Numerical analysis

Notes on the convergence order of gradient schemes for time fractional differential equations

Notes sur l’ordre de convergence de la méthode GD pour les équations fractionnaires en temps

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ARTICLE INFO

Article history:
Received 8 September 2017
Accepted after revision 8 February 2018
Available online 2 March 2018
Presented by Olivier Pironneau

ABSTRACT

We apply the GDM (Gradient Discretization Method), developed recently, as discretization in space to time-fractional diffusion and diffusion-wave equations with a fractional derivative of Caputo type in any space dimension.

In the case of time-fractional diffusion equations, we establish an implicit scheme, and we prove an \( L^\infty (L^2) \)-error estimate. A similar result in a discrete \( L^\infty (H^1_0) \)-norm is also stated.

To construct the numerical scheme for the time-fractional diffusion-wave equation, we write the equation in the form of a system of two low-order equations. We state an a priori estimate result that helps us to derive error estimates in discrete semi-norms of \( L^\infty (H^1) \) and \( H^1 (L^2) \). The convergence is unconditional. Another gradient scheme is also suggested. We state its convergence results, which improve the convergence order proved recently for a SUSHI scheme.

These results hold then for all the schemes within the framework of GDM: conforming and nonconforming finite element, mixed finite element, hybrid mixed mimetic family, some Multi-Point Flux approximation finite volume schemes, and some discontinuous Galerkin schemes.

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RÉSUMÉ

On considère la méthode GD (Gradient Discretization), développée récemment, comme discrétisation dans l'espace pour les équations de diffusion et d'onde fractionnaires en temps avec une dérivée fractionnaire de type Caputo pour toute dimension d'espace. Le temps est discrétisé dans intervalles de pas constant.

Dans le cas des équations de diffusion fractionnaires en temps, nous construisons un schéma implicite et nous prouvons une estimation d'erreur dans la norme \( L^\infty (L^2) \). Un résultat similaire dans la norme \( L^\infty (H^1_0) \)-norm a également été affirmé.

Pour construire le schéma numérique pour l'équation d'onde fractionnaire en temps, on écrit l'équation sous la forme d'un système de deux équations d'ordre plus bas. Nous construisons un schéma implicite, et nous donnons une estimation a priori qui nous permet de montrer des estimations d'erreur dans les semi-normes de \( L^\infty (H^1) \) et

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https://doi.org/10.1016/j.crma.2018.02.006

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1. Introduction

We are concerned with the convergence rate of GDM, developed recently in [5], as discretization in space for the following time-fractional problem:

\[
\partial_t^\alpha u(\mathbf{x}, t) - \Delta u(\mathbf{x}, t) = f(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times (0, T),
\]

(1)

where \( \Omega \) is an open bounded connected subset of \( \mathbb{R}^d \) (\( d \in \mathbb{N}^* \)), \( T > 0 \), and \( f \) is a given function. The operator \( \partial_t^\alpha \) denotes the Caputo derivative of order \( \alpha \) whose formula is, for \( m - 1 < \rho < m \), with \( m \in \mathbb{N}^* \)

\[
\partial_t^\alpha u(t) = \frac{1}{\Gamma(m-\rho)} \int_0^t (t-s)^{m-1-\rho} u^{(m)}(s) \, ds.
\]

(2)

Equation (1) represents the heat equation (resp. wave) when \( \alpha = 1 \) (resp. \( \alpha = 2 \)). We focus in this note on the cases when \( 0 < \alpha < 1 \) and \( 1 < \alpha < 2 \), which refer, respectively, to time-fractional diffusion and diffusion-wave equations.

The initial conditions are given by, for all \( \mathbf{x} \in \Omega \):

\[
\begin{align*}
  u(\mathbf{x}, 0) &= u^0(\mathbf{x}), & \text{when } & 0 < \alpha < 1, \\
  u(\mathbf{x}, 0) &= u^0(\mathbf{x}) & \text{and} & u_t(\mathbf{x}, 0) = u^1(\mathbf{x}), & \text{when } & 1 < \alpha < 2,
\end{align*}
\]

(3, 4)

where \( u^0 \) and \( u^1 \) are given functions defined on \( \Omega \). Homogeneous Dirichlet boundary conditions are given by

\[
u(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in \partial \Omega \times (0, T).
\]

(5)

GDM is a generic framework for the discretization and numerical analysis of different kinds of partial differential equations. It has been developed recently in [5] and it includes, for instance, conforming and nonconforming finite element, mixed finite element, hybrid mixed mimetic family, some Multi-Point Flux approximation finite volume schemes, and some discontinuous Galerkin schemes. It has been applied successfully to approximate numerous models, see for instance [4,6,7] and references therein.

