



Fractional Adams–Bashforth/Moulton methods: An application to the fractional Keller–Segel chemotaxis system



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ABSTRACT

We first formulate a fractional class of explicit Adams–Bashforth (A-B) and implicit Adams–Moulton (A-M) methods of first- and second-order accuracy for the time-integration of ${}^C_0\mathcal{D}_t^\tau u(x, t) = g(t; u)$, $\tau \in (0, 1]$, where ${}^C_0\mathcal{D}_t^\tau$ denotes the fractional derivative in the Caputo sense. In this fractional setting and in contrast to the standard Adams methods, an extra history load term emerges and the associated weight coefficients are τ -dependent. However when $\tau = 1$, the developed schemes reduce to the well-known A-B and A-M methods with standard coefficients. Hence, in terms of scientific computing, our approach constitutes a minimal modification of the existing Adams libraries. Next, we develop an implicit–explicit (IMEX) splitting scheme for linear and nonlinear fractional PDEs of a general advection–reaction–diffusion type, and we apply our scheme to the time–space fractional Keller–Segel chemotaxis system. In this context, we evaluate the nonlinear advection term explicitly, employing the fractional A-B method in the prediction step, and we treat the corresponding diffusion term implicitly in the correction step using the fractional A-M scheme. Moreover, we perform the corresponding spatial discretization by employing an efficient and spectrally-accurate fractional spectral collocation method. Our numerical experiments exhibit the efficiency of the proposed IMEX scheme in solving nonlinear fractional PDEs.

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1. Introduction

The directed movement of cells and microorganisms in response to a diffusible chemical signal is referred to as chemotaxis [1]. Historically, the first mathematical model of chemotaxis was proposed by Evelyn Keller and Lee Segel in order to investigate the aggregation dynamics of the social amoeba *Dictyostelium discoideum* [2]. The model consisted of a nonlinear parabolic system of partial differential equations and is commonly referred to as the Keller–Segel model.

The Keller–Segel model has been analyzed extensively in the last three decades. A comprehensive review of mathematical results on dynamics, existence of solutions, and regularity can be found in the two articles by Horstmann [3,4]. It is well known that in one dimension the Keller–Segel model is well-posed globally in time [5–7]. However, several results that appeared in the 1990s have demonstrated that in higher dimensions, the Keller–Segel model is well-posed only for “small”

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initial data [8–10]. In the presence of “large” initial data, the solutions blow up; in other words, they do not remain bounded [11,12,5,13]. Corrias and Perthame [14] showed that in d dimensions, the Keller–Segel model is critical in $L^{d/2}$, which is to say that the “smallness” or “largeness” of the initial data is determined in terms of the $L^{d/2}$ norm. Similar conditions were derived in [15] for a parabolic-elliptic variation of the Keller–Segel model.

Recent literature has also investigated the influence of substrate heterogeneity on the dynamics of the model. Specifically, Matzavinos and Ptashnyk [16] have investigated the one-dimensional Keller–Segel model in the context of a random heterogeneous domain. In [16], the diffusion and chemotaxis coefficients were assumed to be given by stationary ergodic random fields, and the authors applied stochastic two-scale convergence methods to derive the homogenized macroscopic equations. Matzavinos and Ptashnyk [16] also present numerical algorithms for approximating the homogenized asymptotic coefficients.

The influence of substrate heterogeneity was also investigated in [17–19] by means of fractional calculus [20,21]. Interestingly, Bournaveas and Calvez [17] have shown that the fractional one-dimensional Keller–Segel model exhibits dynamics similar to the classical two-dimensional model. In particular, Bournaveas and Calvez [17] have shown that the solutions of the fractional Keller–Segel model may blow up in finite time, even in the one-dimensional case. In view of these results, the need to develop accurate numerical methods for the fractional Keller–Segel model is apparent.

A variety of numerical methods, originally developed for integer-order PDEs, are currently extended by several authors to fractional partial differential equations (FPDEs) [22–25]. Traditionally, there has been a substantial amount of work in developing finite-difference methods (FDM) for FPDEs. The notion of discretized fractional calculus was originally introduced by Lubich [26,27] and was employed by Sanz-Serna [28] in developing a first-order FDM algorithm for partial integro-differential equations. Since then, a significant amount of work has been devoted to improving the convergence rates of FDM schemes (see e.g., [29–32]).

Of particular interest is the work of Diethelm et al. [33,34], who developed and analyzed an Adams–Bashforth type method. However, this approach consists of a two-step predictor–corrector method, which differs significantly from the standard method, and it additionally requires a considerable modification of existing libraries. Moreover, the rate of convergence is dependent on the range of the fractional order α [35]. Recently, Baffet and Hesthaven have developed high-order local schemes, inspired by the multi-step Adams methods, for fractional differential equations in [36].

In addition to FDM schemes, Sugimoto [37] employed a spectral method to solve the fractional Burgers equation, and Blank [38] adopted a spline-based collocation scheme for a class of fractional ordinary differential equations (FODEs). Li and Xu [39,40] developed a space–time spectral method for a time-fractional diffusion equation with spectral convergence that was based on the early work of Fix and Roop [41]. Subsequently, Khader [42] proposed a Chebyshev collocation method for a space-fractional diffusion equation, while Piret and Hanert [43] developed a radial basis function method for fractional diffusion equations.

The use of spectral methods in FPDEs has been precipitated recently. Various approaches for solving fractional boundary value problems have been proposed, including a Chebyshev spectral method [44], a Legendre spectral method [45], and an adaptive pseudospectral method [46]. Similarly, spectral methods for fractional initial value problems have been proposed, including generalized Laguerre spectral algorithms [47] and Legendre spectral Galerkin methods [48]. It is well known that long-time (and/or adaptive) integration using such spectral schemes becomes computationally intractable. To address this issue, Xu and Hesthaven [49] and Chen et al. [50] have developed stable multi-domain methods for FPDEs. Moreover, a Jacobi tau approximation method has been recently developed by Bhrawy and Zaky for solving multi-term time–space fractional PDEs in [51].

A characteristic of these spectral approaches has been the use of standard integer-order (polynomial) basis functions. Recently, Zayernouri and Karniadakis [52,53] developed spectrally accurate Petrov–Galerkin schemes for both non-delay and delay fractional differential equations. These schemes are based on fractional basis functions (i.e., basis functions of non-integer order), which are termed *Jacobi poly-fractionomials* and were introduced in [54,55] as the eigenfunctions of certain fractional Sturm–Liouville operators. A space–time discontinuous Petrov–Galerkin (DPG) method and a discontinuous Galerkin (DG) method for the time–space fractional advection equation were also introduced in [56]. In [57], Jacobi poly-fractionomials were used to define a new class of *fractional Lagrange interpolants*. These were subsequently employed to numerically solve various FODE and FPDE problems, including multi-term FPDEs, the space-fractional Burgers equation, and variable-order problems [57,58].

The main contribution of the present work is to develop a fractional class of explicit Adams–Bashforth (A-B) and implicit Adams–Moulton (A-M) methods of first- and second-order accuracy for the time integration of FODEs and FPDEs. Our approach seamlessly generalizes the existing family of Adams schemes and requires a minimal modification of the existing Adams libraries, i.e., modifying the weights and adding a history calculator. We obtain the history load exactly up to the accuracy of the scheme via hyper-geometric functions. Moreover, we develop an implicit–explicit (IMEX) splitting scheme for the time–space fractional Keller–Segel chemotaxis system of FPDEs. Even though, the focus of this paper is the fractional Keller–Segel system, our IMEX approach is also applicable to other linear and nonlinear FPDEs.

