Numerical Solutions to Partial Differential Equations

Zhiping Li

LMAM and School of Mathematical Sciences
Peking University

A Model Problem in a 2D Box Region

Let us consider a model problem of parabolic equation:

$$\begin{aligned} u_t &= a\left(u_{xx} + u_{yy}\right), && (x, y) \in \Omega, \quad t > 0, \\ u(x, y, 0) &= u^0(x, y, 0), && (x, y) \in \overline{\Omega}, \\ u(x, y, t) &= 0, && (x, y) \in \partial\Omega, \quad t > 0, \end{aligned}$$

where $a > 0$ is a constant, $\Omega = (0,\ X) \times (0,\ Y) \subset \mathbb{R}^2$.

1. For integers $N_x \geq 1$ and $N_y \geq 1$, let $h_x = \triangle x = X N_x^{-1}$ and $h_y = \triangle y = Y N_y^{-1}$ be the grid sizes in the x and y directions;
2. a uniform parallelopiped grid with the set of grid nodes
$$J_{\Omega \times \mathbb{R}_+} = \{(x_j, y_k, t_m) : 0 \leq j \leq N_x,\ 0 \leq k \leq N_y,\ m \geq 0\},$$
where $x_j = j\, h_x,\ y_k = k\, h_y,\ t_m = m\tau$ ($\tau > 0$ time step size).
3. the space of grid functions
$$U = \{U_{j,k}^m = U(x_j, y_k, t_m) : 0 \leq j \leq N_x,\ 0 \leq k \leq N_y,\ m \geq 0\}.$$

The Forward Explicit Scheme in a 2D Box Region

The forward explicit scheme and its error equation

$$\frac{U_{j,k}^{m+1} - U_{j,k}^{m}}{\tau} = a\left[\frac{U_{j+1,k}^{m} - 2U_{j,k}^{m} + U_{j-1,k}^{m}}{h_x^2} + \frac{U_{j,k+1}^{m} - 2U_{j,k}^{m} + U_{j,k-1}^{m}}{h_y^2}\right].$$

$$e_{j,k}^{m+1} = \left[1 - 2(\mu_x + \mu_y)\right] e_{j,k}^{m} + \mu_x\left(e_{j+1,k}^{m} + e_{j-1,k}^{m}\right) + \mu_y\left(e_{j,k+1}^{m} + e_{j,k-1}^{m}\right) - T_{j,k}^{m}\tau,$$

where $\mu_x = \frac{a\,\tau}{h_x^2}$, $\mu_y = \frac{a\,\tau}{h_y^2}$ are the grid ratios in x and y directions.

The truncation error is

$$Tu(x,y,t) = \frac{1}{2}u_{tt}(x,y,t)\tau - \frac{a}{12}\left(\partial_x^4 u(x,y,t)h_x^2 + \partial_y^4 u(x,y,t)h_y^2\right) + O(\tau^2 + h_x^4 + h_y^4).$$

The Forward Explicit Scheme in a 2D Box Region

1. the condition for the maximum principle: $\mu_x + \mu_y \le \frac{1}{2}$;

2. Fourier modes and amplification factors $\lambda_{\mathbf{l}}$ ($\mathbf{l} = (l_x, l_y)$):
$U_{j,k}^m = \lambda_{\mathbf{l}}^m e^{\mathrm{i}(\alpha_x x_j + \alpha_y y_k)} = \lambda_{\mathbf{l}}^m e^{\mathrm{i}(l_x j\pi N_x^{-1} + l_y k\pi N_y^{-1})}$,
$\alpha_x = \frac{l_x \pi}{X}$, $-N_x + 1 \le l_x \le N_x$, $\alpha_y = \frac{l_y \pi}{Y}$, $-N_y + 1 \le l_y \le N_y$;
(l_x, l_y represent the frequency or wave number in x, y direction.)

