CHAPTER 3

THE FINITE DIFFERENCE METHOD FOR 1-D AND 2-D PARABOLIC EQUATIONS

3.1 Introduction

Many problems in science and engineering are modeled by parabolic equations in one or more dimensions. These so-called partial differential equations (PDE) involve two or more independent variables that determine the behavior of the dependent variable. We shall concentrate on the so-called 1-D and 2-D Parabolic Equations (Douglass & Rachford (1956), Mitchell & Griffiths (1980) and Burden & Douglass (2000)). We begin the chapter by discussing the approximation of derivatives by finite difference method. Section 3.2 and 3.3 discuss the explicit and implicit method. Section 3.4 discusses the iterative solution of the linear system with the formulation of the iterative alternating direction explicit (IADE) scheme on 1-D Parabolic Equation (Sahimi et al., (1993)) and alternating group explicit (AGE) scheme on 1-D are discussed in section 3.5 and 3.6. Section 3.8 and 3.9 treat the explicit and implicit schemes on 2-D Parabolic Equation. Some alternating schemes are included in the subsequent sections.

3.1:1 Crank-Nicolson Method on 1-D (Johnson & Riess (1982))

It is possible to keep the implicit nature of the finite difference scheme for backward difference, whilst improving the accuracy of the scheme by using a central difference in time. That is, using an approximating given by:

$$\frac{U_{i,n+1} - U_{i,n}}{\Delta t} = \frac{U_{i+1,n+1/2} - 2U_{i,n+1/2} + U_{i-1,n+1/2}}{(\Delta x)^2} \qquad (3.1)$$

using such a scheme we have no way of calculating variables at the n+1/2 time level, so we have:

$$\frac{U_{i,n+1}-U_{i,n}}{\Delta t}=\frac{1}{2}\left[\frac{U_{i+1,n+1}-2U_{i,n+1}+U_{i-1,n+1}+U_{i+1,n}-2U_{i,n}+U_{i-1,n}}{(\Delta x)^2}\right] \quad (3.2)$$

that is, variables at the $n+1/2$ time level are replaced by the average of the variables at the n and $n+1$ time levels.

Rearranging (3.2) we obtain:

$$-rU_{i-1,n+1}+(2+2r)U_{i,n+1}-rU_{i+1,n+1}=rU_{i-1,n}+(2-2r)U_{i,n}+rU_{i+1,n} \quad (3.3)$$

where $r=\Delta t/(\Delta x)^2$. Once again we have a tridiagonal system of equations which can be solved using the Thomas algorithm. We can write the system of equations (3.1) as:

$$BU_{n+1}=CU_n+d_n,$$

where $U_n=[U_{1,n},U_{2,n},\cdots,U_{m-1,n}]^T$, $B=2I-rT,\;\; C=2I+rT.$

Here I is the $(m-1)\times(m-1)$ identity matrix and

$$T=\begin{bmatrix}-2 & 1 & & & \\ & -2 & 1 & & \\ & & \cdots & & \\ & & 1 & -2 & 1 \\ & & & 1 & 2\end{bmatrix}_{(m-1)\times(m-1)}$$

The matrix B and C are symmetric and so if B and C commute then $B^{-1}C$ is also symmetric. For matrices of the form: $F(a)=a_oI+a_1A+a_2A^2+\cdots$, that is a polynomial in A, the eigenvalues are given by $f(\lambda)$, where λ is an eigenvalue of A. The eigenvalues of $[f_1(A)]^{-1}f_2(A)$ are given by $f_2(\lambda)/f_1(\lambda)$ where λ is an eigenvalue of A.

3.2 Iterative Solution of the Linear System (Ames 1977)

A system of linear algebraic equations can be sparse and banded. We will typically employ the concise notation

$$Au = b \tag{3.4}$$

to represent such systems and the focus of this section is the study of methods for efficiently solving equation (3.4) on a digital computer. The first iterative methods used for solving large linear systems were based on relaxation of the coordinates. The relaxation steps are aimed at annihilating one or a few components of the residual vector $b - Au$. The convergence of these methods is rarely guaranteed for all matrices, but a large body of theory exists for the case where the coefficient matrix arises from the finite-difference discretization of the PDE. A desirable alternative, which preserve sparseness and can achieve a high degree of accuracy even for large n, is an iterative method such as Jacobi or Gauss-Seidel method.

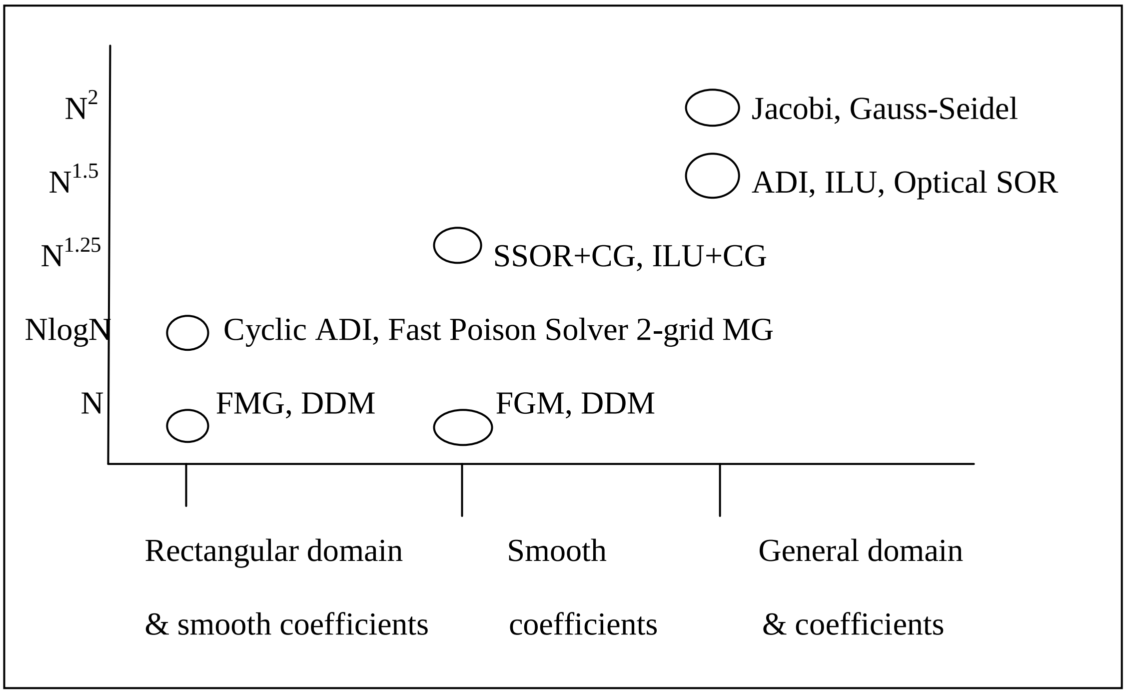

Fig. 3.1: Comparison of required arithmetic for various iterative methods.

Thus, this summary figure by (Young (1967)) indicates that much is involved in selecting a suitable solution method for any specific parabolic boundary value problem.

3.2:1 Basic Theory (Jacobi Method) by (Young (1967))

We begin with the decomposition

$$A = D - E - F, \tag{3.5}$$

in which D is the diagonal of A, $-E$ is the strict lower part and $-F$ is the strict upper part. It is always assumed that the diagonal entries of A are all nonzero. The Jacobi iteration determines the ith component of the next approximation so as to annihilate the ith component of the residual vector.

Thus,

$$(b - Ax_{k+1}) = 0 \tag{3.6}$$

however, recall Eq.(3.4) and note that iterative methods for solving this system of linear equations can essentially always be expressed in the form:

$$U^{(n+1)} = GU^{(n)} + K \tag{3.7}$$

where n is an iterative counter and G is the iteration matrix, it is related to the system matrix A by

$$G = I - Q^{-1}A$$

where I is the identity matrix and Q is generally called the splitting matrix. The Jacobi scheme can be constructed as follows. Firstly, decompose A as in Eq.(3.5), substitute into (3.4) to obtain

$$(D - L - U)U = b, \ or \ DU = (L + U)U + b \tag{3.8}$$

hence, introducing iteration counter, (3.8) becomes

$$U^{(n+1)} = D^{-1}(L + U)U^{n} + D^{-1}b \tag{3.9}$$

from Eq. (3.9) $L + U = D - A$, so $D^{-1}(L + U) = I - D^{-1}A.$

Thus, D is the splitting matrix and Eq.(3.9) is in the form (3.7) with

$$G \equiv D^{-1}(L + U) = 1 - D^{-1}A, \ k = D^{-1}b \tag{3.10}$$

Hence, in matrix terms the definition of the Jacobi method can be expressed as

$$X^{(k+1)} = D^{-1}(L+U)x^{(k)} + D^{-1}b \quad \text{as in Eq.(3.9)}$$

where

$$x_i = \frac{1}{a_{i,j}}(b_i - \sum_{j \neq i} a_{i,j} x_j) \tag{3.11}$$

suggesting an iterative method defined by

$$x_i^{(k+1)} = \frac{1}{a_{i,j}}(b_i - \sum_{j \neq i} a_{i,j} x_j^k) \tag{3.12}$$

3.2:2 Gauss-Seidel (GS) Method (Bertsakas & Tsitsiklis (1998))

Consider again the linear equations; if we proceed as with the Jacobi method but not assume that the equations are examined one at a time in sequence, and that previously computed results are used as soon as they are available we obtain the Gauss-Seidel:

$$X_i^{(k)} = \frac{1}{a_{i,j}}\left[b_i - \sum_{j<i} a_{i,j} x_j^{(k)} - \sum_{j>i} a_{i,j} x_j^{(k-1)}\right] \tag{3.13}$$

the computation appear to be serial, since each component of the new iterate depends upon all previously computed components. The update cannot be done simultaneously as in the Jacobi method. Secondly, the new iterate $x^{(k)}$ depends upon the order in which the equations are examined. The GS is called the "Successive Displacement" to indicate the dependence of iterates on the ordering. A poor choice of ordering can degrade the rate of convergence. In matrix terms, the definition of GS method is:

$$X^{(k)} = (D-L)^{-1}(Ux^{(k-1)} + b) \tag{3.14}$$

consider Eq.(3.4) and $A = D - L - U$ as was done in Eq.(3.5) followed by some rearrangement leads to:

$$(D-L)U^{(n+1)} = U^{(n+1)} + b \tag{3.15}$$

or

$$D(1-D^{-1}L)U^{(n+1)} = U^{(n)} + b,$$

and

$$U^{(n+1)} = (1-D^{-1}L)^{-1}D^{-1}U^{(n)} + (1-D^{-1}L)^{-1}D^{-1}b \tag{3.16}$$

we define

$$L \equiv (1-D^{-1}L)^{-1}D^{-1}U$$

$$K = (1-D^{-1}L)^{-1}D^{-1}b$$

and write

$$U^{(n+1)} = LU^{(n)} + K \tag{3.17}$$

3.2:3 Successive Overrelaxation (SOR) Method (Prasad, (2005))

SOR is obtained from GS iteration by introducing the relaxation parameter ω via the extrapolation:

$$U^{(n+1)} = (1-\omega)U^{(n)} + \omega U^{(n+1)*} \tag{3.18}$$

where $U^{(n+1)*}$ has been obtained from Eq.(3.17). This leads us to the fixed-point formula for SOR iterations:

$$U^{(n+1)} = (1-\omega)U^{(n)} + \omega\left[D^{-1}LU^{(n+1)} + D^{-1}U^{(n)} + D^{-1}b\right]$$

or

$$U^{(n+1)} = (1-\omega D^{-1}L)^{-1}\left[\omega D^{-1}U + (1-\omega)I\right]U^{(n)} + \omega(1-\omega D^{-1}L)^{-1}D^{-1}b \tag{3.19}$$

$$U^{(n+1)*} = D^{-1}LU^{(n+1)} + D^{-1}U^{(n)} + D^{-1}b \tag{3.20}$$

a rearrangement of Eq.(3.15). If we now define

$$\ell\omega \equiv (1-\omega D^{-1}L)^{-1}\left[\omega D^{-1}U + (1-\omega)I\right] \tag{3.21}$$

$$k\omega \equiv \omega(I-\omega D^{-1}L)^{-1}D^{-1}b \tag{3.22}$$

we can write Eq.(3.19) as:

$$U^{(n+1)} = \ell\omega U^{(n)} + k\omega \tag{3.23}$$

the fixed-point form of SOR. The combination Eq.(3.8) and Eq.(3.10) should always be used. Choosing the value of ω, if $\omega = 1$, the SOR method simplifies to the GS method. A theorem due to Kahan (1998) shows that SOR fails to converge if ω is outside the interval $(0,2)$. The term underrelaxation should be used when $0 < \omega < 1$, for convenience the term overrelaxation is now used for any value of $\omega \in (0,2)$. If the coefficient matrix A is symmetric and positive definite, the SOR iteration is guaranteed to converge for any value of ω between 0 and 2, the choice of ω can significantly affect the rate of SOR convergence.

3.3 IADE Scheme on 1-D Parabolic Equation (Sahimi et al., (1993))

Consider a uniform spaced network whose mesh points are $x_i = i\Delta x, t_j = j\Delta t$ for $i = 1,\ldots,m,m+1$ and $j = 0,1,\ldots,n,n+1$ are used with $\Delta x = 1/(m+1)$, $\Delta t = T/(n+1)$ and $\lambda = \Delta t/(\Delta x^2)$, the mesh ratio. That is, the interval $0 < x < 1$ is divided into a grid of points of Δx spacing and the T interval is divided into steps of Δt. The difference operator in Eq.(3.1) is approximated by centred differences. A generalized finite difference to the difference equation Eq.(3.1) at the point $(x_{i,} t_{j+1/2})$ is given by:

$$\begin{aligned} &-\lambda\theta U_{i-1,j+1} + (1+2\lambda\theta)U_{i,j+1} - \lambda\theta U_{i+1,j+1} = \lambda(1-\theta)U_{i-1,j} + \left[1-2\lambda(1-\theta)\right]U_{i,j} + \\ &\lambda(1-\theta)U_{i+1,j},\ i = 1,2,\ldots,m \end{aligned} \tag{3.24}$$

This approximation can be displayed in a more compact matrix form as:

$$\begin{bmatrix} a & b & & & & \\ c & a & b & & & \\ & c & a & b & & \\ & & \ddots & \ddots & \ddots & \\ & & & c & a & b \\ & & & & c & a \end{bmatrix}_{(mxm)} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_{m-1} \\ u_m \end{bmatrix}_{j+1} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ \vdots \\ f_{m-1} \\ f_m \end{bmatrix}$$

i.e,

$$Au = f \tag{3.25}$$

where

$$\begin{aligned} & c = -\lambda\theta \quad a = 1 + 2\lambda\theta \quad b = -\lambda\theta \\ & f_1 = \lambda(1-\theta)(u_{0j} + u_{2j}) + \lambda\theta u_{0,j+1} + [1 - 2\lambda(1-\theta)]u_{1,j} \\ & f_i = \lambda(1-\theta)(u_{i-1,j} + u_{i+1,j}) + [1 - 2\lambda(1-\theta)]u_{i,j} \quad i = 2,3,\ldots,m-2,m-1 \\ & f_m = \lambda(1-\theta)(u_{m-1,j} + u_{m+1,j}) + [1 - 2\lambda(1-\theta)]u_{m,j} + \lambda(1-\theta)u_{m+1,j} + \lambda\theta u_{m+1,j+1} \\ & u = (u_{1,j+1}, u_{2,j+1}, \ldots, u_{m,j+1})^T \; and \;\; f = (f_1, f_2, \ldots, f_3)^T \end{aligned} \tag{3.26}$$

we note that f is a column vector of order m consisting of the boundary values as well as known u at time levels j while u are the values at time level $(j+1)$ which we seek. We also recall that Eq. (3.25) corresponds to the fully implicit, the Crank-Nicolson, the Douglas and the classical explicit methods when θ takes the values $1, \frac{1}{2}, \frac{1}{2}, -1/12\lambda$ and 0, respectively. The corresponding accuracies are of the order: $0[(\Delta x)^2 + \Delta t]$, $0[(\Delta x)^2 + (\Delta t)^2]$, $0[(\Delta x)^4 + (\Delta t)^2]$ and $0[(\Delta x)^2 + \Delta t]$, respectively.

