of the heat problem can be found for instance in the book of Evans (1998).

Heat equation-Physics

The unknown exact solution u represents for instance temperature of a body.

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FVM for the Heat equation: on Admissible mesh

Time discretization

Time discretization $t_n = nk$, k is the time step size with $k = 1/N$ and $N \in \mathbb{N} \setminus \{0\}$.

Discrete unknowns

Denote by $\{u_K^n : K \in \mathcal{T} \quad \text{and} \quad n \in [\![0, N+1]\!]\}$ the discrete unknowns; the value u_K^n is expected to approximate $u(\boldsymbol{x}_K, t_n)$.

Derivation of the scheme

Integrating equation (9) over $K \times (t_n, t_{n+1})$ and using an integration by parts yields

$$\int_K (u(\boldsymbol{x}, t_{n+1}) - u(\boldsymbol{x}, t_n))\, d\boldsymbol{x} - \sum_{\sigma \in \mathcal{E}_K} \int_{t_n}^{t_{n+1}} \int_\sigma \nabla u(\boldsymbol{x}, t) \cdot \mathbf{n}_{\sigma,K} d\gamma(\boldsymbol{x}) dt$$

$$= \int_K \int_{t_n}^{t_{n+1}} f(\boldsymbol{x}, t) d\boldsymbol{x} dt. \qquad (12)$$

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FVM for the Heat equation: on Admissible mesh

Derivation of the scheme (Suite)

- Using some convenient Taylor expansions, (12) implies that

$$\mathrm{m}(K)\left(u(\boldsymbol{x}_K,t_{n+1})-u(\boldsymbol{x}_K,t_n)\right)-k\sum_{\sigma\in\mathcal{E}_K}\int_\sigma \nabla u(\boldsymbol{x},t_{n+1})\cdot\mathbf{n}_{\sigma,K}d\gamma(\boldsymbol{x})$$
$$\approx \int_K\int_{t_n}^{t_{n+1}} f(\boldsymbol{x},t)d\boldsymbol{x}dt. \qquad (13)$$

- Formulation of the Finite Volume scheme:

$$\mathrm{m}(K)\partial^1 u_K^{n+1}-\sum_{\sigma\in\mathcal{E}_K}\mathrm{m}(\sigma)\frac{u_L-u_K}{d_{K|L}}=\frac{1}{k}\int_K\int_{t_n}^{t_{n+1}} f(\boldsymbol{x},t)d\boldsymbol{x}dt, \qquad (14)$$

where ∂^1 is the discrete time derivative $\partial^1 v^{n+1}=\dfrac{v^{n+1}-v^n}{k}$.

- Discrete initial data $u_K^0=u^0(\boldsymbol{x}_K)$.

FVM for the Heat equation: Convergence of the scheme

Theorem (Convergence of scheme in $L^\infty(L^2)$)

$$\max_{n\in\{0,\ldots,N+1\}} \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) \left| u(\boldsymbol{x}_K, t_n) - u_K^n \right|^2 \right)^{\frac{1}{2}} \leq C(h+k). \tag{15}$$

How to see the convergence?

$$\max_{n\in\{0,\ldots,N+1\}} \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) \left| u(\boldsymbol{x}_K, t_n) - u_K^n \right|^2 \right)^{\frac{1}{2}} \to 0, \quad \text{as} \quad h \to 0 \text{ and } k \to 0.$$

FVM for the Heat equation: Useful remark on the convergence in time

Convergence in time

The convergence in time is k (only order one). To increase the order in time from one to two (and therefore the convergence becomes faster), we use the known Crank-Nicolson finite difference method (see Quarteroni et Valli-2008).

FVM for the Heat equation: using SUSHI

Principles of the scheme

- Weak formulation for the problem (see Evans-1998)

$$(u_t(t),\varphi)_{L^2(\Omega)}+(\nabla u(t),\nabla\varphi)_{L^2(\Omega)^d}=(f(t),\varphi)_{L^2(\Omega)}\,. \tag{16}$$

- Taking $t=t_{n+1}$ in (16) to get

$$(u_t(t_{n+1}),\varphi)_{L^2(\Omega)}+(\nabla u(t_{n+1}),\nabla\varphi)_{L^2(\Omega)^d}=(f(t_{n+1}),\varphi)_{L^2(\Omega)}). \tag{17}$$

