Numer Algor (2017) 75:845–878
DOI 10.1007/s11075-016-0223-7

ORIGINAL PAPER

Stability of fully discrete schemes with interpolation-type fractional formulas for distributed-order subdiffusion equations

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Received: 30 November 2015 / Accepted: 11 October 2016 / Published online: 3 November 2016

Abstract Two fully discrete methods are investigated for simulating the distributed-order sub-diffusion equation in Caputo's form. The fractional Caputo derivative is approximated by the Caputo's BDF1 (called L1 early) and BDF2 (or L1-2 when it was first introduced) approximations, which are constructed by piecewise linear and quadratic interpolating polynomials, respectively. It is shown that the first scheme, using the BDF1 formula, possesses the discrete minimum-maximum principle and nonnegativity preservation property such that it is stable and convergent in the maximum norm. The method using the BDF2 formula is shown to be stable and convergent in the discrete H^1 norm by using the discrete energy method. For problems of distributed order within a certain region, the method is also proven to preserve the discrete maximum principle and nonnegativity property. Extensive numerical experiments are provided to show the effectiveness of numerical schemes, and to examine the initial singularity of the solution. The applicability of our numerical algorithms to a problem with solution which lacks the smoothness near the initial time is examined by employing a class of power-type nonuniform meshes.

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Keywords Fractional subdiffusion equations · Caputo derivative · Caputo's BDF formulas · Minimum-maximum principle · Discrete energy method · Stability and convergence

1 Introduction

We propose two numerical methods for solving distributed-order time-fractional subdiffusion equations. Consider a nonnegative function $\rho(\alpha)$ that acts as the weight for the order of fractional differentiation $\alpha \in (0, \beta) \subseteq (0, 1)$ such that $\int_0^\beta \rho(\alpha)\,\mathrm{d}\alpha = \rho_0 > 0$ where $\beta \leqslant 1$ and ρ_0 are positive constants. For the sake of simplicity, we assume that $\rho(\alpha) \in \mathcal{C}([0, \beta])$ and $P_{[g]}(\alpha) \triangleq \rho(\alpha) D_t^\alpha g(t) \in \mathcal{C}_\alpha^2([0, \beta])$ uniformly with respect to $t \geq 0$, where $D_t^\alpha g(t)$ is the fractional Caputo derivative of order α, defined by

$$D_t^\alpha g(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{g'(s)\,\mathrm{d}s}{(t-s)^\alpha}, \quad 0 < \alpha < 1. \tag{1.1}$$

Consider the following initial-boundary value problem

$$_\rho D_t^{[\alpha]} u = \frac{\partial^2 u}{\partial x^2} + f(x, t), \quad x \in \Omega,\ 0 < t \leqslant T, \tag{1.2}$$

$$u(x, t) = u_b(x, t), \quad x \in \partial\Omega,\ 0 < t \leqslant T, \tag{1.3}$$

$$u(x, 0) = \varphi(x), \quad x \in \bar{\Omega} = \Omega \cup \partial\Omega, \tag{1.4}$$

where the domain $\Omega = (0, L)$, $\partial\Omega$ is the boundary, and $_\rho D_t^{[\alpha]} g(t)$ denotes the distributed order fractional derivative of $g(t)$ in time t (with respect to the weight ρ) defined by

$$_\rho D_t^{[\alpha]} g(t) = \int_0^\beta \rho(\alpha) D_t^\alpha g(t)\,\mathrm{d}\alpha = \int_0^\beta P_{[g]}(\alpha)\,\mathrm{d}\alpha. \tag{1.5}$$

Fractional differential equations where the order of differentiation is integrated over a given range have been considered by Caputo [6], where the distributed-order derivative is used to describe the stress-strain relation in dielectrics. Lorenzo and Hartley [24] apply the distributed-order derivative to study the rheological properties of composite materials. Atanackovic [2] proposed a distributed-order viscoelastic model for the uniaxial isothermal deformation of a viscoelastic body, and analyzed a Cauchy problem for distributed-order diffusion-wave equation [3, 4]. The distributed-order model (1.2) often describes retarding sub-diffusion or ultraslow diffusion [7], where the mean squared variance grows logarithmically with time. Compared with single-term or multi-term fractional differential equations, the distributed-order fractional model provides a more flexible and precise tool to describe some real physical phenomena in disordered, viscoelastic media, and composite materials, see [12].

The solution and mathematical analysis of the problem (1.2) has attracted more attentions, see [5, 13, 19, 20, 25, 26, 28]. Bagley and Torvik [5] gave some solutions in series expansion. Kochubei [19] constructed the fundamental solutions of (1.2) and proved their positivity and subordination property. Meerschaert et al. [28] provided explicit strong solutions and their stochastic analogues of the problem. Luchko [25, 26] shown a maximum principle and nonnegativity property of the solution and investigated some uniqueness and existence results of solutions to boundary value problems. By using a functional calculus approach, the well-posedness of a Cauchy problem was discussed in [13] recently. The asymptotic behaviors of the solution for $t \to 0$ and $t \to \infty$ were investigated in [20].

There are also some works focused on numerical methods of the distributed-order differential equations, see [8, 9, 11, 15, 16, 18, 22, 29, 31, 34]. Diethelm and Ford [8] introduced a general framework for distributed-order ordinary differential equations by using the quadrature rule, such as the trapezoidal formula, with some suitable numerical solver for the resulting multi-term fractional equations, while a convergence analysis of the method was discussed in [9]. For a class of distributed-order fractional ordinary differential equations, Katsikadelis [18] applied the trapezoidal quadrature rule for the integral (1.5) and use the analogue equation method to solve the resulting multi-term fractional differential equation. Liao et al. [22] suggested a Du Fort-Frankel-type explicit scheme for solving a distributed-order subdiffusion equation by combining the L1 formula of Riemann-Liouville derivative with the mid-point quadrature of the weighted integral. By using the L1 discrete formula of Caputo derivative and the fractional centred difference of space-fractional Riesz derivative, an implicit method was investigated in [34] for the time distributed-order and Riesz space-fractional diffusions. It shown that the numerical method is convergent in time with an order of $O(\tau^{1+h_\alpha/2})$, where τ is the time-step size and h_α is the spacing of fractional-order interval. By applying the backward difference formula (BDF) for the α-order Caputo derivative (1.1) and the mid-point quadrature rule of (1.5), Morgado and Rebelo [29] developed an implicit difference method for (1.2) with a Lipschitz nonlinear reaction term. It shown that the method is convergent with an temporal order of $O(\tau^{1+h_\alpha/2})$. Mashayekhi et al. [31] established a new approximation for solving distributed-order fractional differential equations by using hybrid functions. Jin et al. [15] proposed two Galerkin finite element methods based on the Laplace transform and a convolution quadrature for Riemann-Liouville derivative generated by the backward Euler method. Optimal convergence rates of the two methods in the L^2 norm were established in terms of the regularity of initial data. The discrete maximum principle of the finite element approximation for subdiffusion models was discussed in [16]. To update the time accuracy, Gao et al. [11] devoted to construct temporally second-order methods for (1.2). They applied the weighted and shifted Grünwald (WSG) formula of Riemann-Liouville derivative, which was proposed in [33], to approximate the involved Caputo derivative, and employed the trapezoid and Simpson formulas of the integral (1.5). Note that, a sufficient condition $\frac{\partial^k u}{\partial t^k}(x, 0) = 0$ ($k = 0, 1, 2, 3, 4$) was imposed in [11] for second-order convergence because of the application of WSG approximation.

The main contribution of this work consists of the following two aspects. At first, the distributed-order Caputo derivative (1.5) is approximated by combining the Caputo's BDF1 (so-called L1) formula of Caputo derivative (1.1) with the mid-point quadrature of the ρ-weighted integral. We call the resulting method CBDF1 method and prove that it preserves the discrete minimum-maximum principle and nonnegative-preserving property (Theorem 3.3), which are basic principles of the continuous model [25, 26]. If the solution is smooth, the temporal accuracy is shown to be of order $O(\tau^{2-\beta}\,|\ln\tau|^{-1})$, see Theorem 3.5. Secondly, we present a new interpretation of the L1-2 formula [10], called Caputo's BDF2 here, of Caputo derivative and apply it to approximate the fractional derivative (1.1). The resulting method, denoted by CBDF2, is shown to be stable and convergent by the H^1 discrete energy analysis, see Theorems 4.6 and 4.7. More interestingly, if $0 < \beta \leqslant 1/3$, we find that the CBDF2 method also preserves the minimum-maximum principle and nonnegative property such that the second-order accuracy will be recovered for smooth solution, see Theorems 4.12 and 4.13.

For simplicity of presentation, only one-dimensional problem is considered because the two- and three-dimensional extensions of our approaches and numerical analysis are straightforward. The rest of this paper is arranged as follows. Two numerical Caputo derivatives and some preliminary lemmas are presented in the next section. The CBDF1 scheme is proposed in Section 3, where the maximum norm stability and convergence are achieved by using the maximum principle. Section 4 witnesses the construction and discrete energy analysis of the CBDF2 method. Also, the maximum principle is applied to improve the error estimate for $0 < \beta \leqslant \frac{1}{3}$. Numerical examples are included in Section 5, and some remarks including two open problems are presented in the concluding section.

2 Numerical Caputo derivative and some preliminary lemmas

For a positive integer N, let the time-step size $\tau = T/N$, $t_n = n\tau$, $0 \leqslant n \leqslant N$, and $t_{n+\frac{1}{2}} = (n + \frac{1}{2})\tau$. The domain $[0, T]$ is covered by $\{t_n | \, 0 \leqslant n \leqslant N\}$. Given any discrete time function $w_\tau = \{w^n | \, 0 \leqslant n \leqslant N\}$, denote $w^{n-\frac{1}{2}} = \left(w^n + w^{n-1}\right)/2$ and $\delta_t w^{n-\frac{1}{2}} = \frac{1}{\tau}\left(w^n - w^{n-1}\right)$.

2.1 Discrete Caputo derivative

The Caputo's BDF1 (L1) approximation of the fractional Caputo derivative $D_t^\alpha g(t_n)$ in the time interval $\cup_{k=1}^n [t_{k-1}, t_k]$ can be obtained by applying the linear interpolating polynomial $\Pi_{1,k} g(t)$ of $g(t)$ in each small interval $[t_{k-1}, t_k](1 \leqslant k \leqslant n)$, that is,

$$D_t^\alpha g(t_n) \approx \mathcal{D}_{B1}^\alpha g^n = \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^{n} \int_{t_{k-1}}^{t_k} \frac{\left(\Pi_{1,k} g(s)\right)' \, \mathrm{d}s}{(t_n - s)^\alpha} = \sum_{k=1}^{n} a_{n-k}^{(\alpha)} \left(\delta_t g^{k-\frac{1}{2}}\right), \tag{2.1}$$

where $g^k = g(t_k)$ for $0 \leqslant k \leqslant n$, and the coefficient $a_k^{(\alpha)}$ defined by

$$a_k^{(\alpha)} = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \left[(k+1)^{1-\alpha} - k^{1-\alpha}\right], \quad k \geq 0. \tag{2.2}$$

This most popular approximation (2.1) was originally studied for the sub-diffusion model in [27] provided that the solution is sufficiently smooth, and was discussed in [17] for more general cases. Without the forcing term, the scheme analyzed in previous two studies is equivalent to the discontinuous Galerkin scheme developed in [32].

To construct high-order approximation of the derivative $D_t^\alpha g(t_n)$, we also define

$$b_k^{(\alpha)} = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\left[\frac{(k+1)^{2-\alpha}-k^{2-\alpha}}{2-\alpha} - \frac{(k+1)^{1-\alpha}+k^{1-\alpha}}{2}\right], \quad k \geq 0. \quad (2.3)$$

The following lemmas states some properties of $a_k^{(\alpha)}$, $b_k^{(\alpha)}$, and the relationship between them.

Lemma 2.1 *The positive coefficient $a_k^{(\alpha)}$ defined by (2.2) fulfils*

$$a_{k-1}^{(\alpha)} > \frac{\tau\, t_k^{-\alpha}}{\Gamma(1-\alpha)} > a_k^{(\alpha)}, \quad a_{k-1}^{(\alpha)} - a_k^{(\alpha)} > a_k^{(\alpha)} - a_{k+1}^{(\alpha)}, \quad k \geq 1\,.$$

Proof The decreasing property of function $x^{-\alpha}$ yields

$$a_{k-1}^{(\alpha)} = \int_{t_{k-1}}^{t_k} \frac{s^{-\alpha}\,\mathrm{d}s}{\Gamma(1-\alpha)} > \frac{\tau\, t_k^{-\alpha}}{\Gamma(1-\alpha)} > a_k^{(\alpha)}, \quad k \geq 1.$$

Lemma 2.2 in [22] shows that $a_k^{(\alpha)}$ is concave and completes the proof. □

Lemma 2.2 *The positive coefficient $b_k^{(\alpha)}$ defined by (2.3) fulfils $b_{k-1}^{(\alpha)} > b_k^{(\alpha)}$, $k \geq 1$.*

Proof Note that $\tau b_{k-1}^{(\alpha)}$ represents numerical error of the trapezoidal formula for the convex function $s^{1-\alpha}/\Gamma(2-\alpha)$ in the cell $[t_{k-1}, t_k]$ and there exists $\xi_k \in (t_{k-1}, t_k)$ $(k \geq 1)$ such that

$$b_{k-1}^{(\alpha)} = \frac{1}{\tau}\int_{t_{k-1}}^{t_k} \frac{s^{1-\alpha}\,\mathrm{d}s}{\Gamma(2-\alpha)} - \frac{t_k^{1-\alpha}+t_{k-1}^{1-\alpha}}{2\Gamma(2-\alpha)} = \frac{\alpha\tau\xi_k^{-1-\alpha}}{12\Gamma(1-\alpha)} > \frac{\alpha\tau t_k^{-1-\alpha}}{12\Gamma(1-\alpha)} > b_k^{(\alpha)} > 0,$$

where the decreasing property of function $x^{-1-\alpha}$ has been used. The proof is completed. □

Lemma 2.3 *For $a_k^{(\alpha)}$ and $b_k^{(\alpha)}$ defined by (2.2) and (2.3), respectively, $b_k^{(\alpha)} < \frac{1}{2}a_k^{(\alpha)}$ for $k \geq 0$.*

Proof The proof of Lemma 3 in [1] implies that

$$\frac{1}{2} < \chi_\alpha(\lambda) \triangleq \frac{(\lambda+1)^{2-\alpha} - \lambda^{2-\alpha} - (2-\alpha)\lambda^{1-\alpha}}{(2-\alpha)\left[(\lambda+1)^{1-\alpha} - \lambda^{1-\alpha}\right]} \leqslant \frac{1}{2-\alpha}, \quad \forall\, \lambda \geq 0.$$

It is easy to check that

$$\frac{(k+1)^{2-\alpha}-k^{2-\alpha}}{2-\alpha} - \frac{(k+1)^{1-\alpha}+k^{1-\alpha}}{2} = \left(\chi_\alpha(k) - \frac{1}{2}\right)\left[(k+1)^{1-\alpha} - k^{1-\alpha}\right], \quad k \geq 0.$$

We apply the definition (2.2) and (2.3) to get

$$b_k^{(\alpha)} = \left(\chi_\alpha(k) - \frac{1}{2}\right)a_k^{(\alpha)} \leqslant \frac{\alpha}{2(2-\alpha)}a_k^{(\alpha)} < \frac{1}{2}a_k^{(\alpha)}, \quad k \geq 0,$$

which ensures the lemma. □

As done in [10], the Caputo's BDF2 approximation $\mathcal{D}_{B2}^{\alpha} g^n$ is constructed as follows. In each cell $[t_{k-1}, t_k]$ $(2 \leqslant k \leqslant n)$, the quadratic interpolating polynomial $\Pi_{2,k} g(t)$ $(2 \leqslant k \leqslant n)$ of three points $(t_{k-2}, g(t_{k-2}))$, $(t_{k-1}, g(t_{k-1}))$, and $(t_k, g(t_k))$ is used and the linear interpolating polynomial $\Pi_{1,1} g(t)$ is applied in the first small cell $[0, t_1]$. Thus, we have

$$\begin{aligned}\mathcal{D}_{B2}^{\alpha} g^n &= \frac{1}{\Gamma(1-\alpha)}\left[\int_{t_0}^{t_1} \frac{\left(\Pi_{1,1} g(s)\right)' \,\mathrm{d}s}{(t_n - s)^{\alpha}} + \sum_{k=2}^{n} \int_{t_{k-1}}^{t_k} \frac{\left(\Pi_{2,k} g(s)\right)' \,\mathrm{d}s}{(t_n - s)^{\alpha}}\right] \\ &= \sum_{k=1}^{n} a_{n-k}^{(\alpha)} \left(\delta_t g^{k-\frac{1}{2}}\right) + \sum_{k=2}^{n} b_{n-k}^{(\alpha)} \left(\delta_t g^{k-\frac{1}{2}} - \delta_t g^{k-\frac{3}{2}}\right), \quad n \geq 1. \end{aligned} \tag{2.4}$$

Here and hereafter, the sums are always set to zero if the upper summation index is less than the lower one. Note that, if $\alpha = 1$, $a_0^{(\alpha)} = 1$, $a_k^{(\alpha)} = 0$ $(k \geq 1)$, $b_0^{(\alpha)} = \frac{1}{2}$ and $b_k^{(\alpha)} = 0$ $(k \geq 1)$. Thus, the discrete formula reduces into the well-known BDF2 approximation of $g'(t)$, $\lim_{\alpha \to 1} \mathcal{D}_{B2}^{\alpha} g^n = \frac{3}{2}\delta_t g^{n-\frac{1}{2}} - \frac{1}{2}\delta_t g^{n-\frac{3}{2}}$, $n \geq 2$. This is why we call (2.4) a Caputo's BDF2 formula. The consistency of the fractional BDF2 formula is stated in the following lemma.