The paper is organized as follows. We first provide some preliminary definitions from fractional calculus in section 2. In section 3, we present our general (fractional) explicit Adams–Bashforth and implicit Adams–Moulton methods for performing time-integration of time-fractional problems. Next, in section 4, we develop a spatial discretization scheme by employing a fractional spectral collocation method. In section 5, we introduce our implicit–explicit (IMEX) time-splitting approach and

apply it to the nonlinear, fractional Keller–Segel model of chemotaxis. Numerical tests on the convergence of our method are presented in section 6. Finally, conclusions and remarks are made in section 7.

2. Definitions

Before defining the problem, we provide some preliminary definitions of fractional calculus following [20,21]. The left-sided Riemann–Liouville integral of order $\mu \in (0, 1)$ is defined as

$$({}_{x_L}I_x^\mu)f(x) = \frac{1}{\Gamma(\mu)} \int_{x_L}^x \frac{f(s)ds}{(x-s)^{1-\mu}}, \quad x > x_L. \tag{1}$$

The corresponding inverse operator of (1), i.e., the left-sided fractional derivative of order μ , is then defined as

$$({}_{x_L}D_x^\mu)f(x) = \frac{d}{dx}({}_{x_L}I_x^{1-\mu}f)(x) = \frac{1}{\Gamma(1-\mu)} \frac{d}{dx} \int_{x_L}^x \frac{f(s)ds}{(x-s)^\mu}, \quad x > x_L. \tag{2}$$

An alternative approach in defining fractional derivatives is to begin with the left-sided Caputo derivative of order $\mu \in (0, 1)$, which is defined as

$$({}_{x_L}^C D_x^\mu f)(x) = ({}_{x_L}I_x^{1-\mu} \frac{df}{dx})(x) = \frac{1}{\Gamma(1-\mu)} \int_{x_L}^x \frac{f'(s)ds}{(x-s)^\mu}, \quad x > x_L. \tag{3}$$

The definitions of the left-sided fractional derivatives of both Riemann–Liouville and Caputo type are linked by the following relationship, which can be derived by a direct calculation

$$({}_{x_L}^{RL} D_x^\mu f)(x) = \frac{f(x_L)}{\Gamma(1-\mu)(x-x_L)^\mu} + ({}_{x_L}^C D_x^\mu f)(x). \tag{4}$$

3. Explicit and implicit time-integration

We first consider a fractional-order problem of the form

$$\begin{aligned} {}_0^C D_t^\tau u(t) &= g(t; u), \quad \tau \in (0, 1], t \in (0, T], \\ u(x, 0) &= u_0, \end{aligned} \tag{5}$$

where $g(t; u)$ could, in general, involve a spatial operator subject to some appropriate boundary conditions. By the definition of the Caputo fractional derivative, we have

$${}_0^C D_t^\tau u = \frac{1}{\Gamma(1-\tau)} \int_0^t \frac{\partial u}{\partial s} \frac{ds}{(t-s)^\tau} = H^k(t) + {}_{t_k}^C D_t^\tau u, \tag{6}$$

where $H^k(t) = \frac{1}{\Gamma(1-\tau)} \int_0^{t_k} \frac{\partial u}{\partial s} \frac{ds}{(t-s)^\tau}$. Moreover,

$${}_{t_k}^C D_t^\tau u = {}_{t_k}^C D_t^\tau (u - u_k + u_k) = {}_{t_k}^C D_t^\tau (u - u_k) = {}_{t_k}^{RL} D_t^\tau (u - u_k), \tag{7}$$

since $(u - u_k)$ vanishes at $t = t_k$ and using (4). Next, by substituting (7) and (6) into (5), we obtain

$${}_{t_k}^{RL} D_t^\tau u(t) = g(t; u) - H^k(t), \quad \tau \in (0, 1], \quad t \in (0, T]. \tag{8}$$

Applying the inverse operator ${}_{t_k}^{RL} I_t^\tau(\cdot)$ to (8) and evaluating at $t = t_{k+1}$, we obtain:

$$u_{k+1} - u_k = \left[{}_{t_k}^{RL} I_t^\tau g(t; u) - \mathcal{H}^k \right] \Big|_{t=t_{k+1}}, \quad \tau \in (0, 1], \tag{9}$$

where $\mathcal{H}^k = {}_{t_k}^{RL} I_t^\tau(H^k)$ will be referred to as the *history load* term in what follows.

In the next section, we introduce fractional generalizations of the Adams–Bashforth (A-B) and Adams–Moulton (A-M) methods through, respectively, an explicit and an implicit extrapolation of the term ${}_{t_k}^{RL} I_t^\tau g(t; u)$.

Table 1
 τ -dependent coefficients of the generalized (fractional) Adams–Bashforth method.

β_j	$J = 0$	$J = 1$	$J = 2$
β_0^{AB}	$\frac{1}{\Gamma(1+\tau)}$	$\frac{1}{\Gamma(1+\tau)} + \frac{1}{\Gamma(2+\tau)}$	$\frac{1}{\Gamma(1+\tau)} + \frac{3/2}{\Gamma(2+\tau)} + \frac{1}{\Gamma(3+\tau)}$
β_1^{AB}	0	$\frac{-1}{\Gamma(2+\tau)}$	$\frac{-2}{\Gamma(2+\tau)} + \frac{-2}{\Gamma(3+\tau)}$
β_2^{AB}	0	0	$\frac{1/2}{\Gamma(2+\tau)} + \frac{1}{\Gamma(3+\tau)}$

3.1. Fractional Adams–Bashforth method

In this method, we apply a time-extrapolation of the right-hand side $g(t; u)$ to the interval $[t_k, t_{k+1}]$ in terms of standard Lagrange interpolants and using “past” grid points in the following manner:

$$g(t; u) \approx \sum_{j=0}^J g(t_{k-j}; u) L_j(t), \quad (10)$$

where $g_{k-j} = g(t_{k-j}; u(t_{k-j}, x))$ and

$$L_j(t) = \prod_{\substack{i=0 \\ i \neq j}}^N \frac{t - t_{k-i}}{t_{k-j} - t_{k-i}}. \quad (11)$$

Hence, we obtain

$$\begin{aligned} {}^{RL}I_t^\tau g(t; u) &\approx \frac{1}{\Gamma(\tau)} \int_{t_k}^{t_{k+1}} \frac{\sum_{j=0}^J g_{k-j} L_j(s) ds}{(t_{k+1} - s)^{1-\tau}} \\ &= (\Delta t)^\tau \sum_{j=0}^J \beta_j^{AB} g_{k-j}, \end{aligned}$$

where β_j^{AB} are the τ -dependent coefficients given in Table 1. Hence, we obtain the fractional A-B method as

$$\boxed{\frac{u_{k+1} - u_k}{(\Delta t)^\tau} = \sum_{j=0}^J \beta_j^{AB} g_{k-j} - \frac{1}{(\Delta t)^\tau} \mathcal{H}^k.} \quad (12)$$

3.2. Fractional Adams–Moulton method

We can alternatively “interpolate” $g(t; u)$ between t_k and t_{k+1} in terms of the following Lagrange interpolants

$$g(t; u) \approx \sum_{j=0}^J g(t_{k+1-j}; u) \mathbb{L}_j(t), \quad (13)$$

where $g_{k+1-j} = g(t_{k+1-j}; u(t_{k+1-j}, x))$ and

$$\mathbb{L}_j(t) = \prod_{\substack{i=0 \\ i \neq j}}^N \frac{t - t_{k+1-i}}{t_{k+1-j} - t_{k+1-i}}. \quad (14)$$

Therefore, we obtain

$$\begin{aligned} {}^{RL}I_t^\tau g(t; u) &\approx \frac{1}{\Gamma(\tau)} \int_{t_k}^{t_{k+1}} \frac{\sum_{j=0}^J g_{k+1-j} \mathbb{L}_j(s) ds}{(t_{k+1} - s)^{1-\tau}} \\ &= (\Delta t)^\tau \sum_{j=0}^J \beta_j^{AM} g_{k+1-j}, \end{aligned}$$

Table 2
 τ -dependent coefficients of the generalized (fractional) Adams–Moulton method.

