The Modified Local Green's Function Method for the solution of the anomalous diffusion equation

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Abstract. The field of fractional calculus is currently gaining momentum in mathematics and has extensive practical applications across several scientific and engineering problems, particularly those that involve nonlocality. This study aims to enhance the discourse surrounding the utilization of numerical techniques for solving problems governed by partial differential equations with fractional time derivatives. To this end, the present work employs an enriched formulation of the Modified Local Green's Function Method (MLGFM) to solve the anomalous diffusion equation in two dimensions. The anomalous, or fractional, diffusion equation presents a time-derivative of non-integer order, in the interval $(0,1]$. When the order of the time-derivative is equal to 1, the classical diffusion equation is recovered, which means that it can be treated as the simplest case of the fractional diffusion equation. To represent the fractional time derivative, the Caputo representation is chosen based on the authors' previous work. The MLGFM is an integral method hybrid of the Finite Element Method (FEM) and the Boundary Element Method (BEM). The method uses the FEM to create discrete projections of the Green's functions and use them as fundamental solutions in BEM formulation. The MLGFM presents high convergence for the potential in the domain, inherited from the FEM, and for the normal flux in the boundary, inherited from the BEM. This paper proposes a trigonometric enrichment based on the Generalized Finite Element technique for the solution of the anomalous diffusion equation. The results are compared with analytical solutions available in the literature.

Keywords: Green's functions, Fractional calculus, Anomalous diffusion

1 Introduction

While the roots of fractional calculus can be traced back to the early days of conventional calculus, it is only in recent times that this particular field of mathematics has attracted significant attention. This growing importance is justified by the various applications of fractional calculus in Engineering, as related in Sun et al. [1] where several applications in Engineering are listed. The fractional calculus is very important, especially when the non-locality is important for the studied phenomena.

This paper deals with the so-called anomalous diffusion equation, where the differential time operator, α, can assume non-integer values in the interval $0 < \alpha \leq 1$. The Caputo representation [2] is chosen to represent the non-integer time operator, based on authors' previous experience [3, 4].

One of the main applications in Civil Engineering is modeling the diffusion of chloride ions in concrete structures. According to Sun et al. [1], given the material porosity, the ideal Fick's law of diffusion is not applicable to describe the diffusion behavior of chloride ion in concrete.

With regard to the formulations of numerical methods in the modeling of problems derived from fractional calculus, one can cite Deng [5], Zheng et al. [6] and Corrêa et al. [3] applying Finite Element formulations, in addition to Katsikadelis [7], Dehghan and Safarpoor [8] and Carrer et al. [2, 9] with Boundary Element applications. In this paper an enriched formulation based on the Modified Local Green's Function Method (MLGFM) [10] is presented.

The MLGFM is an integral hybrid method of the Finite Element Method (FEM) and the Boundary Element

Method (BEM). Its idea is to use the FEM to obtain Green's functions projections and use them as a fundamental solution in BEM formulation. The MLGFM presents good convergence for the primary variables in the domain and for the dual variables in the boundary.

The enrichment technique is based on the Generalized Finite Element Method (GFEM) [11–13], that uses the concepts of the Partition of Unity Method to incorporate a previous acknowledgment about the solution of the problem, enriching the FEM approximation space. In this paper, given the oscillatory nature of the time-dependent answers, a trigonometric enrichment is proposed.

2 The anomalous diffusion equation

The anomalous diffusion equation, for anisotropic media, can be read as:

$$\frac{\partial_{\mathrm{C}}^{\alpha} u}{\partial t^{\alpha}} = D_x \frac{\partial^2 u}{\partial x^2} + D_y \frac{\partial^2 u}{\partial y^2}, \tag{1}$$

where $u = u(\mathbf{x}, t)$ is a scalar field with $\mathbf{x} \in \mathbb{R}^2$, and the variables D_x and D_y are the constant diffusion coefficients in x and y directions, respectively. The time derivative on the left-hand side of Eq. (1), can be written according to Caputo's representation as:

$$\frac{\partial_{\mathrm{C}}^{\alpha} u}{\partial t^{\alpha}} = \frac{1}{\Gamma\left(1-\alpha\right)} \int_0^t \frac{1}{\left(t-\tau\right)^{\alpha}} \frac{\partial u(\mathbf{x},\tau)}{\partial \tau}\, d\tau, \tag{2}$$

where $\Gamma\left(\cdot\right)$ is the Gamma function and $0 < \alpha \leq 1$.

