

**ITERATIVE SOLUTION OF DIFFUSION EQUATION WITH CRANK-NICOLSON
SCHEME USING PAOR METHOD**

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Abstract: In this paper, we solve one-dimensional diffusion equation with second order Crank-Nicholson scheme by PAOR method and this method compared with other methods discussed in this paper through some numerical examples.

Keywords: Finite Difference Method, Crank-Nicolson scheme, AOR, SOR, Gauss-Seidel, Jacobi.

Introduction

Let us consider one dimensional diffusion equation

$$\frac{\partial U}{\partial t} = D \frac{\partial^2 U}{\partial x^2} \quad 0 < x < L, \quad 0 < t < T \quad \dots (1.1)$$

Partitioning the spacial interval $[0, L]$ and temporal interval $[0, T]$ into respective finite grids as

$$x_i = i\Delta x \quad i = 0, 1, 2, 3, \dots, N \quad \text{where } L/N = \Delta x \quad \dots (1.2)$$

$$t_j = j\Delta t \quad j = 0, 1, 2, 3, \dots, M \quad \text{where } T/M = \Delta t \quad \dots (1.3)$$

Denoting the numerical solution of $U(x, t)$ as $U_{i,j} = U(x_i, t_j)$

The Second order Crank-Nicolson scheme of equation (1.1) is

$$\frac{U_{i,j+1} - U_{i,j}}{\Delta t} = \frac{D}{2} \left[\frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{(\Delta x)^2} + \frac{U_{i+1,j+1} - 2U_{i,j+1} + U_{i-1,j+1}}{(\Delta x)^2} \right] \quad \dots (1.4)$$

$$\Rightarrow 2U_{i,j+1} - 2U_{i,j} = \frac{D\Delta t}{(\Delta x)^2} [U_{i+1,j} - 2U_{i,j} + U_{i-1,j} + U_{i+1,j+1} - 2U_{i,j+1} + U_{i-1,j+1}]$$

$$\Rightarrow -\lambda U_{i-1,j+1} + 2(1+\lambda)U_{i,j+1} - \lambda U_{i+1,j+1} = \lambda U_{i-1,j} + 2(1-\lambda)U_{i,j} + \lambda U_{i+1,j} \quad \dots (1.5)$$

where $\lambda = D\Delta t / (\Delta x)^2$

From (1.5), we get for first time level; $i = 1, 2, 3, \dots, N-1, j = 0$

$$-\lambda U_{0,1} + 2(1+\lambda)U_{1,1} - \lambda U_{2,1} = \lambda U_{0,0} + 2(1-\lambda)U_{1,0} + \lambda U_{2,0}$$

$$-\lambda U_{1,1} + 2(1+\lambda)U_{2,1} - \lambda U_{3,1} = \lambda U_{1,0} + 2(1-\lambda)U_{2,0} + \lambda U_{3,0}$$

\vdots

$$-\lambda U_{N-2,1} + 2(1+\lambda)U_{N-1,1} - \lambda U_{N,1} = \lambda U_{N-2,0} + 2(1-\lambda)U_{N-1,0} + \lambda U_{N,0}$$

For second time level; $i = 1, 2, 3, \dots, N-1, j = 1$

$$\begin{aligned}
 -\lambda U_{0,2} + 2(1+\lambda)U_{1,2} - \lambda U_{2,2} &= \lambda U_{0,1} + 2(1-\lambda)U_{1,1} + \lambda U_{2,1} \\
 -\lambda U_{1,2} + 2(1+\lambda)U_{2,2} - \lambda U_{3,2} &= \lambda U_{1,1} + 2(1-\lambda)U_{2,1} + \lambda U_{3,1} \\
 &\vdots \\
 -\lambda U_{N-2,2} + 2(1+\lambda)U_{N-1,2} - \lambda U_{N,2} &= \lambda U_{N-2,1} + 2(1-\lambda)U_{N-1,1} + \lambda U_{N,1}
 \end{aligned}$$

and finally

for nth time level; $i = 1, 2, 3 \dots N-1, j = M-1$

$$\begin{aligned}
 -\lambda U_{0,M} + 2(1+\lambda)U_{1,M} - \lambda U_{2,M} &= \lambda U_{0,M-1} + 2(1-\lambda)U_{1,M-1} + \lambda U_{2,M-1} \\
 -\lambda U_{1,M} + 2(1+\lambda)U_{2,M} - \lambda U_{3,M} &= \lambda U_{1,M-1} + 2(1-\lambda)U_{2,M-1} + \lambda U_{3,M-1} \\
 &\vdots \\
 -\lambda U_{N-2,M} + 2(1+\lambda)U_{N-1,M} - \lambda U_{N,M} &= \lambda U_{N-2,M-1} + 2(1-\lambda)U_{N-1,M-1} + \lambda U_{N,M-1}
 \end{aligned}$$