β_j	$J = 0$	$J = 1$	$J = 2$
β_0^{AM}	$\frac{1}{\Gamma(1+\tau)}$	$\frac{1}{\Gamma(2+\tau)}$	$\frac{1}{2\Gamma(2+\tau)} + \frac{1}{\Gamma(3+\tau)}$
β_1^{AM}	0	$\frac{1}{\Gamma(1+\tau)} - \frac{1}{\Gamma(2+\tau)}$	$\frac{1}{\Gamma(1+\tau)} + \frac{-2}{\Gamma(3+\tau)}$
β_2^{AM}	0	0	$\frac{-1}{2\Gamma(2+\tau)} + \frac{1}{\Gamma(3+\tau)}$

where the coefficients β_j^{AM} are τ -dependent and are given in Table 2. Hence, we obtain the generalized A-M method as

$$\frac{u_{k+1} - u_k}{(\Delta t)^\tau} = \sum_{j=0}^J \beta_j^{AM} g_{k+1-j} - \frac{1}{(\Delta t)^\tau} \mathcal{H}^k. \tag{15}$$

Remark 3.1. We note that the generalized A-B and A-M methods, given in (12) and (15), respectively, share the same history load \mathcal{H}^k . Moreover, $\mathcal{H}^k = 0$ when the temporal fractional order $\tau = 1$; hence, we recover the standard A-B and A-M methods.

3.3. Computation of the history load \mathcal{H}^k

We recall that the history load term is given by $\mathcal{H}^k = {}^{RL}I_t^\tau(H^k)$, where

$$H^k(t) = \frac{1}{\Gamma(1-\tau)} \int_0^{t_k} \frac{\partial u}{\partial s} ds (t-s)^{\tau-1} = \frac{1}{\Gamma(1-\tau)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{\partial u}{\partial s} ds (t-s)^{\tau-1}.$$

In order to approximate $\frac{\partial u}{\partial s}$ in $[t_j, t_{j+1}]$, we employ two interpolation methods to approximate the solution $u(t, \cdot)$.

3.3.1. Linear interpolation of $u(t, \cdot)$

The linear interpolation of u leads to a second-order approximation of the solution in $[t_j, t_{j+1}]$ and leads to

$$\begin{aligned} H^k(t) &\approx H_l^k(t) = \frac{1}{\Gamma(1-\tau)} \sum_{j=0}^{k-1} \left(\frac{u_{j+1} - u_j}{\Delta t} \right) \int_{t_j}^{t_{j+1}} \frac{ds}{(t-s)^\tau} \\ &= \frac{1}{\Gamma(2-\tau)} \sum_{j=0}^{k-1} \left(\frac{u_{j+1} - u_j}{\Delta t} \right) G_j^l(t), \end{aligned}$$

where $G_j^l(t) = (t - t_j)^{1-\tau} - (t - t_{j+1})^{1-\tau}$. Hence,

$$\mathcal{H}^k(t) \approx \mathcal{H}_l^k(t) = \frac{1}{\Gamma(2-\tau)} \sum_{j=0}^{k-1} \left(\frac{u_{j+1} - u_j}{\Delta t} \right) {}^{RL}I_t^\tau \left(G_j^l(t) \right).$$

By evaluating both sides at t_{k+1} , we obtain the corresponding history load as

$$\begin{aligned} \mathcal{H}^k \approx \mathcal{H}_l^k &= \frac{1}{\Gamma(\tau)\Gamma(2-\tau)} \sum_{j=0}^{k-1} \left(\frac{u_{j+1} - u_j}{\Delta t} \right) \left[\int_{t_k}^{t_{k+1}} (t_{k+1} - s)^{\tau-1} (s - t_j)^{1-\tau} ds \right. \\ &\quad \left. - \int_{t_k}^{t_{k+1}} (t_{k+1} - s)^{\tau-1} (s - t_{j+1})^{1-\tau} ds \right], \end{aligned}$$

which can be written as

$$\mathcal{H}^k \approx \mathcal{H}_l^k = \frac{1}{\Gamma(\tau)\Gamma(2-\tau)} \sum_{j=0}^{k-1} \left(\frac{u_{j+1} - u_j}{\Delta t} \right) [\mathcal{A}_{k,j} - \mathcal{A}_{k,j+1}], \tag{16}$$

where $\mathcal{A}_{kj} = \int_{t_k}^{t_{k+1}} (t_{k+1} - s)^{\tau-1} (s - t_j)^{1-\tau} ds$. The latter is obtained analytically in terms of the following hypergeometric functions:

$$\mathcal{A}_{kj} = \begin{cases} -\frac{(\Delta t)^\tau}{\tau} (t_k - t_j)^{1-\tau} \left[-\tau + (\tau - 1) {}_2F_1(1, 1, 1 + \tau, \frac{\Delta t}{t_{k+1} - t_j}) \right], & 0 \leq j < k \\ -(\Delta t)(\tau - 1)\pi \csc(\pi \tau), & j = k. \end{cases} \quad (17)$$

Therefore, the history load \mathcal{H}_I^k is computed exactly in terms of \mathcal{A}_{kj} up to the discretization accuracy of the first derivative of the solution, i.e., $\frac{u_{j+1} - u_j}{\Delta t}$.

3.3.2. Quadratic interpolation of $u(t, \cdot)$

According to standard approximation theory, a third-order approximation of $u(t, \cdot)$ in $[t_j, t_{j+1}]$ yields

$$u(t, \cdot) \approx u_{j+1} \left(\frac{t - t_j}{t_{j+1} - t_j} \right) \left(\frac{t - t_{j-1}}{t_{j+1} - t_{j-1}} \right) + u_j \left(\frac{t - t_{j+1}}{t_j - t_{j+1}} \right) \left(\frac{t - t_{j-1}}{t_j - t_{j-1}} \right) \\ + u_{j-1} \left(\frac{t - t_{j+1}}{t_{j-1} - t_{j+1}} \right) \left(\frac{t - t_j}{t_{j-1} - t_j} \right),$$

where by taking the first partial derivative with respect to time we obtain

$$\frac{\partial u}{\partial t} \approx \left(\frac{\partial u}{\partial t} \right) \Big|_{t=t_{j+1/2}} + \left(\frac{\partial^2 u}{\partial t^2} \right) \Big|_{t=t_{j+1/2}} (t - t_{j+1/2}).$$