The above model is known to describe well the anomalous diffusion phenomena in highly heterogeneous aquifers and complex viscoelastic materials, see [9]. Several numerical schemes, based on the use of different numerical methods in space and several discretizations in time, have been developed to approximate (1)–(5). The aim of these different discretizations in time is to get high convergence rate in time, see a list of some of these discretizations in [10]. As space discretization, finite difference, spectral, finite element, discontinuous Galerkin, finite volume, mixed finite element, and finite volume element methods are used respectively in [16], [13], [10,9,12], [14], [3,15], [17], and [11]. Some of these methods are limited to one or two space dimensions, e.g., [11,12,16,15,17]. However, “the study on the diffusion-wave equation is scarce”, as mentioned in [10, p. 148]. To the best of our knowledge, we are not aware with any existing work on GDM for fractional partial differential equations. We organized this note as follows. In Section 2, we provide some preliminaries concerning the space and time discretizations. In particular, we derive the required properties, summarized in Lemma 2.1, on the time discretization in order to present the convergence analysis of GSs (Gradient Schemes) for time fractional partial differential equations. In Section 3, we present the GS of Definition 3.1 for the time-fractional diffusion equation along with a proof of a convergence order in \( L^\infty(\Omega^2) \)-norm. We also state the new a priori estimate (30) of Remark 1. Some particular schemes that are encompassed by the GS of Definition 3.1 are described in Remark 2. Section 4 is devoted to the analysis of the GS of Definition 4.1 as an approximation for time-fractional diffusion-wave equation along with a proof of a convergence order in several discrete norms. In Remark 4, we quote another possible GS for time-fractional diffusion-wave equations, which recovers the SUSHI scheme of [1] and a Finite Element scheme formulated (but without convergence results) in [12]. In particular, we state in Remark 4 that the conditional convergence proved in [1] can be improved to be unconditional, which is new. This result together with the a priori estimate (30) of Remark 1 and a convergence analysis of the GS of Definition 3.1 in a discrete norm of \( L^\infty(H^1_0(\Omega)) \) will be addressed thoroughly in future papers.
2. Discretization in time and space

**Definition 2.1 (Definition of an approximate gradient discretization, cf. [5]).** Let \( \Omega \) be an open domain of \( \mathbb{R}^d \), where \( d \in \mathbb{N}^* \). An approximate gradient discretization \( D \) is defined by \( D = (\mathcal{X}_D, h_D, \Pi_D, \nabla_D) \), where

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

Then the **coercivity** of the discretization is measured through the constant \( C_D \) given by:

\[
C_D = \max_{v \in \mathcal{X}_D \setminus \{0\}} \frac{\| \Pi_D v \|_{L^2(\Omega)}}{\| \nabla_D v \|_{L^2(\Omega)^d}}.
\]

This yields the following Poincaré inequality, for all \( v \in \mathcal{X}_D \):

\[
\| \Pi_D v \|_{L^2(\Omega)} \leq C_D \| \nabla_D v \|_{L^2(\Omega)^d}.
\]  

The **strong consistency** of the discretization is measured through the interpolation error function \( S_D : H^1_0(\Omega) \to [0, +\infty) \) defined by, for all \( \varphi \in H^1_0(\Omega) \):

\[
S_D(\varphi) = \min_{v \in \mathcal{X}_D} \left( \| \Pi_D v - \varphi \|_{L^2(\Omega)}^2 + \| \nabla_D v - \nabla \varphi \|_{L^2(\Omega)^d}^2 \right)^{1/2}.
\]

The **dual consistency** of the discretization is measured through the conformity error function \( W_D \) defined on \( H_{\text{div}}(\Omega) \) by

\[
W_D(\varphi) = \max_{u \in \mathcal{X}_D \setminus \{0\}} \frac{1}{\| \nabla_D u \|_{L^2(\Omega)^d}} \left| \int_{\Omega} (\nabla_D u(\mathbf{x}) \cdot \varphi(\mathbf{x}) + \Pi_D u(\mathbf{x}) \text{div} \varphi(\mathbf{x})) d\mathbf{x} \right|.
\]

The discretization of \([0, T]\) is performed with a constant time step \( k = \frac{T}{N+1} \), where \( N \in \mathbb{N}^* \), and we shall denote \( t_n = nk \), for \( n \in [0, N + 1] \). We consider the operator \( \tilde{\partial}_t \) of the discrete temporal derivative \( \partial_t u^n = \frac{u^n - u^{n-1}}{k} \), and we denote by \( v^{n+\frac{1}{2}} \) the mean value \( \frac{v^{n+1} + v^n}{2} \).

Throughout this paper, the letter \( C \) stands for a positive constant independent of the parameters of the space and time discretizations.

The schemes we want to present for the diffusion and diffusion-wave equations are based on the following approximation for the fractional derivative \( \tilde{\partial}_t^\beta \varphi \) with \( 0 < \beta < 1 \) (see [5, (4.1)-(4.2), p. 836] and references therein):

\[
\tilde{\partial}_t^\beta \varphi(t_n+1) = \sum_{j=0}^n k \lambda_j^{n+1} \tilde{\partial}_t^1 \varphi(t_{j+1}) + \Upsilon_{n+1}^t(\varphi),
\]

where

\[
\lambda_j^{n+1} = \frac{(n - j + 1)^{1-\beta} - (n - j)^{1-\beta}}{k^\beta \Gamma(2 - \beta)}
\]

and

\[
|\Upsilon_{n+1}^t(\varphi)| \leq C k^{2-\beta} \| \varphi \|_{C^2([0,T])}.
\]

The following properties are either proved in [5] or can be justified easily:

**Lemma 2.1 (Properties of the coefficients \( \lambda_j^{n+1} \)).** For any \( n \in [0, N] \) and for any \( j \in [0, n] \), let \( \lambda_j^{n+1} \) be defined as in (10) where \( 0 < \beta < 1 \). The following properties hold:

\[
k^{-\beta} \frac{1}{\Gamma(2 - \beta)} = \lambda_n^{n+1} > \lambda_{n-1}^{n+1} > \ldots > \lambda_0^{n+1},
\]

\[
\lambda_j^{n+1} \geq \lambda_0 = \frac{T^{-\beta}}{\Gamma(1 - \beta)}, \quad \forall j \in [0, n].
\]
\[ k \sum_{n=1}^{N} (\lambda_{n+1}^j - \lambda_0^j) \leq \frac{k^{1-\beta}}{\Gamma(2-\beta)}, \]  
(14)

and

\[ \sum_{j=0}^{n} k_{j+1} \leq \frac{T^{1-\beta}}{\Gamma(2-\beta)}. \]  
(15)