Lemma 2.4 [10] *Suppose that* $0 < \alpha < 1$ *and* $g(t) \in \mathcal{C}^3[t_0, t_n]$. *For the Caputo's BDF2 formula* $\mathcal{D}_{B2}^{\alpha} g^n$ *defined by* (2.4)*, it holds that*

$$\begin{aligned} \left|D_t^{\alpha} g(t_1) - \mathcal{D}_{B2}^{\alpha} g^1\right| &\leqslant \frac{\tau^{2-\alpha}}{2\Gamma(3-\alpha)} \max_{t_0 \leqslant t \leqslant t_1} \left|g''(t)\right|, \\ \left|D_t^{\alpha} g(t_n) - \mathcal{D}_{B2}^{\alpha} g^n\right| &\leqslant \frac{(t_n - t_1)^{-1-\alpha}\tau^3}{12\Gamma(1-\alpha)} \max_{t_0 \leqslant t \leqslant t_1} \left|g''(t)\right| + \frac{2\tau^{3-\alpha}}{3\Gamma(3-\alpha)} \max_{t_0 \leqslant t \leqslant t_n} \left|g'''(t)\right|, \quad n \geq 2. \end{aligned}$$

Hereafter, any subscripted C, such as C_g, C_ρ, C_{P_g}, and C_{P_u}, denotes a generic positive constant, not necessarily the same at different occurrences, which is always dependent on the solution and the given data but independent of the grid parameters τ, h_α and h.

2.2 Numerical approximation for distributed-order derivatives

For a positive integer N_α, let $h_\alpha = \beta/N_\alpha$ and $\alpha_{\ell-\frac{1}{2}} = (\ell - \frac{1}{2})h_\alpha$, $1 \leqslant \ell \leqslant N_\alpha$. We define the following coefficients

$$a_k \equiv h_\alpha \sum_{\ell=1}^{N_\alpha} a_k^{(\alpha_{\ell-\frac{1}{2}})} \rho(\alpha_{\ell-\frac{1}{2}}), \quad b_k \equiv h_\alpha \sum_{\ell=1}^{N_\alpha} b_k^{(\alpha_{\ell-\frac{1}{2}})} \rho(\alpha_{\ell-\frac{1}{2}}), \quad k \geq 0, \tag{2.5}$$

where $a_k^{(\alpha_{\ell-\frac{1}{2}})}$ and $b_k^{(\alpha_{\ell-\frac{1}{2}})}$ are defined by (2.2) and (2.3), respectively. According to Lemmas 2.1–2.3, one can get the following three lemmas.

Lemma 2.5 *The positive coefficient* a_k *defined by* (2.5) *fulfils*

$$a_{k-1} > \tau \sum_{\ell=1}^{N_\alpha} \frac{h_\alpha \rho(\alpha_{\ell-\frac{1}{2}})}{\Gamma(1-\alpha_{\ell-\frac{1}{2}})} t_k^{-\alpha_{\ell-\frac{1}{2}}} > a_k, \quad a_{k-1} - a_k > a_k - a_{k+1}, \quad k \geq 1\,.$$

Lemma 2.6 *The positive coefficient* b_k *defined by* (2.5) *satisfies* $b_{k-1} > b_k$, $k \geq 1$.

Lemma 2.7 *For the coefficients* a_k *and* b_k *defined by* (2.5), $b_k < \frac{1}{2}a_k$ *for* $k \geq 0$.

For simplcity of presentation, we define

$$d_m(t_k) \triangleq \sum_{\ell=1}^{N_\alpha} \frac{h_\alpha \rho(\alpha_{\ell-\frac{1}{2}})}{\Gamma(m-\alpha_{\ell-\frac{1}{2}})} t_k^{-\alpha_{\ell-\frac{1}{2}}}, \quad m \geq 1, k \geq 1. \tag{2.6}$$

In error analysis, it is necessary to evaluate $d_m(t_k)$ in detail. Now, we establish two inequalities as follows. Note that the positive function $q(x) = \int_0^1 x^{-\alpha}\,\mathrm{d}\alpha$ is decreasing for $x > 0$ such that $q(x) \leqslant q(\frac{1}{2}) = \frac{1}{\ln 2} \leqslant \frac{2}{\ln 2}$ if $x \geq \frac{1}{2}$. If $x \leqslant \frac{1}{2}$, $q(x) = \frac{x^{-1}-1}{\ln(x^{-1})} \leqslant \frac{x^{-1}}{\ln(x^{-1})}$. We get

$$q(x) \leqslant \frac{\max\left(x^{-1}, 2\right)}{\ln\left(\max\left(x^{-1}, 2\right)\right)} \equiv \frac{\mu(x)}{\ln \mu(x)}, \quad x > 0, \tag{2.7}$$

where $\mu(x) \triangleq \max\left(x^{-1}, 2\right)$ here and hereafter. On the other hand, $q(x) = \frac{1-x}{x\ln(x^{-1})} \geq \frac{x^{-1}}{2\ln(x^{-1})}$ if $x \leqslant \frac{1}{2}$. If $x \geq \frac{1}{2}$, $q(x) = x^{-1}\int_0^1 x^{1-\alpha}\,\mathrm{d}\alpha \geq x^{-1}\int_0^1 2^{\alpha-1}\,\mathrm{d}\alpha = \frac{x^{-1}}{2\ln 2}$. Thus,

$$q(x) \geq \frac{x^{-1}}{2\ln \mu(x)}, \quad x > 0. \tag{2.8}$$

It is easy to check that $\frac{t^{-\beta}-1}{\ln(t^{-1})} = \beta q(t^\beta)$. Then, the inequalities (2.7)–(2.8) yield

$$\frac{\beta t^{-\beta}}{2\ln \mu(t^\beta)} \leqslant \frac{t^{-\beta}-1}{\ln(t^{-1})} \leqslant \frac{\beta \mu(t^\beta)}{\ln \mu(t^\beta)}, \quad t > 0. \tag{2.9}$$

Lemma 2.8 *Let* $\rho(\alpha) \in \mathcal{C}([0,\beta])$. *For the coefficients* a_k *and* $d_m(t_k)$ *defined by* (2.5)–(2.6),

(a) $\quad \dfrac{C_\rho \beta}{2t_k^\beta \ln \mu(t_k^\beta)} \leqslant d_m(t_k) \leqslant \dfrac{C_\rho \beta \mu(t_k^\beta)}{\ln \mu(t_k^\beta)}, \quad m \geq 1, k \geq 1;$

(b) $\quad \dfrac{\tau}{a_{k-1}} \leqslant C_\rho \beta^{-1} t_k^\beta \ln \mu(t_k^\beta), \quad k \geq 1;$

(c) $\quad \displaystyle\sum_{k=\nu+1}^{n} a_{n-k} \leqslant \frac{C_\rho \beta t_{n-\nu} \mu(t_{n-\nu}^\beta)}{\ln \mu(t_{n-\nu}^\beta)}, \quad 0 \leqslant \nu \leqslant n-1.$

Proof From the definition (2.6), one has

$$d_m(t_k) \sim \int_0^{\beta} \frac{\rho(\alpha)t_k^{-\alpha}}{\Gamma(m-\alpha)}\,\mathrm{d}\alpha = \frac{\rho(\theta)}{\Gamma(m-\theta)}\int_0^{\beta} t_k^{-\alpha}\,\mathrm{d}\alpha = \frac{\rho(\theta)}{\Gamma(m-\theta)}\frac{t_k^{-\beta}-1}{\ln(t_k^{-1})}, \quad 0<\theta<1.$$

Thus, the inequalities (a) follow from (2.9). Lemma 2.5 and the first inequality of (a) yields the inequality (b), that is, $\frac{\tau}{a_{k-1}} < \frac{1}{d_1(t_k)} \leqslant C_\rho \beta^{-1} t_k^{\beta} \ln\mu(t_k^{\beta})$. From the definitions (2.2) and (2.5), one applies the second inequality of (a) to get

$$\sum_{k=\nu+1}^{n} a_{n-k} = \sum_{\ell=1}^{N_\alpha} \frac{h_\alpha \rho(\alpha_{\ell-\frac{1}{2}}) t_{n-\nu}^{1-\alpha_{\ell-\frac{1}{2}}}}{\Gamma(2-\alpha_{\ell-\frac{1}{2}})} = t_{n-\nu} d_2(t_{n-\nu}) \leqslant \frac{C_\rho \beta t_{n-\nu}\mu(t_{n-\nu}^{\beta})}{\ln\mu(t_{n-\nu}^{\beta})}.$$

Thus, the inequality (c) is verified and the proof is completed. □

Now, we combine the second-order midpoint formula for the weighted integral with the two interpolation-type formulas $\mathcal{D}_{B1}^{\alpha} g^n$ and $\mathcal{D}_{B2}^{\alpha} g^n$ defined above to construct two numerical formulas to approximate the distributed-order fractional derivative ${}_\rho D_t^{[\alpha]} g(t_n)$. The first formula is a distributed-order BDF1 approximation,

$${}_\rho\mathcal{D}_{B1}^{[\alpha]} g^n = h_\alpha \sum_{\ell=1}^{N_\alpha} \rho(\alpha_{\ell-\frac{1}{2}}) \mathcal{D}_{B1}^{\alpha_{\ell-\frac{1}{2}}} g^n = \sum_{k=1}^{n} a_{n-k}\big(\delta_t g^{k-\frac{1}{2}}\big), \quad n \geq 1. \tag{2.10}$$

Note that, if $g(t) \in \mathcal{C}^2([0,t_n])$, the BDF1 formula (2.1) is consistent of order $O(\tau^{2-\alpha})$, see [35],

$$\left|D_t^{\alpha} g(t_n) - \mathcal{D}_{B1}^{\alpha} g^n\right| \leqslant \frac{\tau^{2-\alpha}}{2\Gamma(3-\alpha)} \max_{t_0\leqslant t\leqslant t_n} \left|g''(t)\right|.$$

Thus, one applies Lemma 2.8 (a) with $\tau \leqslant 2^{-1/\beta}$ to get

$$\begin{aligned}
\left|{}_\rho D_t^{[\alpha]} g(t_n) - {}_\rho\mathcal{D}_{B1}^{[\alpha]} g^n\right| &\leqslant \sum_{\ell=1}^{N_\alpha} h_\alpha \rho(\alpha_{\ell-\frac{1}{2}}) \left|D_t^{\alpha_{\ell-\frac{1}{2}}} g(t_n) - \mathcal{D}_{B1}^{\alpha_{\ell-\frac{1}{2}}} g^n\right| + C_{P_g} h_\alpha^2 \\
&\leqslant \max_{t_0\leqslant t\leqslant t_n} \left|g''(t)\right| \tau^2 \sum_{\ell=1}^{N_\alpha} \frac{h_\alpha \rho(\alpha_{\ell-\frac{1}{2}}) \tau^{-\alpha_{\ell-\frac{1}{2}}}}{2\Gamma(3-\alpha_{\ell-\frac{1}{2}})} + C_{P_g} h_\alpha^2 \\
&\leqslant \max_{t_0\leqslant t\leqslant t_n} \left|g''(t)\right| \tau^2 d_3(\tau) + C_{P_g} h_\alpha^2 \leqslant C_\rho \tau^{2-\beta} \left|\ln\tau\right|^{-1} \max_{t_0\leqslant t\leqslant t_n} \left|g''(t)\right| + C_{P_g} h_\alpha^2.
\end{aligned}$$

Thus, we have the following lemma.

Lemma 2.9 *Let $g(t) \in \mathcal{C}^2([0,t_n])$, $\rho(\alpha) \in \mathcal{C}([0,\beta])$ and $P_{[g]}(\alpha) \in \mathcal{C}_\alpha^2[0,\beta]$. Then*

$$\left|{}_\rho D_t^{[\alpha]} g(t_n) - {}_\rho\mathcal{D}_{B1}^{[\alpha]} g^n\right| \leqslant C_\rho \tau^{2-\beta} \left|\ln\tau\right|^{-1} \max_{t_0\leqslant t\leqslant t_n} \left|g''(t)\right| + C_{P_g} h_\alpha^2.$$

By applying the Caputo's BDF2 approximation $\mathcal{D}^{\alpha}_{B2}g^n$ defined in (2.4), we have the following numerical formula to approximate the derivative ${}_{\rho}D_t^{[\alpha]}g(t_n)$,

$$
{}_{\rho}\mathcal{D}^{[\alpha]}_{B2}g^n = h_\alpha \sum_{\ell=1}^{N_\alpha} \rho(\alpha_{\ell-\frac{1}{2}})\mathcal{D}_{B2}^{\alpha_{\ell-\frac{1}{2}}} g^n = \sum_{k=1}^{n} a_{n-k}\big(\delta_t g^{k-\frac{1}{2}}\big) + \sum_{k=2}^{n} b_{n-k}\big(\delta_t g^{k-\frac{1}{2}} - \delta_t g^{k-\frac{3}{2}}\big), \tag{2.11}
$$

where $n \geq 1$. In the analysis of distributed-order BDF2 formula, denote

$$
\Upsilon(t) \triangleq \frac{\beta\mu(t^\beta)}{t\ln\mu(t^\beta)}, \quad t > 0. \tag{2.12}
$$

We have the following estimate for the distributed-order BDF2 formula (2.11).

