AN OPERATIONAL MATRIX FOR SOLVING TIME-FRACTIONAL ORDER CAHN-HILLIARD EQUATION

by

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In the present scientific work, an operational matrix scheme with Laguerre polynomials is applied to solve a space-time fractional order non-linear Cahn-Hilliard equation, which is used to calculate chemical potential and free energy for a non-homogeneous mixture. Constructing operational matrix for fractional differentiation, the collocation method is applied to convert Cahn-Hilliard equation into an algebraic system of equations, which have been solved using Newton method. The prominent features of the manuscript is to providing the stability analysis of the proposed scheme and the pictorial presentations of numerical solution of the concerned equation for different particular cases and showcasing of the effect of advection and reaction terms on the nature of solute concentration of the considered mathematical model for different particular cases.

Key words: *fractional calculus, Cahn-Hilliard equation, Laguerre polynomials, porous мedia, convergence analysis*

Introduction

Some numerical methods based upon Laplace transform [1] and operational matrices of fractional differentiation and integration with B-spline [2], Legendre wavelets [3], *etc.* have been developed for finding the numerical solutions of fractional order differential equations. The functions which are commonly used include Legendre polynomial [4], Laguerre polynomial [5], *etc.* Bhrawy *et al.* [6] proposed a suitable way with the help of shifted Legendre approximation using tau method to find the approximate numerical solution of given fractional differential equation (FDE) with variable coefficient approximating the weighted inner product in tau method with the use of the shifted-Gauss-Lobatto quadrature formula. In [7], the authors have proposed spectral tau approach for obtaining the solution of some given FDE numerically. Pedas [8] have developed a suitable spline collocation method to solve FDE. For finding the spectral solution for a special collection of fractional order initial value problem, a direct technique was introduced by Esmaeili *et al.* [9] with the help of pseudo-spectral method. Moreover, for finding the solution of fractional order differential equation, a technique on computational process which depends on the Muntz polynomials and collocation was presented by Esmaeili *et al.* [10]. In the present work, the basic idea of algorithms is something linked to the ideas used by Bhrawy *et al.* [6] in developing the accurate algorithms for several purposes. During finding the solution of linear FPDE, the authors in [11] have developed an operational matrix

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of Laguerre polynomials for fractional order integration and modified the generalized Laguerre polynomial on semi-infinite intervals.

If ground-water is contaminated overall, then the rehabilitation is deemed to be too difficult and expensive. Careful recognition is very much necessary for recount the problem dominion, boundary conditions and model parameters for creating the numerical groundwater model of field problem. Solute transport through the groundwater is topic encountered in the interdisciplinary branch of science and engineering, called hydrology. The following equation represent solute transport in aquifiers:

$$\frac{\partial u(x,t)}{\partial t} = d\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x} \tag{1}$$

where $u(x, t)$ is solute concentration, $v > 0$, represents the advection coefficient and d represents dispersion coefficient. The aforementioned equation is also called advection dispersion equation. This equation also describes probability density function for location of particles in a continuum. The equation can be used in the groundwater hydrology in which the transport of the passive tracers is carried by the flow of the fluid in the porous media.

The general solute transport model is the reaction-advection-dispersion equation (RADE) since it has the combined effects of advection, dispersion and reaction process due to which solutes are transported down with the stream along the flow also get dispersed and sometimes react with the medium through which it moves. Mathematically it is represented:

$$\frac{\partial u}{\partial t} = \nabla(d\nabla u) - \nabla(vu) + R \tag{2}$$

where R is the reaction term for the species.

The first term on the right-hand side of the eq. (2) is accounting for dispersion phenomena, the second term accounting for the advection process and the last one is the reaction kinetics. When the solute does not react with the medium through which it moves and does not show any type of radioactive decay then it is called conservative system otherwise non-conservative for which reaction term has been encountered in the previous model. If only diffusion process is responsible for the movement of solute, then it is known as diffusion equation.

