Numerical Solutions to PDEs
Lecture Notes #12
— Systems of PDEs in Higher Dimensions —
2D and 3D; Time Split Schemes

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   • Multistep Schemes

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Recap

Last Time

- **Discussion:** Lower Order Terms and Stability
- **Proof:** Dissipation and Smoothness
- **Example:** Crank-Nicolson in Non-Dissipative Mode ($\lambda$ fixed)
- **Example:** Crank-Nicolson in Dissipative Mode ($\mu$ fixed)
- **Boundary Conditions:** accuracy, ghost points
- **Convection-Diffusion:** Grid restrictions due to the **physics** (Reynolds or Peclet number) of the problem; upwinding.
The World is not One-Dimensional!

In order to model interesting physical phenomena, we often are forced to leave the confines of our one-dimensional “toy universe.”

The **good news** is that most of our knowledge from 1D carries over to 2D, 3D, and $nD$ without change. Such is the case for convergence, consistency, stability and order of accuracy.

The **bad news** is that the analysis necessarily becomes a “little” messier — we have to Taylor expand in multiple (space) dimensions, all of which will affect stability, etc...
The World is not One-Dimensional!

From a practical standpoint things also get harder — the computational complexity grows — we go from $O(n)$ to $O(n^d)$ spatial grid-points; and each point has more “neighbors” (1D: 2, 2D: 4/8, 3D: 6/26) ⇒ More computations, more storage, more challenging to visualize in a meaningful way...

<table>
<thead>
<tr>
<th>Grid-points</th>
<th>1D</th>
<th>2D</th>
<th>3D</th>
</tr>
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<tbody>
<tr>
<td>$O(n)$</td>
<td>$O(n^2)$</td>
<td>$O(n^3)$</td>
<td></td>
</tr>
<tr>
<td>Matrix Size</td>
<td>$O(n^2)$</td>
<td>$O(n^4)$</td>
<td>$O(n^6)$</td>
</tr>
<tr>
<td>GE/LU Time</td>
<td>$O(n^3)$</td>
<td>$O(n^6)$</td>
<td>$O(n^9)$</td>
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Table: With $n$ points in each unit-direction, we quickly build very large matrices which are work-intensive to invert (for implicit schemes) using naive Gaussian Elimination / Factorization Methods. Using the fact that most matrix entries are zeros (sparsity), and approximate inversion methods (e.g. Conjugate Gradient), problems can still be propagated fairly quickly.
Figure: First- and second “level” grid neighbors on 1D and 2D grids; for 2D we may consider the “mixed” offsets (rightmost panel). In 2D, we have 4 first-level “pure” \(x\)-, or \(y\)-neighbors; including the “mixed” offsets we have 8; on the second level the numbers are 8 and 24.
Figure: First- and second “level” grid neighbors on a 3D grid. **LEFT:** Only the “pure” $x$-, $y$-, and $z$-directions (6, and 12 neighbors); **MIDDLE:** Including the first level “mixed” offsets (26); and **RIGHT:** including the second level “mixed” offsets (124)
Moving to Higher Dimensions

We start out by discussion stability for systems of equations, both **hyperbolic** and **parabolic**, and then move on to a discussion of these systems in 2 and 3 space dimensions.

The vector versions of our model problems are of the form

\[
\begin{align*}
\tilde{u}_t + A\tilde{u}_x &= 0, & \tilde{u}_t &= B\tilde{u}_{xx}
\end{align*}
\]

where \( \tilde{u} \) is a \( d \)-vector, and the matrices \( A, B \) are \( d \times d \); \( A \) must be diagonalizable with real eigenvalues, and the eigenvalues of \( B \) must have positive real part.

There is very little news here — for instance, The Lax-Wendroff scheme for the vector-one-way-wave-equation and the Crank-Nicolson schemes for both vector equations, look just as in the 1D case, but with the scalars \( a, b \) replaced the matrices \( A, B \).
There is some news in testing for stability: instead of a scalar amplification factor \( g(\theta) \), we get an **amplification matrix**. We obtain this matrix by making the substitution \( \vec{v}_m^n \mapsto G^n e^{im\theta} \).

The **stability condition** takes the form: \( \forall T > 0, \exists C_T \) such that for \( 0 \leq nk \leq T \), we have

\[
\| G^n \| \leq C_T.
\]

Computing the \( G \) to the \( n \)th power may not be a lot of fun for a large matrix \( G \)... For **hyperbolic systems** this simplifies when \( G \) is a polynomial or rational function of \( A \) — this occurs in the Lax-Wendroff and Crank-Nicolson schemes.

