

Fusion Higher -Order Parallel Splitting Methods for Parabolic Partial Differential Equations

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Abstract: A family of numerical methods, based upon a rational approximation to the matrix exponential function, was developed for solving parabolic partial

differential equations. These methods were partially sixth-order precise in space and time, due to combination of sixth-order finite approximations and fifth-order pde's approximations. These methods do not involve the use of complex computation. In these methods second-order spatial derivatives were approximated by sixth-order finite difference approximations. Parallel algorithms were developed and tested on the one, two and three-dimensional heat equations, with constant coefficients, subject to homogeneous boundary conditions and time dependent boundary conditions. It was observed that the results obtained through these methods were highly accurate and can be easily coded on serial or parallel computers.

Keywords: Heat equation, Fifth order numerical methods, Higher order pde's approximations, Method of lines, Parallel algorithm

1 Introduction

Main idea behind the finite-difference methods for obtaining the approximate solution of a given PDE is to approximate the derivatives appearing in the equation by a set of values of the function at a selected number of points. The most usual way to generate these approximations is through the use of Taylor series approximation. The basis of analysis of the finite-difference equations considered here is the modified equivalent PDE approach. It is worth noting that from the truncation error of the modified equivalent equation, it is possible to eliminate the dominant error terms associated with the finite-difference equations that contain weights, thus leading to more accurate techniques. Higher dimensional parabolic initial/boundary-value problems are studied by several authors. Twizell et al. develop families of third and fourth-order methods, which do not require complex arithmetic [5], [6]. M. Dehghan starts working on the concept of parallel splitting method and apply similar techniques for the solution of parabolic and hyperbolic PDEs [3]. Borovykh, Day. W. A and S. Wang also discussed the solution of parabolic PDE but with non-local boundary conditions.

One ways of solving parabolic partial differential equations is by the use of method of lines (MOL), which transform parabolic partial differential equations into a system of ordinary differential equations which can be written in matrix-vector form as

$$\frac{dU(t)}{dt} = A U(t) + v(t) \quad (1)$$

Where A is a square matrix, $v(t)$ results from non-homogeneous boundary conditions and $U(t)$ is the solution vector at time t . Then solution $U(t)$ satisfies the recurrence relation

$$U(t + l) = \exp(lA) U(t) + \int_t^{t+l} \exp((t + l - s)A)v(s) ds; \quad t = 0, l, 2l, \dots \quad (2)$$

when boundary conditions are homogeneous, then recurrence relation takes the form

$$U(t + l) = \exp(lA) U(t); \quad t = 0, l, 2l, \dots \quad (3)$$

2 Derivation of the method

A typical problem in applied mathematics is the one-dimensional homogeneous heat equation with time dependent boundary conditions. This initial/boundary value problem is given by

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < X, \quad t > 0 \tag{4}$$

and the non-local boundary conditions

$$u(0, t) = f_1(t), \quad t > 0 \tag{5}$$

$$u(X, t) = f_2(t), \quad t > 0 \tag{6}$$

subject to the given initial condition

$$u(x, 0) = g(x), \quad 0 \leq x \leq 1 \tag{7}$$

where $g(x)$ is a given continuous function of x . There will exist discontinuities between the initial conditions and the boundary conditions if $g(0) \neq f_1(0)$ and/or $g(X) \neq f_2(0)$. Dividing the interval $[0, X]$ into $N + 1$ subintervals each of width h , so that $(N + 1)h = X$, and the time variable t into time steps each of length l gives a rectangular mesh of points with co-ordinates $(x_m, t_n) = (mh, nl)$ ($m = 0, 1, 2, \dots, N, N + 1$) and ($n = 0, 1, 2, \dots$) covering the region $R = [0 < x < X] \times t$ and its boundary ∂R consisting of the lines $x = 0$, $x = X$ and $t = 0$.

The space derivative in (4) may be approximated to the sixth-order accuracy at some general point (x, t) of the mesh by the expression

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{180 h^2} \{2u(x - 3h, t) - 27u(x - 2h, t) + 270u(x - h, t) - 490u(x, t) + 270u(x + h, t) - 27u(x + 2h, t) + 2u(x + 3h, t)\} - \frac{h^6}{560} \frac{\partial^8 u(x, t)}{\partial x^8} + O(h^7) \tag{8}$$

However, equation (8) is valid only for $(x, t) = (x_m, t_n)$ with $m = 3, 4, \dots, N - 2$ and $n = 0, 1, 2, 3, 4, \dots$. To attain the accuracy at the same points at (x_1, t_n) , (x_2, t_n) , (x_{n-1}, t_n) and (x_n, t_n) special formulas must be developed which approximate $\frac{\partial^2 u(x, t)}{\partial x^2}$ not only to sixth-order but also with dominant error term $-\frac{h^6}{560} \frac{\partial^8 u(x, t)}{\partial x^8}$. It

can be clearly shown that the desired approximations to $\frac{\partial^2 u(x, t)}{\partial x^2}$ are