3. amplification factor
$$\lambda_{\mathbf{l}} = 1 - 4\left[\mu_x \sin^2 \frac{\alpha_x h_x}{2} + \mu_y \sin^2 \frac{\alpha_y h_y}{2}\right] = 1 - 4\left[\mu_x \sin^2 \frac{l_x \pi}{2N_x} + \mu_y \sin^2 \frac{l_y \pi}{2N_x}\right];$$

4. $\mathbb{L}^2$ stable if and only if $\mu_x + \mu_y \le 1/2$;

5. Convergence rate is $O(\tau + h_x^2 + h_y^2)$.

The θ-Scheme in a 2D Box Region

$$\frac{U_{j,k}^{m+1} - U_{j,k}^{m}}{\tau} = (1-\theta)a\left[\frac{\delta_x^2}{h_x^2} + \frac{\delta_y^2}{h_y^2}\right]U_{j,k}^{m} + \theta a\left[\frac{\delta_x^2}{h_x^2} + \frac{\delta_y^2}{h_y^2}\right]U_{j,k}^{m+1}$$

$$= (1-\theta)a\left[\frac{U_{j+1,k}^{m} - 2U_{j,k}^{m} + U_{j-1,k}^{m}}{h_x^2} + \frac{U_{j,k+1}^{m} - 2U_{j,k}^{m} + U_{j,k-1}^{m}}{h_y^2}\right]$$

$$+ \theta a\left[\frac{U_{j+1,k}^{m+1} - 2U_{j,k}^{m+1} + U_{j-1,k}^{m+1}}{h_x^2} + \frac{U_{j,k+1}^{m+1} - 2U_{j,k}^{m+1} + U_{j,k-1}^{m+1}}{h_y^2}\right].$$

The error equation:

$$[(1+2\theta)(\mu_x + \mu_y)]\, e_{j,k}^{m+1} = \theta\left[\mu_x\left(e_{j+1,k}^{m+1} + e_{j-1,k}^{m+1}\right) + \mu_y\left(e_{j,k+1}^{m+1} + e_{j,k-1}^{m+1}\right)\right]$$

$$+ [1 - 2(1-\theta)(\mu_x + \mu_y)]\, e_{j,k}^{m}$$

$$+ (1-\theta)\left[\mu_x\left(e_{j+1,k}^{m} + e_{j-1,k}^{m}\right) + \mu_y\left(e_{j,k+1}^{m} + e_{j,k-1}^{m}\right)\right] - \tau T_{j,k}^{m+\frac{1}{2}},$$

The θ-Scheme in a 2D Box Region

The truncation error

$$T_j^{m+*} = \begin{cases} O(\tau^2 + h_x^2 + h_y^2), & \text{if } \theta = \frac{1}{2}, \\ O(\tau + h_x^2 + h_y^2), & \text{if } \theta \neq \frac{1}{2}, \end{cases}$$

1. the condition for the maximum principle: $2(\mu_x + \mu_y)(1 - \theta) \leq 1$;
2. Fourier modes: $U_{j,k}^m = \lambda_{\mathbf{l}}^m e^{\mathrm{i}(\alpha_x x_j + \alpha_y y_k)} = \lambda_{\mathbf{l}}^m e^{\mathrm{i}\left(\frac{l_x j\pi}{N_x} + \frac{l_y k\pi}{N_y}\right)}$,

   $\mathbf{l} = (l_x, l_y)$, $\alpha_x = \frac{l_x\pi}{X}$, $\alpha_y = \frac{l_y\pi}{Y}$, $\alpha_x x_j = \frac{l_x j\pi}{N_x}$, $\alpha_y y_k = \frac{l_y k\pi}{N_y}$;
3. amplification factor

$$\lambda_{\mathbf{l}} = \frac{1 - 4(1-\theta)\left[\mu_x \sin^2 \frac{l_x\pi}{2N_x} + \mu_y \sin^2 \frac{l_y\pi}{2N_x}\right]}{1 + 4\theta\left[\mu_x \sin^2 \frac{l_x\pi}{2N_x} + \mu_y \sin^2 \frac{l_y\pi}{2N_x}\right]};$$

