Objective. We will continue our discussion on the numerical solution of parabolic partial differential equations. In particular, we will study the stability of the numerical methods we have introduced to solve the canonical parabolic partial differential equation.

Agenda. In today's class, we will discuss the following.

1. Announcements
2. We discuss the material in Chapter 9, Sections 9.2 - 9.6 of LeVeque's book.

Topic: Method of Lines. We can relate our understanding of stability for initial-value problems for ODEs to PDEs using the so-called method of lines. For the method of lines, we implement a spatial discretization only for the PDE. That leaves a finite dimensional system of ODEs in time which we call the semidiscrete equations. For example, if we use a centered, second order finite difference approximation for u_{xx} in the diffusion equation $u_t = u_{xx}$, we obtain for the grid point x_i:

$$U_i'(t) = \frac{1}{h^2}[U_{i-1}(t) - 2U_i(t) + U_{i+1}(t)], \quad i = 1, 2, \cdots, m.$$

If we include the boundary conditions, we can write these semi-discrete equations as the system

$$\mathbf{U}'(t) = A\mathbf{U}(t) + \mathbf{g}(t),$$

with A denoting the tridiagonal matrix corresponding to the centered finite difference approximation and $\mathbf{g}(t)$ corresponding to the Dirichlet boundary conditions: $U_0(t) = g_0(t)$ and $U_{m+1}(t) = g_1(t)$.

In this form, we may apply any of the ODE methods that you have discussed in MATH 231 to solve this problem. The method of lines is rather general. However, we find in practice that more specialized methods tend to be more efficient to solve PDEs.

However, the method of lines is very valuable to studying the stability of a method to solve PDEs. Consider using the forward Euler method to solve the system above. In doing so, we obtain

$$\mathbf{U}^{n+1} = \mathbf{U}^n + kA\mathbf{U}^n + k\mathbf{g}^n,$$

which is the first method we introduced. Instead of forward Euler, suppose we use the trapezoidal method to solve the system of ODEs. For that case, we obtain

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \frac{1}{2}kA\mathbf{U}^{n+1} + \frac{1}{2}kA\mathbf{U}^n + \frac{1}{2}k\mathbf{g}^{n+1} + \frac{1}{2}k\mathbf{g}^n,$$

which is the Crank-Nicolson method.

Now, using our previously acquired knowledge about systems of ODEs, we expect a method to be stable if $k\lambda \in \mathscr{S}$ with λ denoting an eigenvalue of A and $\mathscr{S}$ denoting the stability region of the time stepping method. The eigenvalues of A are known explicitly to be

$$\lambda_p = \frac{2}{h^2}[\cos(p\pi h) - 1], \quad p = 1, 2, \cdots, m,$$

with $h = 1/(m+1)$. Thus, we need to ensure that $k\lambda_p \in \mathscr{S}$ for all p for stability. Since A is symmetric negative-definite, all of its eigenvalues are real and negative. The smallest eigenvalue in magnitude is given by $\lambda_1 \approx -\pi^2$. The largest eigenvalue in magnitude is given by $\lambda_m \approx -4/h^2$. Hence, we require that $-4/h^2 \in \mathscr{S}$.

For the forward Euler method the stability region is given by $|1 + k\lambda_p| \leq 1$ for each p. Since each λ_p is real, we require $-2 \leq k\lambda_p \leq 0$ for each p. Using the largest eigenvalue, we find that

$$-2 \leq -\frac{4k}{h^2} \leq 0,$$

or

$$k \leq \frac{h^2}{2}.$$

This time step restriction is extreme. We must set the time step k to be less than h^2!

Recall for the trapezoidal method that the stability region includes the entire left-half plane. Since the eigenvalues of the system are always negative and real, the Crank-Nicolson method is stable for any $k > 0$. We typically choose $k = O(h)$.

It is for these reasons that we consider the diffusion equation to be stiff. If we look at the stiffness ratio, we find that it is given by

$$\frac{\max|\lambda_p|}{\min|\lambda_p|} \approx \frac{4}{\pi^2 h^2} = O(m^2).$$

We can see why this problem is stiff by looking at its analytical solution with homogeneous Dirichlet boundary conditions: $g_0(t) = g_1(t) = 0$. It is given by a Fourier sine series

$$u(x,t) = \sum_{j=0}^{\infty} a_j e^{-j^2\pi^2 t} \sin(j\pi x),$$

with

$$a_j = 2\int_0^1 \eta(x)\sin(j\pi x)\mathrm{d}x.$$

From this solution, we see that the time scales are given by $\tilde{t} = 1/(j\pi)^2$ for $j = 0, 1, 2, \cdots$. Thus, there are widely varying time scales in this problem associated with the higher spatial frequency modes. Physically, we know that the diffusion equation damps higher frequencies faster than lower ones. It is this spread of time scales that leads to its stiffness.