3.3:1 IADE Scheme MF-DS (Mitchell & Fairweather (1980))

With the Mitchell-Fairweather variant accuracy can be improved by utilizing the following:

$$\begin{aligned} (rI + G_1)u^{(p+1/2)} &= (rI - gG_2)u^{(p)} + f \\ (rI + G_2)u^{(p+1)} &= (rI - gG_1)u^{(p+1/2)} + gf \end{aligned} \tag{3.27}$$

where g = (6 + r) / 6. The coefficient matrix A as in (3.25) however, is decomposed into

$$A = G_1 + G_2 - \frac{1}{6}G_1G_2 \qquad (3.28)$$

to retain the tridiagonal structure of A as in Eq.(3.25), the constituent matrices G_1 and G_2 must be bidiagonal (lower and upper, respectively). Eq.(3.28) leads to:

$$\begin{aligned} e_1 &= \frac{6}{5}(a-1) \\ u_i &= \frac{6}{5}b, \qquad l_i = 6c/(6-e_i); \qquad e_i \neq 6 \\ e_{i+1} &= \frac{6}{5}(a + \frac{1}{6}l_iu_i - 1) \end{aligned} \qquad (3.29)$$

for $i = 1, 2, \cdots, m-1$.

Since G_1 and G_2 are bidiagonal, $(G_1 + rI)$ and $(G_2 + rI)$ can be inverted easily and take a full lower and upper triangular form, respectively.

From (3.27) we have:

$$\begin{aligned} u^{(p+1/2)} &= (rI + G_1)^{-1}(rI - gG_2)u^{(p)} + (rI + G_1)^{-1} f \\ u^{(p+1)} &= (rI + G_2)^{-1}(rI - gG_1)u^{(p+1/2)} + g(rI + G_2)^{-1} f \end{aligned} \qquad (3.30)$$

The IADE scheme is therefore executed at each of the intermediate levels by effecting the following computations:

i) at level (p+1/2)

$$u_i^{(p+1/2)} = (-l_{i-1}u_{i-1}^{(p+1/2)} + s_iu_i^{(p)} + w_iu_{i+1}^{(p)} + f_i)/d \text{ for } i = 1, 2, \cdots, m, \qquad (3.31)$$

where

$$\begin{aligned} d &= 1 + r \\ l_o &= w_m = 0 \\ s_i &= r - ge_i, \qquad i = 1, 2, \ldots, m \\ w_i &= -gu_i, \qquad i = 1, 2, \ldots, m-1 \end{aligned}$$

ii) at level (p+1)

$$u_{m+1-i}^{(p+1)} = (v_{m-1}u_{m-i}^{(p+1/2)} + su_{m+1-i}^{(p+1/2)} + gf_{m+1-i} - u_{m+1-i}u_{m+2-i}^{(p+1)})/d_{m+1-i} \qquad (3.32)$$

for $i = 1, 2, \ldots, m,$ where

$$d_i = r + e_i$$
$$v_o = u_m = 0$$
$$s = r - g,$$
$$v = -gl_i.$$

The IADE algorithm is completed explicitly by Eq.(3.31) and Eq.(3.32) in alternate sweeps along the points in the interval $(0,1)$ until a specified convergence criterion is satisfied.

3.3:2 IADE Scheme of D'Yakonov Fractional Splitting (IADE-DY)

Sahimi et al., (1993) proposed an accurate unconditionally stable 2-step method involving the solution of tridiagonal sets of equations along lines parallel to the x- and y- axes at the first and second steps. Fractional splitting of D'Yakonov was used to obtain accurate, stable and convergent 2-stage iterative procedure for a fixed acceleration parameter *r > 0*. Consider the iterative formula:

$$\begin{aligned}(rI + L)u^{(p+1/2)} &= (rI - gL)(rI - gR)u^{(p)} + hf \\ (rI + R)u^{(p+1)} &= u^{(p+1/2)}\end{aligned} \tag{3.33}$$

and

$$g = \frac{6+r}{6}, \qquad h = \frac{r(12+r)}{6}$$

note that by combining the two equations in (3.33) and eliminating $u^{(p+1/2)}$, we find that as $p \to \infty$, we have:

$$(L + R - \frac{1}{6}LR)u = f \tag{3.34}$$

this suggests that the coefficient matrix A in (3.35) can be decomposed into:

$$A = L + R - \frac{1}{6}LR \tag{3.35}$$

to retain the tridiagonal structure of A. The constituent matrices L and R take the bidiagonal forms (lower and upper, respectively), equating the entries of the matrices in Eq.(3.35) leads to the determination of e_i, u_i, $i=1,2,\ldots,m$, in the recursion form:

$$\begin{aligned} e_1 &= \frac{6(a-1)}{5} \\ u_i &= \frac{6b}{5}, \quad l_i = \frac{6c}{6-e_i}, \quad e_i \neq 6 \\ e_{i+1} &= \frac{6(a+(l_i u_i/6)-1)}{5}, \quad i=1,2,\ldots,m-1 \end{aligned} \tag{3.36}$$

the explicit form of Eq.(3.33) is given by:

$$\begin{aligned} u^{(p+1/2)} &= (rI+L)^{-1}\{(rI-gL)(rL-gR)u^{(p)}+hf\}, \text{ and} \\ u^{(p+1)} &= (rI+R)^{-1}u^{(p+1/2)}, \end{aligned} \tag{3.37}$$

Since L and R are bidiagonal, the inverse of $(rI+L)$ and $(rI+R)$ take a full lower and upper triangular form given by:

$$\alpha_{i,k} = \frac{(-1)^{i-k+2}}{d^{i-(k-1)}} \prod_{j=k}^{i-1} l_j, \qquad i=1,2,\ldots,m, \quad k=1,2,\ldots,i \tag{3.38}$$

with

$$\prod_{j=k}^{i-1} l_j = \begin{cases} l_k l_{k-1} \ldots l_{i-1}, & k < i-1 \\ l_{i-1}, & k = i-1 \\ 1 & k = i \end{cases} \tag{3.39}$$

$$d = 1 + r \tag{3.40}$$

and

$$\beta_{k,j} = (-1)^{j-k} \frac{\prod_{i=k}^{j-1} u_i}{\prod_{i=k}^{j} d_i}, \qquad j=1,2,\ldots,m \quad k=1,2,\ldots,j \tag{3.41}$$

with

$$\prod_{i=k}^{j-1} u_i = \begin{cases} u_k u_{k+1} \quad \ldots \quad u_{j-1}, & k < j-1 \\ u_{j-1}, & k = j-1 \\ 1 & k = j \end{cases} \tag{3.42}$$

and

$$d_i = r + e_i \tag{3.43}$$

by carrying out the relevant multiplication in Eq.(3.8), we obtain the following equations for computation at each of the intermediate levels:

(i) at the $(p+1/2)th$ iterate,

$$\begin{aligned}
u_1^{(p+1/2)} &= \frac{s(s_1 u_1^{(p)} + w_1 u_2^{(p)} + hf_1)}{d} \\
u_i^{(p+1/2)} &= (-l_{i-1} u_{i-1}^{(p+1/2)} + v_{i-1} s_{i-1} u_{i-1}^{(p)} + (v_{i-1} w_{i-1} + ss_i) u_i^{(p)} \\
&\qquad + sw_i u_{i+1}^{(p)} + hf_i)/d \qquad i = 2,3,4,\ldots,m-1 \\
u_m^{(p+1/2)} &= \frac{-l_{m-1} u_{m-1}^{(p+1/2)} + v_{m-1} s_{m-1} u_{m-1}^{(p)} + (v_{m-1} w_{m-1} + ss_m) u_m^{p} + hf_m}{d}
\end{aligned} \tag{3.44}$$

where

$$\begin{aligned}
s &= r - g, & q &= (1+g)r, \\
s_i &= r - ge_i, & i &= 1,2,\ldots,m, \\
w_i &= -gu_i, & i &= 1,2,\ldots,m-1 \\
v_i &= -gl_i, & i &= 1,2,\ldots,m-1
\end{aligned} \tag{3.45}$$

Eq.(3.44) may be written fully in their explicit form as:

$$u_1^{(p+1/2)} = \frac{s(s_1 u_1^{(p)} + w_1 u_2^{(p)} + hf_1}{d}$$

$$u_i^{(p+1/2)} = \frac{(-1)^{i+1} q[\prod_{j=1}^{i-1} l_j s_1 u_1^{(p)}}{d^i} + \frac{\sum_{j=2}^{i-1} (-1)i + j + 1\ q[\prod_{k=j}^{i-1} l_j (l_{j-1} w_{j-1} - sd) u_j^{p}}{d^{i-j+2}}$$

$$\frac{-(l_{i-1} q w_{i-1} - ss_i d) u_i^{(p)}}{d^2} + \frac{sw_i u_{i+1}^{(p)}}{d} + \frac{h \sum_{j=1}^{i} [(-1)^{j+1} f_j \prod_{k=j}^{i-1} l_k}{d^{i-j+1}}, \quad for\ i = 2,3,\ldots,m-1,m.$$

(3.46)

(ii) at the $(p+1)th$ iterate,

$$\begin{aligned}
u_m^{(p+1)} &= \frac{u_m^{(p+1/2)}}{d_m}, \\
u_i^{(p+1)} &= \frac{u_i^{(p+1/2)} - u_i u_{i+1}^{(p+1)}}{d_i}, \quad i = m-1, m-2, \ldots, 2,1
\end{aligned} \tag{3.47}$$

the fully explicit form of (3.47) is given by:

$$u_i^{(p+1)} = \frac{\sum_{k=1}^{m}(-1)^z[\prod_{j=k+1}^{m}(r+e_j)]u_k^{(p+1/2)}\prod_{l=i}^{k-1}u_j}{\prod_{n=1}^{m}(r+e_n)} \tag{3.48}$$

where

$$z = \begin{cases} k+1, & i \ odd \\ k, & i \ even, \quad for \ \ i = 1, 2, \ldots, m \end{cases}$$

The IADE algorithm is executed by using the equations (3.44) and (3.47) in alternate sweeps along the points in the interval $(0,1)$ until a specified convergence criterion is satisfied.

3.3:3 Formulation of the IADE Fourth Order (Mohanty (2004))

A fourth-order Crank-Nicolson type scheme for the numerical solution of Eq.(3.1) is given as follows:

$$\frac{1}{\Delta t}(u_{i,j+1} - u_{i,j}) = \frac{1}{2(\Delta x)^2}\left(\delta_x^2 - \frac{1}{12}\delta_x^4\right)(u_{i,j+1} + u_{i,j}) \tag{3.49}$$

where δ_x is the usual central difference operator. By defining constants such as:

$$a = \frac{\lambda}{24}, b = -\frac{2\lambda}{3}, c = \frac{4+5\lambda}{4}, d = -\frac{2\lambda}{3}, e = \frac{\lambda}{24}, \hat{c} = \frac{4-5\lambda}{4} \tag{3.50}$$

Eq. (3.49) becomes:

$$au_{i-2,j+1} + bu_{i-1,j+1} + cu_{i,j+1} + du_{i+1,j+1} + eu_{i+2,j+1} = -au_{i-2,j} - bu_{i-1,j} + \hat{c}u_{i,j} - du_{i+1,j} - eu_{i+2,j} \qquad i = 2,3,\cdots,m-1$$

The above approximation can be displayed in a matrix form as

$$\begin{bmatrix} c & d & e & & & & \\ b & c & d & e & & 0 & \\ a & b & c & d & e & & \\ & \ddots & \ddots & \ddots & \ddots & & \\ & & a & b & c & d & e \\ & 0 & & a & b & c & d \\ & & & & a & b & c \end{bmatrix}_{(m-2)x(m-2)} \begin{bmatrix} u_2 \\ u_3 \\ \vdots \\ \vdots \\ . \\ u_{m-2} \\ u_{m-1} \end{bmatrix}_{j+1} = \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ \vdots \\ . \\ f_{m-2} \\ f_{m-1} \end{bmatrix}$$

where

$$\begin{aligned} u &= (u_{2,j+1}, u_{3,j+1}, \ldots, u_{m-1,j+1})^T, \qquad f = (f_2, f_3, \ldots f_{m-1})^T \\ f_2 &= -b(u_{1,j} + u_{1,j+1}) + \hat{c}u_{2,j} - du_{3,j} - eu_{4,j} \\ f_3 &= -a(u_{1,j} + u_{1,j+1}) - bu_{2,j} + \hat{c}u_{3,j} - du_{4,j} - eu_{5,j} \\ f_i &= -au_{i-2,j} - bu_{i-1,j} + \hat{c}u_{i,j} - du_{i+1,j} - eu_{i+2,j}, \quad for\ i = 4,5,\ldots,m-3 \\ f_{m-2} &= -au_{m-4,j} - bu_{m-3,j} + \hat{c}u_{m-2,j} - du_{m-1,j} - e(u_{m,j} + u_{m,j+1}) \\ f_{m-1} &= -au_{m-3,j} - bu_{m-2,j} + \hat{c}u_{m-1,j} - d(u_{m,j} + u_{m,j+1}) \end{aligned} \quad (3.51)$$

The column vector f of order $m-2$ consists of boundary values and known u values at time level j. We seek to find the values of u at time level $(j+1)$. The Mitchell-Fairweather variant of the IADE scheme of Sahimi et al (1993) for a fixed acceleration parameter $r > 0$ is given by:

$$\begin{aligned} (rI + G_1)u^{(p+1/2)} &= (rI - gG_2)u^{(p)} + f \\ (rI + G_2)u^{(p+1)} &= (rI - gG_1)u^{(p+1/2)} + gf \end{aligned} \quad (3.52)$$

where

$$g = (6+r)/6 .$$

The coefficient matrix is decomposed into:

$$A = G_1 + G_2 - \frac{1}{6}G_1G_2 \quad (3.53)$$

The constituent matrices G_1 and G_2 must be in the form of lower and upper tridiagonal matrices respectively, in order to retain the pentadiagonal structure of A. Eq.(3.53) leads to:

$$\hat{e}_1 = \frac{6}{5}(c-1)$$
$$\hat{u}_1 = \frac{6}{5}d$$
$$\hat{v}_1 = \frac{6}{5}e, \qquad i = 1,2,\ldots,m-4$$
$$l_1 = \frac{6b}{6-\hat{e}_1}$$
$$\hat{e}_2 = \frac{1}{5}\left(6(c-1)+l_1\hat{u}_1\right)$$
$$for\ \ i = 2,3,\ldots,m-3:$$
$$\hat{u}_1 = \frac{1}{5}\left(6d+l_{i-1}\hat{v}_{i-1}\right),\ \hat{m}_{i-1} = \frac{6a}{6-\hat{e}_i},$$
$$l_i = \frac{1}{6-\hat{e}_i}\left(6b+\hat{m}_{i-1}\hat{u}_{i-1}\right),$$
$$\hat{e}_{i+1} = \frac{1}{5}\left(6(c-1)+l_i\hat{u}_i+\hat{m}_{i-1}\hat{v}_{m-1}\right) \tag{3.54}$$