Lemma 2.10 *Let $g(t) \in \mathcal{C}^3([0, t_n])$, $\rho(\alpha) \in \mathcal{C}([0, \beta])$ and $P_{[g]}(\alpha) \in \mathcal{C}^2_\alpha([0, \beta])$. Then*

$$
\left|\mathcal{R}^1\right| \leqslant C_\rho \tau^{2-\beta} |\ln\tau|^{-1} \max_{t_0\leqslant t\leqslant t_1} \left|g''(t)\right| + C_{P_g} h_\alpha^2,
$$

$$
\left|\mathcal{R}^n\right| \leqslant C_\rho \Upsilon(t_{n-1})\tau^3 \max_{t_0\leqslant t\leqslant t_1} \left|g''(t)\right| + C_\rho\tau^{3-\beta}|\ln\tau|^{-1} \max_{t_0\leqslant t\leqslant t_n} \left|g'''(t)\right| + C_{P_g}h_\alpha^2, \quad n \geq 2,
$$

where $\mathcal{R}^n = {}_{\rho}D_t^{[\alpha]}g(t_n) - {}_{\rho}\mathcal{D}^{[\alpha]}_{B2}g^n$, $n \geq 1$, and $\Upsilon(t_{n-1})$ is defined by (2.12).

Proof Applying and Lemma 2.8 (a) with $\tau \leqslant 2^{-1/\beta}$, one has

$$
\begin{aligned}
\left|\mathcal{R}^1\right| &\leqslant \max_{t_0\leqslant t\leqslant t_1} \left|g''(t)\right| \tau^2 \sum_{\ell=1}^{N_\alpha} \frac{h_\alpha \rho(\alpha_{\ell-\frac{1}{2}})\tau^{-\alpha_{\ell-\frac{1}{2}}}}{2\Gamma(3-\alpha_{\ell-\frac{1}{2}})} + C_{P_g}h_\alpha^2 \\
&\leqslant \tau^2 d_3(\tau) \max_{t_0\leqslant t\leqslant t_1} \left|g''(t)\right| + C_{P_g}h_\alpha^2 \leqslant C_\rho\tau^{2-\beta}|\ln\tau|^{-1} \max_{t_0\leqslant t\leqslant t_1} \left|g''(t)\right| + C_{P_g}h_\alpha^2.
\end{aligned}
$$

Now, consider the case of $n \geq 2$. Applying Lemma 2.8 with $\tau \leqslant 2^{-1/\beta}$, we have

$$
\begin{aligned}
K_{11} &= \frac{\tau^3}{12} \sum_{\ell=1}^{N_\alpha} \frac{h_\alpha \rho(\alpha_{\ell-\frac{1}{2}}) t_{n-1}^{-1-\alpha_{\ell-\frac{1}{2}}}}{\Gamma(1-\alpha_{\ell-\frac{1}{2}})} \leqslant \tau^3 \frac{d_1(t_{n-1})}{t_{n-1}} \leqslant C_\rho \Upsilon(t_{n-1})\tau^3, \\
K_{12} &= \frac{2\tau^3}{3} \sum_{\ell=1}^{N_\alpha} \frac{h_\alpha \rho(\alpha_{\ell-\frac{1}{2}})\tau^{-\alpha_{\ell-\frac{1}{2}}}}{\Gamma(3-\alpha_{\ell-\frac{1}{2}})} \leqslant \tau^3 d_3(\tau) \leqslant C_\rho \tau^{3-\beta}|\ln\tau|^{-1}.
\end{aligned}
$$

Then from Lemma 2.4, we obtain

$$
\begin{aligned}
\left|\mathcal{R}^n\right| &\leqslant \max_{t_0\leqslant t\leqslant t_1} \left|g''(t)\right| K_{11} + \max_{t_0\leqslant t\leqslant t_n} \left|g'''(t)\right| K_{12} + C_{P_g}h_\alpha^2 \\
&\leqslant C_\rho \Upsilon(t_{n-1})\tau^3 \max_{t_0\leqslant t\leqslant t_1} \left|g''(t)\right| + C_\rho\tau^{3-\beta}|\ln\tau|^{-1} \max_{t_0\leqslant t\leqslant t_n} \left|g'''(t)\right| + C_{P_g}h_\alpha^2.
\end{aligned}
$$

It completes the proof. □

3 The scheme using CBDF1 approximation

Let $h = L/M$ for a positive integer M and $x_i = ih$, $0 \leqslant i \leqslant M$. Let the discrete grid $\bar{\Omega}_h = \{x_i \mid 0 \leqslant i \leqslant M\}$, $\Omega_h = \bar{\Omega}_h \cap \Omega$ and the boundary $\partial\Omega_h = \bar{\Omega}_h \cap \partial\Omega$. Given grid function $v_h = \{v_i \mid x_i \in \bar{\Omega}_h\}$, we denote $\delta_x v_{i-\frac{1}{2}} = (v_i - v_{i-1})/h$ and $\delta_x^2 v_i = \left(\delta_x v_{i+\frac{1}{2}} - \delta_x v_{i-\frac{1}{2}}\right)/h$.

Let u_i^n be the numerical approximation of the solution $U_i^n = u(x_i, t_n)$. As done in [29], one has the fractional backward Euler methods for solving (1.2)–(1.4),

$$ {}_\rho\mathcal{D}_{B1}^{[\alpha]} u_i^n = \delta_x^2 u_i^n + f_i^n, \quad x_i \in \Omega_h,\ 1 \leqslant n \leqslant N, \tag{3.1} $$

$$ u_i^n = u_b(x_i, t_n),\ x_i \in \partial\Omega_h,\ 1 \leqslant n \leqslant N; \quad u_i^0 = \varphi(x_i),\ x_i \in \bar{\Omega}_h. \tag{3.2} $$

where ${}_\rho\mathcal{D}_{B1}^{[\alpha]} u_i^n$ is defined by (2.10). For simplicity, we call it the CBDF1 method.

3.1 The minimum-maximum principle

Let $\mathfrak{V}_h = \left\{v_h \,\middle|\, v_h \text{ vanishes on } \partial\Omega_h\right\}$ be the space of grid functions. For any grid function $v_h \in \mathfrak{V}_h$, we introduce $\left\|v\right\|_\infty = \max_{x_i \in \Omega_h} \left|v_i\right|$.

Lemma 3.1 *Assume the function $w_h \in \mathfrak{V}_h$ satisfies $\mathcal{L}_h w_i \equiv d w_i - \delta_x^2 w_i = \xi_i$ for $x_i \in \Omega_h$, where the constant $d > 0$. Then it hold that*

$$ \min\left\{0, \min_{x_j \in \Omega_h} \xi_j/d\right\} \leqslant w_i \leqslant \max\left\{0, \max_{x_j \in \Omega_h} \xi_j/d\right\}, \quad x_i \in \Omega_h. $$

Proof This proof is standard, see [30]. □

Lemma 3.2 *Let $\left\{\omega_l^{(n)} \mid 0 \leqslant l \leqslant n-1, n \geq 1\right\}$ be a time-level-dependent sequence of positive numbers with the decreasing property, that is, $\omega_{l-1}^{(n)} \geq \omega_l^{(n)}$ for $1 \leqslant l \leqslant n-1$, $n \geq 2$. Assume that the grid function $v_h^n \in \mathfrak{V}_h$, $0 \leqslant n \leqslant N$, satisfies*

$$ \sum_{k=1}^{n} \omega_{n-k}^{(n)} (\delta_t v_i^{k-\frac{1}{2}}) - \delta_x^2 v_i^n = \xi_i^n, \quad x_i \in \Omega_h, 1 \leqslant n \leqslant N, \tag{3.3} $$

$$ v_i^0 = \phi_i, \quad x_i \in \bar{\Omega}_h, \tag{3.4} $$

Then it hold that, for $k \geq 1$,

$$ \min\left\{0, \min_{x_j \in \Omega_h} \phi_j + \tau \min_{\substack{x_j \in \Omega_h \\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{\omega_{l-1}^{(l)}}\right\} \leqslant v_i^k \leqslant \max\left\{0, \max_{x_j \in \Omega_h} \phi_j + \tau \max_{\substack{x_j \in \Omega_h \\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{\omega_{l-1}^{(l)}}\right\}, \quad x_i \in \Omega_h. \tag{3.5} $$

Proof For simplicity, denote

$$ E_{min}^k = \min\left\{0, \min_{x_j \in \Omega_h} \phi_j + \tau \min_{\substack{x_j \in \Omega_h \\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{\omega_{l-1}^{(l)}}\right\}, \quad E_{max}^k = \max\left\{0, \max_{x_j \in \Omega_h} \phi_j + \tau \max_{\substack{x_j \in \Omega_h \\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{\omega_{l-1}^{(l)}}\right\}, \quad k \geq 1, $$

such that

$$E_{min}^1 \geq E_{min}^2 \geq \cdots \geq E_{min}^n, \quad E_{max}^1 \leqslant E_{max}^2 \leqslant \cdots \leqslant E_{max}^n .$$

Take $n = 1$, the difference (3.3) reads

$$\frac{\omega_0^{(1)}}{\tau} v^1 - \delta_x^2 v_i^1 = \frac{\omega_0^{(1)}}{\tau} v^0 + \xi_i^1, \quad x_i \in \Omega_h.$$

Then Lemma 3.1 implies (3.5) for $k = 1$. Assuming that (3.5) holds for $1 \leqslant k \leqslant n-1$ $(n \geq 1)$,

$$E_{min}^k \leqslant v_i^k \leqslant E_{max}^k , \quad x_i \in \Omega_h, \ 1 \leqslant k \leqslant n-1 .$$

It is easy to check that

$$\begin{aligned}
\Xi_i^n &\equiv \frac{1}{\omega_0^{(n)}} \sum_{l=1}^{n-1} \left(\omega_{n-l-1}^{(n)} - \omega_{n-l}^{(n)}\right) v_i^l + \frac{\omega_{n-1}^{(n)}}{\omega_0^{(n)}} \left(v_i^0 + \frac{\tau}{\omega_{n-1}^{(n)}} \xi_i^n\right) \\
&\geq \frac{1}{\omega_0^{(n)}} \sum_{l=1}^{n-1} \left(\omega_{n-l-1}^{(n)} - \omega_{n-l}^{(n)}\right) E_{min}^l + \frac{\omega_{n-1}^{(n)}}{\omega_0^{(n)}} E_{min}^n \geq E_{min}^n , \\
\Xi_i^n &\leqslant \frac{1}{\omega_0^{(n)}} \sum_{l=1}^{n-1} \left(\omega_{n-l-1}^{(n)} - \omega_{n-l}^{(n)}\right) E_{max}^l + \frac{\omega_{n-1}^{(n)}}{\omega_0^{(n)}} E_{max}^n \leqslant E_{max}^n .
\end{aligned}$$

We write the difference (3.3) as

$$\frac{\omega_0^{(n)}}{\tau} v_i^n - \delta_x^2 v_i^n = \frac{\omega_0^{(n)}}{\tau} \Xi_i^n, \quad x_i \in \Omega_h .$$

It follows from Lemma 3.1 that

$$E_{min}^n \leqslant \min\left\{0, \min_{x_j \in \Omega_h} \Xi_j^n\right\} \leqslant v_i^n \leqslant \max\left\{0, \max_{x_j \in \Omega_h} \Xi_j^n\right\} \leqslant E_{max}^n , \quad x_i \in \Omega_h .$$

Thus, (3.5) holds for $k = n$. The principle of mathematical induction completes the proof. □

Theorem 3.3 *Let the grid function $v_h^n \in \mathfrak{V}_h$, $0 \leqslant n \leqslant N$, satisfies*

$$\begin{aligned}
{}_\rho\mathcal{D}_{B1}^{[\alpha]} v_i^n &= \delta_x^2 v_i^n + \xi_i^n, \quad x_i \in \Omega_h, 1 \leqslant n \leqslant N, \\
v_i^0 &= \phi_i, \quad x_i \in \bar{\Omega}_h.
\end{aligned}$$

Then it hold that, for $k \geq 1$,

$$\min\left\{0, \min_{x_j \in \Omega_h} \phi_j + \tau \min_{\substack{x_j \in \Omega_h \\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{a_{l-1}}\right\} \leqslant v_i^k \leqslant \max\left\{0, \max_{x_j \in \Omega_h} \phi_j + \tau \max_{\substack{x_j \in \Omega_h \\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{a_{l-1}}\right\}, \quad x_i \in \Omega_h.$$

Proof According to Lemma 2.5, the coefficient a_l is positive and decreasing. We complete the proof by taking $\omega_l^{(n)} = a_l$ $(0 \leqslant l \leqslant n-1)$ in Lemma 3.2. □

3.2 Stability and convergence

If the boundary data $u_b(x,t)=0$, Theorem 3.3 implies that the discrete solution u_h^n of the CBDF1 scheme (3.1)–(3.2) satisfies

$$\left\|u^n\right\|_\infty \leqslant \left\|u^0\right\|_\infty + \max_{1\leqslant \ell\leqslant n} \frac{\tau}{a_{\ell-1}}\left\|f(\cdot,t_\ell)\right\|_\infty, \quad n\ge 1.$$

Furthermore, if $u^0(x)\ge 0$ and $f(x,t)\ge 0$, Theorem 3.3 implies the nonnegativity of the discrete solution, that is, $u_i^n\ge 0$ for $x_i\in\Omega_h$, $n\ge 1$.

Theorem 3.4 *The CBDF1 scheme* (3.1)–(3.2) *is nonnegative-preserving and stable in the maximum norm.*

The error function $e_h^n=U_h^n-u_h^n\in\mathfrak{V}_h$ satisfies the error system

$$\begin{aligned} {}_\rho\mathcal{D}_{B1}^{[\alpha]}e_i^n &= \delta_x^2 e_i^n + (R_1)_i^n, \quad x_i\in\Omega_h,\ 1\leqslant n\leqslant N,\\ e_i^0 &= 0,\ x_i\in\bar{\Omega}_h\,. \end{aligned}$$

According to Lemma 2.9, one has $\left\|(R_1)^k\right\|_\infty \leqslant C_{P_u}(\tau^{2-\beta}\left|\ln\tau\right|^{-1}+h_\alpha^2+h^2)$, $k\ge 1$. Thus, we apply Theorem 3.3 and Lemma 2.8 (b) to find

$$\left\|e^n\right\|_\infty \leqslant \tau\max_{1\leqslant k\leqslant n}\frac{\left\|(R_1)^k\right\|_\infty}{a_{k-1}} \leqslant C_{P_u}\max_{1\leqslant k\leqslant n}\beta^{-1}t_k^\beta\ln\mu(t_k^\beta)(\tau^{2-\beta}\left|\ln\tau\right|^{-1}+h_\alpha^2+h^2)\,. \tag{3.6}$$

Theorem 3.5 *Let* $\rho(\alpha)\in\mathcal{C}([0,\beta])$, $P_{[u]}(\alpha)\in\mathcal{C}_\alpha^2([0,\beta])$ *and* $u(x,t)\in\mathcal{C}_{x,t}^{4,2}(\bar{\Omega}\times[0,T])$ *be a smooth solution of the subdiffusion problem* (1.2)–(1.4). *The numerical solution of the CBDF1 scheme* (3.1)–(3.2) *is convergent in the maximum norm in the sense of* (3.6).

We remark that, the error estimate (3.6) suggest that the first-level solution u_h^1 of the CBDF1 scheme (3.1)–(3.2) is second-order accurate in time, that is,

$$\left\|U^1-u^1\right\|_\infty \leqslant C_{P_u}\left(\tau^2+\tau^\beta\left|\ln\tau\right|(h_\alpha^2+h^2)\right), \tag{3.7}$$

which has been verified by numerical tests for smooth solution, see Fig. 2 in Section 5. Nonetheless, the distributed-order diffusion operator has only limited smoothing property [15]. Actually, for single-term fractional Caputo derivative, the Caputo's BDF1 formula (2.1) is first-order accurate, see Lemma 3.2 in [14], $\left|D_t^\alpha g(t_n)-\mathcal{D}_{B1}^\alpha g^n\right|\leqslant C_g t_n^{-1}\tau$ if $g'(t)=O(t^{\alpha-1})$. If $\beta=1$, the CBDF1 scheme (3.1)–(3.2) maintains first-order temporal accuracy for practical solutions of the subdiffusion problem (1.2)–(1.3) with smooth initial data. In this case, the proof of Lemma 2.9 gives $\left\|(R_1)^k\right\|_\infty \leqslant C_{P_u}(t_k^{-1}\tau + h_\alpha^2 + h^2)$, $k \geq 1$. Then, the minimum-maximum Theorem 3.3 implies the first-order convergence in time,

$$\left\|e^n\right\|_\infty \leqslant C_{P_u} \max_{1\leqslant k\leqslant n} \ln\left(\max(t_k^{-1}, 2)\right)\tau + C_{P_u}(h_\alpha^2 + h^2),$$

which coincides with the temporal error estimate of convolution quadrature approximation generated by the backward Euler method, see Theorem 5.2 in [15].

