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An accurate spectral method for the transverse magnetic mode of Maxwell equations in Cole-Cole dispersive media

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Abstract

In this paper, we propose an accurate numerical means built upon a spectral-Galerkin method in spatial discretization and an enriched multi-step spectral-collocation approach in temporal direction, for the transverse magnetic mode of Maxwell equations in Cole-Cole dispersive media in two-dimensional setting. Our starting point is to derive a new model involving only one unknown field from the original model with three unknown fields: electric, magnetic fields, and the induced electric polarization (described by a global temporal convolution of the electric field). This results in a second-order integral-differential equation with a weakly singular integral kernel expressed by the Mittag-Lefler (ML) function. The most interesting but challenging issue resides in how to efficiently deal with the singularity in time induced by the ML function which is an infinite series of singular power functions with different nature. With this in mind, we introduce a spectral-Galerkin method using Fourierlike basis functions for spatial discretization, leading to a sequence of decoupled temporal integral-differential equations (IDE) with the same weakly singular kernel involving the ML function as the original two-dimensional problem. With a careful study of the regularity of IDE, we incorporate several leading singular terms into the numerical scheme and approximate much regular part of the solution. Then, we solve the IDE by a multi-step well-conditioned collocation scheme together with mapping technique to increase the accuracy and enhance the resolution. We show that such an enriched collocation method is convergent and accurate.

Keywords Cole-Cole media \cdot Dispersive \cdot Spectral method \cdot Non-polynomial approximation

Mathematics Subject Classification (2010) $65N35\cdot 65E05\cdot 65N12\cdot 41A10\cdot 41A25\cdot 41A30\cdot 41A58$

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1 Introduction

In electromagnetism, if the electric permittivity or magnetic permeability depends on the wave frequency, then the medium is called a dispersive medium. The typical models that characterize such a dependence include the Drude mode [44, 45] and the Lorenz model [30, 34]. The Cole-Cole (C-C) dispersive model, distinguishing itself by the nonlocal feature, has been successfully applied to fit experimental dispersion and absorption for a considerable number of liquids and dielectrics [9]. Such a model can be expressed by the empirical formula (cf. [9]):

$$\epsilon(\omega) = \epsilon_0 \left(\epsilon_{\infty} + \frac{\epsilon_s - \epsilon_{\infty}}{1 + (i\,\omega\tau)^{\alpha}} \right), \quad 0 < \alpha \le 1,$$
(1.1)

where τ , ϵ_0 , ϵ_s , ϵ_∞ are all given physics constants. Here, τ is the central relaxation time of the material model, ϵ_0 is the permittivity of vacuum, and ϵ_s and ϵ_∞ are respectively the zero- and infinite-frequency limits of the relative permittivity satisfying $\epsilon_s > \epsilon_\infty \ge 1$. In particular, the model with $\alpha = 1$ leads to the classical Debye dielectric model, or exponential dielectric relaxation.

Since the C-C relaxation model has many applications in diverse fields, such as soil characterization [28], permittivity of biological tissue [12], and the transient nature of electromagnetic radiation in the human body [10, 17], its numerical solution has attracted much attention. Intensive studies have been devoted to the finite difference time domain (FDTD) methods (cf. [8, 26, 27, 37, 38]), and the time-domain finite element methods [2, 15, 20, 23, 39]. Most of them worked on discretization of the Maxwell system directly where the electric field and the induced electric polarization in the model are interconnected and globally dependent (see (2.2)). Although this relation can be transformed into a fractional differential equation (see, e.g., [20, 27, 38]), direct discretization of three fields may result in a large degree of freedoms with a heavy burden of historical dependence in time.

Different from all aforementioned works, we formulate the C-C model as a second-order partial integral-differential equation (PIDE) involving only one unknown field, where the integral part has a weakly singular kernel in terms of the ML function. We then place the emphasis on how to efficiently deal with the temporal singular integral with the kernel function as a series of singular functions in different fractional powers. Without loss of generality, we consider the plane wave geometry of the C-C model and reduce magnetic and electric field vectors to scalar field quantities by polarization, and restrict our attention to the two-dimensional PIDE. We then employ a spectral-Galerkin method using Fourier-like basis functions in space (cf. [21, 22, 33]), and the model boils down to a sequence of decoupled temporal IDE with the same type of singular integrals. As such, unlike the existing methods, we work with a model with the minimum number of unknowns, so the computational cost can be enormously reduced.

We propose a well-conditioned multi-step collocation method for solving the temporal IDE, which is enriched by incorporating a few leading singular terms through a delicate regularity analysis, and integrated with a mapping technique (cf. [41]) for treating the singular integral and nearly singular integrals in the first subinterval. The well-conditioning is achieved by writing the IDE in a first-order damped Hamitonian system and using the Birkhoff-Lagrange interpolating basis (cf. [40]), so the proposed method possesses a long time stability. It is noteworthy that the integral operator in our setting involving the ML function as the singular kernel. Such a kernel is distinct from the usual weakly singular kernel, such as $t^{\alpha-1}$, $0 < \alpha < 1$, in terms of the singular behaviors. We notice that many fast algorithms, stemming from the celebrated fast multipole method, have been recently proposed for the (Riemann-Liouville/Caputo) fractional differential equations (see, e.g., [16, 19, 24]). However, it appears that the extension of these algorithms to our case is nontrivial and largely open due to the completely different nature of the singular kernel.

The rest of the paper is organized as follows. In Section 2, we formulate our new model and present a semi-discretized scheme for the problem of interest. In Section 3, we tackle the challenges of the temporal IDE obtained from the previous section and introduce effective numerical techniques to surmount the obstacles. We also present various numerical results to illustrate various perspectives of the proposed method. We then conclude with discussions and some future work regarding the C-C model in Section 4.

2 Formulation of the model and a semi-discretized scheme

In this section, we derive a new model from the Maxwell system in Cole-Cole media involving three vector fields, and introduce a semi-discretized scheme for the problem of interest.

2.1 Maxwell equations in Cole-Cole media

The time-domain Maxwell's equations in Cole-Cole media take the form (cf. [20, 38]):

$$\epsilon_0 \epsilon_\infty \frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{H} - \frac{\partial \boldsymbol{P}}{\partial t} \quad \text{in } \Omega \times (0, T],$$
 (2.1a)

$$\mu_0 \frac{\partial \boldsymbol{H}}{\partial t} = -\nabla \times \boldsymbol{E} \qquad \text{in } \Omega \times (0, T], \qquad (2.1b)$$

where Ω is a bounded domain in \mathbb{R}^3 with a Lipschitz boundary, and P(x, t) is the induced electric polarization

$$\boldsymbol{P}(\boldsymbol{x},t) = \int_0^t \xi_\alpha(t-s) \boldsymbol{E}(\boldsymbol{x},s) \, ds, \quad \xi_\alpha(t) := \mathscr{L}^{-1} \left\{ \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{1 + (s\tau)^\alpha} \right\}.$$
(2.2)

Here, ξ_{α} is the time-domain susceptibility kernel which involves the inverse Laplace transform \mathscr{L}^{-1} . Note that P(x, 0) = 0 is evident from (2.2). Here, we supplement (2.1)–(2.2) with the initial conditions

$$E(x, 0) = E_0(x), \quad H(x, 0) = H_0(x) \text{ in } \Omega,$$
 (2.3)

and a perfect conducting boundary condition

$$\boldsymbol{n} \times \boldsymbol{E} = \boldsymbol{0} \quad \text{at} \; \partial \Omega \times (0, T).$$
 (2.4)

It is seen that the above Maxwell system contains three unknown vector fields. It is computationally beneficial to eliminate some unknowns. In this paper, we work on the model with one unknown field, as stated in the following lemma.

Lemma 2.1 Define $\mathcal{E} := \epsilon_0 \epsilon_\infty E + P$. Then, a reduced model from (2.1)–(2.4) is

$$\frac{\partial^2 \boldsymbol{\mathcal{E}}}{\partial t^2} = -a\nabla \times \nabla \times \boldsymbol{\mathcal{E}} + b \int_0^t e_{\alpha,\alpha} (-\lambda(t-s)^\alpha) \,\nabla \times \nabla \times \boldsymbol{\mathcal{E}} \, ds \quad in \ \Omega, \ t \in (0,T],$$
(2.5a)

$$\boldsymbol{n} \times \boldsymbol{\mathcal{E}}|_{\partial \Omega} = 0 \quad t \in (0, T], \tag{2.5b}$$

$$\boldsymbol{\mathcal{E}}(\boldsymbol{x},0) = \boldsymbol{\mathcal{E}}_0(\boldsymbol{x}), \quad \boldsymbol{\mathcal{E}}_t(\boldsymbol{x},0) = \boldsymbol{\mathcal{E}}_1(\boldsymbol{x}) \quad in \ \Omega,$$
(2.5c)

where $0 < \alpha < 1$,

$$a = \frac{1}{\mu_0 \epsilon_0 \epsilon_\infty}, \quad b = \frac{\epsilon_s - \epsilon_\infty}{\mu_0 \tau^\alpha \epsilon_0 \epsilon_\infty^2}, \quad \lambda = \frac{\epsilon_s}{\epsilon_\infty \tau^\alpha},$$
 (2.6)

and

$$e_{\alpha,\beta}(-\lambda t^{\alpha}) = t^{\beta-1} E_{\alpha,\beta}(-\lambda t^{\alpha}), \qquad (2.7)$$

with $E_{\alpha,\beta}(t)$ being the standard Mittag-Leffler (ML) function defined by

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha + \beta)}.$$
(2.8)

Proof Firstly, taking derivative with respect to *t* for (2.1a) and $\nabla \times$ for (2.1b), we eliminate *H* and obtain

$$\epsilon_0 \epsilon_\infty \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = -\frac{1}{\mu_0} \nabla \times \nabla \times \boldsymbol{E} - \frac{\partial^2 \boldsymbol{P}}{\partial t^2}.$$
(2.9)

