

Comparative Study of some Numerical Methods to Solve a 3D Advection-Diffusion Equation

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Abstract. In this work, three finite difference methods have been used to solve a three dimensional advection-diffusion equation with given initial and boundary conditions. The three methods are fourth order finite difference method, Crank-Nicolson and Implicit Chapeau Function. We compare the performance of the methods by computing L_2 error, L_∞ error and some performance indices such as mass distribution ratio (MDR), mass conservation ratio (MCR), total mass and R^2 which is a measure of total variation in particle distribution.

Keywords: three dimensional advection-diffusion equation, finite difference methods

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INTRODUCTION

The advection-diffusion equation is one of the most challenging equations in science as it represents two different transport processes: advection and diffusion. It has been used to describe heat transfer in a draining film [1], mass transfer [2], flow in porous media [3] and charge transport in semi-conductor devices [4]. The 3D advection-diffusion equation is given by:

$$\frac{\partial u}{\partial t} + \beta_x \frac{\partial u}{\partial x} + \beta_y \frac{\partial u}{\partial y} + \beta_z \frac{\partial u}{\partial z} = \alpha_x \frac{\partial^2 u}{\partial x^2} + \alpha_y \frac{\partial^2 u}{\partial y^2} + \alpha_z \frac{\partial^2 u}{\partial z^2}, \quad (1)$$

where $\beta_x, \beta_y, \beta_z$ are the velocity components of advection in the direction of x, y and z , respectively, and α_x, α_y , and α_z are diffusivities in the x, y and z directions, respectively.

Yang et al. [5] studied the accuracy of three numerical methods, namely explicit central difference, implicit Crank-Nicolson and implicit Chapeau function methods, for solving advection-diffusion equation as applied to spore and insect dispersal. In this work, we compare the performance of three finite difference methods, namely: fourth Order upwind scheme [6], Crank-Nicolson and Implicit Chapeau function when used to solve the partial differential equation in (1) with initial conditions

$$u(x, y, z, 0) = \exp\left(-\frac{(x-0.5)^2}{\alpha_x} - \frac{(y-0.5)^2}{\alpha_y} - \frac{(z-0.5)^2}{\alpha_z}\right). \quad (2)$$

The analytical solution to this problem is [7]

$$u(x, y, z, t) = \frac{1}{(4t+1)^{3/2}} \exp\left[-\frac{(x-\beta_x t-0.5)^2}{\alpha_x(4t+1)} - \frac{(y-\beta_y t-0.5)^2}{\alpha_y(4t+1)} - \frac{(z-\beta_z t-0.5)^2}{\alpha_z(4t+1)}\right]. \quad (3)$$

The boundary conditions are obtained by direct substitution into Eq. (3). The same approach was done by Yang et al. [5].

To analyse and compare the performance of the three methods, we compute the L_2 and L_∞ errors and some performance indices such as; Total mass, mass conservation ratio (MCR), mass distribution ratio (MDR) and R^2 (which is

a measure of goodness fit) [8]. We next describe how these performances indices are calculated. Let $v_{i,j,k}$ be the exact solution and \bar{v} be its mean, then R^2 , Total mass, MCR and MDR are calculated as

$$R^2 = 1 - \frac{\sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} (v_{i,j,k} - u_{i,j,k})^2}{\sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} (v_{i,j,k} - \bar{v})^2}, \quad \text{Total mass} = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} u_{i,j,k}^n,$$

$$\text{MCR} = \frac{\sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} u_{i,j,k}^n}{\sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} v_{i,j,k}^n}, \quad \text{MDR} = \frac{\sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} (u_{i,j,k}^n)^2}{\sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} (v_{i,j,k}^n)^2}.$$

NUMERICAL METHODS

In this section, three finite difference methods are presented to solve a 3D advection diffusion equation. For simplicity, we use the following notations:

$$c_x = \frac{\beta_x \Delta t}{\Delta x}, \quad c_y = \frac{\beta_y \Delta t}{\Delta y}, \quad c_z = \frac{\beta_z \Delta t}{\Delta z}, \quad s_x = \frac{\alpha_x \Delta t}{\Delta x^2}, \quad s_y = \frac{\alpha_y \Delta t}{\Delta y^2}, \quad s_z = \frac{\alpha_z \Delta t}{\Delta z^2}.$$

