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2nd Order Parallel Splitting Methods for Heat Equation

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Abstract

In this paper, heat equation in two dimensions with non local boundary condition is solved numerically by 2nd order parallel splitting technique. This technique used to approximate spatial derivative and a matrix exponential function is replaced by a rational approximation. Simpson's 1/3 rule is also used to approximate the non local boundary condition. The results of numerical experiments are checked and compared with the exact solution, as well as with the results already existed in the literature and found to be highly accurate.

Keywords: heat equation, 2nd order numerical methods, method of lines, parallel algorithm

Introduction

Several authors have been studied the initial- boundary-value problems (pdes). These equations are mathematical models for real world phenomena which often take the form of equation relating to various quantities and their derivatives. The motion of particle in the straight line, motion of a missile (projectile motion), function of a nuclear reactor, transfer of heat, vibration of a particle and chemical reaction etc. All such problems are governed by elliptic, hyperbolic or parabolic partial differential equations which may or may not be homogenous, in one, two or three dimensions with non local boundary conditions, along with initial conditions existing in the literature. In real life problems, parabolic equations with an integral boundary condition(s) have wide applications, and some time we are required only their numerical solutions. The concentration of a chemical reaction conveniently by employing absorption of light at suitable frequencies. The summation property of electronic and limited availability of light beam, the computational process of used chemical gives rise to quadrature of concentration in spatial region from which the light beam pass through is described by a parabolic equation. We can also use this method for smoothening of data and to calculate time integral of spatial term computation data relating to kinetic rates of chemical reaction. Thus parabolic partial differential equations with nonlocal boundary condition(s) have great impact in diverse fields such as electrochemistry, heat transition, biological and medical sciences and population dynamics. Mostly authors used explicit or Crank-Nikolson finite difference schemes for the numerical solution of these partial differential equations. In 1994

B. J. Noye. et al. have worked out a numerical scheme for the solution of heat equation along with initial condition, boundary conditions and non-local boundary specifications and they used sufficiently smooth data which satisfy the required compatibility conditions in the scheme. They used two different explicit schemes of finite difference which is of second order but for $S = \frac{1}{6}$ this scheme is of fourth order. They have employed the well-known two finite difference scheme 1st is [1], [5] FTCS and 2nd is [1], [9] FTCS, and the integral was approximated by Simpson's 1/3 rule to solve the heat equation. He reduced the time consumed 4330.7 sec to 410.3 sec as well as the results were much better than the previous results existing in the literature [2].

The same problem was also discussed by A.B. Gumel. et al.. They replaced the space derivative by central difference approximants of 2nd order and approximated the quadrature existing in the recurrence relation by the Trapezoidal rule [3] and the matrix exponential in the recurrence relation by Pade's approximant [4]. They suggested a different scheme to solve the heat equation. [3] used the method of line semi discretization and transformed model PDE into the system of linear, 1st order ODE's, and this system of ODE's satisfied a certain recurrence relation. In solution of ODE a matrix exponential term was produced which was approximated with pade approximation, and for unknown $\omega(t)$, he used Trapezoidal rule. [3] also presented the result in relative error form and compared with [1], [5] FTCS explicit method . Yunkang Liu worked on heat equation in one dimension with non local boundary conditions. Several authors have discussed PDE's in one dimension as well as in two dimensions with non local boundary conditions [5]. In 1996 Twizell and Taj introduced a new rational approximation to the matrix exponential function, which creates while solving parabolic partial differential equations. In 1997 Taj and Twizell extends their work to fourth-order parallel splitting methods having all properties as in the third order but with much better error of approximation as compared to previous results. These methods do not require any complex arithmetics and are third-order accurate in space and time as well as L-acceptable, tested and found more accurate than the results existing in the literature [9]-[10]. In 2003 Mehdi Dehghan started working on the theory of parallel splitting method and applied this technique for the solution of hyperbolic and parabolic PDEs. Most of his effort appeared from 2003 to 2005 and he used different methods to get a hold for approximate solutions of the heat equation [8]. In 2008 Jurgen Geiser applied fourth order parallel splitting method for the solution of heat equation by using ADI (Alternating Direction Implicit) methods and LOD (Locally One-Dimensional) methods, which are standard splitting methods of lower order, e.g. second order. He extended this second order to fourth order based on locally higher-order LOD methods. In 2007 the heat equation with boundary integral

specification and mixed order parallel splitting method was discussed by M. A. Rehman. For the numerical solution of non classical PDEs, S. Ali Mardan and M. A. Rehman have introduced a hydride method.