The above system of equations can be written as $AX = b$... (1.6)

Where

$$A = \left[\begin{array}{ccccccccc}
 2(1+\lambda) & -\lambda & & \cdots & & 0 & & & \\
 -\lambda & 2(1+\lambda) & -\lambda & & & \vdots & & & \\
 & & \ddots & & & & & & \\
 \vdots & & -\lambda & 2(1+\lambda) & -\lambda & & & & \\
 0 & \cdots & -\lambda & 2(1+\lambda) & & & & & \\
 -2(1-\lambda) & -\lambda & & \cdots & 0 & 2(1+\lambda) & -\lambda & \cdots & 0 \\
 -\lambda & -2(1-\lambda) & -\lambda & & \vdots & -\lambda & 2(1+\lambda) & -\lambda & \vdots \\
 & & \ddots & & & & \ddots & & \\
 \vdots & & -\lambda & -2(1-\lambda) & -\lambda & & \vdots & & -\lambda & 2(1+\lambda) & -\lambda \\
 0 & \cdots & -\lambda & -2(1-\lambda) & 0 & \cdots & -\lambda & 2(1+\lambda) & \\
 & & & & & \cdots & & & \cdots & & \cdots \\
 & & & & & & -2(1-\lambda) & -\lambda & \cdots & 0 & 2(1+\lambda) & -\lambda & \cdots & 0 \\
 & & & & & & -\lambda & -2(1-\lambda) & -\lambda & \vdots & -\lambda & 2(1+\lambda) & -\lambda & \vdots \\
 & & & & & & & & \ddots & & & & \ddots & \\
 & & & & & & & & \vdots & & -\lambda & -2(1-\lambda) & -\lambda & \vdots & -\lambda & 2(1+\lambda) & -\lambda \\
 & & & & & & & & 0 & \cdots & -\lambda & -2(1-\lambda) & 0 & \cdots & -\lambda & 2(1+\lambda)
 \end{array} \right]$$

$$X = \begin{bmatrix} U_{1,1} \\ U_{2,1} \\ \vdots \\ U_{N-1,1} \\ U_{1,2} \\ U_{2,2} \\ \vdots \\ U_{N-1,2} \\ \vdots \\ U_{1,M} \\ U_{2,M} \\ \vdots \\ U_{N,M} \end{bmatrix}, \quad b = \begin{bmatrix} \lambda U_{0,0} + 2(1-\lambda)U_{1,0} + \lambda U_{2,0} + \lambda U_{0,1} \\ \lambda U_{1,0} + 2(1-\lambda)U_{2,0} + \lambda U_{3,0} \\ \vdots \\ \lambda U_{N-2,0} + 2(1-\lambda)U_{N-1,0} + \lambda U_{N,0} + \lambda U_{N,1} \\ \lambda U_{0,1} + \lambda U_{0,2} \\ 0 \\ \lambda U_{N,1} + \lambda U_{N,2} \\ \vdots \\ \lambda U_{0,M-1} + \lambda U_{0,M} \\ 0 \\ \vdots \\ \lambda U_{N,M-1} + \lambda U_{N,M} \end{bmatrix}$$

Numerical solution of diffusion equation

Splitting the matrix A of (1.6) as $A = I - L - U$... (2.1)

Where I, L, U are unit, a strictly lower and upper triangular parts of A of order $n \times n$ and X & b are unknown and known vectors of order $n \times 1$ respectively.

Parametric Accelerated over relaxation:

The (PAOR) method considered by V.B.Kumar Vatti et.al [7] is

$$X^{(n+1)} = P_{\alpha,r,\omega} X^{(n)} + Q \quad (n = 0, 1, 2, 3, \dots) \quad \dots (2.2)$$

Where

$$P_{\alpha,r,\omega} = [(1+\alpha)I - \omega L]^{-1} \{ (1+\alpha-r)I + (r-\omega)L + rU \} \quad \dots (2.3)$$

$$Q = r[(1+\alpha)I - \omega L]^{-1} b \quad \dots (2.4)$$

$$\text{and } \alpha \neq -1 \quad \dots (2.5)$$

Here, $P_{\alpha,r,\omega}$ is known as an iteration matrix of PAOR method.

