HIGH-PERFORMANCE COMPUTING IN APPLIED MATHEMATICS

Achieving parallelism in high-dimensional PDEs

The operator splitting approach

Numerical solution to high-dimensional PDEs (more than one spatial dimensions) requires efficient implementation of the implicit time integration schemes.

Consider the 2D heat equation:

$$u_t = k(u_{xx} + u_{yy}), \quad 0 < x, y, < L \tag{1}$$

with zero values on the boundary. Discretization on a grid with nodes

$$x_i = i * h, \quad y_j = j * h, \quad i, j = 0 : n$$

where $h = L/n$, results into a large-scale discrete state

$$u_{i,j}, \quad 0 \le i, j \le n$$

that needs to be advanced in time. The explicit FTCS scheme to advance from t^m to $t^{m+1} = t^m + \Delta t$ is

$$u_{i,j}^{m+1} = u_{i,j}^m + k\frac{\Delta t}{h^2}\left[u_{i-1,j}^m + u_{i+1,j}^m + u_{i,j-1}^m + u_{i,j+1}^m - 4u_{i,j}^m\right], \quad 1 \le i, j \le n-1 \tag{2}$$

and it is easy to implement, however it suffers from the stability constraint on the time step:

$$s \stackrel{def}{=} k\frac{\Delta t}{h^2} \le \frac{1}{4}$$

For example, with $k = 1$ and $h = 0.01$, maximum Δt that can be used is 0.25×10^{-4}. Since the computation (2) involves $O(n^2)$ operations, and the time step must satisfy $\Delta t \le \frac{1}{4k}\frac{1}{n^2}$, to get to time $t = 1$ the overall number of arithmetic operations required is of order $O(n^4)$ which is a large number even for moderate values of n, say $n = 100$.

Implicit time integration schemes are unconditionally stable (no restriction on Δt, for example the backward-time central space BTCS

$$u_{i,j}^{m+1} = u_{i,j}^m + s\left[u_{i-1,j}^{m+1} + u_{i+1,j}^{m+1} + u_{i,j-1}^{m+1} + u_{i,j+1}^{m+1} - 4u_{i,j}^{m+1}\right], \quad 1 \le i, j \le n-1 \tag{3}$$

but are not easy to implement.

Notice that the tridiagonal structure from the one dimensional case

$$\begin{bmatrix} 1+2s & -s & 0 & \dots & \dots & 0 \\ -s & 1+2s & -s & 0 & & \vdots \\ 0 & -s & 1+2s & -s & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ & & & & & -s \\ 0 & \dots & & 0 & -s & 1+2s \end{bmatrix} \tag{4}$$

is no longer valid. For example, corresponding to a grid with four interior points, the matrix associated to the BTCS scheme is

$$\mathbf{I}+\mathbf{A}=\begin{bmatrix} 1+4s & -s & -s & 0 \\ -s & 1+4s & 0 & -s \\ -s & 0 & 1+4s & -s \\ 0 & -s & -s & 1+4s \end{bmatrix} \tag{5}$$

and for a grid with 9 interior points the matrix associated to the BTCS scheme is

$$\mathbf{I}+\mathbf{A}=\left[\begin{array}{ccc|ccc|ccc} 1+4s & -s & & -s & & & & & \\ -s & 1+4s & -s & & -s & & & & \\ & -s & 1+4s & & & -s & & & \\ \hline -s & & & 1+4s & -s & & -s & & \\ & -s & & -s & 1+4s & -s & & -s & \\ & & -s & & -s & 1+4s & & & -s \\ \hline & & & -s & & & 1+4s & -s & \\ & & & & -s & & -s & 1+4s & -s \\ & & & & & -s & & -s & 1+4s \end{array}\right]$$

The linear system to be solved is

$$(\mathbf{I}+\mathbf{A})\mathbf{U}^{m+1}=\mathbf{U}^m$$

where $\mathbf{U}$ denotes the $(n-1)\times(n-1)$ matrix with entries $u_{i,j}$ and efficient matrix factorization algorithms such as TRILU may not be directly applied.