Secondly, taking the Laplace transform on both sides of (2.2) leads to

$$\widehat{\boldsymbol{P}}(\boldsymbol{x},s) = \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{1 + (s\tau)^{\alpha}} \widehat{\boldsymbol{E}}(\boldsymbol{x},s), \qquad (2.10)$$

where the notation \widehat{W} stands for the Laplace transform of the field W. Then, a direct calculation (2.10) yields

$$\widehat{E} = \frac{1 + (s\tau)^{\alpha}}{\epsilon_0 \epsilon_\infty (1 + (s\tau)^{\alpha}) + \epsilon_0 (\epsilon_s - \epsilon_\infty)} \widehat{\mathcal{E}} = \frac{1}{\epsilon_0 \epsilon_\infty} \widehat{\mathcal{E}} - \frac{\epsilon_s - \epsilon_\infty}{\epsilon_0 \epsilon_\infty^2 \tau^{\alpha}} \frac{1}{s^{\alpha} + \epsilon_s / (\epsilon_\infty \tau^{\alpha})} \widehat{\mathcal{E}}.$$
(2.11)

Recall the formula of the inverse Laplace transform [13, p. 84]:

$$\mathcal{L}^{-1}\left(\frac{1}{s^{\alpha}+\lambda}\right) = t^{\alpha-1}E_{\alpha,\alpha}(-\lambda t^{\alpha}), \quad \text{if } |\lambda/s^{\alpha}| < 1.$$
(2.12)

Applying the inverse Laplace transform on both sides of (2.11) and using (2.12), we obtain

$$\boldsymbol{E} = \frac{1}{\epsilon_0 \epsilon_\infty} \boldsymbol{\mathcal{E}} - \frac{\epsilon_s - \epsilon_\infty}{\epsilon_0 \epsilon_\infty^2 \tau^\alpha} \int_0^t (t-s)^{\alpha-1} E_{\alpha,\alpha} \left(-\frac{\epsilon_s}{\epsilon_\infty \tau^\alpha} (t-s)^\alpha \right) \boldsymbol{\mathcal{E}}(\boldsymbol{x},s) ds.$$
(2.13)

Substituting (2.13) and $P = \mathcal{E} - \epsilon_0 \epsilon_\infty E$ into (2.9) leads to (2.5a).

With the substitution: $\mathcal{E} = \epsilon_0 \epsilon_\infty E + P$, we can determine the initial and boundary conditions of the new known field \mathcal{E} as follows. By (2.2) and (2.4), we have $n \times P = 0$ at the boundary, so

$$\boldsymbol{n} \times \boldsymbol{\mathcal{E}} = \boldsymbol{0} \quad \text{at} \; \partial \Omega \times (0, T).$$
 (2.14)

Similarly, we can derive the initial conditions from (2.1a), (2.3), and $\mathcal{E} = \epsilon_0 \epsilon_\infty E + P$ as follows

$$\mathcal{E}(\mathbf{x},0) = \epsilon_0 \epsilon_\infty \mathbf{E}_0(\mathbf{x}) := \mathcal{E}_0(\mathbf{x}), \quad \mathcal{E}_t(\mathbf{x},0) = \nabla \times \mathbf{H}_0(\mathbf{x}) := \mathcal{E}_1(\mathbf{x}) \quad \text{in } \Omega$$
(2.15)

This ends the derivation.

Remark 2.1 Note that we can recover the electric field from \mathcal{E} by (2.13):

$$\boldsymbol{E}(\boldsymbol{x},t) = a\mu_0 \,\boldsymbol{\mathcal{E}}(\boldsymbol{x},t) - b\mu_0 \int_0^t e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha}) \boldsymbol{\mathcal{E}}(\boldsymbol{x},s) ds.$$
(2.16)

2.2 Two-dimensional Cole-Cole model

It is seen from (2.5a) that the most interesting but challenging issue lies in the treatment of the singular integral in time. Without loss of generality, we consider the transverse magnetic polarization with E = (0, 0, e(x, y))', so we have $\mathcal{E} = (0, 0, u(x, y))'$. Then, we have the reduced model of (2.5a)–(2.5c):

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} = a\Delta u - b\int_0^t e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})\Delta u(\mathbf{x},s)ds \text{ in } \Omega, \ t \in (0,T],\\ u(\mathbf{x},t)|_{\partial\Omega} = 0 & \text{for } t \in (0,T],\\ u(\mathbf{x},0) = u_0(\mathbf{x}), \quad u_t(\mathbf{x},0) = u_1(\mathbf{x}) & \text{in } \Omega. \end{cases}$$
(2.17)

The existence and uniqueness of a weak solution to (2.17) has been investigated in [18] by a semi-group approach and further explored in [29] using the classic energy argument. However, both studies require $u_0 \in H^1(\Omega)$. In what follows, we shall show L^2 —a priori stability with a minimum requirement of the regularity—that is, $u_0 \in L^2(\Omega)$, which is accomplished by following the spirit of [1].

Theorem 2.1 Let u be the solution of (2.17). If $u_0, u_1 \in L^2(\Omega)$, and $a - b/\lambda \ge 0$, then we have $u \in L^{\infty}(0, T; L^2(\Omega))$ and the following estimate

$$\|u\|_{L^{\infty}(0,T;L^{2}(\Omega))} \leq \sqrt{2} \|u_{0}\|_{L^{2}(\Omega)} + 2T \|u_{1}\|_{L^{2}(\Omega)}.$$
(2.18)

Proof Setting

$$\phi(\mathbf{x},t) = \int_{t}^{\xi} u(\mathbf{x},\theta) d\theta, \quad \xi \in [0,T],$$
(2.19)

one verifies easily that

$$\phi(\mathbf{x},\xi) = 0, \quad \frac{\partial \phi}{\partial t}(\mathbf{x},t) = -u(\mathbf{x},t).$$

Multiplying both sides of the first equation in (2.17) by $\phi(\mathbf{x}, t)$ and integrating in space over Ω , we have

$$(u_{tt},\phi) = -a(\nabla u,\nabla\phi) + b \int_0^t e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})(\nabla u,\nabla\phi)ds.$$
(2.20)

Further integrating both sides with respect to t over $(0, \xi)$ leads to

$$\int_0^{\xi} (u_{tt}, \phi) dt = -a \int_0^{\xi} (\nabla u, \nabla \phi) dt + b \int_0^{\xi} \int_0^t e_{\alpha, \alpha} (-\lambda (t-s)^{\alpha}) (\nabla u, \nabla \phi) ds dt.$$
(2.21)

Next, using integration by parts and the explicit form of ϕ in (2.19), we find

$$\int_{0}^{\xi} (u_{tt}, \phi) dt = \int_{\Omega} \left((u_{t}\phi) \Big|_{0}^{\xi} - \int_{0}^{\xi} u_{t} d\phi \right) dx dy$$

= $\frac{1}{2} \| u(\cdot, \xi) \|_{L^{2}(\Omega)}^{2} - \frac{1}{2} \| u_{0} \|_{L^{2}(\Omega)}^{2} - \int_{\Omega} u_{1}(\mathbf{x}) \phi(\mathbf{x}, 0) dx dy,$
(2.22)

and

$$\int_{0}^{\xi} (\nabla u, \nabla \phi) dt = \int_{0}^{\xi} \int_{t}^{\xi} (\nabla u(\cdot, t), \nabla u(\cdot, \theta)) d\theta dt = \int_{0}^{\xi} \int_{0}^{\theta} (\nabla u(\cdot, t), \nabla u(\cdot, \theta)) dt d\theta$$
$$= \frac{1}{2} \int_{\Omega} \left| \int_{0}^{\xi} \nabla u(\mathbf{x}, t) dt \right|^{2} dx dy, \qquad (2.23)$$

where in the last step, we used the property:

$$\int_{0}^{\xi} \int_{0}^{\theta} g(t)g(\theta)dtd\theta = \int_{0}^{\xi} \int_{t}^{\xi} g(t)g(\theta)d\theta dt = \int_{0}^{\xi} \int_{\theta}^{\xi} g(t)g(\theta)dtd\theta, \quad (2.24)$$

implying

$$\int_{0}^{\xi} \int_{0}^{\theta} g(t)g(\theta)dtd\theta = \frac{1}{2} \int_{0}^{\xi} \int_{0}^{\xi} g(t)g(\theta)d\theta dt = \frac{1}{2} \left| \int_{0}^{\xi} g(t)dt \right|^{2}.$$
 (2.25)

Now, we deal with the singular integral term in (2.21). It is straightforward to verify from the definition (2.8) that

$$\frac{1}{\lambda}\frac{d}{dt}E_{\alpha,1}(-\lambda(t-s)^{\alpha}) = \frac{1}{\lambda}\frac{d}{dt}\sum_{k=0}^{\infty}\frac{(-\lambda)^{k}(t-s)^{k\alpha}}{\Gamma(k\alpha+1)} = \frac{1}{\lambda}\sum_{k=0}^{\infty}\frac{(-\lambda)^{k+1}(t-s)^{k\alpha+\alpha-1}}{\Gamma(k\alpha+\alpha)}$$
$$= -(t-s)^{\alpha-1}E_{\alpha,\alpha}(-\lambda(t-s)^{\alpha}) = -e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha}).$$
(2.26)