Implicit Crank-Nicolson Method (ICN)

Since the 3D implicit methods are costly, we use fractional splitting methods, by splitting the 3D problem into three 1D equations [5].

$$\frac{\partial u}{\partial t} = -\beta_x \frac{\partial u}{\partial x} + \alpha_x \frac{\partial^2 u}{\partial x^2} \quad (4)$$

$$\frac{\partial u}{\partial t} = -\beta_y \frac{\partial u}{\partial y} + \alpha_y \frac{\partial^2 u}{\partial y^2} \quad (5)$$

$$\frac{\partial u}{\partial t} = -\beta_z \frac{\partial u}{\partial z} + \alpha_z \frac{\partial^2 u}{\partial z^2}. \quad (6)$$

At the first fractional time step, i. e., from t_n to $t_{n+1/3}$, Eq. (4) is discretized by first separating into two equations as follows:

$$\frac{1}{2} u_t = -\beta_x u_x \quad (7)$$

$$\frac{1}{2} u_t = \alpha_x u_{xx}. \quad (8)$$

These two equations are discretized as

$$\frac{1}{2} \frac{u_{i,j,k}^{n+1/3} - u_{i,j,k}^n}{\Delta t} = -\beta_x \left(\theta \frac{u_{i+1,j,k}^{n+1/3} - u_{i-1,j,k}^{n+1/3}}{2\Delta x} + (1-\theta) \frac{u_{i+1,j,k}^n - u_{i-1,j,k}^n}{2\Delta x} \right). \quad (9)$$

and

$$\frac{1}{2} \left(\frac{u_{i,j,k}^{n+1/3} - u_{i,j,k}^n}{\Delta t} \right) = \alpha_x \left(\theta \frac{u_{i+1,j,k}^{n+1/3} - 2u_{i,j,k}^{n+1/3} + u_{i-1,j,k}^{n+1/3}}{\Delta x^2} + (1-\theta) \frac{u_{i+1,j,k}^n - 2u_{i,j,k}^n + u_{i-1,j,k}^n}{\Delta x^2} \right), \quad (10)$$

respectively, where $\theta \in [0, 1]$ is temporal weighting factor. Combining Eqs. (9) and (10), we get

$$A_x u_{i-1,j,k}^{n+1/3} + B_x u_{i,j,k}^{n+1/3} + C_x u_{i+1,j,k}^{n+1/3} = D_{i,j,k}^n, \quad (11)$$

where

$$A_x = -\theta c_x - 2\theta s_x, \quad B_x = 2 + 4\theta s_x, \quad C_x = \theta c_x - 2\theta s_x$$

$$D_{i,j,k}^n = (1-\theta)[(c_x + 2s_x)u_{i-1,j,k}^n + (-c_x + 2s_x)u_{i+1,j,k}^n] + [2 - 4(1-\theta)s_x]u_{i,j,k}^n.$$

Following the same approach as the integration procedure in the x -direction, we obtain

$$A_y u_{i,j-1,k}^{n+2/3} + B_y u_{i,j,k}^{n+2/3} + C_y u_{i,j+1,k}^{n+2/3} = D_{i,j,k}^{n+1/3}, \text{ and } A_z u_{i,j,k-1}^{n+1} + B_z u_{i,j,k}^{n+1} + C_z u_{i,j,k+1}^{n+1} = D_{i,j,k}^{n+2/3},$$

at the second and third fractional time steps, respectively.

