NUMERICAL ANALYSIS OF TIME FRACTIONAL THREE DIMENSIONAL DIFUSSION EQUATION

by

Abdon ATANGANA***

Institute for Groundwater Studies, Faculty of Natural and Agricultural Sciences,
University of the Free State, Bloemfontein, South Africa

Original scientific paper
DOI: 10.2298/TSCI15S10S7A

The three dimensional diffusion equations were extended to the scope of fractional order derivative. The fractional operator used here is in Caputo sense. The resulting equation was solved using two numerical approaches: The forward in time and central in space method and the Crank-Nicholson method. The stability analysis of both methods was studied, and the study showed that the Crank-Nicholson method is unconditionally stable while the forward method is stable if some conditions are satisfied.

Key words: *three dimensional diffusion equations, fractional derivative, stability, convergence*

Introduction

The word diffusion is derived from the Latin word, "diffundere" [1, 2], which means "to spread out". If a substance is spreading out it is moving from an area of high concentration to an area of low concentration [1, 2]. A distinguishing feature of diffusion is that it results in mixing or mass transport, without requiring bulk motion. Diffusion is the net movement of a substance for instance, an atom, ion or molecule from a region of high concentration to a region of low concentration. This is also referred to as the movement of a substance down a concentration gradient. A gradient is the change in the value of a quantity for example, concentration, pressure, temperature, with the change in another variable, for instance, distance. For example, a change in concentration over a distance is called a concentration gradient, a change in pressure over a distance is called a pressure gradient, and a change in temperature over a distance is a called a temperature gradient [1, 3]. The concept of diffusion is widely used in: physics, chemistry, biology, sociology, economics, and finance. However, in each case, the object for instance is, atom, idea, and so on, that is undergoing diffusion is spreading out from a point or location at which there is a higher concentration of that object. The equation is usually written as [1-4]:

$$\frac{\partial \varphi(\vec{\mathrm{r}},t)}{\partial t} = \nabla\,[D(\varphi,\vec{\mathrm{r}})\nabla\varphi(\vec{\mathrm{r}},t)] \tag{1}$$

where $\varphi(r, t)$ is the density of the diffusing material at location r and time t, $D(\varphi, r)$ – the collective diffusion coefficient for density φ at location r, and ∇ – the vector differential operator

* Author's e-mail: abdonatangana@yahoo.fr

del. If the diffusion coefficient depends on the density then the equation is non-linear, otherwise it is linear [1-3].

More generally, when D is a symmetric positive definite matrix, the equation describes anisotropic diffusion, which is written (for 3-D diffusion) as [2-4]:

$$\frac{\partial \varphi(\vec{\mathrm{r}},t)}{\partial t} = \sum_{i=1}^{3}\sum_{j=1}^{3}\frac{\partial}{\partial x_i}\left[D_{ij}(\varphi,\vec{\mathrm{r}})\frac{\partial \varphi(\vec{\mathrm{r}},t)}{\partial x_j}\right] \tag{2}$$

If D is constant, then the equation reduces to the linear differential equation:

$$\frac{\partial \varphi(\vec{\mathrm{r}},t)}{\partial t} = D\nabla^2 \varphi(\vec{\mathrm{r}},t) \tag{3}$$

also called the heat equation. Fractional calculus, in understanding of its theoretical and real-world presentations in numerous regulations for example astronomy and manufacturing problems, is discovered to be accomplished of pronouncing phenomena owning long range memory special effects that are challenging to handle through traditional integer-order calculus [5-10]. Nearby has been an increasing concentration in the modification of fractional calculus as a successful modelling instrument for complicated systems, contributing to innovative viewpoints in their dynamical investigation and regulator. This improvement in the methodical knowledge is established by an enormous quantity of evens developing on the subject, manuscripts and presentations in the past years [11, 12]. The aim of this paper is to present the numerical solution of the time-fractional 3-D diffusion equation:

$$\frac{\partial^\alpha \varphi(\vec{\mathrm{r}},t)}{\partial t^\alpha} = D\nabla^2 \varphi(\vec{\mathrm{r}},t) + Q(r,t) \tag{4}$$

The aim of this paper is to solve numerically the eq. (4), here $r = (x, y, z)$. Caputo's definition is illustrated:

$${}_a^C D_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)}\int_a^t \frac{f^{(n)}(\tau)\mathrm{d}\tau}{(t-\tau)^{\alpha+1-n}} \tag{5}$$

Numerical analysis

Consider eq. (4) with initial conditions:

$$u(x,y,z,0) = f(x,y,z), \quad u(0,0,0,t) = u(L_x,L_y,L_z,t) = 0 \tag{6}$$

where $u(x,y,z,t)$, $x\in[a_x,b_x]$, $y\in[a_y,b_y]$, and $z\in[a_z,b_z]$. Suppose satisfies boundary condition in x-, y-, and z-directions. We discretize in time on the uniform grid $t_n = t_0 + n\Delta$, $n = 0, 1, 2,...$ Furthermore, in the x-, y-, and z-directions, we use the uniform grid:

$$x_i = x_0 + i\Delta x, \quad i = 0, ... M, \quad \Delta x = \frac{b_x - a_x}{M+1} \tag{7}$$

$$y_j = y_0 + j\Delta y, \quad j = 0, ..., \quad \Delta y = \frac{b_y - a_y}{N+1} \tag{8}$$

$$z_k = z_0 + k\Delta z, \quad k = 0, ..., \quad \Delta z = \frac{b_z - a_z}{K+1} \tag{9}$$