Since G_1 and G_2 are three banded matrices, then (G_1+rI) and (G_2+rI) can be inverted easily. From Eq.(3.52) we have:

$$\begin{aligned} u^{(p+1/2)} &= (rI+G_1)^{-1}(rI-gG_2)u^{(p)} + (rI+G_1)^{-1}f \\ u^{(p+1)} &= (rI+G_2)^{-1}(rI-gG_1)u^{(p+1/2)} + g(rI+G_2)^{-1}f \end{aligned} \tag{3.55}$$

giving us the following computational formulae at each of the half-iterates

(i) at the $(p+1/2)th$ iterate:

$$\begin{aligned} u_2^{(p+1/2)} &= \frac{1}{R}\left(E_1u_2^{(p)} + W_1u_3^{(p)} + V_1u_4^{(p)} + f_2\right) \\ u_3^{(p+1/2)} &= \frac{1}{R}\left(E_2u_3^{(p)} + W_2u_4^{(p)} + V_2u_3^{(p)} - l_1u_2^{(p+1/2)} + f_3\right) \\ u_i^{(p+1/2)} &= \frac{1}{R}\left(E_{i-1}u_i^{(p)} + W_{i-1}u_{i+1}^{(p)} + V_{i-1}u_{i+2}^{(p)} - \hat{m}_{i-3}u_{i-2}^{(p+1/2)} - l_{i-2}u_{i-1}^{(p+1/2)} + f_i\right), \\ i &= 4,5,\ldots,m-3 \\ u_{m-2}^{(p+1/2)} &= \frac{1}{R}\left(E_{m-3}u_{m-2}^{(p)} + W_{m-3}u_{m-1}^{(p)} - \hat{m}_{m-5}u_{m-4}^{(p+1/2)} - l_{m-4}u_{m-3}^{(p+1/2)} + f_{m-2}\right) \\ u_{m-1}^{(p+1/2)} &= \frac{1}{R}\left(E_{m-2}u_{m-1}^{(p)} - \hat{m}_{m-4}u_{m-3}^{(p+1/2)} - l_{m-3}u_{m-2}^{(p+1/2)} + f_{m-1}\right) \end{aligned} \tag{3.56}$$

with

$$
\begin{aligned}
&R = 1 + r \\
&E_i = r - g\hat{e}_i, \qquad i = 1,2,\ldots,m-2 \\
&W_i = -g\hat{u}_i, \qquad i = 1,2,\ldots,m-3 \\
&V_i = -g\hat{v}_i, \qquad i = 1,2,\ldots,m-4
\end{aligned} \tag{3.57}
$$

(ii) at the $(p+1)th$ iterate:

$$
\begin{aligned}
u_{m-1}^{(p+1)} &= \frac{1}{Z_{m-2}}\left(S_{m-4}u_{m-3}^{(p+1/2)} + Q_{m-3}u_{m-2}^{(p+1/2)} + Pu_{m-1}^{(p+1/2)} + gf_{m-1}\right) \\
u_{m-2}^{(p+1)} &= \frac{1}{Z_{m-3}}\left(S_{m-5}u_{m-4}^{(p+1/2)} + Q_{m-4}u_{m-3}^{(p+1/2)} + Pu_{m-2}^{(p+1/2)} - \hat{u}_{m-3}\,u_{m-1}^{(p+1)} + gf_{m-2}\right) \\
u_{i}^{(p+1)} &= \frac{1}{Z_{i-1}}\left(S_{i-3}u_{i-2}^{(p+1/2)} + Q_{i-2}u_{i-1}^{(p+1/2)} + Pu_{i}^{(p+1/2)} - \hat{u}_{i-1}\,u_{i+1}^{(p+1)} - \hat{v}_{i-1}\,u_{i+2}^{(p+1)} + gf_{i}\right), \\
i &= 4,5,\ldots,m-3 \\
u_{3}^{(p+1)} &= \frac{1}{Z_{2}}\left(Q_1u_{2}^{(p+1/2)} + Pu_{3}^{(p+1/2)} - \hat{u}_2\,u_{4}^{(p+1)} - \hat{v}_2\,u_{5}^{(p+1)} + gf_{3}\right) \\
u_{2}^{(p+1)} &= \frac{1}{Z_{1}}\left(Pu_{2}^{(p+1/2)} - \hat{u}_1\,u_{3}^{(p+1)} - \hat{v}_1\,u_{4}^{(p+1)} + gf_{2}\right)
\end{aligned} \tag{3.58}
$$

with

$$
\begin{aligned}
&P = r - g \\
&Z_i = r + \hat{e}_i, \qquad i = 1,2,\ldots,m-2 \\
&Q_i = -gl_i, \qquad i = 1,2,\ldots,m-3 \\
&S_i = -g\hat{m}_i, \qquad i = 1,2,\ldots,m-4
\end{aligned} \tag{3.59}
$$

the IADE algorithm is completed explicitly by using the required equations at levels $(p+1/2)th$ and $(p+1)th$ in alternate sweeps along all the points in the interval $(0,1)$ until convergence is reached.

3.4 Formulation of the AGE Scheme on 1-D Parabolic Equation (Evans & Sahimi (1989))

If we assume that we have odd (i.e., m odd) number of internal points on the line $0 \le x \le 1$, we can then perform the following splitting of the coefficient in (3.25) as follows:

$$A = G_1 + G_2 \tag{3.60}$$

where

$$G_1 = \begin{bmatrix} \underline{a/2} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} \\ \text{—} & \vdots & \underline{G_s} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} \\ \text{—} & \vdots & \text{—} & \vdots & \underline{G_s} & \vdots & \text{—} & \vdots & \text{—} \\ \text{—} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} \\ & \vdots & & \vdots & & \vdots & & \vdots & G_s \end{bmatrix}_{mxm} \tag{3.61}$$

$$G_2 = \begin{bmatrix} \underline{G_s} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} \\ \text{—} & \vdots & \underline{G_s} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} \\ \text{—} & \vdots & \text{—} & \vdots & \underline{G_s} & \vdots & \text{—} & \vdots & \text{—} \\ \text{—} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} & \vdots & \text{—} \\ & \vdots & & \vdots & & \vdots & & \vdots & a/2 \end{bmatrix}_{mxm} \quad , \quad with\ G_s = \begin{bmatrix} a/2 & b \\ c & a/2 \end{bmatrix}$$

Using the well-known fact of the parabolic correspondence in the earlier text, the following stable and convergent two-stage iterative procedure of the (Peacemn-Rachford (1955)) variant for a fixed acceleration parameter $r > 0$ can be employed (Evans and Sahimi (1988b))

$$(G_1 + rI)u^{(p+1/2)} = (rI - G_2)u^{(p)} + f$$

$$(G_2 + rI)u^{(p+1)} = (rI - G_1)u^{(p+1/2)} + f \tag{3.62}$$

or in the explicit form:

$$u^{(p+1/2)} = (G_1 + rI)^{-1}\left\{(rI - G_2)u^{(p)} + f\right\}$$

$$u^{(p+1)} = (G_2 + rI)^{-1}\left\{(rI - G_1)u^{(p+1/2)} + f\right\} \tag{3.63}$$

Note that $(G_1 + rI)$ and $(G_2 + rI)$ can be easily inverted by merely inverting block diagonal entries. The approximations at each of the intermediate iteration can therefore be computed from (3.63) as follows:

i) at level $(p+1/2)th$

$$\begin{aligned} u_1^{(p+1/2)} &= (r_1 u_1^{(p)} - b u_2^{(p)} + f_1)/r_2 \\ u_i^{(p+1/2)} &= (A u_{i-1}^{(p)} + B u_i^{(p)} + C u_{i+1}^{(p)} + D u_{i+2}^{(p)} + E_i)/\Delta \end{aligned} \tag{3.64}$$

and

$$u_{i+1}^{(p+1/2)} = (A u_{i-1}^{(p)} + B u_i^{(p)} + C u_{i+1}^{(p)} + D u_{i+2}^{(p)} + E_i)/\Delta$$

for $i = 2, 4, \ldots, m-1$ where

$$r_1 = r - \frac{a}{2}, \quad r_2 = r + \frac{a}{2}, \quad \Delta = r_2^2 - bc$$

$$A = -cr_2, \quad B = r_1 r_2, \quad C = -br_1, \quad E_i = r_2 f_i - bf_{i+1}$$

$$D = \begin{cases} 0 & \text{for } i = m-1 \\ b^2 & \text{otherwise} \end{cases}$$

and

$$A = c^2, \quad B = -cr_1, \quad C = r_1 r_2, \quad E_i = r_2 f_{i+2} - cf_i$$

$$D = \begin{cases} 0 & \text{for } i = m-1 \\ -br_2 & \text{otherwise} \end{cases}$$

ii) at level $(p+1)$

$$\begin{aligned} u_i^{(p+1)} &= (P u_{i-1}^{(p+1/2)} + Q u_i^{(p+1/2)} + R u_{i+1}^{(p+1/2)} + S u_{i+2}^{(p+1/2)} + T_i)/\Delta \\ u_{i+1}^{(p+1)} &= (\tilde{P} u_{i-1}^{(p+1/2)} + \tilde{Q} u_i^{(p+1/2)} + \tilde{R} u_{i+1}^{(p+1/2)} + \tilde{S} u_{i+2}^{(p+1/2)} + \tilde{T}_i)/\Delta \end{aligned}$$

for $i = 1, 3, \ldots, m-2$ and

$$u_m^{(p+1)} = (-c u_{m-1}^{(p+1/2)} + r_1 u_m^{(p+1/2)} + f_m)/r_2 \tag{3.65}$$

where

$$P = \begin{cases} 0 & \textit{for } i = 1 \\ -cr_2 & \textit{for } i \neq 1 \end{cases}, \quad Q = r_1 r_2, \quad R = -br_1, \; S = b^2$$

$$T = r_2 f_i - bf_{i+1}$$

and

$$\tilde{P} = \begin{cases} 0 & for \;\; i = 1 \\ c^2 & for \;\; i \neq 1 \end{cases}, \quad \tilde{Q} = -cr_1, \;\; \tilde{R} = Q = r_1 r_2, \;\; \tilde{S} = -br_2$$

$$\tilde{T}_i = -cf_i + r_2 f_{i+1}$$

the AGE algorithm is completed explicitly by using the required equations at levels $(p+1/2)th$ and $(p+1)th$ in alternate sweeps along all the points in the interval $(0,1)$ until a specified convergence criterion is satisfied.

3.4:1 Formulation of the Fourth Order AGE Scheme (Evans & Sahimi (1988b))

Using the Peaceman-Rachford variant (Peaceman & Rachford (1955)), the iterative formulae at the two half iterates are given implicitly as:

$$u^{(p+1/2)} = (G_1 + rI)^{-1}[(rI - G_2)u^{(p)} + f]$$

$$u^{(p+1)} = (G_2 + rI)^{-1}[(rI - G_1)u^{(p+1/2)} + f] \qquad (3.66)$$

where assuming that m is odd, for a fixed acceleration parameter r,

$$A = G_1 + G_2 \qquad (3.67)$$

where

$$K = \begin{pmatrix} \hat{c} & \hat{d} \\ \hat{b} & \hat{c} \end{pmatrix}, \quad L = \begin{pmatrix} \hat{c} & \hat{d} & e & 0 \\ \hat{b} & \hat{c} & d & e \\ a & b & \hat{c} & \hat{d} \\ 0 & a & \hat{b} & \hat{c} \end{pmatrix}, \quad M = \begin{pmatrix} \hat{c} & \hat{d} & e \\ \hat{b} & \hat{c} & d \\ a & b & \hat{c} \end{pmatrix},$$

$$\hat{b} = \frac{b}{2}, \;\; \hat{c} = \frac{c}{2}, \;\; \hat{d} = \frac{d}{2},$$

from Eq. (3.66), we can obtain the following equations at level $(p+1/2)$,

$$u_2^{(p+1/2)} = \frac{1}{\Delta_3}\left[\begin{array}{l}(c_1 r_2 + \hat{d}\hat{b})u_2^{(p)} + (-c_1\hat{d} - r_2\hat{d})u_3^{(p)} + (-c_1 e + d\hat{d})u_4^{(p)} + \hat{d}\, e u_5^{(p)} + \\ c_1 f_2 - \hat{d}\, f_3\end{array}\right]$$

$$u_3^{(p+1/2)} = \frac{1}{\Delta_3}\left[\begin{array}{l}(-\hat{b} r_2 - \hat{b} c_1)u_2^{(p)} + (\hat{b}\hat{d} + c_1 r_2)u_3^{(p)} + (\hat{b} e - c_1 d)u_4^{(p)} - c_1 e u_5^{(p)} - \hat{b}\, f_2 + \\ c_1 f_3\end{array}\right]$$

for $i = 4, 8, 12, \ldots, m-5,$

$$u_i^{(p+1/2)} = \frac{1}{\Delta_1}\left[P u_{i-2}^{(p)} + Q u_{i-1}^{(p)} + R u_i^{(p)} + S u_{i+1}^{(p)} + T u_{i+2}^{(p)} + W u_{i+3}^{(p)} + X u_{i+4}^{(p)} + Y u_{i+5}^{(p)} + Z_i\right]$$

$$u_{i+1}^{(p+1/2)} = \frac{1}{\Delta_1}\left[\bar{P} u_{i-2}^{(p)} + \bar{Q} u_{i-1}^{(p)} + \bar{R} u_i^{(p)} + \bar{S} u_{i+1}^{(p)} + \bar{T} u_{i+2}^{(p)} + \bar{W} u_{i+3}^{(p)} + \bar{X} u_{i+4}^{(p)} + \bar{Y} u_{i+5}^{(p)} + \bar{Z}_i\right]$$

$$u_{i+2}^{(p+1/2)} = \frac{1}{\Delta_1}\left[\hat{P} u_{i-2}^{(p)} + \hat{Q} u_{i-1}^{(p)} + \hat{R} u_i^{(p)} + \hat{S} u_{i+1}^{(p)} + \hat{T} u_{i+2}^{(p)} + \hat{W} u_{i+3}^{(p)} + \hat{X} u_{i+4}^{(p)} + \hat{Y} u_{i+5}^{(p)} + \hat{Z}_i\right]$$

