Numerical Solutions to PDEs

Lecture Notes #13
— Systems of PDEs in Higher Dimensions —
The Alternating Direction Implicit Method

Peter Blomgren,
⟨blomgren.peter@gmail.com⟩

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

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San Diego State University

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Previously

We started looking at multi-dimensional hyperbolic and parabolic problems, first via vector-valued problems with one time and one space dimension, and then to full multi-space dimensional problems.

In terms of definitions, nothing much changed — the concepts of convergence, consistency, stability and order of accuracy are the same.

However, some of the analysis becomes quite challenging. — For instance, we end up needing to bound nth powers of amplification matrices $\|G^n\| \leq C_T$.

In order to be able to say **anything** useful we have to make simplifying assumptions, *e.g* simultaneous diagonalizability.

We looked at **time-split schemes** as a practical way to route around some (size / complexity) of the computational challenges. (Stability and Boundary Conditions are a different story...)

The Alternating Direction Implicit Method

The Alternating Direction Implicit (ADI) method is particularly useful for solving **parabolic equations** on rectangular domains, but can be generalized to other situations.

Given a parabolic equation, $u_t = \nabla \circ (B \nabla u)$,

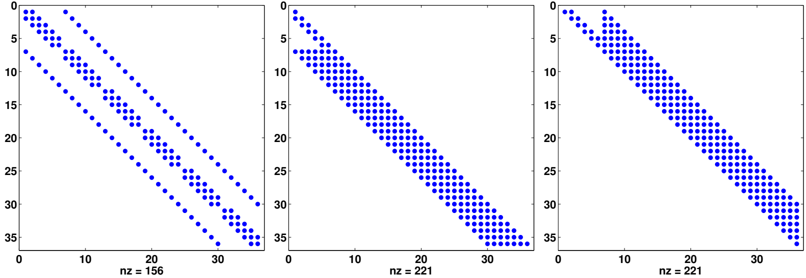
$$u_t = [\partial_x \, \partial_y] \begin{bmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{bmatrix} \begin{bmatrix} \partial_x \\ \partial_y \end{bmatrix} u = b_{11} u_{xx} + 2 b_{12} u_{xy} + b_{22} u_{yy},$$

for which $b_{11}, b_{22} > 0$ and $b_{12}^2 < b_{11} \cdot b_{22}$ for parabolicity; and constant (for now).

Initially, we will consider the case $b_{12} = 0$ (no mixed derivative), on a square domain...

Crank-Nicolson on a Square

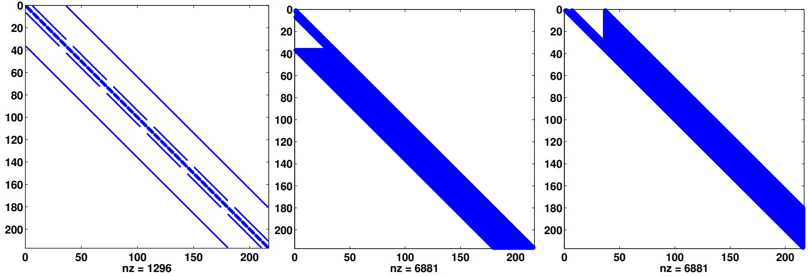
Figure: [LEFT] The matrix which must be inverted in each Crank-Nicolson iteration. If we trade storage of the LU-factorization [CENTER, RIGHT] for speed, then here with 6×6 interior points, we end up needing more than 4 times the storage. For 100×100 interior points, the requirement jumps from 49,600 matrix entries, to just over 2,000,000 (a factor of 40). The band-width grows linearly in n, and the LU-factorization fills in the whole bandwidth. In 3D the story gets even worse — with $n \times n \times n$ interior points, the bandwidth is n^2...



If we use the Crank-Nicolson schemes (for 2 spatial dimensions), we end up having to invert a penta-diagonal matrix in each iteration.