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{180 h^2} \{117u(x - h, t) + 2u(x, t) - 738u(x + h, t) + 1359u(x + 2h, t) - 1300u(x + 3h, t) + 828u(x + 4h, t) - 342u(x + 5h, t) + 83u(x + 6h, t) - 9u(x + 7h, t)\} - \frac{h^6}{560} \frac{\partial^8 u(x, t)}{\partial x^8} + O(h^7) \tag{9}$$

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{180 h^2} \{-9u(x - 2h, t) + 198u(x - h, t) - 322u(x, t) + 18u(x + h, t) + 225u(x + 2h, t) - 166u(x + 3h, t) + 72u(x + 4h, t) - 18u(x + 5h, t) + 2u(x + 6h, t)\} - \frac{h^6}{560} \frac{\partial^8 u(x, t)}{\partial x^8} + O(h^7) \tag{10}$$

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{180 h^2} \{-9u(x + 2h, t) + 198u(x + h, t) - 322u(x, t) + 18u(x - h, t) + 225u(x - 2h, t) - 166u(x - 3h, t) +$$

$$72 u(x - 4h, t) - 18 u(x - 5h, t) + 2u(x - 6h, t)\} - \frac{h^6}{560} \frac{\partial^8 u(x, t)}{\partial x^8} + O(h^7) \quad (11)$$

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{180 h^2} \{117u(x + h, t) + 2 u(x, t) - 738 u(x - h, t) +$$

$$1359u(x - 2h, t) - 1300 u(x - 3h, t) + 828 u(x - 4h, t) - 342 u(x - 5h, t)$$

$$+ 83u(x - 6h, t) - 9u(x - 7h, t)\} - \frac{h^6}{560} \frac{\partial^8 u(x, t)}{\partial x^8} + O(h^7) \quad (12)$$

at the mesh points $(x_1, t_n), (x_{n-2}, t_n), (x_{n-1}, t_n)$ and (x_n, t_n) respectively. Applying (4) with (8)-(12) to the mesh points of the grid at time level $t = t_n$ produces a system of ODE's of the form

$$\frac{dU(t)}{dt} = A U(t) + v(t), \quad t > 0 \quad (13)$$

With initial distribution

$$U(0) = g \quad (14)$$

in which $U(t) = [U_1(t), U_2(t), \dots, U_N(t)]^T$, $g = [g(x_1), g(x_2), \dots, g(x_N)]^T$, T denotes transpose

$$A = \frac{1}{180 h^2} \begin{bmatrix} 2 & -738 & 1359 & -1300 & 828 & -342 & 83 & -9 & \square \\ 198 & -332 & 18 & 225 & -166 & 72 & -18 & 2 & \\ -27 & 270 & -490 & 270 & -27 & 2 & & & \\ 2 & -27 & 270 & -490 & 270 & -27 & 2 & & \\ & 2 & -27 & 270 & -490 & 270 & -27 & 2 & \\ & & & 2 & -27 & 270 & -490 & 270 & -27 & 2 \\ & & & & 2 & -27 & 270 & -490 & 270 & -27 \\ \square & 2 & -18 & 72 & -166 & 225 & 18 & -322 & 198 & \\ & \square & -9 & 83 & -342 & 828 & -1300 & 1359 & -738 & 2 \end{bmatrix}$$

(14a)

with $v(t) = \frac{1}{180 h^2} [124f_1(t), -13f_1(t), 0, \dots, 2f_2(t), 4f_2(t), -9f_2(t), 128f_2(t)]^T$ and the solution of system {(13)-(14)} satisfy the recurrence relation (2). To approximate the matrix exponential function in (2) fifth-order pde's approximation, for a real scalar θ , given by

$$E_5(\theta) = \frac{1+b_1\theta+b_2\theta^2+b_3\theta^3+b_4\theta^4}{1-a_1\theta+a_2\theta^2-a_3\theta^3+a_4\theta^4-a_5\theta^5} \quad (15)$$

where

$$a_5 = \sum_{k=1}^4 (-1)^k \frac{a_k}{(5-k)!} \quad (16)$$

and

$$b_k = \sum_{i=1}^k (-1)^i \frac{a_i}{(k-i)!}, \quad k = 0, 1, 2, 3, 4 \quad (17)$$