Topic: Convergence. We now address the question of the convergence of the numerical solution at a fixed point (X, T) as the spatio-temporal grid is refined. Because we have both space and time in these problems, we need to consider the relative rates by which k and h approach zero. In general, they cannot approach zero at an arbitrary rate that is independent from one another. In fact, we consider a fixed rule of the form $k = \alpha h$ and consider only the limit as $k \to 0$ with the understanding that h will go to zero also according to this rule.

For the forward Euler method, we have the update formula

$$\mathbf{U}^{n+1} = (I + kA)\mathbf{U}^n + k\mathbf{g}^n,$$

and for the Crank-Nicolson method, we have the update formula

$$\mathbf{U}^{n+1} = (I - \frac{1}{2}kA)^{-1}(I + \frac{1}{2}kA)\mathbf{U}^n + (I - \frac{1}{2}kA)^{-1}k\mathbf{g}^n.$$

To study the convergence of these methods, we will need consistency and a suitable form of stability. Consistency is as we discussed before: the local truncation error vanishes as $k \to 0$. For stability, we introduce Lax-Richtmyer stability.

Definition 9.1. *A linear method of the form*

$$\mathbf{U}^{n+1} = B(k)\mathbf{U}^n + \mathbf{b}^n(k)$$

is Lax-Richtmyer stable if, for each time T, there is a constant $C_T > 0$ such that

$$\|B(k)^n\| \leq C_T$$

for all $k > 0$ and integers n for which $kn \leq T$.

With Lax-Richtmyer stability established, we give the Lax Equivalence Theorem.

Theorem 9.2. *A consistent linear method is convergent if and only if it is Lax-Richtmyer stable.*

Informally, we can see how the Lax Equivalence Theorem works. Suppose we have the linear method

$$\mathbf{U}^{n+1} = B(k)\mathbf{U}^n + \mathbf{b}^n(k)$$

with $B(k)$ Lax-Richtmyer stable. If we substitute the exact solution, we obtain

$$\mathbf{u}^{n+1} = B(k)\mathbf{u}^n + \mathbf{b}^n(k) + k\tau^n,$$

with τ^n denoting the local truncation error. Let $\mathbf{E}^n = \mathbf{U}^n - \mathbf{u}^n$ which satisfies

$$\mathbf{E}^{n+1} = B(k)\mathbf{E}^n - k\tau^n.$$

By induction, we find that after N steps, we obtain

$$\mathbf{E}^N = B(k)^N\mathbf{E}^0 - k\sum_{n=1}^{N} B(k)^{N-n}\tau^{n-1}.$$

Thus, it follows that from Lax-Richtmyer stability that

$$\|\mathbf{E}^N\| \leq C_T\|\mathbf{E}^0\| + TC_T \max_{1\leq n\leq N} \|\tau^{n-1}\|.$$

And so, $\|\mathbf{E}^N\| \to 0$ as $k \to 0$ for $Nk \leq T$ as long as $\|\tau\| \to 0$ (consistency) and $\|\mathbf{E}^0\| \to 0$ as $k \to 0$.

For the symmetric matrix A, its 2-norm is its spectral radius. We know the eigenvalues A to be

$$\lambda_p = \frac{2}{h^2}[\cos(p\pi h) - 1], \quad p = 1, 2, \cdots, m.$$

So for the forward Euler method in which

$$B(k) = (I + kA)$$

the matrix $B(k)$ is also symmetric, so its 2-norm is its spectral radius:

$$\rho(B) = \max_{1\leq p\leq m} |1 + k\lambda_p| \approx |1 - k\frac{4}{h^2}|.$$

If we choose $k \leq h^2/2$, then $\rho(B) \leq 1$ and so $\|B\|_2 \leq 1$. Thus, the forward Euler method is Lax-Richtmyer stable and hence, convergent under the restriction that $k \leq h^2/2$.

For the Crank-Nicolson method, the matrix $B(k)$ is given by

$$B(k) = (I - \frac{1}{2}kA)^{-1}(I + \frac{1}{2}kA),$$

and so the eigenvalues of $B(k)$ are given by

$$\frac{1 + k\lambda_p/2}{1 - k\lambda_p/2}.$$

For this reason, the Crank-Nicolson method is Lax-Richtmyer stable in the 2-norm for any $k > 0$.