Crank-Nicolson in a Cube

Figure: [LEFT] The matrix which must be inverted in each Crank-Nicolson iteration. If we trade storage of the LU-factorization [CENTER, RIGHT] for speed, then here with $6 \times 6 \times 6$ interior points, we end up needing more than 10 times the storage. For 20^3 (30^3) interior points, the requirement jumps from 53,600 (183,600) matrix entries, to just over 6,000,000 (47,000,000) — a factor of 114 (256). The band-width grows quadratically $\mathcal{O}(n^2)$, and the LU-factorization fills in the whole bandwidth. $\mathrm{LU}_{\mathrm{time}}^{\mathrm{Matlab}} = 8.5\mathrm{s}$ (143.6s).



If we use the Crank-Nicolson schemes (for 3 spatial dimensions), we end up having to invert a hepta-diagonal matrix in each iteration.

The ADI Method on a Square

The ADI method reduces an n-dimensional problem to a sequence of n one-dimensional problems. We here present the idea in 2D... Let A_1 and A_2 be two linear operators, *e.g.*

$$A_1 u = b_1 \frac{\partial^2}{\partial x^2} u, \quad A_2 u = b_2 \frac{\partial^2}{\partial y^2} u.$$

For the argument to make sense, we must require that we have efficient (convenient) ways of solving the equations

$$w_t = A_i w, \; i = 1, 2,$$

with A_1, and A_2 as above and a Crank-Nicolson step, these solutions are given by inversion of tri-diagonal matrices.

The ADI Method on a Square

The ADI method will give us a way to solve the combined equation

$$u_t = A_1 u + A_2 u,$$

using the available 1D-solvers as building blocks.

Crank-Nicolson applied to the combined equation gives us

$$\frac{u^{n+1} - u^n}{k} = \frac{1}{2}\left[A_1 u^{n+1} + A_1 u^n\right] + \frac{1}{2}\left[A_2 u^{n+1} + A_2 u^n\right] + \mathcal{O}\left(k^2\right).$$

Which, with some rearrangement can be written

$$\left[I - \frac{k}{2}A_1 - \frac{k}{2}A_2\right] u^{n+1} = \left[I + \frac{k}{2}A_1 + \frac{k}{2}A_2\right] u^n + \mathcal{O}\left(k^3\right).$$

The ADI Method on a Square

Now, we notice that

$$(1 \pm A_1)(1 \pm A_2) = 1 \pm A_1 \pm A_2 + A_1 A_2.$$

By adding and subtracting $k^2 A_1 A_2 u^{[*]}$ on both sides of the Crank-Nicolson expression we get

$$\begin{aligned}\left[I - \frac{k}{2}A_1 - \frac{k}{2}A_2 + \frac{k^2}{4}A_1A_2\right] u^{n+1} \\ = \left[I + \frac{k}{2}A_1 + \frac{k}{2}A_2 + \frac{k^2}{4}A_1A_2\right] u^{n} \\ + \frac{k^2}{4}A_1A_2\left[u^{n+1} - u^n\right] + \mathcal{O}\left(k^3\right).\end{aligned}$$

The ADI Method on a Square

We can factor this, and use the fact that $u^{n+1} = u^n + \mathcal{O}(k)$ to embed the last term on the right-hand-side into the $\mathcal{O}(k^3)$-term:

$$\left[I - \frac{k}{2}A_1\right]\left[I - \frac{k}{2}A_2\right]u^{n+1} = \left[I + \frac{k}{2}A_1\right]\left[I + \frac{k}{2}A_2\right]u^n + \mathcal{O}\left(k^3\right).$$

Now, if we want to advance the solution numerically, we can discretize this equation, and here when $A_1 = b_1 u_{xx}$, $A_2 = b_2 u_{yy}$, the matrices corresponding to $I - k/2\, A_i$ will be tridiagonal and can be inverted quickly using the Thomas algorithm.