**Proof.** For the sake of completeness, we give a brief proof for Lemma 2.1. The property (12) stems from the fact that the function \( s \mapsto (s + 1)^{1-\beta} - s^{1-\beta} \) is a decreasing function for \( s > 0 \). The lower bound (13) can be deduced from the fact that \( \lambda_{n+1}^j \geq \lambda_0^j \) (see (12)) and \( \lambda_{n+1}^j = \frac{1}{k^{\beta}(1 - \beta)} \int_{j/n}^{(j+1)/n} s^{\beta} - s \, ds \). This gives \( \lambda_{n+1}^j \geq \frac{C_{\beta}}{k^{\beta}(1 - \beta)} \geq \frac{T^{1-\beta}}{\Gamma(2-\beta)} \). To prove estimate (14), we remark that

\[ k \sum_{n=1}^{N} (\lambda_{n+1}^j - \lambda_0^j) = k \sum_{n=1}^{N} \frac{d_{n-1,\beta} - d_{n,\beta}}{k^{\beta} \Gamma(2-\beta)} = \frac{k(d_{0,\beta} - d_{N,\beta})}{k^{\beta} \Gamma(2-\beta)} \leq \frac{k^{1-\beta} d_{0,\beta}}{\Gamma(2-\beta)}. \]  
(16)

where we have denoted

\[ d_{n-1,\beta} = \lambda_{n+1}^j k^{\beta} \Gamma(2-\beta) = (n-j+1)^{1-\beta} - (n-j)^{1-\beta}. \]  
(17)

Since \( d_{0,\beta} = 1 \), then (16) implies the desired estimate (14). Using the expression (10) yields \( \sum_{n=1}^{N} k_{j+1} \leq \frac{T^{1-\beta}}{\Gamma(2-\beta)} \). This is exactly the desired estimate (15). \( \square \)

The results (9)–(15) will be applied in Sections 3 and 4 with respectively the choices \( \beta = \alpha \) and \( \beta = \alpha - 1 \).

3. **Formulation of a GS for time-fractional diffusion problem and statement of an \( L^\infty(L^2) \)-error estimate**

In this section, we apply the GDM to time-fractional diffusion problem (1) (when \( 0 < \alpha < 1 \), (3), and (5).

**Definition 3.1 (Formulation of a GS for time-fractional diffusion problem).** Assume that \( 0 < \alpha < 1 \). Let \( D = (\mathcal{X}_D, h_D, \Pi_D, \mathcal{V}_D) \) be an approximate gradient discretization in the sense of Definition 2.1 and \( \lambda_{n+1}^j \) be defined as in (10) where \( \beta = \alpha \). We define the following GS as an approximation for problem (1), (3), and (5): Find \( u_D^0 \in \mathcal{X}_D \) such that

\[ \left( \mathcal{V}_D u_D^0, \mathcal{V}_D v \right)_{L^2(\Omega)^d} = - \left( \Delta u_D^0, \Pi_D v \right)_{L^2(\Omega)}, \quad \forall v \in \mathcal{X}_D. \]  
(18)

and for any \( n \in \mathbb{N} \), find \( u^{n+1}_D \in \mathcal{X}_D \) such that, for all \( v \in \mathcal{X}_D \)

\[ \sum_{j=0}^{n} \frac{\lambda_{j+1}}{k} \left( \Pi_D (u^{j+1}_D - u^j_D), \Pi_D v \right)_{L^2(\Omega)} + \left( \mathcal{V}_D u^{n+1}_D, \mathcal{V}_D v \right)_{L^2(\Omega)^d} = (f(t_{n+1}), v)_{L^2(\Omega)}. \]  
(19)

**Theorem 3.1 (\( L^\infty(L^2) \)-error estimate for (18)–(19)).** Let \( \Omega \) be an open bounded connected subset of \( \mathbb{R}^d \), where \( d \in \mathbb{N}^* \). Let \( \alpha \in (0, 1) \) and \( \delta^\alpha u \) be the Caputo derivative given by (2) with \( m = 1 \). Assume that the solution to the fractional diffusion problems (1), (3), and (5) satisfies \( u \in C^2([0, T]; H^2(\Omega)) \). Let \( D = (\mathcal{X}_D, h_D, \Pi_D, \mathcal{V}_D) \) be an approximate gradient discretization in the sense of Definition 2.1 and \( \lambda_{n+1}^j \) be defined as in (10) where \( \beta = \alpha \). Then, there exists a unique solution \( u_D^N \in \mathcal{X}_D \) to the scheme (18)–(19) and the following \( L^\infty(L^2) \)-error estimate holds, for all \( n \in \mathbb{N} \)

\[ \| \Pi_D u^D_D - u(t_n) \|_{L^2(\Omega)} \leq C \left( (1 + C_D)E_{\mathcal{D}}^{\alpha} \| u \|_{C^2([0, T]; L^2(\Omega))} \right), \]  
(20)

where for any function \( \Psi \in C([0, T]; H^2(\Omega)) \), we denote by

\[ E_D^{-1}(\Psi) = \max_{j \in \{0, 1\}} \max_{n \in \{j, N+1\}} E_D(\delta^j \Psi(t_n)) \]  
(21)

and, for any \( \psi \in H^2(\Omega) \), \( E_D(\psi) = \max (W_D(\nabla \psi) + 2S_D(\psi), C_D W_D(\nabla \psi) + (C_D + 1)S_D(\psi)). \)
Sketch of the proof of Theorem 3.1. The existence and uniqueness for schemes (18)–(19) stem from the fact that \( \| \nabla_D \cdot \|_{L^2(\Omega)^d} \) is a norm on \( X_D,0 \). To prove error estimate (20), we compare the solution \((u^n_D)_{n\in[0,N+1]}\) of (18)–(19) with the solution defined by: for any \( n \in \{0, N+1\} \), find \( \tilde{X}_D^n \in X_D,0 \) such that
\[
(\nabla_D \tilde{X}_D^n, \nabla_D v)_{L^2(\Omega)} = - (\Delta u(t_n), \Pi_D D u(t_n))_{L^2(\Omega)}, \quad \forall v \in X_D,0.
\] (22)