4 The scheme using CBDF2 approximation

By applying the distributed-order BDF2 approximation (2.11), we construct the following CBDF2 method for approximating the problem (1.2)–(1.4),

$$_\rho\mathcal{D}_{B2}^{[\alpha]}u_i^n = \delta_x^2 u_i^n + f_i^n, \quad x_i \in \Omega_h,\ 1 \leqslant n \leqslant N, \tag{4.1}$$

$$u_i^n = u_b(x_i, t_n),\ x_i \in \partial\Omega_h,\ 1 \leqslant n \leqslant N; \quad u_i^0 = \varphi(x_i),\ x_i \in \bar{\Omega}_h. \tag{4.2}$$

4.1 Stability

For two grid functions v_h, w_h, define the discrete inner product $\langle v, w\rangle = h\sum_{i=1}^M v_i w_i$ and $\|v\| = \sqrt{\langle v, v\rangle}$. For any grid function $v_h \in \mathfrak{V}_h$, introduce $\|\delta_x v\| = \sqrt{h\sum_{i=1}^M |\delta_x v_{i-\frac{1}{2}}|^2}$ and $\|\delta_x^2 v\| = \sqrt{h\sum_{i=1}^{M-1} |\delta_x^2 v_i|^2}$. For any $v_h \in \mathfrak{V}_h$, we have $\langle v, -\delta_x^2 v\rangle = \|\delta_x v\|^2$ and

$$\|v\| \leqslant \frac{L}{\sqrt{6}}\|\delta_x v\|. \tag{4.3}$$

We present the following lemmas, which are necessary in the discrete energy analysis.

Lemma 4.1 [23] *Let $\{\omega_l \mid l \geq 0\}$ be a sequence of real numbers with the properties,*

$$\omega_l \geq 0, \quad \omega_{l-1} \geq \omega_l, \quad \omega_{l+1} - 2\omega_l + \omega_{l-1} \geq 0.$$

Then for any positive integer n, and real vector $(V_1, V_2, \cdots, V_n)$ with n real entries,

$$\sum_{k=1}^n V_k\left(\sum_{l=1}^k \omega_{k-l}V_l\right) \geq 0.$$

Lemma 4.2 *Let $\{\omega_k \mid k \geq 0\}$ be a positive and decreasing sequence of real numbers. Then for any positive integer n, and real vector $(V_1, V_2, \cdots, V_n)$ with n real entries,*

$$2\sum_{k=\ell}^n V_k \sum_{l=\ell}^k \omega_{k-l}(V_l - V_{l-1}) \geq \sum_{k=\ell}^n \omega_{n-k}V_k^2 - \sum_{k=\ell}^n \omega_{n-k}V_{\ell-1}^2, \quad n \geq \ell \geq 1.$$

Proof Applying the inequality $2ab \geq -a^2 - b^2$, it is not difficult to get

$$2V_k \sum_{l=\ell}^{k} \omega_{k-l}(V_l - V_{l-1}) = 2V_k \left[\omega_0 V_k - \sum_{l=\ell}^{k-1} (\omega_{k-l-1} - \omega_{k-l}) V_l - \omega_{k-\ell} V_{\ell-1} \right]$$

$$\geq 2\omega_0 V_k^2 - \sum_{l=\ell}^{k-1} (\omega_{k-l-1} - \omega_{k-l})(V_l^2 + V_k^2) - \omega_{k-\ell}(V_{\ell-1}^2 + V_k^2)$$

$$\geq \omega_0 V_k^2 - \sum_{l=\ell}^{k-1} (\omega_{k-l-1} - \omega_{k-l}) V_l^2 - \omega_{k-\ell} V_{\ell-1}^2 = \sum_{l=\ell}^{k} \omega_{k-l} V_l^2 - \sum_{l=\ell}^{(k-1)} \omega_{(k-1)-l} V_l^2 - \omega_{k-\ell} V_{\ell-1}^2.$$

Summing the inequality from $k = \ell$ to n, one has

$$2\sum_{k=\ell}^{n} V_k \sum_{l=\ell}^{k} \omega_{k-l}(V_l - V_{l-1}) \geq \sum_{k=\ell}^{n} \omega_{n-k} V_k^2 - \sum_{k=\ell}^{n} \omega_{k-\ell} V_{\ell-1}^2 = \sum_{k=\ell}^{n} \omega_{n-k} V_k^2 - \sum_{k=\ell}^{n} \omega_{n-k} V_{\ell-1}^2.$$

It completes the proof. □

Lemma 4.3 *Let $u_h^n \in \mathfrak{V}_h$, $1 \leqslant n \leqslant N$, solves the CBDF2 method (4.1)–(4.2) with $u_b(x,t) = 0$ and $f(x,t) = 0$. Then it holds that*

$$\left\|\delta_x u^n\right\|^2 \leqslant \tau \sum_{k=2}^{n} b_{n-k} \left\|\delta_t u^{\frac{1}{2}}\right\|^2 + \left\|\delta_x \varphi\right\|^2 \leqslant \frac{\tau}{a_0^2} \sum_{k=2}^{n} b_{n-k} \left\|\delta_x^2 \varphi\right\|^2 + \left\|\delta_x \varphi\right\|^2, \quad n \geq 1.$$

Proof Taking the inner product of the difference (4.1) by $2\tau \delta_t u_i^{n-\frac{1}{2}}$, one applies the first discrete Green's formula to find

$$2\tau \left\langle {}_\rho\mathcal{D}_{B2}^{[\alpha]} u^n, \delta_t u^{n-\frac{1}{2}} \right\rangle + \left\|\delta_x u^n\right\|^2 - \left\|\delta_x u^{n-1}\right\|^2 + \tau^2 \left\|\delta_t \delta_x u^{n-\frac{1}{2}}\right\|^2 = 0, \quad 1 \leqslant n \leqslant N, \tag{4.4}$$

where the equality $2A^n(A^n - A^{n-1}) = (A^n)^2 - (A^{n-1})^2 + (A^n - A^{n-1})^2$ has been used. Summing (4.4) for the index n from 1 to k and replacing k with n, one has

$$2\tau \sum_{k=1}^{n} \left\langle {}_\rho\mathcal{D}_{B2}^{[\alpha]} u^k, \delta_t u^{k-\frac{1}{2}} \right\rangle + \left\|\delta_x u^n\right\|^2 \leqslant \left\|\delta_x \varphi\right\|^2, \quad n \geq 1. \tag{4.5}$$

Lemma 2.5 shows that $a_l \geq 0$, $a_{l-1} \geq a_l$ and $a_{l+1} - 2a_l + a_{l-1} \geq 0$ for $l \geq 1$. Thus, taking $\omega_l = a_l$ and $V_l = \delta_t u_i^{l-\frac{1}{2}}$ in Lemma 4.1, it is not difficult to get

$$K_{21}^n \triangleq 2\tau \sum_{k=1}^{n} \left\langle \sum_{l=1}^{k} a_{k-l}\left(\delta_t u^{l-\frac{1}{2}}\right), \delta_t u^{k-\frac{1}{2}} \right\rangle \geq 0.$$

Lemma 2.6 states that $\{b_k \,|\, k \geq 0\}$ is a positive and decreasing sequence of real numbers. Taking $\ell = 2$, $\omega_l = b_l$ and $V_l = \delta_t u_i^{l-\frac{1}{2}}$ in Lemma 4.2, we can get

$$K_{22}^n \triangleq 2\tau \sum_{k=2}^{n} \left\langle \sum_{l=2}^{k} b_{k-l}\left(\delta_t u^{l-\frac{1}{2}} - \delta_t u^{l-\frac{3}{2}}\right), \delta_t u^{k-\frac{1}{2}} \right\rangle \geq \tau \sum_{k=2}^{n} b_{n-k} \left\|\delta_t u^{k-\frac{1}{2}}\right\|^2 - \tau \sum_{k=2}^{n} b_{n-k} \left\|\delta_t u^{\frac{1}{2}}\right\|^2.$$

Thus applying the definition (2.11), we have

$$2\tau\sum_{k=1}^{n}\left\langle {}_{\rho}\mathcal{D}_{B2}^{[\alpha]}u^k,\delta_t u^{k-\frac{1}{2}}\right\rangle=\sum_{\ell=1}^{2}K_{2\ell}^{n}\geq\tau\sum_{k=2}^{n}b_{n-k}\left\|\delta_t u^{k-\frac{1}{2}}\right\|^2-\tau\sum_{k=2}^{n}b_{n-k}\left\|\delta_t u^{\frac{1}{2}}\right\|^2. \tag{4.6}$$

Inserting the estimate (4.6) into (4.5), one gets

$$\tau\sum_{k=2}^{n}b_{n-k}\left\|\delta_t u^{k-\frac{1}{2}}\right\|^2+\left\|\delta_x u^n\right\|^2\leqslant\tau\sum_{k=2}^{n}b_{n-k}\left\|\delta_t u^{\frac{1}{2}}\right\|^2+\left\|\delta_x\varphi\right\|^2,\quad n\geq 1. \tag{4.7}$$

Recalling ${}_{\rho}\mathcal{D}_{B2}^{[\alpha]}u^1=a_0(\delta_t u^{\frac{1}{2}})$ and taking the inner product of (4.1) with $n=1$ by $-2\tau\delta_t\delta_x^2u_i^{\frac{1}{2}}$, one applies the first discrete Green's formula to get $\left\|\delta_x^2u^1\right\|\leqslant\left\|\delta_x^2\varphi\right\|$. Thus, the (4.1) of $n=1$ gives $\left\|\delta_t u^{\frac{1}{2}}\right\|=a_0^{-1}\left\|\delta_x^2u^1\right\|\leqslant a_0^{-1}\left\|\delta_x^2\varphi\right\|$. Inserting it into (4.7), we obtain the claimed estimate and complete the proof. □

To prove the stability with respect to the external force, we need the following lemma.

Lemma 4.4 *For any* $\varepsilon>0$*, real sequences* $\left\{w^k\,|\,k\geq\ell-1\geq 0\right\}$ *and* $\left\{f^k\,|\,k\geq\ell\geq 1\right\}$*,*

$$2\tau\sum_{l=\ell}^{k}f^l(\delta_t w^{l-\frac{1}{2}})\leqslant\frac{1}{\varepsilon}\left[(w^{\ell-1})^2+\tau\sum_{l=\ell}^{k-1}(w^l)^2+(w^k)^2\right]+\varepsilon\left[(f^\ell)^2+\tau\sum_{l=\ell}^{k-1}(\delta_t f^{l+\frac{1}{2}})^2+(f^k)^2\right].$$

Proof For $k\geq\ell\geq 1$,

$$2\tau\sum_{l=\ell}^{k}f^l(\delta_t w^{l-\frac{1}{2}})=-2w^{\ell-1}f^\ell-2\tau\sum_{l=\ell}^{k-1}w^l\left(\delta_t f^{l+\frac{1}{2}}\right)+2w^kf^k.$$

Thus, the inequality $2ab\leqslant\frac{1}{\varepsilon}a^2+\varepsilon b^2$ yields the claimed result. □

For the simplicity of presentation, given grid function v_h^n, we denote further

$$\left\|v^n\right\|_{\Sigma}\triangleq\sqrt{\left\|v^2\right\|^2+\tau\sum_{l=2}^{n-1}\left\|\delta_t v^{l+\frac{1}{2}}\right\|^2+\left\|v^n\right\|^2},\quad n\geq 2. \tag{4.8}$$

Lemma 4.5 *Let the grid function* $v_h^n\in\mathfrak{V}_h$*,* $0\leqslant n\leqslant N$*, satisfies*

$${}_{\rho}\mathcal{D}_{B2}^{[\alpha]}v_i^n=\delta_x^2v_i^n+\xi_i^n,\quad x_i\in\Omega_h,\ 1\leqslant n\leqslant N, \tag{4.9}$$

$$v_i^0=0,\quad x_i\in\bar{\Omega}_h. \tag{4.10}$$

Then it holds that

$$\left\|\delta_x v^1\right\|^2 \leqslant \frac{\tau}{a_0}\left\|\xi^1\right\|^2, \quad \left\|\delta_x v^n\right\|^2 \leqslant \exp(t_n)\left(\frac{5\tau}{a_0^2}\sum_{k=2}^{n} a_{n-k}\left\|\xi^1\right\|^2 + \frac{2L^2}{3}\left\|\xi^n\right\|_{\Sigma}^2\right), \quad n \geq 2,$$

where $\left\|\xi^n\right\|_{\Sigma}$ *is defined by* (4.8).

Proof Taking the inner product of (4.9) with $n = 1$ by $\tau\delta_t v_i^{\frac{1}{2}}$, one has

$$a_0\tau\left\|\delta_t v^{\frac{1}{2}}\right\|^2 + \left\|\delta_x v^1\right\|^2 \leqslant \tau\left\langle\xi^1, \delta_t v^{\frac{1}{2}}\right\rangle \leqslant \tau\left\|\delta_t v^{\frac{1}{2}}\right\|\left\|\xi^1\right\|,$$

where the zero-valued data (4.10) and the Cauchy-Schwarz inequality has been used. Then

$$\left\|\delta_t v^{\frac{1}{2}}\right\| \leqslant \frac{1}{a_0}\left\|\xi^1\right\|, \quad a_0\tau\left\|\delta_t v^{\frac{1}{2}}\right\|^2 + \left\|\delta_x v^1\right\|^2 \leqslant \frac{\tau}{a_0}\left\|\xi^1\right\|^2. \tag{4.11}$$

It yields the claimed estimate of $n = 1$. Consider the case of $n \geq 2$. Taking the inner product of the (4.9) by $2\tau\delta_t v_i^{n-\frac{1}{2}}$, one applies the first discrete Green's formula to get

$$2\tau\left\langle {}_\rho\mathcal{D}_{B2}^{[\alpha]} v^n, \delta_t v^{n-\frac{1}{2}}\right\rangle + \left\|\delta_x v^n\right\|^2 - \left\|\delta_x v^{n-1}\right\|^2 + \tau^2\left\|\delta_t\delta_x v^{n-\frac{1}{2}}\right\|^2 = 2\tau\left\langle\xi^n, \delta_t v^{n-\frac{1}{2}}\right\rangle.$$

Summing it for the index n from 2 to k and replacing k with n, one has

$$2\tau\sum_{k=2}^{n}\left\langle {}_\rho\mathcal{D}_{B2}^{[\alpha]} v^k, \delta_t v^{k-\frac{1}{2}}\right\rangle + \left\|\delta_x v^n\right\|^2 - \left\|\delta_x v^1\right\|^2 \leqslant 2\tau\sum_{k=2}^{n}\left\langle\xi^k, \delta_t v^{k-\frac{1}{2}}\right\rangle, \quad n \geq 2. \tag{4.12}$$

