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A CHEBYSHEV SPECTRAL METHOD FOR HEAT AND MASS TRANSFER IN MHD NANOFLUID FLOW WITH SPACE FRACTIONAL CONSTITUTIVE MODEL

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ABSTRACT

In some recent studies, it has been suggested that non–Newtonian fluid flow can be modeled by a spatially non–local velocity, whose dynamics are described by a fractional derivative. In this study, we use the space fractional constitutive relation to model heat and mass transfer in a nanofluid. We present a numerically accurate algorithm for approximating solutions of the system of fractional ordinary differential equations describing the nanofluid flow. We present numerically stable differentiation matrices for both integer and fractional order derivatives defined by the one–sided Caputo derivative. The differentiation matrices are based on the series expansion of the unknown functions using a truncated Chebyshev polynomial of the first kind and interpolation using Gauss–Lobatto quadrature. We show that the proposed technique is highly effective for solving the fractional model equations.

Keywords: *Fractional constitutive equations, Spectral method, Chebyshev polynomials, Fractional differentiation matrix*

1. INTRODUCTION

The boundary layer flow of both Newtonian and non–Newtonian fluids has been explored extensively in the literature because of the many industrial and scientific uses of these fluids. Experimental and theoretical investigations of non–Newtonian fluids have shown that they exhibit anomalous behaviours and are generally more complex than viscous fluids. To describe these behaviours, several models have been proposed to mathematically describe and experimentally quantify the stress–strain relationship. These constitutive relations include but are not limited to the power–law, Ellis and Powell–Eyring fluids models. These models and several others have been subjected to experimental and theoretical investigations. In some recent studies, attempts have been made to reconstruct the constitutive relations to incorporate hereditary properties, memory retention and non–local properties of non–Newtonian fluids. The primary objective is to recast the velocity gradient in the momentum transport equation as a fractional derivative.

Fractional calculus can best describe physical models with long term memory and non–locality of the spatial domain. For instance, constitutive relations with time fractional derivative are used to describe memory dependence in dynamical systems (Tarasov, 2013). An investigation and summary of studies on fluid flow problems in which the rheological properties of the fluid are described using fractional calculus is given by Sun *et al.* (2018). In this study, the classical constitutive equation of a viscous fluid was reconstructed so that the velocity gradient is expressed using a non–local spatial derivative. This approach allows for the capture of the non–locality of non–Newtonian fluid and the correlation between the fluid particles. They conducted a theoretical analysis of a steady pipe flow of a laminar incompressible flow, obtaining the frictional head loss, velocity profile and yield stress in terms of the fractional Reynolds number. Chen *et al.* (2015) investigated the fractional boundary layer flow of a Maxwell fluid on an unsteady stretching surface. The constitutive equation was recast so as to introduce space–time dependent fractional derivatives. Research on classical boundary layer flow, heat and mass transfer in magnetohyrodynamics nanofluid has been carried out by, among others, Dhanai *et al.* (2015) and Khan and Pop (2010). By applying the implicit finite difference method, velocity, temperature and nanoparticle concentration profiles were obtained in the study of Dhanai *et al.* (2015) which investigated the combined effects of heat and mass transfer parameters on a steady boundary layer nanofluid flow and examined multiple solutions of the conservation equations. Critical review of literature shows that heat and mass transfer in viscous nanofluid with fractional constitutive relation has not been studied. In this study, a fractional system of equations describing heat and mass transport in an incompressible magnetohydrodynamic viscous nanofluid is developed and solved using a spectral technique that uses Chebyshev polynomials of the first kind as basis functions.

2. MATHEMATICAL FORMULATION

We consider a steady two–dimension boundary layer flow of an incompressible nanofluid with space fractional shear rate induced by an im-

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permeable horizontal wall along the plane $y = 0$, where the y–axis is perpendicular to the wall and the x–axis along the wall. It is assumed that the flow occurs at $y \geq 0$ and a constant magnetic field B is applied in the y–direction. The temperature and nanoparticle volume fraction at the wall (T_w, C_w) are constant and the ambient temperature and concentration are T_∞ and C_∞ respectively as in Fig. 1. By defining the shear stress associated with a fluid with fractional dynamic viscosity coefficient $\mu_\alpha \ (kg/m^{2-\alpha}/s)$ in the following form

$$\tau = \mu_\alpha \frac{\partial^\alpha u}{\partial y^\alpha}, \quad 0 < \alpha < 2, \tag{1}$$
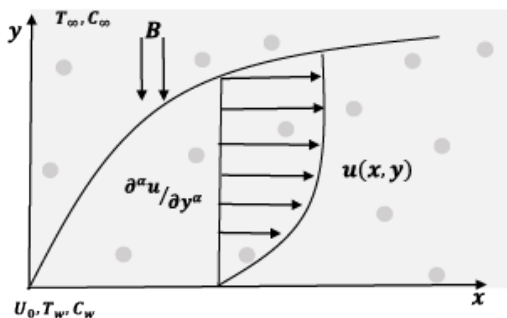

Fig. 1 Coordinate system and flow geometry.

where α is the order of the fractional space derivative, and $\partial^\alpha u/\partial y^\alpha$ denotes the fractional velocity gradient. A reclassification of non–Newtonian fluid based on the fractional constitutive equation (1) was given by (Sun *et al.*, 2018). In the aforementioned study, the case $< \alpha < 1$ was proposed to describe shear thickening fluids, $2 > \alpha > 1$ model shear thinning fluids and $\alpha = 1$, viscous fluids. The partially coupled system of equations describing the transport processes is given as (Chen *et al.*, 2015; Khan and Pop, 2010)