The integral term in (2) is approximated as

$$\int_t^{t+l} \exp((t+l-s)A)v(s) ds = W_1 v(s_1) + W_2 v(s_2) + W_3 v(s_3)$$

$$+ W_4 v(s_4) + W_5 v(s_5) \quad (18)$$

Where $s_1 \neq s_2 \neq s_3 \neq s_4 \neq s_5$ and $W_i (i = 1, 2, 3, 4, 5)$ are matrices. We have

$$\int_t^{t+l} \exp((t+l-s)A) s^{k-1} ds = \sum_{j=1}^s s_j^{k-1} W_j = M_k, \quad k = 1, 2, 3, 4, 5 \quad (19)$$

with

$$M_k = A^{-1} \{ t^{k-1} \exp(lA) - (t+l)^{k-1} I + (k-1)M_{k-1} \}, \quad k = 1, 2, 3, 4, 5 \quad (20)$$

Taking $s_1 = t, s_2 = t + \frac{l}{4}, s_3 = t + \frac{l}{2}, s_4 = t + \frac{3l}{4}, s_5 = t + l$.

Using $\theta = lA$ in (15) and taking $\exp(lA) = PQ^{-1}$, we have (11)

$$P = (I - a_1 lA + a_2 l^2 A^2 - a_3 l^3 A^3 + a_4 l^4 A^4 - a_5 l^5 A^5)^{-1} \quad (21)$$

and

$$Q = I + b_1 lA + b_2 l^2 A^2 + a_3 l^3 A^3 + a_4 l^4 A^4 \quad (22)$$

$$W_1 = \frac{l}{360} \{ 28I + (668 - 3100a_1 + 11520a_2 - 30720a_3 + 46080a_4)lA + (-21 + 100a_1 - 260a_2 + 1920a_4)l^2 A^2 + (18 - 75a_1 + 240a_2 - 540a_3 + 720a_4)l^3 A^3 \} P \quad (23)$$

$$W_2 = \frac{2l}{45} \{ 8I + (-154 + 760a_1 - 2880a_2 + 7680a_3)lA + (1 + 10a_1 - 100a_2 + 480a_3 - 1200a_4)l^2 A^2 + (-1 + 5a_1 - 20a_2 + 60a_3 - 120a_4)l^3 A^3 \} P \quad (24)$$

$$W_3 = \frac{l}{30} \{ 4I + (322 - 1540a_1 + 570a_2 - 15360a_3 + 23040a_4)lA + (23 - 130a_1 + 580a_2 - 1920a_3 + 3840a_4)l^2 A^2 + (3 - 15a_1 + 60a_2 - 180a_3 + 360a_4)l^3 A^3 \} P \quad (25)$$

$$W_4 = \frac{2l}{45} \{ 8I + (-158 + 760a_1 - 2880a_2 + 7680a_3 - 11520a_4)lA + (-21 + 110a_1 - 460a_2 + 1440a_3 - 2640a_4)l^2 A^2 + (-3 + 15a_1 - 60a_2 + 180a_3 - 360a_4)l^3 A^3 \} P \quad (26)$$

$$W_5 = \frac{l}{360} \{ 28I + (640 - 3100a_1 + 11520a_2 - 30720a_3 + 46080a_4)lA + (125 - 640a_1 + 2620a_2 - 7680a_3 + 13440a_4)l^2 A^2 + (25 - 125a_1 + 500a_2 - 1500a_3 + 2640a_4)l^3 A^3 + (3 - 15a_1 + 60a_2 - 180a_3 + 360a_4)l^4 A^4 \} P \quad (27)$$

Algorithm

Assuming that $r_1, r_2, r_3, r_4, r_5 (r_i \neq 0)$ are real distinct zeros of $Q(\theta)$, the denominator of $E_5(\theta)$, then

$$P^{-1} = \prod_{i=1}^5 (I - \frac{l}{r_i} A) \quad (28)$$

$$\exp(lA) = p_j \sum_{j=1}^5 (I - \frac{l}{r_i} A)^{-1} \quad (29)$$

where

$$p_j = \frac{1}{\prod_{\substack{i=1 \\ i \neq j}}^5 (1 - \frac{r_j}{r_i})} \{ 1 + b_1 r_j + b_2 r_j^2 + b_3 r_j^3 + b_4 r_j^4 \}$$

