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Contents

1 Guy's Notes (Part 1)

1.1 Intro

In 228B we will focus on time-dependent problems:

$$
\begin{aligned}
&u_t = D\Delta u \quad \text{(heat/diffusion equation)} \\
&u_t + a u_x = 0 \quad \text{(advection equation)} \\
&u_{tt} = c^2 \Delta u \quad \text{(wave equation)}
\end{aligned}
$$

Also, mixed equations:

$$
\begin{aligned}
&u_t = D\Delta u + R(u) \quad \text{(reaction-diffusion equation)} \\
&u_t + a\nabla u = D\Delta u + R(u) \quad \text{(advection-diffusion-reaction equation)}
\end{aligned}
$$

Nonlinear problems:

$$u_t + u u_x = 0 \quad \text{(Burgers equation)}$$

Conservation laws:

$$u_t + (f(u))_x = 0$$

- The diffusion equation is parabolic
- The advection equation and wave equation are hyperbolic

1.2 Fourier Transforms

For $u \in L^2(\mathbb{R})$, the Fourier transform $\hat{u}(\xi)$ is

$$\hat{u}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} u(x) e^{-i\xi x}\, dx$$

$\hat{u}(\xi)$ is also in L^2, and the inverse transform is

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{u}(\xi) e^{i\xi x}\, dx$$

Parseval's Relation:

$$\|u(x)\|_2 = \|\hat{u}(\xi)\|_2$$

Fourier Transforms of derivatives:

$$
\begin{aligned}
u_x(x) &\to i\xi \hat{u}(\xi) \\
u_{xx}(x) &\to (i\xi)^2 \hat{u}(\xi) = -\xi^2 \hat{u}(\xi)
\end{aligned}
$$

1.3 Forward Time Centered Space Discretization of the Diffusion Equation and Advection Equation

Consider

$$
\begin{aligned}
u_t = Du_{xx} \quad \text{on } x \in [0,1] \\
u(0) = u(1) = 0 \\
u(x,0) = f(x)
\end{aligned}
$$

If we discretize space only we get a system of N couple ODEs:

$$\frac{d}{dt}\mathbf{u}(t) = L\mathbf{u}(t) \quad \mathbf{u}_j(0) = f(x_j)$$

We can use an ODE solver to find the solution. This is called the *method of lines*.

In practice, a solver designed for the particular PDE will be more efficient than an ODE solver. The simplest method for solving ODEs is *forward Euler*. Discretize into time steps Δt so that

$$
\begin{aligned}
t_n &= n\Delta t \\
\frac{d\mathbf{y}}{dt} &= f(\mathbf{y}) \\
\mathbf{y}^{n+1} &= \mathbf{y}^n + f(\mathbf{y}^n)\Delta t
\end{aligned}
$$

The forward Euler discretization for the heat equation is:

$$u_j^n \approx u(x_j, t_n)$$

This is stable *if* the time step is small enough.

The forward Euler discretization for the advection equation is:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\left(\frac{u_{j+1}^n - u_{j-1}^n}{2h}\right) = 0$$

This scheme is unstable for *all* choices of Δt. In other words, $\max_j |u_j^n| \to \infty$ as $n \to \infty$ for any Δt, when we know that $\max_x |u(x)|$ should be bounded.

1.4 Stability Analysis for Forward Euler

Given the ODE $\mathbf{y}' = f(\mathbf{y})$. Suppose we have a method that produces a sequence $\mathbf{y}^n$ given $\mathbf{y}^0$, where $\mathbf{y}^n \approx \mathbf{y}(n\Delta t)$. Apply the method to $y' = \lambda y$. Let $z = \lambda t$, where z may be complex since $y' = Ay$ may have complex eigenvalues. z is in the *region of absolute stability* if $y^n \to 0$ as $n \to \infty$.

$$
\begin{aligned}
\frac{y^{n+1} - y^n}{\Delta t} &= \lambda y^n \\
y^{n+1} &= (1 + \lambda\Delta t)y^n \\
y^n &= (1 + \lambda\Delta t)^n y^0
\end{aligned}
$$

$$y^n \to 0 \text{ if } |1 + \lambda\Delta t| < 1$$

The region of absolute stability is:

$$\{z \in \mathbb{C} \mid |1 + z| < 1\}$$

This is the unit disc of radius 1 centered at -1.

1.5 Analysis of Forward Euler for the Heat/Diffusion Equation

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{D}{h^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n)$$

We need $\lambda\Delta t = z$ in the region of absolute stability for all eigenvalues λ of DL, where L is the discrete Laplacian. The eigenvalues of L are:

$$\lambda_k = \frac{2}{h^2}(\cos(k\pi h) - 1) \quad k = 1, \ldots, N$$

The largest eigenvalue is:

$$\lambda_N = \frac{2}{h^2}(\cos(N\pi h) - 1) \approx -\frac{4}{h^2}$$

Forward Euler is stable on the diffusion equation if

$$\begin{aligned} -\frac{4D\Delta t}{h^2} &> -2 \\ \Delta t &< \frac{h^2}{2} \end{aligned}$$

The diffusion equation is an example of a *stiff* equation, where the ratio of the eigenvalues (similar to the condition number) is large. Since $dy/dt = \lambda y$, λ has dimensions of 1/time. Therefore, λ^{-1} can be thought of as the time scale of change, and so a equation is stiff when it has a wide range of time scales. In the diffusion equation, the fastest time scales are associated with high spatial frequency modes and are damped very quickly.

1.6 FE & CD for the Advection Equation

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{a}{2h}(u_{j+1}^n - uj - 1^n) = 0$$

Consider periodic space and look at the eigenvectors of the centered-difference operator:

$$(D_0 u)_j = \frac{1}{2h}(u_{j+1} - uj - 1)$$

The eigenvectors are

$$u_j = e^{ikx_j}$$

$$\begin{aligned} D_0 e^{ikx_j} &= \frac{1}{2h}(e^{ikx_{j+1}} - e^{ikx_{j-1}}) \\ &= \frac{1}{2h}(e^{ik(x_j+h)} - e^{ik(x_j-h)}) \\ &= e^{ikx_j}\frac{e^{ikh} - e^{-ikh}}{2h} \\ &= \frac{i\sin(kh)}{h}e^{ikx_j} \end{aligned}$$

Since the eigenvalues are pure imaginary, there is no way to choose Δt to that $\lambda\Delta t$ lies in the region of absolute stability.

1.7 Backward Euler

$$\frac{y^{n+1}-y^n}{\Delta t} = f(y^{n+1})$$

- This is an example of an *implicit method*, meaning that we have to solve for y^{n+1}
- This method is very effective for stiff problems

Region of Absolute Stability

$$\begin{aligned} y' &= \lambda y \\ \frac{y^{n+1}-y^n}{\Delta t} &= \lambda y^{n+1} \\ (1-\lambda\Delta t)y^{n+1} &= y^n \\ y^{n+1} &= \frac{1}{1-\lambda\Delta t}y^n \end{aligned}$$

- This is an *A-stable* method, meaning that the region of absolute stability contains the whole left half-plane
- Backward Euler is stable for the heat equation for any time step

1.8 Analysis of Forward Euler, Backward Euler, and the Trapezoidal Rule

Both Forward Euler and Backward Euler are first-order accurate in time. The Forward Euler discretization of the diffusion equation is:

$$\begin{aligned} u_t &= Du_{xx} \\ 0 &= \frac{u_j^{n+1}-u_j^n}{\Delta t} - \frac{D}{h^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) \end{aligned}$$

The local truncation error is:

$$\begin{aligned} \tau_j^n &= \frac{u(x_j,t_{n+1})-u(x_j,t_n)}{\Delta t} - \frac{D}{h^2}\left[u(x_{j-1},t_n) - 2u(x_j,t_n) + u(x_{j+1},t_n)\right] \\ \tau_j^n &= u_t + \frac{\Delta t}{2}u_{tt} + O(\Delta t^2) - D\left[u_{xx} + \frac{h^2}{12}u_{xxxx} + O(h^4)\right] \\ \tau &= \frac{\Delta t}{2}u_{tt} - \frac{Dh^2}{12}u_{xxxx} + \text{higher order terms} \\ \tau &= u_{xxxx}\cdot\left(\frac{\Delta t D^2}{2} + \frac{Dh^2}{12}\right) + \text{higher order terms} \qquad (u_{tt} = D^2 u_{xxxx} \text{ via the ODE}) \end{aligned}$$

For Backward Euler,

$$\tau = u_{xxxx}\cdot\left(-\frac{\Delta t D^2}{2} - \frac{Dh^2}{12}\right) + \text{higher order terms}$$

What about 2nd order in time?

$$\frac{y^{n+1}-y^{n-1}}{2\Delta t} = f(y^n)$$

This is called the *midpoint method*. It is an example of a multi-step method. It is 2nd order accurate, but it has a very restrictive stability region.