Using the above property and integration by parts, we derive

$$\int_{0}^{\xi} \int_{0}^{t} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha}) \left(\nabla u(\cdot,s), \nabla \phi(\cdot,t)\right) ds dt$$

$$= \int_{0}^{\xi} \int_{s}^{\xi} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha}) \left(\nabla u(\cdot,s), \nabla \phi(\cdot,t)\right) dt ds$$

$$= \left(-\frac{1}{\lambda}\right) \int_{0}^{\xi} \int_{s}^{\xi} \left(\nabla u(\cdot,s), \nabla \phi(\cdot,t)\right) dE_{\alpha,1}(-\lambda(t-s)^{\alpha}) ds$$

$$= \frac{1}{\lambda} \int_{0}^{\xi} \left(\nabla u(\cdot,s), \nabla \phi(\cdot,s)\right) ds - \frac{1}{\lambda} \int_{0}^{\xi} \int_{0}^{t} E_{\alpha,1}(-\lambda(t-s)^{\alpha}) \left(\nabla u(\cdot,s), \nabla u(\cdot,t)\right) ds dt. \quad (2.27)$$

Note that the kernel $E_{\alpha,1}(-\lambda t^{\alpha})$ is positive definite (cf. [18, 29]), i.e.,

$$\int_0^{\xi} \int_0^t E_{\alpha,1}(-\lambda(t-s)^{\alpha}) \left(\nabla u(\cdot,s), \nabla u(\cdot,t)\right) ds dt \ge 0.$$

Hence, we obtain from the above inequalities that

$$\frac{1}{2} \|u(\cdot,\xi)\|_{L^{2}(\Omega)}^{2} + \left(\frac{a}{2} - \frac{b}{2\lambda}\right) \int_{\Omega} \left|\int_{0}^{\xi} \nabla u(\boldsymbol{x},t) dt\right|^{2} dx dy$$

$$\leq \frac{1}{2} \|u_{0}\|_{L^{2}(\Omega)}^{2} + \int_{\Omega} u_{1}(\boldsymbol{x}) \phi(\boldsymbol{x},0) dx dy. \qquad (2.28)$$

Therefore, by (2.19), (2.28) and the Cauchy-Schwarz inequality,

$$\begin{split} &\frac{1}{2} \|u(\cdot,\xi)\|_{L^{2}(\Omega)}^{2} + \left(\frac{a}{2} - \frac{b}{2\lambda}\right) \int_{\Omega} \left|\int_{0}^{\xi} \nabla u(\mathbf{x},t) dt\right|^{2} dx dy \\ &\leq \frac{1}{2} \|u_{0}\|_{L^{2}(\Omega)}^{2} + \int_{\Omega} u_{1}(\mathbf{x}) \phi(\mathbf{x},0) dx dy = \frac{1}{2} \|u_{0}\|_{L^{2}(\Omega)}^{2} + \int_{0}^{\xi} \int_{\Omega} u_{1}(\mathbf{x}) u(\mathbf{x},\theta) dx dy d\theta \\ &\leq \frac{1}{2} \|u_{0}\|_{L^{2}(\Omega)}^{2} + \|u_{1}\|_{L^{2}(\Omega)} \int_{0}^{\xi} \|u(\cdot,\theta)\|_{L^{2}(\Omega)} d\theta \leq \frac{1}{2} \|u_{0}\|_{L^{2}(\Omega)}^{2} \\ &+ T \|u_{1}\|_{L^{2}(\Omega)} \|u\|_{L^{\infty}(0,T;L^{2}(\Omega))}. \end{split}$$

Therefore, if $a - b/\lambda \ge 0$, then by the Cauchy-Schwarz inequality,

$$\begin{split} \frac{1}{2} \|u\|_{L^{\infty}(0,T;L^{2}(\Omega))}^{2} &\leq \frac{1}{2} \|u_{0}\|_{L^{2}(\Omega)}^{2} + T \|u_{1}\|_{L^{2}(\Omega)} \|u\|_{L^{\infty}(0,T;L^{2}(\Omega))} \\ &\leq \frac{1}{2} \|u_{0}\|_{L^{2}(\Omega)}^{2} + \frac{1}{4} \|u\|_{L^{\infty}(0,T;L^{2}(\Omega))}^{2} + T^{2} \|u_{1}\|_{L^{2}(\Omega)}^{2}, \end{split}$$

which immediately implies (2.18).

Remark 2.2 Using a standard energy argument, we can follow [5] to derive the estimate:

$$\begin{aligned} \|u_t\|_{L^{\infty}(0,T;L^{2}(\Omega))}^{2} + (a - b/\lambda) \|\nabla u\|_{L^{\infty}(0,T;L^{2}(\Omega))}^{2} \\ &\leq \|u_1\|_{L^{2}(\Omega)}^{2} + \left(a + \frac{b}{\lambda} + \frac{2b^{2}}{(a\lambda - b)\lambda}\right) \|\nabla u_0\|_{L^{2}(\Omega)}^{2}, \end{aligned}$$
(2.29)

under the condition: $a - b/\lambda \ge 0$.

2.3 Spectral-Galerkin discretization using Fourier-like basis in space

As we are mostly interested in dealing with the singular fractional integrals, we consider $\Omega = (-1, 1)$ or $\Omega = (-1, 1)^2$. Let \mathbb{P}_N be the set of all polynomials of degree at most N, and let $\mathbb{P}_N^0 = \{\phi \in \mathbb{P}_N : \phi = 0 \text{ on } \partial\Omega\}$. The spectral-Galerkin approximation of (2.17) in space is to find $u_N(\cdot, t) \in \mathbb{P}_N^0$ such that for any $v_N, w_N, z_N \in \mathbb{P}_N^0$,

$$\begin{cases} (\partial_t^2 u_N, v_N)_{\Omega} + a(\nabla u_N, \nabla v_N)_{\Omega} = b \int_0^t e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha}) (\nabla u_N, \nabla v_N)_{\Omega} \, ds, \\ (u_N(\cdot, 0), w_N)_{\Omega} = (u_0, w_N)_{\Omega}, \quad (\partial_t u_N(\cdot, 0), w_N)_{\Omega} = (u_1, z_N)_{\Omega}. \end{cases}$$

$$(2.30)$$

We next employ the matrix diagonalization technique (cf. [32, Ch. 8]) to reduce (2.30) to a sequence of integral-differential equations in time.

We first look at the one-dimensional case. Define

$$\phi_k(x) = \frac{1}{\sqrt{4k+6}} (L_k(x) - L_{k+2}(x)), \quad k \ge 0,$$
(2.31)

where $L_k(x)$ is the Legendre polynomial of degree k. Then, we have

$$\mathbb{P}_{N}^{0} = \operatorname{span}\{\phi_{k}: \ 0 \le k \le N - 2\}.$$
(2.32)

It is known that under this basis, the stiffness matrix is identify as $(\phi'_k, \phi'_j) = \delta_{kj}$, and the mass matrix *B* with entries $b_{kj} = (\phi_k, \phi_j)_{\Omega}$ is symmetric and pentadiagonal. Moreover, we have $b_{k,k\pm 1} = 0$, so with a separation of even and odd modes, we actually deal with symmetric tridiagonal matrices (cf. [31]). Thus, writing

$$u_N(x,t) = \sum_{k=0}^{N-2} \hat{u}_k(t)\phi_k(x), \quad \hat{\boldsymbol{u}}(t) = (\hat{u}_0(t), \hat{u}_1(t), \cdots, \hat{u}_{N-2}(t))', \quad (2.33)$$

the scheme (2.30) becomes

$$\begin{cases} B\hat{u}''(t) + a\hat{u}(t) = b \int_0^t e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha}) \hat{u}(s) ds, & t \in (0, T], \\ B\hat{u}(0) = \hat{u}_0, & B\hat{u}'(0) = \hat{u}_1, \end{cases}$$
(2.34)

where $\hat{\boldsymbol{u}}_i = ((u_i, \phi_0)_{\Omega}, \dots, (u_i, \phi_{N-2})_{\Omega})'$ for i = 0, 1. Let $\{\lambda_i\}_{i=0}^{N-2}$ be the eigenvalues of *B*, and let *E* be the corresponding eigenvectors of *B*. Note that *E* is an orthonormal matrix, so $E'E = I_{N-1}$. Introducing the change of variables: $\hat{\boldsymbol{u}} = E\boldsymbol{v}$ with $\boldsymbol{v} = (v_0, v_1, \dots, v_{N-2})'$, we can decouple the system (2.34) into

$$\begin{cases} v_i''(t) + a\lambda_i^{-1}v_i(t) = b\lambda_i^{-1}\int_0^t e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})v_i(s)ds, & t \in (0,T], \\ v_i(0) = \lambda_i^{-1}v_{0i}, & v_i'(0) = \lambda_i^{-1}v_{1i}, \end{cases}$$
(2.35)

for $i = 0, \dots, N - 1$, where $\hat{u}_j = E v_j$ with $v_j = (v_{j0}, v_{j1}, \dots, v_{j(N-2)})'$ for j = 0, 1.

Similarly, in the two-dimensional case, we have

$$\mathbb{P}_{N}^{0} = \operatorname{span}\left\{\phi_{i}(x)\phi_{j}(y) : 0 \le i, j \le N - 2\right\}.$$
(2.36)

We write

$$u_N(x,t) = \sum_{i,j=0}^{N-2} \hat{u}_{ij}(t)\phi_i(x)\phi_j(y), \quad \widehat{U}(t) = (\hat{u}_{ij}(t))_{i,j=0,\cdots,N-2}, \quad (2.37)$$

Then, the counterpart of (2.34) becomes

$$\begin{cases} B\widehat{U}''B + a(\widehat{U}B + B\widehat{U}) = b \int_0^t e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})(\widehat{U}B + B\widehat{U})ds, & t \in (0,T], \\ B\widehat{U}B|_{t=0} = \widehat{U}_0, & B\widehat{U}'B|_{t=0} = \widehat{U}_1, \end{cases}$$
(2.38)

Using the full matrix diagonalization technique and setting $\widehat{U} = EWE'$ with $W = (w_{ij})_{i,j=0\cdots,N-2}$ (cf. [32, Ch. 8]), we have

$$\begin{cases} w_{ij}''(t) + a\left(\lambda_i^{-1} + \lambda_j^{-1}\right)w_{ij}(t) = b\left(\lambda_i^{-1} + \lambda_j^{-1}\right)\int_0^t e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})w_{ij}(s)ds, \\ w_{ij}(0) = (\lambda_i\lambda_j)^{-1}w_{ij}^0, \quad v_i'(0) = (\lambda_i\lambda_j)^{-1}w_{ij}^1, \end{cases}$$
(2.39)

for all $t \in (0, T]$, where $\widehat{U}_k = E W^k E'$ and $W^k = \left(w_{ij}^k\right)_{i,j=0,\dots,N-2}$ for k = 0, 1.