The boundary flux is defined by the following expression:

$$q\left(\bar{\mathbf{x}}, t\right) = D_x \frac{\partial u}{\partial x} n_x + D_y \frac{\partial u}{\partial y} n_y, \qquad \bar{\boldsymbol{x}} \in \Gamma \tag{3}$$

where n_x and n_y are the components of the unit outward normal vector to the boundary, and Γ is the problem boundary associated with the domain Ω.

3 The MLGFM formulation for anomalous diffusion equation

The MLGFM approximates both $u\left(\mathbf{x}, t\right)$ and $q\left(\bar{\mathbf{x}}, t\right)$ at the domain and boundary, respectively. These fields can be approximated as:

$$u\left(\mathbf{x}, t\right) = \mathbf{\Psi}^T\left(\mathbf{x}\right) \mathbf{u}(t), \tag{4}$$

$$q\left(\bar{\mathbf{x}}, t\right) = \mathbf{\Phi}^T\left(\bar{\mathbf{x}}\right) \mathbf{q}(t), \tag{5}$$

where $\mathbf{u}(t)$ is the vector of nodal values of $u\left(\mathbf{x}, t\right)$ at time t, $\mathbf{q}(t)$ is the vector of nodal values of $q\left(\bar{\mathbf{x}}, t\right)$ at time t, $\mathbf{\Psi}(\mathbf{x})$ contains the domain FEM or GFEM shape functions, and $\mathbf{\Phi}(\bar{\mathbf{x}})$ contains the boundary shape functions and needs to respect the trace property, that is:

$$\mathbf{\Phi}(\bar{\mathbf{x}}) = \lim_{\mathbf{x} \to \Gamma} \mathbf{\Psi}(\mathbf{x}). \tag{6}$$

Based on MLGFM approach presented by Corrêa et al. [14] , the integral form of Eq. (1) can be written as:

$$\mathbf{K}\,\mathbf{u}(t) = \mathbf{A}\,\mathbf{q}(t) - \mathbf{M}\,\frac{\partial_{\mathrm{C}}^{\alpha}\mathbf{u}(t)}{\partial t^{\alpha}} \tag{7}$$

where the matrices are defined as:

$$\mathbf{K} = \int_{\Omega} \mathbf{B}^{T}\,\mathbf{D}\,\mathbf{B}\,d\Omega, \tag{8}$$

$$\mathbf{M} = \int_{\Omega} \mathbf{\Psi}^{T}\,\mathbf{\Psi}\,d\Omega, \tag{9}$$

$$\mathbf{A} = \int_{\Gamma} \mathbf{\Phi}^{T}\,\mathbf{\Phi}\,d\Gamma, \tag{10}$$

where:

$$\mathbf{B} = \begin{bmatrix} \frac{\partial \mathbf{\Psi}^{T}}{\partial x} \\ \frac{\partial \mathbf{\Psi}^{T}}{\partial y} \end{bmatrix}, \tag{11}$$

$$\mathbf{D} = \begin{bmatrix} D_x & 0 \\ 0 & D_y \end{bmatrix}. \tag{12}$$

In order to solve the Eq. (7), the variable t in Eq. (2) is substituted for a discrete value, denoted as $t_{n+1} = (n+1)\Delta t$, where Δt represents the chosen time interval, with the constraint $0 \leq t \leq t_{n+1}$. Additionally, it is assumed that u exhibits linear variation between successive time steps. This assumption facilitates the analytical computation of the integral in Eq. (2). So after computing the analytical integral in Eq. (2) the resulting expression is:

$$\left.\frac{\partial_{\mathrm{C}}^{\alpha} u}{\partial t^{\alpha}}\right|_{t=t_{n+1}} = \frac{1}{\Gamma(2-\alpha)\Delta t^{\alpha}}\left[u_{n+1} - u_n + \sum_{j=0}^{n-1} b_{(n,j)}(u_{j+1} - u_j)\right], \tag{13}$$

where $b_{(n,j)} = \dfrac{1}{(n+1-j)^{\alpha-1}} - \dfrac{1}{(n-j)^{\alpha-1}}$.