The *operator splitting approach* is introduced as a method to efficiently solve high-dimensional PDEs AND *achieve parallelism*. The idea is to solve the PDE along one direction (x or y) at a time. Notice that the matrix $\mathbf{A}$ in (5) may be written

$$\mathbf{A}=\begin{bmatrix} 4s & -s & -s & 0 \\ -s & 4s & 0 & -s \\ -s & 0 & 4s & -s \\ 0 & -s & -s & 4s \end{bmatrix}=\mathbf{A}_x+\mathbf{A}_y \tag{6}$$

where

$$\mathbf{A}_x=\begin{bmatrix} 2s & -s & 0 & 0 \\ -s & 2s & 0 & 0 \\ 0 & 0 & 2s & -s \\ 0 & 0 & -s & 2s \end{bmatrix}, \quad \mathbf{A}_y=\begin{bmatrix} 2s & 0 & -s & 0 \\ 0 & 2s & 0 & -s \\ -s & 0 & 2s & 0 \\ 0 & -s & 0 & 2s \end{bmatrix} \tag{7}$$

correspond to the discretization of the u_{xx} and u_{yy} derivatives, respectively. So, if only the u_{xx} term would be considered, a linear system with the matrix $\mathbf{I}+\mathbf{A}_x$ would be easily solved since

$$(\mathbf{I}+\mathbf{A}_x)^{-1}=\begin{bmatrix} (\mathbf{I}+\mathbf{A_1})^{-1} & \mathbf{0} \\ \mathbf{0} & (\mathbf{I}+\mathbf{A_1})^{-1} \end{bmatrix}$$

where

$$\mathbf{I}+\mathbf{A}_1=\begin{bmatrix} 1+2s & -s \\ -s & 1+2s \end{bmatrix}$$

Solving the linear system

$$(\mathbf{I} + \mathbf{A}_x)\,\tilde{\mathbf{U}}^{m+1} = \mathbf{U}^m$$

may be then performed in a parallel over the y-dimension index:

$$(\mathbf{I} + \mathbf{A}_1)\tilde{\mathbf{U}}^{m+1}(:,l) = \mathbf{U}^m(:,l), \quad l = 1 : n-1$$

In general the matrix $\mathbf{I} + \mathbf{A}_x$ takes the form

$$\mathbf{I} + \mathbf{A}_1 = \begin{bmatrix} 1+2s & -s & 0 & \dots & \dots & 0 \\ -s & 1+2s & -s & 0 & & \vdots \\ 0 & -s & 1+2s & -s & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ & & & & & -s \\ 0 & \dots & & 0 & -s & 1+2s \end{bmatrix} \tag{8}$$

which is the same as the matrix (4) from the one-dimensional case. The TRILU and TRISOLVE algorithms may be then used to provide the solution at each fixed $l, 1 \le l \le n-1$.

Similarly, from (7) it is noticed that

$$\mathbf{I} + \mathbf{A}_y = \begin{bmatrix} 1+2s & 0 & -s & 0 \\ 0 & 1+2s & 0 & -s \\ -s & 0 & 1+2s & 0 \\ 0 & -s & 0 & 1+2s \end{bmatrix}$$

A linear system involving $\mathbf{I} + \mathbf{A}_y$ may be decomposed into two subsystems: first consisting on eqs. 1 and 3 and second consisting on eqs. 2 and 4 that can be solved in parallel. In general, for each fixed x-index j we solve for $\hat{\mathbf{U}}(j,:)$ the system

$$(\mathbf{I} + \mathbf{A}_1)\hat{\mathbf{U}}^{m+1}(j,:) = \mathbf{U}^m(j,:)$$

The operator splitting performs first a time step in the x-direction to obtain $\tilde{\mathbf{U}}^{m+1}$, then uses the intermediate stage $\tilde{\mathbf{U}}^{m+1}$ as a initial state for the time step in the y-direction to obtain $\hat{\mathbf{U}}^{m+1}$. The approximation of the solution at t^{m+1} is

$$\hat{\mathbf{U}}^{m+1} \approx \mathbf{U}^{m+1}$$

.