The latter expression yields a higher-order approximation of $\frac{\partial u}{\partial t}$ to be employed in the calculation of the history load. Therefore,

$$H^k(t) \approx H_{II}^k(t) = \frac{1}{\Gamma(1 - \tau)} \sum_{j=1}^{k-1} \int_{t_j}^{t_{j+1}} \frac{\left[\left(\frac{\partial u}{\partial s} \right) \Big|_{s=t_{j+1/2}} + \left(\frac{\partial^2 u}{\partial s^2} \right) \Big|_{s=t_{j+1/2}} (s - t_{j+1/2}) \right] ds}{(t - s)^\tau} \\ + \frac{1}{\Gamma(1 - \tau)} \int_0^{t_1} \frac{\left(\frac{\partial u}{\partial s} \right) \Big|_{s=t_{1/2}} ds}{(t - s)^\tau}$$

where we employed the previously obtained lower-order approximation in $[0, t_1]$ corresponding to $j = 0$. Hence,

$$H_{II}^k(t) = \frac{1}{\Gamma(1 - \tau)} \sum_{j=0}^{k-1} \left(\frac{u_{j+1} - u_j}{\Delta t} \right) \int_{t_j}^{t_{j+1}} \frac{ds}{(t - s)^\tau} \\ + \frac{1}{\Gamma(1 - \tau)} \sum_{j=1}^{k-1} \left(\frac{\partial^2 u}{\partial s^2} \right) \Big|_{s=t_{j+1/2}} \int_{t_j}^{t_{j+1}} \frac{(s - t_{j+1/2}) ds}{(t - s)^\tau} \\ = H_I^k(t) + \frac{1}{\Gamma(\tau) \Gamma(2 - \tau)} \sum_{j=1}^{k-1} \left(\frac{u_{j+1} - 2u_j + u_{j-1}}{(\Delta t)^2} \right) G_j^{II}(t), \quad (18)$$

in which the first term is associated with the linear representation of $u(t)$ and the second term in (18) denotes the correction for obtaining a higher-order accuracy. Moreover, $G_j^{II}(t)$ is given by

$$G_j^{II}(t) = -\frac{\Delta t}{2} \left[(t - t_j)^{1-\tau} + (t - t_{j+1})^{1-\tau} \right] + \frac{1}{2 - \tau} \left[(t - t_j)^{2-\tau} - (t - t_{j+1})^{2-\tau} \right] \quad (19)$$

Accordingly, the corresponding load vector is obtained as

$$\mathcal{H}^k \approx \mathcal{H}_{II}^k = {}^{RL}I_{t_k}^\tau {}^{RL}I_{t_{k+1}}^\tau H_{II}^k(t) \\ = {}^{RL}I_{t_k}^\tau {}^{RL}I_{t_{k+1}}^\tau H_I^k(t) + \frac{1}{\Gamma(\tau) \Gamma(2 - \tau)} \sum_{j=1}^{k-1} \left(\frac{u_{j+1} - 2u_j + u_{j-1}}{(\Delta t)^2} \right) {}^{RL}I_{t_k}^\tau {}^{RL}I_{t_{k+1}}^\tau G_j^{II}(t) \quad (20)$$

which can be written as

Table 3

Fractional Adams–Bashforth time-integration of the ${}_0^C \mathcal{D}_t^\tau u(t) = f(t)$ subject to homogeneous initial conditions. (Upper table): fractional A-B ($J = 0$), where the exact solution is $u^{ext} = t^\tau$, (middle table): fractional A-B ($J = 1$), where $u^{ext} = t^{1+\tau}$, and (lower table): fractional A-B ($J = 2$), where $u^{ext} = t^{2+\tau}$. Here, the simulation time is $T = 1$ and $f(t) = \frac{\Gamma(1+\tau+J)}{\Gamma(1+\tau+J-\tau)} t^J$, where $J = 0, 1$, and 2 , respectively.

Fractional A-B, $J = 0, (\mathcal{H}^k \approx \mathcal{H}_1^k)$						
Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/8	0.823385	0.43	0.388225	0.88	0.261049	1.00
1/16	0.613304	0.55	0.211394	0.92	0.129804	1.00
1/32	0.416202	0.70	0.111384	0.96	0.064746	1.00
1/64	0.255626	0.82	0.057415	0.98	0.032357	0.999
1/128	0.144731	0.90	0.029210	0.99	0.016188	0.998

Fractional A-B, $J = 1, (\mathcal{H}^k \approx \mathcal{H}_1^k)$						
Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/8	0.229075	1.65	0.0517457	1.91	0.029365	1.975
1/16	0.073136	1.83	0.013736	1.96	0.000747	1.993
1/32	0.020521	1.90	0.003527	1.978	0.001876	1.998
1/64	0.005516	1.91	0.000895	1.984	0.000469	1.999
1/128	0.001473	1.93	0.000226	1.998	0.000117	2.00

Fractional A-B, $J = 2, (\mathcal{H}^k \approx \mathcal{H}_1^k)$						
Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/8	0.088115	2.72	0.017732	2.92	0.010759	2.92
1/16	0.013366	2.76	0.002345	2.99	0.001423	2.98
1/32	0.001969	2.78	0.000294	3.05	0.000180	3.02
1/64	0.000286	2.90	0.000035	3.12	0.000022	3.09
1/128	0.000038	2.91	4.06×10^{-6}	3.20	2.60×10^{-6}	3.22

$$\mathcal{H}^k \approx \mathcal{H}_{11}^k = \mathcal{H}_1^k + \frac{1}{\Gamma(\tau)\Gamma(2-\tau)} \sum_{j=1}^{k-1} \left(\frac{u_{j+1} - 2u_j + u_{j-1}}{(\Delta t)^2} \right) \left[-\frac{\Delta t(\mathcal{A}_{k,j} + \mathcal{A}_{k,j+1})}{2} + \frac{\mathcal{B}_{k,j} - \mathcal{B}_{k,j+1}}{2-\tau} \right], \quad (21)$$

where $\mathcal{B}_{kj} = \int_{t_k}^{t_{k+1}} (t_{k+1} - s)^{\tau-1} (s - t_j)^{2-\tau} ds$. The latter is computed exactly in terms of the following hypergeometric function:

$$\mathcal{B}_{kj} = \begin{cases} -\frac{(\Delta t)^\tau}{\tau} \frac{(t_k - t_j)^{3-\tau}}{(t_{k+1} - t_j)} \left[{}_2F_1(1, 3, 1 + \tau, \frac{\Delta t}{t_{k+1} - t_j}) \right], & 0 \leq j < k \\ -\frac{(\Delta t)^\tau \pi}{2} (-2 + \tau)(\tau - 1) \csc(\pi \tau), & j = k. \end{cases} \quad (22)$$

Finally, we note that \mathcal{B}_{kj} is constructed only once.

3.4. Numerical tests for the fractional A-B and A-M methods

In Table 3, we examine the performance of the fractional A-B scheme at different values of $J = 0, 1$, and 2 , and for different temporal orders τ . The equation ${}_0^C \mathcal{D}_t^\tau u(t) = f(t)$ is solved subject to homogeneous initial conditions. In the upper table, we present the fractional A-B method with $J = 0$ and $\mathcal{H}^k \approx \mathcal{H}_1^k$. The exact solution in this case is given by $u^{ext} = t^\tau$. In the middle table, we present the fractional A-B method with $J = 1$ and $\mathcal{H}^k \approx \mathcal{H}_{11}^k$, considering $u^{ext} = t^{1+\tau}$. In the lower table, we demonstrate the performance of the fractional A-B method when $J = 2$, $\mathcal{H}^k \approx \mathcal{H}_1^k$, and $u^{ext} = t^{2+\tau}$. The simulation time is $T = 1$ in all cases, and all errors are computed using the L^∞ norm at the final simulation time. The specified exact solutions correspond to the forcing terms $f(t) = \frac{\Gamma(1+\tau+J)}{\Gamma(1+\tau+J-\tau)} t^J$ for $J = 0, 1$, and 2 , respectively. These specific choices of exact solutions are made to illustrate the minimal smoothness requirements in each case. Interestingly, we observe a “ τ -independent” first-, second-, and third-order of accuracy when $J = 0, 1$, and 2 respectively. In other words, the numerical evidence suggests that the fractional A-B method not only generalizes the standard A-B method, but it also preserves the traditional order of accuracy of the A-B methods originally developed for integer-order systems.