If $\underline{\mu}$ and $\bar{\mu}$ are the smallest and the largest eigenvalues of the Jacobi matrix J in magnitude, then the following choices for the parameters are given in [7] as

$$(i) \quad \text{When } \underline{\mu} = \bar{\mu} \quad \omega = \frac{2(1+\alpha)}{1 + \sqrt{1 - \bar{\mu}^2}} \quad \& \quad r = \frac{(1+\alpha)}{\sqrt{1 - \bar{\mu}^2}} \quad \dots (2.6)$$

$$(ii) \quad \text{when } \underline{\mu} \neq \bar{\mu} \text{ and } k > 1$$

$$\omega = \frac{2(1+\alpha)}{1 + \sqrt{1 - \bar{\mu}^2}} \quad \& \quad r = 1 + \alpha + \omega + \frac{\bar{\mu}^2 - \underline{\mu}^2}{2} \quad \dots (2.7)$$

$$(iii) \quad \text{when } \underline{\mu} \neq \bar{\mu} \text{ and } k < 1$$

$$\omega = \frac{2(1+\alpha)}{1 + \sqrt{1 - \bar{\mu}^2}} \quad \& \quad r = \left(1 + \alpha + \omega + \frac{\bar{\mu}^2 - \underline{\mu}^2}{2} \right) / 2 \quad \dots (2.8)$$

$$\text{Where } k = 1 - \sqrt{1 - \bar{\mu}^2} + \frac{\frac{\omega \bar{\mu}^2}{2}}{\frac{\bar{\mu}^2 - \underline{\mu}^2}{2}} \quad \dots (2.9)$$

It can be realized that for the choices of $(\alpha, r, \omega) = (0, r, \omega), (0, \omega, \omega), (0, 1, 1), (0, 1, 0)$ the method (2.5) reduces to AOR, SOR, Gauss-Seidal and Jacobi method respectively.

Numerical Examples

Example 3.1

Let us consider the problem given in [2]

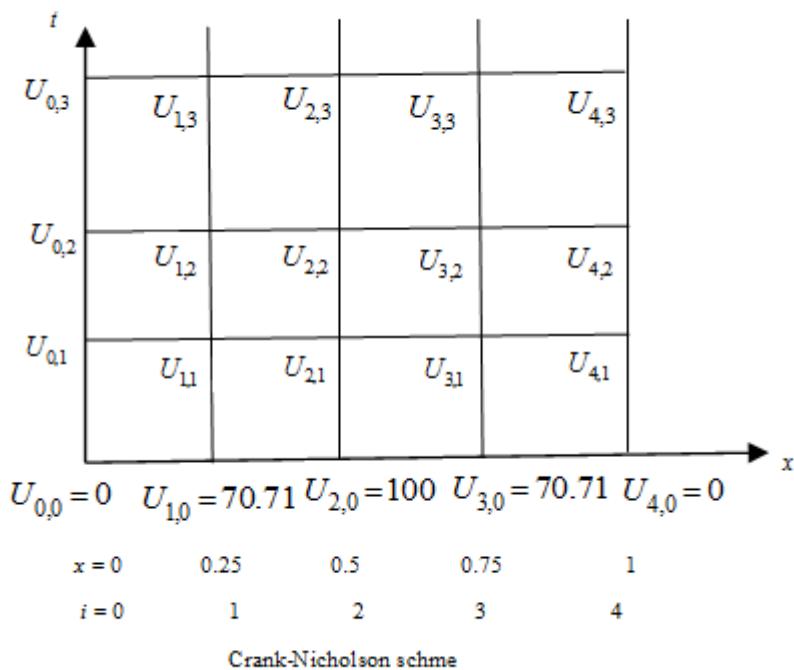
$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} \quad 0 < x < 1, \quad 0 < t < 0.3$$

Subject to the initial condition $U(x, 0) = 100 \sin(\pi x)$

And boundary conditions $U(0, k) = 0$ and $U(1, k) = 0$

Whose exact solution is $U(x, t) = 100 \sin(\pi x) e^{-\pi^2 t}$

If $\Delta x = 0.25$ and $\Delta t = 0.1$, then $\lambda = 1.6$ and one can have the following mesh with 9 internal pivotal points.