**Step 1.** (Comparison between \( u \) and \( \tilde{X}_D^n \)). It is shown in [5, Theorem 3.2, pages 52–53] that
\[
\|u(t_n) - \Pi_D \tilde{X}_D^n\|_{L^2(\Omega)} + \|\nabla(D)u(t_n) - \nabla(D)\tilde{X}_D^n\|_{L^2(\Omega)^d} \leq 2E_D(u(t_n)) \leq 2E_D(u).
\] (23)

Acting \( \partial^1 \) on both sides of (22), we deduce that \( \partial^1 \tilde{X}_D^n \) satisfies the same scheme (22), but with \( \partial^1 u(t_n) \) instead of \( u(t_n) \) in the right-hand side. We are therefore able to apply (23) to get
\[
\|\partial^1 u(t_n) - \Pi_D \partial^1 \tilde{X}_D^n\|_{L^2(\Omega)} + \|\nabla(D)\partial^1 u(t_n) - \nabla(D)\partial^1 \tilde{X}_D^n\|_{L^2(\Omega)^d} \leq 2E_D(\partial^1 u(t_n)) \leq 2E_D(u).
\] (24)

**Step 2.** (Comparison between \( \tilde{X}_D^n \) and \( u^n_D \)). Let us set \( \eta^n_D = u^n_D - \tilde{X}_D^n \). Taking \( n = 0 \) in (22) and comparing the result with \( \frac{18}{} \) (recall that \( u(0) = u^0 \), subject of (3)) yield \( \eta^n_D = 0 \). In addition to this, writing (22) in the level \( n+1 \), subtracting the result from (19), and using (9) together with (1) to get
\[
\sum_{j=0}^{n} \lambda_j^{n+1} (\Pi_D(\eta_{j}^{n+1} - \eta_{j}^{n}), \Pi_D D v)_{L^2(\Omega)} + \|\nabla(D)\eta_{j}^{n+1} - \nabla(D)\eta_{j}^{n}\|_{L^2(\Omega)^d} = (S^{n+1}, \Pi_D D v)_{L^2(\Omega)}.
\] (25)

where \( S^{n+1} = \sum_{j=0}^{n} \lambda_j^{n+1} \|u(t_{j+1}) - \Pi_D \eta_{j}^{n}\|_{L^2(\Omega)^d} + D^{n+1} \). Using the triangle inequality, estimates of \( \|\eta^{n+1}_{j}\| \) and \( \sum_{j=0}^{n} \lambda_j^{n+1} \) given respectively in (11) and (15), and estimate (24) yield
\[
S = \max_{n=0}^{N} \|S^{n+1}\|_{L^2(\Omega)} \leq C \left( 2E_D(u) + k^{2-\alpha} \|u\|_{C^2(0,T;L^2(\Omega)^d)} \right).
\] (26)

Taking \( v = \eta^{n}_{j} \) in (25), re-ordering the sum in the result, using twice inequality \( 2xy \leq x^2 + y^2 \), using the fact that \( \lambda_j^{n+1} - \lambda_j^{n+1} > 0 \) (this stems from (12)) and applying the Poincaré inequality (6) imply that
\[
\lambda_j^{n+1} \|\Pi_D \eta_{j}^{n+1}\|_{L^2(\Omega)^d}^2 + \|\nabla(D)\eta_{j}^{n+1}\|_{L^2(\Omega)^d}^2 \leq \sum_{j=1}^{n} (\lambda_j^{n+1} - \lambda_{j-1}^{n+1}) \|\Pi_D \eta_{j}^{n}\|_{L^2(\Omega)}^2 + C_D(S)^2.
\] (27)

We prove now, by mathematical induction on \( n \) that, for all \( n \in [1,N+1]\)
\[
\|\Pi_D \eta^n\|_{L^2(\Omega)}^2 \leq \frac{C_D S}{\lambda_0},
\] (28)

where \( \lambda_0 \) is given in (13). Taking \( n = 0 \) in (27) yields (28) when \( n = 1 \). Assume that estimate (28) holds for \( n \leq m \) and prove it for \( n = m + 1 \). Taking \( n = m \) in (27) and using (12) and the fact that \( -\lambda_{m+1} < -\lambda_0 \) yield
\[
\lambda_m^{m+1} \|\Pi_D \eta_{m+1}^m\|_{L^2(\Omega)^d}^2 \leq \sum_{j=1}^{m} (\lambda_j^{m+1} - \lambda_{j-1}^{m+1}) \|\Pi_D \eta_{j}^m\|_{L^2(\Omega)}^2 + C_D(S)^2 \leq \lambda_m^{m+1} \left( \frac{C_D S}{\lambda_0} \right)^2.
\] (29)

Gathering now (28), (26), the triangle inequality, and (23) yields the desired estimate (20). \( \square \)

**Remark 1** *(An a priori estimate and an error estimate in a discrete \( L^\infty(H^1_0) \)-norm).* For the sake of simplicity of this note, we only presented and proved an \( L^\infty(L^2) \)-error estimate given in Theorem 3.1. The proof of the \( L^\infty(L^2) \)-error estimate is based on the a priori estimate (28) for the solutions to the discrete problem (25). However, we are able to prove the following new \( L^\infty(H^1_0) \)-estimate
\[
\|\nabla_D \eta^n_D\|_{L^2(\Omega)^d} \leq \left( (C_D)^2 + \frac{1}{\lambda_0} \right) (S)^2.
\] (30)

Estimate (30) will help us to derive and prove a convergence rate in a discrete \( L^\infty(H^1_0) \)-norm. The proof of the a priori estimate (30) is based on additional techniques and on another choice (instead of \( v = \eta^{n+1}_D \)) for the test function \( v \) in (25). This result along with a proof for the convergence of the family of the discrete solutions towards the solution of a weak formulation will be dealt with in [2].