In a similar fashion, we examine the performance of the fractional A-M scheme with different values of J and for different choices of τ in Table 4. We keep the setting as in Table 3 to experimentally observe the order accuracy associated

Table 4

Fractional Adams–Moulton time-integration of the ${}^C_0\mathcal{D}_t^\tau u(t) = f(t)$ subject to homogeneous initial conditions. (Upper table): fractional A-M ($J = 0$), where the exact is solution $u^{\text{ext}} = t^\tau$, (middle table): fractional A-M ($J = 1$), where $u^{\text{ext}} = t^{1+\tau}$, and, (lower table): fractional A-M ($J = 2$), where $u^{\text{ext}} = t^{2+\tau}$. Here, the simulation time is $T = 1$ and $f(t) = \frac{\Gamma(1+\tau+J)}{\Gamma(1+\tau+J-\tau)} t^J$, where $J = 0, 1$, and 2 , respectively.

Fractional A-M, $J = 0, (\mathcal{I}_t^k \approx \mathcal{I}_t^k)$						
Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/8	0.566053	1.82	0.186798	1.32	0.146284	1.19
1/16	0.1602418	1.51	0.074632	1.15	0.063814	1.09
1/32	0.056163	1.28	0.033644	1.07	0.029979	1.04
1/64	0.022971	1.15	0.016002	1.03	0.014544	1.02
1/128	0.010352	1.07	0.007710	1.02	0.007161	1.01
Fractional A-M, $J = 1, (\mathcal{I}_t^k \approx \mathcal{I}_t^k)$						
Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/8	0.051728	2.09	0.037242	2.06	0.031385	2.05
1/16	0.012254	2.02	0.008879	2.03	0.007565	2.02
1/32	0.003004	1.97	0.002171	2.01	0.001859	2.01
1/64	0.000765	1.93	0.000537	2.006	0.000465	2.007
1/128	0.000200	1.94	0.000134	2.00	0.000114	2.00
Fractional A-M, $J = 2, (\mathcal{I}_t^k \approx \mathcal{I}_t^k)$						
Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/8	0.012274	3.00	0.010341	2.94	0.009544	2.92
1/16	0.001528	2.95	0.001351	2.88	0.001260	2.82
1/32	0.000197	2.93	0.000184	2.83	0.000177	2.70
1/64	0.000026	2.91	0.000026	2.78	0.000027	2.57
1/128	3.45×10^{-6}	2.90	3.74×10^{-6}	2.74	4.57×10^{-6}	2.43

with different J 's. Again, we observe a τ -independent first- and second-order of accuracy when $J = 0$ and 1 . However, our results show a τ -dependent accuracy of less than third order when $J = 2$ in contrast to the fractional A-B scheme. This simply highlights the need for a higher-order approximation of the history term, which turns out to be inefficient in terms of computation cost. We remark that the numerical experiments discussed in this section were chosen so that the J -th derivative of the exact solution for $J = 0, 1$, and 2 vanishes at $t = 0$ respectively in each of the methods tested.

4. Spatial discretization via fractional spectral collocation method

In this section, we discuss the spatial discretization of the fractional PDEs that we solve in sections 5 and 6; see equations (34) and (38). In order to efficiently discretize the spatial terms, we employ a fractional spectral collocation method (FSCM), recently developed in [57], which is based on the spectral theory of fractional Sturm–Liouville problems (FSLP), developed in [54]. To this end, we define a set of *interpolation points* $\{x_i\}_{i=1}^N$ on which the corresponding Lagrange interpolants are constructed. Moreover, we require the residual to vanish on the *collocation points*, which coincide with the interpolation points $\{x_i\}_{i=1}^N$.

4.1. Fractional Lagrange interpolants (FLIs)

We represent the solution at time t_k in terms of non-polynomial fractional basis functions, known as *Jacobi poly-fractionomials*, which are the explicit eigenfunctions of the FSLP of first kind, given by

$${}^{(1)}\mathcal{P}_n^\mu(x) = (1+x)^\mu P_{n-1}^{-\mu, \mu}(x), \quad x \in [-1, 1], \quad (23)$$

where $P_{n-1}^{-\mu, \mu}(x)$ denotes the Jacobi polynomial of degree $n - 1$ and parameters $-\mu$ and μ . The left-sided fractional derivative of (23) is given analytically as

$${}_{-1}\mathcal{D}_x^\mu \left({}^{(1)}\mathcal{P}_n^\mu(x) \right) = \frac{\Gamma(n+\mu)}{\Gamma(n)} P_{n-1}(x), \quad (24)$$

where $P_{n-1}(x)$ denotes a Legendre polynomial of order $n - 1$. In our FSCM spatial discretization, we represent the solution at the time t_k via the following poly-fractionomial *nodal expansion* as

$$u_N(x, t_k) = \sum_{j=1}^N u_N(x_j, t_k) h_j^\mu(x), \quad (25)$$

where the functions $h_j^\mu(x)$ denote the *fractional Lagrange interpolants*; these are all of fractional order $(N + \mu - 1)$ and are constructed using the aforementioned interpolation points $-1 = x_1 < x_2 < \dots < x_N = 1$ as:

$$h_j^\mu(x) = \left(\frac{x-x_1}{x_j-x_1}\right)^\mu \prod_{\substack{k=1 \\ k \neq j}}^N \left(\frac{x-x_k}{x_j-x_k}\right), \quad 2 \leq j \leq N-1. \tag{26}$$

Because of the homogeneous Dirichlet boundary conditions in (34) and (38), we only construct $h_j^\mu(x)$ for $j = 2, 3, \dots, N$ when the order ν of the fractional diffusion term is such that $\nu \in (0, 1)$, and we set $u_N(-1) = 0$. Moreover, when $\nu \in (1, 2)$, there are only $(N - 2)$ fractional Lagrange interpolants $h_j^\mu(x)$, $j = 2, 3, \dots, N - 1$, since we impose $u_N(\pm 1) = 0$.