We can get 2nd order accuracy by averaging Forward Euler and Backward Euler:

$$\begin{aligned}\frac{y^{n+1}-y^n}{\Delta t} &= \frac{1}{2}\left(f(y^{n+1})+f(y^n)\right)\\ \frac{1}{2}\left(f(y^{n+1})+f(y^n)\right) &= f(y^{n+1/2})+O(\Delta t^2)\end{aligned}$$

This is called the *trapezoidal rule*. Its absolute stability is:

$$\begin{aligned}\frac{y^{n+1}-y^n}{\Delta t} &= \frac{\lambda}{2}(y^n+y^{n+1})\\ \left(1-\frac{\lambda\Delta t}{2}\right)y^{n+1} &= \left(1+\frac{\lambda\Delta t}{2}\right)y^n\\ y^{n+1} &= \frac{1+z/2}{1-z/2}y^n\\ |2+z| &\le |2-z|\\ \Re(z) &\le 0\end{aligned}$$

Thus, the trapezoidal rule is A-stable.

The trapezoidal rule applied to the heat equation with the standard second-order discrete Laplacian is called *Crank-Nicolson*. It is unconditionally stable, and it is 2nd order accurate in space and time.

1.9 Standard Classes of ODE Methods

1. Runge-Kutta: one step, multi-stage methods
   Example:

$$\begin{aligned}y^* &= y^n+\frac{\Delta t}{2}f(y^n)\\ y^{n+1} &= y^n+\Delta t f(y^*)\\ \text{OR}\qquad y^* &= y^n+\Delta t f(y^n)\\ y^{n+1} &= y^n+\frac{\Delta t}{2}\left(f(y^n)+f(y^*)\right)\end{aligned}$$

   General r-stage Runge-Kutta method:

$$\begin{aligned}Y_i &= y^n+\Delta t\sum_{j=1}^{n}A_{ij}f(t_n+c_j\Delta t, Y_j)\\ y^{n+1} &= y^n+\Delta t\sum_{j=1}^{r}b_jf(t_0+c_j\Delta t, Y_j)\end{aligned}$$

   - A is called the RK matrix
   - bs are the RK weights
   - cs are the RK nodes

For example, the classical 4th order RK matrix is

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array} = \begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b}^T \end{array}$$

2. Linear Multi-Step Methods General r-step method:

$$\sum_{j=0}^{r} \alpha_j y^{n+j} = \Delta t \sum_{j=0}^{r} \beta_j f(y^{n+j})$$

Adams Methods

$$\frac{y^{n+r} - y^{n+r-1}}{\Delta t} = \sum_{j=0}^{r} \beta_j f(y^{n+j})$$

- If $\beta_r = 0 \Rightarrow$ Adams-Bashforth method, explicit (1-step AB method is FE)
- If $\beta_r \neq 0 \Rightarrow$ Adams-Moulton method, implicit (1-step AM is the trapezoidal rule)

Backward Differentiation Formula (BDM) Methods

$$\sum_{j=0}^{n} \alpha_j y^{n+j} = \Delta t \beta_r f(y^{n+r})$$

1-step BDF is Backward Euler: $Y^{n+1} - y^n = \Delta t f(y^{n+1})$
BDF 2 is:

$$3y^{n+2} - 4y^{n+1} + y^n = 2\Delta t f(y^{n+2})$$

This is 2nd order accurate and absolutely stable.

2 Guy's Notes (Part 2)

2.1 Consistency, Stability, and Convergence

We want to know how to ensure that the numerical scheme gives solutions that converge to the solution of the PDE as $\Delta t, h \to 0$.

- **Convergence:** a numerical scheme is *convergent* if for any point x^*, t^* in the domain, $|u_j^n - u(x^*, t^*)| \to 0$ whenever $x_j \to x^*$ and $t_n \to t^*$, i.e. $\Delta t, h \to 0$.

- **Consistency:** the local truncation error $\tau \to 0$ as $\Delta t, h \to 0$.

- **Stability:** a method is *Lax-Richtmyer stable* if for each time T, there is a constant C_T independed of Δt such that
$$\|B^n\| \leq C_T$$
This allows for the solution to grow in time, but not in the number of steps to get a fixed point in time.

Let u^n and v^n be two different solutions to

$$u^{n+1} = Bu^n + b^n \qquad \text{(with different initial conditions, } u^0 \text{ and } v^0\text{)}$$

The method is stable if for each time T, there is a constant K_T, independent of u^0 and v^0, such that

$$\|u^n - v^n\| \leq K_T \|u^0 - v^0\| \quad \forall \; n\Delta t \leq T$$

In other words, if the solutions start close, then they stay close.

2.2 Lax Equivalence Theorem

Theorem 2.1. ***Lax Equivalence Theorem***
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For linear problems,
$$\text{stability} + \text{consistency} \Rightarrow \text{convergence}$$

<u>OR</u>

A linear, consistent difference scheme to a well-posed linear PDE is convergent iff it is stable.

<u>Proof</u>

- Let $u^{n+1} = Bu^n + b^n$ be stable and consistent
- Let $\hat{u}_{\text{sol}}$ be the solution to the PDE at time t_n at the grid points
- Recall: the error is $e^n = u^n - u^n_{\text{sol}}$
- Plug u_{sol} into the difference equation:

$$u^{n+1}_{\text{sol}} = Bu^n_{\text{sol}} + b^n + \Delta t \tau^n$$

- For Forward Euler:

$$\frac{u^{n+1}-u^n}{\Delta t} = Lu^n \quad \Rightarrow \quad u^{n+1} = u^n + \Delta t L u^n$$

$$\frac{u_{\text{sol}}^{n+1}-u_{\text{sol}}^n}{\Delta t} = Lu_{\text{sol}}^n \quad \Rightarrow \quad \underbrace{u_{\text{sol}}^{n+1} = (I+\Delta t L)u_{\text{sol}}^n + \Delta t \tau^n}_{\text{subtract from the difference equation}}$$

$$\begin{aligned}
e^{n+1} &= Be^n - \Delta t \tau^n \\
e^0 &= 0 \quad \text{because we're given the IC} \\
e^1 &= -\Delta t \tau^0 \\
e^2 &= -\Delta t B \tau^0 - \Delta t \tau^1 \\
e^3 &= -\Delta t B^2 \tau^0 - \Delta t \tau^1 - \Delta t \tau^2 \\
&\dots \\
e^n &= -\Delta t \sum_{k=1} n B^{n-k} \tau^{k-1} \\
\|e^n\| &\le \Delta t \sum_{k=1} n \|B^{n-k}\tau^{k-1}\| \\
&\le \Delta t \sum_{k=1} n \|B^{n-k}\| \|\tau^{k-1}\|
\end{aligned}$$

- Let $T = n\Delta t$
- We know that $\|B^{n-k}\| \le C_T$ and $(n-k)\Delta t \le n\Delta t = T$. Thus,

$$\begin{aligned}
\|e^n\| &\le \Delta t C_T \sum_{k=1} n \|\tau^{k-1}\| \\
&\le n \Delta t C_T \max_{1\le k\le n} \|\tau^{k-1}\| = C_T \max_{1\le k\le n} \|\tau^{k-1}\| \to 0 \quad \text{(by consistency)}
\end{aligned}$$

2.3 Stability of Crank-Nicolson in the 2-norm for the 1-D Diffusion Equation

$$\frac{u^{n+1}-u^n}{\Delta t} = \frac{1}{2}(Lu^{n+1} + Lu^n) + \underbrace{f^{n+1/2}}_{\text{or } \frac{1}{2}(f^n+f^{n+1})}$$

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

$$u^{n+1} = \underbrace{\left(I - \frac{\Delta t}{2}L\right)^{-1}\left(I + \frac{\Delta t}{2}L\right)}_{B} u^n + \Delta t \left(I - \frac{\Delta t}{2}L\right)^{-1} f^{n+1/2}$$

- B is symmetric, so $\|B\|_2 = \rho(B)$
- The eigenvalues of L are:

$$\lambda_k = \frac{2}{h^2}\big(\cos(k\pi h) - 1\big) \le 0$$

- The eigenvalues of B are:

$$\lambda_k = \frac{1 + \frac{\Delta t}{2}\lambda_k}{1 - \frac{\Delta t}{2}\lambda_k} \le 1$$

- $\|B\|_2 \le 1$, so $\|B^n\|_2 \le \|B\|_2^n \le 1$, so Crank-Nicolson is stable.