The Equation (13) can be substituted in Eq. (7) as:

$$\mathbf{K}\,\mathbf{u}_{n+1} = \mathbf{A}\,\mathbf{q}_{n+1} - \frac{1}{\Gamma(2-\alpha)\Delta t^{\alpha}}\,\mathbf{M}\left[\mathbf{u}_{n+1} - \mathbf{u}_n + \sum_{j=0}^{n-1} b_{(n,j)}(\mathbf{u}_{j+1} - \mathbf{u}_j)\right], \tag{14}$$

and this system can be reorganized as:

$$\mathbf{K}_{\text{aux}}\,\mathbf{u}_{n+1} = \mathbf{A}\,\mathbf{q}_{n+1} + \frac{1}{\Gamma(2-\alpha)\Delta t^{\alpha}}\,\mathbf{M}\left[\mathbf{u}_n - \sum_{j=0}^{n-1} b_{(n,j)}(\mathbf{u}_{j+1} - \mathbf{u}_j)\right], \tag{15}$$

with:

$$\mathbf{K}_{\text{aux}} = \mathbf{K} + \frac{1}{\Gamma(2-\alpha)\Delta t^{\alpha}}\,\mathbf{M} \tag{16}$$

The system in Eq. (15) can be solved by applying the boundary conditions similarly to the BEM [2] with the results in the previous time steps acting as a domain source.

4 The Enriched Modified Local Green's Function Method

An enriched version of the MLGFM has already been proposed by Silva et al. [15] based on the Hierarchical Finite Element Method. Here, the enrichment is based on GFEM idea and $u(\mathbf{x})$ is approximated as:

$$\tilde{u}(\mathbf{x}) = \sum_{\alpha\in\mathcal{I}_h} u_\alpha\,\mathcal{N}_\alpha(\mathbf{x}) + \sum_{\alpha\in\mathcal{I}_h^e} \mathcal{N}_\alpha(\mathbf{x}) \sum_{j=1}^{n_\alpha} a_{\alpha j}\,\mathcal{L}_{\alpha j}(\mathbf{x}), \tag{17}$$

where $\mathcal{L}_{\alpha j}$ represents an enrichment function assigned to node $\alpha \in \mathcal{I}_h$, $j \in \{1,\ldots,n_\alpha\}$ denotes the index of the enrichment function at that node, and $\mathcal{I}_h^e \subseteq \mathcal{I}_h$ is the set of GFEM enriched nodes. In this paper all nodes are enriched, so $\mathcal{I}_h^e \equiv \mathcal{I}_h$. Alongside the conventional FE shape functions $\mathcal{N}_\alpha$, there are n_α GFEM shape functions corresponding to each node $\alpha \in \mathcal{I}_h^e$, thus u_α are the FEM nodal degrees of freedom and $a_{\alpha j}$ are the enriched degrees of freedom.

The trigonometric enrichment functions are defined as:

$$\boldsymbol{\mathcal{L}}_\alpha = \left\{\sin\left[\pi\left(\frac{x-x_\alpha}{h_\alpha}\right)\right], \sin\left[\pi\left(\frac{y-y_\alpha}{h_\alpha}\right)\right]\right\}, \tag{18}$$

where x_α and y_α are the coordinates of node $\mathbf{x}_\alpha$, $\alpha \in \mathcal{I}_h^e$, and h_α is given by the size of the largest element connected to node α. As FE shape functions, those related to the linear triangular element were used, remembering that the boundary shape functions needs to respect the Eq. (6).

5 Numerical results

Considering a square domain defined in the region $0 \le x, y \le L$, with the boundary conditions:

$$u(0,y,t) = u(L,y,t) = u(x,0,t) = u(x,L,t) = 0, \tag{19}$$

and initial conditions given by:

$$u_0(x,y) = \sin\left(\frac{\pi\,x}{L}\right)\,\sin\left(\frac{\pi\,y}{L}\right), \tag{20}$$

the analytical solution of an anisotropic media is [2, 3]:

$$u(x,y,t) = E_\alpha\left(\nu^2\,t\right)\sin\left(\frac{\pi\,x}{L}\right)\,\sin\left(\frac{\pi\,y}{L}\right), \tag{21}$$

where $E_\alpha(\cdot)$ is the Mittag-Leffler function (see Carrer et al. [2] and Corrêa et al. [3]) and ν is given by:

$$\nu = \frac{\pi}{L}\,\sqrt{D_x + D_y}. \tag{22}$$

In the problem analyzed in this work, the side of the square is $L = 10$ and two media are considered: the first isotropic with $D_x = D_y = 1.0$ and the second anisotropic with $D_x = 1.0$ and $D_y = 0.1$. The meshes used in this example are presented in Fig. 1, which comprise 441 nodes and 800 elements in the domain, and 80 nodes and 80 elements in the boundary. In the analysis, the time step is 0.05s and all the nodes are enriched.

