Chapter 5

Multi-Dimensional Parabolic Problems

5.1 Alternating Direction Implicit (ADI) Methods

We would like to extend the one-dimensional explicit and implicit finite difference schemes that we have been studying to multi-dimensional parabolic problems. As a representative example, consider the three-dimensional heat conduction equation

$$\rho c u_t = \nabla \cdot (k \nabla u) = \frac{\partial}{\partial x}(k \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(k \frac{\partial u}{\partial y}) + \frac{\partial}{\partial z}(k \frac{\partial u}{\partial z}), \qquad (x, y, z) \in \Omega, \qquad t > 0, \tag{5.1.1a}$$

subject to the initial and boundary conditions

$$u(x, y, z, 0) = \phi(x, y, z), \qquad (x, y, z) \in \Omega \cup \partial\Omega, \tag{5.1.1b}$$

$$\alpha u + \beta u_{\mathbf{n}} = \gamma, \qquad (x, y, z) \in \partial\Omega, \qquad t > 0. \tag{5.1.1c}$$

As in one dimension, u is the temperature in a solid having density ρ, specific heat c, and thermal conductivity k. The temperature is to be determined for spatial coordinates (x, y, z) in the three-dimensional region Ω and times $t > 0$. The boundary $\partial\Omega$ of Ω has unit outer normal vector $\mathbf{n}$.

Constructing a mesh for problems such as (5.1.1) on arbitrary regions is a major undertaking. Let's postpone it to Chapter 8 and first tackle problems on rectangular or hexahedral regions. In fact, let's begin with the two-dimensional, constant-coefficient,

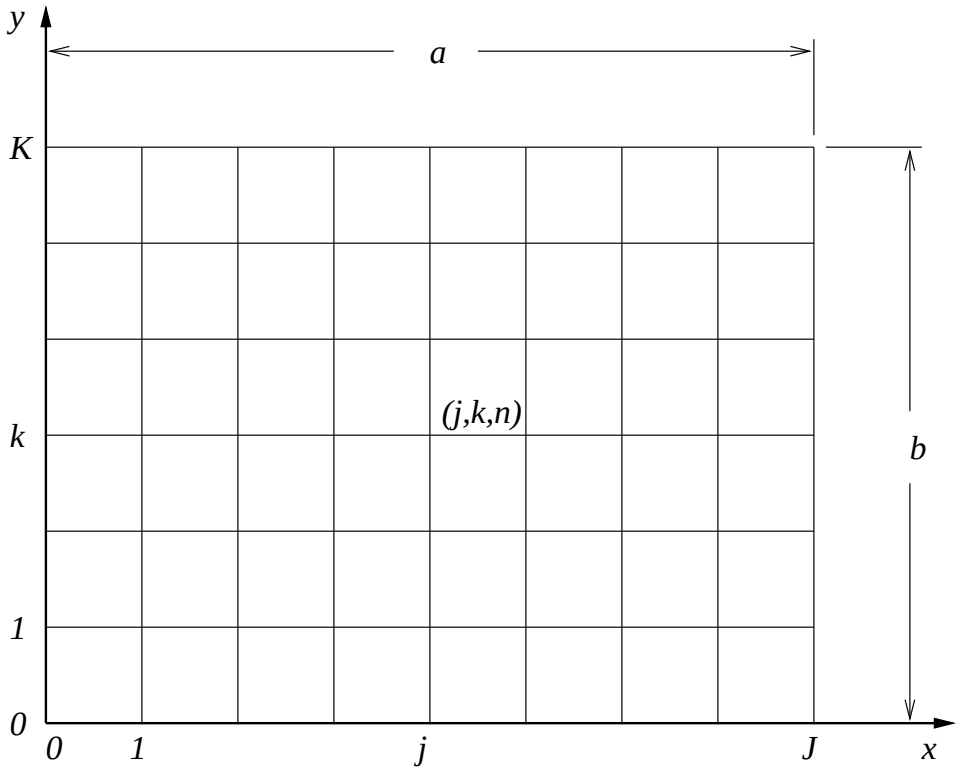

Figure 5.1.1: Two-dimensional rectangular domain Ω and the uniform mesh used for finite difference approximations.

Dirichlet problem

$$u_t = \sigma(u_{xx} + u_{yy}), \qquad (x,y) \in \Omega, \qquad t > 0, \tag{5.1.2a}$$

$$u(x,y,0) = \phi(x,y), \qquad (x,y) \in \Omega \cup \partial\Omega, \tag{5.1.2b}$$

$$u(x,y,t) = \gamma(x,y,t), \qquad (x,y) \in \partial\Omega, \qquad t > 0, \tag{5.1.2c}$$

where Ω is the rectangular region $\{(x,y) \mid 0 < x < a,\ 0 < y < b\}$ shown in Figure 5.1.1.

Introduce a uniform rectangular grid of spacing $\Delta x \times \Delta y$ on Ω with $\Delta x = a/J$ and $\Delta y = b/K$ and partition time into planes parallel to the x, y-plane separated by a distance Δt (Figure 5.1.1. Following the one-dimensional notation, let $U^n_{j,k}$ denote the finite difference approximation of $u^n_{j,k} = u(j\Delta x, k\Delta y, n\Delta t)$.

The extension of the explicit scheme (4.1.2) to two spatial dimensions is straight forward and is given by

$$\frac{U^{n+1}_{j,k} - U^n_{j,k}}{\Delta t} = \sigma \left[\frac{\delta_x^2 U^n_{j,k}}{\Delta x^2} + \frac{\delta_y^2 U^n_{j,k}}{\Delta y^2} \right],$$

where the central difference operators δ_x and δ_y are defined in accordance with Table 2.1.1, but involve differences of the j and k indices, respectively, of $U^n_{j,k}$. Thus,

$$\delta_x^2 U^n_{j,k} = U^n_{j-1,k} - 2U^n_{j,k} + U^n_{j+1,k}, \qquad \delta_y^2 U^n_{j,k} = U^n_{j,k-1} - 2U^n_{j,k} + U^n_{j,k+1}.$$

