Finite Differences for Parabolic PDEs

A. Donev, Courant

Today we consider time-evolving $u(x,t)$ for linear parabolic PDEs

$$u_t = -\mathcal{L}u + f(x,t) + \text{BCs} + \text{ICs} \quad \dots\dots (*)$$

$\mathcal{L}$: elliptic operator

BCs are the same as for elliptic PDEs, e.g., Dirichlet or Neumann if $\mathcal{L}$ is second order (∇^2), on the whole boundary.

Parabolic PDEs are smoothing (inherited from elliptic regularity) and dissipative (all eigenvalues of $-\mathcal{L}$ are real and non-positive, since $\mathcal{L}$ is an elliptic operator).

$$u(x, t \to \infty) \to u_{ell}(x)$$

where $u_{ell}(x)$ solves the elliptic PDE, assuming $f = \text{const}$,

$$\mathcal{L} u_{ell} = f + BCs \ldots \quad (**)$$

i.e., the initial conditions are forgotten / dissipated / erased.

Let a finite-difference (FD) discretization of the elliptic (**) be

$$\overleftrightarrow{A}\,\vec{u} = \vec{f} \quad (t = \text{const})$$

Then, the corresponding method of lines (MOL) discretization of the parabolic (*) is:

$$\frac{d\vec{u}}{dt} = -\overleftrightarrow{A}\,\vec{u} + \vec{f}(t), \quad \vec{u}(0) = \vec{u}_0$$

which is a simple system of linear ODEs! If $f = 0$, then

$$u(t) = \exp(-At)\,\vec{u}_0$$

We are thus back to solving ODEs. But, the # of variables in the ODE is very large (e.g., 10^6 for 3D) and grows as the grid spacing h is reduced.

In the limit $h \to 0$, we get an infinite dimensional system of ODEs, which is troubling!

This is what makes parabolic PDEs much more challenging than (low dimensional) systems of ODEs.

Let's focus for now on (up to) second order accuracy. We could try:

① Forward Euler (explicit)

$$\frac{u^{n+1} - u^n}{\tau} = -Au^n + f(t^n)$$

$$\Rightarrow u^{n+1} = (I - A\tau)u^n + \tau f(t^n)$$

Key advantage of this is that method is explicit so no linear systems need to be solved.

② Implicit midpoint, also called (in physics) Crank–Nicolson

$$\frac{u^{n+1}-u^{n}}{\tau} = -A\left(\frac{u^{n+1}+u^{n}}{2}\right) + f(t^{n+1/2})$$

$$\left(I + \frac{A\tau}{2}\right)u^{n+1} = \left(I - \frac{A\tau}{2}\right)u^{n} + f^{n+1/2}$$

which we need to solve every timestep

$$u^{n+1} = \left(I + \frac{A\tau}{2}\right)^{-1}\left[\left(I - \frac{A\tau}{2}\right)u^{n} + f^{n+1/2}\right]$$

⑥

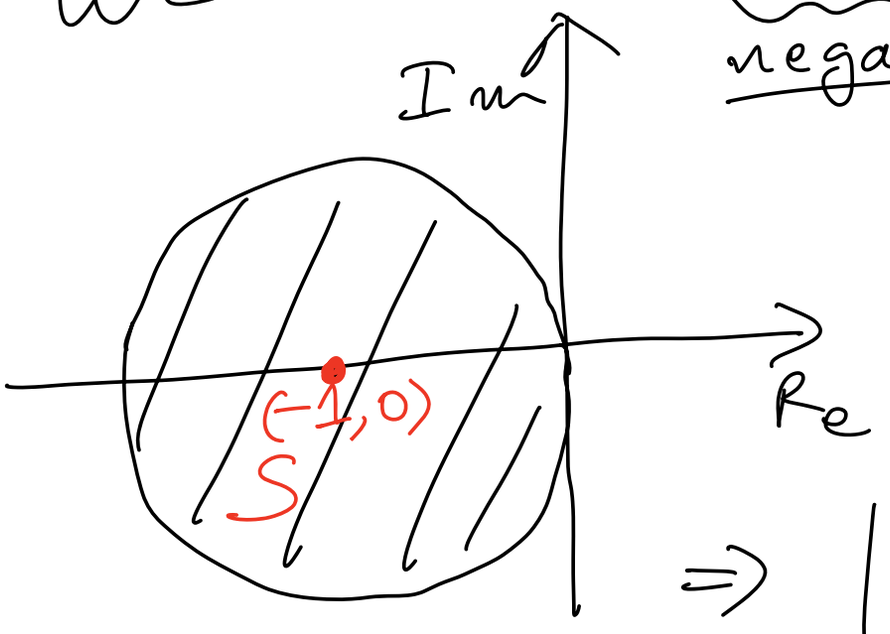
Stability

The key question is, how big can Δt be?