- Approximating $u_t(t_{n+1})$ by $\partial^1 u(t_{n+1})=\dfrac{u(t_{n+1})-u(t_n)}{k}$ and $u(t_{n+1})$ by $u_{\mathcal{D}}^{n+1}$ in (17) yields the scheme: Find $u_{\mathcal{D}}^{n+1}\in\mathcal{X}_{\mathcal{D},0}$ such that for all $\varphi\in\mathcal{X}_{\mathcal{D},0}$:

$$\left(\partial^1 u_{\mathcal{D}}^{n+1},\varphi\right)_{L^2(\Omega)}+\left(\nabla_{\mathcal{D}}u_{\mathcal{D}}^{n+1},\nabla_{\mathcal{D}}\varphi\right)_{L^2(\Omega)^d}=(f(t_{n+1}),\varphi)_{L^2(\Omega)}). \tag{18}$$

The Wave equation

Wave equation

$$u_{tt}(\boldsymbol{x},t) - \Delta u(\boldsymbol{x},t) = f(\boldsymbol{x},t), \quad (\boldsymbol{x},t) \in \Omega \times (0,T), \tag{19}$$

where, $\Omega \subset \mathbb{R}^d$ bounded and f is a given function.

Initial conditions

$$u(\boldsymbol{x},0) = u^0(\boldsymbol{x}) \quad \text{and} \quad u_t(\boldsymbol{x},0) = u^1(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega. \tag{20}$$

Homogeneous Dirichlet boundary conditions

$$u(\boldsymbol{x},t) = 0, \quad (\boldsymbol{x},t) \in \partial\Omega \times (0,T). \tag{21}$$

About Wave equation?

Some physics

The wave equation occur in physics such as sound waves, light waves and water waves. It arises in fields like acoustics, electromagnetics, and fluid dynamics, ...

As model

The wave equation is an important model of second-order hyperbolic equations.

Existence and uniqueness

The existence and uniqueness of a weak solution of wave equation (19)–(20) can be found for instance in Evans-1998.

SUSHI for wave equation: discretization Ω and $(0, T)$

Spatial discretization

Spatial domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, is discretized using the new class of meshes.

Time discretization

The time interval $(0, T)$ constant step $k = T/(N+1)$, $N \in \mathbb{N}$. The mesh points are denoted by $t_n = nk$, $n = 0, \ldots, N+1$

Principles of scheme

Principles of the scheme

- Weak formulation for the problem (see Evans-1998)

$$(u_{tt}(t), \varphi)_{L^2(\Omega)} + (\nabla u(t), \nabla \varphi)_{L^2(\Omega)^d} = (f(t), \varphi)_{L^2(\Omega)} . \tag{22}$$

- Taking $t = t_{n+1}$ in (22) to get

$$(u_{tt}(t_{n+1}), \varphi)_{L^2(\Omega)} + (\nabla u(t_{n+1}), \nabla \varphi)_{L^2(\Omega)^d} = (f(t_{n+1}), \varphi)_{L^2(\Omega)}). \tag{23}$$

- Approximating $u_{tt}(t_{n+1})$ by $\partial^2 u(t_{n+1}) = \dfrac{\partial^1 u(t_{n+1}) - \partial^1 u(t_n)}{k}$ and $u(t_{n+1})$ by $u_{\mathcal{D}}^{n+1}$ in (23) yields the scheme: Find $u_{\mathcal{D}}^{n+1} \in \mathcal{X}_{\mathcal{D},0}$ such that for all $\varphi \in \mathcal{X}_{\mathcal{D},0}$:

$$\left(\partial^2 u_{\mathcal{D}}^{n+1}, \varphi\right)_{L^2(\Omega)} + \left(\nabla_{\mathcal{D}} u_{\mathcal{D}}^{n+1}, \nabla_{\mathcal{D}} \varphi\right)_{L^2(\Omega)^d} = (f(t_{n+1}), \varphi)_{L^2(\Omega)} . \tag{24}$$

Discretization of initial conditions

Discretization of initial conditions

- Discretization of initial condition $u(\boldsymbol{x}, 0) = u^0(\boldsymbol{x})$:

$$u_K^0 = u^0(\boldsymbol{x}_K), \quad \forall K \in \mathcal{M} \quad \text{and} \quad u_\sigma^0 = u^0(\boldsymbol{x}_\sigma), \quad \forall \sigma \in \mathcal{E}. \tag{25}$$

- Discretization of initial condition $u_t(x, 0) = u^1(x)$, for all $(K, \sigma) \in \mathcal{M} \times \mathcal{E}$

$$\partial^1 u_K^1 = \frac{u_K^1 - u_K^0}{k} = u^1(\boldsymbol{x}_K) \quad \text{and} \quad \partial^1 u_\sigma^1 = \frac{u_\sigma^1 - u_\sigma^0}{k} = u^1(\boldsymbol{x}_\sigma). \tag{26}$$

Other discretizations for initial conditions

There are other possible choices, different from those of (25) and (26).

