Numerical Solution of Parabolic Partial Differential Equations via Conjugate Gradient Technique

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Abstract:

Parabolic partial differential equations (PPDEs) arise in many areas of science and engineering, including heat transfer, diffusion, and fluid dynamics. Analytical solutions to these PPDEs are often difficult or impossible to obtain, so numerical methods are needed to approximate the solution. In this research, we investigate the use of the conjugate gradient technique for numerically solving parabolic PDEs. The technique involves discretizing the PPDE with regard to both space and time. The parabolic partial differential equations are then transformed into systems of linear algebraic equations using the Crank-Nicholson centred difference approach. Then, these equations are solved to yield the unknown points in the grids, which are subsequently substituted into the assumed solution to obtain the required estimated solution, which is reported in tabular format. A comparison was made between the conjugate gradient solutions and those produced using the Jacobi preconditioned conjugate gradient technique in terms of the time required and rate of convergence at that point. Results indicate that conjugate gradient techniques are suitable for solving parabolic-type partial differential equations, with Jacobi-preconditioned conjugate gradient technique converging faster. This research has potential applications in various areas of science and engineering where parabolic PDEs arise.

Keywords: Parabolic PDEs, convergence, conjugate gradient approach, preconditioned conjugate gradient technique, Crank-Nicholson approach

1. Introduction

In engineering and research, partial differential equations with parabolic nature are frequently employed to simulate physical processes. These equations describe diverse processes in viscous fluid flow, liquid filtration, gas dynamics, heat conduction, elasticity, biological species, chemical reactions, environmental contamination and so on. [3] [4]. In a few instances, approximations are utilized to transform parabolic PDEs into conventional differential equations or even algebraic equations. This problem's existence and uniqueness are described in the literature. Several numerical strategies for solving this problem have been offered [5]. [6] [7].

Due to their ease of implementation and minimal storage needs, conjugate gradient (CG) approaches have found widespread use in many practical fields, including management sciences

[6], health sciences [16], engineering [30], robotic motion and portfolio selection [4, 8, 28]. They are employed to solve the linear system issue.

$$Hv = p \tag{1}$$

where H is symmetric and positive definite matrix, v is the unknown variable and p is the known values at the right hand side. The conjugate gradient technique is employed to iteratively solve systems of linear equations (1) by efficiently searching for the solution along conjugate directions. It takes advantage of the symmetry and positive definiteness of the coefficient matrix to minimize the residual error. By using a sequence of conjugate directions, it iteratively updates the solution vector until convergence is achieved. The method is widely used in numerical optimization and scientific computing due to its efficiency and ability to handle large systems. In the context of solving parabolic partial differential equations, the conjugate gradient method can be used to solve the resulting linear system of equations obtained after discretizing the PDE using finite difference or finite element methods. Kou [20] developed two novel conjugate gradient algorithms in an effort to develop a technique with both high convergence characteristics and excellent numerical performance. Several strategies have been used to numerically solve partial differential equations with a parabola. [8] [9] [10] [11].
II. Literature Review

2. Methodology

2.1. The Crank Nicholson (CN) Approach

The Crank-Nicolson method is a numerical technique used to solve partial differential equations (PDEs), particularly those that involve diffusion or heat conduction. It's a finite difference method that provides a stable and accurate solution by combining the forward difference scheme and the backward difference scheme. In the approach, the PDE is discretized in both time and space. The time derivative is approximated using a central difference scheme, while the spatial derivatives are approximated using either central difference or other appropriate schemes. The resulting system of equations is solved iteratively to obtain the solution at each time step. What sets the Crank-Nicolson method apart is its implicit nature, which means it accounts for the present and future time steps when updating the solution. This property makes it unconditionally stable, allowing for larger time steps without compromising accuracy. The CN approach provides a balanced compromise between stability and accuracy, making it a popular choice for solving a wide range of PDEs. It has the advantage of been unconditionally stable and disadvantage of having to solve a matrix equation at each time step but on the other hand, the matrix turns out to be tridiagonal and it is very fast algorithm. The CN approach is liked because of averaging both the explicit and implicit time. The concept of Crank Nicholson approach is shown in Figure 1.