The analyses were carried out with $\alpha = 1.0$, $\alpha = 0.8$, $\alpha = 0.5$, $\alpha = 0.2$ and $\alpha = 0.05$. The results for both media are presented in Fig. 2 at $u(L/2, L/2, t)$ and in Fig. 3 at $u(x, L/2, 15)$. The results of the Enriched MLGFM show good agreement with the analytical solution even for small values of the time derivative order α for both analyzed media, isotropic ($D_x = D_y = 1$) and anisotropic ($D_x = 1$ and $D_y = 0.1$).

The condition numbers of the $\mathbf{K}_{\text{aux}}$ matrix in Eq. (15) after applying the boundary condition are presented in Fig. 4. The condition number grows with the time derivative order, but the order of magnitude is almost the same. In other words, time derivative order seems does not have an influence on the method stability.

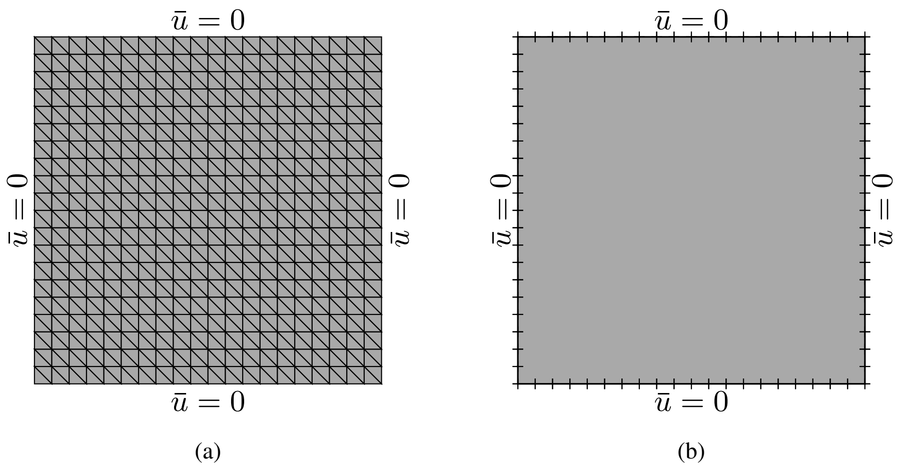

Figure 1. Meshes used in square domain example. (a) domain mesh and (b) boundary mesh

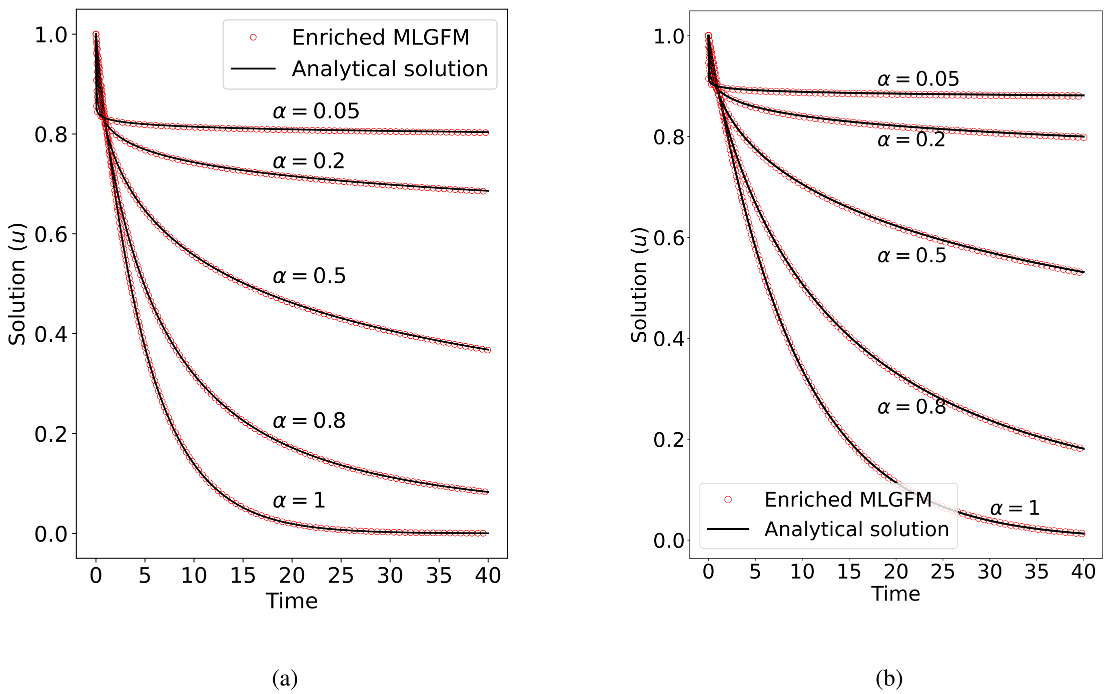

Figure 2. Results at $u(L/2, L/2, 40)$. (a) Isotropic medium and (b) Anisotropic medium.