The θ-Scheme in a 2D Box Region

4. for $\theta \geq 1/2$, unconditionally $\mathbb{L}^2$ stable;
5. for $0 \leq \theta < 1/2$, $\mathbb{L}^2$ stable iff $2(1-2\theta)(\mu_x + \mu_y) \leq 1$;
6. the matrix of the linear system is still symmetric positive definite and diagonal dominant, however, each row has now up to 5 nonzero elements with a band width of the order $O(h^{-1})$;
7. if solved by the Thompson method, the cost is $O(h^{-1})$ times of that of the explicit scheme;
8. in 3D, $\mu_x + \mu_y \Rightarrow \mu_x + \mu_y + \mu_z$, and $O(h^{-1}) \Rightarrow O(h^{-2})$, if solved by the Thompson method, the cost is $O(h^{-2})$ times of that of the explicit scheme.

Alternative Approaches for Solving n-D Parabolic Equations

To reduce the computational cost, we may consider to apply highly efficient iterative methods to solve the linear algebraic equations, for example,

- the preconditioned conjugate gradient method;
- the multi-grid method;
- etc..

Alternatively, to avoid the shortcoming of the implicit difference schemes for high space dimensions, we may develop

- the alternating direction implicit (ADI) schemes;
- the locally one dimensional (LOD) schemes.

A Fractional Steps 2D ADI Scheme by Peaceman and Rachford

1. in the odd fractional steps implicit in x and explicit in y, and in even fractional steps implicit in y and explicit in x:

$$
\begin{aligned}
\left(1 - \frac{1}{2}\mu_x \delta_x^2\right) U_{j,k}^{m+\frac{1}{2}} &= \left(1 + \frac{1}{2}\mu_y \delta_y^2\right) U_{j,k}^{m}, \\
\left(1 - \frac{1}{2}\mu_y \delta_y^2\right) U_{j,k}^{m+1} &= \left(1 + \frac{1}{2}\mu_x \delta_x^2\right) U_{j,k}^{m+\frac{1}{2}},
\end{aligned}
$$

2. numerical boundary conditions are easily imposed directly by those of the original problem, since $U_{j,k}^{m+\frac{1}{2}} \sim u_{j,k}^{m+\frac{1}{2}}$;

A Fractional Steps 2D ADI Scheme by Peaceman and Rachford

3. one step equivalent scheme

$$\left(1 - \frac{1}{2}\mu_x\delta_x^2\right)\left(1 - \frac{1}{2}\mu_y\delta_y^2\right)U_{j,k}^{m+1} = \left(1 + \frac{1}{2}\mu_x\delta_x^2\right)\left(1 + \frac{1}{2}\mu_y\delta_y^2\right)U_{j,k}^{m}.$$

4. Crank-Nicolson scheme

$$\left(1 - \frac{1}{2}\mu_x\delta_x^2 - \frac{1}{2}\mu_y\delta_y^2\right)U_{j,k}^{m+1} = \left(1 + \frac{1}{2}\mu_x\delta_x^2 + \frac{1}{2}\mu_y\delta_y^2\right)U_{j,k}^{m}.$$

5. Since $\mu_x\mu_y\delta_x^2\delta_y^2\delta_t u_{j,k}^{m+\frac{1}{2}} = a^2\,\tau^3\,[u_{xxyyt}]_{j,k}^{m+\frac{1}{2}} + O(\tau^5 + \tau^3(h_x^2 + h_y^2))$, the truncation error of the scheme is $O(\tau^2 + h_x^2 + h_y^2)$.

Stability of the 2D ADI Scheme by Peaceman and Rachford

1. For the Fourier mode $U_{j,k}^m = \lambda_{\mathbf{l}}^m e^{\mathrm{i}(l_x j\pi N_x^{-1} + l_y k\pi N_y^{-1})}$,

$$\lambda_{\mathbf{l}} = \frac{(1 - 2\,\mu_x \sin^2 \frac{l_x\pi}{2N_x})(1 - 2\,\mu_y \sin^2 \frac{l_y\pi}{2N_y})}{(1 + 2\,\mu_x \sin^2 \frac{l_x\pi}{2N_x})(1 + 2\,\mu_y \sin^2 \frac{l_y\pi}{2N_y})},$$

   the scheme is unconditionally $\mathbb{L}^2$ stable;