3 Algorithm development for the integral-differential equation

3.1 Prototype problem

Consider the prototype integral-differential equation:

$$\begin{cases} u''(t) + cu(t) = d \int_0^t e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha}) u(s) ds, & t \in (0,T], \quad 0 < \alpha < 1, \\ u(0) = u_0, \quad u'(0) = u_1, \end{cases}$$
(3.1)

where the constants c, d > 0, and the singular kernel $e_{\alpha,\alpha}(\cdot)$ is defined as in (2.7).

To alleviate ill-conditioning of the following multi-step collocation method, we adopt an ingredient of numerical treatment for Hamiltonian systems (cf. [11]) and rewrite (3.1) into the first-order system:

$$\begin{cases} p'(t) + cq(t) = d \int_0^t e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})q(s)ds; \quad q'(t) = p(t), \quad t \in (0, T], \\ q(0) = u_0, \quad p(0) = u_1, \end{cases}$$
(3.2)

by setting q = u and p = u'.

Similar to Theorem 2.1, we have the following stability of (3.2).

Theorem 3.1 Assume $u_0 = 0$ and $a - b/\lambda \ge 0$ in (3.2). Then, we have the bound

$$p^{2}(t) + (a - b/\lambda)q^{2}(t) \le u_{1}^{2}, \quad \forall t \in [0, T].$$
 (3.3)

Proof The proof is the same as that of Theorem 2.1, and hence is omitted. \Box

Remark 3.1 If $a - b/\lambda \ge 0$, one can define a Hamiltonian

$$H(t) = (u'(t))^{2} + (a - b/\lambda)u^{2}(t), \qquad (3.4)$$

for (3.1) and obtain a damped Hamiltonian system.

The assumption $u_0 = 0$ seems restrictive; however, it is indispensable for this bound. Our numerical experiments show that the Hamiltonian may increase or even outweigh the initial Hamiltonian without the condition (see Fig. 3 below).

3.2 A multi-step collocation method

For simplicity, we partition the interval [0, T] into K subintervals of equal length, that is,

$$I_k = (t_{k-1}, t_k), \quad t_k = kT/K, \quad k = 1, \cdots, K; \quad t_0 = 0.$$

Let $\{x_j\}_{j=0}^N \subseteq [-1, 1]$ be a set of Jacobi-Gauss-Lobatto (JGL) points arranged in ascending order and denote the grids

$$t_j^k = \frac{t_{k-1} + t_k}{2} + \frac{t_k - t_{k-1}}{2} x_j, \quad 0 \le j \le N; \quad 1 \le k \le K.$$
(3.5)

Let $P_N, Q_N \in C^0(0, T)$ be the multi-step spectral-collocation approximations of p, q, respectively, and each consists of K pieces:

$$P_{N}|_{I_{1}} = p_{N}^{1} = p_{*} + \hat{p}_{N}^{1}, \quad Q_{N}|_{I_{1}} = q_{N}^{1} = q_{*} + \hat{q}_{N}^{1}, \quad \hat{p}_{N}^{1}, \hat{q}_{N}^{1} \in \mathbb{P}_{N};$$

$$P_{N}|_{I_{k}} = p_{N}^{k} \in \mathbb{P}_{N}, \quad Q_{N}|_{I_{k}} = q_{N}^{k} \in \mathbb{P}_{N}, \quad k = 2, 3 \cdots, K, \quad (3.6)$$

where p_*, q_* are two pre-defined functions to capture leading singular terms (see Section 3.2.1).

We find these *K* pieces in sequence as follows.

• For k = 1, we find $\{p_N^1, q_N^1\}$ via the collocation scheme:

$$\dot{p}_{N}^{1}(t_{j}^{1}) + cq_{N}^{1}(t_{j}^{1}) = d \int_{0}^{t_{j}^{1}} e_{\alpha,\alpha}(-\lambda(t_{j}^{1} - s)^{\alpha})q_{N}^{1}(s)ds, \quad 1 \le j \le N;$$

$$\dot{q}_{N}^{1}(t_{j}^{1}) = p_{N,1}(t_{j}^{1}), \quad 1 \le j \le N;$$

$$q_{N}^{1}(0) = u_{0}, \quad p_{N}^{1}(0) = u_{1},$$

• For any $k \in \{2, \dots, K\}$, using the computed values $\{p_N^l, q_N^l\}_{l=1}^{k-1}$, we find $\{p_N^k, q_N^k\}$ via the collocation scheme:

$$\dot{p}_{N}^{k}(t_{j}^{k}) + cq_{N}^{k}(t_{j}^{k}) = d \sum_{l=1}^{k-1} \int_{I_{l}} e_{\alpha,\alpha} (-\lambda(t_{j}^{k} - s)^{\alpha}) q_{N}^{l}(s) ds + d \int_{t_{k-1}}^{t_{j}^{k}} e_{\alpha,\alpha} (-\lambda(t_{j}^{k} - s)^{\alpha}) q_{N}^{k}(s) ds, \quad 1 \le j \le N; \dot{q}_{N}^{k}(t_{j}^{k}) = p_{N}^{k}(t_{j}^{k}), \quad 1 \le j \le N; q_{N}^{k}(t_{k-1}) = q_{N}^{k-1}(t_{k-1}), \quad p_{N}^{k}(t_{k-1}) = p_{N}^{k-1}(t_{k-1}).$$
(3.8)

At this point, some important issues need to be addressed.

- (i) It is known that the solution of (3.1) (or (3.2)) has a singular behavior at t = 0. We therefore subtract p_* , q_* from p, q, so that $p - p_*$, $q - q_*$ have higher regularity, leading to globally higher order accuracy. We show below that p_* , q_* can be determined analytically by following the argument in [4, 7].
- (ii) How to accurately compute the integrals involving the singular kernel $e_{\alpha,\alpha}(\cdot)$.

In what follows, we shall resolve these issues (see Sections 3.2.1-3.2.3).

To fix the idea, we restrict our attentions to the Chebyshev approximation. Let $T_n(x) = \cos(n \arccos x)$ be the Chebyshev polynomial of degree *n*, and denote the scaled Chebyshev polynomial by

$$T_n^k(t) = T_n(x), \quad x = \frac{t - t_{k-1}}{t_k - t_{k-1}} + \frac{t - t_k}{t_k - t_{k-1}}, \quad t \in I_k.$$
 (3.9)

Hereafter, $\{x_j\}_{j=0}^N$ are the Chebyshev-Gauss-Lobatto (CGL) points.

3.2.1 Ansatz and the formulation of p_* , q_*

Our starting point is to reformulate (3.1) into the following integral form. This allows us to justify the well-posedness of the problem and derive the desired p_* , q_* that can capture the leading singularities.

Lemma 3.1 Letting z(t) = u''(t), we can rewrite (3.1) as

$$z(t) = \int_0^t \left\{ de_{\alpha,\alpha+2} (-\lambda(t-s)^{\alpha}) - c(t-s) \right\} z(s) ds + f(t),$$
(3.10)

where

$$f(t) = du_0 e_{\alpha, \alpha+1}(-\lambda t^{\alpha}) + du_1 e_{\alpha, \alpha+2}(-\lambda t^{\alpha}) - cu_1 t - cu_0.$$
(3.11)

Then, the problem (3.1) *has a unique solution* $u \in C(\Lambda)$ *.*

Proof Solving u''(t) = z(t) with $u(0) = u_0$ and $u'(0) = u_1$, we find

$$u(t) = u_0 + u_1 t + \int_0^t (t - s)z(s)ds.$$

Therefore, we can rewrite (3.1) as

$$z(t) + c\left(u_0 + u_1t + \int_0^t (t - s)z(s)ds\right) = d\int_0^t e_{\alpha,\alpha}(-\lambda(t - s)^{\alpha})$$
$$\left(u_0 + u_1s + \int_0^s (s - \theta)z(\theta)d\theta\right)ds.$$
(3.12)

Using the identity (cf. [25]): for $t > a, \alpha, \beta > 0$ and r > -1,

$$\int_{a}^{t} e_{\rho,\rho}(-z(t-s)^{\rho})(s-a)^{r} ds = \Gamma(r+1)e_{\rho,\rho+r+1}(-z(t-a)^{\rho}), \qquad (3.13)$$

one verifies readily that

$$\int_0^t e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})ds = e_{\alpha,\alpha+1}(-\lambda t^{\alpha}), \quad \int_0^t s \ e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})ds = e_{\alpha,\alpha+2}(-\lambda t^{\alpha}),$$
(3.14)

and also by the definition (2.16),

$$\int_{0}^{t} \int_{0}^{s} e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha})(s-\theta)z(\theta)d\theta ds = \int_{0}^{t} \int_{\theta}^{t} e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha})(s-\theta)dsz(\theta)d\theta$$
$$= \int_{0}^{t} \left\{ \sum_{k=0}^{\infty} \frac{(-\lambda)^{k}}{\Gamma(k\alpha+\alpha)} \int_{\theta}^{t} (t-s)^{\alpha-1+k\alpha}(s-\theta)ds \right\} z(\theta)d\theta$$
$$= \int_{0}^{t} \sum_{k=0}^{\infty} \frac{(-\lambda)^{k}(t-\theta)^{\alpha+1+k\alpha}}{\Gamma(k\alpha+\alpha+2)} z(\theta) d\theta = \int_{0}^{t} e_{\alpha,\alpha+2} (-\lambda(t-\theta)^{\alpha})z(\theta) d\theta. \quad (3.15)$$

Substituting (3.14)–(3.15) into (3.12) leads to (3.10)–(3.11).