Euler

We want $-\lambda_p \bar{\tau} \in S \quad \forall p$

<u>negative</u> $\Rightarrow$



$$0 \leq \lambda_p \bar{\tau} < 2$$

for stability

$$\Rightarrow |\lambda_{min} \bar{\tau}| < 2$$

For example, consider on $[0,1]$:

$$u_t = k u_{xx} + f(x,t) + \text{Dirichet BCs}$$

$$A = k \begin{bmatrix} -2 & 1 & & & \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & 1 \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{bmatrix}$$

$$\Rightarrow \quad \lambda_p = \frac{2k}{h^2}\left(\cos(p\pi h) - 1\right)$$

$$\Rightarrow \lambda_{min} = \lambda_{p=\frac{1}{h}} \simeq -\frac{4k}{h^2}$$

$$\Rightarrow \boxed{\frac{k\tau}{h^2} = \nu \leq \frac{1}{2}}$$

(stability condition)

Courant-Friedrichs-Lewy (number)

CFL condition & number

Physics: In time τ, diffusion spreads the solution over an average or typical distance $\sqrt{k\tau}$, and we want $\sqrt{k\tau} \sim h$ for stability

For explicit methods, stability requires

$$\Delta t \leq O(1) \frac{h^2}{k}$$

i.e. $\boxed{\nu \leq O(1)}$, where the $O(1)$ constant depends on the specific explicit temporal integrator used.

For forward Euler:

$$\nu \leq \frac{1}{2d}$$ for stability

↖ dimension

Aside: the physics of the CFL condition

$$\gamma \leq \frac{1}{2d}$$ where d = dimension

The diffusion equation comes from random walks. Here is how. Imagine having many many "particles"/points jumping from one grid cell to one of the neighboring $2d$ cells (left/right, up/down in 2D). Imagine that a given cell/node has N particles at time t. Then, the number of particles

$$\left(N_1^+, N_1^-, N_2^+, N_2^-, \ldots, N_d^+, N_d^-, N_0 \right)$$

10.A

that jump from the given grid cell/node to one of the $2d$ neighboring cells/nodes and the number N_0 that stay in the same cell after a time τ is given by the multinomial distribution with parameters $N = N_0 + \sum_{\alpha=1}^{d} (N_\alpha^+ + N_\alpha^-)$, $k = 2d+1$, and probabilities

$$\left(\underbrace{\nu, \nu, \ldots, \nu}_{2d \ \nu\text{'s}}, 1 - 2d\nu \right)$$

Since probabilities are positive,

$1 - 2d\nu \geq 0 \Rightarrow$ $\boxed{\nu \leq \frac{1}{2d}}$ CFL condition

Another physical interpretation of the diffusive CFL limit (but not a derivation per se) is to ask that the mean square displacement of a diffusing particle should be $\leq h^2$:

$$\text{MSD} = \underbrace{2 d k \tau}_{\text{Einstein's formula}} \leq h^2$$

$$\Rightarrow \quad \tau \leq \frac{h^2}{2dk} \quad \Rightarrow \quad \boxed{\nu \leq \frac{1}{2d}}$$

as before

How about accuracy? Let's examine the truncation error:

$$\mathcal{E}(x,t) = \frac{u(x,t+\tau) - u(x,t)}{\tau} - \frac{k}{h^2}\left[u(x-h,t) - 2u(x,t) + u(x+t,h)\right]$$

$$= \frac{1}{2}\tau u_{tt} + O(\tau^2) \leftarrow \text{temporal discretization error}$$

$$- \frac{kh^2}{12} u_{xxxx} + O(h^4) \leftarrow \text{spatial discretization error}$$

where we assumed $f=0$

MOL error = spatial + temporal

$$u_t = k u_{xx} \Rightarrow$$

$$u_{tt} = k(u_{xx})_t = k(u_t)_{xx} \Rightarrow$$

$$u_{tt} = k^2 u_{xxxx} \Rightarrow$$

$$\text{LTE} \quad \varepsilon = k\left(\frac{k\tau}{2} - \frac{h^2}{12}\right) u_{xxxx} + O(\tau^2, h^4)$$

$$\varepsilon = \left(\frac{r}{2} - \frac{1}{12}\right) k h^2 u_{xxxx} \quad \ldots (A)$$