2. the two fractional steps can be equivalently written as

$$(1+\mu_x)U_{j,k}^{m+\frac{1}{2}} = (1-\mu_y)U_{j,k}^m + \frac{\mu_y}{2}\left(U_{j,k-1}^m + U_{j,k+1}^m\right) + \frac{\mu_x}{2}\left(U_{j-1,k}^{m+\frac{1}{2}} + U_{j+1,k}^{m+\frac{1}{2}}\right),$$

$$(1+\mu_y)U_{j,k}^{m+1} = (1-\mu_x)U_{j,k}^{m+\frac{1}{2}} + \frac{\mu_x}{2}\left(U_{j-1,k}^{m+\frac{1}{2}} + U_{j+1,k}^{m+\frac{1}{2}}\right) + \frac{\mu_y}{2}\left(U_{j,k-1}^{m+1} + U_{j,k+1}^{m+1}\right),$$

   thus, the maximum principle holds if $\max\{\mu_x, \mu_y\} \le 1$;

Cost of the 2D ADI Scheme by Peaceman and Rachford

1. order the linear system by $(N_x - 1)\,k + j$ and $(N_y - 1)\,j + k$ in odd and even steps, the corresponding matrixes are tridiagonal;
2. the computational cost: 3 times of that of the explicit scheme.

The Idea of Peaceman and Rachford Doesn't Work for 3D

In 3D, we can still construct fractional step scheme by

1. dividing each time step into 3 fractional steps;
2. introducing $U^{m+\frac{1}{3}}$ and $U^{m+\frac{2}{3}}$ at $t_{m+\frac{1}{3}}$ and $t_{m+\frac{2}{3}}$;
3. in the 3 fractional time steps, applying schemes which are in turn implicit in x-, y- and z-direction and explicit in the other 2 directions respectively.

However, the equivalent one step scheme is, up to a higher order term, the same as the θ-scheme with $\theta = 1/3$, which has a local truncation error $O(\tau + h_x^2 + h_y^2)$ instead of what we expect to have $O(\tau^2 + h_x^2 + h_y^2)$ for an ADI method.

The Key Properties that Make an ADI Scheme Successful

1. Implicit only in one dimension in each fractional time step, thus, if properly ordered, the matrix of the linear algebraic equations is tridiagonal as well as diagonally dominant, hence the computational cost is significantly reduced.

2. In the equivalent one step scheme, the implicit part is the product of 1D implicit difference operators, the explicit part is the product of 1D explicit difference operators (in a half time step, + certain h.o.t. small perturbations), which guarantees the scheme is unconditionally $\mathbb{L}^2$ stable;

3. The difference between the equivalent one step scheme and the Crank-Nicolson scheme is a higher order term, which guarantees that the local truncation error is $O(\tau^2 + h^2)$.

Target Equivalent One Step Schemes of ADI Methods

For the 3D model problem, we aim to develop ADI finite difference schemes which have a one time step equivalent scheme of the form

$$\left(1-\frac{1}{2}\mu_x\delta_x^2\right)\left(1-\frac{1}{2}\mu_y\delta_y^2\right)\left(1-\frac{1}{2}\mu_z\delta_z^2\right)U_{j,k,l}^{m+1}$$
$$=\left(1+\frac{1}{2}\mu_x\delta_x^2\right)\left(1+\frac{1}{2}\mu_y\delta_y^2\right)\left(1+\frac{1}{2}\mu_z\delta_z^2\right)U_{j,k,l}^{m},$$

or

$$\left(1-\frac{1}{2}\mu_x\delta_x^2\right)\left(1-\frac{1}{2}\mu_y\delta_y^2\right)\left(1-\frac{1}{2}\mu_z\delta_z^2\right)U_{j,k,l}^{m+1}$$
$$=\left(1+\frac{1}{2}\mu_x\delta_x^2\right)\left(1+\frac{1}{2}\mu_y\delta_y^2\right)\left(1+\frac{1}{2}\mu_z\delta_z^2\right)U_{j,k,l}^{m}+\text{h.o.t.}$$

