Math 6630: Numerical Solutions of Partial Differential Equations
Finite difference methods for time-dependent problems, Part II

See LeVeque 2007, Chapter 9,
Langtangen and Linge 2017, Chapter 3,

Kreiss, Oliger, and Gustafsson 2013, Chapters 1, 3, 6

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FD for parabolic problems

We've considered the problem and FD discretization,

$$u_t = u_{xx}, \qquad u(x,0) = u_0(x) \quad , x \in [0, 2\pi)$$
$$D^+ u_j^n = D_- D_+ u_j^n,$$

with periodic boundary conditions, and

- Equidistant discretization for x and t
- $x_j = \frac{2\pi j}{M}$, $j \in [M]$. Periodic BC's: we identify $x_M \leftrightarrow x_0$.
  $h = \Delta x = x_{j+1} - x_j$
- $t_n = nk$, $k > 0$ for $n = 0, 1, \ldots$
  $k = \Delta t = t_{k+1} - t_k$
- $u_j^n \approx u(x_j, t_n)$, $\boldsymbol{u}^n = (u_0^n, \ldots, u_{M-1}^n)^T$

Today: Stability, accuracy, convergence, etc.

Method of lines

$$D^+ u_j^n = D_- D_+ u_j^n,$$

The scheme above is fully discrete.

A more transparent understanding of algorithmic behavior can be gained from investigating the semi-discrete scheme:

$$u_t = u_{xx} \quad \xrightarrow{\text{Discretize space}} \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t) = \boldsymbol{A}\boldsymbol{u}(t), \qquad \boldsymbol{u} = (u_1(t), \ldots, u_M(t))^T$$

With periodic boundary conditions, then $\boldsymbol{A}$ is the matrix,

$$h^2 \boldsymbol{A} = \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & & \\ 1 & & & 1 & -2 \end{pmatrix}$$

Method of lines, II

$$u_t = u_{xx} \quad \xrightarrow{\text{Discretize space}} \quad \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t) = \boldsymbol{A}\boldsymbol{u}(t), \qquad \boldsymbol{u} = \left(u_1(t), \ldots, u_M(t)\right)^T$$

This reduction of a *partial* differential equation, to an *ordinary* one through discretization, is called the method of lines.

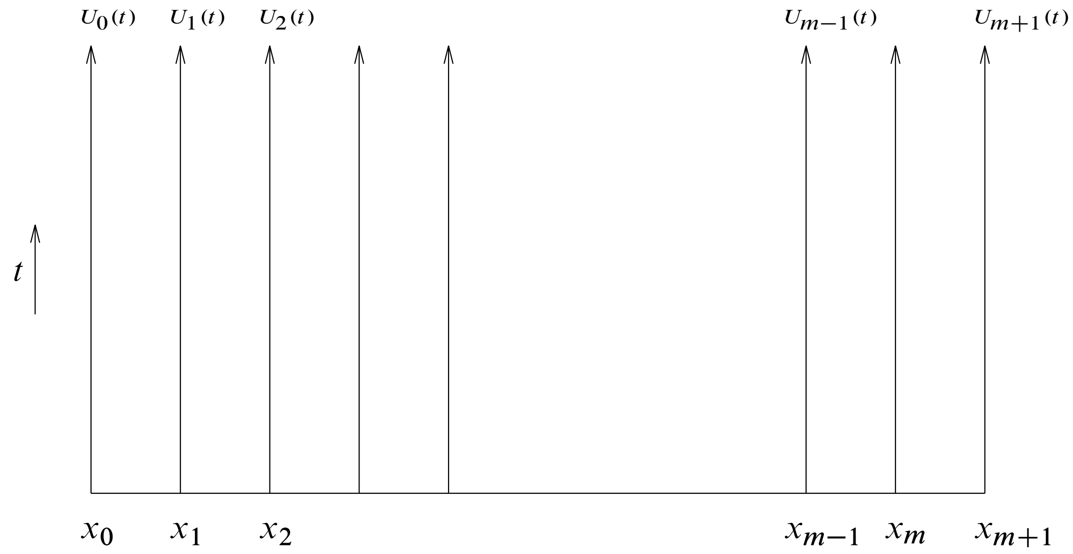

Figure: Method of lines visualization. LeVeque 2007, Figure 9.2

Method of lines, III

$u' = \lambda u$

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The semi-discrete form is useful in *decoupling* space and time.

In particular, it's something we know how to understand from a time-integration point of view:

- Stability (A-stabiltiy, 0-stability)
- Accuracy (time discretization)
- Convergence (conditioned on a fixed spatial discretization)

Convergernce to the solution of the original *PDE solution* does require some interaction of space and time.