Forward in time and central in space method

We shall note that the fractional operator used in this work is the Caputo type. Similar to the first order derivative, the following approximation to the Caputo type was provided in [13, 14]:

$$ {}_{a}^{C}D_{t}^{\alpha}u(x,t_{n+1})=\frac{1}{\Gamma(1-\alpha)}\sum_{l=0}^{n}\int_{t_l}^{t_{l+1}}(t_{l+1}-\tau)^{\alpha}\frac{u(x,y,z,t_{l=1})-u(x,y,z,t_{l-1})}{\Delta t}\mathrm{d}\tau+r_{\delta t}^{n+1} \tag{10}$$

The truncation error is given as:

$$ r_{\Delta t}^{n+1}\le C_u(\Delta t)^{2-\alpha} \tag{11}$$

where C_u is a constant only related to u. Then the Caputo fractional operator can be written:

$$ {}_{a}^{C}D_{t}^{\alpha}u(x,t_{n+1})=\frac{(\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=0}^{n}v_{n-j}u_t(x,y,z,t_l),\quad v_l=(l+1)^{1-\alpha}-l^{1-\alpha} \tag{12}$$

Also, we have that, the second-order spatial derivative is known as [12, 14]:

$$ \frac{\partial^2 u(x_i,y_j,z_k,t_{l+1})}{\partial x^2}=\frac{u(x_{i+1},y_j,z_k,t_{l+1})-2u(x_i,y_j,z_k,t_{l+1})-u(x_{i-1},y_j,z_k,t_{l+1})}{(\Delta x)^2} \tag{13}$$

Replacing eqs. (13) and (12) into eq. (4), we obtain:

$$ \frac{(\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=0}^{n}v_{n-j}u_t(x,y,z,t_l)=D\frac{u(x_{i+1},y_j,z_k,t_l)-2u(x_i,y_j,z_k,t_l)+u(x_{i-1},y_j,z_k,t_l)}{(\Delta x)^2}+$$

$$ +D\frac{u(x_i,y_{j+1},z_k,t_l)-2u(x_i,y_j,z_k,t_l)+u(x_i,y_{j-1},z_k,t_l)}{(\Delta y)^2}+$$

$$ +D\frac{u(x_i,y_j,z_{k+1},t_l)-2u(x_i,y_j,z_k,t_l)+u(x_i,y_j,z_{k-1},t_l)}{(\Delta z)^2}+Q(x_i,y_j,z_k,t_l) \tag{14}$$

For ease, let:

$$ u_{i,j,k}^{l}=u(x_i,y_j,z_k,t_l),\quad Q_{i,j,k}^{l}=Q(x_i,y_j,z_k,t_l) \tag{15}$$

also $\mu=D(\Delta t)^{1-\alpha}/\Gamma(2-\alpha)(\Delta x)^2$, $\beta=D(\Delta t)^{1-\alpha}/\Gamma(2-\alpha)(\Delta y)^2$, and $\gamma=D(\Delta t)^{1-\alpha}/\Gamma(2-\alpha)(\Delta z)^2$. Then, eq. (14) can be reformulated:

$$ u_{i,j,k}^{l+1}=(1-2\mu-2\gamma-2\beta)u_{i,j,k}^{l}+\mu(u_{i+1,j,k}^{l}-u_{i-1,j,k})+\gamma(u_{i,j+1,k}^{l}-u_{i,j,k+1})+$$

$$ +\mu(u_{i+1,j,k}^{l}-u_{i,j,k-1})+\frac{(\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}Q_{i,j,k}^{l}+2u_{i,j,k}^{l-1}+\sum_{m=2}^{l}(u_{i,j,k}^{l+1-m}-u_{i,j,k}^{l-m})v_m \tag{16}$$

We shall now look at the stability of the used scheme. To achieve this, we consider:

$$\varepsilon_{i,j,k}^{n} = g^{n}\mathrm{e}^{k_x x_i + k_y y_j + k_z z_k} \tag{17}$$

Now replace eq. (17) in eq. (16), and after manipulations, we obtain the following relation for the amplification factor $g(k)$:

$$g(k) = 1 - 4\mu\sin^2\left(\frac{k_x\Delta x}{2}\right) - 4\gamma\sin^2\left(\frac{k_y\Delta y}{2}\right) - 4\beta\sin^2\left(\frac{k_z\Delta z}{2}\right) \tag{18}$$

In this case the stability condition reads $|g(k)| \le 1$ for all k:

$$\mu + \beta + \gamma \le \frac{1}{2} \tag{19}$$

This will lead to:

$$\frac{(\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)} \le \frac{\Delta x^2 \Delta y^2 \Delta z^2}{2D(\Delta x^2 + \Delta y^2 + \Delta z^2)} \tag{20}$$