We shall use Simpson's 1/3 rule for approximating the integral condition i.e. non-local boundary condition. One way 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

$$\frac{dU(t)}{dt} = BU(t) + \varphi(t) \quad (1)$$

Where B is a square matrix, $\varphi(t)$ results from non-homogeneous boundary conditions and $U(t)$ is the solution vector at time t .

Development of the Method

Consider two-dimensional heat equation

$$\frac{\partial u(x, y, t)}{\partial t} = \frac{\partial^2 u(x, y, t)}{\partial x^2} + \frac{\partial^2 u(x, y, t)}{\partial y^2}, \quad 0 < x, y < 1, t > 0 \quad (2)$$

Subject to the given initial condition

$$u(x, y, 0) = g(x, y), \quad 0 \leq x, y \leq 1 \quad (3)$$

and the boundary conditions

$$u(0, y, t) = f_0(y, t), \quad t > 0 \quad (4)$$

$$u(1, y, t) = f_1(y, t), \quad t > 0 \quad (5)$$

$$u(x, 1, t) = g_1(x, t), \quad t > 0 \quad (6)$$

$$u(x, 0, t) = g_0(x)\omega(t), \quad t > 0 \quad (7)$$

With nonlocal boundary condition

$$\iint_{00}^{11} u(x, y, t) dx dy = \mu(t) \quad 0 \leq x, y \leq 1 \quad (8)$$

Where

$$f_0(y, t), f_1(y, t), g_0(x, t), g_1(x, t) \text{ and}$$

$\mu(t)$ are functions which are continuous and known, where as u and ω are the unknown functions to be determined.

Discretization

The intervals $0 \leq x \leq 1$ and $0 \leq y \leq 1$ are divided into $N + 1$ subintervals of equal length h and $h = \frac{1}{N+1}$ and t is the time variable and length of each time step is equal and is l , and occupying space $R = [0 < x < 1] \times [0 < y < 1] \times [t > 0]$ gives a cuboidal mesh of cuboids of equal volume $h^2 \times l$ and the co-ordinates of

vertices of each cuboids are $(x_m, y_m, t_n) = (mh, mh, nl)$ where $m = 0, 1, 2, 3, \dots, N + 1$ and $n = 0, 1, 2, 3, \dots$. The boundary ∂R of whole space is consisting of lines $x = 0, x = 1, y = 0, y = 1$ and $t = 0$.

Derivation

The space derivative $\frac{\partial^2 u(x,y,t)}{\partial x^2}$ and $\frac{\partial^2 u(x,y,t)}{\partial y^2}$, are approximated as under

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} = \frac{1}{h^2} \{u(x-h, y, t) - 2u(x, t) + u(x+h, y, t)\} + O(h^3) \quad (9)$$

and

$$\frac{\partial^2 u(x,y,t)}{\partial y^2} = \frac{1}{h^2} \{u(x, y-h, t) - 2u(x, t) + u(x, y+h, t)\} + O(h^3) \quad (10)$$

Applying these approximations to the each mesh points of the grid, at time level $t = t_n$, we get a system of N^2 first-order ordinary differential equations. This may be written in matrix form as

$$\frac{dU(t)}{dt} = BU(t) + \varphi(t), \quad t > 0$$

With initial distribution

$$U(0) = g(x, y)$$

The matrix B is the sum of two square matrices B_1 and B_2 of order N^2 .

$$B_1 = \frac{1}{h^2} \begin{bmatrix} h^2 A & & & O \\ & h^2 A & & \\ & \ddots & \ddots & \ddots \\ & & & h^2 A \\ O & & & & h^2 A \end{bmatrix}$$

where A is given by

$$A = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & & & O \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ O & & & & 1 & -2 \end{bmatrix}$$

and

$$B_2 = \frac{1}{h^2} \begin{bmatrix} -2I & I & & O \\ I & -2I & I & \\ & \ddots & \ddots & \ddots \\ & & I & -2I & I \\ O & & & I & -2I \end{bmatrix}$$

Where both B_1 and B_2 are of order $N^2 \times N^2$ and I is the identity matrix of order N . The vector $\varphi(t)$, sum of two vectors $\varphi_1(t)$ and $\varphi_2(t)$ of order $N^2 \times 1$ arises from the use of the boundary conditions in above two approximation.