To put things together, one time step of the operator splitting approach is

FOR $l = 1 : n-1$ % y-loop parallel

TRISOLVE $(\mathbf{I} + \mathbf{A}_1)\tilde{\mathbf{U}}(:, l) = \mathbf{U}^m(:, l)$

END

FOR $j = 1 : n-1$ % x-loop parallel

TRISOLVE $(\mathbf{I} + \mathbf{A}_2)\mathbf{U}^{m+1}(j, :) = \tilde{\mathbf{U}}(j, :)$

END

Notice that the matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ will not be identical in a general case, for example if different types of boundary conditions are considered on each edge of the domain.

Next we show that operator splitting is *mathematically justified*.

Consider the time continuous problem

$$\frac{dU}{dt} = (A_1 + A_2)U(t) \tag{9}$$

$$U(t_0) = U_0 \tag{10}$$

The operator splitting solution obtained by solving a sequence of subproblems:

$$\frac{d\tilde{U}}{dt} = A_1\tilde{U}(t) \tag{11}$$

$$\tilde{U}(t_0) = U_0 \tag{12}$$

$$\frac{d\hat{U}}{dt} = A_2\hat{U}(t) \tag{13}$$

$$\hat{U}(t_0) = \tilde{U}(t_0 + \tau) \tag{14}$$

and provides an approximation to the "true" solution at $t_0 + \tau$ as:

$$U(t_0 + \tau) \approx \hat{U}(t_0 + \tau) \tag{15}$$

To investigate the order of the error in the approximation (15) we use Taylor series:

$$\begin{aligned} U(t_0+\tau) &= U(t_0)+\tau U'(t_0)+\frac{1}{2}\tau^2 U''(t_0)+O(\tau^3) \\ &= \left[I+\tau(A_1+A_2)+\frac{1}{2}\tau^2(A_1+A_2)^2\right]U_0+O(\tau^3) \\ &= \left[I+\tau(A_1+A_2)+\frac{1}{2}\tau^2(A_1^2+A_1A_2+A_2A_1+A_2^2)\right]U_0+O(\tau^3) \end{aligned} \tag{16}$$

$$\begin{aligned} \hat{U}(t_0+\tau) &= \left[I+\tau A_2+\frac{1}{2}\tau^2 A_2^2\right]\hat{U}(t_0)+O(\tau^3) \\ &= \left[I+\tau A_2+\frac{1}{2}\tau^2 A_2^2\right]\left[I+\tau A_1+\frac{1}{2}\tau^2 A_1^2\right]U_0+O(\tau^3) \\ &= \left[I+\tau(A_1+A_2)+\frac{1}{2}\tau^2(A_1^2+A_2^2+2A_1A_2)\right]U_0+O(\tau^3) \end{aligned} \tag{17}$$

Subtracting (17) from (16) it follows that the error introduced by the splitting approach is

$$U(t_0+\tau)-\hat{U}(t_0+\tau)=\frac{1}{2}\tau^2(A_2A_1-A_1A_2)+O(\tau^3) \tag{18}$$

such that if A_1 and A_2 commute: $A_2A_1 = A_1A_2$ then the error is of third order $O(\tau^3)$. If $A_2A_1 \neq A_1A_2$ then the error is second order $O(\tau^2)$.

Q: Show that the matrices $\mathbf{A}_x$ and $\mathbf{A}_y$ in (7) commute. Conclude that the operator splitting approach applied to the two dimensional heat equation problem with homogeneous boundary conditions is second order accurate in time.