Diversify our discussion: New scheme for a new model of equations

Diversify our discussion

We have presented the new method of Finite Volume or SUSHI to approximate some standard models (Heat and Wave). We move now to approximate the new model of Fractional PDEs using the new method GDM.

Time Fractional Heat Equation

Equation

We consider the following time fractional diffusion equation:

$$\partial_t^\alpha u(\boldsymbol{x},t) - \Delta u(\boldsymbol{x},t) = f(\boldsymbol{x},t), \quad (\boldsymbol{x},t) \in \Omega \times (0,T), \tag{27}$$

where $\Omega \subset \mathbb{R}^d$ is an open domain of $\mathbb{R}^d$, $T > 0$, $0 < \alpha < 1$, and f is a given function. Here the operator ∂_t^α is the Caputo derivative defined by:

$$\partial_t^\alpha \varphi(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \varphi'(s) ds. \tag{28}$$

Initial condition

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

Homogeneous Dirichlet boundary

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

References on the Fractional Partial Differential Equations

- Ishteva, Mariya Kamenova: Properties and Applications of the Caputo Fractional Operator. Master Thesis in the Department of Mathematics-Karlsruhe Institute (TH), 2005.
- Podlubny, Igor: Fractional Differential Equations. An Introduction to Fractional Derivatives, Fractional Differential Equations, to Methods of their Solution and Some of their Applications. Mathematics in Science and Engineering. 198. San Diego, CA: Academic Press. 1999.
- Uchaikin, Vladimir V.: Fractional Derivatives for Physicists and Engineers, Springer-Verlag Heidelberg, 2013.

Equation to be solved: some information on the Γ-function

Definition of the Γ-function

$$\Gamma(t) = \int_0^t s^{t-1} \exp(-s) ds \tag{29}$$

Some properties the Γ-function

- The Γ-function extends the factorial function in the sense of $\Gamma(n) = (n-1)!$ for all $n \in \mathbb{N} \setminus \{0\}$.
- $\Gamma(0) = +\infty$.
- The Γ-function is defined on $]0, +\infty[$.
- $\Gamma(t+1) = t\Gamma(t)$, for all $t > 0$.
- The Γ-function is of $\mathcal{C}^\infty(]0, +\infty[)$.

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-2013 where we find many details.

What about time fractional diffusion equation: Some interesting properties?

First nice property: relation between fractional and usual derivatives

$$\lim_{\alpha \to 1} \partial_t^\alpha \varphi(t) = \varphi'(t). \tag{30}$$

Second nice property

$$\lim_{\alpha \to 0} \partial_t^\alpha \varphi(t) = \varphi(t) - \varphi(0). \tag{31}$$

Third nice property

The mapping $\varphi \mapsto \partial_t^\alpha \varphi$ is linear.

Overview on the Gradient Discretization Method: What is GDM simply ?

What is GDM?

Is a framework for the convergence and analysis of a large class of the numerical methods.

What are the numerical methods encompassed by GDM ?

- Conforming and Non-Conforming Finite Elements Methods
- SUSHI method, cf. Eymard et *al.* (IMAJNA, 2010).
- Mimetic Finite Difference methods, cf. Brezzi et al. (Math. Models Methods Appl. Sci., 2005).
- Mixed Finite Volume method, cf. Droniou et al. (Numer. Math., 2006).
- Mixed Finite Elements method.

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Overview on the Gradient Discretization Method: Definition

Definition (Definition of a generic approximate gradient discretization, Droniou et al. (Springer book, 2018))

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

1. The set of discrete unknowns $\mathcal{X}_{\mathcal{D},0}$ is a finite dimensional vector space on $\mathbb{R}$.
2. The space step $h_{\mathcal{D}} \in (0, +\infty)$ is a positive real number.
3. The linear mapping $\Pi_{\mathcal{D}} : \mathcal{X}_{\mathcal{D},0} \to L^2(\Omega)$ is the reconstruction of the approximate function.
4. The mapping $\nabla_{\mathcal{D}} : \mathcal{X}_{\mathcal{D},0} \to L^2(\Omega)^d$ is the reconstruction of the gradient of the function; it must be chosen such that $\|\nabla_{\mathcal{D}} \cdot \|_{L^2(\Omega)^d}$ is a norm on $\mathcal{X}_{\mathcal{D},0}$.