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{2}$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu_\alpha {}^C_0 D_y^{\alpha+1} u - \frac{\sigma B^2}{\rho} u \tag{3}$$

$$(\rho c)_b \left(u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} \right) = k\frac{\partial^2 T}{\partial y^2} + (\rho c)_p \left(D_B \frac{\partial C}{\partial y} \frac{\partial T}{\partial y} \right.$$
$$\left. + \frac{D_T}{T_\infty} \left(\frac{\partial T}{\partial y} \right)^2 \right) \tag{4}$$

$$u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_B \frac{\partial^2 C}{\partial y^2} + \frac{D_T}{T_\infty} \frac{\partial^2 T}{\partial y^2}, \tag{5}$$

subject to the boundary conditions

$$v = 0, \quad u = U_0, \quad T = T_w, \quad C = C_w \quad \text{at} \quad y = 0,$$
$$u = 0, \quad T = T_\infty, \quad C = C_\infty \quad \text{as} \quad y \to \infty.$$

Here ${}^C_0 D_y^\alpha$ is the Caputo fractional operator of order α of the function $u(y) : (0, \infty) \to \mathbb{R}$, defined as

$${}^C_0 D_y^\alpha u(y) = \begin{cases} \frac{1}{\Gamma(n-\alpha)} \int_0^y \frac{u^n(\tilde{y})}{(y-\tilde{y})^{\alpha+1-n}} d\tilde{y}, & n-1 \leq \alpha < n \in \mathbb{N} \\ \\ \frac{d^n u(y)}{dy^n} & \alpha = n \in \mathbb{N}. \end{cases} \tag{6}$$

The Caputo fractional operator is the most popular in applications due to the ease in imposing conditions on the fractional differential equations. Other fractional operators include the Riemann-Liouville, Riesz and the Canavati fractional derivatives. We note that the Caputo fractional operator is a regularized form of the Riemann-Liouville fractional derivative. The definitions and properties of the Caputo derivative and the aforementioned arbitrary order derivatives can be found in Miller and Ross (1993); Podlubny (1998); Atanackovic *et al.* (2014).

We define u and v (m/s) as the horizontal and vertical velocity components respectively, $\nu_\alpha(m^{1+\alpha}/s) = \mu_\alpha/\rho_b$ is the fractional kinematic viscosity, ρ_b and ρ_p (kg/m^3) are constant basefluid and nanoparticle densities respectively. If we assume the reference length L and velocity U_0, we have the following dimensionless variables

$$(U, V, X, Y, \theta, \phi) = \left(uU_0^{-1}, vU_0^{-1}, xL^{-1}, yL^{-1}, \frac{T - T_\infty}{\Delta T}, \frac{C - C_\infty}{\Delta C} \right), \tag{7}$$

$$(Re_\alpha, M^2, Le, Pr, Nbt, Sc) = \left(\frac{U_0 L^\alpha}{\nu_\alpha}, \frac{\sigma B^2 L}{\rho U_0}, \frac{k}{(\rho c)_p D_B \Delta C}, \right.$$
$$\left. \frac{LU_0(\rho c)_f}{k}, \frac{Nb}{Nt}, \frac{D_B}{LU_0} \right), \tag{8}$$

where Nb and Nt are respectively the Brownian diffusion and thermophoresis parameters, Re_α is the fractional Reynolds number, M is the magnetic parameter, Le is the Lewis number, Pr is the Prandtl number, and Sc is the Schmidt number (Dhanai *et al.*, 2015). Introducing the stream function ψ defined by $U = \partial\psi/\partial Y$ and $V = -\partial\psi/\partial X$, Eqs. (3) to (5) become

$$\frac{\partial\psi}{\partial Y}\frac{\partial^2\psi}{\partial X \partial Y} - \frac{\partial\psi}{\partial X}\frac{\partial^2\psi}{\partial Y^2} = \frac{1}{Re_\alpha}\frac{\partial^{\alpha+2}\psi}{\partial Y^{\alpha+2}} - M^2 \frac{\partial\psi}{\partial Y} \tag{9}$$

$$LePr\left[\frac{\partial\psi}{\partial Y}\frac{\partial\theta}{\partial X} - \frac{\partial\psi}{\partial X}\frac{\partial\theta}{\partial Y} \right] = Le\frac{\partial^2\theta}{\partial Y^2} + \frac{\partial\phi}{\partial Y}\frac{\partial\theta}{\partial Y} + \frac{1}{Nbt}\left(\frac{\partial\theta}{\partial Y} \right)^2 \tag{10}$$

$$Sc\left[\frac{\partial\psi}{\partial Y}\frac{\partial\phi}{\partial X} - \frac{\partial\psi}{\partial X}\frac{\partial\phi}{\partial Y} \right] = \frac{\partial^2\phi}{\partial Y^2} + \frac{1}{Nbt}\frac{\partial^2\theta}{\partial Y^2}. \tag{11}$$

We perform a scaling transformation by introducing the new variables $x, y, \tilde{\psi}, \tilde{\theta}, \tilde{\phi}$ defined as

$$(X, Y, \psi, \theta, \phi) = \left(\lambda^{a_1} x, \lambda^{a_2} y, \lambda^{a_3} \tilde{\psi}, \lambda^{a_4} \tilde{\theta}, \lambda^{a_5} \tilde{\phi} \right). \tag{12}$$