$$u_{i+3}^{(p+1/2)} = \frac{1}{\Delta_1}\left[\tilde{P} u_{i-2}^{(p)} + \tilde{Q} u_{i-1}^{(p)} + \tilde{R} u_i^{(p)} + \tilde{S} u_{i+1}^{(p)} + \tilde{T} u_{i+2}^{(p)} + \tilde{W} u_{i+3}^{(p)} + \tilde{X} u_{i+4}^{(p)} + \tilde{Y} u_{i+5}^{(p)} + \tilde{Z}_i\right]$$

and

$$u_{m-1}^{(p+1/2)} = \frac{1}{c_1}\left[-a u_{m-3}^{(p)} - b u_{m-2}^{(p)} + r_2 u_{m-1}^{(p)} + f_{m-1}\right]$$

where

$$c_1 = \hat{c} + r, \quad r_2 = r - \hat{c}, \quad \Delta_1 = \det(B)$$

$$\text{for } B = \begin{pmatrix} c_1 & \hat{d} & e & 0 \\ \hat{b} & c_1 & d & e \\ a & b & c_1 & \hat{d} \\ 0 & a & \hat{b} & c_1 \end{pmatrix}, \qquad \Delta_3 = c_1^2 - \hat{b}\hat{d},$$

$$P = -B_{11}a, \quad Q = -B_{11}b - B_{12}a, \quad R = B_{11}r_2 - B_{12}\hat{b}, \quad S = -B_{11}\hat{d} + B_{12}r_2, \quad T = B_{13}r_2 - B_{14}\hat{b},$$

$$W = -B_{13}\hat{d} + B_{14}r_2, \quad X = -B_{13}e - B_{14}d, \quad Z_i = B_{11}f_i + B_{12}f_{i+1} + B_{13}f_{i+2} + B_{14}f_{i+3}$$

$$Y = \begin{cases} 0 & \text{if} \quad i = m-5 \\ -B_{14}e & \text{otherwise} \end{cases}$$

$$\bar{P} = -B_{21}a, \quad \bar{Q} = -B_{21}b - B_{22}a, \quad \bar{R} = B_{21}r_2 - B_{22}\hat{b}, \quad \bar{S} = -B_{21}\hat{d} + B_{22}r_2, \quad T = B_{22}r_2 - B_{24}\hat{b},$$

$$\bar{W} = -B_{23}\hat{d} + B_{24}r_2, \quad \bar{X} = -B_{23}e - B_{24}d, \quad \bar{Z} = B_{21}f_i + B_{22}f_{i+1} + B_{23}f_{i+2} + B_{24}f_{i+3}$$

$$\bar{Y} = \begin{cases} 0 & \text{if} \quad i = m-5 \\ -B_{24}e & \text{otherwise} \end{cases}$$

$$\hat{P} = -B_{31}a,\ \ \hat{Q} = -B_{31}b - B_{32}a,\ \ \hat{R} = B_{31}r_2 - B_{32}\hat{b},\ \ \hat{S} = -B_{31}\hat{d} + B_{32}r_2,\ \ \hat{T} = B_{33}r_2 - B_{34}\hat{b},$$

$$\hat{W} = -B_{33}\hat{d} + B_{33}r_2,\quad \hat{X} = -B_{33}e - B_{34}d,\quad \hat{Z}_i = B_{31}f_i + B_{32}f_{i+1} + B_{33}f_{i+2} + B_{34}f_{i+3}$$

$$\hat{Y} = \begin{cases} 0 & if \ \ i = m-5 \\ -B_{34}e & otherwise \end{cases}$$

$$\tilde{P} = -B_{41}a,\ \ \tilde{Q} = -B_{41}b - B_{42}a,\ \ \tilde{R} = B_{41}r_2 - B_{42}\hat{b},\ \ \tilde{S} = -B_{41}\hat{d} + B_{42}r_2,\ \ \tilde{T} = B_{43}r_2 - B_{44}\hat{b},$$

$$\tilde{W} = -B_{43}\hat{d} + B_{44}r_2,\quad \tilde{X} = -B_{43}e - B_{44}d,\quad \tilde{Z}_i = B_{41}f_i + B_{42}f_{i+1} + B_{43}f_{i+2} + B_{44}f_{i+3}$$

$$\tilde{Y} = \begin{cases} 0 & if \ \ i = m-5 \\ -B_{44}e & otherwise \end{cases}$$

and

$$B^{-1} = \frac{1}{\det(B)}(B_{kl})$$

from Eq. (3.126), we obtain the following equations at level $(p+1)$,

$$u_i^{(p+1)} = \frac{1}{\Delta_1}\begin{bmatrix} Au_{i-2}^{(p+1/2)} + Bu_{i-1}^{(p+1/2)} + Cu_i^{(p+1/2)} + Du_{i+1}^{(p+1/2)} + Eu_{i+2}^{(p+1/2)} + Fu_{i+3}^{(p+1/2)} \\ + Gu_{i+4}^{(p+1/2)} + Hu_{i+5}^{(p+1/2)} + J_i \end{bmatrix}$$

$$u_{i+1}^{(p+1)} = \frac{1}{\Delta_1}\begin{bmatrix} \bar{A}u_{i-2}^{(p+1/2)} + \bar{B}u_{i-1}^{(p+1/2)} + \bar{C}u_i^{(p+1/2)} + \bar{D}u_{i+1}^{(p+1/2)} + \bar{E}u_{i+2}^{(p+1/2)} + \bar{F}u_{i+3}^{(p+1/2)} \\ + \bar{G}u_{i+4}^{(p+1/2)} + \bar{H}u_{i+5}^{(p+1/2)} + \bar{J}_i \end{bmatrix}$$

$$u_{i+2}^{(p+1)} = \frac{1}{\Delta_1}\begin{bmatrix} \hat{A}u_{i-2}^{(p+1/2)} + \hat{B}u_{i-1}^{(p+1/2)} + \hat{C}u_i^{(p+1/2)} + \hat{D}u_{i+1}^{(p+1/2)} + \hat{E}u_{i+2}^{(p+1/2)} + \hat{F}u_{i+3}^{(p+1/2)} \\ + \hat{G}u_{i+4}^{(p+1/2)} + \hat{H}u_{i+5}^{(p+1/2)} + \hat{J}_i \end{bmatrix}$$

$$u_{i+3}^{(p+1)} = \frac{1}{\Delta_1}\begin{bmatrix} \tilde{A}u_{i-2}^{(p+1/2)} + \tilde{B}u_{i-1}^{(p+1/2)} + \tilde{C}u_i^{(p+1/2)} + \tilde{D}u_{i+1}^{(p+1/2)} + \tilde{E}u_{i+2}^{(p+1/2)} + \tilde{F}u_{i+3}^{(p+1/2)} \\ + \tilde{G}u_{i+4}^{(p+1/2)} + \tilde{H}u_{i+5}^{(p+1/2)} + \tilde{J}_i \end{bmatrix}$$

$$u_{m-3}^{(p+1)} = \frac{1}{\Delta_2}\begin{bmatrix} -c_{11}au_{m-5}^{(p+1/2)} + (-c_{11}b - c_{12}a)u_{m-4}^{(p+1/2)} + (c_{11}r_2 - c_{12}\hat{b})u_{m-3}^{(p+1/2)} \\ + (-c_{11}\hat{d} + c_{12}r_2)u_{m-2}^{(p+1/2)} + c_{13}r_2u_{m-1}^{(p+1/2)} + c_{11}f_{m-3} + c_{12}f_{m-2} + c_{13}f_{m-3} \end{bmatrix}$$

$$u_{m-2}^{(p+1)} = \frac{1}{\Delta_2}\begin{bmatrix} -c_{21}au_{m-5}^{(p+1/2)} + (-c_{21}b - c_{22}a)u_{m-4}^{(p+1/2)} + (c_{21}r_2 - c_{22}\hat{b})u_{m-3}^{(p+1/2)} \\ + (-c_{21}\hat{d} + c_{22}r_2)u_{m-2}^{(p+1/2)} + c_{23}r_2u_{m-1}^{(p+1/2)} + c_{21}f_{m-3} + c_{22}f_{m-2} + c_{23}f_{m-3} \end{bmatrix}$$

$$u_{m-1}^{(p+1)} = \frac{1}{\Delta_2}\begin{bmatrix} -c_{31}au_{m-5}^{(p+1/2)} + (-c_{31}b - c_{32}a)u_{m-4}^{(p+1/2)} + (c_{31}r_2 - c_{32}\hat{b})u_{m-3}^{(p+1/2)} \\ + (-c_{31}\hat{d} + c_{32}r_2)u_{m-2}^{(p+1/2)} + c_{33}r_2u_{m-1}^{(p+1/2)} + c_{31}f_{m-3} + c_{32}f_{m-2} + c_{33}f_{m-3} \end{bmatrix}$$

where

$$A = \begin{cases} 0 & if \quad i = 2, \\ -B_{11}a & otherwise \end{cases} \qquad B = \begin{cases} 0 & if \quad i = 2, \\ -B_{11}b - B_{12}a & otherwise. \end{cases}$$

$$C = R, \quad D = S, \quad E = T, \quad F = W, \quad G = X, \quad H = -B_{14}e, \quad J_i = Z_i,$$

$$\bar{A} = \begin{cases} 0 & if \quad i = 2, \\ -B_{21} & otherwise. \end{cases} \qquad \bar{B} = \begin{cases} 0 & if \quad i = 2, \\ -B_{21}b - B_{22}a & otherwise. \end{cases}$$

$$\bar{C} = \bar{R}, \quad \bar{D} = \bar{S}, \quad \bar{E} = \bar{T}, \quad \bar{F} = \bar{W}, \quad \bar{G} = \bar{X}, \quad \bar{H} = -B_{14}e, \quad \bar{J}_i = \bar{Z}_i,$$

$$\hat{A} = \begin{cases} 0 & if \quad i = 2, \\ -B_{31} & otherwise. \end{cases} \qquad \hat{B} = \begin{cases} 0 & if \quad i = 2, \\ -B_{31}b - B_{32}a & otherwise. \end{cases}$$

$$\hat{C} = \hat{R}, \quad \hat{D} = \hat{S}, \quad \hat{E} = \hat{T}, \quad \hat{F} = \hat{W}, \quad \hat{G} = \hat{X}, \quad \hat{H} = -B_{34}e, \quad \hat{J}_i = \hat{Z}_i,$$

$$\tilde{A} = \begin{cases} 0 & if \quad i = 2, \\ -B_{41} & otherwise. \end{cases} \qquad \tilde{B} = \begin{cases} 0 & if \quad i = 2, \\ -B_{41}b - B_{42}a & otherwise. \end{cases}$$

$$\tilde{C} = \tilde{R}, \quad \tilde{D} = \tilde{S}, \quad \tilde{E} = \tilde{T}, \quad \tilde{F} = \tilde{W}, \quad \tilde{G} = \tilde{X}, \quad \tilde{H} = -B_{44}e, \quad \tilde{J}_i = \tilde{Z}_i,$$

$$\Delta_2 = \det(C) \quad for \;\; C = \begin{pmatrix} c_1 & \hat{d} & e \\ \hat{b} & c_1 & d \\ a & b & c_1 \end{pmatrix} \quad and \quad C^{-1} = \frac{1}{\det(C)}(c_{kl}).$$

the AGE fourth order algorithm is completed explicitly by using the required equations at levels $(p+1/2)$ and $(p+1)$ in alternate sweeps along the points in the interval $(0,1)$ until convergence is reached.

3.5 Introduction to 2-D Parabolic Equation

In this section we will treat a class of methods for solving the time-dependent heat equation in two space dimensions. This section describes the explicit, implicit, stationary iterative methods, ADI, double sweep IADE and the AGE class of schemes on 2-D Parabolic (Rohalla & Paiviz (2007) and Sahimi et al., (1993)). We will discuss a particular form of a boundary-value problem that can be used to find the temperature distribution $U(x,y,t)$ of a homogeneous plate occupying a region of the x-y plane. In this problem we are given values of U or its normal derivative on the boundary for all $t \geq 0$ and also an initial temperature distribution $U(x,y,0)$. For simplicity we assume that the region R is rectangular, and the specific problem we consider is:

$$\frac{\partial U(x,y,t)}{\partial t} = \alpha^2 \left[\frac{\partial^2 U(x,y,t)}{\partial x^2} + \frac{\partial^2 U(x,y,t)}{\partial y^2} \right] \quad 0 < x < L, 0 < y < K, \; t \geq 0 \qquad (3.68)$$

where $U(x,y,0) = F(x,y)$ is the initial temperature distribution and $U(x,y,t)$ is specified on the boundary of R by $U(x,y,t) = g(x,y)$. As with the one dimensional problem we let $\Delta x = L/M$ for some positive integer M and $x_i = i\Delta x$ for $0 \leq i \leq M$. We do the same in the y- direction: $\Delta y = K/N$ and $y_j = j\Delta y$ for $0 \leq j \leq N$. For simplicity of presentation we assume that M and N are chosen so that $\Delta x = \Delta y$, but this assumption is not necessary. We also choose an increment in $t, \Delta t$, and let $t_n = n\Delta t$ for $n = 0,1,2,\cdots$, we denote $U(x_i, y_j, t_n)$ as $U_{i,j}^n$.

3.6 Explicit Finite Difference Scheme for 2-D Parabolic (Noye (1996))

Using central differences for both U_{xx} and U_{yy} and the forward difference for U_t, we can derive the order $O(\Delta x^2 + \Delta t)$ explicit method given by:

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

or

$$U_{i,j}^{n+1} = r(U_{i-1,j}^n + U_{i+1,j}^n + U_{i,j-1}^n + U_{i,j+1}^n) + (1-4r)U_{i,j}^n \qquad (3.69)$$

where $r = \dfrac{\alpha^2 \Delta t}{(\Delta x)^2}$. The points where approximations are related by Eq.(3.69). In a convergence and stability analysis, thus for (3.69) we must have $r \le 1/4$. If $\Delta x \ne \Delta y$, we need $\alpha^2 \Delta t /((\Delta x)^2 + (\Delta y)^2) \le 1/8$.