**Remark 2** *(Some particular schemes encompassed by GS (18)–(19)).* The following particular schemes are encompassed by GS (18)–(19):
The fully discrete Linear Finite Element Scheme [9, (4.7), page 836], when considering only one time fractional derivative instead of multi-term time fractional derivatives. The discrete gradient $\nabla_D$ and the linear reconstruction $\Pi_D$ involved in (18)–(19) in this case are the gradient $\nabla$ and the interpolation operator. However, it is possible to extend the present results to the case of multi-term time fractional derivatives. This will be detailed in a future work.

The discrete scheme of [9] (see previous item), but with Finite Element spaces given by piecewise polynomials of degree less than or equal to a given natural number $l \geq 2$.

The SUSHI scheme treated in [3]. The operators $\nabla_D$ and $\Pi_D$ involved in (18)–(19) in this case are explicitly given in [8].

4. Formulation of a GS for the time-fractional diffusion-wave problem and statement of its convergence results

In this section, we apply the GDM to the time-fractional diffusion-wave problems (1) (when $1 < \alpha < 2$), (4), and (5). Taking $t = t_{n+1}$ in (1) yields $\partial_t^\alpha u(t_{n+1}) - \Delta u(t_{n+1}) = f(t_{n+1})$, which is equivalent to the system of two equations

$$\partial_t^{\alpha-1} \Pi(t_{n+1}) - \Delta u(t_{n+1}) = f(t_{n+1}) \quad \text{and} \quad \Pi = u_t.$$  

(31)

This system is used, for instance, in [16] to establish a finite difference scheme in one space dimension. Such a scheme is based on a Crank–Nicolson method.

The scheme we want to present in this section is based on two approximations in time:

- the approximation of $\partial_t^{\alpha-1} \Pi(t_{n+1})$, which is given in (9):

$$\partial_t^{\alpha-1} \Pi(t_{n+1}) = \sum_{j=0}^n \lambda_j^{n+1} \partial_t \Pi(t_{j+1}) + T_1^{n+1}(\Pi).$$  

(32)

- the approximation of $\Pi(t_{n+1}) = u_t(t_{n+1})$, which is given by $\frac{3u(t_{n+1}) - 4u(t_n) + u(t_{n-1})}{2k}$. The order of this approximation is $k^2$.

**Definition 4.1 (Definition of a GS for the time-fractional diffusion-wave equation).** Assume that $1 < \alpha < 2$. Let $D = (X_D, h_D, \Pi_D, \nabla_D)$ be an approximate gradient discretization in the sense of Definition 2.1 and $\lambda_j^{n+1}$ be defined as in (10) where $\beta = \alpha - 1$. We define the following GS as an approximation for problems (1), (4), and (5):

- discretization of initial conditions: find $u_0^D, \Pi_0^D \in X_{D,0}$ such that, for all $v \in X_{D,0}$

$$\left(\nabla_D u_0^D, v_D \right)_{L^2(\Omega)} - \left(\Delta u_0, \Pi_D v_D \right)_{L^2(\Omega)} = - \left(\Delta u_0, \Pi_D v_D \right)_{L^2(\Omega)};$$  

(33)

- discretization of equation (1): for any $n \in [0, N]$, find $u_0^{n+1}, \Pi_0^{n+1} \in X_{D,0}$ such that, for all $v \in X_{D,0}$

$$\sum_{j=0}^n \lambda_j^{n+1} \left(\Pi_D(\Pi_j^{n+1} - \Pi_0^D), \Pi_D v_D \right)_{L^2(\Omega)} + \left(\nabla_D u_0^{n+1}, v_D \right)_{L^2(\Omega)} = \left(f(t_{n+1}), \Pi_D v_D \right)_{L^2(\Omega)};$$  

(34)

$$\Pi_0^{n+1} = \partial_t u_0^D \quad \text{and} \quad \Pi_0^{n+1} = \frac{1}{2k} \left(3u_0^{n+1} - 4u_0^D + u_0^{n-1} \right), \quad \forall n \in [1, N].$$  

(35)

**Theorem 4.1 (Error estimates for scheme (33)–(35)).** Let $\Omega$ be an open bounded connected subset of $\mathbb{R}^d$, where $d \in \mathbb{N}^*$. Let $\alpha \in (1, 2)$ and $\partial_t^\alpha$ be the Caputo derivative given by (2) with $m = 2$. Assume that the solution to problems (1), (4), and (5) satisfies $u \in C^2([0, T]; \mathbb{R}^d \times \mathbb{R}^d)$. Let $D = (X_D, h_D, \Pi_D, \nabla_D)$ be an approximate gradient discretization in the sense of Definition 2.1, and $\lambda_j^{n+1}$ be defined as in (10) where $\beta = \alpha - 1$. Then, there exists a unique solution $(u_0^D, \Pi_0^D)_{n=0}^{N+1} \in X_{D,0}^{N+2} \times X_{D,0}^{N+2}$ to (33)–(35), and the following error estimates hold:

