Numerical Solutions to PDEs

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

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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Outline

Last Time

- **Discussion:** Lower Order Terms and Stability
- **Proof:** Dissipation and Smoothness
- **Example:** Crank-Nicolson in Non-Dissipative Mode (λ fixed)
- **Example:** Crank-Nicolson in Dissipative Mode (μ 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 *n*D 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 $\mathcal{O}(n)$ to $\mathcal{O}(n^d)$ spatial grid-points; and each point has more "neighbors" (1D: 2, 2D: 4/8, 3D: 6/26) $\Rightarrow$ More computations, more storage, more challenging to visualize in a meaningful way...

	1D	**2D**	**3D**
Grid-points	$\mathcal{O}(n)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^3)$
Matrix Size	$\mathcal{O}(n^2)$	$\mathcal{O}(n^4)$	$\mathcal{O}(n^6)$
GE/LU Time	$\mathcal{O}(n^3)$	$\mathcal{O}(n^6)$	$\mathcal{O}(n^9)$

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 Metods. 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.

Increased Grid / "Bookkeeping" Complexity

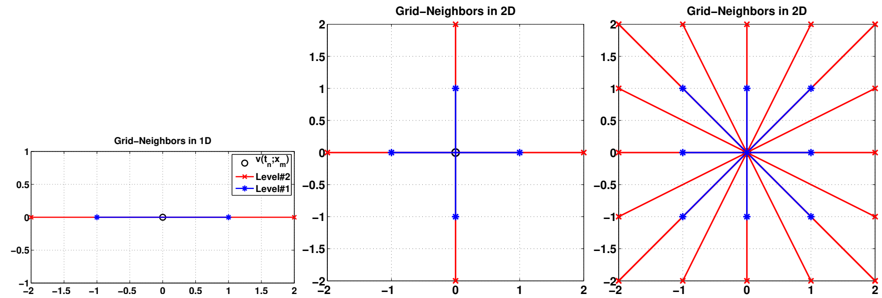


Figure: First- and second "level" grid neighbors on 1D and 2D grids; for 2D we may consider the "mixed" offsets (rightmost panel). In 2D, we have 4 first-level "pure" x-, or y-neighbors; including the "mixed" offsets we have 8; on the second level the numbers are 8 and 24.

Increased Grid / "Bookkeeping" Complexity

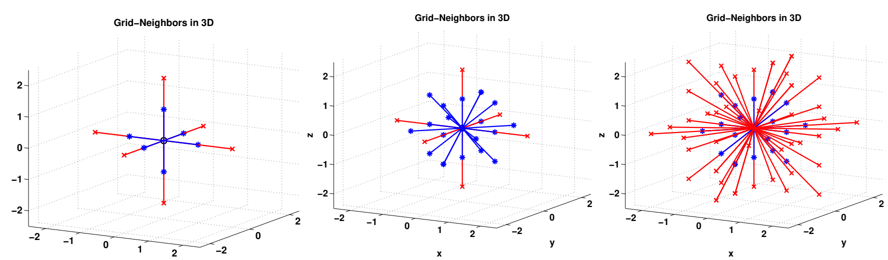


Figure: First- and second "level" grid neighbors on a 3D grid. LEFT: Only the "pure" x-, y-, and z-directions (6, and 12 neighbors); MIDDLE: Including the first level "mixed" offsets (26); and RIGHT: including the second level "mixed" offsets (124)

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

$$\bar{\mathbf{u}}_t + \mathbf{A}\bar{\mathbf{u}}_x = \mathbf{0}, \qquad \bar{\mathbf{u}}_t = \mathbf{B}\bar{\mathbf{u}}_{xx}$$

where $\bar{\mathbf{u}}$ 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.

Moving to Higher Dimensions — Stability, 1 of 2

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 $\bar{\mathbf{v}}_m^n \rightsquigarrow G^n e^{im\theta}$.

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 nth 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 $i = 1, \ldots, d$.

Moving to Higher Dimensions — Stability, 2 of 2

For **parabolic** systems, especially for dissipative schemes with μ constant, similar simplifying methods exist:

The unitary matrix which transforms B to upper triangular form ($\widetilde{B} = U^{-1}BU$) can also be used to transform G to upper triangular form, $\widetilde{G}$. Then if we can find a bound on $\|\widetilde{G}^n\|$, 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_ν of G. However, this condition is **not sufficient** in general.

Example: An Unstable Scheme — 1 of 2

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

$$\begin{aligned} v_m^{n+1} &= v_m^n - \epsilon(w_{m+1}^n - 2w_m^n + w_{m-1}^n) \\ w_m^{n+1} &= w_m^n. \end{aligned}$$

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 — 2 of 2

The eigenvalues of G are both 1, but

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

Hence $\|G^n(\pi)\| = \mathcal{O}(n)$, 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 $\mathcal{O}(k)$ modifications of the amplification matrix, do not affect that stability of the scheme.