Here, λ is the scaling parameter and a_i for $i = 1 \ldots 5$ are constants to be determined such that Eqs. (9) to (11) remain invariant under this group transformation. Upon substituting Eq. (12) into Eqs. (9) to (11), and dropping the tilde for convenience, we get

$$\lambda^{2a_3-2a_2+a_1} \left[\frac{\partial\psi}{\partial y}\frac{\partial^2\psi}{\partial x \partial y} - \frac{\partial\psi}{\partial x}\frac{\partial^2\psi}{\partial y^2} \right] = \lambda^{a_3-(\alpha+2)a_2}\frac{1}{Re_\alpha}\frac{\partial^{\alpha+2}\psi}{\partial y^{\alpha+2}}$$
$$- \lambda^{a_3-a_2} M^2 \frac{\partial\psi}{\partial y} \tag{13}$$

$$\lambda^{a_3-a_2+a_4-a_1} LePr \left[\frac{\partial\psi}{\partial y}\frac{\partial\theta}{\partial x} - \frac{\partial\psi}{\partial x}\frac{\partial\theta}{\partial y} \right] = \lambda^{a_4-2a_2} Le\frac{\partial^2\theta}{\partial y^2}$$
$$+ \lambda^{a_4+a_5-2a_2}\frac{\partial\phi}{\partial y}\frac{\partial\theta}{\partial y} + \lambda^{2a_4-2a_2}\frac{1}{Nbt}\left(\frac{\partial\theta}{\partial y} \right)^2 \tag{14}$$

$$\lambda^{a_3+a_5-a_2-a_1} Sc \left[\frac{\partial\psi}{\partial y}\frac{\partial\phi}{\partial x} - \frac{\partial\psi}{\partial x}\frac{\partial\phi}{\partial y} \right] = \lambda^{a_5-2a_2}\frac{\partial^2\phi}{\partial y^2}$$
$$+ \lambda^{a_4-2a_2}\frac{1}{Nbt}\frac{\partial^2\theta}{\partial y^2}. \tag{15}$$

For the system of equations to remain invariant, we set $a_1 = a_3 = a$ (arbitrary) and $a_2 = a_4 = a_5 = 0$. The characteristics equations associated with the transformation is given as

$$\frac{dx}{ax} = \frac{dy}{0} = \frac{d\psi}{a\psi} = \frac{d\theta}{0} = \frac{d\phi}{0}, \tag{16}$$

which give the similarity functions

$$y = \eta, \quad \psi(x,y) = xf(\eta), \quad \theta(x,y) = \theta(\eta), \quad \phi(x,y) = \phi(\eta). \tag{17}$$

Using the Caputo fractional operator to obtain the fractional derivative of the similarity function $\psi(x,y) = xf(\eta)$ and substituting Eq. (17) into Eqs. (9) to (11) gives the following similarity equations

$$f^{\alpha+2} - Re_\alpha M^2 f' - Re_\alpha f'^2 + Re_\alpha f f'' = 0 \tag{18}$$

$$Le\theta'' + \theta'\phi' + \frac{1}{Nbt}\theta'^2 + LePrf\theta' = 0 \tag{19}$$

$$\phi'' + \frac{1}{Nbt}\theta'' + Scf\phi' = 0, \tag{20}$$

with boundary conditions

$$f(0) = 0, \quad f'(0) = 1, \quad \theta(0) = 1, \quad \phi(0) = 1,$$
$$f'(\eta) = 0, \quad \theta(\eta) = 0, \quad \phi(\eta) = 0 \quad \text{as} \quad \eta \to \infty. \tag{21}$$

We note here that setting $\alpha = 1$, $Re_\alpha = 1$ and $M = 0$, the system of equations reduces to the problem studied in Khan and Pop (2010).

3. NUMERICAL APPROXIMATION

Existing numerical methods for integer order differential equations have been extended to fractional order differential equations. Numerical and approximate methods such as the differential transform, homotopy, Adomian decomposition and finite difference methods have been used to solve fractional differential equations (Wang, 2006; Diethelm et al., 2002; Erjaee et al., 2011; El-Sayed et al., 2010; Momani and Odibat, 2007a,b). Despite the fact that some of these methods are considered accurate and reliable, they have certain limitations. For example, due to the history dependence associated with fractional derivatives, approximations can be computationally expensive. Fractional derivatives are defined globally, hence numerical methods that discretize non–locally would be appropriate in approximating the derivative. One such method is the spectral method. Spectral methods are synonymous with exponential rate of convergence. We discretized the dependent variables and their arbitrary order derivatives using the spectral collocation methods. The Chebyshev spectral collocation method uses trial functions to represent the functions as truncated series expansions. The trial functions are usually orthogonal basis functions such as the Lagrange, Jacobi, Chebyshev and other polynomials. A crucial difference between spectral methods and other methods is that the test functions for spectral methods are inherently continuous and infinitely differentiable global functions. Some recent studies have demonstrated the use of the operational matrix for certain orthogonal polynomials. Ahmadi Darani and Saadatmandi (2017) introduced the operational matrix of a class of fractional order Chebyshev functions using classical Chebyshev polynomials of the first kind. Doha et al. (2011) and Atabakzadeh et al. (2013) presented a matrix operator for shifted Chebyshev polynomials and used it to approximate multi–order fractional ordinary differential equations and Doha et al. (2012) obtained the matrix operator of the Jacobi polynomials. In recent studies by Kazem et al. (2013) and Kayedi-Bardeh et al. (2014), the operational matrices of the fractional Legendre polynomials and fractional Jacobi polynomials are respectively obtained. Direct implementation of the operational matrices

usually lead to accurate solutions. However, dealing with nonlinearity and coupling can be time consuming. Hence, in this study, we follow a different approach by using approximations based on the shifted Chebyshev polynomials of the first kind and integration on the Gauss–Lobatto quadrature to obtain the coefficients of expansion.