We get the discretized ADI scheme

$$\left[I - \frac{k}{2}A_{1,h}\right]\left[I - \frac{k}{2}A_{2,h}\right]v^{n+1} = \left[I + \frac{k}{2}A_{1,h}\right]\left[I + \frac{k}{2}A_{2,h}\right]v^n.$$

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ADI Algorithms: Peaceman-Rachford

There are several approaches to solving the ADI scheme, one commonly used approach is the Peaceman-Rachford algorithm, which also explain the origin of the name **alternating direction implicit method:**

$$
\begin{aligned}
\left[I - \frac{k}{2}A_{1,h}\right] v^{n+1/2} &= \left[I + \frac{k}{2}A_{2,h}\right] v^{n}, \\
\left[I - \frac{k}{2}A_{2,h}\right] v^{n+1} &= \left[I + \frac{k}{2}A_{1,h}\right] v^{n+1/2}.
\end{aligned}
$$

In the first half-step, the x-direction is implicit, and the y-direction explicit, and in the second half-step the roles are reversed.

Is this scheme equivalent to the ADI scheme we derived?!? — It looks quite different!

ADI Algorithms: Peaceman-Rachford

We have,

$$\begin{aligned}
\left[I - \frac{k}{2}A_{1,h}\right] v^{n+1/2} &= \left[I + \frac{k}{2}A_{2,h}\right] v^{n}, \\
\left[I - \frac{k}{2}A_{2,h}\right] v^{n+1} &= \left[I + \frac{k}{2}A_{1,h}\right] v^{n+1/2}.
\end{aligned}$$

Hence,

$$\left[I - \frac{k}{2}A_{1,h}\right]\left[I - \frac{k}{2}A_{2,h}\right] v^{n+1} = \left[I - \frac{k}{2}A_{1,h}\right]\left[I + \frac{k}{2}A_{1,h}\right] v^{n+1/2}$$

$$= \left[I + \frac{k}{2}A_{1,h}\right]\left[I - \frac{k}{2}A_{1,h}\right] v^{n+1/2} = \left[I + \frac{k}{2}A_{1,h}\right]\left[I + \frac{k}{2}A_{2,h}\right] v^{n}.$$

Note that we do not need $A_{1,h}A_{2,h} = A_{2,h}A_{1,h}$ for this to hold.

ADI Algorithms: D'Yakonov

The D'Yakonov scheme is a direct splitting of the ADI scheme we originally derived:

$$\begin{aligned}
\left[I - \frac{k}{2}A_{1,h}\right] v^{n+1/2} &= \left[I + \frac{k}{2}A_{1,h}\right]\left[I + \frac{k}{2}A_{2,h}\right] v^{n} \\
\left[I - \frac{k}{2}A_{2,h}\right] v^{n+1} &= v^{n+1/2},
\end{aligned}$$

Other ADI-type schemes can be derived starting with other basic schemes (we worked from Crank-Nicolson), *e.g.* the **Douglas-Rachford** method (Strikwerda pp. 175–176) is derived based on backward-time central-space.

Boundary Conditions for ADI Schemes

Here, we consider Dirichlet boundary conditions $u = \beta(t, x, y)$ specified at the boundary, in the context of the Peaceman-Rachford scheme

$$\left[I - \frac{k}{2} A_{1,h}\right] v^{n+1/2} = \left[I + \frac{k}{2} A_{2,h}\right] v^n,$$
$$\left[I - \frac{k}{2} A_{2,h}\right] v^{n+1} = \left[I + \frac{k}{2} A_{1,h}\right] v^{n+1/2}.$$

The correct boundary conditions for the half-step quantity is given by

$$v^{n+1/2} = \frac{1}{2}\left[I + \frac{k}{2} A_{2,h}\right] \beta^n + \frac{1}{2}\left[I - \frac{k}{2} A_{2,h}\right] \beta^{n+1}.$$

Where did that come from?!? — Flip the second equation in the scheme, add the two, and solve for $v^{n+1/2}$... And it makes sense, "half" the condition comes from the past, and "half" from the future.

Implementing ADI Methods

We consider Peaceman-Rachford on a grid, where $(x_\ell, y_m) = (\ell\Delta x, m\Delta y)$, $\ell = 0, \dots, L$, $m = 0, \dots, M$. We let $\mu_x = k/\Delta x^2$, $\mu_y = k/\Delta y^2$. Further, we let $v_{\ell,m}$ denote the full-step quantity, and $w_{\ell,m}$ denote the half-step quantity; if we are not interested in saving the results for all $t = kn$, we can overwrite these quantities...