Multistep Schemes as Systems

We can analyze multi-step schemes by converting them into systems form, *e.g.* the scheme

$$\widehat{v}^{n+1}(\xi) = \sum_{\nu=0}^{K} a_\nu(\xi)\widehat{v}^{n-\nu}(\xi),$$

can be written in as a $K+1$ system

$$\widehat{V}^{n+1} = G(\theta)\widehat{V}^n,$$

where $\widehat{V}^n = [\widehat{v}^n(\xi), \dots \widehat{v}^{n-K}(\xi)]^T$. The matrix $G(\theta)$ is the **companion matrix** of the polynomial with coefficients $-a_\nu(\xi)$, given by...

Multistep Schemes as Systems

$$G(\theta) = \begin{bmatrix} a_0 & a_1 & \dots & a_{K-1} & a_K \\ I & 0 & \dots & 0 & 0 \\ 0 & I & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & I & 0 \end{bmatrix}$$

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

$$\bar{\mathbf{u}}_t + A\bar{\mathbf{u}}_x + B\bar{\mathbf{u}}_y = 0$$

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

$$\frac{v_{\ell,m}^{n+1} - v_{\ell,m}^{n-1}}{2k} + A\left[\frac{v_{\ell+1,m}^n - v_{\ell-1,m}^n}{2h_1}\right] + B\left[\frac{v_{\ell,m+1}^n - v_{\ell,m-1}^n}{2h_2}\right] = 0.$$

Leapfrogging Along in 2D

In order to perform the stability analysis, we introduce the Fourier transform solution $\widehat{v}^n(\bar{\xi}) = \widehat{v}^n(\xi_1, \xi_2)$, formally we can let $v^n_{\ell,m} \rightsquigarrow G^n e^{i\ell\theta_1} e^{im\theta_2}$, 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

$$\widehat{v}^{n+1} + 2i\left(\lambda_1 A \sin(\theta_1) + \lambda_2 B \sin(\theta_2)\right)\widehat{v}^n - \widehat{v}^{n-1} = 0,$$

i.e. we are interested in the amplification matrix G, which satisfies

$$G^2 + 2i\left(\lambda_1 A \sin(\theta_1) + \lambda_2 B \sin(\theta_2)\right) G - I = 0.$$

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 $\|G^n\| \leq C_T$... However, it is very difficult to get reasonable conditions without making some assumptions on A and B...

Leapfrogging Along in 2D

The most common assumption, which rarely has any connection to reality, is that A and B are **simultaneously diagonalizable**.

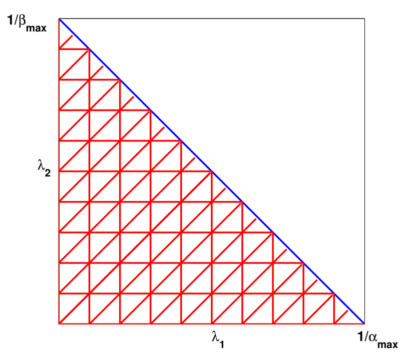
That is, we assume there exists a matrix P for which both PAP^{-1} and PBP^{-1} are diagonal matrices. We let α_ν and β_ν be the diagonal entries of these matrices, and note that with the linear transform $\bar{\mathbf{w}} = P\bar{\mathbf{v}}$, we get d uncoupled scalar relations

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

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

$$\lambda_1|\alpha_\nu| + \lambda_2|\beta_\nu| < 1, \quad \nu = 1, \dots, d.$$

Leapfrogging Along in 2D



The most pessimistic stability region is given by

$$\lambda_1|\alpha|_{\max} + \lambda_2|\beta|_{\max} < 1$$

where $|\alpha|_{\max}$ and $|\beta|_{\max}$ are computed from the separate diagonalizations of A and B.

The Abarbanel-Gottlieb Scheme

A resource-saving modification to the leapfrog scheme, which allows for larger time-steps, is given by

$$\frac{v^{n+1}_{\ell,m} - v^{n-1}_{\ell,m}}{2k} + A\delta_{0x}\Bigg[\underbrace{\frac{v^n_{\ell,m+1} + v^n_{\ell,m-1}}{2}}_{\textit{Average in } y}\Bigg] + B\delta_{0y}\Bigg[\underbrace{\frac{v^n_{\ell+1,m} + v^n_{\ell-1,m}}{2}}_{\textit{Average in } x}\Bigg] = 0.$$

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...

The Abarbanel-Gottlieb Scheme

Since, "obviously,"

$$
\begin{aligned}
&|\lambda_1\alpha_\nu \sin(\theta_1)\cos(\theta_2) + \lambda_2\beta_\nu \sin(\theta_2)\cos(\theta_1)| \\
&\qquad \leq \max\left\{\lambda_1|\alpha_\nu|,\ \lambda_2|\beta_\nu|\right\} \left(|\sin(\theta_1)|\,|\cos(\theta_2)| + |\sin(\theta_2)|\,|\cos(\theta_1)|\right) \\
&\quad \leq \max\left\{\lambda_1|\alpha_\nu|,\ \lambda_2|\beta_\nu|\right\} \left(\left(\sin^2(\theta_1)+\cos^2(\theta_1)\right)^{1/2}\left(\sin^2(\theta_2)+\cos^2(\theta_2)\right)^{1/2}\right) \\
&\qquad\qquad = \max\left\{\lambda_1|\alpha_\nu|,\ \lambda_2|\beta_\nu|\right\}.
\end{aligned}
$$

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...