$j = 1, 2, 3, 4, 5$ and

$$p_{j+5} = \frac{1}{\prod_{\substack{i=1 \\ i \neq j}}^5 (1 - \frac{r_j}{r_i})} \times$$

$$\{28 + (668 - 3100a_1 + 11520a_2 - 30720a_3 + 46080a_4)r_j + (-21 + 100a_1 - 260a_2 + 1920a_4)r_j^2 + (18 - 75a_1 + 240a_2 - 540a_3 + 720a_4)r_j^3\}$$

$$p_{j+10} = \frac{1}{\prod_{\substack{i=1 \\ i \neq j}}^5 (1 - \frac{r_j}{r_i})} \times$$

$$\{8 + (-154 + 760a_1 - 2880a_2 + 7680a_3 - 11520a_4)r_j + (1 + 10a_1 - 100a_2 + 480a_3 - 1200a_4)r_j^2 + (-1 + 5a_1 - 20a_2 + 60a_3 - 120a_4)r_j^3\}$$

$$p_{j+15} = \frac{1}{\prod_{\substack{i=1 \\ i \neq j}}^5 (1 - \frac{r_j}{r_i})} \times$$

$$\{4 + (322 - 1540a_1 + 570a_2 - 15360a_3 + 23040a_4)r_j + (23 - 130a_1 + 580a_2 - 1920a_3 + 3840a_4)r_j^2 + (3 - 15a_1 + 60a_2 - 180a_3 + 360a_4)r_j^3\}$$

$$p_{j+20} = \frac{1}{\prod_{\substack{i=1 \\ i \neq j}}^5 (1 - \frac{r_j}{r_i})} \times$$

$$\{8 + (-158 + 760a_1 - 2880a_2 + 7680a_3 - 11520a_4)r_j + (-21 + 110a_1 - 460a_2 + 1440a_3 - 2640a_4)r_j^2 + (-3 + 15a_1 - 60a_2 + 180a_3 - 360a_4)r_j^3\}$$

$$p_{j+25} = \frac{1}{\prod_{\substack{i=1 \\ i \neq j}}^5 (1 - \frac{r_j}{r_i})} \times$$

$$\{28 + (640 - 3100a_1 + 11520a_2 - 30720a_3 + 46080a_4)r_j + (125 - 640a_1 + 2620a_2 - 7680a_3 + 13440a_4)r_j^2 + (25 - 125a_1 + 500a_2 - 1500a_3 + 2640a_4)r_j^3 + (3 - 15a_1 + 60a_2 - 180a_3 + 360a_4)r_j^4\}$$

Hence equation (14) becomes

$$U(t+l) = \sum_{i=1}^5 A_i^{-1} \left[p_i U(t) + \frac{l}{360} \left\{ \begin{aligned} & p_{i+5} v(t) + 16p_{i+10} v\left(t + \frac{l}{4}\right) + 12p_{i+15} v\left(t + \frac{l}{2}\right) \\ & + 16p_{i+20} v\left(t + \frac{3l}{4}\right) + p_{i+25} v(t+l) \end{aligned} \right\} \right]$$

where

$$A_i = I - \frac{l}{r_i} A_i, i = 1,2,3,4,5$$

Hence

$$U(t+l) = \sum_{i=1}^5 y_i(t)$$

where $y_i, i = 1,2,3,4,5$ are the solutions of the systems

$$A_i y_i = p_i U(t) + \frac{l}{360} \left\{ \begin{array}{l} p_{i+5} v(t) + 16p_{i+10} v\left(t + \frac{l}{4}\right) + 12p_{i+15} v\left(t + \frac{l}{2}\right) \\ + 16p_{i+20} v\left(t + \frac{3l}{4}\right) + p_{i+25} v(t+l) \end{array} \right\}$$

2 Extension to two-space dimension

The above method cannot be extended to two/three-space dimensions with time-dependent boundary conditions. Consider the two-dimensional heat equation with constant coefficients

$$\frac{\partial u(x,y,t)}{\partial t} = \frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2}, \quad 0 < x, y < X, \quad t > 0 \tag{30}$$

subject to the given initial condition

$$u(x, y, 0) = g(x, y), \quad 0 \leq x \leq X \tag{31}$$

where $g(x, y)$ is some continuous function of x and y and the boundary conditions

$$u(0, y, t) = u(X, y, t) = 0, \quad t > 0 \tag{32}$$

$$u(x, 0, t) = u(x, X, t) = 0, \quad t > 0 \tag{33}$$

Discretizing $0 \leq x, y \leq X$ as in the one-dimensional case using equal space steps and replacing the space derivatives in the PDE (30) by the appropriate fifth-order approximations and applying to all N^2 -interior mesh points at time level $t = nl$ ($n = 0, 1, 2, 3, \dots$) gives a system of N^2 first-order differential equations which may be written in matrix-vector form as

$$\frac{dU(t)}{dt} = B U(t), \quad t > 0 \tag{34}$$

With initial distribution

$$U(0) = g \tag{35}$$

In which

$$U(t) = [U_{1,1}(t), U_{2,1}(t), U_{3,1}(t), \dots, U_{N,1}(t), \dots, U_{1,N}(t), U_{2,N}(t), \dots, U_{N,N}(t)]^T,$$