- an estimate on the gradient approximation, i.e. $L^\infty(0, T; H^1(\Omega))$-estimate. For any $n \in [0, N + 1]$

$$\|\nabla_D u_0^D - \nabla u(t_n)\|_{L^2(\Omega)}^{d} \leq C \left(\varepsilon_D^k(u_t) + \varepsilon_D^k(u) + (C_D + 1)k^{3-\alpha} \|u\|_{C^2(0, T; \mathbb{R}^d)}\right),$$  

(36)

- an $H^1_0(0, T; L^2(\Omega))$-estimate

$$\left(\sum_{n=0}^{N+1} k\|\Pi_D(\Pi_0^D - u_t(t_n))\|_{L^2(\Omega)}^{d} \right)^{1/2} \leq C \left(\varepsilon_D^k(u_t) + (C_D + 1)k^{3-\alpha} \|u\|_{C^2(0, T; \mathbb{R}^d)}\right),$$  

(37)

where $\varepsilon_D^k$ is defined in (21).
To prove Theorem 4.1, we first give a technical lemma whose proof will be detailed in a future paper and an *a priori* estimate result.

**Lemma 4.1.** For any \( (\eta^n_D)_{n=0}^{N+1} \subset \mathcal{L}_{D,0}^{N+2} \), the following inequality holds, for all \( n \in [1, N] \)

\[
\left( \nabla_D \eta^{n+1}_D, \nabla_D \left( 3 \eta^n_D - 4 \eta^n_D + \eta^{n-1}_D \right) \right)_{L^2(\Omega)^d} \geq \mathbb{E}^{n+1} - \mathbb{E}^n,
\]

where \( \mathbb{E}^{n+1} = | \nabla_D (\eta^{n+1}_D - \eta^n_D) |^2 \|_{L^2(\Omega)^d} + \frac{3}{2} \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d}^2 - \frac{1}{2} \| \nabla_D \eta^n_D \|_{L^2(\Omega)^d}^2 \). In addition to this,

\[
\mathbb{E}^{n+1} \geq \frac{1}{2} \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d}^2.
\]

**Lemma 4.2 (Discrete a priori estimate).** We assume that there exists \( (\eta_D^n, \pi_D^n)_{n=0}^{N+1} \subset \mathcal{L}_{D,0}^{N+2} \times \mathcal{L}_{D,0}^{N+2} \) such that, for all \( v \in \mathcal{L}_{D,0}^1 \) and for all \( n \in [1, N] \)

\[
\sum_{j=0}^n \lambda_j^{n+1} \left( \Pi_D (\eta^{j+1}_D - \eta^{j}_D), \Pi_D v \right)_{L^2(\Omega)} + \left( \nabla_D \eta^{n+1}_D, \nabla_D v \right)_{L^2(\Omega)^d} = (S^{n+1}, \Pi_D v)_{L^2(\Omega)},
\]

where, for all \( n \in [0, N] \), \( S^{n+1} \in \mathcal{L}^1(\Omega) \), and \( \eta_D^0 = \eta_D^1 = 0 \). Let \( S \) be given by \( S = \max_{n=0}^N \| S^{n+1} \|_{L^2(\Omega)} \).

Then the following estimate holds:

\[
\max_{n=0}^N \| \nabla_D \eta_D^n \|_{L^2(\Omega)^d} + \left( \sum_{n=0}^{N+1} k \| \Pi_D \eta^n_D \|_{L^2(\Omega)}^2 \right)^{\frac{1}{2}} \leq C S,
\]

where \( S = S + \max_{n=0}^N \| \nabla_D (\eta^{n+1}_D - \frac{3\mathbb{E}^{n+1} - 4 \| \eta^n_D \|_{L^2(\Omega)^d}}{2k} \| \eta^n_D - \eta^{n-1}_D \|_{L^2(\Omega)^d}^2 + \| \nabla_D (\eta^{n+1}_D - \eta^{n-1}_D) \|_{L^2(\Omega)^d}^2.)
\]

**Sketch of the proof of Lemma 4.2.** Taking \( v = \eta_D^{n+1} \) in (40), reordering the sum in the result, and using the inequality \( 2xy \leq x^2 + y^2 \) and the fact that \( \lambda_j^{n+1} - \lambda_{j-1}^{n+1} > 0 \) imply that

\[
\lambda_n^{n+1} \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)}^2 + 2 \left( \nabla_D \eta^{n+1}_D, \nabla_D \left( \frac{3 \eta^{n+1}_D - 4 \eta^n_D + \eta^{n-1}_D}{2k} \right) \right)_{L^2(\Omega)^d}
\]

\[
\leq \sum_{j=1}^n (\lambda_j^{n+1} - \lambda_{j-1}^{n+1}) \| \Pi_D \eta^j_D \|_{L^2(\Omega)}^2 + 2S \left( \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)} + \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d} \right).
\]

Summing (42) over \( n \in [1, J-1] \), where \( J \in [2, N+1] \), and using (38)-(39), the fact that \( \sum_{n=1}^J \sum_{j=1}^n (\lambda_j^{n+1} - \lambda_{j-1}^{n+1}) \| \Pi_D \eta^j_D \|_{L^2(\Omega)}^2 \leq \sum_{n=1}^J \sum_{j=2}^n (\lambda_j^{n+1} - \lambda_{j-1}^{n+1}) \| \Pi_D \eta^j_D \|_{L^2(\Omega)}^2 \) and (14) to get

\[
k \sum_{n=1}^J \lambda_n^{n+1} \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)}^2 + \frac{1}{2} \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d}^2 \leq k \sum_{n=1}^J \sum_{j=2}^n (\lambda_j^{n+1} - \lambda_{j-1}^{n+1}) \| \Pi_D \eta^j_D \|_{L^2(\Omega)}^2
\]

\[
+ 2kS \sum_{n=1}^J \left( \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)} + \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d} \right) + C \left( \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)}^2 + \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d} \right).
\]