Solving for $U^{n+1}_{j,k}$,

$$U^{n+1}_{j,k} = r_x(U^n_{j-1,k} + U^n_{j+1,k}) + r_y(U^n_{j,k-1} + U^n_{j,k+1}) + (1 - 2r_x - 2r_y)U^n_{j,k}, \tag{5.1.3a}$$

where

$$r_x = \frac{\sigma \Delta t}{\Delta x^2}, \qquad r_y = \frac{\sigma \Delta t}{\Delta y^2}. \tag{5.1.3b}$$

The computational stencil for (5.1.3) is shown in Figure 5.1.2. The scheme is used exactly as in one dimension. Thus, beginning with the initial conditions

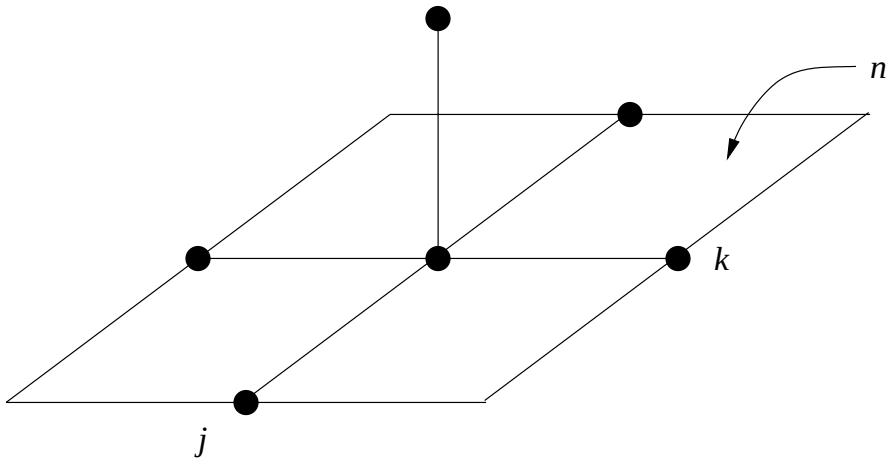

Figure 5.1.2: Computational stencil for the explicit scheme (5.1.3).

$$U^0_{j,k} = \phi(j\Delta x, k\Delta y), \qquad j = 0, 1, \ldots, J, \qquad k = 0, 1, \ldots, K, \tag{5.1.3c}$$

and assuming that the solution $U^n_{j,k}$, $j = 0, 1, \ldots, J$, $k = 0, 1, \ldots, K$, has been calculated, (5.1.3a) is used to compute $U^{n+1}_{j,k}$ at all interior points $j = 1, 2, \ldots, J-1$, $k = 1, 2, \ldots, K-1$. The boundary conditions

$$U^{n+1}_{j,k} = \gamma(j\Delta x, k\Delta y, (n+1)\Delta t), \qquad j = 0, J, \qquad k = 0, K, \tag{5.1.3d}$$

furnish the solution on $\partial\Omega$.

Absolute stability of (5.1.3a) is assured in the maximum norm when

$$r_x + r_y \leq 1/2.$$

If $\Delta x = \Delta y$ the stability requirement is $\sigma \Delta t / \Delta x^2 \leq 1/4$, which is more restrictive than in one dimension. Thus, there is an even greater motivation to study implicit methods in two dimensions.

When the Crank-Nicolson method is applied to (5.1.2), we find

$$\frac{U_{j,k}^{n+1} - U_{j,k}^{n}}{\Delta t} = \sigma \left[\frac{\delta_x^2}{\Delta x^2} \frac{(U_{j,k}^{n+1} + U_{j,k}^{n})}{2} + \frac{\delta_y^2}{\Delta y^2} \frac{(U_{j,k}^{n+1} + U_{j,k}^{n})}{2} \right],$$

or

$$[1 - \frac{r_x \delta_x^2 + r_y \delta_y^2}{2}] U_{j,k}^{n+1} = [1 + \frac{r_x \delta_x^2 + r_y \delta_y^2}{2}] U_{j,k}^{n}. \tag{5.1.4a}$$

The computational stencil of (5.1.4a) is shown in Figure 5.1.3.

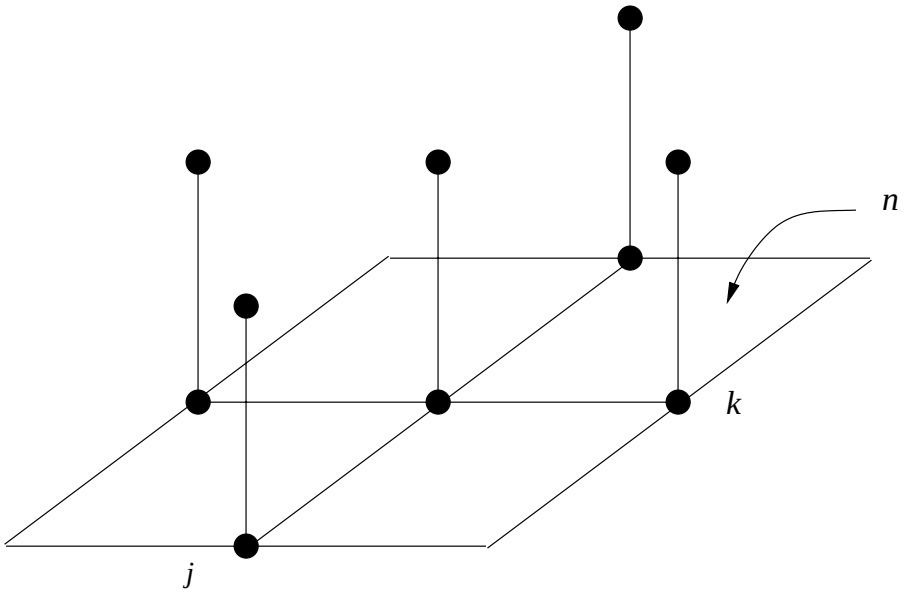

Figure 5.1.3: Computational stencil for the Crank-Nicolson scheme (5.1.4).