As done in the proof of Lemma 4.3, we have

$$2\tau\sum_{k=2}^{n}\left\langle\sum_{l=1}^{k} a_{k-l}\left(\delta_t v^{l-\frac{1}{2}}\right), \delta_t v^{k-\frac{1}{2}}\right\rangle \geq -2a_0\tau\left\|\delta_t v^{\frac{1}{2}}\right\|^2,$$

$$2\tau\sum_{k=2}^{n}\left\langle\sum_{l=2}^{k} b_{k-l}\left(\delta_t v^{l-\frac{1}{2}} - \delta_t v^{l-\frac{3}{2}}\right), \delta_t v^{k-\frac{1}{2}}\right\rangle \geq \tau\sum_{k=2}^{n} b_{n-k}\left\|\delta_t v^{k-\frac{1}{2}}\right\|^2 - \tau\sum_{k=2}^{n} b_{n-k}\left\|\delta_t v^{\frac{1}{2}}\right\|^2,$$

and then

$$2\tau\sum_{k=1}^{n}\left\langle {}_\rho\mathcal{D}_{B2}^{[\alpha]} v^k, \delta_t v^{k-\frac{1}{2}}\right\rangle \geq \tau\sum_{k=2}^{n} b_{n-k}\left\|\delta_t v^{k-\frac{1}{2}}\right\|^2 - \tau\sum_{k=2}^{n} b_{n-k}\left\|\delta_t v^{\frac{1}{2}}\right\|^2 - 2a_0\tau\left\|\delta_t v^{\frac{1}{2}}\right\|^2. \tag{4.13}$$

We apply Lemma 4.4 with $\varepsilon = 3L^2$ and the embedding inequality (4.3) to obtain

$$\begin{aligned} 2\tau\sum_{k=2}^{n}\left\langle\xi^k, \delta_t v^{k-\frac{1}{2}}\right\rangle &\leqslant \frac{3}{L^2}\left(\left\|v^1\right\|^2 + \tau\sum_{l=2}^{n-1}\left\|v^l\right\|^2 + \left\|v^n\right\|^2\right) + \frac{L^2}{3}\left\|\xi^n\right\|_{\Sigma}^2 \\ &\leqslant \frac{1}{2}\left\|\delta_x v^n\right\|^2 + \frac{\tau}{2}\sum_{l=2}^{n-1}\left\|\delta_x v^l\right\|^2 + \frac{1}{2}\left\|\delta_x v^1\right\|^2 + \frac{L^2}{3}\left\|\xi^n\right\|_{\Sigma}^2. \end{aligned} \tag{4.14}$$

Inserting the estimates (4.13)–(4.14) into (4.12), we apply the first-level estimate (4.11) and Lemma 2.7 to find

$$\begin{aligned}\left\|\delta_x v^n\right\|^2 &\leqslant \tau\sum_{l=2}^{n-1}\left\|\delta_x v^l\right\|^2+2\tau\sum_{k=2}^{n}b_{n-k}\left\|\delta_t v^{\frac12}\right\|^2+4a_0\tau\left\|\delta_t v^{\frac12}\right\|^2+3\left\|\delta_x v^1\right\|^2+\frac{2L^2}{3}\left\|\xi^n\right\|_\Sigma^2\\ &\leqslant \tau\sum_{l=2}^{n-1}\left\|\delta_x v^l\right\|^2+\frac{2\tau}{a_0^2}\sum_{k=2}^{n}b_{n-k}\left\|\xi^1\right\|^2+\frac{4\tau}{a_0}\left\|\xi^1\right\|^2+\frac{2L^2}{3}\left\|\xi^n\right\|_\Sigma^2\\ &\leqslant \tau\sum_{l=2}^{n-1}\left\|\delta_x v^l\right\|^2+\frac{5\tau}{a_0^2}\sum_{k=2}^{n}a_{n-k}\left\|\xi^1\right\|^2+\frac{2L^2}{3}\left\|\xi^n\right\|_\Sigma^2.\end{aligned}$$

The discrete Gronwall inequality yields the claimed estimate and completes the proof. □

Lemmas 4.3 and 4.5 imply the following result.

Theorem 4.6 *The CBDF2 scheme* (4.1)–(4.2) *is stable in the discrete H^1 norm.*

4.2 Convergence

The error function $e_h^n = U_h^n - u_h^n \in \mathfrak{V}_h$ satisfies the following error system

$$_\rho\mathcal{D}_{B2}^{[\alpha]}e_i^n = \delta_x^2 e_i^n + (R_2)_i^n, \quad x_i\in\Omega_h,\ 1\leqslant n\leqslant N, \tag{4.15}$$

$$e_i^0 = 0,\ x_i\in\bar\Omega_h\,, \tag{4.16}$$

where $(R_2)_i^n$ denotes the truncation error at time $t = t_n$. According to Lemma 2.10, one has

$$\left|(R_2)^1\right| \leqslant C_{P_u,0}(\tau^{2-\beta}\left|\ln\tau\right|^{-1}+h_\alpha^2+h^2)\,, \tag{4.17}$$

$$\left|(R_2)^n\right| \leqslant C_{P_u,0}\Upsilon(t_{n-1})\tau^3+C_{P_u}(\tau^{3-\beta}\left|\ln\tau\right|^{-1}+h_\alpha^2+h^2),\quad n\geq 2, \tag{4.18}$$

where the first-level-dependent factor $\Upsilon(t_{n-1})$ is defined by (2.12).

Taking small time-step $\tau \leqslant 2^{-1/\beta}$, we apply Lemma 2.8 (b) to get $\frac{\tau}{a_0} \leqslant C_\rho\tau^\beta\left|\ln\tau\right|$. Thus, Lemma 4.5 together with the truncation error (4.17) yields the first-level error estimate,

$$\left\|\delta_x e^1\right\| \leqslant \sqrt{\frac{\tau}{a_0}}\left\|(R_2)^1\right\| \leqslant C_{P_u}\big(\tau^{2-\frac{\beta}{2}}\left|\ln\tau\right|^{-\frac12}+h_\alpha^2+h^2\big). \tag{4.19}$$

Assuming further that $g(t)\in\mathcal{C}^4([t_2,T])$, Lemma 2.10 also yields

$$\left|{}_\rho D_t^{[\alpha]}g'(t_{k+\frac12})-{}_\rho\mathcal{D}_{B2}^{[\alpha]}(\delta_t g^{k+\frac12})\right|\leqslant C_{P_g,0}\Upsilon(t_{k-\frac12})\tau^3+C_{P_g}(\tau^{3-\beta}\left|\ln\tau\right|^{-1}+h_\alpha^2+h^2),\ k\geq 2.$$

Then, following the technique in [21], one can apply the formula of Taylor expansion with integral remainder to obtain

$$\left\|\delta_t(R_2)^{k+\frac12}\right\| \leqslant C_{P_u,0}\Upsilon(t_{k-\frac12})\tau^3+C_{P_u}(\tau^{3-\beta}\left|\ln\tau\right|^{-1}+h_\alpha^2+h^2)\,,\quad k\geq 2.$$

It follows from the definition (4.8) that

$$\left\|(R_2)^n\right\|_{\Sigma_2} \leqslant C_{P_u,0}\Upsilon(t_{n-1})\tau^3 + C_{P_u}(\tau^{3-\beta}\left|\ln\tau\right|^{-1} + h_\alpha^2 + h^2), \quad n \geq 2. \quad (4.20)$$

From (2.12), $\Upsilon(t_{n-1}) = \frac{2\beta}{\ln 2}t_{n-1}^{-1}$ if $t_{n-1}^{\beta} \geq \frac{1}{2}$ and $\Upsilon(t_{n-1}) \leqslant \frac{\beta}{\ln 2}t_{n-1}^{-1-\beta}$ if $t_{n-1}^{\beta} < \frac{1}{2}$. Thus,

$$\Upsilon(t_{n-1}) \leqslant \frac{\beta}{\ln 2}\, t_{n-1}^{-1}\mu(t_{n-1}^{\beta}), \quad n \geq 2\,. \quad (4.21)$$

Furthermore, applying Lemma 2.8 (b)-(c) with $\tau \leqslant 2^{-1/\beta}$, it is not difficult to obtain

$$\frac{\tau}{a_0^2}\sum_{k=2}^{n} a_{n-k} \leqslant C_\rho\tau^{2\beta-1}\left|\ln\tau\right|^2\frac{\beta t_{n-1}\mu(t_{n-1}^{\beta})}{\ln\mu(t_{n-1}^{\beta})} \leqslant C_\rho\beta\tau^{2\beta-1}\left|\ln\tau\right|^2 t_{n-1}\mu(t_{n-1}^{\beta}), \quad n \geq 2. \quad (4.22)$$

Therefore, we apply Lemma 4.5 and the embedding inequality (4.3) to find

$$\begin{aligned}\left\|\delta_x e^n\right\| &\leqslant \exp\left(\frac{t_n}{2}\right)\sqrt{\frac{5\tau}{a_0^2}\sum_{k=2}^{n}a_{n-k}\left\|(R_2)^1\right\|^2 + \frac{2L^2}{3}\left\|(R_2)^n\right\|_{\Sigma}^2}\\ &\leqslant C_{P_u,0}\sqrt{\max\left(t_{n-1}^{1-\beta}, 2t_{n-1}\right)}\,\tau^{\beta-\frac{1}{2}}\left|\ln\tau\right|\left(\tau^{2-\beta}\left|\ln\tau\right|^{-1} + h_\alpha^2 + h^2\right)\\ &\quad + C_{P_u,0}\max\left(t_{n-1}^{-\beta}, 2\right)t_{n-1}^{-1}\tau^3 + C_{P_u}\left(\tau^{3-\beta}\left|\ln\tau\right|^{-1} + h_\alpha^2 + h^2\right), \quad n \geq 2,\end{aligned} \quad (4.23)$$

where the estimates (4.17)–(4.20) of truncation errors and (4.21)–(4.22) has been applied.

Theorem 4.7 *Assume that* $\rho(\alpha) \in \mathcal{C}([0,\beta])$, $P_{[u]}(\alpha) \in \mathcal{C}_\alpha^2([0,\beta])$ *and the subdiffusion problem* (1.2)–(1.4) *admits a smooth solution* $u(x,t) \in \mathcal{C}_{x,t}^{4,3}(\bar{\Omega}\times[0,T]) \cap \mathcal{C}_{x,t}^{4,4}(\bar{\Omega}\times(0,T])$. *The solution of the CBDF2 scheme* (4.1)–(4.2) *is convergent in the sense of* (4.19) *and* (4.23).

It is seen that the first-level-dependent factor $\Upsilon(t_{n-1})$ dominates the global error when the integration time t_n is close to $t = 0$ such that the main lose of temporal accuracy in (4.23) is due to the application of Caputo's BDF1 formula (2.1) at $t = t_1$. However, numerical tests in next section show that, in resolving smooth solutions, the CBDF2 scheme (4.1)–(4.2) is second-order accurate in time. Maybe, the lose of theoretical accuracy is only a fault of the present H^1 discrete energy analysis rather than practical effectiveness of the CBDF2 method. To see it more clearly, in next subsection, we apply the method of maximum principle to resolve the theoretical deficiency partly.

4.3 Improved analysis for $\beta \leqslant 1/3$

The fractional BDF2 formula (2.4) also takes the form of

$$\mathcal{D}_{B2}^{\alpha}g^n = \sum_{k=1}^{n}c_{n-k}^{(n,\alpha)}\left(\delta_t g^{k-\frac{1}{2}}\right), \quad n \geq 1,$$

The coefficient $c_k^{(n,\alpha)}$ is defined by [10]

$$c_0^{(1,\alpha)} = a_0^{(\alpha)}; \qquad c_k^{(n,\alpha)} = \begin{cases} a_0^{(\alpha)} + b_0^{(\alpha)}, & k = 0, \\ a_k^{(\alpha)} + b_k^{(\alpha)} - b_{k-1}^{(\alpha)}, & 1 \leqslant k \leqslant n-2, \\ a_{n-1}^{(\alpha)} - b_{n-2}^{(\alpha)}, & k = n-1, \end{cases} \quad n \geq 2; \tag{4.24}$$

where $a_k^{(\alpha)}$ and $b_k^{(\alpha)}$ are defined by (2.2) and (2.3), respectively. We have the following results.

Lemma 4.8 *For* $0 < \alpha < 1$ *and* $x \geq 1$, $p_1(x) = \frac{(x+2)^{1-\alpha}+x^{1-\alpha}}{2} - \frac{(x+1)^{2-\alpha}-x^{2-\alpha}}{2-\alpha} > 0$.

Proof Consider the consistency error of the trapezoidal formula for $s^{1-\alpha}$ in $[x, x+1]$,

$$\int_x^{x+1} s^{1-\alpha}\,\mathrm{d}s - \frac{(x+1)^{1-\alpha}+x^{1-\alpha}}{2} = \frac{\alpha(1-\alpha)}{12(x+\mu_1)^{1+\alpha}}, \quad 0 < \mu_1 < 1.$$

Then, we apply the mean-value theorem to get

$$\begin{aligned} p_1(x) &= \frac{(x+2)^{1-\alpha}+x^{1-\alpha}}{2} - \int_x^{x+1} s^{1-\alpha}\,\mathrm{d}s = \frac{(x+2)^{1-\alpha}-(x+1)^{1-\alpha}}{2} - \frac{\alpha(1-\alpha)}{12(x+\mu_1)^{1+\alpha}} \\ &= \frac{1-\alpha}{2(x+\mu_2)^{\alpha}} - \frac{\alpha(1-\alpha)}{12(x+\mu_1)^{1+\alpha}} \geq \frac{1-\alpha}{2(x+\mu_2)} - \frac{\alpha(1-\alpha)}{12(x+\mu_1)} \\ &= \frac{(1-\alpha)\left[(6-\alpha)x+6\mu_1-\alpha\mu_2\right]}{12(x+\mu_1)(x+\mu_2)} \geq \frac{(1-\alpha)\left(6+6\mu_1-3\alpha\right)}{12(x+\mu_1)(x+\mu_2)} > 0, \quad x \geq 1, \end{aligned}$$

where $0 < \mu_1 < 1 < \mu_2 < 2$. The proof is completed. □

Lemma 4.9 *For positive constants* d_0 *and* d_1, $p_2(d_0, d_1; s) = d_0 2^{-s} - d_1 3^{-s} - 1$ *is increasing monotonously for* $s \leqslant s^*$ *and decreasing for* $s > s^*$, *where* $s^* = \ln\left(\frac{d_1 \ln 3}{d_0 \ln 2}\right)/\ln(\frac{3}{2})$.

Proof The claimed result follows from the fact, $\frac{\mathrm{d}p_2}{\mathrm{d}s} = 3^{-s} d_0 \ln 2 \left(\frac{d_1 \ln 3}{d_0 \ln 2} - \left(\frac{3}{2}\right)^s\right)$. □

Lemma 4.10 *If* $0 < \alpha \leqslant 1/3$, *the coefficient* $c_l^{(n,\alpha)}$ *defined by* (4.24) *is positive and fulfils*

$$(a) \quad c_{n-1}^{(n,\alpha)} \geq \frac{1}{2} a_{n-1}^{(\alpha)}, \quad n \geq 1; \qquad (b)\; c_{l-1}^{(n,\alpha)} \geq c_l^{(n,\alpha)}, \quad 1 \leqslant l \leqslant n-1, \; n \geq 2.$$

Proof In this proof, the definitions (2.2), (2.3), and (4.24) of $a_k^{(\alpha)}$, $b_k^{(\alpha)}$, and $c_k^{(n,\alpha)}$ will be used frequently and they will be not mentioned every time. If $n \leqslant 2$, $c_0^{(1,\alpha)} - \frac{1}{2}a_0^{(\alpha)} = \frac{1}{2}a_0^{(\alpha)} > 0$,

$$c_1^{(2,\alpha)} - \frac{1}{2}a_1^{(\alpha)} = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\left(2^{-\alpha} - \frac{1}{2-\alpha}\right) \geq \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\left(\frac{1}{\sqrt{2}} - \frac{2}{3}\right) > 0, \quad \forall\, 0 < \alpha \leqslant \frac{1}{2}.$$

For the case of $n \geq 3$, we apply Lemma 4.8 to get

$$c_{n-1}^{(n,\alpha)} - \frac{1}{2}a_{n-1}^{(\alpha)} = \frac{1}{2}a_{n-1}^{(\alpha)} - b_{n-2}^{(\alpha)} = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\, p_1(n-2) > 0, \quad n \geq 3.$$

Thus, the inequality (a) has been verified.