Since $\nu \leq \frac{1}{2}$ for stability,

we see that for forward Euler,

$\nu = 1/6$ makes the spatial and temporal discretization/truncation errors (approximately) equal in magnitude

this is a good choice for ν!

$$\tau \sim \frac{h^2}{[4-6]k} \Rightarrow LTE \sim (k u_{xxxx}) h^2$$

$\bar{\tau} = O(h^2) \Rightarrow LTE = O(h^2)$ for Euler

So the method is second-order accurate in the grid spacing h!
Even though we used a first order temporal integrator, we (expect to) get 2nd order in space-time. Since $\bar{\tau} \sim h^2$, we say that the error is 2nd order under space-time refinement.
(or 2nd order in space-time)

CRANK-NICOLSON (implicit)

We know that implicit midpoint is A-stable, so the method is unconditionally stable.

But of course τ cannot be arbitrarily large for accuracy.

For CN, we have

$$LTE = \underbrace{O(h^2)}_{\text{spatial}} + \underbrace{O(\tau^2)}_{\text{temporal}}$$

We want $|\text{spatial}| \simeq |\text{temporal}|$

$\tau = O(h) \Rightarrow LTE = O(h^2)$ for CN

As $h \to 0$, $O(h^2) << O(h)$, so CN can take a much larger time step size than Euler for fine grids (high accuracy)! But, each time step is more expensive because we need to solve. Order of accuracy is the same, so the choice of method is dictated by computational cost!

To compare computational cost, however, we need to estimate:

① The constant C in $\bar{\tau} = C h / k$

② How expensive it is to solve the linear system in CN.

Let's start with the easier question #2, solving

$$\left(I + \frac{A\bar{\tau}}{2}\right) u^{n+1} = \left(I - \frac{A\bar{\tau}}{2}\right) u^{n} + f^{n+1/2}$$

What types of solvers might we use?

What if we used an iterative solver like (P)CG?

Condition number:

$$\kappa_2\left(I + \frac{\tau A}{2}\right) = \left| \frac{1 + \tau/2\, \lambda_{max}^{(A)}}{1 - \tau/2\, \lambda_{min}^{(A)}} \right|$$

$$\simeq \frac{1 + \frac{8k\tau}{2h^2}}{1 + \frac{\pi^2 k\tau}{2L^2}} \simeq 1$$

$$\simeq 1 + 4\nu$$

L: length of domain

$$K_2 \sim 1 + \frac{4k\tau}{h^2} = 1 + \frac{4C}{h}$$

As $h \to 0$, $\nu \to \infty$ for CN, so for small h we have

$$\boxed{K_2 \sim 4\nu} > 1$$

The number of iterations required to reach a certain tolerance in CG is $\sim \sqrt{K}$

$$\#\text{ iterations} \sim 2\sqrt{\nu} = 2\sqrt{\frac{k2}{h^2}} = 2\sqrt{\frac{C}{h}}$$

Each iteration of CG costs the same as a step of forward Euler (roughly), so

CN step $\Leftrightarrow$ $\sqrt{\frac{c}{h}}$ Euler steps

So we are back to question #1, how large can c be?

This is a little bit of a tricky question. We will answer it using physical intuition instead of (tedious) math

Let us denote the smallest relevant length scale in the specific physical problem of interest with $l < L$. This is problem specific and one must use physical understanding instead of trying to derive some sort of universal or a priori error estimate (this is again why PDEs are different/harder than ODEs!)

The time step size should resolve the dynamics at scale ℓ, and the grid should resolve the scale ℓ. So at the coarsest sensible grid,

$$h \sim \frac{\ell}{r}, \quad \tau = \frac{1}{r} \frac{\ell^2}{k}$$

where the resolution factor

$$r \sim [2-8] \text{ or so.}$$

$$\tau = \frac{ch}{k} = \frac{ck}{rk} = \frac{l^2 k}{rk}$$

$$\Rightarrow c \approx l \Rightarrow \boxed{\tau \sim \frac{lh}{k}}$$

$$\Rightarrow \text{CN step} \simeq \sqrt{\frac{l}{h}} \text{ Euler steps}$$

To reach time T, we need

$$\frac{T}{\tau} = \begin{cases} \frac{6Tk}{h^2} & \text{Euler steps} \\ \frac{Tk}{lh} & \text{CN steps} \end{cases}$$

Total computational cost:

$\frac{6Tk}{h^2}$ · (FD apply) for Euler

$\frac{Tk}{\ell h}$ · $\sqrt{\frac{\ell}{h}}$ · (FD apply) for CN

$$\frac{CPU_{Euler}}{CPU_{CN}} = \frac{\frac{6T\cancel{k}}{h^2}}{\frac{T\cancel{k}}{h\sqrt{\ell h}}} = 6\sqrt{\frac{\ell}{h}} > 1$$

often $>> 1$

So CN always beats Euler,

and really beats Euler if $h \ll l$ (well-resolved simulation).