Note that the operator

$$\mathscr{T}_{\alpha}[z] := \int_0^t \left\{ de_{\alpha,\alpha+2}(-\lambda(t-s)^{\alpha}) - c(t-s) \right\} z(s) ds$$

is continuous, so it is a Hilbert-Schimit operator. It also implies \mathscr{T}_{α} is compact from $C(\Lambda)$ to $C(\Lambda)$ [43, p. 277]. The existence and uniqueness of the solution to (3.10) immediately follows from the Fredholm alternative.

It is important to point out that Brunner (cf. [4, Thm 6.1.6]) studied a class of integral equations with the weakly singular kernel $(t - s)^{-\mu}K(s, t)$, where $0 < \mu < 1$ and K is smooth, and formally characterized the singular behavior of the solutions. Although the result therein cannot be directly applied to (3.10), we can use the formulation of the singularity as an *ansatz* to extract the most singular part of the solution of (3.10).

Theorem 3.2 For small t > 0, the solution of (3.1) has the form

$$u(t) = \sum_{\substack{i,j\\i+j\alpha \ge 2}} \gamma_{ij} t^{i+j\alpha} + u_1 t + u_0,$$
(3.16)

where $\{\gamma_{ij}\}$ are real coefficients. Here, the first several most singular terms of u(t) can be worked out as follows:

$$\begin{split} u(t) &= u_{*}(t) + \phi(t) \\ &\coloneqq \sum_{j} \left\{ du_{1} \frac{(-\lambda)^{j-3/\alpha-1}}{\Gamma(j\alpha+1)} \mathbb{1}_{\{3/\alpha \in \mathbb{N}, 4/\alpha > j > 3/\alpha\}} \\ &+ du_{0} \frac{(-\lambda)^{j-2/\alpha-1}}{\Gamma(j\alpha+1)} \mathbb{1}_{\{2/\alpha \in \mathbb{N}, 4/\alpha > j > 2/\alpha\}} \right\} t^{j\alpha} \\ &+ \sum_{j} \left\{ du_{1} \frac{(-\lambda)^{j-2/\alpha-1}}{\Gamma(j\alpha+2)} \mathbb{1}_{\{2/\alpha \in \mathbb{N}, 3/\alpha > j > 2/\alpha\}} \\ &+ du_{0} \frac{(-\lambda)^{j-1/\alpha-1}}{\Gamma(j\alpha+2)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}, 3/\alpha > j > 1/\alpha\}} \right\} t^{1+j\alpha} \\ &+ \sum_{0 < j < 2/\alpha} \left\{ du_{0} \frac{(-\lambda)^{j-1}}{\Gamma(j\alpha+3)} + du_{1} \frac{(-\lambda)^{j-1/\alpha-1}}{\Gamma(j\alpha+3)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}, j > 1/\alpha\}} \right\} t^{2+j\alpha} \\ &+ \sum_{0 < j < 1/\alpha} \left\{ du_{1} \frac{(-\lambda)^{j-1}}{\Gamma(j\alpha+4)} + du_{0} \frac{(-\lambda)^{j+1/\alpha-1}}{\Gamma(j\alpha+4)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}\}} \right\} t^{3+j\alpha} + \phi(t), \end{split}$$
(3.17)

where $\mathbb{1}_S$ is the indicator function of the set S and $\phi(t) \in C^4(\Lambda)$ and u_1, u_0, d are the same as in (3.1). With this, we take q_*, p_* in (3.6) to be

$$q_*(t) = u_*(t), \quad p_*(t) = u'_*(t).$$
 (3.18)

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Proof Suppose that there exists a term of the form t^{θ} , $\theta < 2$ in the ansatz. Substituting the term into (3.1) and letting *t* approach 0, one easily concludes that the left-hand side of (3.1) blows up, contradicting the right-hand side, which is 0. As a result, non-integer powers of the form t^{θ} , $\theta < 2$ are expelled in the ansatz of u(t).

On the other hand, it is impossible for us to extract the explicit expression of γ_{ij} for all $t^{i+j\alpha}$ as it is extremely tedious and complicated. Hence, we can restrict our attention to exploiting the coefficients γ_{ij} of term $t^{i+j\alpha}$, $2 < i + j\alpha < 4$.

Substituting (3.16) into (3.2) and using (3.13) yield

$$\sum_{\substack{i,j\\i+j\alpha\geq 2}} \gamma_{ij}(i+j\alpha)(i-1+j\alpha)t^{i-2+j\alpha} + c \left\{ \sum_{\substack{i,j\\i+j\alpha\geq 2}} \gamma_{ij}t^{i+j\alpha} + u_{1}t + u_{0} \right\}$$

= $du_{1} \sum_{k=0}^{\infty} \frac{(-\lambda)^{k}}{\Gamma(k\alpha+\alpha+2)} t^{(k+1)\alpha+1} + du_{0} \sum_{k=0}^{\infty} \frac{(-\lambda)^{k}}{\Gamma(k\alpha+\alpha+1)} t^{(k+1)\alpha}$
+ $d \sum_{\substack{i,j\\i+j\alpha\geq 2}} \Gamma(i+1+j\alpha)\gamma_{ij} \sum_{k=0}^{\infty} \frac{(-\lambda)^{k}}{\Gamma(k\alpha+\alpha+i+1+j\alpha)} t^{(k+1+j)\alpha+i}.$ (3.19)

Now, we equate powers of lower order terms $t^{1+j\alpha}$, $t^{j\alpha}$, $t^{j\alpha-1}$ and $t^{j\alpha-2}$ for the following four cases respectively. It is noteworthy to point out that monomials are excluded out of our consideration for these cases.

Case 1: $\{j : 3 + j\alpha < 4, j \in \mathbb{N}\}$

We consider similar terms of the form $t^{1+j\alpha}$. Note that the candidates in the righthand side of (3.19) which could have the form are $t^{(k+1)\alpha+1}$ and $t^{(k+1)\alpha}$. Let

$$\begin{cases} 1+j\alpha = (k+1)\alpha + 1 \quad \Rightarrow \quad k = j-1, \\ 1+j\alpha = (k+1)\alpha \qquad \Rightarrow \quad k = j-1+1/\alpha, \text{ if } 1/\alpha \in \mathbb{N}. \end{cases}$$

Hence, equating coefficients of $t^{1+j\alpha}$ on both sides of (3.19) yields

$$\gamma_{3j}(3+j\alpha)(2+j\alpha) = du_1 \frac{(-\lambda)^{j-1}}{\Gamma(j\alpha+2)} + du_0 \frac{(-\lambda)^{j+1/\alpha-1}}{\Gamma(j\alpha+2)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}\}},$$

$$\gamma_{3j} = du_1 \frac{(-\lambda)^{j-1}}{\Gamma(j\alpha+4)} + du_0 \frac{(-\lambda)^{j+1/\alpha-1}}{\Gamma(j\alpha+4)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}\}}.$$
(3.20)

Case 2: $\{j : 2 + j\alpha < 4, j \in \mathbb{N}\}$

Now, we consider similar terms of the form $t^{j\alpha}$. Similar as the previous case by considering two candidates $t^{(k+1)\alpha+1}$ and $t^{(k+1)\alpha}$ of the right-hand side of (3.19), we have

$$\begin{cases} j\alpha = (k+1)\alpha \qquad \Rightarrow \quad k = j - 1, \\ j\alpha = (k+1)\alpha + 1 \qquad \Rightarrow \quad k = j - 1 - 1/\alpha, \text{ if } 1/\alpha \in \mathbb{N} \text{ and } j > 1/\alpha. \end{cases}$$

Equating coefficients for $t^{j\alpha}$ on both sides of (3.19) implies

$$\gamma_{2j}(2+j\alpha)(1+j\alpha) = du_0 \frac{(-\lambda)^{j-1}}{\Gamma(j\alpha+1)} + du_1 \frac{(-\lambda)^{j-1/\alpha-1}}{\Gamma(j\alpha+1)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}, j > 1/\alpha\}},$$

$$\gamma_{2j} = du_0 \frac{(-\lambda)^{j-1}}{\Gamma(j\alpha+3)} + du_1 \frac{(-\lambda)^{j-1/\alpha-1}}{\Gamma(j\alpha+3)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}, j > 1/\alpha\}}.$$

(3.21)

Case 3: $\{j : 1 + j\alpha < 4, j \in \mathbb{N}\}$

For the term $t^{j\alpha-1}$, we follow the same fashion to have

$$\begin{cases} j\alpha - 1 = (k+1)\alpha + 1 & \Rightarrow \quad k = j - 2/\alpha - 1, \text{ if } 2/\alpha \in \mathbb{N} \text{ and } j > 2/\alpha \\ j\alpha - 1 = (k+1)\alpha & \Rightarrow \quad k = j - 1/\alpha - 1, \text{ if } 1/\alpha \in \mathbb{N} \text{ and } j > 1/\alpha. \end{cases}$$