6 Final remarks

In this paper, an enriched formulation of the MLGFM was presented and applied to the anomalous diffusion equation. This class of problems belongs to the branch of fractional calculus and, as mentioned before, is especially important when the nonlocality is important to the studied phenomena.

The choice of the enrichment functions was based on the fact that, in some time-dependent problems like this, the results have an oscillatory nature. With this idea, a trigonometric enrichment was proposed. The construction of the enriched functions was based on the Partition of the Unity idea, as in the GFEM.

The Enriched MLGFM results present good agreement with the analytical solution, even for small values of the order of time derivative α. In the literature, the difficulty of obtaining precise results for small values of α [9] is observed, but this formulation was able to achieve this. The good results show the potential of the MLGFM enriched by the proposed trigonometric functions for more applications in the anomalous diffusion equation and other time-dependent problems.

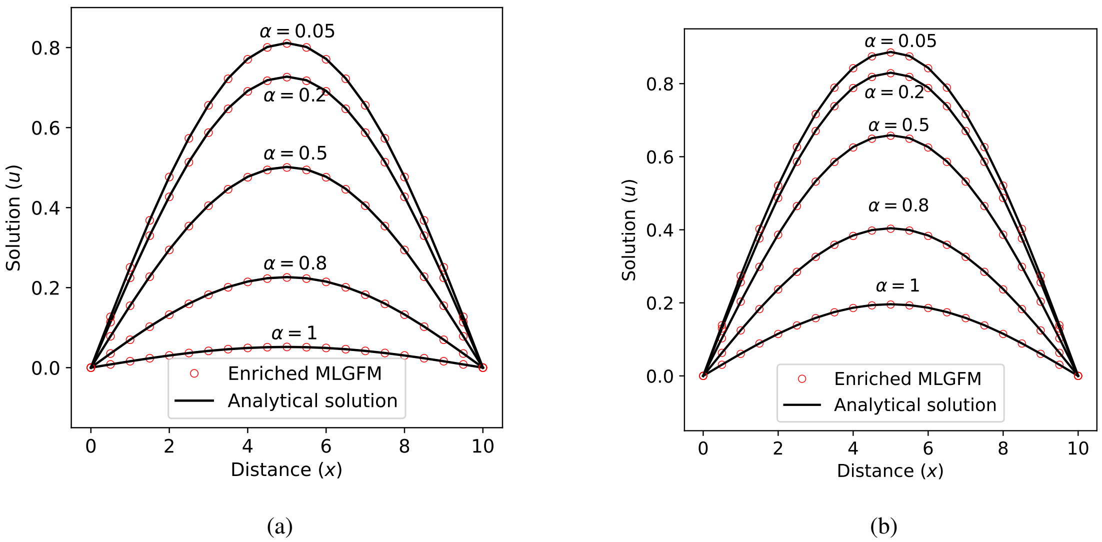

Figure 3. Results at $u(x, L/2, 15)$. (a) Isotropic medium and (b) Anisotropic medium.

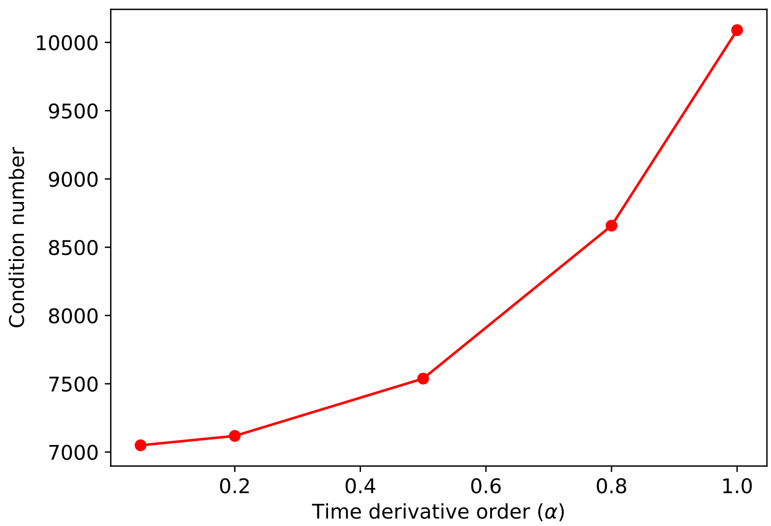

Figure 4. Condition number for different values of α.

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