An Extendable ADI Scheme Proposed by D'yakonov

For the 3D model problem, the ADI Scheme of D'yakonov is

$$\left(1 - \frac{\mu_x}{2}\delta_x^2\right) U_{j,k,l}^{m+*} = \left(1 + \frac{\mu_x}{2}\delta_x^2\right)\left(1 + \frac{\mu_y}{2}\delta_y^2\right)\left(1 + \frac{\mu_z}{2}\delta_z^2\right) U_{j,k,l}^{m},$$

$$\left(1 - \frac{\mu_y}{2}\delta_y^2\right) U_{j,k,l}^{m+**} = U_{j,k,l}^{m+*},$$

$$\left(1 - \frac{\mu_z}{2}\delta_z^2\right) U_{j,k,l}^{m+1} = U_{j,k,l}^{m+**}.$$

The scheme obviously has all the key properties. However, there is one thing need to be taken care of: U^{m+*}, U^{m+**} are not approximate solutions, their boundary conditions may not be directly derived from that of the original problem.

Numerical Boundary Conditions for U^{m+*}, U^{m+**}

Since $U_{j,k,l}^{m+1} \sim u_{j,k,l}^{m+1}$, $U_{j,k,l}^{m+1} = u_{j,k,l}^{m+1}$ on the boundary ($j = 0, N_x$, or $k = 0, N_y$, or $l = 0, N_z$). Thus, the boundary condition

$$\{U_{j,k,l}^{m+**} : j = 0, N_x,\ 0 \le k \le N_y,\ 0 < l < N_z, \text{or}\ \ k = 0, N_y;\ 0 \le j \le N_x,\ 0 < l < N_z\}$$

can be obtained from $U_{j,k,l}^{m+**} = \left(1 - \frac{\mu_z}{2}\delta_z^2\right) U_{j,k,l}^{m+1}$.

The boundary condition

$$\left\{U_{j,k,l}^{m+*} : j = 0, N_x,\ 0 < k < N_y,\ 0 < l < N_z\right\}.$$

can be obtained from $U_{j,k,l}^{m+*} = \left(1 - \frac{\mu_y}{2}\delta_y^2\right) U_{j,k,l}^{m+**}$ and the boundary values for $U_{j,k,l}^{m+**}$ on the nodes $j = 0, N_x$.

An Extendable ADI Scheme Proposed by Douglas and Rachford

For the 3D model problem, the Scheme is of the form

$$\begin{aligned}
U_{j,k,l}^{m+1*} &= U_{j,k,l}^{m} + \frac{1}{2}\mu_x\delta_x^2\left(U_{j,k,l}^{m+1*} + U_{j,k,l}^{m}\right) + \mu_y\delta_y^2 U_{j,k,l}^{m} + \mu_z\delta_z^2 U_{j,k,l}^{m},\\
U_{j,k,l}^{m+1**} &= U_{j,k,l}^{m+1*} + \frac{1}{2}\mu_y\delta_y^2\left(U_{j,k,l}^{m+1**} + U_{j,k,l}^{m}\right) - \mu_y\delta_y^2 U_{j,k,l}^{m},\\
U_{j,k,l}^{m+1} &= U_{j,k,l}^{m+1**} + \frac{1}{2}\mu_z\delta_z^2\left(U_{j,k,l}^{m+1} + U_{j,k,l}^{m}\right) - \mu_z\delta_z^2 U_{j,k,l}^{m}.
\end{aligned}$$

Since U^{m+1*} and U^{m+1**} are approximate solutions at t_{m+1}, their boundary conditions can be directly derived from that of the original problem.The scheme has all the key properties with the h.o.t.$= -\frac{1}{4}\mu_x\mu_y\mu_z\delta_x^2\delta_y^2\delta_z^2 U_{j,k,l}^{m}$.

The Idea of the ADI Scheme of Douglas and Rachford

The construction of the scheme may be viewed as a prediction-correction process, which may also be explained as follows:

In the 1st fractional step, Crank-Nicolson to x, explicit to y, z.