2.4 Stability of FE for Diffusion in the ∞-norm

$$\begin{aligned}\frac{u^{n+1}-u^n}{\Delta t} &= Lu^n + f^n \\ u^{n+1} &= (I+\Delta t L)u^n + \Delta t f^n\end{aligned}$$

- $\|B\|_\infty = \text{max row sum} = \frac{\Delta t}{h^2} + \left|1 - \frac{2\Delta t}{h^2}\right| + \frac{\Delta t}{h^2}$
- Assume $\quad 1 - \frac{2\Delta t}{h^2} > 0 \quad \Rightarrow \quad \Delta t \leq \frac{h^2}{2}$
- $\|B\|_\infty = 1$, so $\|B^n\|_\infty \leq \|B\|_\infty^n = 1$, so FE is stable for diffusion in the ∞-norm.

3 1-18-11

3.1 Stability Analysis for Growing Solutions

$$u^{n+1} = Bu^n + b^n$$

$$\text{This is stable if: } \|B\| \le C_T$$
$$n\Delta t \le T$$

But what if the solution is supposed to grow?

If there is a constant α, independent of Δt (for Δt sufficiently small) such that

$$\|B\| \le 1 + \alpha\Delta t$$

then the scheme is *Lax-Richtmyer* stable.
Suppose

$$\|B\| \le 1 + \alpha\Delta t$$
$$\|B^n\| \le \|B\|^n \le (1+\alpha\Delta t)^n \le e^{\alpha(n\Delta t)} \le e^{\alpha T}$$

$$1 + \alpha\Delta t \le e^{\alpha\Delta t} \qquad (1 + \alpha\Delta t \text{ are the first 2 terms in the Taylor expansion})$$

for $n\Delta t \le T$. T can depend on time, but not on the number of time steps.
Consider

$$u_t = u_{xx} + bu$$

If b is positive, we may expect growth of the solution.

Forward Euler:

$$u^{n+1} = (I + \Delta tL + \Delta tbI)\, u^n$$

Suppose $\Delta t \le h^2/2$.

$$\|I + \Delta tL + \Delta tbI\|_\infty = \frac{2\Delta t}{h^2} + \left|1 - \frac{2\Delta t}{h^2} + \Delta tb\right|$$
$$\le 1 + \Delta t|b|$$

This is stable for any b. This is good for $b > 0$, but if $b < 0$ the solution should not grow (for suitable boundary conditions).

If $b < 0$, Guy would enforce $\|B\| \le 1$ (strong stability). This way you aren't allowing for growth when the solution shouldn't be growing.

3.2 von Neumann Analysis

It is often difficult to compute norms of matrices. Recall how we used the Fourier transform to solve the diffusion equation on the real line. The same idea works for any linear constant coefficient PDE, and it also works for constant coefficient linear difference equations on the whole real line or for periodic boundaries.

Discretized real line:

$$x_j = jh, \qquad j = -\infty, \ldots, \infty$$

Note that $e^{i\xi x_j}$ are eigenfunctions of constant coefficient difference operators.
Centered Difference Operator (D_0):

$$\begin{aligned}
(D_0 u)_j &= \frac{u_{j+1} - u_{j-1}}{2h} \\
\left(D_0 e^{i\xi x_j}\right)_j &= \frac{e^{i\xi x_{j+1}} - e^{i\xi x_{j-1}}}{2h} = \frac{e^{i\xi(x_j+h)} - e^{i\xi(x_j-h)}}{2h} = e^{i\xi x_j}\left(\frac{e^{i\xi h)} - e^{-i\xi h)}}{2h}\right) \\
&= \frac{i\sin(\xi h)}{h} e^{i\xi x_j}
\end{aligned}$$

Second Difference Operator (D_+D_-):

$$\begin{aligned}
(D_+D_-u)_j &= \frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} \\
\left(D_+D_-e^{i\xi x_j}\right)_j &= \frac{2}{h^2}\left(\cos(\xi h) - 1\right) e^{i\xi x_j} \\
&= -\frac{4}{h^2}\sin^2\left(\frac{\xi h}{2}\right) e^{i\xi x_j}
\end{aligned}$$

Let v_j be a discrete function on the discrete real line. The Fourier transform of v_j is:

$$\hat{v}(\xi) = \frac{h}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} v_j e^{-i\xi x_j} \qquad \text{for } -\pi \le \xi h \le \pi \ \Rightarrow\ -\frac{\pi}{h} \le \xi \le \frac{\pi}{h}$$

The inverse Fourier transform is:

$$v_j = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{v}(\xi) e^{i\xi x_j}\, d\xi$$

Thus, we have:

$$\mathcal{F} : \underbrace{\frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{v}(\xi) e^{i\xi x_j}\, d\xi}_{v_j} \mapsto \hat{v}(\xi)$$

$$\mathcal{F}^{-1} : \underbrace{\frac{h}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} v_j e^{-i\xi x_j}}_{\hat{v}(\xi)} \mapsto v_j$$

Note:

$$\underbrace{\text{real space (bounded)}}_{\text{discrete}} \to \underbrace{\text{Fourier space (discrete)}}_{\text{bounded}}$$

Parseval's relation holds:

$$\|\hat{v}\|_2 = \|v\|_2 = \left(\sum_j |v_j|^2\right)^{1/2}$$

To show the stability of $u^{n+1} = Bu^n$, we can show that

$$\|B\|_2 \le 1 + \alpha\Delta t$$

This is equivalent to

$$\|u_{n+1}\|_2 \le (1 + \alpha\Delta t)\|u_n\|_2$$

By Parseval's relation, we can show stability by showing that

$$\|\hat{u}_{n+1}\| \le (1 + \alpha\Delta t)\|\hat{u}_n\|_2$$

3.3 Forward Euler for the Diffusion Equation

$$
\begin{aligned}
u_j^{n+1} &= u_j^n + \frac{D\Delta t}{h^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) \\
u_j^n &= \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{u}^n(\xi) e^{i\xi x_j}\, d\xi && \text{(definition of Inverse Fourier Transform)} \\
&\uparrow \text{ plug this into the difference scheme} \\
u_j^{n+1} &= \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{u}^n(\xi) \left(e^{i\xi x_j} + \frac{D\Delta t}{h^2}\left(e^{i\xi x_{j-1}} - 2e^{i\xi x_j} + e^{i\xi x_{j+1}}\right)\right) d\xi \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} \hat{u}^n(\xi) \left(1 - \frac{4D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right)\right) e^{i\xi x_j}\, d\xi \\
\hat{u}^{n+1} &= \left(1 - \frac{4D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right)\right)\hat{u}^n && \text{(apply } \mathcal{F} \text{ to both sides)} \\
&= g(\xi)\hat{u}^n
\end{aligned}
$$

$g(\xi)$ is called the *amplification factor*. The von Neumann condition is

$$|g(\xi)| \leq 1 + \alpha\Delta t \quad \forall\ \xi$$

If this is met, then

$$\|\hat{u}^{n+1}\|_2 \leq (1 + \alpha\Delta t)\|\hat{u}^n\|_2$$

and so the scheme is stable.

For Forward Euler, we require:

$$
\begin{aligned}
\left|1 - \frac{4D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right)\right| &\leq 1 \\
-1 \leq 1 - \frac{4D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right) &\leq 1 \\
0 \leq \frac{4D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right) &\leq 2 \\
\Delta t &\leq \frac{h^2}{2D}
\end{aligned}
$$

To perform von Neumann analysis, assume a solution of the form

$$u_j^n = e^{i\xi x_j}$$

and compute

$$u_j^{n+1} = g(\xi)e^{i\xi x_j}$$

More generally,

$$u_j^n = g(\xi)^n e^{i\xi x_j}$$

For example, the von Neumann analysis of the leapfrog (midpoint) scheme for diffusion is:

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = \frac{D}{h^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n)$$

$$\left(\frac{g^{n+1} - g^{n-1}}{2\Delta t}\right) \cancel{e^{i\xi x_j}} = \frac{D}{h^2} g^n \left(-4\sin^2\left(\frac{\xi h}{2}\right)\right) \cancel{e^{i\xi x_j}}$$

$$g^2 - 1 = -\frac{8D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right) g$$

$$g^2 + \frac{8D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right) g - 1 = 0$$

$$g_\pm(\xi) = \frac{-\frac{8D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right) \pm \sqrt{\left(\frac{8D\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right)\right) + 4}}{2}$$

$$|g_\pm| \geq 1 \ \forall \ \xi \quad \Rightarrow \quad \text{unconditionally stable}$$

4 1-20-11

4.1 Stability and Discretization

Idea: sometimes instability is a local phenomenon.