The series form of shifted Chebyshev polynomials $T_{l,n}$ of degree $n > 0$, where l is the truncation of the positive half domain, is defined (Abramowitz and Stegun, 1965; Doha et al., 2011; Ahmadi Darani and Saadatmandi, 2017) as

$$T_{l,n} = n\sum_{j=0}^{n} \frac{(-1)^{n-j}(n+j-1)!2^{2j}}{(n-j)!(2j)!l^j}\eta^j, \tag{22}$$

and satisfies the orthogonality condition

$$\int_0^l T_{l,n}(\eta)T_{l,m}(\eta)w_l(\eta)d\eta = \delta_{mn}h_n. \tag{23}$$

We discretized the dependent variables using the shifted Chebyshev Gauss Lobatto grid points $\eta \in [0, l]$

$$\eta = \frac{l}{2}\left(1 - \cos\frac{\pi i}{N}\right), \qquad i = 0, \ldots, N. \tag{24}$$

The weight function $w_l(\eta)$ for the shifted Chebyshev polynomials is given by $1/\sqrt{l\eta - \eta^2}$ and $h_n = c_n\pi/2$, with $c_0 = 2$ and $c_n = 1$ for $n \geq 1$. If we assume $F(\eta) = \{f(\eta), \theta(\eta), \phi(\eta)\}$, to be a square integrable and smooth function defined over the truncated semi infinite interval $[0, l]$, then the function can be approximated as $N + 1$ terms of the shifted Chebyshev polynomials

$$F_N(\eta) = \sum_{n=0}^{N} F_n T_{l,n}(\eta), \tag{25}$$

the coefficients F_n satisfy the orthogonality condition

$$F_n = \frac{1}{h_n}\sum_{j=0}^{N}\frac{\pi}{c_j N}T_{l,n}(\eta_j)F(\eta_j), \quad n = 0, \ldots, N. \tag{26}$$

If $F(\eta)$ is approximated using the shifted Chebyshev polynomials and evaluated at the shifted Gauss-Lobatto collocation points, then any arbitrary order derivative of $F(\eta)$ is given as

$$\mathsf{D}^\alpha F_N(\eta) = \sum_{j=0}^{N} \mathsf{D}_{j,p}^\alpha F(\eta_j). \tag{27}$$

Here,

$$\mathsf{D}_{j,p}^\alpha = \frac{\pi}{c_j N}\sum_{n=0}^{N}\sum_{k=0}^{N}\frac{1}{h_n}T_{l,n}(\eta_j)\mathsf{D}_{n,k}^{(\alpha)}T_{l,k}(\eta_p), \quad j, p = 0, 1, \ldots, N. \tag{28}$$

and

$$\mathsf{D}_{n,k}^{(\alpha)} = n\sum_{j=0}^{n}\frac{(-1)^{n-j}(n+j-1)!2^{2j}}{(n-j)!(2j)!l^j}\frac{\Gamma(j+1)}{\Gamma(j-\alpha+1)}q_{j,k}, \tag{29}$$

where $q_{j,k}$ are entries of a matrix defined as (Ahmadi Darani and Saadatmandi, 2017; Ahmadi-Darani and Nasiri, 2013; Atabakzadeh et al., 2013; Doha et al., 2011)

$$q_{j,k} = \begin{cases} 0 & j = 0, 1, \ldots, \lceil \alpha \rceil - 1, \\ \frac{k\sqrt{\pi}}{h_k} \sum_{r=0}^{k} \frac{(-1)^{k-r}(k+r-1)!2^{2r}}{(k-r)!(2r)!} l^{j-\alpha} \frac{\Gamma(j-\alpha+r+1/2)}{\Gamma(j-\alpha+r+1)} & j = \lceil \alpha \rceil, \lceil \alpha \rceil + 1, \ldots, N; \\ & k = 0, 1, \ldots, N. \end{cases} \tag{30}$$

We note here that if $\alpha = 1$, Eq. (27) is equivalent to

$$\mathrm{D}F_N(\eta) = \sum_{j=0}^{N} \left[\frac{2w_{l,j}}{\pi} \sum_{n=1}^{N} \frac{n}{c_n} T_{l,n}(\eta_j) S_{l,n-1}(\eta_k) \right] F(\eta_j),$$
$$k = 0, \ldots, N, \tag{31}$$

where $S_{l,n}$ is the shifted second kind Chebyshev polynomials of degree $n \geq 1$. In order to approximate $f(\eta)$ in terms of the Chebyshev polynomials, it has been assumed that $f(\eta)$ is a smooth function, so it is safe to take advantage of the semi–group property of the Caputo fractional operator, therefore when approximating $f^{\alpha+2}(\eta)$, we can have (Matlob and Jamali, 2017; Dabiri and Butcher, 2018)

$$\frac{d^2}{d\eta^2} \left({}_0^C D_\eta^\alpha f(\eta) \right) = {}_0^C D_\eta^\alpha \left(\frac{d^2 f(\eta)}{d\eta^2} \right) = {}_0^C D_\eta^{2+\alpha} f(\eta). \tag{32}$$