Equating coefficients for $t^{j\alpha-1}$ yields

$$\gamma_{1j}(1+j\alpha)(j\alpha) = du_1 \frac{(-\lambda)^{j-2/\alpha-1}}{\Gamma(j\alpha)} \mathbb{1}_{\{2/\alpha \in \mathbb{N}, 3/\alpha > j > 2/\alpha\}} + du_0 \frac{(-\lambda)^{j-1/\alpha-1}}{\Gamma(j\alpha)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}, 3/\alpha > j > 1/\alpha\}}, \gamma_{1j} = du_1 \frac{(-\lambda)^{j-2/\alpha-1}}{\Gamma(j\alpha+2)} \mathbb{1}_{\{2/\alpha \in \mathbb{N}, 3/\alpha > j > 2/\alpha\}} + du_0 \frac{(-\lambda)^{j-1/\alpha-1}}{\Gamma(j\alpha+2)} \mathbb{1}_{\{1/\alpha \in \mathbb{N}, 3/\alpha > j > 1/\alpha\}}.$$
(3.22)

Case 4: $\{j : j\alpha < 4, j \in \mathbb{N}\}$

Finally, we consider the term $t^{j\alpha-2}$,

$$\begin{cases} j\alpha - 2 = (k+1)\alpha + 1 \qquad \Rightarrow \quad k = j - 3/\alpha - 1, \text{ if } 3/\alpha \in \mathbb{N} \text{ and } j > 3/\alpha, \\ j\alpha - 2 = (k+1)\alpha \qquad \Rightarrow \quad k = j - 2/\alpha - 1, \text{ if } 2/\alpha \in \mathbb{N} \text{ and } j > 2/\alpha. \end{cases}$$

Equating coefficients for $t^{j\alpha-2}$ leads to

$$\begin{split} \gamma_{0j}(j\alpha)(j\alpha-1) \\ &= du_1 \frac{(-\lambda)^{j-3/\alpha-1}}{\Gamma(j\alpha-1)} \mathbb{1}_{\{3/\alpha \in \mathbb{N}, 4/\alpha > j > 3/\alpha\}} + du_0 \frac{(-\lambda)^{j-2\alpha-1}}{\Gamma(j\alpha-1)} \mathbb{1}_{\{2/\alpha \in \mathbb{N}, 4/\alpha > j > 2/\alpha\}}, \\ \gamma_{1j} &= du_1 \frac{(-\lambda)^{j-3/\alpha-1}}{\Gamma(j\alpha+1)} \mathbb{1}_{\{3/\alpha \in \mathbb{N}, 4/\alpha > j > 3/\alpha\}} + du_0 \frac{(-\lambda)^{j-2/\alpha-1}}{\Gamma(j\alpha+1)} \mathbb{1}_{\{2/\alpha \in \mathbb{N}, 4/\alpha > j > 2/\alpha\}}. \end{split}$$

Once lower order terms (i.e., $t^{i+j\alpha}$ with $i+j\alpha < 4$) are determined, the remainder is wrapped up into $\phi(t) \in C^4(\Lambda)$.

Remark 3.2 We exclude the cases $i + j\alpha \in \mathbb{N}$ *in that polynomials can be absorbed into* $\phi(t)$ *.*

3.2.2 Mapping techniques for evaluating weakly singular integrals

In the implementation of the scheme (3.7)–(3.8), we have to deal with singular integrals of type I:

$$\mathcal{I}_{\alpha}^{I}(t) = \int_{t_{k-1}}^{t} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})g(s) \, ds,$$

for $g(s) = s^{\beta}, \ t = t_{j}^{1} \in (t_{0}, t_{1}], \ k = 1,$
or $g(s) = T_{n}^{k}(s), \ t = t_{j}^{k} \in (t_{k-1}, t_{k}], \ k = 1, 2, \cdots, K,$ (3.23)

and the nearly singular integers of type II:

$$\mathcal{I}_{\alpha}^{\mathbb{I}}(t) = \int_{t_{k-1}}^{t_k} e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha}) g(s) \, ds,$$

for $g(s) = s^{\beta}, \ t > t_1, \ t \approx t_1, \ k = 1;$
or $g(s) = T_n^k(s), \ t > t_k, \ t \approx t_k; \ k = 1, 2, \cdots, K,$ (3.24)

where $\beta \in \mathbb{R}$ relates to the aforementioned ansatz p_*, q_* in the first subinterval $[0, t_1]$.

The difficulty of approximating both types resides in the fact that the kernel $e_{\alpha,\alpha}(\cdot)$ has infinitely many terms of singular powers with different singular behaviors (cf. (2.8) and (2.7)). As a result, a numerical quadrature, e.g., Jacobi-Gauss quadrature, involving a single weight function cannot provide the satisfactory accuracy. Indeed, we depict in Fig. 1 the integrands with several parameters, and observe that the integrands exhibit heavy boundary layers at one end of the interval.

To surmount this obstacle, we resort to the mapping technique that can redistribute the quadrature points to the end of the interval where they are mostly needed to resolve the boundary layer. Following the idea of [41], we introduce the one-sided singular mapping:

$$t = h(y; r) = t_r + (t_l - t_r) \left(\frac{1 - y}{2}\right)^{1 + r}, \quad y \in [-1, 1], \quad t \in [t_l, t_r], \quad r \in \mathbb{N}.$$
(3.25)

Let $\{y_i, \omega_i\}_{i=0}^N$ be the Gauss-Legendre quadrature points and weights on [-1, 1], and define the mapped points $\{t_i = h(y_i; r)\}_{i=0}^N$. Denote by f(t) a generic integrand on (t_l, t_r) with a singular layer near $t = t_r$. Basically, we have

$$\int_{t_l}^{t_r} f(t)dt = c_r \int_{-1}^{1} f(h(y;r)) \left(\frac{1-y}{2}\right)^r dy \approx c_r \sum_{i=0}^{N} f(t_i) \left(\frac{1-y_i}{2}\right)^r \omega_i,$$
(3.26)

where $c_r = (r + 1)\frac{t_r - t_l}{2}$. We see that with the factor $(1 - y)^r$, the integrand much better behaved in y. On the other hand, more and more points are clustered near $t = t_r$ as r increases. To demonstrate the gain of the mapping technique, we consider two examples of different types: (i) $f(t) = e_{0.6,0.6}(-(0.7 - t)^{0.6})T_n^1(t), t \in (0, 0.7)$, and (ii) $f(t) = e_{0.6,0.6}(-(1.01 - t)^{0.6})T_n^1(t), t \in (0, 1)$. Note that we can calculate the exact values of two integrals by using the property of ML functions.



Fig. 1 (Left): A plot of $e_{0,6,0,6}(-(0.7 - s)^{0.6})T_n^1(s), n = 1$ or $2, s \in [0, 0.7]$. (Right): A plot of $e_{0,6,0,6}(-(1.01 - s)^{0.6})T_n^1(s), n = 1$ or $2, s \in [0, 1]$

In Fig. 2, we depict the error curves of the usual quadrature and the mapped approaches (i.e., r = 0 and r = 3) against various N. We observe a much faster decay of the errors from the mapped approach. Therefore, with the mapping, we can compute the singular/nearly singular integrals much more accurately.

3.2.3 Well-conditioned collocation matrix

The third issue of marching collocation scheme is that the condition number of standard collocation matrix D associated with the second-order term u_{tt} grows like $\mathcal{O}(N^4)$, where N is the number of collocation points. To circumvent the difficulty, we first rewrite (3.1) into a damped Hamiltonian system with only first-order derivatives and then construct the explicit inverse matrix B for first-order collocation matrix through Birkhoff interpolation.

Here, we only list the explicit form of $B = B_j(x_i)$, $1 \le i, j \le N$. On the standard interval [-1, 1] and given Chebyshev collocation points and its associated weights $\{x_i, w_i\}_{i=0}^N$ with increasing order, $B_j(x)$ has the following form.

$$B_j(x) = \sum_{k=0}^{N-1} w_j [T_k(x_j) - T_N(x_j)(-1)^{N+k}] \partial_x^{-1} T_k(x), \qquad (3.27)$$



Fig. 2 Errors of Gauss-Legendre quadrature (G-L) and mapped G-L quadrature (with r = 3). Left: case (i); right: case (ii)

where $\partial_x^{-1} T_k(x) = \int_{-1}^x T_k(y) dy$, and

$$\partial_x^{-1} T_0(x) = 1 + x, \quad \partial_x^{-1} T_1(x) = \frac{x^2 - 1}{2},$$

$$\partial_x^{-1} T_k(x) = \frac{T_{k+1}(x)}{2(k+1)} - \frac{T_{k-1}(x)}{2(k-1)} - \frac{(-1)^k}{k^2 - 1}, \quad k \ge 2.$$
(3.28)

The readers are referred to [40] for the details, where the computation of *B* is stable even for thousands of collocation points.

3.3 Numerical experiments

Example 3.1 Consider the equation

$$\begin{cases} u''(t) + 4u(t) = 3 \int_0^t e_{\alpha,\alpha}(-1.5(t-s)^{0.6})u(s)ds, & t \in [0, 20], \\ u(0) = 0, & u'(0) = 2. \end{cases}$$
(3.29)

We partition the domain into 20 equidistant subintervals. Since the solution is singular near t = 0, we take advantage of the ansatz (3.17) for the first subinterval and use the approximation (3.7). For other intervals, we apply standard polynomial approximation (3.8). Clearly, we can define the Hamiltonian $H(t) = p^2(t) + 2q^2(t)$.

Indeed, as we observe from Fig. 3, the Hamiltonian decreases as time increases. The system stays at the origin when it reaches the steady state.



Fig. 3 (Left): A phase plot for (3.29) with u(0) = 0, $u_t(0) = 2$ by using 20 collocation points on each time interval. (Right): A plot of Hamiltonian decay with respect to time

To validate the necessity of condition $u_0 = 0$ in Theorem 3.1, we switch the initial condition of (3.29) to u(0) = 2, $u_t(0) = 0$ and obtain Fig. 4. One can easily observe that as time proceeds, the Hamiltonian may exceed the initial one, which contracts Theorem 3.1.