The alternating directions implicit (ADI) method

In a general formulation, we consider an ODEs system

$$\frac{dU}{dt} = (A_1+A_2)U \tag{19}$$

$$U(0) = U^0 \tag{20}$$

where $U(t)$ is an N-dimensional vector. The operator A_1 may represent for example, the discretization in x-direction, whereas A_2 may represent the discretization in y-direction.

The implicit trapezoidal method applied to (19) is written

$$U^{m+1}=U^m+\frac{\Delta t}{2}\left[(A_1+A_2)U^{m+1}+(A_1+A_2)U^m\right] \tag{21}$$

or equivalently,

$$\left[I - \frac{\Delta t}{2}(A_1 + A_2)\right] U^{m+1} = \left[I + \frac{\Delta t}{2}(A_1 + A_2)\right] U^m \qquad (22)$$

so the matrix $I - \frac{\Delta t}{2}(A_1 + A_2)$ needs to be factorized (LU).

The main idea of the ADI method is to proceed in two stages, treating only one operator implicitly at each stage. First a half-step is taken implicitly in the direction A_1 and explicitly in the direction A_2 followed by a half-step is taken implicitly in the direction A_2 and explicitly in the direction A_1. When applied to the general problem (19) the equations for the ADI method are written

$$\begin{aligned} U^{m+1/2} &= U^m + \frac{\Delta t}{2}\left[A_1 U^{m+1/2} + A_2 U^m\right] \\ U^{m+1} &= U^{m+1/2} + \frac{\Delta t}{2}\left[A_1 U^{m+1/2} + A_2 U^{m+1}\right] \end{aligned}$$

which are equivalent to

$$\left(I - \frac{\Delta t}{2}A_1\right) U^{m+1/2} = \left(I + \frac{\Delta t}{2}A_2\right) U^m \qquad (23)$$

$$\left(I - \frac{\Delta t}{2}A_2\right) U^{m+1} = \left(I + \frac{\Delta t}{2}A_1\right) U^{m+1/2} \qquad (24)$$

Q: Show that the ADI equations (23-24) are equivalent to

$$\left(I - \frac{\Delta t}{2}A_1\right)\left(I - \frac{\Delta t}{2}A_2\right) U^{m+1} = \left(I + \frac{\Delta t}{2}A_1\right)\left(I + \frac{\Delta t}{2}A_2\right) U^m \qquad (25)$$

Q: From (25) and (22) deduce that the ADI scheme is second order accurate in time.

Case study: 2D heat equation

Corresponding to the space discretization of the 2D heat equation using central differences formula,

$$(A_1 U)_{j,l} = \frac{1}{(\Delta x)^2}\left[U_{j-1,l} - 2U_{j,l} + U_{j+1,l}\right]$$

$$(A_2 U)_{j,l} = \frac{1}{(\Delta x)^2}\left[U_{j,l-1} - 2U_{j,l} + U_{j,l+1}\right]$$

The first stage of the ADI method, given by equation (23) is written

$$(1+2s)U_{j,l}^{m+1/2} - sU_{j-1,l}^{m+1/2} - sU_{j+1,l}^{m+1/2} = (1-2s)U_{j,l}^m + sU_{j,l-1}^m + sU_{j,l+1}^m, \quad j = 1, \ldots, Nx; l = 1, \ldots, Ny \qquad (26)$$

where

$$s = \frac{\Delta t}{2(\Delta x)^2}$$

and Nx, Ny are the number of interior grid points in the x and y directions, respectively.