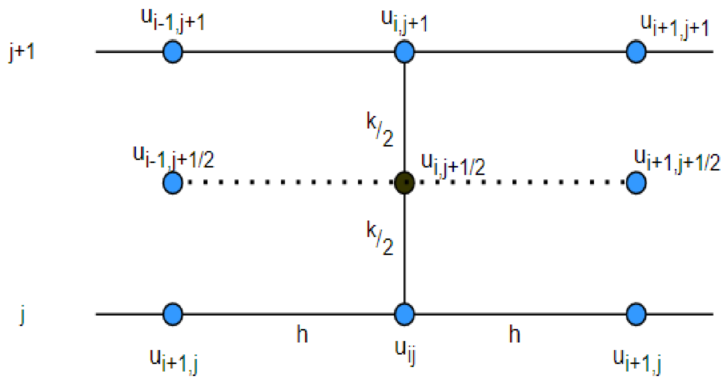

Figure 1: Illustration of Crank Nicholson concept

Based on the CN approach for solving a one-dimension parabolic equations in (2)

$$\frac{\partial \cup(x,t)}{\partial t} - \frac{\partial^2 \cup(x,t)}{\partial x^2} = 0 \tag{2}$$

A centred and backward finite difference can be employed to obtain the CN scheme for the heat equation considered in (2) as follows;

$$\frac{u(x-s,t) - 2u(x,t) + u(x+s,t)}{s^2} = \frac{u(x,t) - u(x,t-\kappa)}{\kappa} \tag{3}$$

$$-\frac{\kappa}{s^2}\left[u(x-s,t) + \left(1+\frac{\kappa}{s^2}\right)u(s,t)\right] - \frac{\kappa}{s^2}u(x+s,t) = u(x,t-\kappa) \tag{4}$$

Setting $\lambda = \frac{\kappa}{s^2}$, we arrive at

$$-s\left[u(x-s,t) + (1+2\lambda)u(s,t)\right] - \lambda u(x+s,t) = u(x,t-\kappa) \tag{5}$$

By replacing the coordinates (x,t) with (i, j), equation (5) becomes (6)

$$-\lambda u_{i-1,j} + (1+2\lambda)u_{i,j} - \lambda u_{i+1,j} = u_{i,j-1} \tag{6}$$

The relation in (6) is the Crank Nicholson scheme for a one-dimensional Parabolic problems.

2.2. Conjugate Gradient (CG) Procedure

The conjugate gradient method is an iterative algorithm used for solving large linear systems of equations. Specifically, it is used to solve systems of the form $Hv = p$. The conjugate gradient method iteratively improves an initial guess for the solution vector, approximating it in a sequence of steps until a desired tolerance or number of iterations is achieved. At each iteration, the method computes a search direction that is conjugate to the previous search directions. This means that the search directions are orthogonal with respect to the matrix H, which allows the method to converge more quickly than other methods that use non-orthogonal search directions. The algorithm associated with CG technique is presented in the next section.

2.2.1. Algorithm for Conjugate gradient technique

1. Input initial estimate $v_0 = 0$
2. Set $r_0 = p - Hv_0$, $s_0 = r_0$ and $y = 0$
3. While r_y is not equal zero, construct the step size $\alpha_y = \frac{r_y^T r_y}{s_y^T s_y}$
4. Construct next iterate by stepping in direction s_y; $v_{y+1} = v_y + \alpha_y s_y$
5. Construct new residual $r_{y+1} = r_y - \alpha_y H s_y$
6. Construct scalar for linear combination for next direction $\beta_y = \frac{r_{y+1}^T r_{y+1}}{r_y^T r_y}$
7. Construct next conjugate vector $s_{y+1} = r_y + 1 + \beta_y s_y$
8. Increment $y = y + 1$
9. End the iteration and return v_{y+1} as the result