We get, the first half-stage

$$
\begin{aligned}
-\left[\frac{b_1\mu_x}{2}\right] w_{\ell-1,m} + \left[1 + b_1\mu_x\right] w_{\ell,m} - \left[\frac{b_1\mu_x}{2}\right] w_{\ell+1,m} \\
= \left[\frac{b_2\mu_y}{2}\right] v_{\ell,m-1} + \left[1 - b_2\mu_y\right] v_{\ell,m} + \left[\frac{b_2\mu_y}{2}\right] v_{\ell,m+1},
\end{aligned}
$$

for $\ell = 1, \dots, L-1$, and $m = 1, \dots, M-1$.

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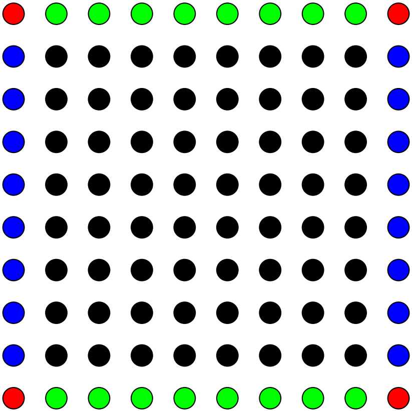
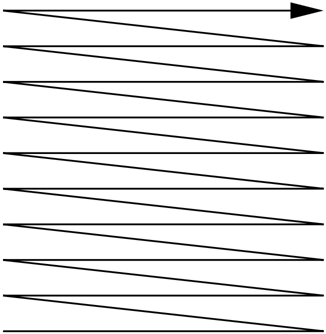
Implementing ADI Methods

Figure: "Active" points in the first half-step, the interior points are active both for the old v-layer and the w-layer which is being computed. Also, the boundary values at the top $v_{\ell,M}$ and bottom $v_{\ell,0}$ boundaries are active, and so are $w_{0,m}$ (left) and $w_{L,m}$ (right).



Implementing ADI Methods

If we enumerate our grid-points in the following (LEXIOGRAPHICAL) way



then we get $(M-1)$ tridiagonal systems (one for each "row"), with $(L-1)$ unknowns.

Implementing ADI Methods

We also need the missing boundary conditions for w

$$w_{0,m} = \left[\frac{b_2\mu_y}{4}\right]\beta^n_{0,m-1} + \left[\frac{1-b_2\mu_y}{2}\right]\beta^n_{0,m} + \left[\frac{b_2\mu_y}{4}\right]\beta^n_{0,m+1}$$
$$- \left[\frac{b_2\mu_y}{4}\right]\beta^{n+1}_{0,m-1} + \left[\frac{1+b_2\mu_y}{2}\right]\beta^{n+1}_{0,m} - \left[\frac{b_2\mu_y}{4}\right]\beta^{n+1}_{0,m+1}.$$

$$w_{L,m} = \left[\frac{b_2\mu_y}{4}\right]\beta^n_{L,m-1} + \left[\frac{1-b_2\mu_y}{2}\right]\beta^n_{L,m} + \left[\frac{b_2\mu_y}{4}\right]\beta^n_{L,m+1}$$
$$- \left[\frac{b_2\mu_y}{4}\right]\beta^{n+1}_{L,m-1} + \left[\frac{1+b_2\mu_y}{2}\right]\beta^{n+1}_{L,m} - \left[\frac{b_2\mu_y}{4}\right]\beta^{n+1}_{L,m+1}.$$

For $m = 1, \ldots, M-1$ ($m = 0$, and $m = M$ are not needed).

Implementing ADI Methods

The second half-stage is given by

$$-\left[\frac{b_2\mu_y}{2}\right] v_{\ell,m-1} + \left[1 + b_2\mu_y\right] v_{\ell,m} - \left[\frac{b_2\mu_y}{2}\right] v_{\ell,m+1}$$
$$= \left[\frac{b_1\mu_x}{2}\right] w_{\ell-1,m} + \left[1 - b_1\mu_x\right] w_{\ell,m} + \left[\frac{b_1\mu_x}{2}\right] - w_{\ell+1,m},$$