We can obtain an order $O((\Delta x)^2 + \Delta t)$ implicit method by using a backward-difference approximation for $U_t(x_i, y_j, t_n)$ yields

$$\frac{V_{i,j}^{n+1} - V_{i,j}^{n}}{\Delta t} = \alpha^2 \frac{(V_{i-1,j}^{n} - 2V_{i,j}^{n} + V_{i+1,j}^{n}) + (V_{i,j-1}^{n} - 2V_{i,j}^{n} + V_{i,j+1}^{n})}{(\Delta x)^2}$$

or

$$V_{i,j}^{n} = -rV_{i-1,j}^{n+1} - rV_{i,j-1}^{n+1} + (1+4r)V_{i,j}^{n+1} - rV_{i,j}^{n+1} - rV_{i+1,j}^{n+1} \tag{3.70}$$

3.7 Implicit Crank-Nicholson on 2-D Parabolic (Smith (1985))

To improve the order to $O((\Delta x)^2 + (\Delta t)^2)$ as in Crank-Nicolson, we again average the forward-difference approximation Eq.(3.69) with the backward-difference approximation Eq.(3.70) to yield:

$$V_{i,j}^{n+1} - V_{i,j}^{n} = \frac{r}{2}\begin{bmatrix} (V_{i-1,j}^{n+1} - 2V_{i,j}^{n+1} + V_{i+1,j}^{n+1}) + (V_{i-1,j}^{n} - 2V_{i,j}^{n} + V_{i+1,j}^{n}) + \\ (V_{i,j-1}^{n+1} - 2V_{i,j}^{n+1} + V_{i,j+1}^{n+1}) + (V_{i,j-1}^{n} - 2V_{i,j}^{n} + V_{i,j+1}^{n}) \end{bmatrix} \tag{3.71}$$

the Crank-Nicolson method Eq.(3.71) is unconditionally stable but requires the solution of an $[(M-1)(N-1) \times (M-1)(N-1)]$ linear system of equations to advance to $t = t_n + 1$ from $t = t_n$. The Eq.(3.71) involves five unknowns:

$$(V_{i-1,j}^{n+1}, V_{i,j-1}^{n+1}, V_{i,j}^{n+1}, V_{i+1,j}^{n+1}, V_{i,j+1}^{n+1}),$$

and hence the system is no longer tridiagonal and can lead to more computations. This drawback is corrected by a modification known as the (Peaceman-Rachford (1955)) ADI scheme. The Truncation error (TE) is given by:

$$TE(i\Delta x, n\Delta t) = \frac{\Delta t}{2}\frac{\partial^2 U}{\partial t} + O(\Delta t)^2 - \frac{\sigma}{12}(\Delta x)^2\frac{\partial^4 U}{\partial x^4} + (\Delta y)^2\frac{\partial U^4}{\partial x^4} + O(\Delta x^4, \Delta y^4) \qquad (3.72)$$

where U is the exact solution of the PDE.

3.8 Stationary Iterative Methods on 2-D Parabolic Equation (Ames 1977)

This section begins with methods involving splitting the sparse matrix that arises from finite differencing and then iterating until a solution is found as in (Ames 1977). The platform uses the finite-difference method which provides approximation solutions for the Parabolic Equation such that the derivatives at a point are approximated by difference quotients over a small interval (Smith 1985). We seek to discretize the second order Parabolic Equation as used in (Lee & Riess 1991) Eq.(3.128):

3.8:1 Jacobi Scheme (McDonough (1994)):

If we use the central differences for both U_{xx} and U_{yy} and the forward difference for U_t, into (3.1), and let $\Delta x^2 = \Delta y^2 = \Delta^2$ we have:

$$U_{i,j}^{n+1} = U_{i,j}^{n} + \frac{\Delta t}{\Delta^2}\left(U_{i+1,j}^{n} + U_{i-1,j}^{n} + U_{i,j+1}^{n} + U_{i,j-1}^{n} - 4U_{i,j}^{n}\right) i = 1\ldots, n,\ j = 1\ldots, m \qquad (3.73)$$

it is stable in one spatial dimension only if $\Delta t/\Delta^2 \le 1/2$. In two dimensions this becomes $\Delta t/\Delta^2 \le 1/4$. Suppose we try to take the largest possible time step, and set $\Delta t = \Delta^2/4$. Then equation (3.73) becomes:

$$U_{i,j}^{n+1} = \frac{1}{4}\left(U_{i+1,j}^{n} + U_{i-1,j}^{n} + U_{i,j+1}^{n} + U_{i,j-1}^{n}\right) \qquad (3.74)$$

thus the algorithm consists of using the average of U at its four nearest neighbor points on the grid (plus contribution from the source). This procedure is then iterated until convergence. This method is in fact a classical method with origins dating back to the last century, called “Jacobi’s method”. The method is impractical because it converges too slowly. However, it is the basis for understanding the modern methods, which are always compared with it.

3.8:2 Gauss-Seidel Scheme (McDonough (1994)):

Another classical method is the Gauss-Seidel method. Here we make use of updated values of U on the right hand side of (3.74) as soon as they become available. In other words, the averaging is done “in place” instead of being “copied” from an earlier time step to a later one. If we proceed along the rows, incrementing j for fixed i, we write the computing formula Eq.(3.74) as:

$$U_{i,j}^{n+1} = \frac{1}{4}(U_{i+1,j}^{n} + U_{i-1,j}^{n+1} + U_{i,j+1}^{n} + U_{i,j-1}^{n+1}) \quad (3.75)$$

This method is also slowly converging and only of theoretical interest, but some analysis of it will be instructive. If we have approximate values of the unknowns at each grid point, this equation can be used to generate new values. We call $U^{(n)}$ the current values of the unknowns at each iteration k and $U^{(n+1)}$ the value in the next iteration. Moreover, the new values are used in this equation as soon as they become available. The pseudocode for this method is:

Procedure *Seidel* $(a_x, a_y, n_x, n_y, h, itmax, (U_{ij}))$

Real array $(U_{ij})0{:}\ n_x, 0{:}n_y$

Integer $i,\ j,\ k,\ n_x, n_y,\ itmax$

for $k = 1$ ***to*** *itmax* ***do***

  for $j = 1$ ***to*** $ny - 1$ ***do***

    $y \leftarrow a_y + jh$

for *i = 1* ***to*** *n_x – 1 do*

$x = a_x + ih$
$v = U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}$
$U_{i,j} = (v)/4$

end for

end for

end for

end procedure Seidel

In using this procedure, one must decide on the number of iterative steps to be computed, *itmax*.

3.8:3 Successive Over-relaxation (SOR) (McDonough (1994))

To show how successive overrelaxation can be applied to the 2-D Parabolic Equation, we begin with Eq. (3.75), adding superscripts to show that a new value is computed from previous iterates,

$$U_{i,j}^{n+1} = \frac{1}{4}(U_{i+1,j}^{n} + U_{i-1,j}^{n+1} + U_{i,j+1}^{n} + U_{i,j-1}^{n+1})$$

We now both add and subtract $U_{i,j}^{(n)}$ on the right-hand side, getting

$$U_{i,j}^{(n+1)} = U_{i,j}^{(n)} + \left[\frac{U_{i+1,j}^{(n)} + U_{i-1,j}^{(n+1)} + U_{i,j+1}^{(n)} + U_{i,j-1}^{(n+1)} - 4U_{i,j}^{(n)}}{4}\right]. \quad (3.76a)$$

The term in brackets is called the "residual". We can consider the bracketed term in Eq. (3.76a) to be an adjustment to the old value $U_{i,j}^{(n)}$, to give the new and improved value $U_{i,j}^{(n+1)}$. If, instead of adding just the bracketed term, we add a larger value (thus "overrelaxing"), we get the new iterating relation

$$U_{i,j}^{(n+1)} = U_{i,j}^{(n)} + \omega\left[\frac{U_{i+1,j}^{(n)} + U_{i-1,j}^{(n+1)} + U_{i,j+1}^{(n)} + U_{i,j-1}^{(n+1)} - 4U_{i,j}^{(n)}}{4}\right]. \qquad (3.76b)$$

Maximum acceleration is obtained for some optimum value of ω. This optimum value will always lie between 1.0 and 2.0. We define a scalar $\omega_n (0 < \omega_n < 2)$ and apply Eq.(3.75) to all interior points (i, j) and call it $U_{i,j}^{/}$. Hence, we have:

$$U_{i,j}^{n+1} = \omega_n U_{i,j}^{/} + (1-\omega_n)U_{i,j}^{n} \qquad (3.76c)$$

3.9 ADI Method on 2-D Parabolic Equation

In this section we treat a class of method introduced by Peaceman & Rachford (1955), for solving the time-dependent heat equation in two space dimensions. It was quickly recognized that the unconditional stability of the method might render it effective due to the possibility of employing large steps for pseudo-time marching (McDonough 1994). At each pseudo-time step the discrete equations are implicitly solved first in one spatial direction, then in the other, leading to the terminology (ADI). The obtained two Systems of Linear Algebraic Equations (SLAE), in the $(n+1/2)$ time-layer are band tridiagonal matrices, while the second one obtained in the $(n+1)$ time layer is a block tridiagonal matrix (Jiang & Wong (1991)). In order to solve the SLAE in the $(n+1/2)$ time-layer in parallel, we have to transform the corresponding matrix by means of permutation of rows to a block tridiagonal matrix. This transformation involves transposition of the right hand side (rhs) of the equation we solve when the rhs is represented as a matrix. It is clear that such a transposition entails communication which may be reduced if a parallel tridiagonal solver is exploited. Solving 2-D Parabolic Equations using the ADI method, there are three main steps in constructing an ADI method in this context: i) discretization of the PDE, ii) factorization of the discrete equation and iii) splitting of the factored equations. Many implementations of the ADI methods have been developed such as Kellogg (1964), Dahlquist (1978) and Douglass & Rachford (1956). The equation is parabolic in time and thus the solution can be obtained by marching along the t-direction. Using the regular finite difference method, we have:

$$(U_t)_{i,j}{}^n = \frac{U_{i,j}{}^{n+1} - U_{i,j}{}^n}{\Delta t}, \qquad (U_{xx})_{i,j}{}^n = \frac{U_{i+1,j}{}^n - 2U_{i,j}{}^n + U_{i-1,j}{}^n}{(\Delta x)^2}$$
$$(U_{yy})_{i,j}{}^n = \frac{U_{i,j+1}{}^n - 2U_{i,j}{}^n + U_{i,j-1}{}^n}{(\Delta y)^2}. \tag{3.77}$$

Eq. (3.68) becomes:

$$U_{i,j}{}^{n+1} = F_x(U_{i+1,j}{}^n + U_{i-1,j}{}^n) + F_y(U_{i,j+1}{}^n + U_{i,j-1}{}^n) + (1 - 2F_x - 2F_y)U_{i,j}{}^n, \tag{3.78}$$

where $F_x = \frac{c^2 \Delta t}{(\Delta x)^2}$ and $F_y = \frac{c^2 \Delta t}{(\Delta y)^2}$ are the two grid Fourier numbers, and the subscripts i, j and the subscript n denote the numbers of x, y and t intervals respectively. The stability requirement can be shown to be

$$\frac{c^2 \Delta t}{(\Delta x)^2 + (\Delta y)^2} \le \frac{1}{8}$$

for accuracy, Δx and Δy are small, then Δt is much smaller for stability. Due to drawbacks, associated with the C-N methods, the ADI method was introduced. A time-step $(n \to n+1)$ is provided into two half time steps $(n \to (n+1/2) \to n+1)$. In the first half time step $(n \to (n+1/2)$, central difference in x is expressed at the end $(n+1/2)$, and central difference in y is expressed at the start n. Therefore,

$$\frac{U_{i,j}^{n+1/2} - U_{i,j}^n}{\Delta t / 2} = c^2 \left[\frac{U_{i+1,j}^{n+1/2} - 2U_{i,j}^{n+1/2} + U_{i-1,j}^{n+1/2}}{(\Delta x)^2} + \frac{U_{i,j+1}^n - 2U_{i,j}^n + U_{i,j-1}^n}{(\Delta y)^2} \right] \tag{3.79}$$

In the second half-time step, $\partial^2 U / \partial x^2$ is expressed at the start $(n+1/2)$ and $\partial^2 U / \partial y^2$ is expressed at the end $(n+1)$. Therefore,

$$\frac{U_{i,j}^{n+1} - U_{i,j}^{n+1/2}}{\Delta t/2} = c^2\left[\frac{U_{i+1,j}^{n+1/2} - 2U_{i,j}^{n+1/2} + U_{i-1,j}^{n+1/2}}{(\Delta x)^2} + \frac{U_{i,j+1}^{n+1} - 2U_{i,j}^{n+1} + U_{i,j-1}^{n+1}}{(\Delta y)^2}\right] \quad (3.80)$$

to see why the two spatial derivatives can be written at different time in the two half-time steps in (3.79) and (3.80), we add them to get:

$$\frac{U_{i,j}^{n+1} - U_{i,j}^{n}}{2(\Delta t/2)} = c^2\left[\frac{U_{i+1,j}^{n+1/2} - 2U_{i,j}^{n+1/2} + U_{i-1,j}^{n+1/2}}{(\Delta x)^2} + \frac{1}{2}\left(\frac{U_{i,j+1}^{n} - 2U_{i,j}^{n} + U_{i,j-1}^{n}}{(\Delta y)^2} + \frac{U_{i,j+1}^{n+1} - 2U_{i,j}^{n+1} + U_{i,j-1}^{n+1}}{(\Delta y)^2}\right)\right] \quad (3.81)$$

this shows that by going through the two half-time steps, the PDE is effectively represented at the half-time step $(n+1/2)$, using the central difference for the time derivative, central difference for x-derivative, and central difference for y-derivative by averaging at the $n-$ and $(n+1)th$ time-steps. The ADI method for one complete time step is thus second-order accurate in both time and space. Rearranging Eq.(3.79) we have:

$$F_x U_{i-1,j}^{n+1/2} - (2F_x + 2)U_{i,j}^{n+1/2} + F_x U_{i+1,j}^{n+1/2} = -F_y U_{i,j-1}^{n} + (2F_y - 2)U_{i,j}^{n} - F_y U_{i,j+1}^{n} \quad (3.82)$$

$$F_y U_{i,j-1}^{n+1} - (2F_y + 2)U_{i,j}^{n+1} + F_y U_{i,j+1}^{n+1} = -F_x U_{i-1,j}^{n+1/2} + (2F_x - 2)U_{i,j}^{n+1/2} - F_x U_{i+1,j}^{n+1/2} \quad (3.83)$$

where, $F_x = c\Delta t/(\Delta x)^2$, $F_y = c\Delta t/(\Delta y)^2$.

The ADI method gives us an opportunity to exploit any method to solve the SLAE obtained in the $(n+1/2)$ and the $(n+1)$ time layers. In this thesis, we use the tridiagonal solver for the SLAE. Let us denote A for solving the system (3.68) with SLAE.

$A_k X_k = B_k, \qquad k = 1, 2, \ldots$ *can be represented in the following manner*

1. *Compute* B_1 *in the* $(n+1/2)$ *time layer using* $(2.8a)$ *with the initial conditions.*
2. *Make permutations of vectors* $X_1^{(0)}, B_1$, *where* $X_1^{(0)}$ *is initial solution in* $(n+1/2)$ *layer.*
3. *Solve* $A_1 X_1 = B_1$ *in the* $(n+1/2)$ *layer with the tridiagonal solves.*
4. *Compute* B_2 *in the* $(n+1)-st$ *time layer, using* $(2.8b)$ *from step* 1
5. *Solve* $A_2 X_2 = B_2$ *in the* $(n+1)-st$ *time layer with the tridiagonal solves.*
6. *March in the time direction by repeating steps* 1 *to* 5 *with the values obtained in the previous time* $-$ *steps.*

The rhs of (3.82) and (3.83) has three coefficients of three consecutive grid points. Thus, N systems and M tridiagonal equation are required to be stored in step 3 and M systems of N tridiagonal equations are required to be solved in step 5. The systems in each step can be combined so that only one system of $M \times N$ tridiagonal equations is required to be solved in each step. The ADI method is second-order accurate. Since it has the tridiagonal feature, it is fast and does not require excessive storage.