It is in position to prove the decreasing property of $c_k^{(n,\alpha)}$. If $n = 2$, Lemma 2.1 shows that $c_0^{(2,\alpha)} - c_1^{(2,\alpha)} = a_0^{(\alpha)} + 2b_0^{(\alpha)} - a_1^{(\alpha)} > 0$. For the case of $n \geq 3$, Lemma 2.2 in [10] gives the following results,

$$c_0^{(n,\alpha)} > \left|c_1^{(n,\alpha)}\right|, \quad c_0^{(n,\alpha)} > c_2^{(n,\alpha)} \geq c_3^{(n,\alpha)} \geq \cdots \geq c_{n-1}^{(n,\alpha)} > 0, \quad n \geq 3.$$

Moreover, Lemma 2.2 means that $c_1^{(3,\alpha)} - c_2^{(3,\alpha)} = c_1^{(n,\alpha)} - c_2^{(n,\alpha)} + b_2^{(\alpha)} > c_1^{(n,\alpha)} - c_2^{(n,\alpha)}$, $n \geq 4$. Thus, it remains to prove that $c_1^{(n,\alpha)} > c_2^{(n,\alpha)}$ is valid for $n \geq 4$ and $0 < \alpha \leqslant \frac{1}{3}$.

Thanks to Lemma 4.9, the maximum point of $p_2(2,1;\alpha)$ is $\alpha^* = \ln\left(\frac{\ln 3}{\ln 4}\right)/\ln(\frac{3}{2}) < 0$ so that $p_2(2,1;\alpha) \leqslant p_2(2,1;0) = 0$ for $0 \leqslant \alpha \leqslant 1$; while the maximum point of $p_2(3,2;\alpha)$ locates at $\alpha^\star = \ln\left(\frac{\ln 9}{\ln 8}\right)/\ln(\frac{3}{2}) > 0$ and $p_2(3,2;\alpha) \geq \min\{p_2(3,2;0), p_2(3,2;\frac{1}{4})\} = p_2(3,2;0) = 0$ for $0 \leqslant \alpha \leqslant \frac{1}{4}$. Then, for $n \geq 4$, we have (see the curves of $P_2(\alpha,\alpha)$ and $P_2(0,\alpha)$ in Fig. 1)

$$\begin{aligned}\Gamma(3-\alpha)\tau^{\alpha-1}\left(c_1^{(n,\alpha)} - c_2^{(n,\alpha)}\right) &= \Gamma(3-\alpha)\tau^{\alpha-1}\left[a_1^{(\alpha)} - a_2^{(\alpha)} - b_2^{(\alpha)} + 2b_1^{(\alpha)} - b_0^{(\alpha)}\right] \\ &= 6p_2(3,2;\alpha) - \frac{3\alpha}{2}\, p_2(2,1;\alpha) \geq 6p_2(3,2;\alpha) \geq 0, \quad 0 \leqslant \alpha \leqslant \frac{1}{4}.\end{aligned}$$

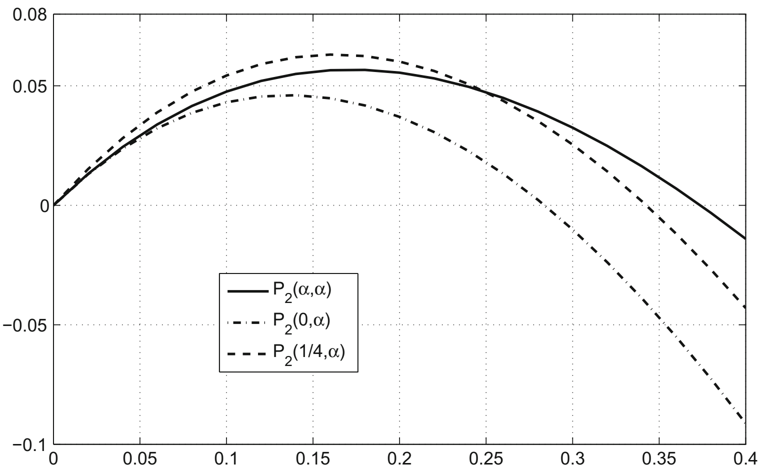

Fig. 1 Curves of $P_2(\lambda,\alpha) = 6p_2(3,2;\alpha) - \frac{3\lambda}{2}\, p_2(2,1;\alpha)$ for $\lambda = \alpha$, 0 and $1/4$

Take $\bar{d}_0 = \frac{46}{15}$ and $\bar{d}_1 = \frac{31}{15}$ such that the maximum point of $p_2(\bar{d}_0, \bar{d}_1; \alpha)$ locates near $\alpha^\star > 0$ and $p_2(\bar{d}_0, \bar{d}_1; \alpha) \geq \min\{p_2(\bar{d}_0, \bar{d}_1; 0), p_2(\bar{d}_0, \bar{d}_1; \frac{1}{3})\} = p_2(\bar{d}_0, \bar{d}_1; 0) = 0$ for $0 \leqslant \alpha \leqslant \frac{1}{3}$. It follows that (see the curves of $P_2(\alpha, \alpha)$ and $P_2(1/4, \alpha)$ depicted in Fig. 1)

$$\begin{aligned}\Gamma(3-\alpha)\tau^{\alpha-1}\big(c_1^{(n,\alpha)} - c_2^{(n,\alpha)}\big) &= 6p_2(3,2;\alpha) - \frac{3\alpha}{2}\, p_2(2,1;\alpha) \geq 6p_2(3,2;\alpha) - \frac{3}{8}\, p_2(2,1;\alpha)\\ &= \frac{45}{8}\, p_2(\bar{d}_0, \bar{d}_1; \alpha) \geq 0, \qquad \frac{1}{4} \leqslant \alpha \leqslant \frac{1}{3}\,,\ n \geq 4.\end{aligned}$$

Therefore, we obtain (b) and complete the proof. □

Now, define the following coefficient

$$c_k^{(n)} \equiv h_\alpha \sum_{\ell=1}^{N_\alpha} c_k^{(n,\alpha_{\ell-\frac{1}{2}})} \rho(\alpha_{\ell-\frac{1}{2}})\,, \quad 1 \leqslant k \leqslant n-1,\ n \geq 1. \tag{4.25}$$

where $c_k^{(n,\alpha_{\ell-\frac{1}{2}})}$ is defined by (4.24). Then Lemma 4.10 yields

Lemma 4.11 *If $0 < \beta \leqslant 1/3$, the coefficient $c_l^{(n)}$ defined by (4.25) is positive and fulfils*

(a) $c_{n-1}^{(n)} \geq \frac{1}{2} a_{n-1}, \quad n \geq 1;$ *(b)* $c_{l-1}^{(n)} \geq c_l^{(n)}, \quad 1 \leqslant l \leqslant n-1,\ n \geq 2\,.$

Also, the distributed-order BDF2 formula (2.11) reads ${}_\rho\mathcal{D}_{B2}^{[\alpha]} g^n = \sum_{k=1}^{n} c_{n-k}^{(n)} \big(\delta_t g^{k-\frac{1}{2}}\big)$. Thanks to Lemma 4.11, one can take $\omega_l^{(n)} = c_l^{(n)}$ $(0 \leqslant l \leqslant n-1)$ in Lemma 3.2 to get the following minimum-maximum principle.

Theorem 4.12 *Assume that $0 < \beta \leqslant \frac{1}{3}$ and the function $v_h^n \in \mathfrak{V}_h$, $0 \leqslant n \leqslant N$, satisfies*

$$\begin{aligned}{}_\rho\mathcal{D}_{B2}^{[\alpha]} v_i^n &= \delta_x^2 v_i^n + \xi_i^n, \quad x_i \in \Omega_h, 1 \leqslant n \leqslant N,\\ v_i^0 &= \phi_i, \quad x_i \in \bar{\Omega}_h.\end{aligned}$$

Then it holds that, for $k \geq 1$,

$$\min\Big\{0, \min_{x_j \in \Omega_h} \phi_j + 2\tau \min_{\substack{x_j \in \Omega_h\\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{a_{l-1}}\Big\} \leqslant v_i^k \leqslant \max\Big\{0, \max_{x_j \in \Omega_h} \phi_j + 2\tau \max_{\substack{x_j \in \Omega_h\\ 1 \leqslant l \leqslant k}} \frac{\xi_j^l}{a_{l-1}}\Big\}, \quad x_i \in \Omega_h.$$

It means that, if $0 < \beta \leqslant \frac{1}{3}$, the CBDF2 scheme (4.1)–(4.2) is nonnegative-preserving and stable in the maximum norm.

Recalling the definition (2.12), we apply Lemma 2.8 (b) and $t_k \leqslant 2t_{k-1}$ $(k \geq 2)$ to find

$$\frac{\tau}{a_{k-1}}\Upsilon(t_{k-1}) = \frac{t_k^\beta \mu(t_{k-1}^\beta)\ln\mu(t_k^\beta)}{t_{k-1}\ln\mu(t_{k-1}^\beta)} \leqslant 2^{1+\beta} t_{k-1}^{\beta-1}, \quad \text{if} \quad t_{k-1}^\beta \geq \frac{1}{2}, \ k \geq 2,$$

and $\frac{\tau}{a_{k-1}}\Upsilon(t_{k-1}) \leqslant 2^\beta t_{k-1}^{-1}$ if $t_{k-1}^\beta \leqslant \frac{1}{2}$, $k \geq 2$. Thus, it follows that

$$\frac{\tau}{a_{k-1}}\Upsilon(t_{k-1}) \leqslant 2^\beta t_{k-1}^{-1} \max\left(1, 2t_{k-1}^\beta\right), \quad k \geq 2. \tag{4.26}$$

We apply Theorem 4.12 to the error system (4.15)–(4.16) of the CBDF2 method and obtain

$$\begin{aligned}\left\|e^n\right\|_\infty &\leqslant 2\tau \max_{1\leqslant k\leqslant n} \frac{\left\|(R_2)^k\right\|_\infty}{a_{k-1}} \leqslant C_\rho \tau^\beta |\ln\tau| \left\|(R_2)^1\right\|_\infty + 2\tau \max_{2\leqslant k\leqslant n} \frac{\left\|(R_2)^k\right\|_\infty}{a_{k-1}} \\ &\leqslant C_{P_u,0}\tau^\beta |\ln\tau| \left(\tau^{2-\beta}|\ln\tau|^{-1} + h_\alpha^2 + h^2\right) + C_{P_u,0}\tau^3 \max_{2\leqslant k\leqslant n} \frac{\tau}{a_{k-1}}\Upsilon(t_{k-1}) \\ &\quad + C_{P_u} \max_{2\leqslant k\leqslant n} t_k^\beta \beta^{-1} \ln\mu(t_k^\beta)\left(\tau^{3-\beta}|\ln\tau|^{-1} + h_\alpha^2 + h^2\right) \\ &\leqslant C_{P_u,0}\tau^2 + C_{P_u} \max_{2\leqslant k\leqslant n} t_k^\beta \beta^{-1} \ln\mu(t_k^\beta)\left(\tau^{3-\beta}|\ln\tau|^{-1} + h_\alpha^2 + h^2\right), \quad n \geq 1,\end{aligned} \tag{4.27}$$

where the estimates (4.17)–(4.18) of truncation errors and (4.26) have been used. Obviously, it improves the error estimate (4.23) derived by the H^1 discrete energy analysis. In general, the CBDF2 scheme would not attain the time accuracy $O(\tau^{3-\beta})$ because the first-level solution u_h^1 is only second-order accurate in time, see (3.7).

Theorem 4.13 *Let* $0 < \beta \leqslant \frac{1}{3}$, $\rho(\alpha) \in \mathcal{C}([0,\beta])$, $P_{[u]}(\alpha) \in \mathcal{C}_\alpha^2([0,\beta])$, *and the distributed-order subdiffusion problem* (1.2)–(1.4) *admits a smooth solution* $u(x,t) \in \mathcal{C}_{x,t}^{4,3}(\bar{\Omega}\times[0,T])$. *The numerical solution of the CBDF2 scheme* (4.1)–(4.2) *is second-order convergent in the maximum norm in the sense of* (4.27).

5 Numerical experiments

We examine the proposed CBDF1 (3.1)–(3.2) and CBDF2 (4.1)–(4.2) schemes by running them on MATLAB in a PC with 4GB RAM. In this section, the temporal convergence rate will be focused on since the standard second-order spatial discretization has been well examined, see [11], for example. In our computations, the fractional-order interval $(0,\beta)$ and spatial domain $\Omega = (0, L)$ are divided uniformly into N_α and M subintervals, respectively, with the grid lengths $h_\alpha = \beta/N_\alpha$ and $h = L/M$. Also, the time interval $[0, T]$ is divided into N uniform parts with the step size $\tau =$

T/N. As usual, the maximum norm solution error $e(N, N_\alpha, M) = \|U(\cdot, T) - u^N\|_\infty$ at the final time $t = T$, is recorded in each run.

5.1 Accuracy verification

Example 1 The smooth solution $u(x,t) = x(1-x)(1+t^3)$ solves the following problem,

$$\int_0^\beta \Gamma(4-\alpha) D_t^\alpha u(x,t)\,\mathrm{d}\alpha = \frac{\partial^2 u}{\partial x^2} + f(x,t), \quad 0 < x < 1,\ 0 < t \leqslant T,$$
$$u(0,t) = 0,\ u(1,t) = 0,\ 0 < t \leqslant T; \qquad u(x,0) = x(1-x),\ 0 \leqslant x \leqslant 1,$$

where $f(x,t) = 2(t^3+1) + \frac{6x(1-x)}{\ln t} t^3(t^{-\beta} - 1)$ and $T = 1$.

We examine the solution error and convergence order by running the CDBF1 and CBDF2 method for Example 1 with $\beta = 1/3, 1/2$ and 1. Fixed the grid spacings $h_\alpha = 1/1200$ and $h = 1/1000$, values small enough such that the spatial and fractional-order error is negligible as compared with the temporal error, or $e(N, N_\alpha, M) \approx e(N)$. Tables 1 and 2 list the solution errors on the gradually refined grids with the coarsest grid of $N = 8$. The experimental rate (listed as Rate in tables) of convergence, in τ, is estimated by $q_\tau \approx \log_2 [e(N)/e(2N)]$. It is observed that the CBDF1 scheme (3.1)–(3.2) is of order $O(\tau^{2-\beta})$ in time, which supports Theorem 3.5 experimentally. Table 2 implies that the time accuracy of the CBDF2 method (4.1)–(4.2) is of order $O(\tau^{3-\beta})$; however, it is mysterious to us. At least, the second-order convergence for the case of $\beta = 1$ is confirmed numerically.

Since the two methods have the same approximation for the integral with respect to the fractional-order α, we only test it by using the CBDF2 scheme with $\beta = 1$. Given small time and spatial steps $\tau = 2 \times 10^{-4}$ and $h = 10^{-3}$ such that $e(N, N_\alpha, M) \approx e(N_\alpha)$, Table 3 lists the CBDF2 solution errors on the gradually halving grids with the coarsest grid of $N_\alpha = 4$. The experimental rate of convergence, in h_α, is estimated by $q_\alpha \approx \log_2 [e(N_\alpha)/e(2N_\alpha)]$. We see that the CBDF2 (or CBDF1) scheme is second-order accurate in h_α.