Elementary tools

Definition: The fractional order derivative operator D^α of the given order $\alpha > 0$ in the Caputo form is discussed [12]:

$$(D^\alpha X)(t) = \begin{cases} \dfrac{d^m X(t)}{dx^m}, & \text{if } \alpha = m \in N \\ \dfrac{1}{\Gamma(m-\alpha)}\displaystyle\int_0^t (t-\rho)^{m-\alpha-1} X^{(m)}(\rho) \quad d\rho, & \text{if } m-1 < \alpha < m \end{cases} \tag{3}$$

Proposed Cahn-Hilliard model

Due to the property of diverse phenomena of the equation of continuity and Fick's first law in phase transition and its application in soft matter to complex areas the scientiests are applying the equation in Navier-Stokes equation of fluid-flow [13, 14]. This has motivated the authors to study the physical behaviour of the model (4) in fractional order system, which being non-morkovian in nature will generate Brownion motion and will have long term memory. Thus the non-local fractional order C-H equation for system with the presence of reaction and advection terms:

$$\frac{\partial^\alpha u}{\partial t^\alpha} = D\frac{\partial^2}{\partial x^2}\left(-u + u^3 - \gamma\frac{\partial^2 u}{\partial x^2}\right) + v\frac{\partial u}{\partial x} + k(-u+1)u \tag{4}$$

where $0 \le x \le 1$, $0 \le \alpha \le 1$, and $0 \le t \le 1$, with boundary conditions $u(x, 0) = (-x + 1)x$, $u(1, t) = 0$, $u(0, t) = 0$. In the aforementioned expressions, D is the diffusion coefficient, v – the advection coefficient, and k – the reaction coefficient.

Basic properties of Laguerre polynomials

Consider an interval T and corrosponding weight function as $z(x) = \mathrm{e}^{-x}$ in usual way. Further, Construct a set $L_z^2(T) = \{R|R$ is a measurable function on T and $\mathrm{PRP}_z < \infty\}$ and equipped it with the considered operation of inner product and its norm:

$$(R,S)_z = \int_T R(x)S(x)z(x)dx, \quad \mathrm{PSP}_z = (R,S)_z^{1/2}$$

Moreover, the Laguerre polynomials of degree q is defined and denoted:

$$L_q(x) = \frac{1}{q!}\mathrm{e}^x \partial_x^q (x^q \mathrm{e}^{-x}), \quad q = 0,1,...; \tag{5}$$

Further, analytical outlines of the n^{th} degree Laguerre polynomials the semi-half interval $T = (0, \infty)$:

$$L_h(x) = \sum_{\rho=0}^{h} \frac{h!(-1)^\rho}{(-\rho+h)!(\rho!)^2} x^h, \quad h = 0,1,...; \tag{6}$$

From eq. (6), we can be found a special term in the following manner, which can be of used further:

$$D^\alpha L_m(0) = (-1)^\alpha \sum_{i=0}^{m-\alpha} \frac{(-i-1+m)!}{(m-i-\alpha)!(\alpha-1)!} \tag{7}$$

where α is a natural number.

Laguerre operational matrix for fractional differentiation

Consider $R(x) \in L_z^2(T)$ and expressed it in the terms of famous Laguerre polynomials:

$$R(x) = \sum_{h=0}^{\infty} u_h L_h(x), \quad u_h = \int_0^\infty R(x)L_h(x)z(x)\mathrm{d}x, \quad h = 0,1,2,...; \tag{8}$$

In customary, we use mainly the initial $(N + 1)$-terms of Laguerre polynomials:

$$R_N(x) = \sum_{n=0}^{N} u_n L_n(x) = C^T S(x) \tag{9}$$

The coefficient of Laguerre vector C and the mentioned Laguerre vector in the aforementioned equation:

$$C^T = [c_0, c_1, ..., c_N], \quad S(x) = [L_0(x), L_1(x), ..., L_N(x)]^T \tag{10}$$