Sometimes, however, our simulations may be under-resolved, and then $h \sim l$ and CN is not more efficient but is a lot more work to implement (e.g., linear solver + BCs is hard in 3D!). So both methods have their place. But most codes use CN.

Convergence of FD methods

For a linear PDE any one-step method will take the form

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

e.g.

$$B = \begin{cases} \left(I + \frac{\tau A}{2}\right)^{-1}\left(I - \frac{\tau A}{2}\right) & \text{CN} \\ \left(I - \tau A\right) & \text{FE} \\ \left(I + \tau A\right)^{-1} & \text{BE} \end{cases}$$

Def: A method is Lax–Richtmyer stable if

$\forall T > 0$, $\exists C_T > 0$ s.t.

$$\boxed{\| B^n(\tau) \| \leq C_T} \qquad \forall n \leq \frac{T}{\tau}$$

$$\forall \tau > 0$$

A fundamental result (obtained at Courant) is the Lax equivalence thm:

A consistent method is convergent iff it is (Lax–Richtmyer) stable

consistency + stability $\Leftrightarrow$ convergence

Proof sketch:

Error $E^n = U^n - \hat{U}^n$ ← true solution

$$E^{n+1} = BE^n - \Sigma * (LTE)^n$$

$$\Rightarrow \|E^N\| \leq T C_T \max_n \|(LTE)^n\|$$

So if $LTE = O(h^p) \Rightarrow$

$$\|E^N\| \leq T C_T \cdot O(h^p)$$

and the method is p-th order accurate

The weakest possible condition for L.-R. stability is

$$\|B(\bar{\tau})\| \leq 1 + \alpha\bar{\tau}$$

$$\Rightarrow \|B^n\| \leq (1+\alpha T)^{T/\bar{\tau}} \leq e^{\alpha T} = C_T$$

But often we prefer methods that satisfy strong stability

$$\|B\| \leq 1$$

For example, absolutely stable methods are strongly stable.

But, interestingly, absolute stability is <u>not</u> required per se for convergence. We will see an example for hyperbolic eqs. with forward Euler soon.

Zero stability is not meaningful for PDEs, we seek instead absolute (strong) stability.

$\tau \sim h^q$, eigenvalues of ODE depend on h, so <u>not</u> guaranteed that $\tau \lambda_{max} \to 0$ as $h \to 0$!

This is in contrast with ODEs, where $\tau \lambda_{max} \to 0$ as $\tau \to 0$, so one-step methods always converge. Furthermore, there are very few cases where convergence can be proven / guaranteed for nonlinear PDEs, but this can be done for general (low-dimensional) ODEs.

von Neumann stability analysis

As a first step when analyzing FD methods, we cousider periodic BCs and use a Fourier transform, to obtain the trivial ODEs:

$$\frac{d\hat{U}_k}{dt} = -\lambda_k \hat{U}_k + f_k(t)$$

λ_k: symbol of FD elliptic operator

Any scheme will give ($f=0$):

$$\hat{U}_k^{n+1} = g(k;\tau)\,\hat{U}_k^{n}, \qquad k \in [0, \tfrac{\pi}{h})$$

$g(k;\tau)$: amplification factor

L.-R. stability requires

$$|g(k;\tau)| \le 1 + \alpha\tau$$

which is a very general result that is NOT limited to MOL methods or to parabolic PDEs (e.g., it applies to space-time methods for hyperbolic PDEs)

For example, for $u_t = K u_{xx}$ in 1D we get

$$\hat{L}_k = \frac{1}{h^2}\left(e^{ikh} - 2 + e^{-ikh}\right)$$

$$= \frac{2}{h^2}\left(\cos(kh) - 1\right), \quad |k| < \frac{\pi}{h}$$

$$|g_k| = |1 + \tau \hat{L}_k| \leq 1 \quad \text{for strong stability}$$

$$\Rightarrow \left|1 - \frac{4K\tau}{h^2}\right| \leq 1 \Rightarrow \tau \leq \frac{h^2}{2K}$$

At home: Find stability limit on τ in 2D for 5 pt Laplacian