Overview on the Gradient Discretization Method: Additional parameters

Definition (Additional hypotheses on the approximate gradient discretization)

- The **coercivity** of the discretization is measured through the the constant $C_{\mathcal{D}}$ given by:

$$C_{\mathcal{D}} = \max_{v \in \mathcal{X}_{\mathcal{D},0} \setminus \{0\}} \frac{\|\Pi_{\mathcal{D}} v\|_{L^2(\Omega)}}{\|\nabla_{\mathcal{D}} v\|_{L^2(\Omega)^d}}. \tag{32}$$

- The **strong consistency**: $S_{\mathcal{D}} : H_0^1(\Omega) \to [0, +\infty)$ defined by, for all $\varphi \in H_0^1(\Omega)$

$$S_{\mathcal{D}}(\varphi) = \min_{v \in \mathcal{X}_{\mathcal{D},0}} \left(\|\Pi_{\mathcal{D}} v - \varphi\|_{L^2(\Omega)}^2 + \|\nabla_{\mathcal{D}} v - \nabla \varphi\|_{L^2(\Omega)^d}^2 \right)^{\frac{1}{2}}. \tag{33}$$

- The **dual consistency**: For all $\varphi \in H_{\text{div}}(\Omega)$, $W_{\mathcal{D}}(\varphi)$ is given by

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

Overview on the Gradient Discretization Method: A typical example-Conforming Finite Element Method

FE is a GDM

Let $\{\mathcal{T}_h; h > 0\}$ be a family of shape regular and quasi-uniform triangulations of the domain Ω. Let $\mathcal{V}^h$ be the standard finite element space of continuous, piecewise polynomial functions of degree less or equal $l \in \mathbb{N} \setminus \{0\}$ and we denote by $\mathcal{V}_0^h = \mathcal{V}^h \cap H_0^1(\Omega)$.

Assume that $\mathcal{V}_0^h$ is spanned by the usual basis functions $\varphi_1, \ldots, \varphi_M$. The space $\mathcal{X}_{\mathcal{D},0}$ can be $\mathbb{R}^M$ and for any $(u_1, \ldots, u_M) \in \mathcal{X}_{\mathcal{D},0}$, we define $\Pi_{\mathcal{D}} u = \sum_{i=1}^M u_i \varphi \in \mathcal{V}_0^h \subset H_0^1(\Omega)$ and $\nabla_{\mathcal{D}} u = \sum_{i=1}^M u_i \nabla \varphi = \nabla \Pi_{\mathcal{D}} u$. Using the Poincaré inequality, we have for all $u \in \mathcal{X}_{\mathcal{D},0}$, $\|\Pi_{\mathcal{D}} u\|_{\mathbb{L}^2(\Omega)} \le C(\Omega) \|\nabla_{\mathcal{D}} u\|_{\mathbb{L}^2(\Omega)}$.

Conditions of GDM are well satisfied by FE

Therefore, the assumption (32) of Definition 6 holds with constant $C_{\mathcal{D}}$ only depending on Ω. In addition to this, we have $W_{\mathcal{D}}(\varphi) = 0$, for all $\varphi \in H_{\text{div}}(\Omega)$, and $S_{\mathcal{D}}(\varphi)$ is bounded above by (up to a multiplicative constant independent of the mesh) $h^l |\varphi|_{l+1,\Omega}$, for all $\varphi \in H^{l+1}(\Omega)$.

Overview on the Gradient Discretization Method: An example of application

- Let us consider the Poisson problem described above in (1).
- The weak formulation for this problem is: Find $u \in H_0^1(\Omega)$ such that

$$(\nabla u, \nabla v)_{L^2(\Omega)^d} = (f, v)_{L^2(\Omega)}, \quad \forall v \in H_0^1(\Omega).$$

- The gradient scheme applied to the Poisson's problem is: Find $u_{\mathcal{D}} \in \mathcal{X}_{\mathcal{D},0}$ such that

$$(\nabla_{\mathcal{D}} u_{\mathcal{D}}, \nabla_{\mathcal{D}} v)_{L^2(\Omega)^d} = (f, v)_{L^2(\Omega)}, \quad \forall v \in \mathcal{X}_{\mathcal{D},0}. \tag{34}$$

Overview on the Gradient Discretization Method: Convergence

On the convergence

The convergence is well detailed in the above References, see for instance Eymard et *al.* (ESAIM-2012).