Time Split Schemes

Much of the work when it comes to devising **practically useful** schemes in higher dimensions, is in the direction of dimension reduction; *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 $\left[A\frac{\partial}{\partial x}\right]$ act with twice the strength during half of the time-step, with $\left[B\frac{\partial}{\partial y}\right]$ "turned off", and then switch, *i.e.*

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

$$u_t + 2\left[B\frac{\partial}{\partial y}\right]u = 0, \qquad t_0 + k/2 \leq t \leq t_0 + k.$$

Time Split Schemes

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]).

Time Split Schemes — 3 of 3

References — For More Details

[1] D. Gottlieb, *Strang-type Difference Schemes for Multidimensional Problems*, SIAM Journal on Numerical Analysis, **9** (1972), pp. 650–661.

[2] G. Strang, *On the Construction and Comparison of Difference Schemes*, SIAM Journal on Numerical Analysis, **5** (1968), pp. 506–517.

[3] R.J. LeVeque and J. Oliger, *Numerical Methods Based on Additive Splittings for Hyperbolic Partial Differential Equations*, Mathematics of Computation, **40** (1983), pp. 469–497.

A Quick Note on Strang-Splitting — 1 of 3

After Fourier transformation we have

$$\widehat{u}_t = -i(A\omega_x + B\omega_y)\widehat{u}$$

so that

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

In the time-split case

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

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).

A Quick Note on Strang-Splitting — 2 of 3

True Solution

$$\begin{aligned} e^{(A+B)k} &\sim I + k(A+B) + \frac{k^2}{2}(A+B)^2 + \mathcal{O}\left(k^3\right) \\ &\sim I + k(A+B) + \frac{k^2}{2}(A^2+B^2+AB+BA) + \mathcal{O}\left(k^3\right) \end{aligned}$$

Standard Split

$$\begin{aligned} e^{Ak}e^{Bk} &\sim \left[I + kA + \frac{k^2}{2}A^2 + \mathcal{O}\left(k^3\right)\right]\left[I + kB + \frac{k^2}{2}B^2 + \mathcal{O}\left(k^3\right)\right] \\ &\sim I + k(A+B) + \frac{k^2}{2}(A^2+B^2+2AB) + \mathcal{O}\left(k^3\right) \end{aligned}$$

Strang Split

$$\begin{aligned} e^{Ak/2}e^{Bk}e^{Ak/2} &\sim \left[I + \frac{k}{2}A + \frac{k^2}{8}A^2 + \mathcal{O}\left(k^3\right)\right]\left[I + kB + \frac{k^2}{2}B^2 + \mathcal{O}\left(k^3\right)\right]\left[I + \frac{k}{2}A + \frac{k^2}{8}A^2 + \mathcal{O}\left(k^3\right)\right] \\ &\sim I + k(A+B) + \frac{k^2}{2}(A^2+B^2+AB+BA) + \mathcal{O}\left(k^3\right) \end{aligned}$$

A Quick Note on Strang-Splitting — 3D — 3 of 3

True Solution

$$\begin{aligned} e^{(A+B+C)k} &\sim I + k(A+B+C) + \frac{k^2}{2}(A+B+C)^2 + \mathcal{O}\left(k^3\right) \\ &\sim I + k(A+B+C) + \\ &\frac{k^2}{2}(A^2+B^2+C^2+(AB+BA)+(AC+CA)+(BC+CB)) + \mathcal{O}\left(k^3\right) \end{aligned}$$

Strang Split

$$\begin{aligned} e^{Ak/2}e^{Bk/2}e^{Ck}e^{Bk/2}e^{Ak/2} &\sim \left[I + \frac{k}{2}A + \frac{k^2}{8}A^2 + \mathcal{O}\left(k^3\right)\right]\left[I + \frac{k}{2}B + \frac{k^2}{8}B^2 + \mathcal{O}\left(k^3\right)\right] \\ &\left[I + kC + \frac{k^2}{2}C^2 + \mathcal{O}\left(k^3\right)\right]\left[I + \frac{k}{2}B + \frac{k^2}{8}B^2 + \mathcal{O}\left(k^3\right)\right]\left[I + \frac{k}{2}A + \frac{k^2}{8}A^2 + \mathcal{O}\left(k^3\right)\right] \\ &\sim I + k(A+B+C) + \frac{k^2}{2}(A^2+B^2+C^2+(AB+BA)+(AC+CA)+(BC+CB)) + \mathcal{O}\left(k^3\right) \end{aligned}$$

Homework #3 — Due 3/9/2018

Strikwerda-6.3.2 — Theoretical

Strikwerda-6.3.10 — Numerical

Strikwerda-6.3.14 — Theoretical