3. Computational Experiments

Experiment 1: We apply the Crank Nicholson scheme (6) to compute the solution of the Parabolic PDE

$$\frac{\partial^2 \cup(x,t)}{\partial x^2} - \frac{\partial \cup(x,t)}{\partial t} = 0$$

$$\cup(0,t) = \cup(1,t) = 0,\ \cup(\mathrm{x},0) = \sin(\pi x)$$

$$\mathrm{h} = 0.25,\ \mathrm{k} = 0.25,\quad \mathrm{x} \in [0,1]\ \ and\ \ t \in [0,1],\ \lambda = \frac{k}{h^2} = 4$$

The discretized format of the above PDE problem is shown in Figure 2

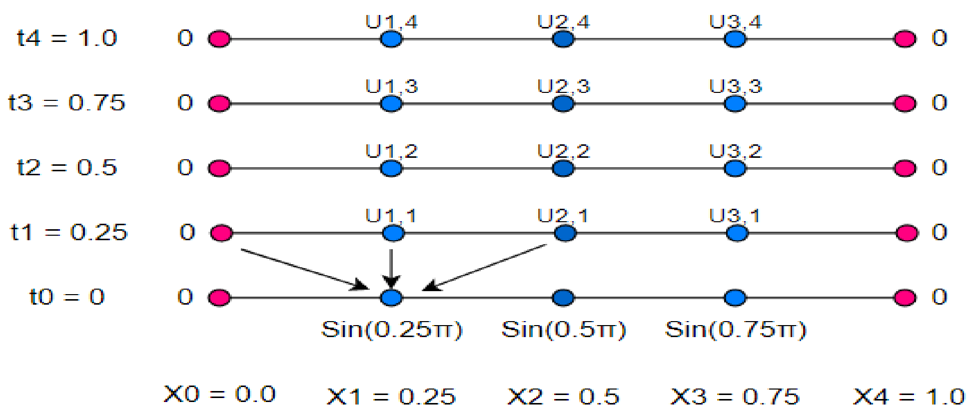

Figure 2: Discretized form of Experiment 1

After analyzing the discretized grids above using equation (1), it generated the following linear equations.

$$\begin{array}{l} -4U_{0,1}+9U_{1,1}-4U_{2,1}=U_{1,0} \\ -4U_{1,1}+9U_{2,1}-4U_{3,1}=U_{2,0} \\ -4U_{2,1}+9U_{3,1}-4U_{4,1}=U_{3,0} \end{array} \Rightarrow \begin{array}{r} 9U_{1,1}-4U_{2,1}+\quad 0=\sin(\pi/4) \\ -4U_{1,1}+9U_{2,1}-4U_{3,1}=\sin(\pi/2) \\ 0-\ 4U_{4,1}+\ 9U_{3,1}=\sin(3\pi/4) \end{array}$$

The solution at row 1 at $t_1 = 0.25$ is the solution of $Hv = p$:

$$\begin{pmatrix} 9 & -4 & 0 \\ -4 & 9 & -4 \\ 0 & -4 & 9 \end{pmatrix}\begin{pmatrix} v_{1,1} \\ v_{2,1} \\ v_{3,1} \end{pmatrix}=\begin{pmatrix} \sin(0.25\pi) \\ \sin(0.5\pi) \\ \sin(0.75\pi) \end{pmatrix} \Rightarrow \begin{pmatrix} v_{1,1} \\ v_{2,1} \\ v_{3,1} \end{pmatrix}=\begin{pmatrix} 0.21151 \\ 0.29912 \\ 0.21151 \end{pmatrix}$$

The solution at row 2 when $t_2 = 0.5$ gives.