In the 2nd fractional step, to improve stability and accuracy in y, the y-direction is corrected by the Crank-Nicolson scheme:

$$\begin{aligned} U_{j,k,l}^{m+1**} = U_{j,k,l}^{m} &+ \frac{1}{2}\mu_x\delta_x^2\left(U_{j,k,l}^{m+1*} + U_{j,k,l}^{m}\right) \\ &+ \frac{1}{2}\mu_y\delta_y^2\left(U_{j,k,l}^{m+1**} + U_{j,k,l}^{m}\right) + \mu_z\delta_z^2 U_{j,k,l}^{m}. \end{aligned}$$

Note, this minus the 1st equation gives the second in the scheme.

The Idea of the ADI Scheme of Douglas and Rachford

In the 3rd, z-direction is corrected by the Crank-Nicolson scheme:

$$
\begin{aligned}
U_{j,k,l}^{m+1} = U_{j,k,l}^{m} &+ \frac{1}{2}\mu_x \delta_x^2 \left(U_{j,k,l}^{m+1*} + U_{j,k,l}^{m} \right) \\
&+ \frac{1}{2}\mu_y \delta_y^2 \left(U_{j,k,l}^{m+1**} + U_{j,k,l}^{m} \right) + \frac{1}{2}\mu_z \delta_z^2 \left(U_{j,k,l}^{m+1} + U_{j,k,l}^{m} \right).
\end{aligned}
$$

Note, the 3rd equation in the scheme is simply the difference of the above two equations.

Since $U_{j,k,l}^{m+1*}$ and $U_{j,k,l}^{m+1**}$ are approximations of $U_{j,k,l}^{m+1}$, numerical boundary conditions can be directly derived from those of the original problem.

An Extendable Locally One Dimensional (LOD) Scheme

1. In the ith fractional step, the problem is treated as a one dimensional problem of the ith dimension.
2. 1D Crank-Nicolson scheme is applied to each fractional step.
3. For the 3D model problem, the LOD scheme is given as

$$\begin{aligned}
\left(1-\frac{1}{2}\mu_x\delta_x^2\right)U_{j,k,l}^{m+*} &= \left(1+\frac{1}{2}\mu_x\delta_x^2\right)U_{j,k,l}^{m}, \\
\left(1-\frac{1}{2}\mu_y\delta_y^2\right)U_{j,k,l}^{m+**} &= \left(1+\frac{1}{2}\mu_y\delta_y^2\right)U_{j,k,l}^{m+*}, \\
\left(1-\frac{1}{2}\mu_z\delta_z^2\right)U_{j,k,l}^{m+1} &= \left(1+\frac{1}{2}\mu_z\delta_z^2\right)U_{j,k,l}^{m+**}.
\end{aligned}$$

4. The scheme has all of the key properties.

Impose Boundary Conditions for the LOD Scheme

However, U^{m+*}, U^{m+**} are nonphysical, their boundary conditions must be handled with special care.

1. multiplying $(1 - \frac{1}{2}\mu_z\delta_z^2)$ on the 3rd equation leads to

$$\left(1 - \frac{1}{4}\mu_z^2\delta_z^4\right) U_{j,k,l}^{m+**} = \left(1 - \mu_z\delta_z^2 + \frac{1}{4}\mu_z^2\delta_z^4\right) U_{j,k,l}^{m+1},$$

Hence, by omitting the $O(\tau^2)$ order terms, the boundary condition for U^{m+**} can be given by:

$$U_{j,k,l}^{m+**} = \left(1 - \mu_z\delta_z^2\right) U_{j,k,l}^{m+1},$$
$$k = 0, N_y,\ 0 \le j \le N_x,\ 0 < l < N_z,$$
$$j = 0, N_x,\ 0 \le k \le N_y,\ 0 < l < N_z.$$