$$g = [g_{1,1}, g_{2,1}, g_{3,1}, \dots, g_{N,1}, \dots, g_{1,N}, g_{2,N}, \dots, g_{N,N}]^T, \quad T \text{ denoting the transpose,}$$

the matrix B is the sum of two square matrices B_1 and B_2 of order N^2 , given by

$$B_1 = \frac{1}{180h^2} \begin{bmatrix} 180h^2 A & & & \\ & 180h^2 A & & \\ & & \ddots & \\ & & & 180h^2 A \end{bmatrix}_{N^2 \times N^2}$$

Where matrix A is given by (14a) and



$$B_2 = \frac{1}{180h^2} \begin{bmatrix} 2I & -738I & 1359I & -1300I & 828I & -342I & 83I & -9I & \square \\ 198I & -332I & 18I & 225I & -166I & 72I & -18I & 2I & \\ -27I & 270I & -490I & 270I & -27I & 2I & & & \\ 2I & -27I & 270I & -490I & 270I & -27I & 2I & & \\ & 2I & -27I & 270I & -490I & 270I & -27I & 2I & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & 2I & -27I & 270I & -490I & 270I & -27I & 2I \\ & & & & 2I & -27I & 270I & -490I & 270I & -27I \\ & 2I & -18I & 72I & -166I & 225I & 18I & -322I & 198I & \\ \square & -9I & 83I & -342I & 828I & -1300I & 1359I & -738I & 2I & \end{bmatrix}$$

Where I is identity matrix of order N and the solution of system (34), (35) satisfies the recurrence relation (3) Clearly B_1 and B_2 commute. □

Development of Algorithm

Since $B = B_1 + B_2$, replacing A by B in equation (3) gives
 $U(t + l) = \exp(lB_1) \exp(lB_2) U(t), \quad t = 1,2,3, \dots$ (36)
 to the fifth order. Using (29) in (36) gives

$$U(t + l) = \left(p_j \sum_{j=1}^5 (I - \frac{l}{r_i} B_1)^{-1} \right) \left(p_j \sum_{j=1}^5 (I - \frac{l}{r_i} B_2)^{-1} \right) U(t) \quad (37)$$

Let

$$z_i(t) = p_j \sum_{j=1}^5 (I - \frac{l}{r_i} B_1)^{-1} U(t), \quad i = 1,2,3,4,5 \quad (38)$$

Then the linear systems

$$\left(I - \frac{l}{r_i} B_2 \right) z_i(t) = p_i U(t) \quad i = 1,2,3,4,5 \quad (39)$$

can be solved for vectors $z_i (i = 1,2,3,4,5)$ of order N^2 of five different process simultaneously. Assuming that

$$Z(t) = \sum_{i=1}^5 z_i(t) \quad (40)$$

Equation (37) can be written as

$$U(t + l) = \left(p_j \sum_{i=1}^5 (I - \frac{l}{r_i} B_1)^{-1} \right) Z(t)$$

or

$$U(t + l) = \sum_{j=1}^5 w_i(t) \quad (41)$$

in which $w_i (i = 1,2,3,4,5)$, the solution of linear systems

$$\left(I - \frac{l}{r_i} B_1 \right) w_i(t) = p_i Z(t), \quad (i = 1,2,3,4,5) \quad (42)$$

can be computed on five different processors simultaneously.

Tabular form of algorithm

Steps	Processors ($i = 1,2,3,4,5$)
1= input	l, B_1, B_2, U_0, r_i
2= compute	$p_i, \left(I - \frac{l}{r_i} B_1\right), \left(I - \frac{l}{r_i} B_2\right)$
3=Decompose	$I - \frac{l}{r_i} B_1 = L_i U_i, \quad I - \frac{l}{r_i} B_2 = P_i Q_i$
4= Solve	$P_i Q_i z_i(t) = p_i U(t)$
5= Calculate	$Z(t) = \sum_{j=1}^5 z_j(t)$
6=Solve	$L_i U_i w_i(t) = p_i Z(t)$
7= Calculate	$U(t + l) = \sum_{j=1}^5 w_j(t)$
	Go to Step 4 for next time step