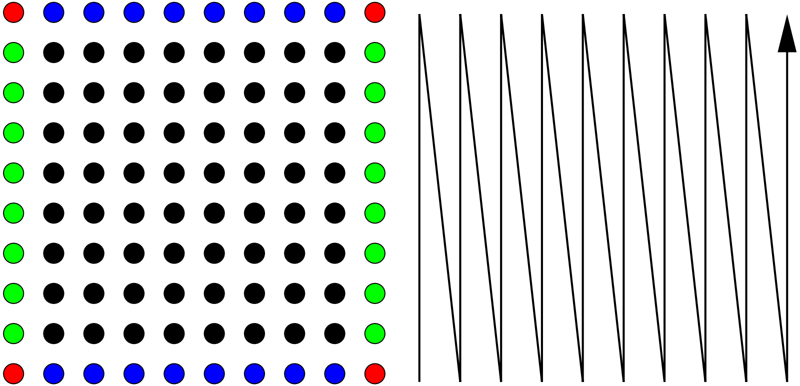
for $\ell = 1, \ldots, L-1$, and $m = 1, \ldots, M-1$.

With the correct grid-ordering, we get $(L-1)$ tridiagonal systems of size $(M-1)$.

Boundary conditions for v are given at time-level $(n+1)$.

Implementing ADI Methods

Figure: "Active" points in the second half-step [left], and the appropriate enumeration order of the grid-points [right].



The Mitchell-Fairweather Scheme

In Strikwerda (pp. 180–181), there is a discussion of the Mitchell-Fairweather scheme, which is an ADI scheme which is second order in time, and fourth order accurate in space:

$$\left[1 - \frac{1}{2}\left(b_1\mu_x - \frac{1}{6}\right) h^2\delta_x^2\right] v^{n+1/2} = \left[1 + \frac{1}{2}\left(b_2\mu_y + \frac{1}{6}\right) h^2\delta_y^2\right] v^n,$$

$$\left[1 - \frac{1}{2}\left(b_2\mu_y - \frac{1}{6}\right) h^2\delta_y^2\right] v^{n+1} = \left[1 + \frac{1}{2}\left(b_1\mu_x + \frac{1}{6}\right) h^2\delta_x^2\right] v^{n+1/2},$$

with Dirichlet boundary conditions for $v^{n+1/2}$

$$v^{n+1/2} = \frac{1}{2b_1\mu_x}\left\{ \left(b_1\mu_x + \frac{1}{6}\right)\left[1 + \frac{1}{2}\left(b_2\mu_y + \frac{1}{6}\right) h^2\delta_y^2\right]\beta^n \right.$$
$$\left. + \left(b_1\mu_x - \frac{1}{6}\right)\left[1 - \frac{1}{2}\left(b_2\mu_y - \frac{1}{6}\right) h^2\delta_y^2\right]\beta^{n+1} \right\}.$$

ADI with Mixed (u_{xy}) Derivative Terms

It has been shown that no ADI scheme involving only the time levels $n+1$ and n can be second-order accurate when $b_{12} \neq 0$ (*i.e.* when we have mixed derivatives).

A second-order accurate modification of the Peaceman-Rachford scheme is given by

$$\left[1 - \frac{k}{2} b_{11} \delta_x^2\right] v^{n+1/2} = \left[1 + \frac{k}{2} b_{22} \delta_y^2\right] v^n + k b_{12} \delta_{0x} \delta_{0y} \left[\frac{3}{2} v^n - \frac{1}{2} v^{n-1}\right],$$

$$\left[1 - \frac{k}{2} b_{22} \delta_y^2\right] v^{n+1} = \left[1 + \frac{k}{2} b_{11} \delta_x^2\right] v^{n+1/2} + k b_{12} \delta_{0x} \delta_{0y} \left[\frac{3}{2} v^n - \frac{1}{2} v^{n-1}\right],$$

with Dirichlet boundary conditions for $v^{n+1/2}$

$$v^{n+1/2} = \frac{1}{2} \left(1 + \frac{k}{2} b_{22} \delta_y^2\right) \beta^n + \frac{1}{2} \left(1 - \frac{k}{2} b_{22} \delta_y^2\right) \beta^{n+1}.$$

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