4.2. Spatial differentiation matrices \mathbf{D}^σ and $\mathbf{D}^{1+\sigma}$, $\sigma \in (0, 1)$

We note that FLIs satisfy the Kronecker delta property $h_j^\mu(x_k) = \delta_{jk}$ at interpolation points, and they vary as a poly-fractionomial between the interpolation points. With each FLI, we associate fractional differentiation matrices \mathbf{D}^σ and $\mathbf{D}^{1+\sigma}$, $\sigma \in (0, 1)$, which are obtained as follows:

$$\mathbf{D}_{ij}^\sigma = \frac{1}{(x_j+1)^\mu} \sum_{n=1}^N \beta_n^j \sum_{q=\lceil \sigma-\mu \rceil}^{n-1} b_{nq} (x_i+1)^{q+\mu-\sigma} \tag{27}$$

and

$$\mathbf{D}_{ij}^{1+\sigma} = \frac{1}{(x_j+1)^\mu} \left[\sum_{n=1}^N \beta_n^j \sum_{q=\lceil \sigma-\mu \rceil}^{n-1} b_{nq} (q+\mu-\sigma) (x_i+1)^{q+\mu-\sigma-1} \right], \tag{28}$$

in which $\lceil \sigma - \mu \rceil$ denotes the integer ceiling of $\sigma - \mu$, and

$$b_{nq} = (-1)^{n+q-1} \binom{1}{2}^q \binom{n-1+q}{q} \binom{n-1+\mu}{n-1-q} \frac{\Gamma(q+\mu+1)}{\Gamma(q+\mu-\sigma+1)}. \tag{29}$$

We remark that the coefficients are obtained only *once* through the following poly-fractionomial expansion

$$\prod_{\substack{k=1 \\ k \neq j}}^N \left(\frac{x-x_k}{x_j-x_k}\right) = \sum_{n=1}^N \beta_n^j P_{n-1}^{-\mu, \mu}(x) \tag{30}$$

and can be computed efficiently since the Jacobi polynomials $P_{n-1}^{-\mu, \mu}(x)$ are orthogonal with respect to the weight function $w(x) = (1-x)^{-\mu}(1+x)^\mu$. Hence, taking the polynomial $p_j(x) = \prod_{\substack{k=1 \\ k \neq j}}^N \left(\frac{x-x_k}{x_j-x_k}\right)$, the coefficients β_n^j are given exactly by the following Gauss-Lobatto–Jacobi quadrature rule:

$$\begin{aligned} \beta_n^j &= \frac{1}{\lambda_n} \int_{-1}^1 w(x) p_j(x) P_{n-1}^{-\mu, \mu}(x) dx \\ &= \frac{1}{\lambda_n} \sum_{q=1}^Q \omega_q p_j(x_q) P_{n-1}^{-\mu, \mu}(x_q), \end{aligned} \tag{31}$$

where $\{x_q\}_{q=1}^Q$ and $\{\omega_q\}_{q=1}^Q$ are the associated quadrature points and weights corresponding to the Jacobi weight $w(x)$; moreover, λ_n denotes the orthogonality constant of the Jacobi poly-fractionomials given by $\lambda_n = \frac{2}{2k-1} \frac{\Gamma(n-\mu)\Gamma(n+\mu)}{(n-1)!\Gamma(n)}$. We remark that the coefficients β_n^j are given exactly by the Gauss-Lobatto–Jacobi quadrature rule when $Q \geq (N - 1) + 3/2$.

Remark 4.1. When $\sigma = \mu$ (the interpolation parameter), the above differentiation matrices are simply obtained as

$$\mathbf{D}_{ij}^\mu = \frac{1}{(x_j+1)^\mu} \sum_{n=1}^N \frac{\Gamma(n+\mu)}{\Gamma(n)} \beta_n^j P_{n-1}(x_i) \tag{32}$$

and

$$\mathbf{D}_{ij}^{1+\mu} = \frac{1}{(x_j+1)^\mu} \sum_{n=2}^N \beta_n^j \left[\frac{\Gamma(n+\mu)}{\Gamma(n)} \frac{n}{2} P_{n-2}^{1,1}(x_i) \right]. \tag{33}$$

Table 5

Convergence study of the spatial operators. Here, $u^{ext}(x) = (2^{1/6}(1+x)^{4+1/3} - (1+x)^{4+1/2})$.

$\mu = 1/10$				
N	${}_{-1}^{RL}I_x^\mu u(x) = f(x)$	${}_{-1}^{RL}D_x^\mu u(x) = f(x)$	${}_{-1}^{RL}D_x^{1+\mu} u(x) = f(x)$	${}_{-1}^{RL}D_x^{1+\mu} u(x) - u(x) = f(x)$
3	0.0143673	0.0175926	3.88583	0.368123
7	0.0000103311	0.0000106009	0.0000947525	0.000594943
11	2.31×10^{-8}	2.306×10^{-8}	4.18×10^{-7}	2.27×10^{-6}
$\mu = 1/2$				
N	${}_{-1}^{RL}I_x^\mu u(x) = f(x)$	${}_{-1}^{RL}D_x^\mu u(x) = f(x)$	${}_{-1}^{RL}D_x^{1+\mu} u(x) = f(x)$	${}_{-1}^{RL}D_x^{1+\mu} u(x) - u(x) = f(x)$
3	0.043334	0.102084	0.866727	0.346067
7	0.00009786	0.0000794	0.0002552	0.00141853
11	1.54×10^{-6}	9.1×10^{-7}	5.8×10^{-6}	0.00002033
$\mu = 9/10$				
N	${}_{-1}^{RL}I_x^\mu u(x) = f(x)$	${}_{-1}^{RL}D_x^\mu u(x) = f(x)$	${}_{-1}^{RL}D_x^{1+\mu} u(x) = f(x)$	${}_{-1}^{RL}D_x^{1+\mu} u(x) - u(x) = f(x)$
3	0.0528279	0.209984	0.423576	0.263411
7	0.000078243	0.0000256864	0.000969232	0.00179444
11	3.81×10^{-6}	7.43×10^{-7}	0.0000430498	0.0000925764

As the collocation/interpolation points, the roots of ${}_{-1}D_x^\mu [{}^{(1)}P_M^\mu(x)]$ that represent the (fractional) critical points of the Jacobi poly-fractional functions lead to the fastest rates of convergence and minimal condition number of the resulting system.

In order to demonstrate the spectral accuracy of the corresponding spatial discretization, we have performed a convergence study of the spatial operators for the following three differential problems: ${}_{-1}^{RL}I_x^\mu u(x) = f(x)$, ${}_{-1}^{RL}D_x^\mu u(x) = f(x)$, ${}_{-1}^{RL}D_x^{1+\mu} u(x) = f(x)$, and ${}_{-1}^{RL}D_x^{1+\mu} u(x) - u(x) = f(x)$. In each problem the reaction term $f(x)$ was chosen so as the exact solution is given by $u^{ext}(x) = (2^{1/6}(1+x)^{4+1/3} - (1+x)^{4+1/2})$. The accuracy of the method for each problem is shown in Table 5.

5. Fractional-order splitting scheme: semi-discrete form

We consider a time-space fractional PDE of the form:

$$\begin{aligned} {}_0\mathcal{D}_t^\tau u(x, t) &= (\mathcal{N}_x^\sigma + \mathcal{L}_x^\alpha)u(x, t) + F(u), \quad x \in [-1, 1], \\ u(x, 0) &= h(x), \\ u(\pm 1, t) &= 0, \end{aligned} \tag{34}$$

where $\tau, \sigma \in (0, 1]$, $\alpha \in (1, 2]$. Moreover, $\mathcal{N}_x^\sigma u$ represents a *nonlinear* (e.g., convective) differential operator. \mathcal{L}_x^α denotes a *linear* (e.g., diffusive) operator, and $F(u)$ is the corresponding reaction term. Equation (34) should be compared with equation (38) in the following section. In the semi-discrete form, we evaluate the nonlinear and reaction terms “explicitly” by employing the fractional explicit A-B method, see (12), while we treat the corresponding diffusion term “implicitly” using the fractional A-M scheme in (15) as

$$\begin{aligned} \frac{u(x, t_{k+1}) - u(x, t_k)}{(\Delta t)^\tau} &= \sum_{j=0}^J \beta_j^{AB} \left[\mathcal{N}_x^\sigma u(x, t_{k-j}) + F(u(x, t_{k-j})) \right] \\ &+ \sum_{j=0}^J \beta_j^{AM} \mathcal{L}_x^\alpha u(x, t_{k+1-j}) - \frac{\mathcal{H}^k}{(\Delta t)^\tau}. \end{aligned} \tag{35}$$