For simplicity, assume that trivial boundary data is prescribed, *i.e.*, $\gamma = 0$ in (5.1.2c); order the equations (5.1.4a) and unknowns by rows; and write (5.1.4a) in the matrix form

$$(\mathbf{I} + \frac{1}{2}\mathbf{C})\mathbf{U}^{n+1} = (\mathbf{I} - \frac{1}{2}\mathbf{C})\mathbf{U}^{n}, \tag{5.1.4b}$$

where

$$\mathbf{U}^n = [U^n_{1,1}, \ldots, U^n_{J-1,1}, U^n_{1,2}, \ldots, U^n_{J-1,2}, \ldots, U^n_{1,K-1}, \ldots, U^n_{J-1,K-1}]^T, \tag{5.1.4c}$$

$$\mathbf{C} = \begin{bmatrix} \mathbf{D}_x & \mathbf{D}_y & & \\ \mathbf{D}_y & \mathbf{D}_x & \mathbf{D}_y & \\ & & \ddots & \\ & & \mathbf{D}_y & \mathbf{D}_x \end{bmatrix}, \tag{5.1.4d}$$

$$\mathbf{D}_x = \begin{bmatrix} a & b & & \\ b & a & b & \\ & & \ddots & \\ & & b & a \end{bmatrix}, \qquad \mathbf{D}_y = \begin{bmatrix} c & & & \\ & c & & \\ & & \ddots & \\ & & & c \end{bmatrix}, \tag{5.1.4e}$$

and

$$a = 2(r_x + r_y), \qquad b = -r_x, \qquad c = -r_y. \tag{5.1.4f}$$

The matrices $\mathbf{D}_x$ and $\mathbf{D}_y$ are $(J-1)\times(J-1)$ tridiagonal and diagonal matrices, respectively, so $\mathbf{C}$ is a $(J-1)(K-1)\times(J-1)(K-1)$ block tridiagonal matrix. This system may be solved by an extension of the tridiagonal algorithm (Figure 4.1.4) to block systems ([3], Chapter 2); however, this method requires approximately $(5/3)KJ^3$ multiplications per time step. This would normally be too expensive for practical computation. Iterative solution techniques can reduce the computational cost and we will reconsider these in Chapter 9. For the present, let us discuss a solution scheme called the *alternating direction implicit (ADI)* method. Variations of this method were introduced by Douglas [1] and Peaceman and Rachford [5].

The ADI method is a *predictor-corrector* scheme where part of the difference operator is implicit in the initial (prediction) step and another part is implicit in the final (correction) step. In the Peaceman-Rachford [5] variant of ADI, the predictor step consists of solving (5.1.2) for a time step $\Delta t/2$ using the backward Euler method for the x derivative terms and the forward Euler method for the y derivative terms, *i.e.*,

$$U^{n+1/2}_{j,k} = U^n_{j,k} + \frac{r_x}{2}\delta_x^2 U^{n+1/2}_{j,k} + \frac{r_y}{2}\delta_y^2 U^n_{j,k}. \tag{5.1.5a}$$

The corrector step completes the solution process for a time step by using the forward Euler method for x derivative terms and the backward Euler method for y derivative terms; thus,

$$U_{j,k}^{n+1} = U_{j,k}^{n+1/2} + \frac{r_x}{2}\delta_x^2 U_{j,k}^{n+1/2} + \frac{r_y}{2}\delta_y^2 U_{j,k}^{n+1}. \tag{5.1.5b}$$

The computation stencils for both the predictor and corrector steps are shown in Figure 5.1.4. The predictor (5.1.5a) is implicit in the x direction and the corrector (5.1.5b) is implicit in the y direction.

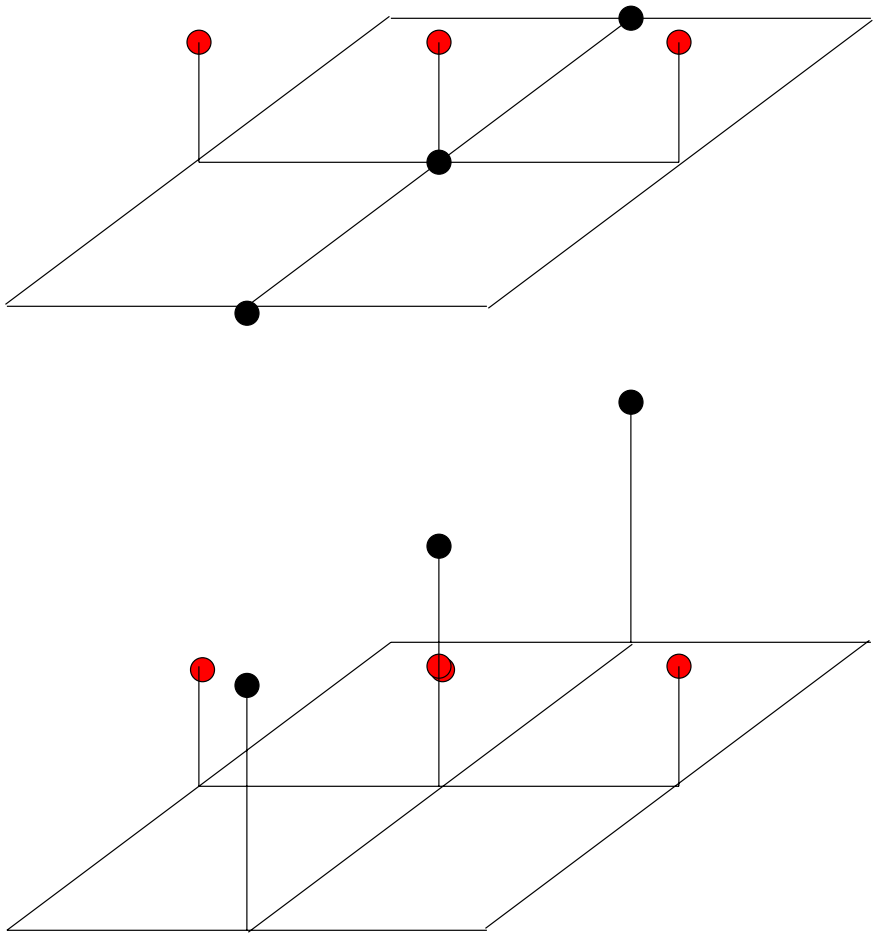

Figure 5.1.4: Computational stencil for the predictor (top) and corrector (bottom) steps of the ADI method (5.1.5a, 5.1.5b). Predicted solutions are shown in red and corrected solutions are black.