Stability

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t) = \boldsymbol{A}\boldsymbol{u}(t), \qquad\qquad \boldsymbol{u} = (u_1(t), \ldots, u_M(t))^T$$

We understand how to generate reasonable schemes for this: any 0-stable method could suffice.

To fix some details, one typically initially considers the simplest scheme to understand the system: Forward Euler.

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + k\boldsymbol{A}\boldsymbol{u}^n.$$

This is a *linear* ODE, and so one simple concept to explore is A-stability.

Is it reasonable to expect behavior of the discrete solution corresponding to A-stability?

To determine stability, the eigenvalues/vectors of $\boldsymbol{A}$ are explicitly computable:

$$\lambda_j(\boldsymbol{A}) = -\frac{4}{h^2}\sin^2\left(\frac{\pi\widetilde{j}}{2M}\right), \qquad \widetilde{j} := \begin{cases} j-1, & j \text{ odd} \\ j, & j \text{ even} \end{cases} \qquad j \in [M]$$

Note that the eigenvalues all have negative real parts ... as we hope for.

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Stiffness

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All these eigenvalues lie in the left half-plane, on the real axis. In particular,

$$\lambda_{\min}(\boldsymbol{A}) = -\frac{4}{h^2} \sim 4M^2 \qquad \lambda_{\max}(\boldsymbol{A}) \sim -1$$

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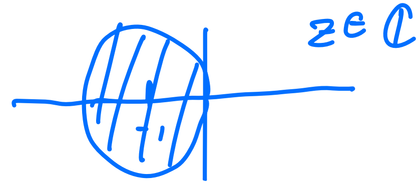
$$\lambda_{\min}(\boldsymbol{A}) = -\frac{4}{h^2} \sim 4M^2 \qquad \lambda_{\max}(\boldsymbol{A}) \sim -1$$

Therefore, there are some parts of the solution that vary slowly (small $|\lambda|$) and other parts of the solution that vary quickly (large $|\lambda|$).

This is a classic sign of stiffness of an ODE – since even moderate M causes large values of $\lambda_{\min}/\lambda_{\max}$, this is a stiff system for those values of M.

Although we have attempted to separate space and time, our choice of spatial discretization will impact our time discretization.

Stability



$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t) = \boldsymbol{A}\boldsymbol{u}(t), \qquad \boldsymbol{u} = (u_1(t), \ldots, u_M(t))^T$$

What does A-stability tell us about the time discretization? For Forward Euler, recall that the region of stability is defined by,

$$|z+1| \leqslant 1, \qquad z = \lambda k,$$

$u' = \lambda u$

with λ being the eigevalues of $\boldsymbol{A}$.

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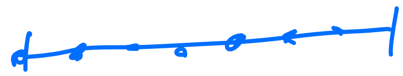
Since $z = \lambda k$ is real-valued (and negative in this case), we really have the condition,

$$z \geqslant -2 \quad \Longrightarrow \quad k|\lambda_{\min}(\boldsymbol{A})| \leqslant 2 \quad \Longrightarrow \quad k \leqslant \frac{h^2}{2}$$

Note that this is a rather disappointing stability requirement. (Consider, say, $h = 0.01$)

Stability



$u_{xx} \approx \frac{1}{h^2}(\cdots)$

u_{xxxx}

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For this PDE, violating this notion of stability is bad: this PDE dissipates energy. Violating stability causes energy to grow.

Note that changing the type of explicit time-stepping scheme (RK, multi-step, etc) does not really change this stability condition, up to some $\mathcal{O}(1)$ constants.

The only real remedy is an A-stable (implicit) scheme.

Local truncation error

$$u_t = u_{xx}, \qquad\qquad u(x,0) = u_0(x)$$
$$D^+ u_j^n = D_- D_+ u_j^n,$$

For computing the local truncation error, considering the semi-discrete scheme does not provide much benefit.

The LTE is the scheme residual when the exact (smooth) solution is inserted:

$$\mathrm{LTE}^n = D^+ u(x_j, t_n) - D_- D_+ u(x_j, t_n) \sim \mathcal{O}(h^2 + k).$$

As before, we say a scheme is consistent if $\lim_{k,h\downarrow 0} \mathrm{LTE}^n = 0$.

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Without directly considering cost of space vs time discretization, one would logically want to balance the LTE by choosing $k \sim h^2$, which is similar to the stability condition.

However, we've already seen that this is not really an attractive strategy for choosing k, motivating that this scheme is not really a good one.