3.1. Error bound estimation

If $F(\eta)$ is a square integrable function and $w_l(\eta)$ is a Lebesque integrable function defined in the interval $(0, l)$, we can define a $L_{w_l}^2$ space in which $F(\eta)$ is measurable and the norm of $F(\eta)$ associated with the space is defined as

$$\|F(\eta)\|_{w_l} = \left(\int_0^l |F(\eta)|^2 w_l(\eta) d\eta \right)^{\frac{1}{2}}, \quad \text{finite}, \tag{33}$$

and this norm is induced by the inner product

$$\langle F(\eta), \tilde{F}(\eta) \rangle = \int_0^l F(\eta)\tilde{F}(\eta)w_l(\eta)d\eta. \tag{34}$$

If we consider $\mathbf{T}_N$, the space of all Chebyshev polynomials of degree $\leq N$, such that $\mathbf{T}_N F(\eta)$ is the approximation of $F(\eta)$ on the shifted Chebyshev–Gauss–Lobatto nodes. Assume that the derivative $F^{N+1}(\eta)$ exist and is continuous on the interval $(0, l)$, and using the error term of the generalized Taylor's approximation of $F(\eta)$, for any η, the error bound is defined as

$$\|\varepsilon_N\|_{w_l} = \|F(\eta) - \mathbf{T}_N F(\eta)\|_{w_l}^2 \tag{35}$$
$$\leq \frac{1}{(\Gamma(N+2))^2} Q_N \int_0^l \frac{\eta^{2N+2}}{\sqrt{l\eta - \eta^2}} d\eta \tag{36}$$
$$= \frac{1}{(\Gamma(N+2))^2} Q_N l^{2N+2} \frac{\Gamma(2N+5/2)}{\Gamma(2N+3)}, \tag{37}$$

where $Q_N = \left(\max_{0 < \eta \leq l} F^{N+1}(\eta) \right)^2$. For sufficiently large N, we can see that $\|\varepsilon_N\|_{w_l} \to 0$.

4. NUMERICAL RESULTS

In this section, we obtain approximate solutions of the equations describing heat and mass transfer in a nanofluid with space fractional constitutive relation using the technique described in Section 3. The aim is to obtain approximate solutions of the system of differential Eqs. (18) to (20) rather than giving an analysis of the effects of the flow parameters. The parametric analysis of heat and mass transfer process has been given in studies such as Dhanai et al. (2015); Khan and Pop (2010); Fang and Zhang (2009); Chen et al. (2015). Some results obtained using the above

scheme are compared with results in these studies. The nonlinear system is first linearized using quasilinearization as in Bellman and Kalaba (1965); Motsa et al. (2011, 2014) [see Appendix A for the discretization of the equations]. In developing numerical schemes, a pertinent question often asked centers around the accuracy of the numerical scheme. For an approximation method, it is expected that when the approximate solutions and their derivatives are substituted in Eqs. (18) to (20), the residual errors should vanish. That is, given the points $\eta_j \in [0, l]$ for $j = 0, \ldots, N$, we should expect

$$\varepsilon_f = \left| {}_0^C D_\eta^{\alpha+2} f(\eta_j) - Re_\alpha M^2 \frac{df}{d\eta}(\eta_j) - Re_\alpha \left(\frac{df}{d\eta}(\eta_j) \right)^2 \right.$$
$$\left. + Re_\alpha f(\eta_j) \frac{d^2 f}{d\eta^2}(\eta_j) \right|_{L_{w_l}^2} \approx 0 \tag{38}$$

$$\varepsilon_\theta = \left| Le \frac{d^2\theta}{d\eta^2}(\eta_j) + \frac{d\theta}{d\eta}(\eta_j)\frac{d\phi}{d\eta}(\eta_j) + \frac{1}{Nbt}\left(\frac{d\theta}{d\eta}(\eta_j) \right)^2 \right.$$
$$\left. + LePr f(\eta_j)\frac{d\theta}{d\eta}(\eta_j) \right|_{L_{w_l}^2} \approx 0 \tag{39}$$

$$\varepsilon_\phi = \left| \frac{d\phi}{d\eta}(\eta_j) + \frac{1}{Nbt}\frac{d^2\theta}{d\eta^2}(\eta_j) + Sc f(\eta_j)\frac{d\phi}{d\eta}(\eta_j) \right|_{L_{w_l}^2} \approx 0. \tag{40}$$

Tables 1 to 3 show the solutions obtained for different values of N and α and the residual errors as defined in Eqs. (38) to (40). The approximate solutions are obtained with $Nt = Nb = 0.5, Le = Pr = 5, Re_\alpha = 1, M = 0$. It can be seen that the errors are bounded between 10^{-16} and 10^{-13}.