In this case, the matrix which diagonalizes \( A \), also diagonalizes \( G \), and the stability only depends on the eigenvalues, \( a_i \) of \( A \), e.g. for Lax-Wendroff we must have \( |a_i \lambda| \leq 1 \), for \( i = 1, \ldots, d \).
For parabolic systems, especially for dissipative schemes with $\mu$ constant, similar simplifying methods exist:

The unitary matrix which transforms $B$ to upper triangular form ($\tilde{B} = U^{-1}BU$) can also be used to transform $G$ to upper triangular form, $\tilde{G}$. Then if we can find a bound on $\|\tilde{G}^n\|$, a similar bound applies to $\|G^n\|$.

For more general schemes, the situation is more complicated. A necessary condition for stability is

$$|g_\nu| \leq 1 + Kk,$$

for all eigenvalues $g_\nu$ of $G$. However, this condition is not sufficient in general.
We consider the ("somewhat" artificial, but simple) example

\[
\begin{bmatrix}
u_1 \\
u_2
\end{bmatrix}_t = \begin{bmatrix} 0 \\
0 \end{bmatrix},
\]

and the first order accurate scheme

\[
\begin{align*}
v_{m}^{n+1} &= v_{m}^{n} - \epsilon(w_{m+1}^{n} - 2w_{m}^{n} + w_{m-1}^{n}) \\
w_{m}^{n+1} &= w_{m}^{n}.
\end{align*}
\]

The corresponding amplification matrix is

\[
G = \begin{bmatrix} 1 & 4\epsilon \sin^2 \left(\frac{\theta}{2}\right) \\
0 & 1 \end{bmatrix}.
\]
Example: An Unstable Scheme

The eigenvalues of $G$ are both 1, but

$$G^n = \begin{bmatrix} 1 & 4n\epsilon \sin^2 \left( \frac{\theta}{2} \right) \\ 0 & 1 \end{bmatrix}$$

Hence $\|G^n(\pi)\| = O(n)$, which shows that the scheme is unstable. □

The good news is that the straight-forward extensions of (stable) schemes for single equations to systems usually results in stable schemes.

As for scalar equations, lower order terms resulting in $O(k)$ modifications of the amplification matrix, do not affect that stability of the scheme.
We can analyze multi-step schemes by converting them into systems form, e.g. the scheme

\[ \hat{v}^{n+1}(\xi) = \sum_{\nu=0}^{K} a_\nu(\xi) \hat{v}^{n-\nu}(\xi), \]

can be written in as a \( K + 1 \) system

\[ \hat{V}^{n+1} = G(\theta) \hat{V}^n, \]

where \( \hat{V}^n = [\hat{v}^n(\xi), \ldots, \hat{v}^{n-K}(\xi)]^T \). The matrix \( G(\theta) \) is the **companion matrix** of the polynomial with coefficients \(-a_\nu(\xi)\), given by...
We note that this form of the companion matrix, seems to be somewhat non-standard — both PlanetMath.org and mathworld.wolfram.com give a slightly different (but equivalent) form.
Some Comments

For scalar finite difference schemes, the algorithm given in the context of *simple von Neumann polynomials* and *Schur polynomials* is usually much easier than trying to verify an estimate like $\|G^n\| \leq C_T$.

For **multi-step schemes** applied to **systems of equations**, there is no working extension of the theory of Schur polynomials, so writing the scheme in the form of a one-step scheme for an enlarged system is usually the best route in determining the stability for such schemes.
Finite Difference Schemes in Two and Three Dimensions

As stated earlier, our definitions for convergence, consistency, and stability carry over to multiple dimensions; however, the von Neumann stability analysis becomes quite challenging... We consider two examples:

First, we consider the leapfrog scheme for the system

\[ \ddot{u}_t + A \dot{u}_x + B \dot{u}_y = 0 \]

where \( A, B \) are \( d \times d \) matrices. We write the scheme

\[
\frac{v_{\ell,m}^{n+1} - v_{\ell,m}^{n-1}}{2k} + A \left[ \frac{v_{\ell+1,m}^n - v_{\ell-1,m}^n}{2h_1} \right] + B \left[ \frac{v_{\ell,m+1}^n - v_{\ell,m-1}^n}{2h_2} \right] = 0.
\]
In order to perform the stability analysis, we introduce the Fourier transform solution \( \hat{v}^n(\xi) = \hat{v}^n(\xi_1, \xi_2) \), formally we can let 
\[
v^n_{\ell,m} \sim G^n e^{i\ell\theta_1 e^{im\theta_2}},
\]
where \( \theta_i = h_i \xi_i, \ i = 1, 2 \). With \( \lambda_1 = k/h_1 \), and \( \lambda_2 = k/h_2 \), we get the recurrence relation
\[
\hat{v}^{n+1} + 2i (\lambda_1 A \sin(\theta_1) + \lambda_2 B \sin(\theta_2)) \hat{v}^n - \hat{v}^{n-1} = 0,
\]
\( i.e. \) we are interested in the amplification matrix \( G \), which satisfies
\[
G^2 + 2i (\lambda_1 A \sin(\theta_1) + \lambda_2 B \sin(\theta_2)) G - I = 0.
\]
The scheme can be rewritten as a one-step scheme for a larger system, and we can derive an expression for \( G \) for that system, and check \( \|G^n\| \leq C_T \ldots \) However, it is very difficult to get reasonable conditions without making some assumptions on \( A \) and \( B \).
The most common assumption, which rarely has any connection to reality, is that $A$ and $B$ are **simultaneously diagonalizable**.