Convergence, I

As usual, the holy grail is convergence. The idea for how to proceed is similar to what we've seen before:

Suppose numerical solution satisfies the scheme exactly:

$$\boldsymbol{u}^{n+1} = \boldsymbol{B}\boldsymbol{u}^{n} + \boldsymbol{f}^{n},$$

where

- $\boldsymbol{B}$ is a matrix such $\boldsymbol{k}\boldsymbol{A}$ for the Forward Euler method
- $\boldsymbol{f}^n$ is any inhomogeneity in the equation (e.g., the term f in $u_t = u_{xx} + f(x,t)$)

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The exact solution $u(x,t)$ at the grids points $\boldsymbol{U}(t)$ satisfies the scheme with an LTE correction $\boldsymbol{\tau}_n$:

$$\boldsymbol{U}(t_{n+1}) = \boldsymbol{B}\boldsymbol{U}(t_n) + \boldsymbol{f}^n + k\boldsymbol{\tau}^n,$$

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Subtracting these two, the error $\boldsymbol{e}_n := \boldsymbol{U}(t_n) - \boldsymbol{u}^n$ satisfies,

$$\boldsymbol{e}_{n+1} = \boldsymbol{B}\boldsymbol{e}_n + k\boldsymbol{\tau}^n,$$

Convergence, II

$$\begin{aligned} \boldsymbol{u}^{n+1} &= \boldsymbol{B}\boldsymbol{u}^n + \boldsymbol{f}^n, \\ \boldsymbol{U}(t_{n+1}) &= \boldsymbol{B}\boldsymbol{U}(t_n) + \boldsymbol{f}^n + k\boldsymbol{\tau}^n, \\ \boldsymbol{e}_{n+1} &= \boldsymbol{B}\boldsymbol{e}_n + k\boldsymbol{\tau}^n, \end{aligned}$$

Iterating the error equation, we conclude,

$$\boldsymbol{e}_n = \boldsymbol{B}^n \boldsymbol{e}_0 + k \sum_{j=1}^{n} \boldsymbol{B}^{n-j} \boldsymbol{\tau}^{j-1}$$

NB: the superscripts n and $n-j$ on $\boldsymbol{B}$ *are* exponents.

Convergence, III

Therefore,

$$\|\boldsymbol{e}_n\| = \|\boldsymbol{B}^n\| \|\boldsymbol{e}_0\| + k \sum_{j=1}^{n} \|\boldsymbol{B}^{n-j}\| \|\boldsymbol{\tau}^{j-1}\|$$

Convergence, III

Therefore,

$$\|\boldsymbol{e}_n\| = \|\boldsymbol{B}^n\| \|\boldsymbol{e}_0\| + k \sum_{j=1}^{n} \|\boldsymbol{B}^{n-j}\| \|\boldsymbol{\tau}^{j-1}\|$$

This reveals that we need to control $\boldsymbol{B}^n$, motivating a new definition.

Definition

A numerical scheme of the form $\boldsymbol{u}^{n+1} = \boldsymbol{B}\boldsymbol{u}^n + \boldsymbol{f}^n$ for computing a solution up to terminal time T is Lax-Richtmyer stable if

$$\|\boldsymbol{B}^n\| \leqslant C(T),$$

for all k sufficiently small and all time indices n satisfying $nk \leqslant T$.

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$$\|\boldsymbol{B}^n\| \leqslant C(T), \qquad \|B\| \leq 1$$

for all k sufficiently small and all time indices n satisfying $nk \leqslant T$.

In practice, showing $\|\boldsymbol{B}\| \leqslant 1 + Ck$ for some constant C independent of k is enough.

$$\|B^n\| \leq \|B\|^n \leq \left(1 + \frac{T}{N} \cdot \frac{1}{T} C\right)^n \sim e^{C/T}$$

Lax-Richtmyer, redux

Convergence of the scheme, under consistency and (Lax-Richtmyer) stability follows:

$$
\begin{aligned}
\|\boldsymbol{e}_n\| &= \|\boldsymbol{B}^n\| \|\boldsymbol{e}_0\| + k \sum_{j=1}^{n} \|\boldsymbol{B}^{n-j}\| \|\boldsymbol{\tau}^{j-1}\| \\
&\stackrel{\text{stability}}{\leqslant} C(T) \left[\|\boldsymbol{e}_0\| + kn \max_{j \in [n]} \|\boldsymbol{\tau}^{j-1}\| \right], \\
&\leqslant C(T) \left[\|\boldsymbol{e}_0\| + T \max_{j \in [n]} \|\boldsymbol{\tau}^{j-1}\| \right], \\
&\xrightarrow{k,h \downarrow 0+ \text{ consistency}} 0,
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where we additionally need $\boldsymbol{e}^0 \to 0$ as $k \downarrow 0$.