We recall from Remark 3.1 that the corresponding history load terms in the A-B and A-M methods are identical. Next, we split (35) in the following fashion: (i) in the *prediction step*, we keep the nonlinear and reaction terms to explicitly obtain an “intermediate” solution $u_p(x, t_{k+1})$ while ignoring the diffusion term:

$$\boxed{\frac{u_p(x, t_{k+1}) - u(x, t_k)}{(\Delta t)^\tau} = \sum_{j=0}^J \beta_j^{AB} \left[\mathcal{N}_x^\sigma u(x, t_{k-j}) + F(u(x, t_{k-j})) \right] - \frac{\mathcal{H}^k}{(\Delta t)^\tau},} \tag{36}$$

and (ii) in the *correction step*, we include the diffusion term to implicitly solve for the (corrected) solution at the new time-step t_{k+1} as

$$\frac{u(x, t_{k+1}) - u_p(x, t_{k+1})}{(\Delta t)^\tau} = \sum_{j=0}^J \beta_j^{AM} \mathcal{L}_x^\alpha u(x, t_{k+1-j}). \tag{37}$$

Here, we choose the order of discretization (i.e., J) in the prediction A-B and correction A-M steps to be the same (i.e., $J = 3$).

In the following, we employ the splitting scheme of (36) and (37) in the context of the time- and space-fractional Keller–Segel chemotaxis system.

5.1. Fractional Keller–Segel chemotaxis system

We consider the following time–space fractional Keller–Segel model:

$$\begin{aligned} {}_0^C \mathcal{D}_t^\tau u(x, t) &= -K_{c-1} \mathcal{D}_x^\mu \left[u \mathcal{D}_x^\beta C(x, t) \right] + K_{-1} \mathcal{D}_x^{1+\sigma} u + f(x, t; u), \\ u(x, 0) &= h(x), \\ u(\pm 1, t) &= 0, \end{aligned} \tag{38}$$

in which τ, σ, μ , and $\beta \in (0, 1)$. Equation (38) is coupled to the following elliptic fractional (in space) equation of order $\gamma \in (1, 2)$:

$$\begin{aligned} K_{e-1} \mathcal{D}_x^\gamma C(x, t) &= -u(x, t) \\ C(-1, t) &= 0 \\ \frac{\partial C}{\partial x} \Big|_{x=-1} &= 0 \end{aligned} \tag{39}$$

The corresponding fully discretized problem is obtained by collocating (38) on the collocation points $\{x_i\}_{i=1}^N$ and employing the differentiation matrices in (32) and (33) as

$$\begin{aligned} \frac{\bar{\mathbf{u}}_p(t_{k+1}) - \bar{\mathbf{u}}(t_k)}{(\Delta t)^\tau} &= -K_c \sum_{j=0}^J \beta_j^{AB} \left[\mathbf{D}^\mu \left(\text{diag}\{\bar{\mathbf{u}}(t_{k-j})\} \mathbf{D}^\beta \bar{\mathbf{C}}(t_{k-j}) \right) + f(\bar{\mathbf{u}}(t_{k-j})) \right] \\ &\quad + K \sum_{j=0}^J \beta_j^{AM} \mathbf{D}^{1+\mu} \bar{\mathbf{u}}(t_{k+1-j}) - \frac{\bar{\mathcal{H}}^k}{(\Delta t)^\tau}, \end{aligned} \tag{40}$$

where $\bar{\mathbf{u}}$ denotes the solution vector at the interpolation points and $\text{diag}\{\bar{\mathbf{u}}(t_{k-j})\}$ represents a diagonal matrix whose entries are the components of the solution vector $\bar{\mathbf{u}}$ at the time step t_{k-j} . In order to decouple (38), at each time-step t_k we use (25) to obtain

$$\begin{aligned} K_{e-1} \mathcal{D}_x^\gamma C(x, t_k) &= -u(x, t_k) = -\sum_{j=1}^N u(x_j, t_k) h_j^\mu(x) \\ &= -\sum_{j=1}^N u(x_j, t_k) \frac{1}{(x_j + 1)^\mu} \sum_{n=1}^N \beta_n^j (1+x)^\mu P_{n-1}^{-\mu, \mu}(x) \\ &= -\sum_{j=1}^N \left(\frac{u(x_j, t_k)}{(x_j + 1)^\mu} \sum_{n=1}^N \beta_n^{j(1)} \mathcal{P}_n^\mu(x) \right). \end{aligned}$$

Since ${}^{(1)}\mathcal{P}_n^\mu(-1) = 0$, we directly obtain ${}_{-1}\mathcal{D}_x^\beta C(x, t)$ by applying the inverse operator i.e., a fractional integration of order $\eta = \gamma - \beta \in (0, 1)$ as

$${}_{-1}\mathcal{D}_x^\beta C(x, t) = -\frac{1}{K_e} \sum_{j=1}^N \left(\frac{u(x_j, t_k)}{(x_j + 1)^\mu} \sum_{n=1}^N \beta_{n-1}^j I_x^\eta \left[{}^{(1)}\mathcal{P}_n^\mu(x) \right] \right) \tag{41}$$

where ${}_{-1}I_x^\eta \left[{}^{(1)}\mathcal{P}_n^\mu(x) \right]$ is derived exactly as

$${}_{-1}I_x^\eta \left[{}^{(1)}\mathcal{P}_n^\mu(x) \right] = \frac{\Gamma(n + \mu)}{\Gamma(n + \mu + \eta)} (1+x)^{n+\mu} P_{n-1}^{-\mu-\eta, \mu+\eta}(x). \tag{42}$$

Table 6

IMEX simulation of Keller–Segel chemotaxis system subject to homogeneous initial/boundary conditions. The parameter values used are given by $\mu = \sigma = \beta = 4/7$, $\gamma = 1 + 4/7$, also $K = 10^{-3}$ and $\frac{K_c}{K_e} = 10^{-4}$. We consider the exact solution to be $u^{ext}(t, x) = \sin(t^{3+1/2})(2^{1/6}(1+x)^{4+1/3} - (1+x)^{3+1/2})$ with the simulation time $T = 2$.

Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/16	0.38225007	1.93	0.38074322	1.70	0.50777938	1.82
1/32	0.10051565	2.06	0.11783198	2.0	0.14348360	2.14
1/64	0.02416292	2.06	0.02946394	2.10	0.03259522	2.21
1/128	0.00580067	2.03	0.00687303	2.18	0.00699726	2.35
1/256	0.0014200	1.97	0.00151012	2.36	0.00137238	2.8
1/512	0.00036249	*	0.00029442	*	0.00019696	*

Table 7

IMEX simulation of Keller–Segel chemotaxis system subject to homogeneous initial/boundary conditions. The parameter values used are given by $\mu = \sigma = \beta = 4/7$, $\gamma = 1 + 4/7$, $K = 10^{-3}$, and $\frac{K_c}{K_e} = 10^{-4}$. We consider the exact solution to be $u^{ext}(t, x) = t^\tau \sin(t) \exp(-2t)[2^{1/6}(1+x)^{4+1/3} - (1+x)^{3+1/2}]$, where $\tau \in (0, 1)$ is the temporal derivative order and the simulation time $T = 2\pi$.