On a rectangular region, the predictor equations (5.1.5a) are solved by the tridiagonal algorithm with the unknowns ordered by rows. Thus, assuming that Dirichlet boundary

data is prescribed, we write (5.1.5a) at all interior points $j = 1, 2, \ldots, J-1$, in a given row k to obtain

$$(\mathbf{I} + \mathbf{C}_x)\mathbf{U}_k^{n+1/2} = \mathbf{g}_{y,k}^n, \tag{5.1.6a}$$

where

$$\mathbf{U}_k^{n+1/2} = \begin{bmatrix} U_{1,k}^{n+1/2} \\ U_{2,k}^{n+1/2} \\ \vdots \\ U_{J-1,k}^{n+1/2} \end{bmatrix}, \qquad \mathbf{C}_x = \frac{r_x}{2}\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & \\ & & -1 & 2 \end{bmatrix}, \tag{5.1.6b}$$

$$\mathbf{g}_{y,k}^n = \begin{bmatrix} U_{1,k}^n + r_y\delta_y^2 U_{1,k}^n/2 \\ \vdots \\ U_{J-1,k}^n + r_y\delta_y^2 U_{J-1,k}^n/2 \end{bmatrix}. \tag{5.1.6c}$$

Thus, $\mathbf{U}_k^{n+1/2}$ is determined by solving (5.1.6) using the tridiagonal algorithm for all interior rows $k = 1, 2, \ldots, K-1$.

The corrector system (5.1.5b) is solved by ordering the unknowns by columns. In particular, writing (5.1.5b) for all interior points in column j gives

$$(\mathbf{I} + \mathbf{C}_y)\mathbf{U}_j^{n+1} = \mathbf{g}_{x,j}^{n+1/2}, \tag{5.1.7}$$

where $\mathbf{U}_j^n$, $\mathbf{C}_y$, and $\mathbf{g}_{x,j}^{n+1/2}$ follow from (5.1.6b, 5.1.6c) upon replacement of x by y and k by j and interchange of the spatial subscripts. Equation (5.1.7) is then solved by columns for $j = 1, 2, \ldots, J-1$, using the tridiagonal algorithm.

The horizontal predictor sweep requires the solution of $K-1$ tridiagonal systems of dimension $J-1$. Each tridiagonal system requires approximately $5J$ operations, where an operation is one multiplication or division plus one addition or subtaction (*cf.* Section 4.1). Thus, the predictor step requires approximately $5JK$ operations. Similarly, in the corrector step, we have to solve $J-1$ tridiagonal systems of dimension $K-1$, which also require approximately $5JK$ operations. Therefore, the total operation count per time step is $10JK$ operations, which would normally be far less than the $(5/3)KJ^3$ operations needed for the block tridiagonal algorithm.

The local discretization error for multi-dimensional problems is defined exactly the same as for one-dimensional problems (Definition 3.1.1). The intermediate ADI solution introduces an added complication; thus, we have to either combine separate estimates of the local discretization errors of the predictor and corrector steps or eliminate $U_{j,k}^{n+1/2}$ from (5.1.5b). The latter course is the simpler of the two for this application since $U_{j,k}^{n+1/2}$ may be eliminated by adding and subtracting (5.1.5a) and (5.1.5b). The result is

$$U_{j,k}^{n+1} - U_{j,k}^{n} = r_x \delta_x^2 U_{j,k}^{n+1/2} + \frac{r_y}{2}\delta_y^2 (U_{j,k}^{n+1} + U_{j,k}^{n}),$$

$$U_{j,k}^{n+1/2} = \frac{1}{2}(U_{j,k}^{n+1} + U_{j,k}^{n}) - \frac{r_y}{4}\delta_y^2 (U_{j,k}^{n+1} - U_{j,k}^{n}).$$

Substituting the second equation into the first

$$U_{j,k}^{n+1} - U_{j,k}^{n} = \frac{1}{2}(r_x\delta_x^2 + r_y\delta_y^2)(U_{j,k}^{n+1} + U_{j,k}^{n}) - \frac{r_x r_y}{4}\delta_x^2\delta_y^2 (U_{j,k}^{n+1} - U_{j,k}^{n}).$$

Dividing by Δt, gathering all terms on the right side, replacing the numerical approximation by any smooth function, *e.g.*, the exact solution of the differential equation, and subtracting the result from the differential equation (5.1.2a) yields the local discretization error as

$$\Delta t \tau_{j,k}^{n} = \Delta t(u_t - \sigma u_{xx} - \sigma u_{yy})|_{j,k}^{n} - (1 - \frac{r_x}{2}\delta_x^2 - \frac{r_y}{2}\delta_y^2)u_{j,k}^{n+1} + (1 + \frac{r_x}{2}\delta_x^2 + \frac{r_y}{2}\delta_y^2)u_{j,k}^{n}$$
$$-\frac{r_x r_y}{4}\delta_x^2\delta_y^2(u_{j,k}^{n+1} - u_{j,k}^{n}).$$

Remark 1. The term $\Delta t\tau_{j,k}^{n}$ is not the local error. Since this scheme is implicit, the expression for the local error is more complex.

The first three terms of the above expression are the product of Δt and the local discretization error of the Crank-Nicolson scheme (5.1.4a), *i.e.*,

$$\Delta t(\tau_{j,k}^{n})_{CN} = \Delta t(u_t - \sigma u_{xx} - \sigma u_{yy})|_{j,k}^{n} - (1 - \frac{r_x}{2}\delta_x^2 - \frac{r_y}{2}\delta_y^2)u_{j,k}^{n+1} + (1 + \frac{r_x}{2}\delta_x^2 + \frac{r_y}{2}\delta_y^2)u_{j,k}^{n}.$$

A Taylor's series expansion would reveal that

$$(\tau_{j,k}^{n})_{CN} = O(\Delta x^2) + O(\Delta y^2) + O(\Delta t^2).$$

Expanding the remaining term in a Taylor's series yields

$$\frac{r_x r_y}{4}\delta_x^2\delta_y^2(u_{j,k}^{n+1} - u_{j,k}^{n}) = \frac{r_x r_y}{4}\delta_x^2\delta_y^2\delta_t u_{j,k}^{n+1/2} = \frac{\sigma^2}{4}\Delta t^3[(u_{txxyy})_{j,k}^{n+1/2} + \ldots].$$

Thus, the local discretization error of the ADI method is

$$\tau_{j,k}^n = (\tau_{j,k}^n)_{CN} + O(\Delta t^2) = O(\Delta x^2) + O(\Delta y^2) + O(\Delta t^2),$$

which is the same order as that of the Crank-Nicolson method.