Consider the variable coefficient diffusion equation:

$$\begin{aligned} u_t &= (D(x)u_x)_x \leftarrow \text{ conservation form} \\ &= -J_x \end{aligned}$$

For diffusion:

$$\begin{aligned} &\text{1-D: } J = -Du_x \\ &\text{higher dimensions: } \mathbf{u}_t = -\nabla \cdot \mathbf{J}, \quad \mathbf{J} = -D\nabla \mathbf{u} \end{aligned}$$

We want our discretization to mimic the conservation form.

Discretize a line with points $\ldots, x_{j-1}, x_j, x_{j+1}, \ldots$

$$u_t = -J_x \qquad u_j \approx u(x_j)$$

Approximate J_x at the grid points.
Approximate J at the edges.

$$\begin{aligned} J_{j+\frac{1}{2}} &\approx J(x_{j+\frac{1}{2}}) \\ (J_x)_j &\approx \frac{J_{j+\frac{1}{2}} - J_{j-\frac{1}{2}}}{h} \\ \frac{\partial u_j}{\partial t} = u_t &= \frac{J_{j-\frac{1}{2}} - J_{j+\frac{1}{2}}}{h} \\ J_{j+\frac{1}{2}} &= -D_{j+\frac{1}{2}} \left(\frac{u_{j+1} - u_j}{h} \right) \\ ((D(x)u_x)_x)_j &\approx \frac{D_{j+\frac{1}{2}} \left(\frac{u_{j+1}-u_j}{h} \right) - D_{j-\frac{1}{2}} \left(\frac{u_j - u_{j-1}}{h} \right)}{h} \\ &\approx \frac{D_{j-\frac{1}{2}} u_{j-1} - \left(D_{j-\frac{1}{2}} + D_{j+\frac{1}{2}} \right) u_j + D_{j+\frac{1}{2}} u_{j+1}}{h^2} \end{aligned}$$

von Neumann Analysis

Analyze the constant coefficient problem

$$\Delta t \leq \frac{h^2}{2D} \text{ for some } \overline{D}$$

Pick $\overline{D} = \max D(x)$.
Use the $\|\cdot\|_\infty$ norm to analyze stability.

$$u^{n+1} = (I + \Delta t L)u^n$$

$$\|I + \Delta t \tilde{L}\|_\infty = \max_j \left(\frac{\Delta t}{h^2} \left(D_{j-\frac{1}{2}} + D_{j+\frac{1}{2}} \right) + \left| 1 - \frac{\Delta t}{h^2} \left(D_{j-\frac{1}{2}} + D_{j+\frac{1}{2}} \right) \right| \right)$$

Impose that

$$1 - \frac{\Delta t}{h^2} \left(D_{j-\frac{1}{2}} + D_{j+\frac{1}{2}} \right) \geq 0 \quad \Rightarrow \quad \Delta t \leq \frac{h^2}{D_{j-\frac{1}{2}} + D_{j+\frac{1}{2}}} \quad \forall\, j$$

Then

$$\|I + \Delta t \tilde{L}\|_\infty = 1$$

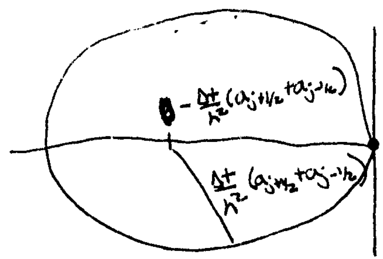
Question: Is Crank-Nicolson for this variable coefficient problem unconditionally stable?

$$\left(I - \Delta t \tilde{L}\right) u^{n+1} = \left(I + \Delta t \tilde{L}\right) u^n$$

$$\frac{du}{dt} = \tilde{L} u$$

If $\tilde{L}$ is negative definite, then it is stable.
Check:

$$u^T \tilde{L} u \le 0$$



4.2 Implicit Methods for Diffusion

Solve a linear system at each time step.
For example, Crank-Nicolson:

$$\left(I - \frac{\Delta t D}{2} L\right) u^{n+1} = \left(I + \frac{\Delta t D}{2}\right) u^n + \Delta t f^{n+\frac{1}{2}}$$

In 1-D, factor in $O(N)$ work to solve the tridiagonal system.

Higher Dimensions
Forward Euler time step restriction:

- 1-D: $\Delta t \le \frac{h^2}{2D}$
- 2-D: $\Delta t \le \frac{h^2}{4D}$
- 3-D: $\Delta t \le \frac{h^2}{6D}$

In 2- or 3-D, how do we solve

$$\left(I - \frac{\Delta t}{2} L\right) u^{n+1} = r$$

We can use an iterative scheme, such as SOR, CG, or MG. Or we can use direct solve.

$\left(I - \frac{\Delta t}{2} L\right)$ has the same eigenvectors as L, and the eigenvalues are just the shifted eigenvalues of L.
The condition number of $I - \frac{\Delta t}{2} L = O(\Delta t / h^2)$.

As $\Delta t \to 0$, h fixed, $I - \frac{\Delta t}{2} L \to I$, and we expect convergence in 1 step.

As $\Delta t \to \infty$, h fixed, $I - \frac{\Delta t}{2} L$ blows up.

$$\left(\frac{1}{\Delta t} - \frac{1}{2} L\right) u = \frac{1}{\Delta t} r, \qquad r \text{ is } O(\Delta t)$$

$$-L u^{n+1} = O(1) \leftarrow \text{ Poisson equation}$$

$$r = \left(I + \frac{\Delta t}{2} L\right) + \Delta t f^{n+1/2}$$

$$\Delta t \to 0, \qquad \frac{\Delta t}{h} \text{ fixed}, \qquad \frac{\Delta t}{h^2} \to \infty$$

We have a good initial guess for u^{n+1}:

$$u^{n+1} = u^n + O(\Delta t)$$

There is another way to approximately solve the system that was not available for time-independent problems. . .

4.3 ADI & LOD

Recall:

$$\Delta = \partial_x^2 + \partial_y^2 \qquad L = L_x + L_y$$

What if we diffuse in the x-direction and then in the y-direction ⇒ LOD scheme (Locally One-Dimensional)

$$\left(I - \frac{\Delta t}{2} L_x\right) u^* = \left(I + \frac{\Delta t}{2} L_x\right) u^n$$
$$\left(I - \frac{\Delta t}{2} L_y\right) u^{n+1} = \left(I + \frac{\Delta t}{2} L_y\right) u^*$$

What about 1 dimension implicit and 1 dimension explicit ⇒ ADI (Alternating Direction Implicit)
Common ADI scheme "Peaceman-Rachford":

$$\left(I - \frac{\Delta t}{2} L_x\right) u^* = \left(I + \frac{\Delta t}{2} L_y\right) u^n$$
$$\left(I - \frac{\Delta t}{2} L_y\right) u^{n+1} = \left(I + \frac{\Delta t}{2} L_x\right) u^*$$

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5.1 LOD & ADI (Continued)

- First substep
  - Solve a tridiagonal system on each line $\Rightarrow$ $O(N)$ work
  - Do this N_y times $\Rightarrow$ $O(N_xN_y)$ work
- Second substep
  - $O(N_y)$ work done N_x times $\Rightarrow$ $O(N_xN_y)$ work

Questions: Accuracy? Stability? Boundary conditions?