Then solution $U(t)$ satisfies the recurrence relation

$$U(t + l) = \exp(lB) U(t) + \int_t^{t+l} \exp((t + l - s)B) \varphi(s) ds; \quad t = 0, l, 2l, \dots$$

Where l is constant time step in the descretization. To approximate the matrix exponential function in a new rational approximate, for a real scalar θ , given by

$$E_2(\theta) = \frac{1 + (1 - a)\theta +}{1 - a\theta + (a - \frac{1}{2})\theta^2}$$

The unknown U^n will be ordered in the form

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

$$g = [g_{1,1}, g_{2,1}, g_{3,1}, \dots, g_{N,1}, \dots, g_{1,N}, g_{2,N}, \dots, g_{N,N}]^T,$$

and the solution of system satisfy the recurrence relation (2). Where

$$\int_t^{t+l} \exp((t + l - s)B) \varphi(s) ds = W_1 \varphi(s_1) + W_2 \varphi(s_2)$$

Where $s_1 \neq s_2$ and weights $W_i (i = 1, 2, \dots)$ are matrices. It can easily be shown that when

$$\varphi(s) = [1, 1, 1, \dots, 1]^T, \text{ then}$$

$$W_1 + W_2 = M_1$$

where

$$M_1 = \{B^{-1}(\exp(lB) - I)\}$$

and when

$$\varphi(s) = [s, s, s, \dots, s]^T, \text{ then}$$

$$S_1 W_1 + S_2 W_2 = M_2$$

where $M_2 = B^{-1} \{t \exp(lB) - (t+l)I + B^{-1}(\exp(lB) - I)\}$

$$\text{Using } \theta = lB \text{ in } E_2(\theta) = \frac{1+(1-\alpha)\theta + \exp(lB) = PQ \text{ we have}}{1-\alpha\theta + (\alpha - \frac{1}{2})\theta^2}$$

$$P(lB) = (I - \alpha lB + ((\alpha - \frac{1}{2})l^2 B^2)^{-1}$$

and

$$Q(lB) = I + (1 - \alpha)lB$$

Taking $s_1 = t, s_2 = t + l$
and then solving and replacing by $\exp(lB)$ gives

$$U(t+l) = \exp(lB)U(t) + \frac{l}{2} [G(lB)\varphi(t) + K(lB)\varphi(t+l)]; t = 0, l, 2l, \dots$$

$$\text{In which, } G(lB) = \left[I - \alpha lB + (\alpha - \frac{1}{2})(lB)^2 \right]^{-1}$$

And

$$K(lB) = \left[I - \alpha lB + (\alpha - \frac{1}{2})(lB)^2 \right]^{-1} \left[I - 2(\alpha - \frac{1}{2})lB \right]$$

Parallel Algorithm

In parallel Algorithm $\exp(lB)$, $G(lB)$ and (lB) are decomposed in their partial fraction form given below

$$\exp(lB) = \sum_{i=1}^2 q_i (I - \lambda_i lB)^{-1}$$

Where

$$q_1 = \frac{1 - \alpha + \lambda_1}{\lambda_1 - \lambda_2}, q_2 = \frac{1 - \alpha + \lambda_2}{\lambda_2 - \lambda_1}$$

and

$$G(lB) = \sum_{i=1}^2 q_{i+2} (I - \lambda_i lB)^{-1}$$

Where

$$q_3 = \frac{\lambda_1}{\lambda_1 - \lambda_2}, q_4 = \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

$$K(lB) = \sum_{i=1}^2 q_{i+4} (I - \lambda_i lB)^{-1}$$

where

$$q_5 = \frac{1-2\alpha + \lambda_1}{\lambda_1 - \lambda_2}, q_6 = \frac{1-2\alpha + \lambda_2}{\lambda_2 - \lambda_1}$$

Where λ_1 and λ_2 are given below

$$\lambda_1 = \frac{2\alpha - 1}{\alpha + \sqrt{\alpha^2 - 4\alpha + 2}}$$

and

$$\lambda_2 = \frac{2\alpha - 1}{\alpha - \sqrt{\alpha^2 - 4\alpha + 2}}$$

Hence equation

$$U(t+l) = \exp(lB)U(t) + \frac{l}{2}[G(lB)\varphi(t) + K(lB)\varphi(t+l)]; t = 0, l, 2l, \dots$$

become

$$U(t+l) = \sum_{i=1}^2 A_i^{-1}(q_i U(t) + \frac{l}{2}(q_{i+2}\varphi(t) + q_{i+4}\varphi(t+l)))$$

Where

$$A_i = (I - \lambda_i l B)^{-1}, i = 1, 2$$

Hence

$$U(t+l) = \sum_{i=1}^2 y_i(t)$$

Where y_i are the solutions of the system.

$$A_i y_i = q_i U(t) + \frac{l}{2}\{q_{i+2}\varphi(t) + q_{i+4}\varphi(t+l)\}$$

Numerical Experiment

$$u(x, y, t) = e^{x+y}$$

$$u(0, y, t) = e^{y+2t}$$

$$u(1, y, t) = e^{1+y+2t}$$

$$u(x, 1, t) = e^{1+x+2t}$$

$$u(x, 0, t) = g_0(x)\omega(t)$$

$$g_0(x) = e^x$$

$$\mu(t) = (e-1)^2 e^{2t}$$

$$\omega(t) = e^{2t}$$

The analytical solution of the problem is

$$u(x, y, t) = e^{x+y+2t}$$

Table 1.