3.10 Double Sweep Two-Stage IADE Scheme on 2-D Parabolic Equation

The double sweep method is generally used to reduce a two-dimensional problem to a succession of one-dimensional problems which form tridiagonal system of equations. At each time increment, the execution of the method constitutes a horizontal sweep along lines parallel to the x axis, followed by a vertical sweep along lines parallel to the y axis. Here we shall solve the two-dimensional parabolic problem by using the double sweep methods of Peaceman and Rachford (1955) (DS-PR) and Mitchell and Fairweather (1964) (DS-MF). Each method involves the solution of sets of tridiagonal equations along lines parallel to the x and y axes at the first and second time steps, respectively. The Iterative Alternating Decomposition Explicit method of D'Yakonov (IADE-DY) is executed by employing fractional splitting strategy applied alternatively at each intermediate time step to the solution of the equations.

We use two approaches of numerical schemes to approximate a two-dimensional parabolic problem. The first is by employing the double sweep method of Peaceman and Rachford (DS-PR) (1955), while the second is the Mitchell and Fairweather (DS-MF) (1964). The tridiagonal system of equations that arises from the difference method applied is then solved by using the two-stage Iterative Alternating Decomposition Explicit method of D'Yakonov (IADE-DY) which was developed by Sahimi et al., (2001). By fractional splitting, each time step in the double sweep methods of DS-PR and DS-MF is split into two steps of size $\Delta t/2$. In the horizontal sweep, Eq. (3.1) advances from t_k to $t_{k+1/2}$ by using a difference approximation that is implicit in only the x-direction. Specifically, past values in the y-direction along the grid line $x = x_i$ are used, to yield the intermediate value $u_{i,j,k+1/2}$. Then, in the vertical sweep from $t_{k+1/2}$ to t_{k+1}, the solution is obtained by using an approximation implicit in only the y-direction and uses past values in the x-direction along the grid line $y = y_j$, to yield the final value $u_{i,j,k}$.

3.10:1 Peaceman and Rachford Double Sweep Method (DS-PR)

At the $(k+1/2)$ time level of the DS-PR method, the solution of Eq. (3.128) uses a backward-difference approximation as in Eq. (3.144).

$$u_{i,j,k+1/2} - u_{i,j,k} = \frac{\lambda}{2}\delta_x^2 u_{i,j,k+1/2} + \frac{\lambda}{2}\delta_y^2 u_{i,j,k} \qquad (3.84)$$

where δ_x *and* δ_y are the usual central difference operators in the *x* and *y* coordinates respectively.

i.e.: $u_{i,j,k+1/2} - u_{i,j,k} = \frac{\lambda}{2}(u_{i-1,j,k+1/2} - 2u_{i,j,k+1/2} + u_{i+1,j,k+1/2}) + \frac{\lambda}{2}(u_{i,j-1,k} - 2u_{i,j,k} + u_{i,j+1,k})$

$$-\frac{\lambda}{2}u_{i-1,j,k+1/2}+(1+\lambda)u_{i,j,k+1/2}-\frac{\lambda}{2}u_{i+1,j,k+1/2}=\frac{\lambda}{2}u_{i,j+1,k}+(1-\lambda)u_{i,j,k}+\frac{\lambda}{2}u_{i,j-1,k} \qquad (3.85)$$

from Eq. (3.85), for $j=1,2,\ldots,n$

$$i=1: \quad (1+\lambda)u_{1,j,k+1/2}-\frac{\lambda}{2}u_{2,j,k+1/2}=\frac{\lambda}{2}u_{0,j,k+1/2}+\frac{\lambda}{2}u_{1,j+1,k}+(1-\lambda)u_{1,j,k}+\frac{\lambda}{2}u_{1,j-1,k} \qquad (3.86)$$

$$i=2,3,\cdots,m-1: -\frac{\lambda}{2}u_{i-1,j,k+1/2}+(1+\lambda)u_{i,j,k+1/2}-\frac{\lambda}{2}u_{i+1,j,k+1/2}= \\ \frac{\lambda}{2}u_{i,j+1,k}+(1-\lambda)u_{i,j,k}+\frac{\lambda}{2}u_{i,j-1,k} \qquad (3.87)$$

$$i=m: -\frac{\lambda}{2}u_{m-1,j,k+1/2}+(1+\lambda)u_{m,j,k+1/2}=\frac{\lambda}{2}u_{m+1,j,k+1/2}+ \\ \frac{\lambda}{2}u_{m,j-1,k}+(1-\lambda)u_{m,j,k}+\frac{\lambda}{2}u_{m,j+1,k} \qquad (3.88)$$

let $a=1+\lambda,\ b=c=-\frac{\lambda}{2}$. Eq. (3.86) – (3.88) can be written in a more compact matrix form as:

$$Au_j^{(k+1/2)}=f_k, \quad j=1,2,\ldots,n. \qquad (3.89)$$

where

$$\begin{aligned} &u=(u_{1,j},u_{2,j},\ldots,u_{m,j})^T, \quad f=(f_{1,j},f_{2,j},\ldots,f_{m,j})^T \\ &f_{1,j}=\frac{\lambda}{2}u_{1,j+1,k}+(1-\lambda)u_{1,j,k}+\frac{\lambda}{2}(u_{1,j-1,k}+u_{0,j,k+1/2}) \\ &f_{i,j}=\frac{\lambda}{2}u_{i,j+1,k}+(1-\lambda)u_{i,j,k}+\frac{\lambda}{2}u_{i,j-1,k} \quad i=2,3,\ldots,m-1 \\ &f_{m,j}=\frac{\lambda}{2}u_{m,j+1,k}+(1-\lambda)u_{m,j,k}+\frac{\lambda}{2}(u_{m,j-1,k}+u_{m+1,j,k+1/2}) \end{aligned} \qquad (3.90)$$

at the (k+1) time level, Eq. (3.68) is approximated by:

$$u_{i,j,k+1}-u_{i,j,k+1/2}=\frac{\lambda}{2}\delta_x^2u_{i,j,k+1/2}+\frac{\lambda}{2}\delta_y^2u_{i,j,k+1} \qquad (3.91)$$

$$u_{i,j,k+1}-u_{i,j,k+1/2}=\frac{\lambda}{2}(u_{i-1,j,k+1/2}-2u_{i,j,k+1/2}+u_{i+1,j,k+1/2})+ \\ \frac{\lambda}{2}(u_{i,j-1,k+1}-2u_{i,j,k+1}+u_{i,j+1,k+1}) \qquad (3.92)$$

$$-\frac{\lambda}{2}u_{i,j-1,k+1}+(1+\lambda)u_{i,j,k+1}-\frac{\lambda}{2}u_{i,j+1,k+1}= \frac{\lambda}{2}u_{i-1,j,k+1/2}+(1-\lambda)u_{i,j,k+1/2}+\frac{\lambda}{2}u_{i+1,j,k+1/2} \tag{3.93}$$

from Eq. (3.93), for i = 1, 2, . . . , m.

$$j=1:(1+\lambda)u_{i,1,k+1}-\frac{\lambda}{2}u_{i,2,k+1}=\frac{\lambda}{2}u_{i-1,1,k+1/2}+(1-\lambda)u_{i,1,k+1/2}+ \frac{\lambda}{2}u_{i+1,1,k+1/2}+\frac{\lambda}{2}u_{i,0,k+1} \tag{3.94}$$

$$j=2,3,\cdots,n-1$$

$$-\frac{\lambda}{2}u_{i,j-1,k+1}+(1+\lambda)u_{i,j,k+1}-\frac{\lambda}{2}u_{i,j+1,k+1}=\frac{\lambda}{2}u_{i-1,j,k+1/2}+ (1-\lambda)u_{i,j,k+1/2}+\frac{\lambda}{2}u_{i+1,j,k+1/2} \tag{3.95}$$

$$j=n:-\frac{\lambda}{2}u_{i,n-1,k+1}+(1+\lambda)u_{i,n,k+1}=\frac{\lambda}{2}u_{i-1,n,k+1/2}+ (1-\lambda)u_{i,n,k+1/2}+\frac{\lambda}{2}u_{i+1,n,k+1/2}+\frac{\lambda}{2}u_{i,n+1,k+1} \tag{3.96}$$

let $a=1+\lambda,\ b=c=-\frac{\lambda}{2}$. Eq. (3.94) – Eq. (3.96) can be displayed in a more compact matrix form as:

$$Bu_i^{(k+1)}=g_{k+1/2}, \qquad i=1,2,\ldots,m \tag{3.97}$$

where $u_i^{(k+1)}=(u_{i,1},u_{i,2},\ldots u_{i,n})^T$, $g=(g_{i,1},g_{i,2},\ldots,g_{i,n})^T$

$$\begin{aligned}
g_{i,1}&=\frac{\lambda}{2}u_{i+1,1,k+1/2}+(1-\lambda)u_{i,1,k+1/2}+\frac{\lambda}{2}(u_{i-1,1,k+1/2}+u_{i,0,k+1})\\
g_{i,j}&=\frac{\lambda}{2}u_{i+1,j,k+1/2}+(1-\lambda)u_{i,j,k+1/2}+\frac{\lambda}{2}u_{i-1,j,k+1/2} \quad j=2,3,\ldots,n-1\\
g_{i,n}&=\frac{\lambda}{2}u_{i+1,n,k+1/2}+(1-\lambda)u_{i,n,k+1/2}+\frac{\lambda}{2}(u_{i-1,n,k+1/2}+u_{i,n+1,k+1})
\end{aligned} \tag{3.98}$$

3.10:2 IADE-DY (Sahimi et al., (2001))

The matrices A and B are respectively tridiagonal of size $(m \times m)$ and $(n \times n)$. Hence, at each of the $(k+1/2)$ and $(k+1)$ time levels, these matrices can be decomposed into $G_1 + G_2 - \frac{1}{6}G_1G_2$, where G_1 *and* G_2 lower and upper bidiagonal matrices are given respectively by:

$$G_1 = [l_i, 1], \qquad and \quad G_2 = [e_i, u_i],$$

where

$$e_1 = \frac{6}{5}(a-1),\ u_i = \frac{6}{5}b,\ e_{i+1} = \frac{6}{5}(a + \frac{1}{6}l_iu_i - 1),\ l_i = \frac{6c}{6-e_i}\ (e_i \neq 6)\ i = 1, 2, \ldots, m-1$$

hence, by taking p as an iteration index, and for a fixed acceleration parameter $r > 0$, the two-stage IADE-DY scheme of the form:

$$\begin{aligned} (rI + G_1)u^{(p+1/2)} &= (rI - gG_1)(rI - gG_2)u^{(p)} + hf \quad and \\ (rI + G_2)u^{(p+1)} &= u^{(p+1/2)} \end{aligned} \tag{3.99}$$

can be applied on each of the sweeps Eq. (3.84) and Eq. (3.91). Based on the fractional splitting strategy of D'Yakonov, the iterative procedure is accurate and found to be stable and convergent. By carrying out the relevant multiplications in Eq. (3.99), the following equations for computation at each of the intermediate levels are obtained:

(i) at the $(p+1/2)th$ iterate,

$$\begin{aligned} u_1^{(p+1/2)} &= \frac{1}{\hat{d}}(s_1\hat{s}u_1^{(p)} + w_1\hat{s}u_2^{(p)} + hf_1) \\ u_i^{(p+1/2)} &= \frac{1}{\hat{d}}(-l_{i-1}u_{i-1}^{(p+1/2)} + v_{i-1}s_{i-1}u_{i-1}^{(p)} + (v_{i-1}w_{i-1} + s_i\hat{s})u_i^{(p)} + w_i\hat{s}u_{i+1}^{(p)} + hf_i), \\ i &= 2, 3, \ldots, m-1 \\ u_m^{(p+1/2)} &= \frac{1}{\hat{d}}(-l_{m-1}u_{m-1}^{(p+1/2)} + v_{m-1}s_{m-1}u_{m-1}^{(p)} + (v_{m-1}w_{m-1} + s_m\hat{s})u_m^{(p)} + hf_m) \end{aligned} \tag{3.100}$$

where,

$$g=\frac{6+r}{6},\ h=\frac{r(12+r)}{6},\ \hat{d}=1+r,\ \hat{s}=r-g,\ s_i=r-ge_i,\ i=1,2,\ldots,m$$

and

$$v_i=-gl_i,\ w_i=-gu_i \quad i=1,2,\ldots,m-1.$$

(ii) at the $(p+1)th$ iterate,

$$u_m^{(p+1)}=\frac{u_m^{(p+1/2)}}{d_m},$$

$$u_i^{(p+1)}=\frac{1}{d_i}(u_i^{(p+1/2)}-\hat{u}_i\,u_{i+1}^{(p+1)}),\ where\ d_i=r+e_i,\ i=m-1,m-2,\ldots,2,1 \tag{3.101}$$

the two-stage iterative procedure in the IADE-DY algorithm corresponds to sweeping through the mesh involving at each iterates the solution of an explicit equation. This is continued until convergence is reached, that is when the convergence requirement $\left\|u^{(p+1)}-u^{(p)}\right\|\le\in$ is met, where $\in$ is the convergence criterion.

3.10:3 DS-MF (Mitchell & Fairweather (1964))

The numerical representative of Eq. (3.128) using the Mitchell and Fairweather scheme is as follows:

$$\left(1-\frac{1}{2}\left(\lambda-\frac{1}{6}\right)\delta_x^2\right)u_{i,j,k+1/2}=\left(1+\frac{1}{2}\left(\lambda+\frac{1}{6}\right)\delta_y^2\right)u_{i,j,k} \tag{3.102}$$

$$\left(1-\frac{1}{2}\left(\lambda-\frac{1}{6}\right)\delta_y^2\right)u_{i,j,k+1}=\left(1+\frac{1}{2}\left(\lambda+\frac{1}{6}\right)\delta_x^2\right)u_{i,j,k+1/2} \tag{3.103}$$

the horizontal sweep Eq. (3.102) and the vertical sweep Eq. (3.103) formulas can be manipulated and written in a compact matrix form as in Eq. (3.89) and Eq. (3.97) respectively. At the $(k+1/2)$ time level, for $j=1,2,\cdots,n$, we have:

$$f_{1,j}=\left(\frac{1}{12}+\frac{\lambda}{2}\right)\left(u_{1,j-1,k}+u_{1,j+1,k}\right)+\left(\frac{5}{6}-\lambda\right)u_{1,j,k}-\left(\frac{1}{12}-\frac{\lambda}{2}\right)u_{0,j,k+1/2}$$
$$f_{i,j}=\left(\frac{1}{12}+\frac{\lambda}{2}\right)\left(u_{i,j-1,k}+u_{i,j+1,k}\right)+\left(\frac{5}{6}-\lambda\right)u_{i,j,k},\ i=2,3,\ldots,m-1 \qquad (3.104)$$
$$f_{m,j}=\left(\frac{1}{12}+\frac{\lambda}{2}\right)\left(u_{m,j-1,k}+u_{m,j+1,k}\right)+\left(\frac{5}{6}-\lambda\right)u_{m,j,k}-\left(\frac{1}{12}-\frac{\lambda}{2}\right)u_{m+1,j,k+1/2}$$

and at the $(k+1)$ time level, for $i=1,2,\cdots,m$, we have:

$$g_{i,1}=\left(\frac{1}{12}+\frac{\lambda}{2}\right)\left(u_{i-1,1,k+1/2}+u_{i+1,1,k+1/2}\right)+\left(\frac{5}{6}-\lambda\right)u_{i,1,k+1/2}-\left(\frac{1}{12}-\frac{\lambda}{2}\right)u_{i,0,k+1}$$
$$g_{i,j}=\left(\frac{1}{12}+\frac{\lambda}{2}\right)\left(u_{i-1,j,k+1/2}+u_{i+1,j,k+1/2}\right)+\left(\frac{5}{6}-\lambda\right)u_{i,j,k+1/2},\ j=2,3,\ldots,n-1 \qquad (3.105)$$
$$g_{i,n}=\left(\frac{1}{12}+\frac{\lambda}{2}\right)\left(u_{i-1,n,k+1/2}+u_{i+1,n,k+1/2}\right)+\left(\frac{5}{6}-\lambda\right)u_{i,n,k+1/2}-\left(\frac{1}{12}-\frac{\lambda}{2}\right)u_{i,n+1,k+1/2}$$

by defining $a=\frac{5}{6}+\lambda$ and $b=c=\frac{1}{12}-\frac{\lambda}{2}$, the resulting tridiagonal system of equations are solved using similar iterative procedure as in the DS-PR, that is, the two-stage IADE-DY algorithm.