That is, we assume there exists a matrix $P$ for which both $PAP^{-1}$ and $PBP^{-1}$ are diagonal matrices. We let $\alpha_\nu$ and $\beta_\nu$ be the diagonal entries of these matrices, and note that with the linear transform $\tilde{w} = P\tilde{v}$, we get $d$ uncoupled scalar relations

$$
\tilde{w}_\nu^{n+1} + 2i (\lambda_1 \alpha_\nu \sin(\theta_1) + \lambda_2 \beta_\nu \sin(\theta_2)) \tilde{w}_\nu^n - \tilde{w}_\nu^{n-1} = 0,
$$

where $\nu = 1, \ldots, d$. This is somewhat more tractable (we can reuse our previous knowledge), and we can conclude that the scheme is stable if and only if

$$
\lambda_1 |\alpha_\nu| + \lambda_2 |\beta_\nu| < 1, \quad \nu = 1, \ldots, d.
$$
The most pessimistic stability region is given by

\[ \lambda_1 |\alpha|_{\text{max}} + \lambda_2 |\beta|_{\text{max}} < 1 \]

where \(|\alpha|_{\text{max}}\) and \(|\beta|_{\text{max}}\) are computed from the separate diagonalizations of \(A\) and \(B\).
A resource-saving modification to the leapfrog scheme, which allows for larger time-steps, is given by

\[
\frac{v_{\ell,m}^{n+1} - v_{\ell,m}^{n-1}}{2k} + A\delta_{0x} \left[ \frac{v_{\ell,m+1}^{n} + v_{\ell,m-1}^{n}}{2} \right] + B\delta_{0y} \left[ \frac{v_{\ell+1,m}^{n} + v_{\ell-1,m}^{n}}{2} \right] = 0.
\]

With the simultaneous diagonalizable assumption, the stability condition is given by

\[
|\lambda_1 \alpha_{\nu} \sin(\theta_1) \cos(\theta_2) + \lambda_2 \beta_{\nu} \sin(\theta_2) \cos(\theta_1)| < 1.
\]

A sequence of inequalities can make some sense out of this...
Since, “obviously,”

\[
|\lambda_1 \alpha \nu \sin(\theta_1) \cos(\theta_2) + \lambda_2 \beta \nu \sin(\theta_2) \cos(\theta_1)| \\
\leq \max \left\{ \lambda_1 |\alpha \nu|, \lambda_2 |\beta \nu| \right\} (|\sin(\theta_1)| |\cos(\theta_2)| + |\sin(\theta_2)| |\cos(\theta_1)|) \\
\leq \max \left\{ \lambda_1 |\alpha \nu|, \lambda_2 |\beta \nu| \right\} \left( (\sin^2(\theta_1) + \cos^2(\theta_1))^{1/2} (\sin^2(\theta_2) + \cos^2(\theta_2))^{1/2} \right) \\
= \max \left\{ \lambda_1 |\alpha \nu|, \lambda_2 |\beta \nu| \right\}. 
\]

The two conditions

\[
\lambda_1 |\alpha \nu| < 1, \quad \lambda_2 |\beta \nu| < 1,
\]

are sufficient for stability (and also necessary).
More General Stability Conditions

It is possible to derive more general stability conditions, without simultaneous diagonalization. If the problem is hyperbolic (easiest argued from the physics), then the matrix function $A\xi_1 + B\xi_2$ is uniformly diagonalizable, i.e. we can find a matrix $P(\xi)$ with uniformly bounded condition number so that

$$P(\xi)(A\xi_1 + B\xi_2)P(\xi)^{-1} = D(\xi),$$

is a diagonal matrix with real eigenvalues. The stability condition becomes

$$\max_{1 \leq i \leq d} \max_{\theta_1, \theta_2} |D_i(\lambda_1 \sin(\theta_1), \lambda_2 \sin(\theta_2))| < 1.$$ 

Sometimes this can be done with reasonable effort, in other cases it is a big task...
Much of the work when it comes to devising \textbf{practically useful} schemes in higher dimensions, is in the direction of dimension reduction; \textit{i.e.} reducing the problem to a sequence of lower-dimensional problems.