The stability of (5.1.5) can be analyzed by the von Neumann method. The two-dimensional form of the discrete Fourier series is

$$U_{j,k}^n = \sum_{p=0}^{J-1} \sum_{q=0}^{K-1} A_{p,q}^n e^{2\pi i(pj/J + qk/K)}. \tag{5.1.8a}$$

Substituting into (5.1.5 and proceeding as in one dimension, we find

$$A_{p,q}^n = (M_{p,q})^n A_{p,q}^0, \tag{5.1.8b}$$

where $A_{p,q}^0$ is a Fourier component of the initial data and $M_{p,q}$ is the amplification factor. Again, following the one-dimensional analysis, we verify that $|M_{p,q}| \leq 1$ for all positve r_x and r_y; hence, the Peaceman-Rachford version of the ADI method (5.1.5) is unconditionally stable.

5.2 Operator Splitting Methods

The ADI approach is often difficult to extend to problems on non-rectangular domains, to nonlinear problems, and to problems having mixed derivatives such as u_{xy}. The dimensional reduction developed for the ADI method can be viewed as an approximate factorization of the differential or discrete operator. Let us motivate the factorization by first examining the ordinary differential equation

$$\frac{dy}{dt} = (a + b)y$$

which, of course, has the solution

$$y(t) = e^{t(a+b)}y(0) = e^{ta}e^{tb}y(0).$$

The latter form suggests that the solution of the initial value problem may be obtained by first solving $dy/dt = by$ to time t with $y(0)$ prescribed as initial data, and then solving

$dy/dt = ay$ subject to the initial condition $e^{tb}y(0)$. This interpretation, however, does not extend to vector systems of the form

$$\frac{d\mathbf{y}}{dt} = (\mathbf{A} + \mathbf{B})\mathbf{y}$$

unless $\mathbf{A}$ and $\mathbf{B}$ commute. Thus, we may write the solution of the vector problem as

$$\mathbf{y}(t) = e^{t(\mathbf{A}+\mathbf{B})}\mathbf{y}(0),$$

where

$$e^{t\mathbf{C}} = \mathbf{I} + t\mathbf{C} + \frac{t^2}{2!}\mathbf{C}^2 + \dots .$$

However,

$$\mathbf{y(t)} = \mathbf{e^{t(A+B)}y(0)} \neq \mathbf{e^{tA}e^{tB}y(0)}$$

unless $\mathbf{AB} = \mathbf{BA}$. Nevertheless, let's push on and consider a linear partial differential equation

$$u_t = \mathcal{L}u = (\mathcal{L}_1 + \mathcal{L}_2)u, \tag{5.2.1}$$

where $\mathcal{L}$ is a spatial differential operator that has been split into the sum of $\mathcal{L}_1$ and $\mathcal{L}_2$. We'll think of $\mathcal{L}_1$ as being associated with x derivatives and $\mathcal{L}_2$ as being associated with y derivatives, but this is not necessary. Any splitting will do.

The solution of the linear partial differential equation can also be written as the exponential

$$u(x, y, t) = e^{t\mathcal{L}}u(x, y, 0)$$

when $\mathcal{L}$ is independent of t. The interpretation of the exponential of the operator $\mathcal{L}$ follows from a Taylor's series expansion of u in powers of t, *i.e.*,

$$u(x, y, t) = u(x, y, 0) + tu_t(x, y, 0) + \frac{t^2}{2!}u_{tt}(x, y, 0) + \ldots = e^{t\frac{\partial}{\partial t}}u(x, y, 0)$$

or, using the partial differential equation,

$$u(x, y, t) = u(x, y, 0) + t\mathcal{L}u(x, y, 0) + \frac{t^2}{2!}\mathcal{L}^2u(x, y, 0) + \ldots = e^{t\mathcal{L}}u(x, y, 0).$$

The above manipulations are similar to those used to obtain the Lax-Wendroff scheme of Section 3.3.

Unfortunately, once again,

$$u(x,y,t) = e^{t(\mathcal{L}_1+\mathcal{L}_2)}u(x,y,0) \neq e^{t\mathcal{L}_1}e^{t\mathcal{L}_2}u(x,y,0),$$

unless the operators $\mathcal{L}_1$ and $\mathcal{L}_2$ commute. Let us verify this by using Taylor's series expansions of both sides of the above expression; thus,

$$e^{t(\mathcal{L}_1+\mathcal{L}_2)}u(x,y,0) = [\mathbf{I} + t(\mathcal{L}_1+\mathcal{L}_2) + \frac{t^2}{2}(\mathcal{L}_1^2 + \mathcal{L}_1\mathcal{L}_2 + \mathcal{L}_2\mathcal{L}_1 + \mathcal{L}_2^2) + \ldots]u(x,y,0)$$

and

$$e^{t\mathcal{L}_1}e^{t\mathcal{L}_2}u(x,y,0) = (\mathbf{I} + t\mathcal{L}_1 + \frac{t^2}{2}\mathcal{L}_1^2 + \ldots)(\mathbf{I} + t\mathcal{L}_2 + \frac{t^2}{2}\mathcal{L}_2^2 + \ldots)u(x,y,0)$$

or

$$e^{t\mathcal{L}_1}e^{t\mathcal{L}_2}u(x,y,t) = [(\mathbf{I} + t(\mathcal{L}_1+\mathcal{L}_2) + \frac{t^2}{2}(\mathcal{L}_1^2 + 2\mathcal{L}_1\mathcal{L}_2 + \mathcal{L}_2^2) + \ldots]u(x,y,0).$$

Hence,

$$[e^{t(\mathcal{L}_1+\mathcal{L}_2)} - e^{t\mathcal{L}_1}e^{t\mathcal{L}_2}]u(x,y,0) = [\frac{t^2}{2}(\mathcal{L}_2\mathcal{L}_1 - \mathcal{L}_1\mathcal{L}_2) + O(t^3)]u(x,y,0).$$