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where we additionally need $\boldsymbol{e}^0 \to 0$ as $k \downarrow 0$.
We have just shown part of the following result:

Theorem (Lax-Richtmyer Equivalence)

A linear scheme is convergent if and only if it is consistent and (Lax-Richtmyer) stable.

I.e.,

$$\text{Stability} + \text{Consistency} = \text{Convergence}$$

Achieving stability

How would we achieve (Lax-Richtmyer) stability? The general form is,

$$\boldsymbol{u}^{n+1} = \boldsymbol{B}\boldsymbol{u}^n + \boldsymbol{f}^n,$$

and our Forward Euler in time, central difference in space approximation is,

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + k\boldsymbol{A}\boldsymbol{u}^n = \left(\boldsymbol{I} + k\boldsymbol{A}\right)\boldsymbol{u}^n,$$

so for stability, say in the 2-norm, we require,

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Since all eigenvalues of $\boldsymbol{A}$ are real and negative, this is ensured via,

$$k|\lambda_{\min}(\boldsymbol{A})| \leqslant 2 \quad \Longrightarrow \quad k \leqslant \frac{h^2}{2}$$

which is *exactly* the same requirement we obtained from A-stability.

Scheme convergence

Thus, we have that

$$u_t = u_{xx} \quad \longrightarrow \quad D^+ u_j^n = D_+ D_- u_j^n$$

has an LTE and stability criterion:

$$\mathrm{LTE}_n = \mathcal{O}(k^2 + h)$$
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This explain many "weird" issues we observed when naively trying to ascertain convergence of this method:

- Things are unstable if we don't satisfy $k \lesssim h^2$. In particular $k \sim h$ is not useful.
- How would we numerically verify h convergence? We'd need to
  - Pick a smallest h, say $h_{\min}$
  - Fix $k \leqslant h_{\min}^2/2$
  - Compare errors for $h = h_{\min}, 2h_{\min}, 4h_{\min}, 8h_{\min}, \ldots$
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- Fix k, and varying h to satisfy $k \leqslant h^2/2$ would allow us to detect h-convergence
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If we alternatively use Crank-Nicholson:

- Stability is unconditional ($\|\boldsymbol{B}^n\| \leqslant 1$ is automatic)
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- Fix k, varying h to satisfy $k \leqslant h$ would allow us to detect h-convergence
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Von Neumann stability, I

We've seen that it's possible to directly verify Lax-Richtmyer stability.

But in even slightly more complicated scenarios, a similar analysis is quite difficult.

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A similar computation is true for reasonable spatial discretizations of derivatives.

Then a reasonable (somewhat empirical) notion of (Von Neumann) stability for a scheme would assert that the scheme does *not amplify* eigenfunctions in time.

Von Neumann stability, II

The general strategy for von Neumann stability on linear problems is to consider the scheme,

$$u_j^{n+1} = B(\boldsymbol{u}^n)$$

for a linear operator B acting on the degrees of freedom at time step j. If we make the ansatz,

$$\boldsymbol{u}^n = e^{i\omega \boldsymbol{x}} \quad \longrightarrow \quad u_j^n = e^{i\omega x_j} = e^{i\omega j h},$$

then we expect that plugging this into scheme will yield the expression,

$$u_j^{n+1} = g(\omega) e^{i\omega j h},$$

for some constant $g(\omega)$.[1]

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The function g is called the (Von Neumann) *amplification factor* of the scheme.

The scheme will be (Von Neumann) stable if $|g(\omega)| \leqslant 1$.[2]

[1] In principle g can depend on j, but it will not if the discretization is spatially homogeneous.
[2] Like for Lax-Richtmyer stability, we'll actually just need $|g(\omega)| \leqslant 1 + Ck$.

Examples

Example

Compute the Von Neumann stability condition for

$$D^+ u_j^n = D_0 u_j^n$$

Setting $u_j^n = e^{i\omega jh}$, and $u_j^{n+1} = g(\omega)e^{i\omega jh}$, then we have,

$$u_j^{n+1} = u_j^n + \frac{k}{h^2}\left[u_{j+1}^n - 2u_j^n + u_{j-1}^n\right]$$

$$\downarrow$$

$$g(\omega)e^{i\omega jh} = e^{i\omega jh} + \frac{k}{h^2}e^{i\omega jh}\left[e^{i\omega h} - 2 + e^{-i\omega h}\right],$$

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Since $-2 \leqslant (\cos\omega h - 1) \leqslant 0$, then $|g(\omega)| \leqslant 1$ if

$$\frac{2k}{h^2} \leqslant 1 \quad \Longrightarrow \quad k \leqslant \frac{h^2}{2}$$

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