Δt	$\tau = 1/10$	Order	$\tau = 1/2$	Order	$\tau = 9/10$	Order
1/16	0.00090994	1.18	0.01015426	1.77	0.03877761	2.04
1/32	0.00040271	2.02	0.002987301	2.35	0.00939105	2.25
1/64	0.00009962	2.41	0.00058501	2.37	0.00196767	2.11
1/128	0.00001880	2.48	0.00011303	2.20	0.00045476	2.03
1/256	3.37×10^{-6}	2.43	0.00002458	2.12	0.00011098	2.03
1/512	6.26×10^{-7}	*	5.63×10^{-6}	*	0.00002702	*

We note that the enforcement of $\partial C / \partial x = 0$ at $x = -1$ is guaranteed by the construction of the fractional Lagrange interpolants in (25). Hence, by plugging (42) into (41), we obtain at each time step t_k the coupling term ${}_{-1}\mathcal{D}_x^\beta C(x, t_n)$ in (40) as

$${}_{-1}\mathcal{D}_x^\beta C(x, t) = -\frac{1}{K_e} \sum_{j=1}^N \left(\frac{u(x_j, t_n)}{(x_j + 1)^\mu} \sum_{n=1}^N \beta_n^j \frac{\Gamma(n + \mu)}{\Gamma(n + \mu + \eta)} (1 + x)^{\eta + \mu} P_{n-1}^{-\mu - \eta, \mu + \eta}(x) \right). \tag{43}$$

Next, by evaluating ${}_{-1}\mathcal{D}_x^\beta C(x, t)$ at the spatial collocation points $\{x_i\}_{i=1}^N$, we explicitly obtain the i -th entry of $\mathbf{D}^\beta \vec{C}$ at the time-step t_k as

$${}_{-1}\mathcal{D}_x^\beta C(x_i, t_k) = \frac{1}{K_e} \sum_{j=1}^N \{\mathbb{I}^\eta\}_{ij} u(x_j, t_k), \tag{44}$$

or equivalently in the matrix-vector product form,

$$\mathbf{D}^\beta \vec{C} = \frac{1}{K_e} \mathbb{I}^\eta \vec{\mathbf{u}}(t_k). \tag{45}$$

Here, \mathbb{I}^η represents the “fractional integration matrix” the entries of which are obtained as

$$\{\mathbb{I}^\eta\}_{ij} = -\frac{1}{(x_j + 1)^\mu} \sum_{n=1}^N \beta_n^j \frac{\Gamma(n + \mu)}{\Gamma(n + \mu + \eta)} (1 + x_i)^{\eta + \mu} P_{n-1}^{-\mu - \eta, \mu + \eta}(x_i). \tag{46}$$

We note that \mathbb{I}^η is constructed only once and is used in each time-step. By virtue of (45), the splitting method is decoupled in the prediction step as

$$\frac{\vec{\mathbf{u}}_p(t_{k+1}) - \vec{\mathbf{u}}(t_k)}{(\Delta t)^\tau} = -\frac{K_c}{K_e} \sum_{j=0}^J \beta_j^{AB} \left[\mathbf{D}^\mu \left(\text{diag}\{\vec{\mathbf{u}}(t_{k-j})\} \mathbb{I}^\eta \vec{\mathbf{u}}(t_{k-j}) \right) + f(\vec{\mathbf{u}}(t_{k-j})) \right] - \frac{\vec{\mathcal{H}}^k}{(\Delta t)^\tau}, \tag{47}$$

which is followed by the corresponding correction step as

$$\frac{\vec{\mathbf{u}}(t_{k+1}) - \vec{\mathbf{u}}_p(t_{k+1})}{(\Delta t)^\tau} = K \sum_{j=0}^J \beta_j^{AM} \mathbf{D}^{1+\mu} \vec{\mathbf{u}}(t_{k+1-j}). \tag{48}$$

6. Numerical tests

We have examined the IMEX splitting method by solving the system of equations (38) and (39). The results of two distinct numerical experiments are shown in Tables 6 and 7. In both experiments, $\sigma = \beta = 4/7$ and $\gamma = 1 + 4/7$. In addition, we have chosen $K = 10^{-3}$ and $\frac{K_c}{K_e} = 10^{-4}$. We remark that the parameter regime in these experiments is consistent with various applications of the Keller–Segel model where K_e is usually much larger than K_c and K [59]. The source term in (38) has been chosen so that the exact solutions are (i) $u^{ext}(t, x) = \sin(t^{3+1/2})(2^{1/6}(1+x)^{4+1/3} - (1+x)^{3+1/2})$ in Table 6 and (ii) $u^{ext}(t, x) = t^\tau \sin(t) \exp(-2t)[2^{1/6}(1+x)^{4+1/3} - (1+x)^{3+1/2}]$ in Table 7.

While the spectral accuracy of the spatial discretization has been already tested in Table 5, here we keep the polynom order $N = 16$ and perform a time-grid refinement. In this simulation, we employ the A-B and A-M methods corresponding to $J = 1$, which leads to an observable second-order of accuracy in time. Our experiment showed that employing higher-order A-B and A-M methods, corresponding to $J = 2$, would not help increase the accuracy. This can be explained by the splitting error introduced by the method.

7. Summary and discussion

In this work, we generalized the first- and second-order accurate standard Adams schemes to a fractional class of explicit Adams–Bashforth (A-B) and implicit Adams–Moulton (A-M) methods for time-fractional problems. In this approach, we obtained the corresponding weight coefficients as τ -dependent, which reduced to the well-known A-B and A-M methods with standard coefficients when $\tau = 1$. In addition, we obtained the history load exactly up to the accuracy of the scheme via hyper-geometric functions. We remark that most of the existing finite-difference methods for fractional differential equations are designed around an *implicit* discretization of *linear* FODEs/FPDEs. The use of these methods in the context of IMEX methods leads to *at most* first-order accuracy for general nonlinear problems, in which explicit treatment is needed. In contrast, our approach consistently provides the proper explicit and implicit Adams schemes, preserving their first-order (for $J = 0$) and second-order (for $J = 1$) accuracy.

We further remark that in the case $J = 0$ our scheme appears to require only a τ -th order Caputo derivative in order for the method to be first order accurate. Similarly, as our numerical experiments indicate, second order convergence is attained by our scheme when the exact solution has a $(1 + \tau)$ -th order Caputo derivative.

Another important aspect of the present work is that our generalized family of Adams schemes can be easily implemented on top of existing libraries by modifying the standard weights and adding a new history calculator. This is in contrast to previous attempts to generalize these types of schemes for the fractional case [33,34]. Indeed previous generalizations consisted of two-step predictor–corrector methods, which differ significantly from the classical Adams schemes and require a considerable modification of existing libraries.

In this paper, we employed our generalized A-B and A-M methods to further develop an implicit–explicit (IMEX) splitting scheme for linear and nonlinear FPDEs. We particularly examined the fractional Keller–Segel chemotaxis system, in which the nonlinear advection term was evaluated explicitly by employing the fractional A-B formulation in the prediction step, and then, the diffusion term was treated implicitly in the correction step using the corresponding fractional A-M method. In order to discretize the spatial operator, a spectrally-accurate fractional spectral collocation method was employed.

The focus of the paper has been on the development of the numerical schemes and the numerical experimentation that was indicative of the efficiency of the scheme. In future work, we aim to carry out the theoretical study including error estimates and stability analysis of the present IMEX schemes. In addition, we aim to employ a strategy for treating data near the lower integration limit in the time-fractional derivative in order to obtain higher-order schemes. Further improvement of the presented schemes would make it possible to formulate more efficient methods to compute the history load term \mathcal{H}_k in each time-step to achieve higher efficiency. This has the potential to further generalize the schemes developed in this paper to higher-order methods.

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