Similarly, any arbitrary function $u(x, t)$ from $L_z^2(T) \times L_z^2(T)$ of two variables can be approximated in the form of Laguerre polynomials:

$$u(x,t) = \sum_{l=0}^{N}\sum_{m=0}^{N} u_{lm} L_l(x) L_m(t) \tag{11}$$

where $V = [u_{im}]$ and $u_{im} = \{L_l(x), [u(x, t), L_m(t)]\}$. Now, the derivative of the Laguerre vector $S(x)$ can be written:

$$\frac{\mathrm{d}S(x)}{\mathrm{d}x} = G^{(1)}S(x) \tag{12}$$

In eq. (12) $G^{(1)}$ is an operational matrix of Laguerre polynomials of $(N + 1) \times (N + 1)$ order for the derivative. Further, by the use of eq. (12):

$$\frac{\mathrm{d}^n S(x)}{\mathrm{d}x^n} = \left[G^{(1)}\right]^n S(x) \tag{13}$$

where n is a natural value and the superscript in $G^{(1)}$ denotes the powers of matrix. Thus $G^{(\mathrm{m})} = [G^{(1)}]^m$, $m = 1, 2...$;

Lemma 1. Suppose that $L_m(x)$ be the Laguerre polynomial of order m:

$$G^\alpha L_m(x) = 0, \quad m = 0,1,...,\lceil\alpha\rceil - 1, \quad \alpha > 0 \tag{14}$$

where $\lceil\alpha\rceil$ be the ceiling function. We are going to generalize the operational matrix for fractional order differentian in view of eq. (12) in the following theorems.

Theorem 1. Suppose that $S(x)$ be the Laguerre vector which is given in eq. (10) and $\alpha > 0$:

$$G^\alpha S(x) = G^{(\alpha)} S(x) \tag{15}$$

where $G^{(\alpha)}$ is the operational matrix of $(N + 1) \times (N + 1)$ order for differentiation of order α in the Caputo definition:

$$G^{(\alpha)} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \\ Y_\alpha(\lceil\alpha\rceil,0) & Y_\alpha(\lceil\alpha\rceil,1) & Y_\alpha(\lceil\alpha\rceil,2) & \cdots & Y_\alpha(\lceil\alpha\rceil,N) \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ Y_\alpha(i,0) & Y_\alpha(i,1) & Y_\alpha(i,2) & \cdots & Y_\alpha(i,N) \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ Y_\alpha(N,0) & Y_\alpha(N,1) & Y_\alpha(N,2) & \cdots & Y_\alpha(N,N) \end{bmatrix} \tag{16}$$

where

$$Y_\alpha(f,g) = \sum_{k=\lceil\alpha\rceil}^{f}\sum_{l=0}^{g} \frac{(-1)^{k+l} f!g!\Gamma(k-\alpha+l+1)}{(f-k)!\Gamma(k-\alpha+1)k!(g-l)!(l!)^2} \tag{17}$$

In previous expression, it is observed that in $G^{(\alpha)}$, the initial $\lceil\alpha\rceil$ rows vanishes [15].

Application of proposed scheme on concerned model

In this whole section of the manuscript, our primary motive is to provide the collocation scheme in an atttractive way, using operational matrix of Laguerre polynomials, such that propsed scheme can be applied effectively to find the solution of our considered problem. Further, we can approximate $u(x, t)$ in form of Laguerre polynomials:

$$u(x,t) = \sum_{a=0}^{N}\sum_{b=0}^{N} c_{ab} L_a(x) L_b(t) \tag{18}$$

where c_{ab} is unknowns which will be calculated latter. The eq. (18):

$$u(x,t) = R^T(x).C.R(t) \tag{19}$$

where $C = [c_{ab}]$ is $(N + 1) \times (N + 1)$ order matrix of unknown coefficients which is calculated later and $R(t) = [L_0(t), L_1(t)...L_N(t)]^T$ is a column vector. Now, taking the fractional derivatives of order β with respect to x on previous equation and applying *Theorem 1*:

$$\frac{\partial^\beta u}{\partial x^\beta} = G^\beta u(x,t) = G^\beta R^T(x).C.R(t) \tag{20}$$