Implicit Chapeau function Method (ICF)

In this section we refer to Yang et al. [5]. We follow the same procedure as that of the Crank Nicolson method where (7) and (8) are discretized, respectively by

$$\frac{1}{12\Delta t} \left[(u_{i-1,j,k}^{n+1/3} - u_{i-1,j,k}^n) + 4(u_{i,j,k}^{n+1/3} - u_{i,j,k}^n) + (u_{i+1,j,k}^{n+1/3} - u_{i+1,j,k}^n) \right] = -\beta_x \left(\theta \frac{u_{i+1,j,k}^{n+1/3} - u_{i-1,j,k}^{n+1/3}}{2\Delta x} + (1-\theta) \frac{u_{i+1,j,k}^n - u_{i-1,j,k}^n}{2\Delta x} \right). \quad (12)$$

and

$$\frac{1}{12\Delta t} \left[(u_{i-1,j,k}^{n+1/3} - u_{i-1,j,k}^n) + 4(u_{i,j,k}^{n+1/3} - u_{i,j,k}^n) + (u_{i+1,j,k}^{n+1/3} - u_{i+1,j,k}^n) \right] = \alpha_x \left[\theta \left(\frac{u_{i+1,j,k}^{n+1/3} - 2u_{i,j,k}^{n+1/3} + u_{i-1,j,k}^{n+1/3}}{\Delta x^2} \right) + (1-\theta) \left(\frac{u_{i+1,j,k}^n - 2u_{i,j,k}^n + u_{i-1,j,k}^n}{\Delta x^2} \right) \right]. \quad (13)$$

Combining (12) and (13), we get

$$A_x u_{i-1,j,k}^{n+1/3} + B_x u_{i,j,k}^{n+1/3} + C_x u_{i+1,j,k}^{n+1/3} = D_{i,j,k}^n, \quad (14)$$

where $A_x = 2 - 6\theta c_x - 12\theta s_x$, $B_x = 8 + 24\theta s_x$, $C_x = 2 + 6\theta c_x - 12\theta s_x$ and

$$D_{i,j,k}^n = [2 + (1-\theta)(6c_x + 12s_x)]u_{i-1,j,k}^n + (8 - 24(1-\theta)s_x)u_{i,j,k}^n + [2 + (1-\theta)(-6c_x + 12s_x)]u_{i+1,j,k}^n$$

Using the same procedures as in the first fractional time step for the integrations in the y -direction and z -direction, we obtain

$$A_y u_{i,j-1,k}^{n+2/3} + B_y u_{i,j,k}^{n+2/3} + D_y u_{i,j+1,k}^{n+2/3} = D_{i,j,k}^{n+1/3}, \text{ and } A_z u_{i,j,k-1}^{n+1} + B_z u_{i,j,k}^{n+1} + D_z u_{i,j,k+1}^{n+1} = D_{i,j,k}^{n+2/3}.$$

Fourth Order Finite Difference Method (FOM)

Using the fourth order finite difference method [6] at the first fractional time step, we obtain

$$u_{i,j,k}^{n+1/3} = A_x u_{i-2,j,k}^n + B_x u_{i-1,j,k}^n + C_x u_{i,j,k}^n + D_x u_{i+1,j,k}^n + E_x u_{i+2,j,k}^n, \quad (15)$$

where

$$\begin{aligned} A_x &= \frac{1}{24} \left(12s_x(s_x + c_x^2) + 2s_x(6c_x - 1) + c_x(c_x - 1)(c_x + 1)(c_x + 2) \right), \\ B_x &= -\frac{1}{6} \left(12s_x(s_x + c_x^2) + 2s_x(3c_x - 4) + c_x(c_x - 2)(c_x + 1)(c_x + 2) \right), \\ C_x &= \frac{1}{4} \left(12s_x(s_x + c_x^2) - 10s_x + (c_x - 1)(c_x - 2)(c_x + 1)(c_x + 2) \right), \\ D_x &= -\frac{1}{6} \left(12s_x(s_x + c_x^2) - 2s_x(3c_x + 4) + c_x(c_x - 2)(c_x - 1)(c_x + 2) \right), \\ E_x &= \frac{1}{24} \left(12s_x(s_x + c_x^2) - 2s_x(6c_x + 1) + c_x(c_x - 1)(c_x + 1)(c_x - 2) \right). \end{aligned}$$

In a similar way, we obtain

$$u_{i,j,k}^{n+2/3} = A_y u_{i,j-2,k}^{n+1/3} + B_y u_{i,j-1,k}^{n+1/3} + C_y u_{i,j,k}^{n+1/3} + D_y u_{i,j+1,k}^{n+1/3} + E_y u_{i,j,k+2}^{n+1/3}$$

and

$$u_{i,j,k}^{n+1} = A_z u_{i,j,k-2}^{n+2/3} + B_z u_{i,j,k-1}^{n+2/3} + C_z u_{i,j,k}^{n+2/3} + D_z u_{i,j,k+1}^{n+2/3} + E_z u_{i,j,k+2}^{n+2/3}.$$

at the second and third fractional time steps, respectively.