Notice that in equations (26) only the x-index varies in the left side, that is the equatons are implicit in the x-direction only. For a fixed index l, the vector $U^{m+1/2}(:,l)$ may be found by solving the tridiagonal system

$$AU^{m+1/2}(:,l) = b \tag{27}$$

where the matrix A is tridiagonal,

$$\mathbf{A} = \begin{bmatrix} 1+2s & -s & 0 & 0 & 0 & 0 & 0 \\ -s & 1+2s & -s & 0 & 0 & 0 & 0 \\ 0 & -s & 1+2s & -s & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \dots & \dots & 0 & 0 \\ 0 & 0 & 0 & -s & 1+2s & -s & 0 \\ 0 & 0 & 0 & 0 & -s & 1+2s & -s \\ 0 & 0 & 0 & 0 & 0 & -s & 1+2s \end{bmatrix} \tag{28}$$

and b is an Nx-dimensional vector with components

$$b(j) = (1-2s)U^m_{j,l} + sU^m_{j,l-1} + sU^m_{j,l+1}, \quad j = 1 : Nx$$

Stage 1 of the ADI method is then implemented in a loop over the y-direction:

for $l = 1 : Ny$
  for $j = 1 : Nx$
    $b(j) = (1-2s)U_{j,l} + sU_{j,l-1} + sU_{j,l+1}$
  end
  TRISOLVE $AU^{new}(:,l) = b$
end

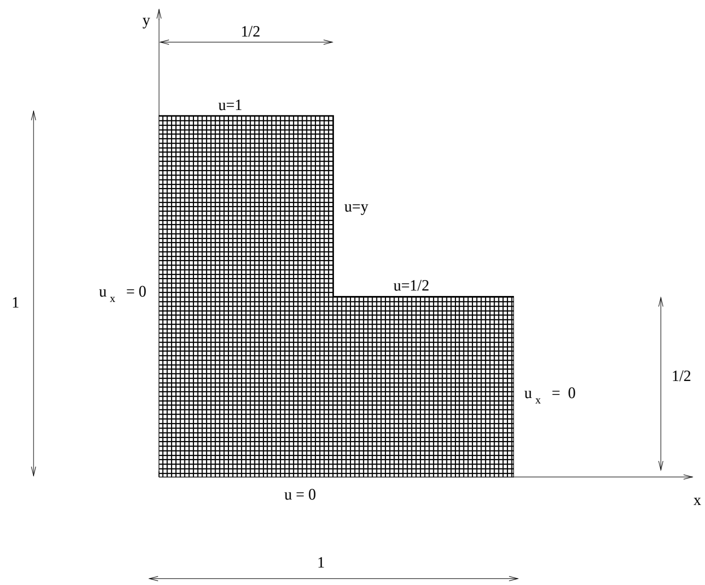
So in this stage a tridiagonal system of dimension Nx is solved Ny times. By analogy, Stage 2 of the ADI method is implemented in a loop over the x-direction:

for $j = 1 : Nx$
  for $l = 1 : Ny$
    $b(l) = (1-2s)U^{new}_{j,l} + sU^{new}_{j-1,l} + sU^{new}_{j+1,l}$
  end
  TRISOLVE $AU(j,:) = b$
end

So in this stage a tridiagonal system of dimension Ny is solved Nx times.

Execution of Stage 1 followed by Stage 2 advances the solution with a Δt step in time, overwritting U. U^{new} is an intermediate stage.

Application: 2D heat flow problem in an L-shaped domain $\mathcal{D}$ as indicated in the figure below.



Mathematically, the problem is formulated as the PDE

$$u_t = \alpha(u_{xx} + u_{yy}), \qquad (x, y) \in \mathcal{D}, \quad t > 0 \tag{29}$$

with boundary conditions

$$\begin{aligned}
u(x, 0, t) &= 0, && 0 \leq x \leq 1, \quad t > 0 && (30)\\
u_x(0, y, t) &= 0, && 0 < y < 1, \quad t > 0 && (31)\\
u(x, 1, t) &= 1, && 0 \leq x \leq 0.5, \quad t > 0 && (32)\\
u(0.5, y, t) &= y, && 0.5 \leq y \leq 1, \quad t > 0 && (33)\\
u(x, 0.5, t) &= 0.5, && 0.5 \leq x \leq 1, \quad t > 0 && (34)\\
u_x(1, y, t) &= 0, && 0 < y < 0.5, \quad t > 0 && (35)
\end{aligned}$$