3 Extension to three- space dimension

Consider the three-dimensional heat equation with constant coefficients

$$\frac{\partial u(x,y,z,t)}{\partial t} = \frac{\partial^2 u(x,y,z,t)}{\partial x^2} + \frac{\partial^2 u(x,y,z,t)}{\partial y^2} + \frac{\partial^2 u(x,y,z,t)}{\partial z^2}, \quad 0 < x, y, z < X, \quad t > 0 \quad (43)$$

subject to the given initial condition

$$u(x, y, z, 0) = g(x, y, z), \quad 0 \leq x, y, z \leq X \quad (44)$$

where $g(x, y, z)$ is some continuous function of x, y and z and the boundary conditions

$$u(0, y, z, t) = u(X, y, z, t) = 0, \quad 0 \leq y, z \leq X, \quad t > 0 \quad (45)$$

$$u(x, 0, z, t) = u(x, X, z, t) = 0, \quad 0 \leq x, z \leq X, \quad t > 0 \quad (46)$$

$$u(x, y, 0, t) = u(x, y, X, t) = 0, \quad 0 \leq x, y \leq X, \quad t > 0 \quad (47)$$

Discretizing $0 \leq x, y, z \leq X$ as in the one-dimensional case and replacing the space derivatives in the PDE (43) by the appropriate sixth-order approximations and applying to all N^3 -interior mesh points at time level $t = nl$ ($n = 0,1,2,3, \dots$) gives a system of N^3 first-order differential equations which may be written in matrix-vector form as

$$\frac{dU(t)}{dt} = C U(t), \quad t > 0 \quad (48)$$

With initial distribution

$$U(0) = g \quad (49)$$

In which

$U(t) = [U_{1,1,1}(t), U_{2,1,1}(t), U_{3,1,1}(t), \dots, U_{N,1,1}(t), U_{1,2,1}(t), U_{2,2,1}(t), \dots, U_{N,N,N}(t)]^T$,
 $g = [g_{1,1,1}, g_{2,1,1}, g_{3,1,1}, \dots, g_{N,1,1}, g_{1,2,1}, g_{2,2,1}, \dots, g_{N,N,N}]^T$, T denoting the transpose, the matrix C is the sum of three square matrices C_1, C_2 and C_3 of order N^3 , given by

$$C_1 = \frac{1}{180h^2} \begin{bmatrix} 180h^2 A & & & & \\ & 180h^2 A & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 180h^2 A \end{bmatrix}_{N^3 \times N^3}$$

Where matrix A is given by (14a) and is a block diagonal matrix with N^2 diagonal blocks. □

$$C_2 = \frac{1}{180h^2} \begin{bmatrix} 180h^2 B_2 & & & & \\ & 180h^2 B_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 180h^2 B_2 \end{bmatrix}_{N^3 \times N^3}$$

Where B_2 is a block-diagonal matrix with N diagonal blocks and □

$$C_3 = \frac{1}{180h^2} \begin{bmatrix} 2I^* & -738I^* & 1359I^* & -1300I^* & 828I^* & -342I^* & 83I^* & -9I^* & \square \\ 198I^* & -332I^* & 18I^* & 225I^* & -166I^* & 72I^* & -18I^* & 2I^* & \\ -27I^* & 270I^* & -490I^* & 270I^* & -27I^* & 2I^* & & & \\ 2I^* & -27I^* & 270I^* & -490I^* & 270I^* & -27I^* & 2I^* & & \\ & 2I^* & -27I^* & 270I^* & -490I^* & 270I^* & -27I^* & 2I^* & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & 2I^* & -27I^* & 270I^* & -490I^* & 270I^* & -27I^* & 2I^* \\ & & & & 2I^* & -27I^* & 270I^* & -490I^* & 270I^* & -27I^* \\ \square & & 2I^* & -18I^* & 72I^* & -166I^* & 225I^* & 18I^* & -322I^* & 198I^* \\ & & -9I^* & 83I^* & -342I^* & 828I^* & -1300I^* & 1359I^* & -738I^* & 2I^* \end{bmatrix}$$

Where I^* is the identity matrix of order N^2 . □

Development of Algorithm

Since $C = C_1 + C_2 + C_3$, replacing A by C in equation (3) gives $U(t+l) = \exp(lC_1) \exp(lC_2) \exp(lC_3) U(t), \quad t = 1,2,3, \dots$ (50)

So $\exp(lC) = \sum_{j=1}^5 p_j (I - \frac{l}{r_i} A)^{-1}$ (51)

and $U(t+l) = (p_j \sum_{j=1}^5 (I - \frac{l}{r_i} C_1)^{-1}) (p_j \sum_{j=1}^5 (I - \frac{l}{r_i} C_2)^{-1}) (p_j \sum_{j=1}^5 (I - \frac{l}{r_i} C_3)^{-1}) U(t)$ (52)

Let $z_i(t) = p_j (I - \frac{l}{r_i} C_3)^{-1} U(t), \quad i = 1,2,3,4,5$ (53)