$$\begin{pmatrix} 9 & -4 & 0 \\ -4 & 9 & -4 \\ 0 & -4 & 9 \end{pmatrix}\begin{pmatrix} v_{1,2} \\ v_{2,2} \\ v_{3,2} \end{pmatrix}=\begin{pmatrix} 0.21151 \\ 0.29912 \\ 0.21151 \end{pmatrix} \Rightarrow \begin{pmatrix} v_{1,2} \\ v_{2,2} \\ v_{3,2} \end{pmatrix}=\begin{pmatrix} 0.063267 \\ 0.089473 \\ 0.063267 \end{pmatrix}$$

Similarly, a $t_3 = 0.75\,\text{secs}$ in row 3.

$$\begin{pmatrix} 9 & -4 & 0 \\ -4 & 9 & -4 \\ 0 & -4 & 9 \end{pmatrix}\begin{pmatrix} v_{1,3} \\ v_{2,3} \\ v_{3,3} \end{pmatrix}=\begin{pmatrix} 0.063267 \\ 0.089473 \\ 0.063267 \end{pmatrix} \Rightarrow \begin{pmatrix} v_{1,3} \\ v_{2,3} \\ v_{3,3} \end{pmatrix}=\begin{pmatrix} 0.018924 \\ 0.026763 \\ 0.018924 \end{pmatrix}$$

For $t_4 = 1.0\,\text{sec}$ in row 4, the solution is obtained.

$$\begin{pmatrix} 9 & -4 & 0 \\ -4 & 9 & -4 \\ 0 & -4 & 9 \end{pmatrix}\begin{pmatrix} v_{1,4} \\ v_{2,4} \\ v_{3,4} \end{pmatrix} = \begin{pmatrix} 0.018924 \\ 0.026763 \\ 0.018924 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} v_{1,4} \\ v_{2,4} \\ v_{3,4} \end{pmatrix} = \begin{pmatrix} 0.0056606 \\ 0.0080053 \\ 0.0056606 \end{pmatrix}$$

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Experiment 2: The Crank Nicholson scheme (6) is applied to find $\cup_{i,j}$ for $i = 0,1,2,3,4$ and $j = 0,1,2$ of the Parabolic partial differential equation.

$$\frac{\partial^2 \cup(x,t)}{\partial^2 x} - \frac{\partial \cup(x,t)}{\partial t} = 0$$

$$\cup(0,t) = 0,\ \cup(4,t) = 0, \cup(\mathrm{x},0) = \frac{x}{3}\left(16 - x^2\right)$$

$$\mathrm{h} = 1,\ \mathrm{k} = 1,\quad \mathrm{x} \in [0,4]\ \textit{and}\ t \in [0,2],\ \lambda = \frac{k}{h^2} = 1$$

Evaluation of the boundary conditions are presented in Table 1.

Table 1: Discretized PDE with boundary points for Experiment 2

t \ x	0	1	2	3	4
0	0	5	8	7	0
1	0	$\cup_1$	$\cup_2$	$\cup_3$	0
2	0	$\cup_4$	$\cup_5$	$\cup_6$	0

Application of equation (1) to the discretized PDE, generated the linear systems $(Hv = p)$.

$$\begin{aligned} 4\cup_1 - \cup_2 + 0 &= 8 \\ -\cup_1 + 4\cup_2 - \cup_3 &= 12 \\ 0 - \cup_2 + 4\cup_3 &= 8 \end{aligned} \quad \text{such that} \quad \begin{aligned} 4\cup_4 - \cup_5 + 0 &= \cup_1 \\ -\cup_4 + 4\cup_5 - \cup_6 &= \cup_2 \\ 0 - \cup_5 + 4\cup_6 &= \cup_3 \end{aligned}$$

where

$$H = \begin{pmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix}, v = \begin{pmatrix} \cup_1 \\ \cup_2 \\ \cup_3 \end{pmatrix} \quad \textit{and} \quad p = \begin{pmatrix} 8 \\ 12 \\ 8 \end{pmatrix}$$

The solution obtained for row 3 is

$$\begin{pmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix}\begin{pmatrix} \cup_1 \\ \cup_2 \\ \cup_3 \end{pmatrix} = \begin{pmatrix} 8 \\ 12 \\ 8 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} \cup_1 \\ \cup_2 \\ \cup_3 \end{pmatrix} = \begin{pmatrix} 3.14286 \\ 4.57143 \\ 3.14286 \end{pmatrix}$$