Stability: Both LOD and ADI are unconditionally stable.
von Neumann Analysis:

$$
\begin{aligned}
\hat{u}^* &= \frac{1-\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_2 h}{2}\right)}{1+\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_1 h}{2}\right)}\hat{u}^n \\
\hat{u}^{n+1} &= \frac{1-\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_1 h}{2}\right)}{1+\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_2 h}{2}\right)}\hat{u}^* \\
&= \underbrace{\frac{\left(1-\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_1 h}{2}\right)\right)\left(1-\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_2 h}{2}\right)\right)}{\left(1+\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_1 h}{2}\right)\right)\left(1+\frac{4\Delta t}{h^2}\sin^2\left(\frac{\xi_2 h}{2}\right)\right)}}_{g(\xi_1,\xi_2)}\hat{u}^n
\end{aligned}
$$

$$|g(\xi_1,\xi_2)| \le 1 \ \forall \xi_1, \xi_2$$

Accuracy of ADI:
Multiply the first equation by $(I+\frac{\Delta t}{2}L_x)$ and use the fact that $(I-\frac{\Delta t}{2}L_x)$ and $(I+\frac{\Delta t}{2}L_x)$ commute to get:

$$\left(I-\frac{\Delta t}{2}L_x\right)\left(I+\frac{\Delta t}{2}L_x\right)u^* = \left(I+\frac{\Delta t}{2}L_x\right)\left(I+\frac{\Delta t}{2}L_y\right)u^n$$

Use the second equation to eliminate u^*:

$$
\begin{aligned}
\left(I-\frac{\Delta t}{2}L_x\right)\left(I-\frac{\Delta t}{2}L_y\right)u^{n+1} &= \left(I+\frac{\Delta t}{2}L_x\right)\left(I+\frac{\Delta t}{2}L_y\right)u^n \\
\left(I-\frac{\Delta t}{2}(L_x+L_y)+\frac{\Delta t^2}{4}L_xL_y\right)u^{n+1} &= \left(I+\frac{\Delta t}{2}(L_x+L_y)+\frac{\Delta t^2}{4}L_xL_y\right)u^n \\
\frac{u^{n+1}-u^n}{\Delta t} &= \frac{1}{2}(Lu^{n+1}+Lu^n)+\frac{\Delta t}{4}L_xL_y(u^n-u^{n+1})
\end{aligned}
$$

As $\Delta t \to 0$:

$$
\begin{aligned}
\frac{\Delta t^2}{4}L_xL_y\left(\frac{u^n-u^{n+1}}{\Delta t}\right) &\approx -\frac{\Delta t^2}{4}\frac{\partial^5 u}{\partial x^2\partial y^2\partial t} \\
u_t = \Delta u + \underbrace{O(\Delta t^2)+O(h^2)}_{\text{from Crank-Nicolson}} &+ \underbrace{O(\Delta t^2)}_{\text{from ADI}}
\end{aligned}
$$

Boundary Conditions:
We are using Forward Euler in the y-direction and Backward Euler in the x-direction.

$$u^* \not\approx u^{n+1} \qquad u^* = u^{n+\frac{1}{2}} + O(\Delta t^2)$$

Boundary conditions:

$$u^*_{0j} = u^{n+\frac{1}{2}}_{0j} \qquad u^*_{Nx+1,j} = u^{n+\frac{1}{2}}_{Nx+1,j}$$

Another way: Add the 2 ADI (Peaceman-Rachford) equations

$$\begin{aligned} 2u^* &= \left(I + \frac{\Delta t}{2} L_y\right) u^n + \left(I - \frac{\Delta t}{2} L_y\right) u^{n+1} \\ u^* &= \frac{u^n + u^{n+1}}{2} - \frac{\Delta t}{4} L_y \left(u^{n+1} - u^n\right) \\ \frac{u(x, t+\Delta t) - u(x,t)}{\Delta t} &= \frac{1}{h^2}\left(u(x-h,t) - 2u(x,t) + u(x+h,t)\right) + \underbrace{\tau}_{O(\Delta t)} \\ u^{n+1} &= u(x, t_n) + \Delta t L u(x, t_n) \\ u(x, t_{n+1}) &= u^{n+1} \end{aligned}$$

$$\begin{aligned} y' &= f(y) \\ y^{n+1} &= y(t_n) + \Delta t f(y(t_n)) \\ y(t_n + \Delta t) &= y(t_n) + \Delta t y'(t_n) + O(\Delta t^2) \\ &= \underbrace{y(t_n) + \Delta t f(y(t_n))}_{y^{n+1}} + O(\Delta t^2) \end{aligned}$$

u^* on the boundary on LOD

$$\begin{aligned} \left(I - \frac{\Delta t}{2} L_x\right) u^* &= \left(I + \frac{\Delta t}{2} L_x\right) u^n \\ \left(I_{\frac{\Delta t}{2}} L_y\right) u^{n+1} &= \left(I + \frac{\Delta t}{2} L_y\right) u^n \end{aligned}$$

u^* does not approximate the solution.
We can solve the 2nd equation on the boundary after finding some approximation to u^* at the corners.

3-D, second order ADI is known as the "Douglass-Gunn scheme"

LOD is an example of a fractional stepping method.

5.2 Fractional Step Schemes

e.g. the reaction-diffusion equation:

$$u_t = D\Delta u + R(u)$$

- $D\Delta u$: transport by diffusion
- $R(u)$: chemical reaction

e.g. Fisher's equation:

$$u_t = Du_{xx} + ku(1-u)$$

How to solve this numerically?
Try a Crank-Nicolson scheme:

$$\begin{aligned}
\frac{u^{n+1}-u^n}{\Delta t} &= \frac{1}{2}\left(Lu^{n+1} + Lu^n\right) + \frac{1}{2}\left(R(u^n) + R(u^{n+1})\right) \\
\underbrace{\left(I - \frac{\Delta t}{2}L\right)u^{n+1} - \frac{\Delta t}{2}R(u^{n+1})}_{\text{this is nonlinear}} &= \left(I - \frac{\Delta t}{2}L\right)u^n + \frac{\Delta t}{2}R(u^n)
\end{aligned}$$

We can use Newton's method to solve it.

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$$u_t = u_x x + R(u)$$
$$\left(I - \frac{\Delta t}{2}L\right)u^{n+1} - \frac{\Delta t}{2}R(u^{n+1}) = \left(I + \frac{\Delta t}{2}L\right)u^n + \frac{\Delta t}{2}R(u^n)$$

6.1 Newton's Method

Newton's method for a scalar equation is a way of finding solutions u to $f(u) = 0$. Guess a solution, then linearize the equation and solve for the zero in the linear equation

$$u^{k+1} = u^k - \frac{f(u^k)}{f'(u^k)}$$

How should this be generalized for a system of equations?

$$\begin{aligned} \mathbf{F}(\mathbf{u}) &= 0 \\ f'(u^k)(u^{k+1} - u^k) &= -f(u^k) \\ f'(u^k)\delta^k &= -f(u^k) \\ u^{k+1} &= u^k + \delta^k \end{aligned}$$

The Jacobian of $\mathbf{F}$ at $\mathbf{u}^k$ takes the role of $f'(u^k)$.

$$J^k \delta^k = -\mathbf{F}(\mathbf{u}^k)$$

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \delta^k$$

<u>Example:</u> Reaction Diffusion (with $b = 1$)

$$F(u) = \left(I - \frac{\Delta t}{2}L\right)u - \frac{\Delta t}{2}R(u) - \left(I + \frac{\Delta t}{2}L\right)u^n - \frac{\Delta t}{2}R(u^n)$$

Want to find u^{n+1} so that $F(u^{n+1}) = 0$, where $n \equiv$ time step and $k \equiv$ Newton's method iteration.

$$\begin{aligned} F'(u) &= \left(I - \frac{\Delta t}{2}L\right) - \frac{\Delta t}{2}R'(u) \\ F'(u^{n+1,k})\delta^k &= -F(u^{n+1,k}) \leftarrow \text{solve this linear system} \end{aligned}$$

Note that R is a diagonal matrix, so R' is obtained by differentiating each entry.

$$u^{n+1,k+1} = u^{n+1,k} + \delta^k \leftarrow \text{update } u$$

Check:

1. $\|\delta\| < \text{tol}$
2. $\|F(u^{n+1,k+1})\| < \text{tol}$

6.2 Alternate Method: Fractional Step Method

$$\frac{du}{dt} = Lu + R(u)$$

Advance in 2 steps

- Start with u^n and update $\frac{du}{dt} = Lu$ over time length Δt to get u^*
- Start at u^* and update $\frac{du}{dt} = R(u)$ over time length Δt to get u^{n+1}

Is this easier?

If I take 2 substeps with second-order accurate in time methods, do we get a second-order scheme?
$\Rightarrow$ In general, no.

Consider $u_t = A(u) + B(u)$
The simplest fractional stepping scheme is:

- Solve $u_t = A(u)$ to get u^*
- Solve $u_t = B(u)$ to get u^{n+1} (with initial condition (guess?) u^*)

We can analyze without considering what numerical scheme we use in each substep.

Look at the linear problem

$$\frac{du}{dt} = u_t = Au + Bu$$

Start at $u(t_n)$:

$$u(t_{n+1}) = e^{(A+B)\Delta t}u(t_n)$$

Use fractional stepping:

$$u^* = e^{A\Delta t}u(t_n)$$
$$u^{n+1} = e^{B\Delta t}u^* = e^{B\Delta t}e^{A\Delta t}u(t_n)$$

If A and B are matrices, $e^{A+B} \neq e^A e^B$ in general.