Impose Boundary Conditions for the LOD Scheme

2. Similarly, multiplying $(1 - \frac{1}{2}\mu_y \delta_y^2)$ on the 2nd equation, omitting the $O(\tau^2)$ and higher order terms, the boundary condition for U^{m+*} can be given by:

$$U_{j,k,l}^{m+*} = \left(1 - \mu_y \delta_y^2\right) U_{j,k,l}^{m+**},$$
$$j = 0, N_x,\ 0 < k < N_y,\ 0 < l < N_z.$$

General Domain and Boundary Conditions

1. Approximate boundary conditions can be established with the similar methods used in § 1.3.4 for elliptic problems.
2. Approximate boundary conditions can further restrict the stability condition for explicit schemes, thus implicit schemes are even more preferable.
3. ADI and LOD schemes are in more complicated forms.
4. Some special regions with non-planar boundaries can be transformed into box regions by curvilinear coordinate systems, say, the polar coordinate system can be used for a circular region; and the cylindrical coordinate system can be used for cylindrical regions, etc...

Variable-coefficient and nonlinear Equations

1. ADI and LOD schemes can also be extended to high dimensional variable-coefficient linear, and even certain nonlinear problems.

2. In such cases, the difference operators $(1 \pm \frac{1}{2}\mu_x\delta_x^2)$ and $(1 \pm \frac{1}{2}\mu_y\delta_y^2)$ are generally noncommutative, *i.e.*

$$\left(1 \pm \frac{1}{2}\mu_x\delta_x^2\right)\left(1 \pm \frac{1}{2}\mu_y\delta_y^2\right) \neq \left(1 \pm \frac{1}{2}\mu_y\delta_y^2\right)\left(1 \pm \frac{1}{2}\mu_x\delta_x^2\right),$$

and this will introduce the so called splitting error.

3. Boundary conditions are more difficult to handle.

Implicit, Semi-implicit Schemes

For nonlinear problems, nonlinear algebraic equations derived from implicit schemes need to be solved with iterative methods, such as semi-implicit schemes.

The idea is to

- apply an implicit scheme only to the principal linear part of the nonlinear equation;
- approximate the residual nonlinear part by an explicit scheme.

Implicit, Semi-implicit Schemes and Elliptic Solver

To apply the implicit schemes to linear parabolic problems and the semi-implicit schemes to nonlinear parabolic problems, **it is a sequence of linear algebraic systems corresponding to certain elliptic problems we actually need to solve in the end**.

So, Fast solvers for elliptic problems play important roles in solving parabolic problems.

Asymptotic Analysis and Extrapolation Methods

The asymptotic analysis and extrapolation methods introduced in § 1.5 for elliptic problems can also be extended to analyze the finite difference approximation error for parabolic problems.

In particular, the error bounds can be estimated by the numerical solutions obtained on grids with different mesh sizes.

For example, for the explicit scheme of the heat equation, let $\tau = \mu h^2$, $\mu \leq 1/2$, then, we have $U^m_{(h)j} = u^m_{(h)j} + O(h^2) + O(h^4)$,

$$U^{(1)m}_j \triangleq \frac{4U^{4m}_{(h/2)2j} - U^m_{(h)j}}{3} = u^m_{(h)j} + O(h^4).$$

n-D 1st Order Linear Hyperbolic Partial Differential Equation:

1. Scalar case ($u \in \mathbb{R}^1$), $\quad u_t + \sum_{i=1}^{n} a_i\, u_{x_i} + b\, u = \psi_0,$

   where a_i, b and ψ_0 are real functions $x = (x_1, \ldots, x_n)$ and t.

2. Vector case ($\mathbf{u} = (u_1, \cdots, u_p)^T \in \mathbb{R}^p$),

$$\mathbf{u}_t + \sum_{i=1}^{n} A_i\, \mathbf{u}_{x_i} + B\, \mathbf{u} = \boldsymbol{\psi}_0,$$

   where A_i, $B \in \mathbb{R}^{p \times p}$, $\boldsymbol{\psi}_0 \in \mathbb{R}^p$ are real functions of t and $x = (x_1, \ldots, x_n)$, and $\forall \boldsymbol{\alpha} \in \mathbb{R}^n$, $A(x,t) = \sum_{i=1}^{n} \alpha_i A_i(x,t)$ is real diagonalizable, *i.e.* $A(x,t)$ has p linearly independent eigenvectors corresponding to real eigenvalues.