Table 1 Numerical accuracy in τ of CBDF1 solutions for Example 1 with $h_\alpha = 1/1200$, $h = 1/1000$, and $\beta = 1/3, 1/2, 1$

	$\beta = 1/3$		$\beta = 1/2$		$\beta = 1$	
N	$e(N)$	Rate	$e(N)$	Rate	$e(N)$	Rate
8	2.9979e-04	1.6196	7.3591e-04	1.5287	4.2924e-03	1.1908
16	9.7560e-05	1.6534	2.5506e-04	1.5573	1.8803e-03	1.1930
32	3.1014e-05	1.6757	8.6665e-05	1.5742	8.2243e-04	1.1856
64	9.7078e-06	1.6911	2.9105e-05	1.5840	3.6156e-04	1.1741
128	3.0064e-06	*	9.7085e-06	*	1.6023e-04	*

Table 2 Numerical accuracy in τ of CBDF2 solutions for Example 1 with $h_\alpha = 1/1200$, $h = 1/1000$, and $\beta = 1/3, 1/2, 1$

	$\beta = 1/3$		$\beta = 1/2$		$\beta = 1$	
N	$e(N)$	Rate	$e(N)$	Rate	$e(N)$	Rate
8	2.4999e-05	2.6830	6.2390e-05	2.5885	4.0603e-04	2.2296
16	3.8928e-06	2.6972	1.0373e-05	2.5965	8.6573e-05	2.2112
32	6.0024e-07	2.7074	1.7151e-06	2.6008	1.8696e-05	2.1928
64	9.1899e-08	2.7149	2.8273e-07	2.6024	4.0893e-06	2.1755
128	1.3997e-08	*	4.6558e-08	*	9.0521e-07	*

5.2 Numerical comparisons

Example 2 [11] The solution $u(x,t) = (2t)^\kappa \sin x$ solves the following problem,

$$\int_0^1 \Gamma(\kappa + 1 - \alpha) D_t^\alpha u(x,t)\,\mathrm{d}\alpha = \frac{\partial^2 u}{\partial x^2} + f(x,t), \quad 0 < x < \pi,\ 0 < t \leqslant T,$$
$$u(0,t) = 0,\ u(\pi,t) = 0,\ 0 < t \leqslant T; \qquad u(x,0) = 0,\ 0 \leqslant x \leqslant \pi,$$

where $f(x,t) = 2^\kappa t^{\kappa-1} \sin x \big[t + \Gamma(\kappa+1)\frac{(t-1)}{\ln t}\big]$ and $T = 0.5$.

Note that the second-order CBDF2 scheme (4.1)–(4.2) computes the first-level solution by using the CBDF1 scheme (3.1)–(3.2) such that a second-order accurate solution u_h^1 will be needed. The first-level error of the CBDF1 solution is now examined by taking $\kappa = 2$ in Example 2 with $\frac{\partial^2 u}{\partial t^2} = O(1)$. Taking small grid lengths $h = h_\alpha = 10^{-3}$ such that the time error dominates the solution error, Fig. 2 depicts $\log_2 \|U^1 - u^1\|_\infty$ against $\log_2 \tau$ for time-steps $\tau = 2^{-k}$ ($k = 6, 7, 8, 9, 10$). By doing a least square fitting, we get

$$\log_2 \|U^1 - u^1\|_\infty \approx 1.9402 \log_2 \tau - 0.9684\,,$$

which suggests the solution u_h^1 is about second-order accuracy in time. The first-level error estimate (3.7) is confirmed experimentally.

Now, we compare the CBDF2 method with a second-order WSG scheme, see (3.11)–(3.13) in [11], which is constructed by applying a weighted and shifted Grünwald formula to approximating the fractional derivative. Note that the two schemes are only different in numerical approximations of fractional derivative such

Table 3 Accuracy in h_α of CBDF2 solution for Example 1 with $N = 5000$, $M = 1000$

N_α	$e(N_\alpha)$	Rate
4	4.2653e-06	2.0115
8	1.0578e-06	2.0015
16	2.6418e-07	1.9949
32	6.6282e-08	*

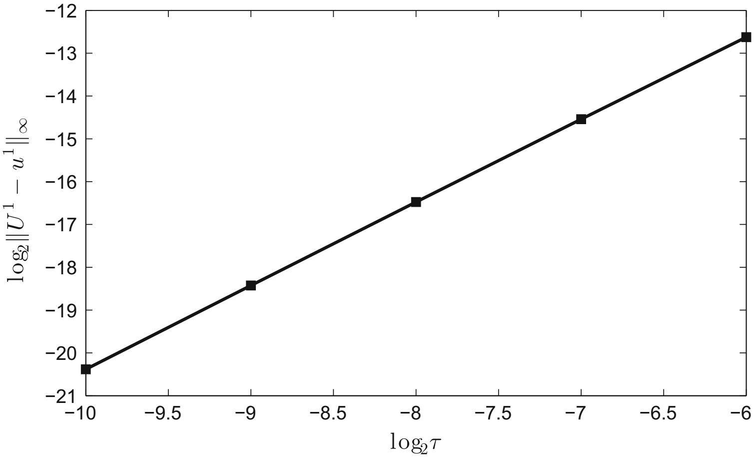

Fig. 2 Initial error at $t_1 = 2^{-k}$ $(k = 6, 7, 8, 9, 10)$ of CBDF1 solution

that the computational cost of them is about the same. Table 4 reports the maximum norm solution errors of three different solutions in Example 2 by setting $M = N_\alpha = 10^3$. It is observed that the time accuracy of CBDF2 scheme is comparable with that of WSG scheme for $\kappa = 2$ and $3/2$, while for $\kappa = 1$, the WSG scheme has a lose of accuracy and the CBDF2 scheme has no temporal error.

Actually, for the solution of $\kappa = 1$, $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^3 u}{\partial t^3} = 0$ such that the distributed-order BDF2 formula (2.11) has no temporal error, see Lemma 2.10, and the CBDF2 scheme is exact in time direction. The numerical behavior for the case of $\kappa = 3/2$ may also be explained by our theory. In this case, $\frac{\partial^2 u}{\partial t^2} = O(t^{-1/2})$ such that the time truncation error of $(R_2)^1$ in (4.17) would degrade into $O(\tau^{\frac{1}{2}} |\ln \tau|)$ and the first-level error (4.19) becomes $O(\tau^{\frac{3}{2}})$. Thus, the whole temporal accuracy can not exceed the order of $O(\tau^{\frac{3}{2}})$. On the other hand, Lemma 2.10 implies that, to recover second-order time accuracy for this type of solutions, one would improve the resolution for some of solutions near $t_0 = 0$ but not only the first-level solution. In next subsection, we will improve the resolution by employing nonuniform meshes.

5.3 Nonuniform mesh and initial behaviors

In resolving the solution which lacks the smoothness near the initial time, nonuniform meshes that concentrate the grid points near $t = 0$ would be necessary. We consider a class of nonuniform grid, $0 = t_0 < t_1 < \cdots < t_N = T$ with $t_n = (n\tau)^m$, where the constant $m \geq 1$ and $\tau = T^{1/m}/N$. The larger the value of m, the stronger must be the concentration of time levels near $t = 0$. Appendix presents the Caputo's BDF1 and BDF2 formulas on nonuniform mesh for approximating the Caputo derivative (1.1) and distributed-order derivative (1.5).

Taking $m = 1.5$ and small grid spacings h_α, h such that $e(N, N_\alpha, M) \approx e(N)$, Table 5 lists the nonuniform CBDF2 solution errors on the gradually refined meshes

Table 4 Numerical accuracy in τ of solutions for Example 2 with $M = N_\alpha = 10^3$

		Second-order WSG [11]		CBDF2	
κ	N	$e(N)$	Rate	$e(N)$	Rate
	8	6.2773e-03	2.0295	1.5102e-03	2.2967
	16	1.5375e-03	2.0078	3.0737e-04	2.2191
$\kappa = 2$	32	3.8230e-04	1.9916	6.6015e-05	2.1636
	64	9.6135e-05	1.9548	1.4734e-05	2.0805
	128	2.4799e-05	*	3.4835e-06	*
	8	6.4055e-04	1.6556	8.4038e-04	1.6990
	16	2.0332e-04	1.6435	2.5883e-04	1.6265
$\kappa = \frac{3}{2}$	32	6.5077e-05	1.6383	8.3830e-05	1.5936
	64	2.0906e-05	1.6479	2.7776e-05	1.5652
	128	6.6709e-06	*	9.3863e-06	*
	8	5.1877e-03	1.3421	3.3671e-07	−0.0036
	16	2.0462e-03	1.2537	3.3754e-07	−0.0023
$\kappa = 1$	32	8.5812e-04	1.2020	3.3807e-07	−0.0012
	64	3.7300e-04	1.1684	3.3836e-07	−0.0006
	128	1.6595e-04	*	3.3851e-07	*

with the coarsest grid of $N = 8$. The experimental rate of convergence, in τ, is also estimated by computing $q_N \approx \log_2 [e(N)/e(2N)]$. We see that, for the solution $u(x,t) = (2t)^{3/2} \sin x$, the CBDF2 scheme (4.1)–(4.2) on nonuniform mesh is second-order accurate in time. It is not mysterious although a mathematical analysis is not available. Roughly speaking, the nonuniform time mesh equals to make a transform $t = \xi^{3/2}$ for this solution, $u(x,t) = v(x,\xi) = \sqrt{8}\,\xi^{9/4} \sin x$. Thus, the resolution of $v(x,\xi_n)$ near $\xi_0 = 0$ will be improved essentially in the uniform grid of $\xi_n = n\tau$ due to the fact, $\frac{\partial^2 v}{\partial \xi^2} = O(\xi^{\frac{1}{4}})$.

Table 5 Improved accuracy in τ for $u = (2t)^{3/2} \sin x$ with $m = 1.5$, $M = N_\alpha = 10^3$

N	$e(N)$	Rate
8	1.1966e-03	2.0360
16	2.9178e-04	2.0525
32	7.0340e-05	2.0772
64	1.6669e-05	2.1452
128	3.7684e-06	*

Table 6 Numerical accuracy in τ of CBDF1 solution in resolving Example 3 with initial data $\varphi_1(x)$ for grid parameters $M = N_\alpha = 10^3$ and $m = 1, 1.5, 2$

	$m = 1.0$		$m = 1.5$		$m = 2.0$	
N	$\bar{e}(N)$	Rate	$\bar{e}(N)$	Rate	$\bar{e}(N)$	Rate
8	1.9132e-04	1.1274	1.1232e-04	1.3826	9.1884e-05	1.4383
16	8.7575e-05	1.0626	4.3079e-05	1.2544	3.3905e-05	1.3025
32	4.1929e-05	1.0343	1.8057e-05	1.1878	1.3746e-05	1.2335
64	2.0472e-05	1.0204	7.9266e-06	1.1514	5.8460e-06	1.1894
128	1.0092e-05	*	3.5684e-06	*	2.5633e-06	*
256	*	*	*	*	*	*

Example 3 Consider the following initial-boundary value problem

$$\int_0^1 D_t^\alpha u(x,t)\,\mathrm{d}\alpha = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1,\ 0 < t \leqslant 1,$$
$$u(0,t) = 0,\ u(1,t) = 0,\ 0 < t \leqslant 1; \qquad u(x,0) = \varphi_k(x),\ 0 \leqslant x \leqslant 1,$$

where the initial data $\varphi_k(x)$ $(k = 1, 2)$ are defined by

$$\varphi_1(x) = x(1-x); \qquad \varphi_2(x) = \begin{cases} 2x, & 0 \leqslant x \leqslant 1/2, \\ 2(1-x), & 1/2 < x \leqslant 1. \end{cases}$$

We have no analytic solutions $u(x,t)$ for this example.

Now, we examine the numerical behaviors of CBDF1 and CBDF2 schemes in resolving Example 3 with two different initial data $\varphi_1(x)$ and $\varphi_2(x)$. As proven in [15], this type of distributed-order diffusion problems always has limited smoothing property near the initial time even with smooth initial data.

However, as remarked in the last part of Section 3, the CBDF1 scheme would also have first-order accurate in time direction, see Tables 6 and 7, in which the CBDF1

Table 7 Numerical accuracy in τ of CBDF1 solution in resolving Example 3 with initial data $\varphi_2(x)$ for grid parameters $M = N_\alpha = 10^3$ and $m = 1, 1.5, 2$

	$m = 1.0$		$m = 1.5$		$m = 2.0$	
N	$\bar{e}(N)$	Rate	$\bar{e}(N)$	Rate	$\bar{e}(N)$	Rate
8	6.1084e-04	1.1266	3.5720e-04	1.3840	2.9066e-04	1.4399
16	2.7976e-04	1.0621	1.3687e-04	1.2562	1.0713e-04	1.3032
32	1.3398e-04	1.0340	5.7297e-05	1.1892	4.3413e-05	1.2337
64	6.5429e-05	1.0202	2.5128e-05	1.1521	1.8460e-05	1.1896
128	3.2258e-05	*	1.1307e-05	*	8.0935e-06	*
256	*	*	*	*	*	*

Table 8 Numerical accuracy in τ of CBDF2 solution in resolving Example 3 with initial data $\varphi_2(x)$ for grid parameters $M = N_\alpha = 10^3$ and $m = 1, 1.5, 2$

	$m = 1.0$		$m = 1.5$		$m = 2.0$	
N	$\bar{e}(N)$	Rate	$\bar{e}(N)$	Rate	$\bar{e}(N)$	Rate
8	3.4635e-04	1.0153	7.0083e-05	1.4627	2.8787e-04	1.8182
16	1.7135e-04	1.1095	2.5427e-05	1.2812	8.1634e-05	1.9909
32	7.9412e-05	1.1841	1.0462e-05	1.4280	2.0537e-05	2.0148
64	3.4949e-05	1.2415	3.8883e-06	1.5909	5.0821e-06	2.0135
128	1.4781e-05	*	1.2908e-06	*	1.2587e-06	*
256	*	*	*	*	*	*

solution is computed on the gradually refined nonuniform meshes with the coarsest grid of $N = 8$. Since the exact solution is not available, the convergence rate $\bar{q}$ on the nonuniform meshes is determined as follows. Assume that $\left\|U(\cdot, T) - u^N(N)\right\|_\infty \approx C_u N^{-\bar{q}}$, where $u_h^n(N)$ denotes the solution at $t = t_n$ on nonuniform grid with N points. Thus, the triangle inequality gives $\bar{e}(N) \triangleq \left\|u^N(N) - u^{2N}(2N)\right\|_\infty \approx C_u N^{-\bar{q}}(1+2^{-\bar{q}})$. Then, the experimental rate $\bar{q}$ of convergence can be approximated by $\bar{q} \approx \log_2\left[\bar{e}(N)/\bar{e}(2N)\right]$.

We see that, compared with the CBDF1 solution on uniform mesh, the nonuniform CBDF1 solution, especially when $m = 2$, has little improvement of the convergence rate. It may be owing to that certain nonuniform grid recovers the accuracy $O(\tau^{2-\alpha})$ of the BDF1 formula (2.1) for the α-order Caputo derivative (1.1).