The solution obtained for row 4 is

$$\begin{pmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix}\begin{pmatrix} U_4 \\ U_5 \\ U_6 \end{pmatrix} = \begin{pmatrix} 3.14286 \\ 4.57143 \\ 3.14286 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} U_4 \\ U_5 \\ U_6 \end{pmatrix} = \begin{pmatrix} 1.22449 \\ 1.75510 \\ 1.22449 \end{pmatrix}$$

Table 2: Comparison Result for Experiment 1

Time steps	Techniques	Iterations	CPU Time (sec)
t_1	CG	1	0.0090
	JPCG	1	0.0089
	JACOBI	26	0.0299
	GAUSS SEIDEL	14	0.0300
t_2	CG	1	0.0130
	JPCG	1	0.0070
	JACOBI	23	0.0241
	GAUSS SEIDEL	13	0.0180
t_3	CG	1	0.0080
	JPCG	1	0.0090
	JACOBI	21	0.0290
	GAUSS SEIDEL	11	0.0200
t_4	CG	1	0.0070
	JPCG	1	0.0080
	JACOBI	18	0.0240
	GAUSS SEIDEL	10	0.0343

Table 3: Comparison Result for Experiment 2

Time steps	Techniques	Iterations	CPU Time (sec)
t_1	CG	2	0.0139
	JPCG	2	0.0039
	JACOBI	15	0.0299
	GAUSS SEIDEL	11	0.0245
t_2	CG	2	0.0499
	JPCG	2	0.0070
	JACOBI	13	0.0289
	GAUSS SEIDEL	8	0.0209

4. Discussion of Computational Results

From Table 1, it is observed that the Conjugate Gradient (CG) technique and Jacobi Preconditioned Conjugate Gradient (JPCG) techniques consistently required only 1 iteration across all time steps, making them the fastest methods in terms of iteration count. Jacobi and Gauss Seidel showed improvement in iteration count over time steps, with Gauss Seidel consistently requiring fewer iterations compared to Jacobi. The Central Processing Unit (CPU) time varied for all methods and showed fluctuations between time steps. However, CG and JPCG generally had lower CPU times compared to Jacobi and Gauss Seidel. The results from Table 3 indicate that Conjugate Gradient technique and Jacobi Preconditioned Conjugate Gradient technique consistently required 2 iterations for both time steps. JPCG was the fastest method in terms of CPU time for the first-time and second-timestep. Jacobi showed improvement in the number of iterations between the two-time steps, while the CPU time varied for all methods.

5. Conclusion

The research investigated the application of the conjugate gradient technique for solving parabolic partial differential equations (PPDEs) numerically. The study utilized the Crank-Nicholson approach to discretize the PPDEs and transform them into systems of linear algebraic equations. The conjugate gradient method was then employed to solve these equations and obtain the estimated solutions. The results demonstrated that the conjugate gradient technique, along with the Jacobi preconditioned conjugate gradient technique, was effective in solving parabolic-type PDEs. The methods exhibited convergence and provided accurate solutions within a minimal number of iterations. The Jacobi preconditioned conjugate gradient technique demonstrated faster convergence compared to the standard conjugate gradient method.

The research findings have significant implications for various scientific and engineering fields where parabolic PDEs arise. The efficient numerical solution of these equations can facilitate simulations and analysis of physical processes, including heat transfer, diffusion, fluid dynamics, and more. The conjugate gradient technique offers a viable approach for solving such problems, and the Jacobi preconditioned variant can further enhance the convergence rate.

In conclusion, the research highlights the suitability of the conjugate gradient technique, particularly the Jacobi preconditioned variant, for numerically solving parabolic PDEs. The methods provide accurate solutions with faster convergence, making them valuable tools in scientific and engineering applications involving parabolic-type partial differential equations.

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