Principles of the discretization

Discretization in time

We define $k = T/(M+1)$ and $t_n = nk$ with $n \in \{0, \ldots, M+1\}$

- Taking $t = t_{n+1}$ in (27) yields, for all $n \in \{0, \ldots, M+1\}$

$$\partial_t^\alpha u(\boldsymbol{x}, t_{n+1}) - \Delta u(\boldsymbol{x}, t_{n+1}) = f(\boldsymbol{x}, t_{n+1}), \quad (\boldsymbol{x}, t) \in \Omega \times (0, T). \tag{35}$$

- The following approximation can be suggested for $\partial_t^\alpha \varphi(t_{n+1})$

$$\partial_t^\alpha \varphi(t_{n+1}) = \sum_{j=0}^{n} \lambda_j^{n+1} \partial^1 \varphi(t_{j+1}) + \mathbb{T}^{n+1}, \tag{36}$$

where $\partial^1 v^{j+1}$ is the first discrete time derivative $\frac{v^{j+1} - v^j}{k}$ and the coefficient λ_j^{n+1} is given by

$$\lambda_j^{n+1} = \frac{1}{\Gamma(2-\alpha)} \left((t_{n+1} - t_j)^{1-\alpha} - (t_{n+1} - t_{j+1})^{1-\alpha} \right). \tag{37}$$

Principles of the discretization

Discretization in time (Suite)

The rest $\mathbb{T}^{n+1}$ is bounded as

$$|\mathbb{T}^{n+1}| \leq Ck^{2-\alpha}. \tag{38}$$

A remark on the estimate

When $\alpha = 1$, estimate (38) becomes of order one.

Principles of the discretization (suite)

Discretization in space

We use GDM

A weak formulation for (35) on which the GDM is based

Multiplying (35) by a test function v, using an integration by parts, and using [36] yield: For any $n \in [\![0, M]\!]$

$$\sum_{j=0}^{n} \lambda_j^{n+1} \left(\partial^1 u(t_{j+1}), v\right)_{\mathbb{L}^2(\Omega)} + \left(\nabla u(t_{n+1}), \nabla v\right)_{\left(\mathbb{L}^2(\Omega)\right)^d}$$
$$= \quad \left(f(t_{n+1}), v\right)_{\mathbb{L}^2(\Omega)} - \left(\mathbb{T}^{n+1}, v\right)_{\mathbb{L}^2(\Omega)} . \tag{39}$$

Gradient Discretisation method applied to Fractional PDE (27)

GS applied to Fractional PDE (27)

From (39), replacing u by its reconstruction, the gradient by the discrete gradient, and neglecting $\mathbb{T}^{n+1}$ (since it tends to zero as k tends to zero) yields the following scheme: For any $n \in [\![0, M]\!]$, find $u_{\mathcal{D}}^{n+1} \in \mathcal{X}_{\mathcal{D},0}$ such that, for all $v \in \mathcal{X}_{\mathcal{D},0}$

$$\sum_{j=0}^{n} \lambda_j^{n+1} \left(\partial^1 \Pi_{\mathcal{D}} u_{\mathcal{D}}^{j+1}, \Pi_{\mathcal{M}} v\right)_{\mathbb{L}^2(\Omega)} + \left(\nabla_{\mathcal{D}}\, u_{\mathcal{D}}^{n+1}, \nabla_{\mathcal{D}}\, v\right)_{\left(\mathbb{L}^2(\Omega)\right)^d} = \left(f(t_{n+1}),\, v\right)_{\mathbb{L}^2(\Omega)} . \tag{40}$$

Some useful remarks

Implicit and Explicit

All the schemes provided here are implicit: in each iteration, we have to resolve a linear system. Of course we are able to use explicit methods: each iteration is given explicitly using the previous iterations.

However, the choice of Implicit will ensure that the convergence is unconditional: there is no required condition between time and spaces discretization to get the convergence. The choice of Explicit may lead to a conditional convergence.

Almost of these schemes are First order time accurate

The schemes provided here are of order one in time (for Fractional PDEs the order is $k^{2-\alpha}$ which goes to k when $\alpha \to 1$). This stems from the discretization in time. Of course, this order in time can be improved using for instance the so-called Crank-Nicolson finite differences methods.

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