The backward in time and central in space for 3-D diffusion equation is stable if and only if the inequality is satisfied:

$$\frac{(\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)} \le \frac{\Delta x^2 \Delta y^2 \Delta z^2}{2D(\Delta x^2 + \Delta y^2 + \Delta z^2)} \tag{21}$$

The Crank-Nicolson method

An implicit scheme, introduced by Crank and Nicolson in 1947 [14] is based on the central approximation. The approximation used for the space derivative is just an average of approximations in points (x_i, $t_i + 0.5\ \Delta t$):

$$\frac{\partial^2 u(x_i, y_j, z_k, t_{l+1})}{\partial x^2} = \frac{u_{i+1,j,k}^{l+1} - 2u_{i,j,k}^{l+1} + u_{i-1,j,k}^{l+1} + u_{i+1,j,k}^{l} - 2u_{i,j,k}^{l} + u_{i-1,j,k}^{l}}{(\Delta x)^2} \tag{22}$$

Replacing eqs. (22) and (12) into eq. (4) to obtain:

$$\frac{(\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=0}^{n} v_{n-j}u_t(x,y,z,t_l) = D\frac{u_{i+1,j,k}^{l+1} - 2u_{i,j,k}^{l+1} + u_{i-1,j,k}^{l+1} + u_{i+1,j,k}^{l} - 2u_{i,j,k}^{l} + u_{i-1,j,k}^{l}}{(\Delta x)^2} +$$

$$+D\frac{u_{i,j+1,k}^{l+1} - 2u_{i,j,k}^{l+1} + u_{i,j-1,k}^{l+1} + u_{i,j+1,k}^{l} - 2u_{i,j,k}^{l} + u_{i,j-1,k}^{l}}{(\Delta y)^2} +$$

$$+D\frac{u_{i,j,k+1}^{l+1} - 2u_{i,j,k}^{l+1} + u_{i,j,k-1}^{l+1} + u_{i,j,k+1}^{l} - 2u_{i,j,k}^{l} + u_{i,j,k-1}^{l}}{(\Delta z)^2} + Q(x_i, y_j, z_k, t_l) \tag{23}$$

Equation (23) can be rewritten:

$$u_{i,j,k}^{l+1}(1+2\mu+2\gamma+2\alpha)=$$
$$=(1-2\mu-2\gamma-2\beta)u_{i,j,k}^{l}+\mu(u_{i+1,j,k}^{l}-u_{i-1,j,k}^{l})+\gamma(u_{i,j+1,k}^{l}-u_{i,j,k+1}^{l})+$$
$$+\beta(u_{i+1,j,k}^{l}-u_{i,j,k-1}^{l})+\frac{(\Delta t)^{1-\alpha}}{\Gamma(2-\alpha)}Q_{i,j,k}^{l}+2u_{i,j,k}^{l-1}+\sum_{m=2}^{l}(u_{i,j,k}^{l+1-m}-u_{i,j,k}^{l-m})v_m+$$
$$+\mu(u_{i+1,j,k}^{l+1}-u_{i-1,j,k}^{l-1})+\gamma(u_{i,j+1,k}^{l+1}-u_{i,j-1,k}^{l-1})+$$
$$+\beta(u_{i+1,j,k}^{l+1}-u_{i,j,k-1}^{l-1}) \tag{24}$$

To study the stability of the Crank-Nicholson scheme for time fractional 3-D diffusion equation, we consider the equation:

$$\varepsilon_{i,j,k}^{n}=g^{n}\mathrm{e}^{k_x x_i+k_y y_j+k_z z_k} \tag{25}$$

Now replacing it into eq. (24) and after simplification and manipulations, we obtain the amplification factor:

$$g(k)=\frac{1-4\mu\sin^2\left(\frac{k_x\Delta x}{2}\right)-4\gamma\sin^2\left(\frac{k_y\Delta y}{2}\right)-4\beta\sin^2\left(\frac{k_z\Delta z}{2}\right)}{1+4\mu\sin^2\left(\frac{k_x\Delta x}{2}\right)+4\gamma\sin^2\left(\frac{k_y\Delta y}{2}\right)+4\beta\sin^2\left(\frac{k_z\Delta z}{2}\right)} \tag{26}$$

The denominator of eq. (26) is always greater than the numerator. That is, the absolute value of g is less than one, that implies, the Crank Nicholson scheme for time fractional 3-D diffusion equation is unconditionally stable.

Conclusions

The aim of the work was to study the numerical analysis of the 3-D time fractional diffusion equation. To achieve this, we made use of two different numerical techniques namely: The Crank-Nicholson and the forward scheme. The efficiency of these methods was tested *via* the stability analysis, which revealed that, the Crank-Nicholson is more efficient than the forward.

Nomenclature

D – diffusion coefficient,
$Q(r, t)$ – source term representing capacity of internal sources, [–]
t – time, [s],
x, y, z – special coordinates, [m]
∇^2 – the Laplace operator

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Paper submitted: October 10, 2014
Paper revised: March 15, 2015
Paper accepted: March 18, 2015