The CBDF2 errors on nonuniform meshes for the initial data φ_2 are listed in Table 8. Observation shows that the nonuniform meshes improve the resolution and

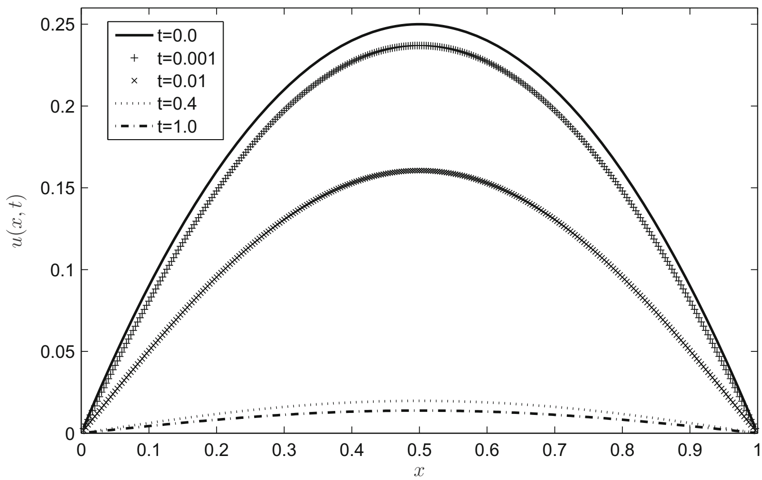

Fig. 3 Numerical solution of Example 3 with initial data $\varphi_1(x)$

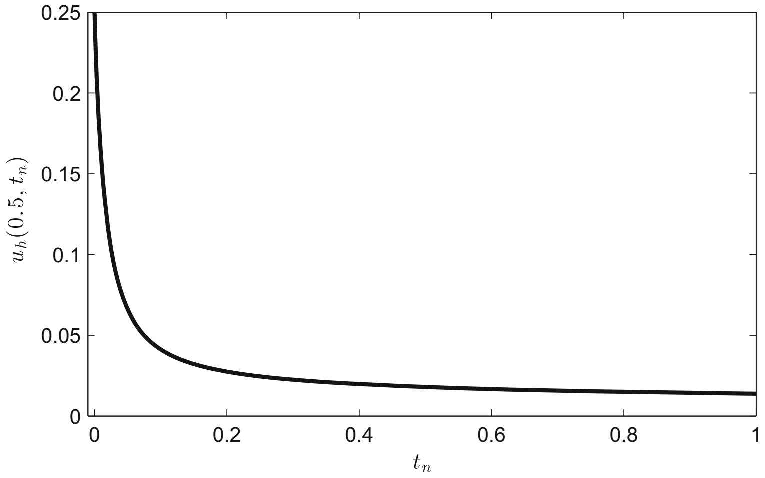

Fig. 4 Numerical solution $u_h(0.5, t_n)$ of Example 3 with data $\varphi_1(x)$

convergence rate of solution evidently, and the case of $m = 2$ recovers the second-order temporal accuracy of our CBDF2 method (4.1)–(4.2). For the initial data φ_1, we get similar results but omit them here. It is to note that, if a larger m is applied, numerical precision of solution will be affected since it introduces a larger maximum time-step $\tau_N = (N\tau)^m - ((N-1)\tau)^m \approx mT/N$. Always, a practical choice of parameter m is a trade-off between the numerical precision and convergence rate of solution.

Lastly, we apply the suggested methods with $m = 2$ to compute the solutions in Example 3 with the two nonnegative initial data. Note that, due to the resolution

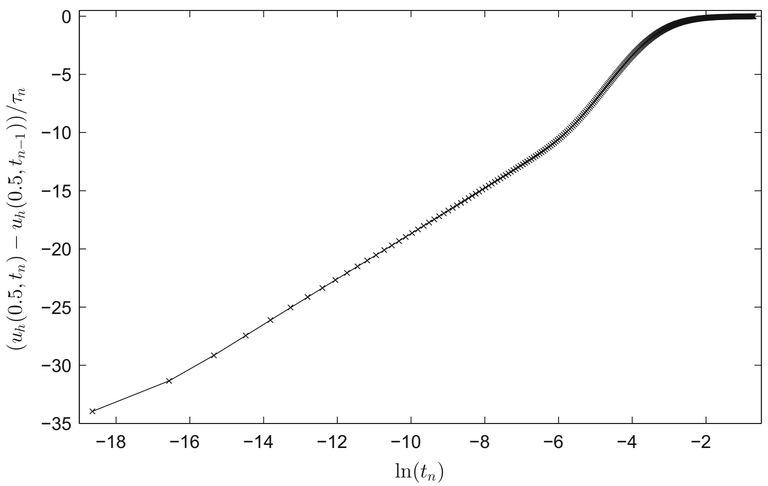

Fig. 5 Discrete derivative $\delta_t u_h(t_{n-\frac{1}{2}})$ of Example 3 with data $\varphi_1(x)$

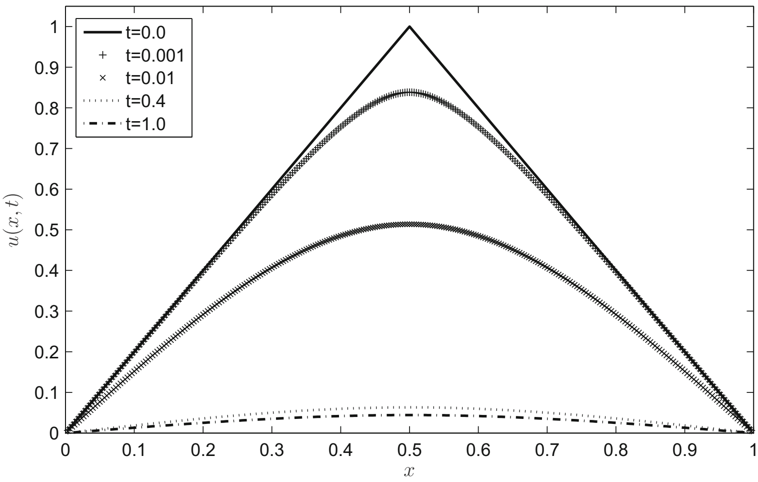

Fig. 6 Numerical solution of Example 3 with initial data $\varphi_2(x)$

of figures, the solutions generated by the CBDF1 and CBDF2 methods cannot be distinguished in the following curves such that we do not specify the concrete algorithm in each run. Taking small grid lengths $h = h_\alpha = 10^{-3}$ and the initial data $u(x, 0) = \varphi_1(x)$, we depict the numerical solution u_h^n in Fig. 3 at five different time $t_n = 0, 0.001, 0.01, 0.4$, and 1.0. As predicted by Theorems 3.4 and 4.12, the discrete solutions are nonnegative and decaying. Focusing on $x = 0.5$, for an instance, we observe

$$-\frac{u_h(0.5, 0.01) - u_h(0.5, 0)}{0.01} \gg -\frac{u_h(0.5, 1.0) - u_h(0.5, 0.4)}{0.6}.$$

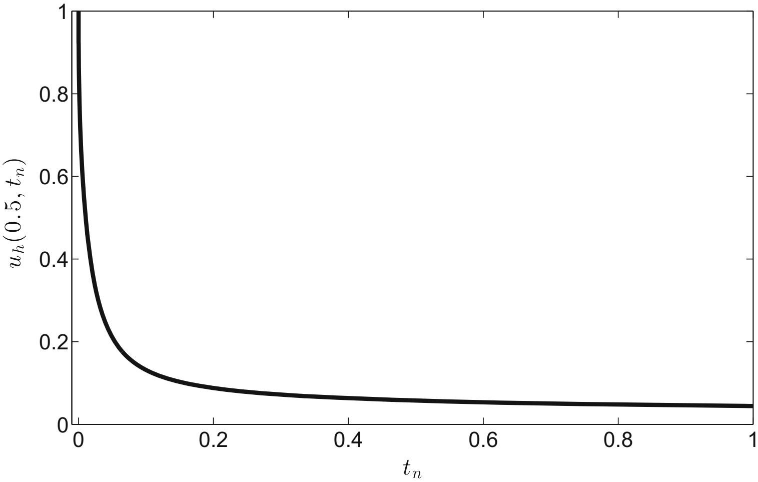

Fig. 7 Numerical solution $u_h(0.5, t_n)$ of Example 3 with data $\varphi_2(x)$

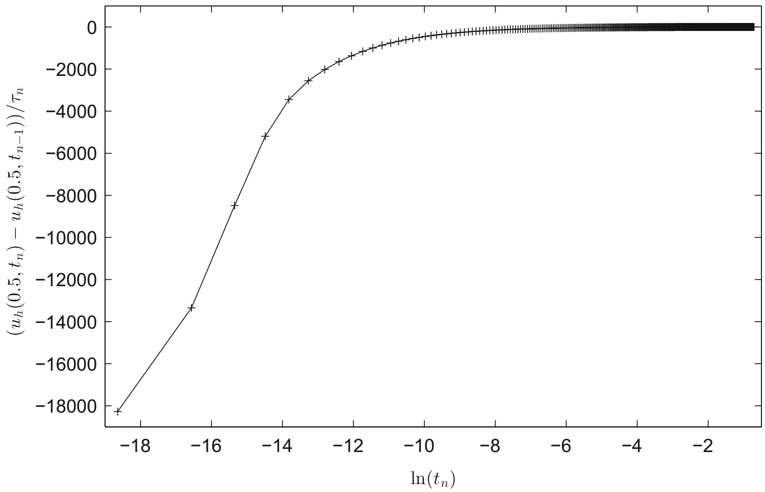

Fig. 8 Discrete derivative $\delta_t u_h(t_{n-\frac{1}{2}})$ of Example 3 with data $\varphi_2(x)$

It means that the solution near $t = 0$ decays much more faster than that away from $t = 0$.

To see the asymptotic behavior of the solution near $t = 0$, the solution $u_h(0.5, t_n)$ is listed in Fig. 4 for $t_n \in (t_1, 1)$, and the time derivative $\delta_t u_h(0.5, t_{n-\frac{1}{2}})$ is depicted in Fig. 5 with respect to $\ln(t_n)$ for $t_n \in (t_1, 0.5)$. In the two plots, we take $m = 3$ such that more mesh points can be concentrated in the initial time layer. One observes that $\left|\frac{\partial u}{\partial t}\right| = O(\ln(t^{-1}))$ as the time $t \in (0, 10^{-2})$, in which there have about 200 grid points. It supports the asymptotic estimate, see Theorem 2.2 in [20] or Theorem 2.1 in [15], for smooth initial data.

The curves in Figs. 6, 7, and 8, where the solution of Example 3 with the hat-like initial data $\varphi_2(x)$ are reported, are computed analogue to those in Figs. 3, 4, and 5. It is seen that the solution near $t = 0$ decays much more faster than that away from $t = 0$ and, by comparing Fig. 8 with Fig. 5, the module of time derivative $\left|\frac{\partial u}{\partial t}\right|$ is much greater than that generated by smooth data $\varphi_1(x)$. It increases the numerical difficulty in resolving the solution near the initial time. Actually, comparing the last two columns in Table 7 (Table 9) with those in Table 6 (Table 8), one can find that the lose of numerical precision near $t = 0$ pollutes the resolution of numerical solution evidently.

6 Concluding remarks

By using two Caputo's BDF formulas of fractional Caputo derivative, we proposed two stable implicit difference scheme for solving distributed-order subdiffusion equation. It is proven that the CBDF1 method satisfies the discrete minimum-maximum principle such that it is nonnegative-preserving and stable in the maximum norm. By using the discrete energy analysis, the CBDF2 scheme is shown to be stable and convergent in the discrete H^1 norm. Due to a low-order scheme employed at the first-time level, there is a theoretical lose of convergence order. For a certain region of the fractional-order, $\beta \in (0, 1/3]$, we also apply the maximum principle to prove that the CBDF2 scheme is nonnegative-preserving and second-order convergent in time.

Extensive experiments are presented to verify our theoretical results and show the effectiveness of the proposed methods. It is observed that the solution of distributed-order subdiffusion admits a weak initial singularity even for smooth initial data. Although the initial singularity is not well resolved theoretically, a class of nonuniform meshes which concentrates time-levels near $t = 0$ is suggested to recover the convergence rate of numerical methods.

There are a number of issues to be further studied. Firstly, it remains unknown how to recover the second-order accuracy theoretically for the CBDF2 method with $\beta = 1$. Secondly, numerical tests show that the CBDF2 scheme is always nonnegative-preserving. However, it remains open how to prove the nonnegative property for $\beta = 1$. At last, it is of practical interest to develop error estimates, reflecting the regularity of solutions, on nonuniform grids.

Acknowledgments This research is partially supported by the research grant 010/2015/A from FDCT of Macao, the research grant MYRG2015-00064-FST from University of Macau, the grants No. 11001271, 91530204, and 11372354 from the National Science Foundation of China, and the grant DRA2015518 from 333 High-level Personal Training Project of Jiangsu Province.

Appendix: approximate fractional derivatives on nonuniform grid

In a nonuniform time mesh, we denote $\tau_n = t_n - t_{n-1}$ and $\delta_t w^{n-\frac{1}{2}} = (w^n - w^{n-1})/\tau_n$. Let $\eta_k = t_n - t_{k-1} = \sum_{l=k}^{n} \tau_l$, $1 \leqslant k \leqslant n$, $n \geq 1$. We define the following coefficients

$$a_{n-k}^{(n,\alpha)} = \frac{\eta_k^{1-\alpha} - \eta_{k+1}^{1-\alpha}}{\Gamma(2-\alpha)}, \quad 1 \leqslant k \leqslant n\,;$$

$$b_{n-k}^{(n,\alpha)} = \frac{2}{\Gamma(3-\alpha)} \frac{\eta_k^{2-\alpha} - \eta_{k+1}^{2-\alpha}}{\tau_k + \tau_{k-1}} - \frac{\tau_k}{\tau_k + \tau_{k-1}} \frac{\eta_k^{1-\alpha} + \eta_{k+1}^{1-\alpha}}{\Gamma(2-\alpha)}\,, \quad 1 \leqslant k \leqslant n\,,$$

where $\eta_{n+1} = 0$. The nonuniform BDF1 and BDF2 formulas of Caputo derivative (1.1) reads

$$\mathcal{D}_{B1}^{\alpha} g^n = \sum_{k=1}^{n} a_{n-k}^{(n,\alpha)} \left(\delta_t g^{k-\frac{1}{2}}\right), \quad n \geq 1,$$

$$\mathcal{D}_{B2}^{\alpha} g^n = \sum_{k=1}^{n} a_{n-k}^{(n,\alpha)} \left(\delta_t g^{k-\frac{1}{2}}\right) + \sum_{k=2}^{n} b_{n-k}^{(n,\alpha)} \left(\delta_t g^{k-\frac{1}{2}} - \delta_t g^{k-\frac{3}{2}}\right), \quad n \geq 1.$$

To approximate the distributed-order derivative ${}_{\rho}D_t^{[\alpha]} g(t_n)$, we also define

$$a_{n-k}^{(n)} = h_{\alpha} \sum_{\ell=1}^{N_{\alpha}} a_{n-k}^{(n,\alpha_{\ell-\frac{1}{2}})} \rho(\alpha_{\ell-\frac{1}{2}})\,, \quad b_{n-k}^{(n)} = h_{\alpha} \sum_{\ell=1}^{N_{\alpha}} b_{n-k}^{(n,\alpha_{\ell-\frac{1}{2}})} \rho(\alpha_{\ell-\frac{1}{2}})\,, \quad 1 \leqslant k \leqslant n.$$

Then, the distributed-order BDF1 and BDF2 formulas on nonuniform grid take the form of

$$
\begin{aligned}
{}_{\rho}\mathcal{D}_{B1}^{[\alpha]}g^n &= \sum_{k=1}^{n} a_{n-k}^{(n)}\big(\delta_t g^{k-\frac{1}{2}}\big), \quad n \geq 1,\\
{}_{\rho}\mathcal{D}_{B2}^{[\alpha]}g^n &= \sum_{k=1}^{n} a_{n-k}^{(n)}\big(\delta_t g^{k-\frac{1}{2}}\big) + \sum_{k=2}^{n} b_{n-k}^{(n)}\big(\delta_t g^{k-\frac{1}{2}} - \delta_t g^{k-\frac{3}{2}}\big), \quad n \geq 1.
\end{aligned}
$$

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