An analytic solution of the momentum equation for $\alpha = 1$ and $Re_\alpha = 1$ was obtained by Fang and Zhang (2009) as

$$f(\eta) = \frac{1}{\sqrt{1+M^2}} \left(1 - e^{-\sqrt{1+M^2}\eta} \right), \tag{41}$$

and so the skin friction is given as
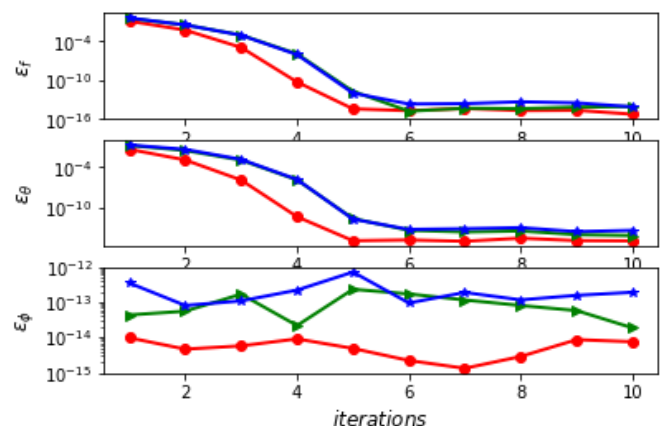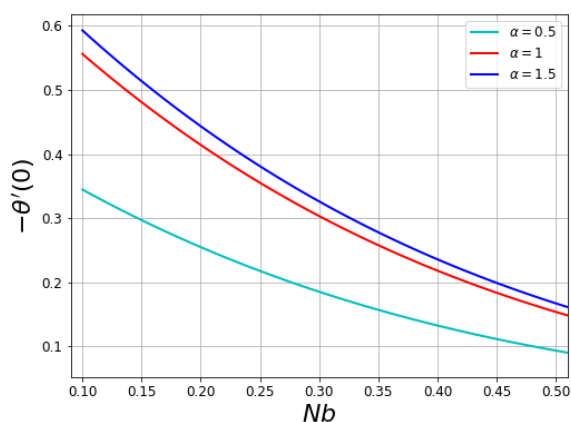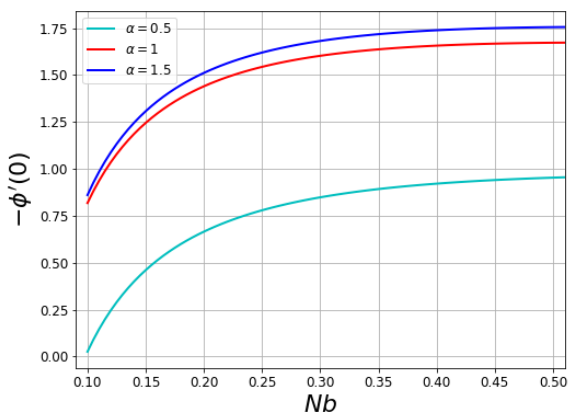
$$f''(0) = -\sqrt{1+M^2}. \tag{42}$$

Fig. 2 The $L_{w_l}^2$ norm error of the numerical solutions to the model equations using different number of collocation points. The blue line corresponds to $N = 10$, green line to $N = 15$ and red line corresponds to $N = 20$ for $\alpha = 0.2$.

(a)

(b)

Fig. 3 Variation of heat and mass transfer rates with Nb for different values of fractional order α.

Table 3 Approximate solution of $\phi(\eta)$ and the maximum residual error for $l = 2$.

α	N	$\phi(\eta)$	ε_ϕ
0.5	4	$[1, 0.5661, 0.1631, 0.0565, 0]^T$	$5.55e^{-16}$
	6	$[1, 0.7769, 0.3273, 0.0650, -0.0047, -0.0107, 0]^T$	$1.54e^{-14}$
1	4	$[1, 0.5749, 0.2088, 0.0752, 0]^T$	$1.55e^{-15}$
	6	$[1, 0.7658, 0.3564, 0.1916, 0.0928, 0.0140, 0]^T$	$1.50e^{-14}$
1.5	4	$[1, 0.5443, 0.2174, 0.0348, 0]^T$	$2.66e^{-15}$
	6	$[1, 0.7457, 0.3362, 0.1917, 0.0665, 0.0010, 0]^T$	$7.55e^{-15}$

Table 4 Comparison of the shear stress at the wall $f^{\alpha+1}(0)$ for $\alpha = 1$ between the exact solution as obtained by Fang and Zhang, 2009 and approximate solutions based on the proposed method.

M	Exact	Approximate
0	-1.0000	-1.000039
0.1	-1.0049	-1.004979
0.2	-1.0198	-1.019658
0.3	-1.0440	-1.043674
0.4	-1.0770	-1.076404
0.5	-1.1180	-1.117066

Table 1 Computation results of $f'(\eta)$ and the maximum residual error for $l = 2$.