Relative errors for $n = 49$ and $l = \frac{1}{15000}$ when $\omega(t)$ is given

Node points $x = y$	Theoretical solution	2nd order finite difference [3]	New Scheme
0:1	9.0250	$2:5562 \times 10^{-7}$	1.171×10^{-6}
0:2	11.0232	$2:8302 \times 10^{-6}$	2.881×10^{-6}
0:3	13.4637	$4:1114 \times 10^{-6}$	4.151×10^{-6}
0:4	16.4446	$4:6798 \times 10^{-6}$	4.714×10^{-6}
0:5	20.0855	$4:5541 \times 10^{-6}$	4.586×10^{-6}
0:6	24.5325	$3:8804 \times 10^{-6}$	3.913×10^{-6}
0:7	29.9641	$2:8540 \times 10^{-6}$	2.890×10^{-6}
0:8	36.5982	$1:6804 \times 10^{-6}$	1.722×10^{-6}
0:9	44.7012	$1:0154 \times 10^{-6}$	6.340×10^{-7}

The Treatment of Non Local Boundary Condition

By using Simpson's 1/3 Rule.

$$\int_0^1 \int_0^1 u(x, y, t) dx dy \approx \frac{h^2}{9} \sum_{i=0}^M \sum_{j=0}^M b_i b_j U_{i,j}$$

Where

$$M = N + 1$$

$$b_0 = b_M = 1$$

$$c_i = 4 \text{ for odd } i \text{ and } c_i = 2 \text{ for even } i$$

Above equation may be written as

$$\int_0^1 \int_0^1 u(x, y, t) dx dy \approx \frac{h^2}{9} \sum_{i=0}^M c_i U_{i,0} + R(t)$$

Where

$$R(t) = \frac{h^2}{9} \sum_{i=0}^M \sum_{j=1}^M c_i c_j U_{i,j}$$

Integrating the boundary condition with respect to x it gives

$$\int_0^1 u(x, 0, t) = \omega(t) \int_0^1 g_0(x) dx$$

Once again use Simpson's Rule we get

$$\frac{h}{3} \sum_{i=0}^M c_i U_{i,0} \approx \omega(t) \int_0^1 g_0(x) dx$$

$$\omega(t) = \frac{\mu(t) - R(t)}{\frac{h}{3} \left(\int_0^1 \int_0^1 g_0(x) dx \right)}$$

Table2.

Relative errors for $n = 49$ and $l = \frac{1}{15000}$ When $\omega(t)$ is unknown

Node points $x = y$	Theoretical solution	2nd order finite difference [3]	New Scheme with Simpson's rule
0:1	9.0250	$3:3994 \times 10^{-4}$	6.049×10^{-6}
0:2	11.0232	$3:0427 \times 10^{-6}$	3.207×10^{-6}
0:3	13.4637	$2:6002 \times 10^{-4}$	5.420×10^{-7}
0:4	16.4446	$1:8408 \times 10^{-4}$	1.422×10^{-6}
0:5	20.0855	$1:1595 \times 10^{-4}$	2.512×10^{-6}
0:6	24.5325	$6:3782 \times 10^{-5}$	2.764×10^{-6}
0:7	29.9641	$2:9338 \times 10^{-5}$	2.349×10^{-6}
0:8	36.5982	$5:1982 \times 10^{-6}$	1.526×10^{-6}
0:9	44.7012	$3:3960 \times 10^{-6}$	5.940×10^{-7}

Conclusion

Using given algorithm the problems are solved for $n = 49$ and $l = \frac{1}{15000}$. We have developed 2nd order parallel splitting method for heat equation in two dimensions and non local boundary condition was approximated by Simpson's 1/3 rule and exponential term in recurring relation by new rational approximate. First we solved the problem when the value of $\omega(t)$ was given and then for unknown $\omega(t)$. The method is L_0 stable and used for two dimensional heat equation with non local boundary conditions. The results for relative error obtained by using above numerical method compared with the results [3], which are better. It is also observed that there is no oscillation over the entire interval and the method behaved smoothly.

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