Both of these examples led to $\|B\| \leq 1$ which corresponds to strong stability. For Lax-Richtmyer stability, however, it is sufficient if there exists a constant α so that a bound of the form

$$\|B(k)\| \leq 1 + \alpha k$$

holds. This is true because

$$\|B(k)^n\| \leq (1 + \alpha k)^n \leq e^{\alpha T}.$$

Topic: Von Neumann Analysis. One way to analyze the PDE discretization is to study the Cauchy problem for either problems over the whole line $-\infty < x < \infty$ or for a periodic problem with periodic boundary conditions. For that case, we introduce the so-called eigengridfunction

$$W_j = e^{\mathrm{i}jh\xi}.$$

Consider the second order, centered finite difference approximation applied to W_j:

$$\begin{aligned} D^2 W_j &= \frac{1}{h^2}(W_{j-1} - 2W_j + W_{j+1}) \\ &= \frac{1}{h^2}(e^{\mathrm{i}(j-1)h\xi} - 2e^{\mathrm{i}jh\xi} + e^{\mathrm{i}(j+1)h\xi}) \\ &= \frac{1}{h^2}(e^{-\mathrm{i}h\xi} - 2 + e^{\mathrm{i}h\xi})W_j \\ &= \frac{2}{h^2}(\cos(h\xi) - 1)W_j. \end{aligned}$$

We obtain a result proportional to W_j with eigengridvalue $\frac{2}{h^2}(\cos(h\xi) - 1)$.

To explain why we would use this eigengridfunction, consider the Cauchy problem over the whole line $-\infty < x < \infty$. Now suppose a grid function V_j defined at grid points $x_j = jh$ for $j = 0, \pm 1, \pm 2, \cdots$ is an l_2 function:

$$\|V\|_2 = \left(h \sum_{j=-\infty}^{\infty} |V_j|^2 \right)^{1/2} < \infty.$$

Then, we can represent V_j as a linear combination of the eigengridfunctions $W_j = e^{\mathrm{i}jh\xi}$ for all

$\xi \in [-\pi/h, \pi/h]$ since functions with larger wave number ξ cannot be resolved on this grid. Thus, we have

$$V_j = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{V}(\xi) e^{\mathrm{i}jh\xi} \mathrm{d}\xi,$$

with

$$\hat{V}(\xi) = \frac{h}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} V_j e^{-\mathrm{i}jh\xi}.$$

We refer to this expression as the discrete Fourier transform. For the discrete Fourier transform, we still have Parseval's relation

$$\|\hat{V}\|_2 = \|V\|_2$$

with

$$\|V\|_2 = \left(h \sum_{j=-\infty}^{\infty} |V_j|^2 \right)^{1/2}$$

and

$$\|\hat{V}\|_2 = \left(\int_{-\pi/h}^{\pi/h} |\hat{V}(\xi)|^2 \right)^{1/2}.$$

Now, recall that to have Lax-Richtmyer stability in the 2-norm, it is sufficient that there exists a constant α such that

$$\|U^{n+1}\|_2 \leq (1 + \alpha k)\|U^n\|_2.$$

Using Parseval's relation, we obtain

$$\|\hat{U}^{n+1}\|_2 \leq (1 + \alpha k)\|\hat{U}^n\|_2.$$

The utility of working in the Fourier domain is that we obtain a decoupled system of the form

$$\hat{U}^{n+1} = g(\xi)\hat{U}^n,$$

with $g(\xi)$ called the amplification factor. Thus, if we show that

$$|g(\xi)| \leq 1 + \alpha k$$

with some α independent of ξ then it follows that the method is stable since

$$|\hat{U}^{n+1}| \leq (1 + \alpha k)|\hat{U}^n|$$

will hold for all ξ which implies that

$$\|\hat{U}^{n+1}\|_2 \leq (1+\alpha k)\|\hat{U}^n\|_2.$$

Effectively, what Von Neumann stability analysis does is diagonalizes the method so that we can determine its stability more easily.

For the forward Euler method:

$$U_j^{n+1} = U_j^n + kD^2U_j^n,$$

we set $U_j^n = e^{\mathrm{i}jh\xi}$ and $U_j^{n+1} = g(\xi)e^{\mathrm{i}jh\xi}$ to obtain

$$g(\xi)e^{\mathrm{i}jh\xi} = e^{\mathrm{i}jh\xi} + \frac{2k}{h^2}(\cos(h\xi)-1)e^{\mathrm{i}jh\xi}.$$

Therefore,

$$g(\xi) = 1 + \frac{2k}{h^2}(\cos(h\xi)-1).$$

Since $-1 \leq \cos(h\xi) \leq 1$, we determine that

$$1 - \frac{4k}{h^2} \leq g(\xi) \leq 1.$$

To guarantee that $|g(\xi)| \leq 1$ for all ξ, we must require that

$$\frac{4k}{h^2} \leq 2,$$

which is the result we arrived at earlier.

We will be using Von Neumann analysis throughout this semester.