Similarly:

$$\frac{\partial^\alpha u}{\partial t^\alpha} = G^\alpha u(x,t) = R^T(x).C.G^\alpha R(t) \tag{21}$$

Thus the boundary conditions can also be written as $R^T(x).C.R(0) = x(1 - x)$, $R^T(1).C.R(\mathrm{t}) = 0$, $R^T(0).C.R(\mathrm{t}) = 0$. Now collocating eq. (4) using the aforementioned transformed boundary conditions at points $x_p = p/N$ for $p = 0, 1, 2,..., N$ and $tp = p/N$ for $p = 0, 1, 2,...,N$. Thus using the previous collcoations, we find a system of non-linear algebraic equations. On solving this algebraic systems, we get the matrix C, and numerical solution can be calculated by substituting C in eq. (19).

Convergence analysis

The notable attention given here is to calculate upper bound of the error occurs in the proposed approximation.

Theorem 2. For generalized Laguerre polynomial $L_h^{(\omega)}(t)$, the global uniform bounds is estimated:

$$|L_h^{(\omega)}(t)| \le \begin{cases} \dfrac{(\omega+1)_h}{h!}\mathrm{e}^{t/2}, & \text{if } \omega \ge 0, t \ge 0, h = 0,1,2,...; \\ \left(2-\dfrac{(\omega+1)_h}{h!}\right)\mathrm{e}^{t/2}, & \text{if } -1 < \omega \le 0, t \ge 0, h = 0,1,2,...; \end{cases} \tag{22}$$

where $(f)_h : = f(f + 1)(f + 2)...(f + h - 1)$, $h = 1, 2, 3...$

Proof. Szego provided these global uniform bounds in [16], also these estimates were discussed in [17].

Remark. The ordinary Laguerre polynomial is a particular case of the generalized Laguerre polynomial, and can be found by using $\omega = 0$, *i. e.*:

$$L_h^{(0)}(t) = L_h(t) \tag{23}$$

Thus the global uniform bounds (22), for the Laguerre polynomial takes the form:

$$|L_h(t)| \le \frac{1}{h!}\mathrm{e}^{t/2}, \quad t \ge 0, \quad h = 0,1,2,... \tag{24}$$

Theorem 3. Let $u(x, t)$ be the sufficiently smooth function on the region P, $(\partial^\alpha u/\partial t^\alpha)_N$ be the approximation of $(\partial^\alpha u/\partial t^\alpha)$. Then the error in approximating $(\partial^\alpha u/\partial t^\alpha)$ by $(\partial^\alpha u/\partial t^\alpha)_N$ is bounded:

$$|E_r(N)| \le \sum_{a=N+1}^{\infty}\sum_{b=N+1}^{\infty} \frac{c_{ab}}{a!.m!}\chi_{mbN}\mathrm{e}^{(x+t)/2}, \quad t,x \ge 0, \quad b,a = 0,1,2,... \tag{25}$$

where $\chi_{mbN} = \sum_{m=0}^{N} Y_\alpha(b,m)$.

Proof. In the sight of eq. (18):

$$u(x,t)=\sum_{a=0}^{\infty}\sum_{b=0}^{\infty}c_{ab}L_a(x)L_b(t),\quad v(x,t)=\sum_{h=0}^{\infty}\sum_{k=0}^{\infty}c'_{hk}L_h(x)L_k(t) \tag{26}$$

truncating it upto $(N+1)$ term:

$$u_N(x,t)=\sum_{a=0}^{N}\sum_{b=0}^{N}c_{ab}L_a(x)L_b(t),\quad v_N(x,t)=\sum_{h=0}^{N}\sum_{k=0}^{N}c'_{hk}L_h(x)L_k(t) \tag{27}$$