Fractional stepping error: $u^{n+1} - u(t_{n+1})$

Taylor expand u^{n+1} and $u(t_{n+1})$ as $\Delta t \to 0$:

$$\begin{aligned}
e^{(A+B)\Delta t} &= I + \Delta t(A+B) + \frac{\Delta t^2}{2}(A+B)^2 + O(\Delta t^3) \\
e^{B\Delta t}e^{A\Delta t} &= \left(I + \Delta t B + \frac{\Delta t^2}{2}B^2 + O(\Delta t^3)\right)\left(I + \Delta t A + \frac{\Delta t^2}{2}A^2 + O(\Delta t^3)\right) \\
&= I + \Delta t A + \Delta t B + \frac{\Delta t^2}{2}A^2 + \Delta t^2 BA + \frac{\Delta t^2}{2}B^2 + O(\Delta t^3) \\
&= I + \Delta t(A+B) + \frac{\Delta t^2}{2}(A^2 + 2BA + B^2) + O(\Delta t^3)
\end{aligned}$$

$(A+B)^2 = (A+B)(A+B) = A^2 + AB + BA + B^2 \neq A^2 + 2BA + B^2$ in general, unless A & B commute

$$u^{n+1} - u(t_{n+1}) = O(\Delta t^2)$$

This fractional stepping gives a first order accurate scheme. This is because there is $O(\Delta t^2)$ error per step, and there are $O(\Delta t^{-1})$ total steps.

How to get smaller splitting errors, resulting in a more accurate scheme?

6.3 Strang Splitting

1. Half-Step: $u_t = A(u)$
2. Full-Step: $u_t = B(u)$
3. Half-Step: $u_t = A(u)$

$$e^{\frac{\Delta t}{2}A} e^{\Delta t B} e^{\frac{\Delta t}{2}A} = e^{\Delta t(A+B)} + O(\Delta t^3)$$

The overall solution is second-order.

Another scheme (cheaper than Strang):

$$1) \quad \left.\begin{aligned} u_t &= A(u) \\ u_t &= B(u) \end{aligned}\right\} \text{first order}$$

$$2) \quad \left.\begin{aligned} u_t &= B(u) \\ u_t &= A(u) \end{aligned}\right\} \text{first order}$$

The overall scheme is second order. In other words, u^{n+1} is first order and u^{n+2} is second order.

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7.1 Intro

$$u_t = A(u) + B(u)$$

Suppose A is stiff and B is not.

- Use implicit time methods for stiff problems
- Use explicit time methods for not stiff problems

7.2 IMEX Methods

A different approach from fractional stepping is IMEX $\Rightarrow$ mix an implicit scheme and an explicit scheme.

For example, use trapezoidal rule for A and 2nd order AB (Adams Bashforth) $\Rightarrow$ becomes a 3 order scheme.

$$\frac{u^{n+1} - u^n}{\Delta t} = \underbrace{\frac{1}{2}\left(A(u^n) + A(u^{n+1}\right)}_{\text{trapezoidal}} + \underbrace{\frac{3}{2}B(u^n) - \frac{1}{2}Bu^{n-1})}_{\text{Adams Bashforth}}$$

- With fractional stepping, it's very difficult to get better than 2nd order accuracy.
- For this scheme, we can use FE for the first step, since it is 2nd order

7.3 LOD for Diffusion

Recall:

$$\left(I - \frac{\Delta t}{2}L_x\right)u^* = \left(I + \frac{\Delta t}{2}L_x\right)u^n$$
$$\left(I - \frac{\Delta t}{2}L_y\right)u^{n+1} = \left(I + \frac{\Delta t}{2}L_y\right)u^*$$

In terms of fractional stepping:

$$u_t = L_x u + L_y u$$

This is 2nd order in time if L_x and L_y commute. In general, L_x and L_y commute on the interior but not near the boundaries. But if we have a constant coefficicient on a periodic domain, then they commute.

Crank-Nicolson:

$$\left(I - \frac{\Delta t}{2}(L_x + L_y)\right)u^{n+1} = \left(I + \frac{\Delta t}{2}(L_x + L_y)\right)u^n$$

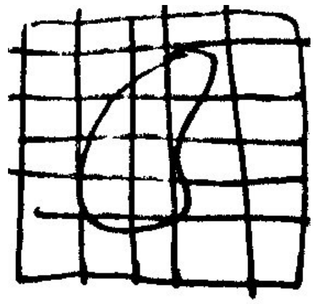
LOD can be used as an effective preconditioner if you want to use conjugate gradient to apply the inverse of the matrix.

7.4 Nonrectangular Domains

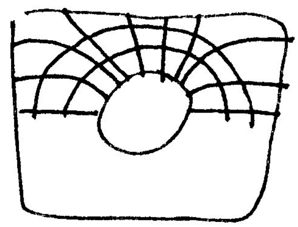
$$u_t = D\Delta u$$

Different Approaches to Discretization

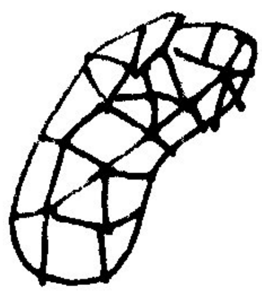
1. Cartesian grid: put the odd-shaped domain in a big box and discretize the box.
   Challenge: figuring out how to modify the discretization to account for the curved boundary.



2. Use body fitted mesh, where the gridpoints are the points on the mesh.
   Use coordinates that deform with the boundary.

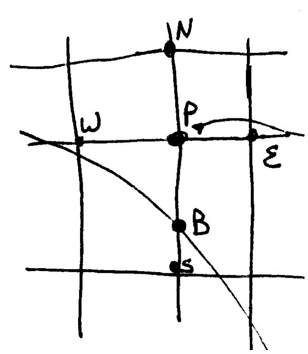


3. Use an unstructured mesh
   Put down some points on the interior and the boundary, triangulate the domain. Often used with the Finite Element Method. Can be automated fairly easily.



7.5 Cartesian Grid

- **Regular Point:** its 4 neighbors lie within the domain
- **Irregular Point:** at least one neighbor lies outside the domain



Suppose we have Dirichlet boundary conditions. Think of $L = L_x + L_y$. For this example, L_x does not need to be modified. There are 2 ways to do this:

1. Use a 3-point discretization of L_y using N, P, B
2. Quadratically extrapolate the data from N, P, B to S and use the regular stencil at P

In simple cases, these give the same discretization for L_y
For strategy 1, the main question is how do we modify the notation?
Let $d(P, B) = \alpha h$.

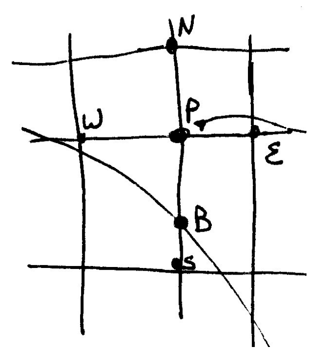
$$y_P - y_B = \alpha h, \quad 0 < \alpha < 1$$

Then the 3-point approximation to u_{yy} is

$$\begin{aligned} u_{yy} &\approx \frac{2}{(\alpha+1)h^2} u_N - \frac{2}{\alpha h^2} u_P + \frac{2}{\alpha(\alpha+1)h^2} u_B \\ &= \frac{2\alpha u_N - 2(\alpha+1)u_P + 2u_B}{\alpha(\alpha+1)h^2} \end{aligned}$$

Need to store the stencil of the discrete Laplacian at the irregular points (at least).
Outside the domain?
Stability:
We want to avoid explicit time schemes, even when

$$\frac{h^2}{4D} \text{ is not small}$$



The stability restriction is:

$$\Delta t \leq \frac{h^2}{2\left(\frac{1}{\alpha} + \frac{1}{\beta}\right) D}$$

Accuracy:
The 3-point approximation to the 2nd derivative is 1st order accurate for non-uniform spacing. At irregular points, the LTE is $O(h)$. At regular points, the LTE is $O(h^2)$. However, since irregular points are near the boundary (1-D) and regular points are in the interior (2-D), we have a lot more regular points than irregular points. Recall: in 228a we showed that in 1-D, an $O(h)$ discretization adjacent to the boundary contributed $O(h^3)$ to the total error. The same result holds in 2-D.