Then solving the linear systems

$$\left(I - \frac{l}{r_i} C_3\right) z_i(t) = p_i U(t), \quad i = 1,2,3,4,5 \quad (54)$$

for $z_i(i = 1,2,3,4,5)$

$$U(t + l) = \sum_{i=1}^5 p_j \left(I - \frac{l}{r_i} C_1\right)^{-1} p_j \left(I - \frac{l}{r_i} C_2\right)^{-1} Z(t) \quad (55)$$

where

$$Z(t) = \sum_{j=1}^5 z_j(t) \quad (56)$$

Let

$$y_i(t) = p_i \left(I - \frac{l}{r_i} C_2\right)^{-1} Z(t), \quad (i = 1,2,3,4,5) \quad (57)$$

then the solution of the linear system

$$\left(I - \frac{l}{r_i} C_2\right) y_i(t) = p_i Z(t), \quad (i = 1,2,3,4,5) \quad (58)$$

Gives

$$Y(t) = \sum_{j=1}^5 y_j(t) \quad (59)$$

Then

$$U(t + l) = \sum_{j=1}^5 w_j(t) \quad (60)$$

In which $w_j(i = 1,2,3,4,5)$ are the solution of the linear systems

$$\left(I - \frac{l}{r_i} C_1\right) w_i(t) = p_i Y(t), \quad (i = 1,2,3,4,5) \quad (61)$$

The algorithm used here is given in tabular form as

Tabular form of algorithm

Steps	Processors $(i = 1,2,3,4,5)$
1= input	$l, C_1, C_2, C_3, U_0, r_i$
2= compute	$p_i, \left(I - \frac{l}{r_i} C_1\right), \left(I - \frac{l}{r_i} C_2\right), \left(I - \frac{l}{r_i} C_3\right)$
3=Decompose	$I - \frac{l}{r_i} C_1 = L_i U_i, I - \frac{l}{r_i} C_2 = F_i G_i, I - \frac{l}{r_i} C_3 = P_i Q_i$
4= Solve	$P_i Q_i z_i(t) = p_i U(t)$
5= Calculate	$Z(t) = \sum_{j=1}^5 z_j(t)$
6=Solve	$F_i G_i y_i(t) = p_i Z(t)$
7= Calculate	$Y(t) = \sum_{j=1}^5 y_j(t)$
8= Solve	$L_i U_i w_i(t) = p_i Y(t)$
9= Calculate	$U(t + l) = \sum_{j=1}^5 w_j(t)$
	Go to Step 4 for next time step

4 Numerical experiments

Using above given algorithms these problem are solved for different values of $N \geq 9$ and l . In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq X$ and no oscillations are observed. Now the developed numerical methods were applied to different problems from the literature by taking

$$a_1 = 4.5500, a_2 = 4.0083, a_3 = 1.3375, a_4 = 1.9194e - 001, \\ a_5 = 1.0000e - 002, r_1 = 6.6385, r_2 = 5.4014, r_3 = 4.8497, \\ r_4 = 2.0202, r_5 = 2.8466e - 001$$

Example 1 (One-dimensional Problem)

Consider the Second order PDE problem (1) with $X = 1$, $f_1(t) = 0$, $f_2(t) = \exp(-\frac{\pi^2}{4}t)$ and $g(x) = \sin(\frac{\pi}{2}x)$. This problem which has analytical solution

$$u(x, t) = \exp(-\frac{\pi^2}{4}t) \sin(\frac{\pi}{2}x)$$

has a time-dependent boundary condition but does not have discontinuities between the initial conditions and boundary conditions. The maximum value of the analytical solution of this problem at time $t = 1.0$ occurs for $x = 1.0$ and is approximately $8.418664873971583e - 002$

Example 2 (One-dimensional Problem)

Consider the Second order PDE problem with $X = 1$, $f_1(t) = t$, $f_2(t) = 0$ and $g(x) = 1$. This problem which has analytical solution

$$u(x, t) = (1 - x)t - \frac{1}{6}(x^3 - 3x^2 + 2x) \\ + \sum_{n=1}^{\infty} 2 \left\{ 1 - (-1)^n + \frac{1}{n^2\pi^2} \right\} \exp\left(\frac{-n^2\pi^2 t \sin(n\pi x)}{n\pi}\right)$$

has discontinuities between the initial conditions and boundary conditions at $x = 0$ and $x = 1$. The maximum value of the analytical solution of this problem at $t = 1.0$ occurs for $x = 0$ and is $9.003351750986498e - 001$

Example 3 (One-dimensional Problem)