3.11 Formulation of the AGE Scheme on 2-D Parabolic

In Evans & Sahimi (1988a), the Alternating Group explicit (AGE) method was introduced for the solution of parabolic partial differential equations in one space dimension and applied on 2-D problem in Evans & Yousif (1993). This technique was extended to problems involving parabolic and hyperbolic partial differential equations in Evans and Sahimi (1988). The AGE method can be readily extended to higher space dimensions (see Abdullah (1991)). To ensure unconditional stability, the Douglas-Rachford (DR) variant is used instead of Peaceman-Rachford (PR) formula.

In two space dimensions, for example, the specific problem we are considering is Eq. (3.68) where for simplicity we assume that the region *R* of the *xy*-plane is a rectangle.

Based on the AGE concept for the one-dimensional case, the formulation for higher dimensional problems can be done in very much the same way by employing the operator fractional splitting strategy introduced by Yanenko (1971).

A weighted finite-difference approximation to (3.68) at the point $((i, j, k+\frac{1}{2})$ is given by:

$$\frac{\Delta_t u_{i,j,k}}{\Delta t} = \frac{1}{(\Delta x)^2}\left\{\theta(\delta_x^2 + \delta_y^2)u_{i,j,k+1} + (1-\theta)(\delta_x^2 + \delta_y^2)u_{i,j,k}\right\} + h_{i,j,k+1/2} \tag{3.107}$$

which leads to the five-point formula:

$$\begin{aligned} &-\lambda\theta u_{i-1,j,k+1} + (1+4\lambda\theta)u_{i,j,k+1} - \lambda\theta u_{i,j,k+1} \\ &-\lambda\theta u_{i,j-1,k+1} - \lambda\theta u_{i,j+1,k+1} = \lambda(1-\theta)u_{i-1,j,k} + (1-4\lambda(1-\theta))u_{i,j,k} + \lambda(1-\theta)u_{i+1,j,k} \\ &+\lambda(1-\theta)u_{i,j-1,k} + \lambda(1-\theta)u_{i,j+1,k} + \Delta t h_{i,j,k+1/2}, \\ &for \;\; i = 1,2,\ldots,m; \;\; j = 1,2,\ldots,n. \end{aligned} \tag{3.108}$$

we note that when θ takes the values $0, 1/2$ and 1, we obtain the classical explicit, the Crank-Nicolson and the fully implicit schemes whose truncation errors are $0([\Delta x]^2 + \Delta t),\ 0([\Delta x]^2 + [\Delta t]^2)$ *and* $0([\Delta x]^2 + \Delta t)$ respectively. The explicit scheme is stable only for $\lambda \le \frac{1}{4}$ $(if\, \Delta x \ne \Delta y, we\, need\, \Delta t \big/ [(\Delta x)^2 + (\Delta y)^2] \le \frac{1}{8})$. The fully implicit and the Crank-Nicolson schemes are, however, unconditionally stable.

The weighted finite-difference Eq. (3.108) can be expressed in the more compact matrix form as:

$$\begin{aligned} Au_{(r)}^{[k+1]} &= Bu_{(r)}^{[k]} + b + g, \\ &= f \end{aligned} \tag{3.109}$$

where $u_{(r)}^{[k]}$ are the unknown u-values at time level k ordered row-wise as denoted by the suffix r and

$$u_{(r)} = (u_1, u_2, \ldots, u_n)^T \;\; with \; u_j = (u_{1j}, u_{2j}, \ldots, u_{mj})^T,\; j = 1,2,\ldots,n.$$

thus, the mn internal mesh points on the rectangular grid system R are ordered row-wise. The vector b consists of the boundary values where

$$b = (b_1, b_2, \ldots, b_n)^T$$

with

$$\begin{aligned}
b_1 &= (\lambda(1-\theta)[u_{0,1,k} + u_{1,0,k}] + \lambda\theta[u_{0,1,k+1} + u_{1,0,k+1}], \\
&\qquad \lambda(1-\theta)u_{2,0,k} + \lambda\theta u_{2,0,k+1} \ldots, \lambda(1-\theta)u_{m-1,0,k} + \lambda\theta u_{m-1,0,k+1,} \\
&\qquad \lambda(1-\theta)[u_{m,0,k} + u_{m+1,1,k}] + \lambda\theta[u_{m,0,k+1} + u_{m+1,1,k+1}])^T; \\
b_j &= (\lambda(1-\theta)u_{0,j,k} + \lambda\theta u_{0,j,k+1}, 0, \ldots, 0\lambda(1-\theta)u_{m+1,j,k} + \lambda\theta u_{m+1,j,k+1})T \\
&\quad for \quad j = 2, 3, \ldots, n-1; \\
&and \\
b_n &= (\lambda(1-\theta)[u_{o,n,k} + u_{1,n+1,k}] + \lambda\theta[u_{0,n,k+1} + u_{1,n+1,k+1}], \\
&\qquad \lambda(1-\theta)u_{2,n+1,k} + \lambda\theta u_{2,n+1,k+1}, \ldots, \lambda(1-\theta)u_{m-1,n+1,k} \\
&\qquad + \lambda\theta u_{m-1,n+1,k+1}, \; \lambda(1-\theta)[u_{m,n+1,k} + u_{m+1,n,k}] \\
&\qquad + \lambda\theta[u_{m,n+1,k+1} + u_{m+1,n,k+1}])^T
\end{aligned}$$

and the vector g contains the source term of Eq. (3.108) given by:

$$g = (g_1, g_2, \ldots, g_n)^T$$

with

$$\begin{aligned}
g_j &= (g_{1j}, g_{2j}, \ldots, g_{mj})^T \\
&= \Delta t(h_{1,j,k+1/2}, h_{2,j,k+1/2}, \ldots, h_{m,j,k+1/2})^T \quad for \quad j = 1, 2, \ldots, n.
\end{aligned}$$

the coefficient matrix A in Eq. (3.109) takes the block tri-diagonal form.

$$A_2 = diag(a_1) \quad of \;\; order \quad (m \times m)$$

where

$$c = 1 + 4\lambda\theta \quad and \quad a_1 = -\lambda\theta$$

Similarly, the matrix B is of the form:

$$B_2 = diag(e_1) \quad of \;\; order \quad (m \times m)$$

where

$$d = 1 - 4\lambda(1-\theta) \quad and \quad e_1 = \lambda(1-\theta)$$

if we split A into the sum of its constituent symmetric and positive definite matrices G_1, G_2, G_3 and G_4, we have:

$$A = G_1 + G_2 + G_3 + G_4, \tag{3.110}$$

with

$$diag(G_1 + G_2) = \frac{1}{2} diag(A)$$

and

$$diag(G_3 + G_4) = \frac{1}{2} diag(A) .$$

in particular, we let,

$$A_4 = diag(c/2) \ of \ order \ (m \times m), \ we \ have$$

The Douglas-Rachford formula for the AGE fractional scheme then takes the form:

$$\left.\begin{aligned}(G_1 + rI)u_{(r)}^{(p+1/4)} &= (rI - G_1 - 2G_2 - 2G_3 - 2G_4)u_{(r)}^{(p)} + 2f, \\ (G_2 + rI)u_{(r)}^{(p+1/2)} &= G_2 u_{(r)}^{(p)} + ru_{(r)}^{(p+1/4)}, \\ (G_3 + rI)u_{(r)}^{(p+3/4)} &= G_3 u_{(r)}^{(p)} + ru_{(r)}^{(p+1/2)}, \\ (G_4 + rI)u_{(r)}^{(p+1)} &= G_4 u_{(r)}^{(p)} + ru_{(r)}^{(p+3/4)}.\end{aligned}\right\} \tag{3.111}$$

we now consider the above iterative formulae at each of the four intermediate levels:

i) At the first intermediate level (the $(p+1/4)th$ iterate)

since $A = G_1 + G_2 + G_3 + G_4,$ then using the first expression of Eq. (3.111) and Eq. (3.109) we obtain:

$$(G_1 + rI)u_{(r)}^{(p+1/4)} = ((rI + G_1) - 2A)u_{(r)}^{(p)} + 2Bu_{(r)}^{[k]} + 2(b+g)$$

or

$$u_{(r)}^{(p+1/4)} = (G_1 + rI)^{-1}[((rI + G_1) - 2A)u_{(r)}^{(p)} + 2Bu_{(r)}^{[k]} + 2(b+g)]. \tag{3.112}$$

without loss of generality we assume that the size of the matrix is odd. By writing $D_1 = C_1 - 2A_1,\ D_2 = C_2 - 2A_1,\ E_1 = -2A_2,\ F_1 = 2B_1\ and\ F_2 = 2B_2$ hence, using we obtain the following set of equations for computation of the AGE algorithm at the $(p+1/4)th$ iterate:

$$u_{j(r)}^{(p+1/4)} = C_1^{-1}(D_1 u_{1(r)}^{(p)} + E_1 u_{2(r)}^{(p)} + F_1 u_{1(r)}^{[k]} + F_2 u_{2(r)}^{[k]} + 2(b_1 + g_1)); \qquad (3.113)$$

$$\begin{aligned} u_{j(r)}^{(p+1/4)} &= C_2^{-1}(E_1(u_{(j-1)(r)}^{(p)} + u_{(j+1)(r)}^{(p)}) + D_2 u_{j(r)}^{(p)} + F_2(u_{(j-1)(r)}^{[k]} + u_{(j+1)(r)}^{[k]}) \\ &\quad + F_1 u_{j(r)}^{[k]} + 2(b_j + g_j)), \quad for \quad j = 2, 4, \ldots, n-1; \end{aligned} \qquad (3.114)$$

$$\begin{aligned} u_{j(r)}^{(p+1/4)} &= C_1^{-1}(E_1(u_{(j-1)(r)}^{(p)} + u_{(j+1)(r)}^{(p)}) + D_1 u_{j(r)}^{(p)} + F_2(u_{(j-1)(r)}^{[k]} + u_{(j+1)(r)}^{[k]} \\ &\quad + F_1 u_{j(r)}^{[k]} + 2(b_j + g_j)), \quad for \quad j = 3, 5, \ldots, n-2; \end{aligned} \qquad (3.115)$$

$$u_{n(r)}^{(p+1/4)} = C_1^{-1}(E_1 u_{(n-1)(r)}^{(p)} + D_1 u_{n(r)}^{(p)} + F_2 u_{(n-1)(r)}^{[k]} + F_1 u_{n(r)}^{[k]} + 2(b_n + g_n)). \qquad (3.116)$$

let $\alpha_1 = r_1 - 2c,\ \ \alpha_2 = -2a_1,\ \ \alpha_3 = 2d\ \ and\ \ \alpha_4 = 2e_1$. When the above equations are written component-wise, we have:

(a) for Eq. (3.113)

$$\left.\begin{aligned} u_{11}^{(p+1/4)} &= \left[\alpha_1 u_{11}^{(p)} + \alpha_2(u_{21}^{(p)} + u_{12}^{(p)} + \alpha_3 u_{11}^{[k]} + \alpha_4(u_{21}^{[k]} + u_{12}^{[k]}) + 2(b_{11} + g_{11)}\right] / r_1 \\ u_{i1}^{(p+1/4)} &= \left[r_1 v_i - a_1 \bar{v}_i\right] \Big/ \Delta \Big\} \\ u_{i+1,1}^{(p+1/4)} &= [-a_1 v_i + r_1 \bar{v}_i \Big/ \Delta \qquad for \quad i = 2, 4, \ldots, m-1, \end{aligned}\right. \qquad (3.117)$$

where

$$\begin{aligned} v_i &= -a_1 u_{i+1,1}^{(p)} + \alpha_1 u_{i,1}^{(p)} + \alpha_2(u_{i-1,1}^{(p)} + u_{i2}^{(p)} + \alpha_3 u_{i1}^{[k]} \\ &\qquad \alpha_4(u_{i-1,1}^{[k]} + u_{i+1,1}^{[k]} + u_{i2}^{[k]} + 2(g_{i1} + b_{i1}) \\ &and \\ \bar{v}_i &= -a_1 u_{i1}^{(p)} + \alpha_1 u_{i+1,1}^{(p)} + \alpha_2(u_{i+2,1}^{(p)} + u_{i+1,2}^{(p)}) + \alpha_3 u_{i+1,1}^{[k]} \\ &\qquad \alpha_4(u_{i1}^{[k]} + u_{i+2,1}^{[k]} + u_{i+1,2}^{[k]}) + 2(b_{i+1,1} + g_{i+1,1}) \\ &with\ u_{i1} = 0\ \ for\ \ i \succ m; \end{aligned}$$

b) for Eq. (3.114)

$$\left.\begin{aligned} u_{i,j}^{(p+1/4)} &= \left[r_1 v_{i,j} - a_1 \bar{v}_{i,j} \right] \Big/ \Delta \\ u_{i+1,j}^{(p+1/4)} &= \left[-a_1 v_{i,j} + r_1 \bar{v}_{i,j} \right] \Big/ \Delta \end{aligned} \right\} j = 2, 4, \ldots, n-1, \ i = 1, 3, \ldots, m-2,$$

$$\begin{aligned} u_{mj}^{(p+1/4)} &= [\alpha_1 u_{mj}^{(p)} + \alpha_2 (u_{m-1,j}^{(p)} + u_{m,j-1}^{(p)} + u_{m,j+1}^{(p)}) + \alpha_3 u_{mj}^{[k]} \\ &\quad + \alpha_4 (u_{m-1,j}^{[k]} + u_{m,j-1}^{[k]} + u_{m,j+1}^{[k]}) + 2(b_{mj} + g_{mj})] / r_1, \\ &\qquad j = 2, 4, \ldots, n-1. \end{aligned} \tag{3.118}$$

where

$$\begin{aligned} v_{i,j} &= \alpha_1 u_{i,j}^{(p)} + \alpha_2 (u_{i,j-1}^{(p)} + u_{i,j+1}^{(p)} + u_{i-1,j}^{(p)}) + \alpha_3 u_{i,j}^{[k]} \\ &\quad + \alpha_4 (u_{i,j-1}^{[k]} + u_{i,j+1}^{[k]} + u_{i+1,j}^{[k]} + u_{i-1,j}^{[k]}) - a_1 u_{i+1,j}^{(p)} + 2(b_{i+1,j} + g_{i+1,j}) \end{aligned}$$