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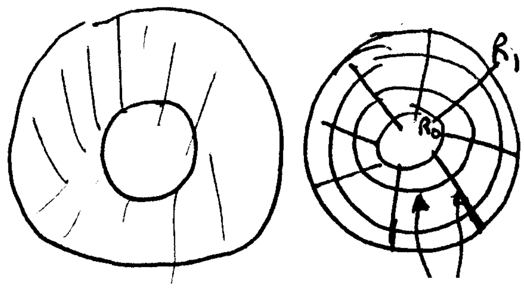
8.1 Boundary Fitted Mesh

Idea: map the physical domain to a rectangular domain, discretize the transformed domain, and solve.



$$x = r\cos\theta$$
$$y = r\sin\theta$$

Use polar coordinates to transform from (r,θ) coordinates to (x,y). Discretize using equally spaced points in r and θ. The circles are lines of constant r, and the outward rays are lines of constant θ. If we plot this discretized domain in r-θ space, we are working with a rectangle. We also have to transform the PDE (Laplacian):

$$\Delta = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}$$

The "price" of using transformed coordinates is an equation that depends on the new coordinates.

Let $\mathbf{x} = (x_1, x_2)$ be the original coordinates.
Let $\xi = (\xi_1, \xi_2)$ be the transform coordinates.
Let $\mathbf{x} = \mathbf{F}(\xi)$ $\quad\leftarrow$ the challenge is to find this map.

$$J_{ij} = \frac{\partial F_i}{\partial x_j} \qquad g = J^T J$$

Once we have our trnsformation $\mathbf{F}$, the transformed Laplacian in ξ coordinates is

$$\Delta u = \sum_i \sum_j \frac{1}{\sqrt{|g|}}\frac{\partial}{\partial \xi_i}\left(\sqrt{|g|}g_{ij}^{-1}\frac{\partial u}{\partial \xi_j}\right)$$

This is easy if you have the map. We often don't have the map, but it can be generated numerically.

8.2 Hyperbolic Problems

Intuitive sense: propogation of information requires a finite amount of time.

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

is *hyperbolic* if A has real eigenvalues and is diagonalizable.

In 2-D:

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

Non-Linear

$$\mathbf{u}_t + \nabla \cdot \mathbf{F}(\mathbf{u}) = 0$$

Start with the advection equation:

$$u_t + au_x = 0$$

Solution is

$$u(x,t) = u_0(x - at)$$

on the real line with initial condition

$$u(x,0) = u_0(x)$$

The initial data just translates.

The diffusion equation is forgiving because data smoothes out, but this does not happen with the advection equation.

We showed previously that forward time, centered space discretizationis unstable.

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\left(\frac{u_{j+1}^n - u_{j-1}^n}{2h}\right) = 0$$

von Neumann analysis:

$$g(\xi) = 1 - \frac{a\Delta t}{h}\sin(\xi h) i$$

$$|g(\xi)| > 1 \text{ for some } \xi$$

However, a growing solution does not imply unstable. (Provided that the solution grows exponentially slowly and is bounded by some rate.) This scheme is actually stable as long as $\Delta t \to 0$ sufficiently faster than h.

Note: absolute stability does not allow a solution to grow, but Lax Richtmeyer does.

Suppose we take $\Delta t = h^2$ for our refinement path.

$$\begin{aligned} |g(\xi)|^2 &= 1 + \frac{a^2 \Delta t^2}{h^2}\sin^2(\xi h) \\ &= 1 + \Delta t\left(\frac{a^2\Delta t}{h^2}\sin^2(\xi h)\right) \\ &\leq 1 + \Delta t a^2 \end{aligned}$$

This is stable, but we would never do this because there are stable, explicit schemes with $\Delta t = O(h)$.

Write this discretization as

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{2h}\left(u_{j+1}^n - u_{j-1}^n\right)$$

With a slight modification, we get the Lax-Friedrichs scheme (which is stable):

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n - \frac{\Delta t a}{2h}(u_{j+1}^n - u_{j-1}^n)$$

$$\text{Let } \nu = \frac{\Delta t a}{h}$$

ν is called the *Courant number*. Then we can rewrite Lax-Friedrichs as:

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n) - \frac{\nu}{2}(u_{j+1}^n - u_{j-1}^n)$$

von Neumann analysis:

$$\begin{aligned} g(\xi) &= \frac{1}{2}(e^{i\xi h} + e^{-i\xi h}) - \frac{\nu}{2}(e^{i\xi h} - e^{-i\xi h}) \\ &= \cos(\xi h) - i\nu \sin(\xi h) \end{aligned}$$

$$|g(\xi)|^2 = \cos^2(\xi h) + \nu^2 \sin^2(\xi h)$$

This is stable provided that

$$\begin{aligned} \nu^2 &\leq 1 \\ |\nu| &\leq 1 \end{aligned}$$

9 2-8-11

9.1 Comments on HW1, Problem 2

Crank-Nicoloson for diffusion equation with initial data

$$u(t=0) = \begin{cases} 1 & 0 \le x \le 0.5 \\ 0 & 0.5 < x \le 1 \end{cases}$$

Let's look at the regions of absolute stability for the trapezoidal rule and backward Euler. (Crank-Nicolson is the application of the trapezoidal rule to diffusion with the standard 3-point discretization.)

$$\begin{aligned} y' &= \lambda y \\ y^{n+1} &= R(z) y^n, \quad \text{where } z = \lambda \Delta t \end{aligned}$$

This is absolutely stable if $|R(z)| \le 1$.

For Trapezoidal Rule:

$$R(z) = \frac{1 + z/2}{1 - z/2} \tag{9.1}$$

For Backward Euler:

$$R(z) = \frac{1}{1 - z} \tag{9.2}$$

Method Of Lines aplied to

$$\frac{du}{dt} = Lu$$

where L is the discrete Laplacian.

$$\lambda_k = -\frac{4}{h^2} \sin^2\left(\frac{k\pi h}{2}\right), \quad k = 1, \ldots, N$$

If we plot λ_k vs. k, we see that the largest magnitude eigenvalues correspond to large k, i.e. high spatial frequencies.

What does it mean to have large negative eigenvalues? It means "those things" decay very rapidly.

As $h \to 0$, $\lambda_N \to -\infty \Rightarrow z \to -\infty$ along the real axis (note: z is/can be complex). For the Trapezoidal Rule, $R(z) \to -1$ (see (9.1)). For Backward Euler, $R(z) \to 0$ (see (9.2)). This is telling us that the high frequency modes in trapezoidal rule decay and oscillate in discrete time.

Both Backward Euler and Trapezoidal Rule are A-stable, but backward Euler is *L-stable* (stronger).

- If $|R(z)| \le 1 \; \forall \; z$ such that $\Re(z) \le 0$, then the method is *A-stable*.
- If $|R(z)| \to 0$ as $|z| \to \infty$, then the method is *L-stable*.
  - Note: L-stable $\not\Leftarrow$ A-stable

When applying Crank-Nicolson, be aware of your initial conditions.

All BDF methods are L-stable.
BDF 1 & 2 are both A-stable.
BDF 1 is Backward Euler.
BDF 2 is

$$\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t} = f(u^{n+1})$$

What is the extra cost of BDF 2 compared to Backward Euler? More storage (you have to store 1 more time level).

Implicit Runge-Kutta is L- & A-stable and 2nd order accurate.

$$u^* = y^n + \frac{\Delta t}{4}\left(f(u^n) + f(u^*)\right)$$

where u^* approximates $u^{n+1/2}$.

$$u^{n+1} = \frac{1}{3}\left(4u^* - u^n + \Delta t f(u^{n+1})\right)$$

Let's look at the amplification factor for Crank-Nicolson:

$$g(\xi) = \frac{1 - \frac{2\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right)}{1 + \frac{2\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right)}, \qquad \xi h = \theta, \quad -\pi \le \theta \le \pi$$

$$g(\theta) = \frac{1 - \delta\sin^2\left(\frac{\theta}{2}\right)}{1 + \delta\sin^2\left(\frac{\theta}{2}\right)} \quad \text{where } \delta = \frac{2\Delta t}{h^2}$$

We can get rid of oscillations by making $\delta \approx 1 \Rightarrow \Delta t \approx h^2/2$. But this is the stability restriction for Forward Euler.