Taking $\lambda = 1.6$ in (1.5) and for the 3 time levels, we obtain the following systems to solve for the 9 unknowns as obtained in the previous section.

$$\begin{bmatrix} 5.2 & -1.6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1.6 & 5.2 & -1.6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1.6 & 5.2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.2 & -1.6 & 0 & 5.2 & -1.6 & 0 & 0 & 0 & 0 \\ -1.6 & 1.2 & -1.6 & -1.6 & 5.2 & -1.6 & 0 & 0 & 0 \\ 0 & -1.6 & 1.2 & 0 & -1.6 & 5.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.2 & -1.6 & 0 & 5.2 & -1.6 & 0 \\ 0 & 0 & 0 & -1.6 & 1.2 & -1.6 & -1.6 & 5.2 & -1.6 \\ 0 & 0 & 0 & 0 & -1.6 & 1.2 & 0 & -1.6 & 5.2 \end{bmatrix} \begin{bmatrix} U_{1,1} \\ U_{2,1} \\ U_{3,1} \\ U_{1,2} \\ U_{2,2} \\ U_{3,2} \\ U_{1,3} \\ U_{2,3} \\ U_{3,3} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

For this system is calculated that $\underline{\mu} = 8.49676997596072e-07$, $\bar{\mu} = 0.435145833164668$ and $k = 0.186501934239268$

$$f_1 = 1.6U_{0,0} - 1.2U_{1,0} + 1.6U_{2,0} + 1.6U_{0,1}$$

$$f_2 = 1.6U_{1,0} - 1.2U_{2,0} + 1.6U_{3,0}$$

$$f_3 = 1.6U_{2,0} - 1.2U_{3,0} + 1.6U_{4,0} + 1.6U_{4,1}$$

Table 1

S.N0	Method	Choices of parameters	Number of iterations	error
1	AOR	$r = 1.05243217865689$ $\omega = 1.05243217865689$	19	0.5×10^{-14}
2	PAOR	$r = 1.07355406335841$ $\omega = 1.05243217865689$	17	0.5×10^{-14}
3	SOR	$r = 1.05243217865689$ $\omega = 1.05243217865689$	19	0.5×10^{-14}
4	G.S	-	27	0.5×10^{-14}
5	J	-	52	0.5×10^{-14}

Example 3.2

Let us consider the problem given in [8]

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} \quad 0 < x < 1, \quad t > 0$$

Subject to the initial condition $U(x, 0) = \sin(\pi x)$

and boundary conditions $U(0, k) = 0$ and $U(1, k) = 0$

Whose exact solution is $U(x, t) = \sin(\pi x) e^{-\pi^2 t}$

If $\Delta x = 0.2$ and $\Delta t = 0.08$, then $\lambda = 2$ and one can have the following mesh with 12 internal pivotal points.

Taking $\lambda = 2$ in (1.5) and for the 3 time levels, we obtain the following system to solve for the 12 unknowns as obtained in the previous section.

$$\begin{bmatrix} 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 & -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & -1 & 0 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 & -1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 3 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & -1 & 0 & -1 & 3 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 3 \end{bmatrix} \begin{bmatrix} U_{1,1} \\ U_{2,1} \\ U_{3,1} \\ U_{4,1} \\ U_{1,2} \\ U_{2,2} \\ U_{3,2} \\ U_{4,2} \\ U_{1,3} \\ U_{2,3} \\ U_{3,3} \\ U_{4,3} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Where

$$f_1 = U_{0,0} - U_{1,0} + U_{2,0} + U_{0,1}$$

$$f_2 = U_{1,0} - U_{2,0} + U_{3,0}$$

$$f_3 = U_{2,0} - U_{3,0} + U_{4,0}$$

$$f_4 = U_{3,0} - U_{4,0} + U_{5,0} + U_{5,1}$$

For this system, it is calculated that $\underline{\mu} = 0.206010077891906$, $\bar{\mu} = 0.53934608689934$ and

Table 2

S.N0	Method	Choices of parameters	Number of iterations	error
1	AOR	$r = 1.085726700693682$ $\omega = 1.085726700693682$	20	0.5×10^{-14}
2	PAOR	$r = 1.104976862661991$ $\omega = 1.085726700693682$	19	0.5×10^{-14}
3	SOR	$r = 1.085726700693682$ $\omega = 1.085726700693682$	20	0.5×10^{-14}
4	G.S	-	32	0.5×10^{-14}
5	J	-	64	0.5×10^{-14}

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