The difference between the the two expressions is $O(t^2)$ unless $\mathcal{L}_1\mathcal{L}_2 u = \mathcal{L}_2\mathcal{L}_1 u$. The factorization "almost" works when t is small; hence, we can replace t by a small time increment Δt to obtain

$$u(x,y,\Delta t) = e^{\Delta t(\mathcal{L}_1+\mathcal{L}_2)}u(x,y,0) = [e^{\Delta t\mathcal{L}_1}e^{\Delta t\mathcal{L}_2} + \frac{\Delta t^2}{2}(\mathcal{L}_2\mathcal{L}_1 - \mathcal{L}_1\mathcal{L}_2) + O(\Delta t^3)]u(x,y,0).$$

To obtain a numerical method, we (i) discretize the spatial operators $\mathcal{L}_1$ and $\mathcal{L}_2$, (ii) neglect the local error terms, and (iii) use the resulting method from time step-to-time step. Thus,

$$\mathbf{U}^{n+1} = e^{\Delta t\mathbf{L}_{1,\Delta}}e^{\Delta t\mathbf{L}_{2,\Delta}}\mathbf{U}^n, \tag{5.2.2}$$

where $\mathbf{L}_{1,\Delta}$ and $\mathbf{L}_{2,\Delta}$ are discrete approximations of $\mathcal{L}_1$ and $\mathcal{L}_2$. This technique, often called the *method of fractional steps* or *operator splitting*, has several advantages:

1. If the operators $\mathbf{L}_{1,\Delta}$ and $\mathbf{L}_{2,\Delta}$ satisfy the von Neumann conditions

$$\|e^{\Delta t\mathbf{L}_{k,\Delta}}\| \leq 1 + c_k\Delta t, \qquad k = 1,2,$$

then the combined scheme is stable, since, using (5.2.2)

$$\|\mathbf{U}^{n+1}\| \leq \|e^{\Delta t \mathbf{L}_{1,\Delta}}\| \|e^{\Delta t \mathbf{L}_{2,\Delta}}\| \|\mathbf{U}^{n}\| \leq (1 + c\Delta t)\|\mathbf{U^n}\|.$$

Similarly, if the individual operators are absolutely stable, the combined scheme will be absolutely stable.

2. With operator splitting, the local error is $O(\Delta t^2)$ unless the operators $\mathcal{L}_1$ and $\mathcal{L}_2$ commute, in which case it is $O(\Delta t^3)$.

Let us examine some possibilities

Example 5.2.1. In order to solve (5.2.1) by operator splitting, we solve

$$u_t = \mathcal{L}_2 u$$

for a time step and then repeat the time step solving

$$u_t = \mathcal{L}_1 u.$$

If we discretize the partial differential equations with Crank-Nicolson approximations, we have

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})\hat{U}_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n}, \tag{5.2.3a}$$

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})U_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})\hat{U}_{j,k}^{n+1}. \tag{5.2.3b}$$

We have used a $\hat{}$ to denote the "predicted solution" of (5.2.3a).

Remark 1. If the operators $\mathbf{L}_{1,\Delta}$ and $\mathbf{L}_{2,\Delta}$ commute, then we may easily verify that (5.2.3) is equivalent to the Peaceman-Rachford form of ADI (5.1.5) for the heat conduction equation. Unlike the Peaceman-Rachford implementation, however, a portion of the operator is neglected at each step.

Let's apply (5.2.3) to the variable-coefficient heat conduction equation

$$u_t = (\sigma u_x)_x + (\sigma u_y)_y$$

where $\sigma = \sigma(x, y)$. Suppose that we select

$$\mathcal{L}_1 u = (\sigma u_x)_x, \qquad \mathcal{L}_2 u = (\sigma u_y)_y,$$

We discretize each operator using (4.4.4) and introduce the shorthand notation

$$\mathbf{L}_{1,\Delta}U^n_{j,k} = \frac{\hat{\delta}^2_x U^n_{j,k}}{\Delta x^2} \equiv \frac{\delta_x(\sigma_{j,k}\delta_x U^n_{j,k})}{\Delta x^2}$$

where

$$\delta_x(\sigma_{j,k}\delta_x U^n_{j,k}) = \sigma_{j+1/2,k}(U^n_{j+1,k} - U^n_{j,k}) - \sigma_{j-1/2,k}(U^n_{j,k} - U^n_{j-1,k}).$$

A similar formula may be written for $\mathbf{L}_{2,\Delta}$. Upon using (5.2.3)

$$(\mathbf{I} - \frac{r^0_y}{2}\hat{\delta}^2_y)\hat{U}^{n+1}_{j,k} = (\mathbf{I} + \frac{r^0_y}{2}\hat{\delta}^2_y)U^n_{j,k}, \tag{5.2.4a}$$

$$(\mathbf{I} - \frac{r^0_x}{2}\hat{\delta}^2_x)U^{n+1}_{j,k} = (\mathbf{I} + \frac{r^0_x}{2}\hat{\delta}^2_x)\hat{U}^{n+1}_{j,k} \tag{5.2.4b}$$

where

$$r^0_x = \Delta t/\Delta x^2, \qquad r^0_y = \Delta t/\Delta y^2. \tag{5.2.4c}$$

The combined method (5.2.4a, 5.2.4b) is solved in alternating directions, like the ADI method (5.1.5). The way that we have split the operator, (5.2.4a) would be solved by columns and (5.2.4b) would be solved by rows. Proceeding in the opposite manner is acceptable.