α	N	$f'(\eta)$	ε_f
0.5	4	$[1, 0.7111, 0.0007, -0.2103, 0]$	$1.33e^{-15}$
	6	$[1, 0.7734, 0.1885, -0.0036, -0.0526, -0.1339, 0]^T$	$1.09e^{-14}$
1	4	$[1, 0.7439, 0.3115, 0.0675, 0]^T$	$6.11e^{-16}$
	6	$[1, 0.8671, 0.5768, 0.3046, 0.1236, 0.0288, 0]^T$	$4.40e^{-14}$
1.5	4	$[1, 1.001, 0.6175, 0.1164, 0]^T$	$7.77e^{-16}$
	6	$[1, 0.9702, 0.7793, 0.4531, 0.18308, 0.0391, 0]^T$	$1.07e^{-13}$

Table 2 Numerical results of $\theta(\eta)$ and norm of the residual error for $l = 2$

α	N	$\theta(\eta)$	ε_θ
0.5	4	$[1, 0.9219, 0.5083, 0.1128, 0]^T$	$4.44e^{-16}$
	6	$[1, 0.9863, 0.8981, 0.6650, 0.3585, 0.1035, 0]^T$	$4.10e^{-15}$
1	4	$[1, 0.9052, 0.3961, 0.0301, 0]^T$	$8.05e^{-16}$
	6	$[1, 0.9770, 0.8048, 0.4140, 0.1170, 0.0214, 0]^T$	$6.14e^{-15}$
1.5	4	$[1, 0.8571, 0.2085, 0.0310, 0]^T$	$8.33e^{-16}$
	6	$[1, 0.9757, 0.7606, 0.3093, 0.0562, 0.0124, 0]^T$	$3.43e^{-15}$

Table 5 Comparison of the heat and mass transfer coefficients at the wall for different values of Nt and Nb with $\alpha = 1$ and fixed values for $Pr = Le = 10$, $Re_\alpha = 1$ and $M = 0$

Nt	Nb	$-\theta'(0)$		$-\phi'(0)$	
		Present Study	Khan and Pop (2010)	Present Study	Khan and Pop (2010)
0.2	0.2	0.36572	0.3654	2.49971	2.5152
	0.3	0.18262	0.1816	2.50181	2.5150
	0.4	0.08745	0.0859	2.46878	2.4807
0.3	0.2	0.27395	0.2371	2.63457	2.6555
	0.3	0.13639	0.1355	2.59230	2.6068
	0.4	0.06496	0.0641	2.53433	2.5486
0.4	0.2	0.21160	0.2110	2.75631	2.7818
	0.3	0.10507	0.1046	2.66824	2.6876
	0.4	0.04996	0.0495	2.58740	2.6038

Table 6 Numerical values of the shear stress at the wall, rate of heat and mass transfer coefficients for different values of the fractional order α, magnetic parameter M, and Prandtl number Pr when $Le = 5$, $Nt = Nb = 0.5$.

M	α	Pr	$f^{\alpha+1}(0)$	$-\theta'(0)$	$-\phi'(0)$
0	0.5	0.7	12.31787	0.37124	1.04856
		10	12.31714	0.00415	1.46487
	1	0.7	-1.05859	0.42433	1.59908
		10.	-1.06348	0.03665	1.81565
	1.5	0.7	-2.19141	0.44243	1.70113
		10	-2.17969	0.03934	1.95014
0.5	0.5	0.7	12.34448	0.36922	1.02365
		10	12.34473	0.00340	1.45313
	1	0.7	-1.16309	0.42146	1.58259
		10	-1.16406	0.03584	1.79791
	1.5	0.7	-2.38672	0.44005	1.69217
		10	-2.40234	0.03960	1.93226

To establish the accuracy of the numerical scheme, we compare Equation (42) with the approximate solutions. Table 4 shows the comparison between the exact and approximate values of the skin friction coef-
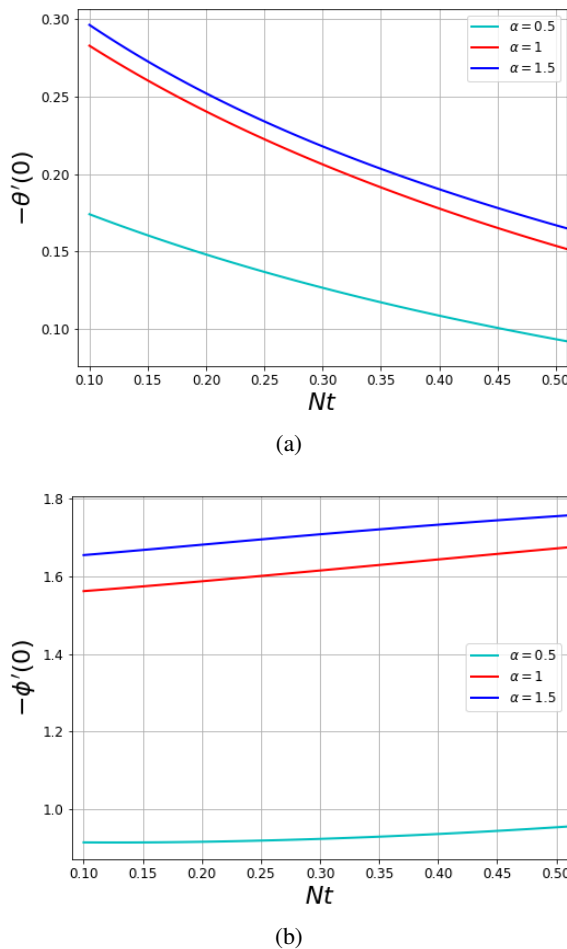
(a)

(b)

Fig. 4 Variation of heat and mass transfer rates with Nt for different values of fractional order α.