Consider

$$u_t + \left[ A \frac{\partial}{\partial x} \right] u + \left[ B \frac{\partial}{\partial y} \right] u = 0.$$ 

One way to simplify this is to let \( A \frac{\partial}{\partial x} \) act with twice the strength during half of the time-step, with \( B \frac{\partial}{\partial y} \) “turned off”, and then switch, \textit{i.e.}

$$u_t + 2 \left[ A \frac{\partial}{\partial x} \right] u = 0, \quad t_0 \leq t \leq t_0 + k/2,$$

$$u_t + 2 \left[ B \frac{\partial}{\partial y} \right] u = 0, \quad t_0 + k/2 \leq t \leq t_0 + k.$$
The analysis of time-split schemes becomes quite “interesting,” to say the least.

- If we use second-order accurate difference schemes, the overall scheme is second-order accurate only if the order of the splitting is reversed on alternate time steps.
- Stability for split-time schemes do not necessarily follow from the stability of each of the steps. Only in the case where the amplification factors (if being matrices) commute is this true (see [1], and [2]).
- Prescribing appropriate boundary conditions is a challenge (see [3]).
References — For More Details


After Fourier transformation we have

\[ \hat{u}_t = -i(A\omega_x + B\omega_y)\hat{u} \]

so that

\[ \hat{u}_t(t+k; \omega_x, \omega_y) = e^{-i(A\omega_x + B\omega_y)k} \hat{u}(t; \omega_x, \omega_y) = e^{(\tilde{A}+\tilde{B})k} \hat{u}(t; \omega_x, \omega_y). \]

In the time-split case

\[ \hat{u}_t(t + k; \omega_x, \omega_y) = e^{\tilde{A}k} e^{\tilde{B}k} \hat{u}(t; \omega_x, \omega_y). \]

Next, we consider the Taylor expansions of the propagators \( e^{(\tilde{A}+\tilde{B})k} \) and \( e^{\tilde{A}k} e^{\tilde{B}k} \) (dropping the tildes).
True Solution
\[ e^{(A+B)k} \sim I + k(A + B) + \frac{k^2}{2}(A + B)^2 + \mathcal{O}(k^3) \]
\[ \sim I + k(A + B) + \frac{k^2}{2}(A^2 + B^2 + AB + BA) + \mathcal{O}(k^3) \]

Standard Split
\[ e^{Ak} e^{Bk} \sim \left[ I + kA + \frac{k^2}{2}A^2 + \mathcal{O}(k^3) \right] \left[ I + kB + \frac{k^2}{2}B^2 + \mathcal{O}(k^3) \right] \]
\[ \sim I + k(A + B) + \frac{k^2}{2}(A^2 + B^2 + 2AB) + \mathcal{O}(k^3) \]

Strang Split
\[ e^{Ak/2} e^{Bk} e^{Ak/2} \sim \left[ I + \frac{k}{2}A + \frac{k^2}{8}A^2 + \mathcal{O}(k^3) \right] \left[ I + kB + \frac{k^2}{2}B^2 + \mathcal{O}(k^3) \right] \left[ I + \frac{k}{2}A + \frac{k^2}{8}A^2 + \mathcal{O}(k^3) \right] \]
\[ \sim I + k(A + B) + \frac{k^2}{2}(A^2 + B^2 + 2AB + BA) + \mathcal{O}(k^3) \]
True Solution

\[ e^{(A+B+C)k} \sim I + k(A + B + C) + \frac{k^2}{2}(A + B + C)^2 + \mathcal{O}(k^3) \]

\[ \sim I + k(A + B + C) + \frac{k^2}{2}(A^2 + B^2 + C^2 + (AB + BA) + (AC + CA) + (BC + CB)) + \mathcal{O}(k^3) \]

Strang Split

\[ e^{Ak/2} e^{Bk/2} e^{Ck/2} e^{Ak/2} \sim \left[ I + \frac{k}{2} A + \frac{k^2}{8} A^2 + \mathcal{O}(k^3) \right] \left[ I + \frac{k}{2} B + \frac{k^2}{8} B^2 + \mathcal{O}(k^3) \right] \left[ I + \frac{k}{2} C + \frac{k^2}{8} C^2 + \mathcal{O}(k^3) \right] \left[ I + \frac{k}{2} A + \frac{k^2}{8} A^2 + \mathcal{O}(k^3) \right] \]

\[ \sim I + k(A + B + C) + \frac{k^2}{2}(A^2 + B^2 + C^2 + (AB + BA) + (AC + CA) + (BC + CB)) + \mathcal{O}(k^3) \]
Homework #3 — Due 3/10/2017

Strikwerda-6.3.2 — Theoretical
Strikwerda-6.3.10 — Numerical
Strikwerda-6.3.14 — Theoretical