Example 5.2.2. Consider the Taylor's series expansions about time level $n + 1/2$

$$u^{n+1}_{j,k} = [\mathbf{I} + \frac{\Delta t}{2}\mathcal{L} + \frac{\Delta t^2}{4 \cdot 2!}\mathcal{L}^2 + O(\Delta t^3)]u^{n+1/2}_{j,k},$$

$$u^n_{j,k} = [\mathbf{I} - \frac{\Delta t}{2}\mathcal{L} + \frac{\Delta t^2}{4 \cdot 2!}\mathcal{L}^2 + O(\Delta t^3)]u^{n+1/2}_{j,k}.$$

Adding and subtracting

$$u^{n+1}_{j,k} - u^n_{j,k} = [\Delta t\mathcal{L} + O(\Delta t^3)]u^{n+1/2}_{j,k},$$

$$u^{n+1}_{j,k} + u^n_{j,k} = 2[\mathbf{I} + \frac{\Delta t^2}{4 \cdot 2!}\mathcal{L}^2 + O(\Delta t^3)]u^{n+1/2}_{j,k}.$$

Eliminating $u^{n+1/2}_{j,k}$

$$u^{n+1}_{j,k} - u^n_{j,k} = \frac{\Delta t}{2}\mathcal{L}(u^{n+1}_{j,k} + u^n_{j,k}) + O(\Delta t^3).$$

Splitting the operator into its component parts

$$[\mathbf{I} - \frac{\Delta t}{2}\mathcal{L}_1 - \frac{\Delta t}{2}\mathcal{L}_2]u_{j,k}^{n+1} = [\mathbf{I} + \frac{\Delta t}{2}\mathcal{L}_1 + \frac{\Delta t}{2}\mathcal{L}_2]u_{j,k}^{n} + O(\Delta t^3).$$

This is just the trapezoidal rule integration of (5.2.1) for a time step. Indeed, were we to discretize the spatial operators $\mathcal{L}_1$ and $\mathcal{L}_2$ using centered differences, we would obtain the same Crank-Nicolson scheme (5.1.4a) that we rejected. Now, instead, let's factor each operator as

$$\mathbf{I} \pm \frac{\Delta t}{2}\mathcal{L}_1 \pm \frac{\Delta t}{2}\mathcal{L}_2 = (\mathbf{I} \pm \frac{\Delta t}{2}\mathcal{L}_1)(\mathbf{I} \pm \frac{\Delta t}{2}\mathcal{L}_2) - \frac{\Delta t^2}{4}\mathcal{L}_1\mathcal{L}_2.$$

Thus, we have

$$(\mathbf{I} - \frac{\Delta t}{2}\mathcal{L}_1)(\mathbf{I} - \frac{\Delta t}{2}\mathcal{L}_2)u_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathcal{L}_1)(\mathbf{I} + \frac{\Delta t}{2}\mathcal{L}_2)u_{j,k}^{n} +$$
$$\frac{\Delta t^2}{4}\mathcal{L}_1\mathcal{L}_2(u_{j,k}^{n+1} - u_{j,k}^{n}) + O(\Delta t^3).$$

We have already shown that the next-to-last term on the right is $O(\Delta t^3)$; thus, it may be combined with the discretization error to obtain

$$(\mathbf{I} - \frac{\Delta t}{2}\mathcal{L}_1)(\mathbf{I} - \frac{\Delta t}{2}\mathcal{L}_2)u_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathcal{L}_1)(\mathbf{I} + \frac{\Delta t}{2}\mathcal{L}_2)u_{j,k}^{n} + O(\Delta t^3).$$

If we neglect the local discretization error and discretize the spatial operators, we obtain

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})(\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n} \tag{5.2.5}$$

Peaceman and Rachford [5] solved (5.2.3) as

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})U_{j,k}^{n+1/2} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n}, \tag{5.2.6a}$$

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})U_{j,k}^{n+1/2}. \tag{5.2.6b}$$

When applied to the heat conduction equation with centered spatial differences, this scheme is also identical to the ADI scheme (5.1.5).

Let us verify that (5.2.5) and (5.2.6) are equivalent. Thus, operate on (5.2.6b) with $\mathbf{I} - \Delta t\mathbf{L}_{1,\Delta}/2$ to obtain

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n+1} = (\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})(\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})U_{j,k}^{n+1/2}.$$

The operators on the right may be interchanged to obtain

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})U_{j,k}^{n+1/2}.$$

Using (5.2.6a) yields (5.2.5).

Example 5.2.3. D'Yakonov (*cf.* [4], Section 2.12) introduced the following scheme for solving (5.2.5)

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})\hat{U}_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{1,\Delta})(\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n} \tag{5.2.7a}$$

$$(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta})U_{j,k}^{n+1} = \hat{U}_{j,k}^{n+1}. \tag{5.2.7b}$$

This scheme has the same order of accuracy and characteristics as the Peaceman-Rachford ADI scheme (5.2.6).

Example 5.2.4. Douglas and Rachford [2] developed an alternative scheme for (5.2.1) using backward-difference approximations. Thus, consider integrating (5.2.1) for a time step by the backward Euler method to obtain

$$(\mathbf{I} - \Delta t\mathcal{L}_1 - \Delta t\mathcal{L}_2)u_{j,k}^{n+1} = u_{j,k}^{n} + O(\Delta t)^2.$$

Let us rewrite this as

$$(\mathbf{I} - \Delta t\mathcal{L}_1 - \Delta t\mathcal{L}_2 + \Delta t^2\mathcal{L}_1\mathcal{L}_2)u_{j,k}^{n+1} = (\mathbf{I} + \Delta t^2\mathcal{L}_1\mathcal{L}_2)u_{j,k}^{n} +$$

$$\Delta t^2\mathcal{L}_1\mathcal{L}_2(u_{j,k}^{n+1} - u_{j,k}^{n}) + O(\Delta t)^3.$$

As in Example 5.2.2, we may show that the next-to-last term on the right is $O(\Delta t^3)$ and, hence, may be neglected. Also neglecting the temporal discretization error term, discretizing the operators $\mathcal{L}_1$ and $\mathcal{L}_2$, and factoring the left side gives

$$(\mathbf{I} - \Delta t\mathbf{L}_{1,\Delta})(\mathbf{I} - \Delta t\mathbf{L}_{2,\Delta})U_{j,k}^{n+1} = (\mathbf{I} + \Delta t^2\mathbf{L}_{1,\Delta}\mathbf{L}_{2,\Delta})U_{j,k}^{n}.$$

Douglas and Rachford [2] factored this as

$$(\mathbf{I} - \Delta t\mathbf{L}_{1,\Delta})\hat{U}_{j,k}^{n+1} = (\mathbf{I} + \Delta t\mathbf{L}_{2,\Delta})U_{j,k}^{n} \tag{5.2.8a}$$

$$(\mathbf{I} - \Delta t \mathbf{L}_{2,\Delta}) U_{j,k}^{n+1} = \hat{U}_{j,k}^{n+1} - \Delta t \mathbf{L}_{2,\Delta} U_{j,k}^{n} \tag{5.2.8b}$$

Assuming that the discrete spatial operators are second-order accurate, the local discretization error is $O(\Delta t) + O(\Delta x^2) + O(\Delta y^2)$. This is lower order than the $O(\Delta t^2)$ local discretization error that would be obtained from the ADI factorization (5.2.6); however, backward differencing gives greater stability than (5.2.6) which may be useful for nonlinear problems.