and

$$\begin{aligned} \bar{v}_{i,j} &= \alpha_1 u_{i+1,j}^{(p)} + \alpha_2 (u_{i+1,j-1}^{(p)} + u_{i+1,j+1}^{(p)} + u_{i+2,j}^{(p)}) + \alpha_3 u_{i+1,j}^{[k]} \\ &\quad + \alpha_4 (u_{i,j}^{[k]} + u_{i+1,j-1}^{[k]} + u_{i+1,j+1}^{[k]} + u_{i+2,j}^{[k]}) - a_1 u_{i,j}^{(p)} + 2(b_{i+1,j} + g_{i+1,j}) \end{aligned}$$

with $u_{0j} = 0.$

c) for Eq. (3.115)

$$\begin{aligned} u_{1j}^{(p+1/4)} &= [\alpha_1 u_{1j}^{(p)} + \alpha_2 (u_{1,j-1}^{(p)} + u_{1,j+1}^{(p)} + u_{2,j}^{(p)}) + \alpha_3 u_{1,j}^{[k]} \\ &\quad + \alpha_4 (u_{1,j-1}^{[k]} + u_{1,j+1}^{[k]} + u_{2,j}^{[k]}) + 2(b_{1j} + g_{1j})] / r_1, \\ &\qquad j = 3, 5, \ldots, n-2, \end{aligned} \tag{3.119}$$

$$\left.\begin{aligned} u_{ij}^{(p+1/4)} &= [r_1 w_{ij} - a_1 \bar{w}_{ij}] / \Delta, \\ u_{i+1,j}^{(p+1/4)} &= [-a_1 w_{ij} + r_1 \bar{w}_{ij}] / \Delta \end{aligned} \right\} \ for \ \ j = 3, 5, \ldots, n-2; \ i = 2, 4, \ldots, m-1, \tag{3.120}$$

where,

$$\begin{aligned} w_{ij} &= \alpha_1 u_{ij}^{(p)} + \alpha_2 (u_{i-1,j}^{(p)} + u_{i,j-1}^{(p)} + u_{i,j+1}^{(p)}) + \alpha_3 u_{ij}^{[k]} \\ &\quad + \alpha_4 (u_{i-1,j}^{[k]} + u_{i,j-1}^{[k]} + u_{i,j+1}^{[k]} + u_{i+1,j}^{[k]}) - a_1 u_{i+1,j}^{(p)} + 2(b_{ij} + g_{ij}) \end{aligned}$$

and

$$\begin{aligned} \bar{w}_{ij} &= \alpha_1 u_{i+1,j}^{(p)} + \alpha_2 (u_{i+1,j-1}^{(p)} + u_{i+1,j+1}^{(p)} + u_{i+2,j}^{(p)}) + \alpha_3 u_{i+1,j}^{[k]} \\ &\quad + \alpha_4 (u_{i,j}^{[k]} + u_{i+1,j-1}^{[k]} + u_{i+1,j+1}^{[k]} + u_{i+2,j}^{[k]}) - a_1 u_{i,j}^{(p)} + 2(b_{i+1,j} + g_{i+1,j}) \end{aligned}$$

with $u_{i,j} = 0$ *for* $i > m,$

d) for Eq. (3.116)

$$u_{1n}^{(p+1/4)} = [\alpha_1 u_{1n}^{(p)} + \alpha_2 (u_{1,n-1}^{(p)} + u_{2,n}^{(p)}) + \alpha_3 u_{1,n}^{[k]} +$$
$$\alpha_4 (u_{1,n-1}^{[k]} + u_{2,n}^{[k]}) + 2(b_{1n} + g_{1n})] / r_1$$

$$\left.\begin{aligned} u_{in}^{(p+1/4)} &= [r_1 z_i - a_1 \bar{z}_i] / \Delta, \\ u_{i+1,n}^{(p+1/4)} &= [-a_1 z_i + r_1 \bar{z}_i] / \Delta \end{aligned}\right\} \; for\ i = 2, 4, \ldots, m-1, \tag{3.121}$$

$$z_i = \alpha_1 u_{i,n}^{(p)} + \alpha_2 (u_{i-1,n}^{(p)} + u_{i,n-1}^{(p)}) + \alpha_3 u_{i,n}^{[k]}$$
$$+ \alpha_4 (u_{i-1,n}^{[k]} + u_{i,n-1}^{[k]} + u_{i+1,n}^{[k]}) - a_1 u_{i+1,n}^{(p)} + 2(b_{i,n} + g_{i,n})$$

and

$$\bar{z}_i = \alpha_1 u_{i+1,n}^{(p)} + \alpha_2 (u_{i+1,n-1}^{(p)} + u_{i+2,n}^{(p)}) + \alpha_3 u_{i+1,n}^{[k]}$$
$$+ \alpha_4 (u_{i,n}^{[k]} + u_{i+1,n-1}^{[k]} + u_{i+2,n}^{[k]}) - a_1 u_{i,n}^{(p)} + 2(b_{i+1,n} + g_{i+1,n})$$

with $u_{i,n} = 0$ *for* $i > m$.

ii) At the second intermediate level (the $(p+1/2)th$ iterate):

From the second equation of Eq. (3.173) we have:

$$u_{(r)}^{p+1/2)} = (G_2 + rI)^{-1} [G_2 u_{(r)}^{(p)} + r u_{(r)}^{(p+1/4)}] \tag{3.122}$$

let $\hat{C}_1 \equiv C_1$ with the diagonal elements r_1 replaced by $c/4$ and $\hat{C}_2 \equiv C_2$ with the diagonal elements r_1 replaced by $c/4$. For computational purposes, we will then have:

$$\left.\begin{aligned} u_{j(r)}^{(p+1/2)} &= C_2^{-1} [\bar{C}_2 u_{j(r)}^{(p)} + r u_{j(r)}^{(p+1/4)}], \\ u_{(j+1)(r)}^{(p+1/2)} &= C_1^{-1} [\bar{C}_1 u_{(j+1)(r)}^{(p)} + r u_{(j+1)(r)}^{(p+1/4)}], \end{aligned}\right\} \quad j = 1, 3, \ldots, n-2, \tag{3.123}$$

and

$$u_{n(r)}^{(p+1/2)} = C_2^{-1} [\bar{C}_2 u_{n(r)}^{(p)} + r u_{n(r)}^{(p+1/4)}]. \tag{3.124}$$

by denoting $r_2 = c/4r_1$ and $r_3 = r/r_1$ the above equations can be written component-wise as follows:

a) for Eq. (3.123) and Eq. (3.124),

$$\left.\begin{aligned} u_{ij}^{(p+1/2)} &= [r_1 v_{ij} - a_1 \bar{v}_{ij}]/\Delta \\ u_{i+1,j}^{(p+1/2)} &= [-a_1 v_{ij} + r_1 \bar{v}_{ij}]/\Delta \end{aligned}\right\} \; for \quad j = 1,3,\ldots,n; \; i = 1,3,\ldots,m-2, \qquad (3.125)$$

and

$$u_{mj}^{(p+1/2)} = r_2 u_{mj}^{(p)} + r_3 u_{mj}^{(p+1/4)}, \quad j = 1,3,\ldots,n.$$

where

$$v_{ij} = \frac{c}{4} u_{ij}^{(p)} + a_1 u_{i+1,j}^{(p)} + r u_{ij}^{(p+1/4)}$$
$$and$$
$$\bar{v}_{ij} = a_1 u_{ij}^{(p)} + \frac{c}{4} u_{i+1,j}^{(p)} + r u_{i+1,j}^{(p+1/4)}.$$

b) for the second Eq. (3.123)

$$u_{1j}^{(p+1/2)} = r_2 u_{1j}^{(p)} + r_3 u_{1j}^{(p+1/4)}, \quad j = 2,4,\ldots,n-1,$$

$$\left.\begin{aligned} u_{ij}^{(p+1/2)} &= [r_1 v_{ij} - a_1 \bar{v}_{ij}]/\Delta \\ u_{i+1,j}^{(p+1/2)} &= [-a_1 v_{ij} - r_1 \bar{v}_{ij}]/\Delta \end{aligned}\right\} \; j = 2,4,\ldots,n-1; \; i = 2,4,\ldots,m-1, \qquad (3.126)$$

where v_{ij} and $\bar{v}_{ij}$ are given as in Eq. (3.125).

iii) At the third intermediate level (the (p + ¾)th iterate):

if we reorder the mesh points column-wise parallel to the y-axis, we have, by using the suffix c,

$$u_{(c)} = (u_1, u_2, \ldots, u_m)^T \quad with \quad u_i = (u_{i1}, u_{i2}, \ldots u_{in})^T \quad for \; i = 1,2,\ldots,m.$$

We also find that:

$$(G_3 + G_4) u_{(r)} = (\bar{G}_1 + \bar{G}_2) u_{(c)}$$
$$and \qquad (3.127)$$
$$G_3 u_{(r)} = \bar{G}_1 u_{(c)}, G_4 u_{(r)} = \bar{G}_2 u_{(c)}.$$

hence the third equation of (3.111) is transformed to:

$$(\bar{G}_1 + rI)u_{(c)}^{(p+3/4)} = \bar{G}_1 u_{(c)}^{(p)} + ru_{(c)}^{(p+1/2)}$$
$$or \qquad (3.128)$$
$$u_{(c)}^{(p+3/4)} = (\bar{G}_1 + rI)^{-1}[\bar{G}_1 u_{(c)}^{(p)} + ru_{(c)}^{(p+1/2)}].$$

let the matrices P_1 and P_2 be exactly as the same forms as C_1 and C_2 but of order $(n \times n)$ we will then have:

$$\bar{P}_1 = P_1 \quad with\ r_1\ replaced\ by\ \frac{c}{4}$$

and

$$\bar{P}_2 = P_2 \ with\ r_1\ replaced\ by\ \frac{c}{4}.$$

The following equations are therefore obtained for computation at the $(p+\frac{3}{4})th$

$$u_{i(c)}^{(p+3/4)} = P_1^{-1}[\bar{P}_1 u_{i(c)}^{(p)} + ru_{i(c)}^{(p+1/2)}] \ \ for\ i = 1,3,\ldots,m \qquad (3.129)$$

and

$$u_{i(c)}^{(p+3/4)} = P_2^{-1}[\bar{P}_2 u_{i(c)}^{(p)} + ru_{i(c)}^{(p+1/2)}] \ for\ i = 2,4,\ldots,m-1. \qquad (3.130)$$

which component-wise yields:

a) for Eq. (3.129):

$$u_{i1}^{(p+3/4)} = r_2 u_{i1}^{(p)} + r_3 u_{i1}^{(p+1/2)}, \quad i = 1,3,\ldots,m.$$

$$\left.\begin{aligned} u_{i,j}^{(p+3/4)} &= [r_1 w_{ij} - a_1 \bar{w}_{ij}]/\Delta, \\ u_{i,j+1}^{(p+3/4)} &= [-a_1 w_{ij} + r_1 \bar{w}_{ij}]/\Delta, \end{aligned}\right\} \ i = 1,3,\ldots,m; \quad j = 2,4,\ldots,n-1, \qquad (3.131)$$

where

$$w_{ij} = \frac{c}{4}u_{ij}^{(p)} + a_1 u_{i,j+1}^{(p)} + ru_{ij}^{(p+1/2)}$$

and

$$\bar{w}_{ij} = a_1 u_{ij}^{(p)} + \frac{c}{4}u_{i,j+1}^{(p)} + ru_{i,j+1}^{(p+1/2)},$$

b) for Eq. (3.131):

$$\left.\begin{aligned} u_{i,j}^{(p+3/4)} &= [r_1 w_{ij} - a_1 \bar{w}_{ij}]/\Delta, \\ u_{i,j+1}^{(p+3/4)} &= [-a_1 w_{ij} + r_1 \bar{w}_{ij}]/\Delta, \end{aligned}\right\} \; i = 2,4,\ldots,m-1; \quad j = 1,3,\ldots,n-2,$$

$$u_{i,n}^{(p+3/4)} = r_2 u_{i,n}^{(p)} + r_3 u_{i,n}^{(p+1/2)}, \tag{3.132}$$

where $w_{ij} = \bar{w}_{ij}$ are given as in Eq. (3.132).

iv) at the fourth intermediate level (the (p+1)th iterate:

The last equation of (3.111) is transformed to:

$$(\bar{G}_2 + rI)u_{(c)}^{(p+1)} = \bar{G}_2\, u_{(c)}^{(p)} + ru_{(c)}^{(p+3/4)}$$

or

$$u_{(c)}^{(p+1)} = (\bar{G}_2 + rI)^{-1}[\bar{G}_2\, u_{(c)}^{(p)} + ru_{(c)}^{(p+3/4)}]$$

which leads to the following formulae:

$$u_{i(c)}^{(p+1)} = P_2^{-1}[\bar{P}_2\, u_{i(c)}^{(p)} + ru_{i(c)}^{(p+3/4)}], \; i = 1,3,\ldots,m, \tag{3.133}$$

and

$$u_{i(c)}^{(p+1)} = P_1^{-1}[\bar{P}_1\, u_{i(c)}^{(p)} + ru_{i(c)}^{(p+3/4)}], \quad i = 2,4,\ldots,m-1. \tag{3.134}$$

for computational purposes, we have:

a) for Eq. (3.133):

$$\left.\begin{aligned} u_{i,j}^{(p+1)} &= [r_1 z_{ij} - a_1 \bar{z}_{ij}]/\Delta, \\ u_{i,j+1}^{(p)} &= [-a_1 z_{ij} + r_1 \bar{z}_{ij}]/\Delta, \end{aligned}\right\} \; i = 1,3,\ldots,m; \quad j = 1,3,\ldots,n-2,$$

$$u_{i,n}^{(p+1)} = r_2 u_{i,n}^{(p)} + r_3 u_{i,n}^{(p+3/4)}, \quad i = 1,3,\ldots,m \tag{3.135}$$

and

b) for Eq. (3.134):

$$u_{i,1}^{(p+1)} = r_2 u_{i,1}^{(p)} + r_3 u_{i,1}^{(p+3/4)}, \quad i = 2,3,\ldots,m-1. \tag{3.136}$$

$$\left.\begin{aligned} u_{i,j}^{(p+1)} &= [r_1 z_{ij} - a_1 \bar{z}_{ij}]/\Delta, \\ u_{i,j+1}^{(p+1)} &= [-a_1 z_{ij} + r_1 \bar{z}_{ij}]/\Delta, \end{aligned}\right\} \quad i = 1, 2, 4, \ldots, m-1; \quad j = 2, 4, \ldots, n-1,$$

where

$$z_{ij} = \frac{c}{4} u_{ij}^{(p)} + a_1 u_{i,j+1}^{(p)} + r u_{ij}^{(p+3/4)}$$

and

$$\bar{z}_{ij} = a_1 u_{ij}^{(p)} + \frac{c}{4} u_{i,j+1}^{(p)} + r u_{i,j+1}^{(p+3/4)}.$$

Hence, the AGE scheme corresponds to sweeping through the mesh parallel to the coordinate x and y axes involving at each stage the solution of 2 x 2 block systems. The iterative procedure is $\left| u_{ij}^{(p+1)} - u_{ij}^{(p)} \right| \le \varepsilon$ is met where ε is the convergence criterion.