Example 3.2 To validate the special treatment of our algorithm in the first subinterval, we consider the equation

$$\begin{cases} \ddot{u}(t) + cu(t) = d \int_0^t e_{\alpha,\alpha} (-\lambda(t-s)^{\alpha}) u(s) ds + g(t), \\ u(0) = u_0, \quad \dot{u}(0) = u_1, \end{cases}$$
(3.30)

where initial conditions and source term g(t) are chosen such that

$$u(t) = t^{2+\alpha} + t^{3+2\alpha} + \begin{cases} (t-1)^5, & t \in [0,1], \\ -(t-1)^5, & t \in (1,2]. \end{cases}$$
(3.31)

Here, we aim to mimic the ansatz in Proposition 3.2. From our algorithm, $\tau = 2$ implies direct polynomial approximation for u(t), $\tau = 3$ leads to polynomial approximation for the last two terms of u(t), and $\tau = 5$ indicates polynomial approximation for the last term. Numerical results are shown in Fig. 5. The number in the parentheses means the slope of associated reference line.



Fig.4 (Left): A phase plot for (3.29) with u(0) = 2, $u_t(0) = 0$ by using 20 collocation points on each time interval. (Right): A plot of Hamiltonian decay with respect to time. Note that under this initial condition, the decay is not strict



Fig.5 (Left): Numerical error for interval refinement with nine frozen collocation points. (Right): Numerical error of approximation with two equal-length subintervals, on which various collocation points are applied

Remark 3.3 Note that our scheme equations (3.7)–(3.8) with N = 2 and j = 2 (but without using the techniques described in Sections 3.2.1–3.2.3) turn out to be a second-order finite difference (FD) scheme. We carry out the following test for our collocation scheme and FD scheme for this example. We first divide the interval [0, 2] into two subintervals and collocate 10 points on each subinterval. An accuracy of 5.2158×10^{-8} in L^{∞} -norm is achieved for the proposed scheme within 0.64 s. Next, we divide the interval [0, 2] into 20 subintervals and apply the finite difference method for the equation. It takes 7.5 s on the same machine to produce the accuracy 0.0091. This shows the remarkable advantages of the new technique.

3.4 Error analysis

To begin with, we present an important result on Chebyshev-Gauss-Lobatto interpolation of the singular function: $h(t) = (t + 1)^{\theta}, t \in [-1, 1]$ and real $\theta > 0$.

Lemma 3.2 Let I_N be the interpolation operator on the Chebyshev-Lobatto points $\{t_i\}_{i=0}^N$. Then

$$\|h - I_N h\|_{\infty} \le 2N^{-2\theta}.$$
 (3.32)

Proof Let a_n denote the exact Chebyshev expansion coefficient of h(t), i.e., $a_n = \int_{-1}^{1} h(t)T_n(t)w(t)dt$, where $w(t) = (1 - t^2)^{-1/2}$. Then, a careful computation (cf. [14, Lemma 4] implies

$$a_n = \mathcal{O}(n^{-1-2\theta}). \tag{3.33}$$

Furthermore, denote $I_N h(t) = \sum_{n=0}^{N} {}^{\prime\prime} b_n T_n(x)$, where double prime means the first and the last terms are to be taken by a factor of 1/2. Apply [3, Theorem 21] to get

$$\|u - I_N u\|_{\infty} \le 2 \sum_{n=N+1}^{\infty} |a_n| = 2N^{-2\theta}.$$
(3.34)

This ends the proof.

Remark 3.4 We note that [32, Theorem 3.40] provides a convergence rate for Chebyshev interpolation for rather general functions. However, by taking advantage of the concrete form of h(t), we can get significantly better convergence rates.

For the sake of analysis, we define the operators $\mathcal{A}^j, \mathcal{B}^j : C(I_j) \to C(I_j)$ on each I_j by

$$(\mathcal{A}^{j}u)(t) = \int_{I_{j}} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})u(s)ds, \quad t > t_{j},$$
(3.35)

and

$$(\mathcal{B}^{j}u)(t) = \int_{t_{j-1}}^{t} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})u(s)ds, \ t \in I_{j}.$$
(3.36)

Then, there exists a best polynomial $\pi_N(\mathcal{B}^j u)$ of order N such that (cf. [14, Lemma 7])

$$\|\mathcal{K}^{j}u - \pi_{N}(\mathcal{B}^{j}u)\|_{\infty} \le CN^{-\alpha}\|u\|_{\infty}.$$
(3.37)

Theorem 3.3 Assume the ansatz (3.16) for u when $t \to 0$ and $u \in H^m(0, T]$ for some m > 5/2, and $c - d/\lambda \ge 0$, $\tau = 4$. Then, for our marching scheme on the whole time span [0, T], there holds

$$\|p - p_N\|_{\infty} + (c - d/\lambda)\|q - q_N\|_{\infty} \le CN^{-\min\{4, m-5/2\}},$$
(3.38)

where C depends on u, T but is independent of N.

Proof Define the error function on I_i by

$$e_{p,j}(t) = p^{j}(t) - p_{N}^{j}(t), e_{q,j}(t) = q^{j}(t) - q_{N}^{j}(t), t \in I_{j}.$$

Recall from (3.17) that on the interval I_1 , we denote

$$q^{1}(t) = q_{*}(t) + \phi(t), \quad p^{1}(t) = p_{*}(t) + \phi'(t).$$
 (3.39)

Hence, we have

$$e_{p,1}(t) = p^{1}(t) - p_{N}^{1}(t) = \phi'(t) - \hat{p}_{N}^{1}(t), e_{q,1}(t) = q^{1}(t) - q_{N}^{1}(t) = \phi(t) - \hat{q}_{N}^{1}(t).$$

Then, on each I_j , substituting (3.7) or (3.8) into (3.2), and subtracting the resulted equation from (3.2), we have

$$\begin{cases} \dot{p}^{j}(\xi_{i}) - \dot{p}_{N}^{j}(\xi_{i}) = -cq^{j}(\xi_{i}) + cq_{N}^{j}(\xi_{i}) + d\sum_{k=1}^{j-1} \int_{I_{k}} e_{\alpha,\alpha}(-\lambda(\xi_{i} - s)^{\alpha})e_{q,k}(s)ds \\ + d\int_{I_{j-1}}^{\xi_{i}} e_{\alpha,\alpha}(-\lambda(\xi_{i} - s)^{\alpha})e_{q,j}(s)ds, \\ \dot{q}^{j}(\xi_{i}) - \dot{q}_{N}^{j}(\xi_{i}) = p^{j}(\xi_{i}) - p_{N}^{j}(\xi_{i}), \\ e_{p,j}(t_{j-1}) = e_{p,j-1}(t_{j-1}), e_{q,j}(t_{j-1}) = e_{q,j-1}(t_{j-1}), \end{cases}$$
(3.40)

where $\{\xi_i\}_{i=0}^N$ is the Chebyshev-Lobatto collocation points on I_j . Multiply both sides of (3.40) by $l_i(t)$ and sum over *i*, where $l_i(t)$ is the Lagrange interpolation basis associated with ξ_i to obtain

$$I_N \dot{p}^j - \dot{p}_N^j = -aI_N q^j + aq_N^j + bI_N \sum_{k=1}^{j-1} \mathcal{A}^k e_{q,k} + bI_N \mathcal{B}^j e_{q,j},
 I_N \dot{q}^j - \dot{q}_N^j = I_N p^j - p_N^j.$$
(3.41)

Since $e_{p,j} = p^j - I_N p^j + I_N p^j - p_N^j$ and $e_{q,j} = q^j - I_N q^j + I_N q^j - q_N^j$, we therefore have the error function

$$\begin{cases} \dot{e}_{p,j}(t) = -ae_{q,j}(t) + b \int_{t_{j-1}}^{t} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})e_{q,j}(s)ds + F(t), \\ \dot{e}_{q,j}(t) = e_{p,j}(t) + G(t), \\ e_{p,j}(t_{j-1}) = e_{p,j-1}(t_{j-1}), e_{q,j}(t_{j-1}) = e_{q,j-1}(t_{j-1}), \end{cases}$$
(3.42)

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where

$$F(t) = \underbrace{\dot{p}^{j} - I_{N}\dot{p}^{j}}_{F_{1}} + \underbrace{a(q^{j} - I_{N}q^{j})}_{F_{2}} + \underbrace{bI_{N}\sum_{k=1}^{j-1}\mathcal{A}^{k}e_{q,k}}_{F_{3}} + \underbrace{b(I_{N} - I)\mathcal{B}^{j}e_{q,j}(s)}_{F_{4}}, (3.43)$$

$$G(t) = \underbrace{\dot{q}^{j} - I_{N}\dot{q}^{j}}_{G_{1}} + \underbrace{I_{N}p^{j} - p^{j}}_{G_{2}}.$$
(3.44)

Integrating both sides of (3.42) from 0 to ξ and following the proof of Theorem 2.1, we obtain

$$e_{p,j}^{2}(\xi) + (a - b/\lambda)e_{q,j}^{2}(\xi)$$

$$\leq e_{p,j}^{2}(t_{j-1}) + (a - b/\lambda)e_{q,j}^{2}(t_{j-1}) - \frac{2be_{q,j}(t_{j-1})}{\lambda} \int_{t_{j-1}}^{\xi} \dot{e}_{q,j}(t)E_{\alpha,1}(-\lambda t^{\alpha})dt$$

$$+ \int_{t_{j-1}}^{\xi} F(t)e_{p,j}(t)dt + a \int_{t_{j-1}}^{\xi} G(t)e_{q,j}(t)dt.$$
(3.45)