Re-ordering the sum to get

\[
\sum_{n=2}^J \sum_{j=2}^n (\lambda_j^{n+1} - \lambda_{j-1}^{n+1}) \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)}^2 = \sum_{n=1}^J (\lambda_{n+1}^2 - \lambda_n^2) \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)}^2,
\]

gathering this with (43), and the fact that \( \lambda_{n+1}^2 = \lambda_n^2 \) imply that

\[
k \sum_{n=1}^J \lambda_n^2 \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)}^2 + \frac{1}{2} \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d}^2 \leq 2kS \sum_{n=1}^J \left( \| \Pi_D \eta^{n+1}_D \|_{L^2(\Omega)}^2 + \| \nabla_D \eta^{n+1}_D \|_{L^2(\Omega)^d} \right). \]
\begin{equation}
    k\lambda_0 \sum_{n=1}^{j-1} \| \Pi_D \bar{\eta}_D^{n+1} \|^2_{L^2(\Omega)} + \| \nabla_D \eta_D^n \|^2_{L^2(\Omega)^d} \leq \sum_{n=2}^{j-1} k\| \nabla_D \eta_D^n \|^2_{L^2(\Omega)^d} + C\Lambda,
\end{equation}

where $\Lambda = \| \Pi_D \bar{\eta}_D^0 \|^2_{L^2(\Omega)} + \| \nabla_D \eta_D^0 \|^2_{L^2(\Omega)^d} + \bar{\mathcal{S}}^2$. Using a discrete version of the Gronwall’s lemma, (45) implies that $\| \nabla_D \eta_D^n \|^2_{L^2(\Omega)^d}$, for all $n \in [0, N + 1]$, and $\sum_{n=0}^{N+1} k\| \Pi_D \bar{\eta}_D^n \|^2_{L^2(\Omega)}$ are bounded above by $C\Lambda$. Let us now find an upper bound for $\Lambda$. Taking $n = 0$ in (40) and replacing $v$ by $\bar{\eta}_D$, in the result yield

\begin{equation}
    \lambda_0 \| \Pi_D \bar{\eta}_D^0 \|^2_{L^2(\Omega)} + \frac{2}{k} \| \nabla_D \eta_D^0 \|^2_{L^2(\Omega)^d} = (S^1, \Pi_D v)_{L^2(\Omega)} + 2 \left( \nabla_D \eta_D^0, \nabla_D \left( \partial^1 \eta_D^0 - \bar{\eta}_D^0 \right) \right)_{L^2(\Omega)^d}.
\end{equation}

Using Young’s inequality (46) implies that $\Lambda \leq C\bar{\mathcal{S}}^2$. This yields the desired estimate (41).

**Sketch of the proof of Theorem 4.1.** The existence and uniqueness for schemes (33)–(35) stem from the fact that $\| \nabla_D \cdot \|^2_{L^2(\Omega)^d}$ is a norm on $X_{D,0}$. To prove error estimates (36)–(37), we compare the solution $(u^n_D, \bar{\eta}_D^n)_{n \in [0, N + 1]}$ with the solutions of (22) and the following auxiliary problem: for any $n \in [0, N + 1]$, find $\Upsilon_D^n \in X_{D,0}$ such that, for all $v \in X_{D,0}$

\begin{equation}
    \left( \nabla_D \Upsilon_D^n, \nabla_D v \right)_{L^2(\Omega)^d} = - \left( \Delta u^n_D(t_n), \Pi_D v \right)_{L^2(\Omega)}.
\end{equation}

**Step 1.** (Comparison of $u(t_n)$ with $\Xi_D^n$ and $u(t_n)$ with $\Upsilon_D^n$). The same reasoning quoted to obtain (23)–(24) can also be applied on the scheme (47) to get

\begin{equation}
    \| u^n_D(t_n) - \Pi_D \Upsilon_D^n \|^2_{L^2(\Omega)} + \| \partial^1 (u(t_n) - \Pi_D \Upsilon_D^n) \|^2_{L^2(\Omega)} \leq 2E^k_D(u).
\end{equation}

**Step 2.** (Comparison of $\Xi_D^n$ with $u^n_D$ and $\Upsilon_D^n$ with $\bar{\eta}_D^n$). We set $\eta_D^n = u^n_D - \Xi_D^n$, and $\Upsilon_D^n = \Xi_D^n - \eta_D^n$. Taking $n = 0$ in schemes (22) and (47) and comparing the results with (33) yield $\eta_D^0 = \Upsilon_D^0 = 0$. In addition to this, writing (22) in the level $n + 1$, subtracting the result from (34), and using (31)–(32) to get

\begin{equation}
    \sum_{j=0}^{n} \lambda_j^{n+1} \left( \Pi_D (\bar{\eta}_D^{j+1} - \bar{\eta}_D^j), \Pi_D v \right)_{L^2(\Omega)} + \left( \nabla_D \eta_D^{n+1}, \nabla_D v \right)_{L^2(\Omega)^d} = \left( S^{n+1}, \Pi_D v \right)_{L^2(\Omega)},
\end{equation}

where $S^{n+1} = \sum_{j=0}^{n} \lambda_j^{n+1} \partial^1 (u(t_{j+1}) - \Pi_D \Upsilon_D^{j+1}) + \bar{\mathcal{S}}^{n+1}$. Applying a priori estimate (41) yields

\begin{equation}
    \sum_{n=0}^{N+1} \| \nabla_D \eta_D^n \|^2_{L^2(\Omega)^d} + \left( \sum_{n=0}^{N+1} k\| \Pi_D \bar{\eta}_D^n \|^2_{L^2(\Omega)} \right)^{\frac{1}{2}} \leq C\bar{\mathcal{S}}.
\end{equation}