Consider the Second order PDE problem with $X = 2$, $f_1(t) = 0$, $f_2(t) = 0$ and $g(x) = 1$. This problem which has analytical solution

$$u(x, t) = \sum_{n=1}^{\infty} \{1 - (-1)^k\} \frac{2}{k\pi} \sin\left(\frac{k\pi x}{2}\right) \exp\left(\frac{-k^2\pi^2 t}{4}\right)$$

has discontinuities between the initial conditions and boundary conditions at $x = 0$ and $x = 2$. The maximum value of the analytical solution of this problem at $t = 1.0$ is $1.071897702241022e-001$

Example 4 (Two-dimensional Problem)

Consider the two space dimensional heat equation with constant coefficients with $X = 2$ and $g(x, y) = \sin(\frac{\pi}{2}y)$ the model problem has theoretical solution

$$u(x, y, t) = \sin\left(\frac{\pi}{2}y\right) \sum_{n=1}^{\infty} \{1 - (-1)^k\} \frac{2}{k\pi} \sin\left(\frac{k\pi x}{2}\right) \exp\left(\frac{-(k^2 + 1)\pi^2 t}{4}\right)$$

The maximum value of the analytic solution occurs at $t = 1.0$ for $(x, y) = (1, 1)$ and is approximately $9.156990281594897e - 003$

Example 5 (Three-dimensional Problem)

Consider the three space dimensional heat equation with constant coefficients with $X = 2$ and $g(x, y, z) = \sin\left(\frac{\pi}{2}x\right) \sin\left(\frac{\pi}{2}y\right) \sin\left(\frac{\pi}{2}z\right)$ the model problem has theoretical solution

$$u(x, y, z, t) = \sin\left(\frac{\pi}{2}x\right) \sin\left(\frac{\pi}{2}y\right) \sin\left(\frac{\pi}{2}z\right) \exp\left(\frac{-3\pi^2t}{4}\right)$$

The maximum value of the analytic solution occurs at $t = 0.1$ for $(x, y, z) = (1, 1, 1)$ and is approximately $4.770088045530259e - 001$

5 Conclusion

It is observed that the results obtained using new scheme are highly accurate and the method developed is fifth-order accurate in space and time. This technique can be coded easily on serial or parallel computers. It is worth mentioning that the methods using real arithmetic and multiprocessor architecture especially in multi-dimensional problems will save remarkable CPU time rather than the complex arithmetic based methods.

Table 1. Maximum absolute error for Example 1

N	9	10	11	12
$l = 0.1$	1.0639e-007	1.0730e-007	1.0666e-007	1.0702e-007
$l = 0.05$	6.3776e-009	6.1424e-009	5.9921e-009	5.9214e-009
$l = 0.0125$	6.3226e-010	3.5483e-010	2.1615e-010	1.3754e-010
$l = 0.01$	6.2462e-010	3.4733e-010	2.0866e-010	1.3005e-010

Table 2. Maximum absolute error for Example 2

N	9	10	11	12
$l = 0.1$	9.6619e-007	9.0298e-007	9.4470e-007	9.1731e-007
$l = 0.05$	4.3550e-008	4.2881e-008	4.3204e-008	4.2821e-008
$l = 0.0125$	6.2747e-010	3.9542e-010	2.8125e-010	2.1149e-010
$l = 0.01$	5.7169e-010	3.4071e-010	2.2636e-010	1.5670e-010

Table 3. Maximum absolute error for Example 3

N	9	10	11	12
$l = 0.1$	8.6519e-007	8.2892e-007	8.4009e-007	8.2871e-007
$l = 0.05$	9.7619e-008	6.2673e-008	4.5581e-008	3.6804e-008
$l = 0.0125$	6.4374e-008	2.9766e-008	1.4691e-008	8.8700e-009
$l = 0.01$	6.4347e-008	2.9738e-008	1.4698e-008	8.8766e-009

N	9	10	11	12
$l = 0.1$	1.6480e-007	1.4939e-007	1.4760e-007	1.4205e-007
$l = 0.05$	3.4890e-008	2.1569e-008	1.5399e-008	1.1505e-008
$l = 0.0125$	2.9251e-008	1.6044e-008	9.7598e-009	5.9483e-009
$l = 0.01$	2.9246e-008	1.6039e-008	9.7550e-009	5.9436e-009

N	9	10	11	12
$l = 0.1$	1.6346e-006	1.3369e-006	1.2495e-006	1.1504e-006
$l = 0.05$	6.1743e-007	3.5207e-007	2.3545e-007	1.5880e-007
$l = 0.0125$	5.7276e-007	3.0913e-007	1.9120e-007	1.1562e-007
$l = 0.01$	5.7272e-007	3.0910e-007	1.9117e-007	1.1558e-007

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