Again, the second mean value theorem implies there exists a $\xi_0 \in (t_{j-1}, \xi)$ such that

$$-\frac{2be_{q,j}(t_{j-1})}{\lambda} \int_{t_{j-1}}^{\xi} \dot{e}_{q,j}(t) E_{\alpha,1}(-\lambda t^{\alpha}) dt = -\frac{2be_{q,j}(t_{j-1}) E_{\alpha,1}(-\lambda t_{j-1}^{\alpha})}{\lambda} \int_{t_{j-1}}^{\xi_{0}} \dot{e}_{q,j}(t) dt$$
$$= \frac{2be_{q,j}(t_{j-1}) E_{\alpha,1}(-\lambda t_{j-1}^{\alpha})}{\lambda} (e_{q,j}(t_{j-1}) - e_{q,j}(\xi_{0}))$$
$$\leq \left(\frac{2b}{\lambda} + \frac{b}{\lambda\epsilon}\right) e_{q,j}^{2}(t_{j-1}) + \frac{b\epsilon}{\lambda} \|e_{q,j}\|_{\infty}^{2}, \tag{3.46}$$

where ϵ is an arbitrarily small positive number. Hence,

$$e_{p,j}^{2}(\xi) + (a - b/\lambda)e_{q,j}^{2}(\xi) \leq e_{p,j}^{2}(t_{j-1}) + (a + b/\lambda + b/\lambda\epsilon)e_{q,j}^{2}(t_{j-1}) + b\epsilon/\lambda \|e_{q,j}\|_{\infty}^{2} + \frac{1}{2}\|F\|_{\infty}^{2} + \frac{1}{2}\|e_{p,j}\|_{\infty}^{2} + \frac{(a - b/\lambda)}{2}\|e_{q,j}\|_{\infty}^{2} + \frac{a^{2}}{2(a - b/\lambda)}\|G\|_{\infty}^{2}.$$
 (3.47)

Since the inequality holds for all $\xi \in I_i$, we clearly have for $\epsilon \to 0$

 $\|e_{p,j}\|_{\infty}^{2} + (a-b/\lambda)\|e_{q,j}\|_{\infty}^{2} \leq C(e_{p,j}^{2}(t_{j-1}) + e_{q,j}^{2}(t_{j-1}) + \|F\|_{\infty}^{2} + \|G\|_{\infty}^{2}), \quad (3.48)$ where

$$C = \max\left\{2, 2a + \frac{2b}{\lambda} + \frac{2b}{\lambda\epsilon}, \frac{a^2}{a - b/\lambda}\right\}$$

With the stability inequality at our disposal, we next prove the convergence rate on I_j by induction.

When j = 1, it is obvious that $e_{p,1}(0) = 0 = e_{q,1}(0)$. Next, let us bound $||F||_{\infty}$ and $||G||_{\infty}$. Note that in this case, $F_3 = 0$, and then, Lemma 3.2 immediately indicates

$$||F_1||_{\infty} = ||\phi'' - I_N \phi''||_{\infty} \le CN^{-4}.$$
(3.49)

Similarly, we have $||F_2||_{\infty} \leq CN^{-8}$, $||G_1||_{\infty} \leq CN^{-6}$, and $||G_2||_{\infty} \leq CN^{-6}$. Moreover,

$$\|F_4\|_{\infty} = b\|(I - I_N)\mathcal{B}e_{q,1}(s)\|_{\infty} \le C\|(I - I_N)(\mathcal{B}e_{q,1} - B_N\mathcal{B}e_{q,1})\|_{\infty} \le C(1 + \log N)\|\mathcal{B}e_{q,1} - B_N\mathcal{B}e_{q,1}\|_{\infty} \le C(1 + \log N)N^{-\alpha}\|e_{q,1}\|_{\infty},$$
(3.50)

where $\log N$ is the Lebesgue constant of the operator I_N .

Combining (3.49)–(3.50), we have

$$\|e_{p,1}\|_{\infty}^{2} + (a - b/\lambda)\|e_{q,1}\|_{\infty}^{2} \le CN^{-8} + C(1 + \log N)N^{-2\alpha}\|e_{q,1}\|_{\infty}^{2}.$$
 (3.51)

For sufficiently large N, we can always have $(1 + \log N)^2 N^{-2\alpha} \le (a - b/\lambda)/2C$. Therefore,

$$||e_{p,1}||_{\infty} \le CN^{-4}$$
, and $||e_{q,1}||_{\infty} \le CN^{-4}$. (3.52)

Hence, (3.38) is true for j = 1.

Suppose our estimate is true for all $j = 1, \dots, k$, let us consider the case j = k + 1. From (3.48), the argument is similar to the case j = 1, except for the use of [6, (5.5.28)]:

$$\begin{aligned} \|F_1\|_{\infty} &= \|\dot{p}^j - I_N \dot{p}^j\|_{\infty} \le CN^{5/2-m}, \quad \|F_2\|_{\infty} = \|q^j - I_N q^j\|_{\infty} \le CN^{1/2-m}, \\ \|G_1\|_{\infty} &= \|\dot{q}^j - I_N \dot{q}^j\|_{\infty} \le CN^{3/2-m}, \quad \|G_2\|_{\infty} = \|p - I_N p\|_{\infty} \le CN^{3/2-m}. \end{aligned}$$

$$(3.53)$$

Since $E_{\alpha,1}(-\lambda(t-s)^{\alpha})$ is increasing on *s*, we conclude $e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha}) \ge 0$. Thus,

$$\|F_{3}\|_{\infty} = \left\|\sum_{n=1}^{k} \int_{t_{n-1}}^{t_{n}} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})e_{q,n}(s)ds\right\|_{\infty}$$

$$\leq \max_{1 \leq n \leq k} \|e_{q,n}\|_{\infty} \int_{0}^{t_{k}} e_{\alpha,\alpha}(-\lambda(t-s)^{\alpha})ds$$

$$= \max_{1 \leq n \leq k} \|e_{q,n}\|_{\infty} [E_{\alpha,1}(-\lambda(t-t_{n})^{\alpha}) - E_{\alpha,1}(-\lambda t^{\alpha})]$$

$$\leq \max_{1 \leq n \leq k} \|e_{q,n}\|_{\infty} \leq CN^{-\min\{4,m-5/2\}}.$$
(3.54)

Therefore,

$$\|e_{p,k+1}\|_{\infty}^{2} + (a - b/\lambda)\|e_{q,k+1}\|_{\infty}^{2} \le CN^{-\min\{8,2m-5\}},$$
(3.55)

where C depends on u, a, b, λ , and T, but independent of N. This ends the proof. \Box

Remark 3.5 If u(t) satisfies the condition that it has an absolutely continuous (m - 1)st derivative $u^{(m-1)}$ on [0, T] for some m > 2 with $u^{(m-1)}(t) = m^{(m-1)}(0) + \int_0^T g(y) dy$, where g is absolutely integrable and of bounded variation $Var(g) < \infty$ on [0, T], we can easily improve the result (3.38) to

$$||p - p_N||_{\infty} + (a - b/\lambda)||q - q_N||_{\infty} \le CN^{-\min\{4, m-2\}}$$

by using [42, Theorem 4.5].



Fig. 6 Left: initial profile. Middle: evolution of E(x, t) at time points t = 0 (blue), t = 0.375 (green), t = 0.75 (black), and t = 1.275 (red). Right: 3D solution illustration of E(x, t)

3.5 Numerical experiments

Example 3.3 Consider the one-dimensional Cole-Cole model (2.17) with $x \in [0, 2]$. At t = 0, we choose an initial square impulse on $x \in [0.9, 1.1]$ and $u_t(x, 0) = 0$.

To be consistent with the parameters used in numerical experiments of [8, p. 61], we take c = 1 and d = 74/75. Clearly, we observe that the electric field propagate E evolves in a similar fashion as solution of classical wave equation in a finite interval domain (cf. [36, p. 63]), which is, a wave bounces back and forth many times. Unlike the classical problem, the magnitude of E in our example damps along with time because of energy loss. The time evolution of electric field E of (2.16) for $\alpha = 0.6$, T = 1.5 is presented in Fig. 6. In the experiment, we use a polynomial degree of order 200 in spatial approximation and collocation points of number 20 on each time subinterval of length 0.3.

Example 3.4 We consider the two-dimensional Cole-Cole model (2.17) for $(x, y) \in [0, 2]^2$ with smooth initial pulse $u(x, y, 0) = \sin(2\pi x) \sin(\pi y/2)$.

In Fig. 7, we depict the numerical solutions at different time and record the evolution of numerical energy. Observe that the numerical solutions at different times have very similar shapes, but the magnitude seems to decrease as time increases. Although the numerical energy does not decay monotonically, it is bounded by the initial energy (cf. Theorem 3.1 and Remark 3.1).



Fig. 7 Numerical solution of (2.17) with 20 collocation points on each time interval for time T = 0, 5, 10, 15, and 20, respectively. The last figure is for numerical energy evolution with respect to time

4 Discussion and conclusion

In this paper, we have shown that the high-dimensional Cole-Cole model can be transformed into a temporal PIDE with weakly singular kernel through the adoption of a new auxiliary variable and electric polarization. Furthermore, by taking advantage of the special feature of the PIDE, we apply a domain separation technique to convert the equation into a set of ordinary integro-differential equations, so the model can be solved more efficiently. Moreover, we have carefully exploited the singular behavior of solution of a typical ordinary integro-differential equation and designed a catered numerical algorithm for it. It is noteworthy that to combat the singular integral in our algorithm, some technical mapped Gauss-Jacobi numerical quadrature seems indispensable.

Another aspect of our algorithm that needs investigation is its fast algorithm counterpart. Similar to the fast algorithm for weakly singular kernel integration [19] or Caputo fractional derivative [16], a promising way is to apply the fast multipole method to find an accurate approximation for the Laplace transform of the kernel $e_{\alpha,\alpha}(-\lambda t^{\alpha}), 0 < \alpha < 1, \lambda > 0$, or the function $1/(\lambda + s^{\alpha})$. Runge's approximation theorem (cf. [35, p. 61]) assures the existence of such an approximation. We hope to report this in a forthcoming research paper.

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