3. If $A(x,t) = \sum_{i=1}^{n} \alpha_i A_i(x,t)$ has p mutually different real eigenvalues, the system is called strictly hyperbolic.

n-D 2nd Order Linear Hyperbolic Partial Differential Equation

- A general 2nd order scalar equation ($u \in \mathbb{R}^1$),

$$u_{tt} + 2\sum_{i=1}^{n} a_i\, u_{x_i t} + b_0\, u_t - \sum_{i,j=1}^{n} a_{ij}\, u_{x_i x_j} + \sum_{i=1}^{n} b_i\, u_{x_i} + cu = \psi_0,$$

  where a_i, a_{ij}, b_i, c and ψ_0 are real functions $x = (x_1, \ldots, x_n)$ and t, (a_{ij}) is real symmetric positive definite.

- Define $v = u$, $v_0 = u_t$, $v_i = u_{x_i}$, then the above 2nd order scalar equation transforms into a first order linear system of partial differential equations for $\mathbf{v} = (v, v_0, v_1, \cdots, v_n)^T$

$$A\mathbf{v}_t + \sum_{i=1}^{n} A_i \mathbf{v}_{x_i} + B\mathbf{v} = \boldsymbol{\psi}_0,$$

n-D 2nd Order Scalar Transforms to n-D 1st Order System ($p = n + 2$)

$$A = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & a_{11} & \cdots & a_{1n} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & a_{n1} & \cdots & a_{nn} \end{bmatrix}, \qquad A_i = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 2a_i & -a_{1i} & \cdots & -a_{ni} \\ 0 & -a_{1i} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & -a_{ni} & & & \end{bmatrix},$$

$$B = \begin{bmatrix} 0 & -1 & 0 & \cdots & 0 \\ c & b_0 & b_1 & \cdots & b_n \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, \qquad \psi_0 = \begin{bmatrix} 0 \\ \psi_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

n-D 2nd Order Scalar Transforms to n-D 1st Order System ($p = n + 2$)

1. Let $R^T A R = I$ (A is real symmetric positive definite);
2. Introduce a new variable $\mathbf{w} = R^{-1}\mathbf{v}$;
3. Denote $\hat{A}_i = R^T A_i R$, $\hat{B} = R^T B R$, $\hat{\psi}_0 = R^T \psi$;
4. $\hat{A}(x,t) = \sum_{i=1}^n \alpha_i \hat{A}_i(x,t)$ is a real symmetric matrix and thus is real diagonizable for all real α_i, $i = 1, \ldots, n$;
5. The 2nd order scalar equation now transforms into a 1st order linear hyperbolic system of partial differential equations for $\mathbf{w} \in \mathbb{R}^{(n+2)}$:
$$\mathbf{w}_t + \sum_{i=1}^{n} \hat{A}_i \mathbf{w}_{x_i} + \hat{B}\mathbf{w} = \hat{\psi}_0.$$

Standard Form of *n*-D 1st Order Linear Hyperbolic Equations

1. The standard form of 1st order linear hyperbolic equation:

$$u_t + \sum_{i=1}^{n} a_i\, u_{x_i} = \psi, \quad (\psi = \psi_0 - b\, u).$$

2. The standard form of 1st order linear hyperbolic system:

$$\mathbf{u}_t + \sum_{i=1}^{n} A_i\, \mathbf{u}_{x_i} = \boldsymbol{\psi}, \quad (\boldsymbol{\psi} = \boldsymbol{\psi}_0 - B\, \mathbf{u});$$

3. The equation (system) is said to be homogeneous, if $\psi = 0$;

Standard Form of *n*-D 1st Order Linear Hyperbolic Equations

4. In general, a higher order linear hyperbolic equation (system of equations) can always be transformed into a first order linear hyperbolic system of equations.

5. An equation (system) is said to be nonlinear, if at least one of the coefficients depends on the unknown or the right hand side term is a nonlinear function of the unknown.

Thank You!

习题 2：20，21