Using estimates of the $\eta_D^n$ and $k\sum_{j=0}^{n} \lambda_j^{n+1}$ given respectively in (11) and (15) and estimate (48) yield

\begin{equation}
    S = \max_{n=0}^{N} \| S^{n+1} \|^2_{L^2(\Omega)} \leq C \left( E^k_D(u) + k^3 \| u \|_{C^3([0,T];L^2(\Omega))} \right).
\end{equation}

Using (35) implies that $\eta_D^1 - \partial^1 \eta_D^1 = -\Upsilon_D^1 + \partial^1 \Xi_D^1$. On the other hand, from (22) and (47), we deduce that

\begin{equation}
    \left( \nabla_D \left( \partial^1 \Xi_D^1 - \Upsilon_D^1 \right), \nabla_D v \right)_{L^2(\Omega)^d} = - \left( \Delta \left( \partial^1 u(t_1) - \frac{u(t_1) + u(t_0)}{2} \right), \Pi_D v \right)_{L^2(\Omega)}, \quad \forall v \in X_{D,0}.
\end{equation}

Taking $v = \partial^1 \Xi_D^1 - \Upsilon_D^1$ in (52), using the Cauchy–Schwarz inequality together with (6) and a convenient Taylor expansion imply that

\begin{equation}
    \left\| \nabla_D \left( \eta_D^1 - \partial^1 \eta_D^1 \right) \right\|_{L^2(\Omega)^d} \leq C D^2 \| u \|_{C^3([0,T];C^2(\Omega))}. \quad \text{In the same manner, we can prove that}
\end{equation}

\begin{equation}
    \left\| \nabla_D \left( \eta_D^{n+1} - \frac{1}{2k} (3\eta_D^{n+1} - 4\eta_D^n + \eta_D^{n-1}) \right) \right\|_{L^2(\Omega)^d} \leq C D^2 \| u \|_{C^3([0,T];C^2(\Omega))}.
\end{equation}

Therefore,

\begin{equation}
    \bar{\mathcal{S}} \leq C \left( E^k_D(u) + (D + 1) k^3 \| u \|_{C^3([0,T];C^2(\Omega))} \right).
\end{equation}

This with estimate (50) and error estimates (23) and (48) imply the desired estimates (36)–(37). \square
Remark 3 (On the convergence order). Assume that there exists $C > 0$ such that following estimates hold (they are satisfied by some important examples of GSs, see [5, Page 53])

\[ C_D \leq C, \]
\[ S_D(\varphi) \leq C h_D \| \varphi \|_{C^2(\Omega)}, \quad \forall \varphi \in C^2(\Omega) \cap H^1_0(\Omega), \]
\[ W_D(\varphi) \leq C h_D \| \varphi \|_{C^1(\Omega)}^d, \quad \forall \varphi \in C^1(\Omega)^d \subset H^1(\Omega). \]

Using the representation $\partial^1 \Psi(t_{n+1}) = \frac{1}{\nu} \int_{t_n}^{t_{n+1}} \Psi(t) \, dt$, and (54)-(55) imply that $\mathbb{E}_D^h(u)$, given by (21), is of order $h_D$. Therefore, under hypotheses (53)-(55), error estimates (20) and (36)-(37) imply that

- Scheme (18)-(19) is of order $k^{2-\alpha} + h_D$ in a discrete $L^\infty(L^2)$-norm;
- Scheme (33)-(35) is of order $k^{3-\alpha} + h_D$ in discrete semi-norms of $L^\infty(H^1)$ and $H^1(L^2)$.

Remark 4 (Another GS for time-fractional diffusion-wave equations). Another possible GS, instead of (33)-(35), for time-fractional diffusion-wave equations, i.e. $1 < \alpha < 2$ in (1), is the following: for any $n \in \{0, N\}$, find $u_D^{n+1} \in \mathcal{X}_{D,0}$ such that for all $v \in \mathcal{X}_{D,0}$

\[
\lambda_n^{n+1} \left( \partial^1 \Pi_D u_D^{n+1}, \Pi_D v \right)_{L^2(\Omega)} + \sum_{j=1}^N \left( \lambda_j^{n+1} - \lambda_j^n \right) \left( \partial^1 \Pi_D u_D^j, \Pi_D v \right)_{L^2(\Omega)} + \left( \nabla_D u_D^{n+1} + \nabla_D v \right)_{L^2(\Omega)} = \left( f^{n+1} + \lambda_0^{n+1} u_0^1, \Pi_D v \right)_{L^2(\Omega)},
\]

where $u_D^0$ is given as in (33).

This scheme is based on a Crank–Nicolson method. In addition to the SUSHI scheme of [1], the Finite Element scheme [12, (3.9), p. 475] is also encompassed by (56). It is possible to show the following convergence result for scheme (56) with $u_D^0$ given by (33), under assumptions (53)-(55):

\[
\| \nabla_D u_D^n - \nabla u(t_n) \|_{L^2(\Omega)} \leq C \left( k^{3-\alpha} + h_D \right) \| u \|_{L^2(0,T; C^2(\Omega))}.
\]

This convergence is unconditional and it is similar to that of (33)-(35), see Remark 3. This improves the conditional convergence proved in [1, Theorem 1, p. 394]. These convergence results will be detailed in [2].

Acknowledgements

The author would like to thank the anonymous referees for their valuable advice and comments that helped not only to improve the paper, but also to open some new perspectives for the present work.

References