Now, the partial derivative of $u(x, t)$ and $u_N(x, t)$ of order α w.r.t. t:

$$\frac{\partial^\alpha u}{\partial t^\alpha}=\sum_{a=0}^{\infty}\sum_{b=0}^{\infty}c_{ab}L_a(x)\frac{\partial^\alpha L_b(t)}{\partial t^\alpha},\quad \left(\frac{\partial^\alpha u}{\partial t^\alpha}\right)_N=\sum_{a=0}^{N}\sum_{b=0}^{N}c_{ab}L_a(x)\frac{\partial^\alpha L_b(t)}{\partial t^\alpha} \tag{28}$$

from the previous equation, we can write:

$$E_r(N)=\frac{\partial^\alpha u}{\partial t^\alpha}-\left(\frac{\partial^\alpha u}{\partial t^\alpha}\right)_N=\sum_{a=N+1}^{\infty}\sum_{b=N+1}^{\infty}c_{ab}L_a(x)\frac{\partial^\alpha L_b(t)}{\partial t^\alpha} \tag{29}$$

Using derivative of Laguerre polynomials, previous equation reduces:

$$|E_r(N)|=|\sum_{a=N+1}^{\infty}\sum_{b=N+1}^{\infty}c_{ab}L_a(x)\left[\sum_{m=0}^{N}\Upsilon_\alpha(b,m)L_m(t)\right]| \tag{30}$$

or

$$|E_r(N)|=\sum_{a=N+1}^{\infty}\sum_{b=N+1}^{\infty}c_{ab}.\chi_{mbN}\,|L_m(t)|.|L_a(t)| \tag{31}$$

Applying eq. (24):

$$|E_r(N)|\le\sum_{a=N+1}^{\infty}\sum_{b=N+1}^{\infty}c_{ab}\chi_{mbN}\frac{1}{m!}\mathrm{e}^{t/2}\frac{1}{a!}\mathrm{e}^{x/2} \tag{32}$$

or

$$|E_r(N)|\le\sum_{a=N+1}^{\infty}\sum_{b=N+1}^{\infty}\frac{c_{ab}}{a!.m!}\chi_{mbN}\mathrm{e}^{(x+t)/2},\quad t,x\ge 0,\quad b,a=0,1,2,... \tag{33}$$

Which is the required *proof*.

Error analysis of proposed scheme

In this section of the article, we will apply Laguerre polynomial operational matrix method for the fractional order differentiation solve fractional order 1-D non-linear PDE to illustrate the accuracy and applicability of the proposed scheme and compared the obtained result with the exact solution of the given example.

Example. The 1-D non-linear PDE:

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+u(1-u) \tag{34}$$

with the initial and boundary conditions as:

$$u(x,0)=\frac{1}{4}\left(1-\tanh\left[\frac{x}{2\sqrt{6}}\right]\right)^2,\ u(0,t)=\frac{1}{4}\left\{1-\tanh\left[\frac{1}{2\sqrt{6}}\left(-\frac{5t}{\sqrt{6}}\right)\right]\right\}^2$$

$$u(1,t)=\frac{1}{4}\left\{1-\tanh\left[\frac{1}{2\sqrt{6}}(1-\frac{5t}{\sqrt{6}})\right]\right\}^2$$

has the exact solution as

$$u(x,t)=\frac{1}{4}\left\{1-\tanh\left[\frac{1}{2\sqrt{6}}\left(x-\frac{5t}{\sqrt{6}}\right)\right]\right\}^2$$

The absolute error between solutions is depicted through fig. 1.

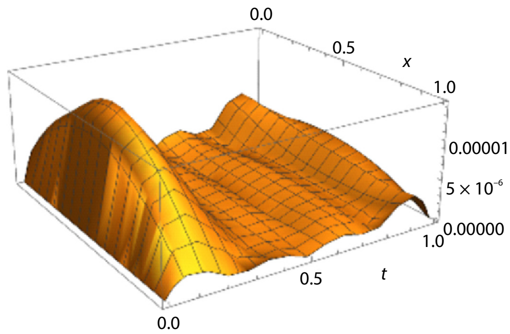

Figure 1. Plots of the absolute error between the numerical and exact solutions *vs.* *x* and *t*

Results and discussion

The variations of the solute concentration $u(x, t)$ *vs*. the column length x at $t = 1$ for various values of the fractional order time parameter for conservative case ($k = 0$) and non-conservative case ($k \neq 0$) in the absence/presence of the advection term are found numerically taking $\gamma = 1$ and the obtained results are displayed through figs. 2-5.