TABLE 1. $h = 0.05$ and $k = 0.001$, $T = 0.05$.

| Method | L_2 - error | L_∞ | Total mass | R^2 | MCR | MDR | min u | max u |
|--------|-------------------------|------------|------------|--------|-----|--------|---------------------------|---------|
| Exact | 0 | 0 | 44.5466 | 1 | 1 | 1 | 1.6640×10^{-32} | 0.7419 |
| ICN | 0.0032 | 0.0799 | 44.5465 | 0.9932 | 1 | 1.0129 | -3.9948×10^{-5} | 0.7145 |
| ICF | 5.8236×10^{-4} | 0.0210 | 44.5466 | 0.9998 | 1 | 0.9870 | -1.2857×10^{-10} | 0.7209 |
| FOM | 8.3415×10^{-4} | 0.0226 | 44.5466 | 0.9995 | 1 | 1.0013 | -1.2422×10^{-4} | 0.7330 |

TABLE 2. $h = 0.05$ and $k = 0.001$, $T = 0.2$.

| Method | L_2 - error | L_∞ | Total mass | R^2 | MCR | MDR | min u | max u |
|--------|-------------------------|------------|------------|--------|--------|--------|---------------------------|---------|
| Exact | 0 | 0 | 44.5400 | 1 | 1 | 1 | 1.2227×10^{-32} | 0.4072 |
| ICN | 0.0052 | 0.0916 | 44.3273 | 0.9658 | 0.9952 | 1.0238 | -0.0027 | 0.4059 |
| ICF | 7.7228×10^{-4} | 0.0163 | 44.8431 | 0.9992 | 1.0068 | 0.9778 | -5.0893×10^{-10} | 0.3910 |
| FOM | 9.6606×10^{-4} | 0.0181 | 44.5894 | 0.9988 | 1.0011 | 1.0016 | 1.2227×10^{-32} | 0.4110 |

NUMERICAL RESULTS

The numerical results obtained using the three numerical methods at time $T = 0.05$ and 0.2 are shown in Tables 1-2. For all computations, we consider the spatial step sizes $\Delta x = \Delta y = \Delta z = h = 0.05$ and the temporal step size, $\Delta t = k = 0.001$, where the advection and diffusion coefficients are given by $\beta_x = \beta_y = \beta_z = 0.8$ and $\alpha_x = \alpha_y = \alpha_z = 0.01$. These three methods are stable at these values of $\Delta x, \Delta y, \Delta z, \Delta t, \beta_x, \beta_y, \beta_z, \alpha_x, \alpha_y$ and α_z .

Conclusion

In this paper, three numerical methods have been used to solve a 3D advection-diffusion problem, with spatial step size, $h = 0.05$ and temporal step size, $k = 0.001$ at two different times; $T = 0.05, 0.2$. We compare $L_2, L_\infty, \text{MCR}, \text{MDR}$, Minimum and Maximum values of u using the three methods and also the corresponding exact values. We observe that as we progress in time, the maximum value of u decreases as expected as the partial differential equation has dissipative terms. Table 1 shows the errors at $h = 0.05, k = 0.001$ and $T = 0.05$. Based on L_2 and L_∞ errors, ICF is best scheme followed by FOM followed by ICN. Based on the positive definite character, ICF is best scheme out of the three methods, though it is not completely positive definite. MDR values from ICN and FOM are respectively 1.0129 and 1.0013 while this value from ICF is 0.9870. MDR is affected by mass spreading into areas of the grid that should remain free of mass, by damping of the peak concentration, by negative ripples or by diffusive events in the solution [9]. Table 2 shows errors at $h = 0.05, k = 0.001$ and $T = 0.2$. Based on L_2, L_∞ errors, MDR values, most efficient scheme is ICF followed by FOM. We conclude that in general ICF is quite an efficient method to solve the problem.

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