ficient for different values of M. The approximate values are found to be close to the exact values. The approximate values in Table 4 are obtained with $N = 10$ and $l = 5.9$. The heat and mass transfer coefficients $\{\theta'(0), \phi'(0)\}$ obtained using this method are compared with earlier results by Khan and Pop (2010). Table 5 shows that the new results are in agreement with the published data. Figure 2 shows that the solutions converge for different number of collocation points, especially in the equation where we have the fractional order. In Table 6, the approximate values of the skin friction and heat and mass transfer rates are presented. Figs. 3 and 4 respectively show the variation in the heat and mass transfer rates with the Brownian diffusion and thermophoresis parameters for different values of the fractional order α. It can be clearly seen that the heat and mass transfer rates increase as α increases. Fig. 3(a) shows that the heat transfer rate decreases as the mass diffusion parameter Nb increases, while Fig. 3(b) shows that the mass transfer rate is a monotonically increasing function of Nb. From Fig. 4, we can see that the mass transfer rate decreases as the thermal diffusion parameter increases, while the heat transfer rate strictly decreases. Previous studies have suggested that increasing the number of collocation points for spectral methods does not necessarily improves the accuracy (Dabiri and Butcher, 2017b,a; Zayernouri and Karniadakis, 2014).

5. CONCLUSION

This study proposed a new numerical technique for finding solutions of fractional differential equations. The method uses Chebyshev polynomials as basis function for the series solution and interpolating using Gauss–Lobatto quadrature. Differentiation matrices for fractional and integer

order derivatives were introduced. To test its accuracy, the method was used to solve the model equations that describe momentum, heat and mass transfer in a nanofluid with fractional constitutive relation. The residual error norms in the solutions were found to be less or equal to 10^{-13}, thus demonstrating the accuracy and convergence of the method.

APPENDIX A: DISCRETIZATION OF THE MODEL EQUATIONS

In this appendix, we describe the full discretization of the coupled system of the equations (18) to (20). We obtain the numerical solution $f(\eta)$ by solving Eq. (18) independent of Eqs. (19) and (20) and then Eqs. (19) and (20) are solved as coupled system. In order to linearize each equation, we apply the quasilinearization method of Bellman and Kalaba (1965). The linearization method is a generalization method of the Newton–Raphson method and is constructed using the Taylor's series expansion about an initial guess of the solution. Applying the linearization on Eqs. (18), we have

$$f_{r+1}^{\alpha+1} + (Re_\alpha f_r)f''_{r+1} + (-2Re_\alpha f'_r - Re_\alpha M^2)f'_{r+1}$$
$$+ (Re_\alpha f''_r)f_{r+1} = R_r^f, \tag{43}$$

where $R_r^f = Re_\alpha f''_r f_r - Re_\alpha f'^2_r$ and f_r and f_{r+1} are solutions $f(\eta)$ at two successive iterations. The linearization method assumes that the difference between these solutions approaches zero as $r \to \infty$ (Bellman and Kalaba, 1965). If we now apply the Chebyshev approximation on the linearized Eq. (43) by substituting Eqs. (25), (27), and (31) where appropriate and using the semi–group property, so that we have

$$\left[D^\alpha D^2 + diagflt[Re_\alpha f_r]D^2 + diagflt[-2Re_\alpha f'_r - Re_\alpha M^2]D \right.$$
$$\left. + diagflt[Re_\alpha f''_r] \right] f_{N,r+1} = R_r^f, \tag{44}$$

in which $diagflt[\dots]$ constructs a two–dimensional matrix with the input as a diagonal. upon obtaining the solution $f_{N,r+1}(\eta)$, we use the known solution in the linearization of Eqs. (19) and (20) which is solved as system. The linearized form of Eqs. (19) and (20) is given as

$$Le\theta''_{r+1} + (\phi'_r + (2/Nbt)\theta'_r + LePrf_{r+1})\theta'_{r+1} + (\theta'_r)\phi'_{r+1} = R_r^\theta \tag{45}$$
$$(1/Nbt)\theta''_{r+1} + \phi''_{r+1} + (Scf_{r+1})\phi'_{r+1} = 0, \tag{46}$$

where $R_r^\theta = \phi'_r\theta'_r + (1/Nbt)\theta'^2_r$. Again we apply the Chebyshev approximation to the linearized coupled system and this yields

$$\left[LeD^2 + diagflt[\phi'_r + (2/Nbt)\theta'_r + LePrf_{r+1}]D \right] \theta_{N,r+1}$$
$$+ \left[diagflt[\theta'_r]D \right] \phi_{N,r+1} = R_r^\theta \tag{47}$$
$$\left[(1/Nbt)D^2 \right] \theta_{N,r+1} + \left[D^2 + diagflt[Scf_{r+1}]D \right] \phi_{N,r+1} = O, \tag{48}$$

where O is a zero matrix of size $(N+1) \times 1$. Note also that the right hand side of Eqs. (44) and (47) are expressed in terms of the $N + 1$–truncated shifted Chebyshev approximation. As stated earlier, the semi–infinite domain $[0, \infty)$ has been truncated to $[0, l]$, therefore, the coupled linearized system of algebraic equations are solved subject to

$$f_{N,r+1}(\eta_0) = 0, \quad D_{0,q}f_{N,r+1}(\eta_0) = 1, \quad \theta_{N,r+1}(\eta_0) = 1,$$
$$\phi_{N,r+1}(\eta_0) = 1$$
$$D_{N,q}f_{N,r+1}(\eta_N) = 0, \quad \theta_{N,r+1}(\eta_N) = 0, \quad \phi_{N,r+1}(\eta_N) = 0 \tag{49}$$

to obtain a consistent system.

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