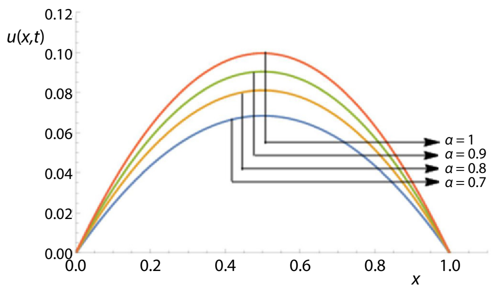

Figure 2. Plots of field variable $u(x, t)$ *vs.* x at $t = 1$ for $k = 0$, $v = 0$ and different values of α

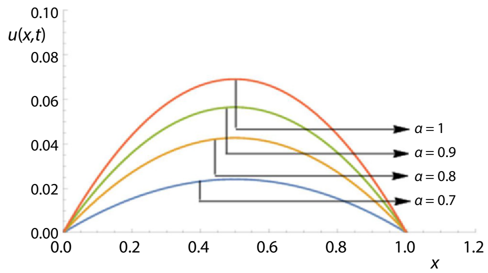

Figure 3. Plots of field variable $u(x, t)$ *vs.* x at $t = 1$ for $k = -1, v = 0$ and different values of α

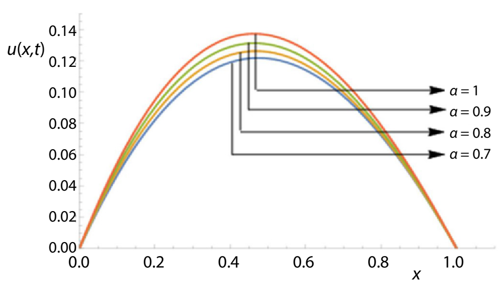

Figure 4. Plots of field variable $u(x, t)$ *vs.* x at $t = 1$ for k = 0, $v = -1$ and different values of α

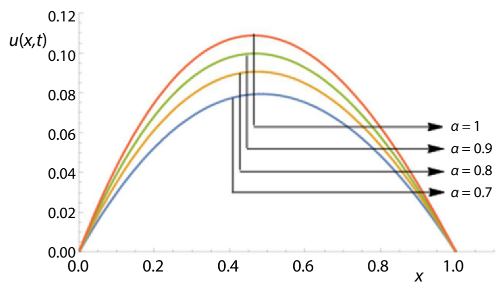

Figure 5. Plots of field variable $u(x, t)$ *vs.* x at $t = 1$ for $k = -1$, $v = -1$ and different values of α

The effect of reaction term on the solution profile during the absences of advection term for different values of the fractional order time derivative and also those during the presence of advection term can be found by comparing the numerical results shown in fig. 3 with figs. 2 and 5 with fig. 4, respectively. It is seen that the overshoots of sub-diffusion are decreased as the system approaches from standard order to fractional order. It is also seen from the figures that damping are found in both cases due to the presence of sink term. Again the overshoots of the probability density function $u(x, t)$ increases due to the presence of advection term. It is also seen that as γ decreases the overshoots of sub-diffusion increases for various α. This can be physically interpreted as the concentration increases with the increase decrease of the separation of the transition regions between the domains.

Conclusion

The present scientific contribution has achieved three important goals. First one is finding the numerical solution of the solute concentration $u(x, t)$ of famous Cahn-Hilliard equation of integer order as well as fractional order by the use of powerful and efficient technique Laguerre operational matrix. Second one is the pictorial conferrals of the nature of overshoots during sub-diffusion due to existence of advection and reaction terms. The third one is the pictorial conferrals of the damping nature of the solute concentration when the system go close from standard order to fractional order in the presence of sink term.

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