Example 5.2.5. The previous examples suggest a simplicity that is not always present. Boundary conditions must be treated very carefully since the intermediate solutions or $\mathbf{U}^{n+1/2}$ or $\hat{\mathbf{U}}^{n+1}$ need not be consistent approximations of $u(x, (n+1/2)\Delta t)$ or $u(x, (n+1)\Delta t)$. Yanenko [8] presents a good example of the complications that can arise at boundaries. Strikwerda [7], Section 7.3, suggests using a combination of $\mathbf{U}^n$ and $\mathbf{U}^{n+1}$ to get the intermediate boundary condition. Let us illustrate this for the Dirichlet problem (5.1.2) using the Peaceman-Rachford ADI scheme (5.2.6). During the horizontal sweep (5.2.6a), we need boundary conditions for $\mathbf{U}^{n+1/2}$ at $x = 0$ and 1. Adding (5.2.6a) and (5.2.6b) gives

$$U_{j,k}^{n+1/2} = \frac{1}{2}(\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{2,\Delta}) U_{j,k}^{n} + \frac{1}{2}(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta}) U_{j,k}^{n+1}.$$

Using the boundary condition (5.1.2c)

$$U_{j,k}^{n+1/2} = \frac{1}{2}(\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}_{2,\Delta}) \gamma_{j,k}^{n} + \frac{1}{2}(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}_{2,\Delta}) \gamma_{j,k}^{n+1} \tag{5.2.9}$$

which can be used as a boundary condition for $\mathbf{U}^{n+1/2}$. The obvious boundary condition

$$U_{j,k}^{n+1/2} = \frac{\gamma_{j,k}^{n} + \gamma_{j,k}^{n+1}}{2}$$

is only first-order accurate as apparent from (5.2.9).

Boundary conditions for the Douglas-Rachford scheme can be obtained from the corrector equation (5.2.8b) and the boundary condition (5.1.2c) as

$$\hat{U}_{j,k}^{n+1} = (\mathbf{I} - \Delta t \mathbf{L}_{2,\Delta}) \gamma_{j,k}^{n+1} + \Delta t \mathbf{L}_{2,\Delta} \gamma_{j,k}^{n}. \tag{5.2.10}$$

Example 5.2.6. Strang [6] developed a factorization technique that has a faster rate of convergence than the splitting (5.2.2) when the operators $\mathcal{L}_1$ and $\mathcal{L}_2$ do not commute.

Strang computes

$$U_{j,k}^{n+1} = e^{(\Delta t/2)\mathcal{L}_2} e^{\Delta t \mathcal{L}_1} e^{(\Delta t/2)\mathcal{L}_2} U_{j,k}^n. \tag{5.2.11}$$

This scheme appears to require an extra solution per step; however, if results are output every n time steps then

$$U_{j,k}^n = (e^{(\Delta t/2)\mathcal{L}_2} e^{\Delta t \mathcal{L}_1} e^{(\Delta t/2)\mathcal{L}_2})(e^{(\Delta t/2)\mathcal{L}_2} e^{\Delta t \mathcal{L}_1} e^{(\Delta t/2)\mathcal{L}_2}) \ldots (e^{(\Delta t/2)\mathcal{L}_2} e^{\Delta t \mathcal{L}_1} e^{(\Delta t/2)\mathcal{L}_2}) U_{j,k}^0$$

or

$$U_{j,k}^n = e^{(\Delta t/2)\mathcal{L}_2} e^{\Delta t \mathcal{L}_1} e^{\Delta t \mathcal{L}_2} e^{\Delta t \mathcal{L}_1} \ldots e^{(\Delta t/2)\mathcal{L}_2} U_{j,k}^0.$$

Hence, the factorization (5.2.11) is the same as the simpler splitting (5.2.2) except for the first and last time steps.

Let us estimate the local error; thus, assuming that $U_{j,k}^n = u_{j,k}^n$,

$$U_{j,k}^{n+1} = (\mathbf{I} + \frac{\Delta t}{2}\mathcal{L}_2 + \frac{\Delta t^2}{8}\mathcal{L}_2^2 + \ldots)(\mathbf{I} + \Delta t \mathcal{L}_1 + \frac{\Delta t^2}{2}\mathcal{L}_1^2 + \ldots)$$
$$(\mathbf{I} + \frac{\Delta t}{2}\mathcal{L}_2 + \frac{\Delta t^2}{8}\mathcal{L}_2^2 + \ldots) u_{j,k}^n$$

or

$$U_{j,k}^{n+1} = [\mathbf{I} + \Delta t(\mathcal{L}_1 + \mathcal{L}_2) + \frac{\Delta t^2}{2}(\mathcal{L}_1^2 + \mathcal{L}_1\mathcal{L}_2 + \mathcal{L}_2\mathcal{L}_1 + \mathcal{L}_2^2) + O(\Delta t^3)] u_{j,k}^n.$$

Thus,

$$u_{j,k}^{n+1} - U_{j,k}^{n+1} = [e^{\Delta t(\mathcal{L}_1 + \mathcal{L}_2)} - e^{(\Delta t/2)\mathcal{L}_2} e^{\Delta t \mathcal{L}_1} e^{(\Delta t/2)\mathcal{L}_1}] u_{j,k}^n = O(\Delta t^3).$$

Problems

1. Although operator splitting has primarily been used for dimensional splitting, it may be used in other ways. Consider the nonlinear reaction-diffusion problem

$$u_t = \sigma u_{xx} + u(1-u), \qquad 0 < x < 1, \qquad t > 0,$$

$$u(0,t) = u(1,t) = 0, \qquad t > 0,$$

$$u(x,0) = \phi(x), \qquad 0 \le x \le 1.$$

Develop a procedure for solving this problem that involves splitting the diffusion (σu_{xx}) and reaction ($u(1-u)$) operators. Discuss its stability and local discretization errors.

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