9.2 Comments on HW1, Problem 4

In 4(a), many claimed

$$|g(\xi)|^2 \le 1 + \frac{|a|}{h}\Delta t \quad \Rightarrow \quad \text{stability}$$

This does not take into account the path that $\Delta t/h$ must take. It merely says that as $\Delta t \to 0$ with h fixed, it is stable.

$$\mu = \frac{b\Delta t}{h^2} \le \frac{1}{2}$$

9.3 Lax-Friedrich for $u_t + au_x = 0$

$$u_t + au_x = 0$$

$$\begin{aligned}
u_j^{n+1} &= \frac{u_{j-1}^n + u_{j+1}^n}{2} - \frac{a\Delta t}{2h}\left(u_{j+1}^n - u_{j-1}^n\right)\\
\frac{u_j^{n+1} - u_j^n}{\Delta t} &= \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{2\Delta t} - \frac{a}{2h}\left(u_{j+1}^n - u_{j-1}^n\right)\\
u_t + O(\Delta t) &= \frac{h^2}{2\Delta t}\left(\frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{2\Delta t}\right) - au_x + O(h^2)\\
u_t + O(\Delta t) &= \frac{h^2}{2\Delta t}u_x x + O\left(\frac{h^4}{\Delta t}\right) - au_x + O(h^2)
\end{aligned}$$

$$u_t + au_x = \underbrace{O(\Delta t) + O(h^2) + O\left(\frac{h^2}{\Delta t}\right)}_{\text{Local Truncation Error}}$$

Let $\Delta t, h \to 0$ and $h^2/\Delta t \to 0$. For stability, we require that

$$\left|\frac{a\Delta t}{h}\right| \le 1$$

Take $\Delta t/h =$ constant. This effectively makes the last term $O(h) \to 0$ as $h \to 0$, so the scheme is constant. Therefore, Lax-Friedrich converges.

Why did that one tweak give us a stable scheme? It introduced a small diffusion into the problem. Therefore, we could think of Lax-Friedrich as a discretization of

$$u_t + au_x = \epsilon u_{xx}, \qquad \epsilon = \frac{h^2}{2\Delta t}$$

In our homework we showed that Forward Euler with centered difference is stable if

$$\nu^2 \le 2\mu \le 1$$

$$\nu^2 = \frac{a^2 \Delta t^2}{h^2}, \qquad \mu = \frac{\epsilon \Delta t}{h^2}$$

$$2\mu = 2\left(\frac{h^2}{2\Delta t}\right)\frac{\Delta t}{h^2} = 1$$

$$\text{Stability Constraint:} \quad \nu^2 = 1$$

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Courant Number: $\nu = \frac{a\Delta t}{h}$
For Lax-Friedrichs, we require $|\nu| \leq 1$

10.1 CFL Condition

(Stands for Courant-Friedrichs-Lewy)

In hyperbolic equations, there is a finite speed of proprogation. We can use this idea in designing numerical schemes.

The domain of dependence of the point (x, t) is the set of points that determine the solution, $u(x, t)$, at (x, t).

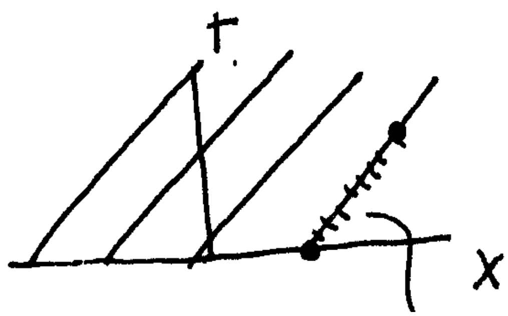
For

$$u_t + au_x = 0$$

Our solution is of the form

$$u(x, t) = u_0(x - at)$$

The solution is constant on the curves (lines) $x - at = x_0$.

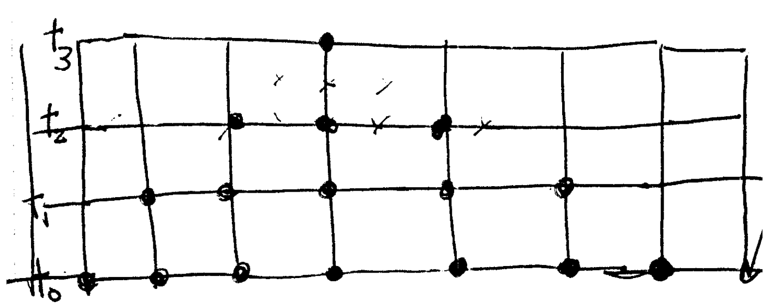


The Domain of Dependence (DoD) of (x, t) is $(x - at, 0)$, i.e. a single point. If we had a nonhomogeneous equation, the DoD would be the line.

DoD for $u_t = u_{xx}$ on $\mathbb{R}$: the whole spatial domain (i.e. the whole real line)

For numerical methods, we are interested in the numerical (discrete) domain of dependence. That is, the set of points in discrete space and time which determine the numerical solution u_j^n at (x_j, t_n).

Suppose we use a 3-point centered explicit time scheme.



The filled in points are the numerical DoD.

What happens to the numerical DoD as we refine space and time with $r = \frac{\Delta t}{h}$ fixed?
$\Rightarrow$ The number of points increases, but they occupy the same region of space-time.

At time t_0, the points in the numerical domain of dependence are contained within the interval $\left[X - \frac{h}{\Delta t}T, X + \frac{h}{\Delta t}T\right] = [X - T/r, X + T/r]$.

It is reasonable to expect that for the scheme to converge, we need the domain of dependence of the PDE to be contained within the DoD of the numerical scheme.

The CFL Condition: $D_a \subseteq D_N$ as $\Delta t, h \to 0$.

For $u_t + au_{xx} = 0$, the DoD is

$$x - at \in \left[X - \frac{T}{r}, X + \frac{T}{r}\right]$$

$$X - \frac{T}{r} \le X - aT \le X + \frac{T}{r}$$

$$-T \le -raT \le T$$

$$-1 \le ra \le 1$$

$$|ra| \le 1$$

$$\left|\frac{\Delta ta}{h}\right| \le 1$$

$$|\nu| \le 1$$

This is the CFL condition for this equation with this stencil.

CFL is a *necessary* condition for convergence, but it is not *sufficient*.

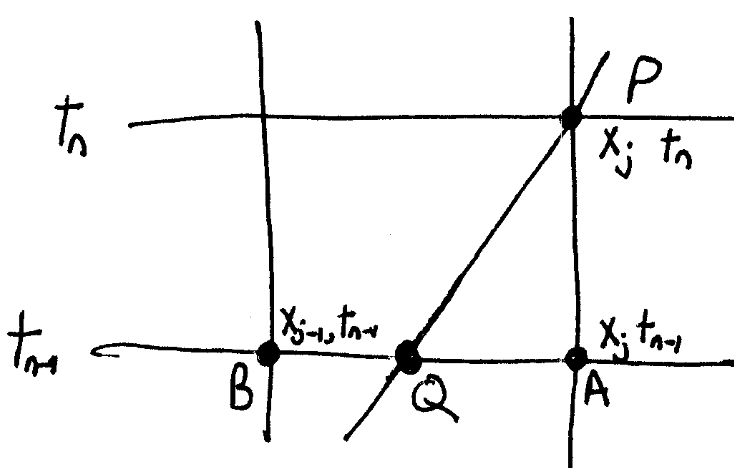
For example, forward time centered-space is not stable even when $|\nu| \le 1$, if $\Delta t = O(h)$.

Generally, we think about CFL for hyperbolic problems, not for parabolic problems.

10.2 Upwinding

$$u_t + au_{xx} = 0$$

Suppose $a > 0$, i.e. information is moving to the right. Why use the centered space scheme?



$$\text{Suppose } \nu = \frac{a\Delta t}{h} < 1$$

If we know the solution at Q, then we know it at P because $u(P) = u(Q)$. Question: where is Q?

$$\begin{aligned} x_j - at_{n+1} &= x_Q - at_n \\ x_Q &= x_j - a\Delta t \leftarrow \text{in general, this is not on the grid} \end{aligned}$$

Use the numerical solution at points A & B to interpolate to point Q.

$$\begin{aligned} QA &= x_j - (x_j - a\Delta t) = \frac{a\Delta t}{h} h = \nu h \\ QB &= x_j - a\Delta t - x_{j-1} = h - a\Delta t = h - \nu h = (1-\nu)h \end{aligned}$$

$$\begin{aligned} u(P) &= u(Q) \\ &\approx \frac{(1-\nu)hu(Q) + \nu h u(B)}{h} \\ &\approx (1-\nu)u(A) + \nu u(B) \end{aligned}$$

The upwinding numerical scheme is

$$\begin{aligned} u_j^{n+1} &= (1-\nu)u_j^n + \nu u_{j-1}^n \\ &= u_j^n - \nu(u_j^n - u_{j-1}^n) \\ &= u_j^n - \frac{a\Delta t}{h}(u_j^n - u_{j-1}^n) \end{aligned}$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\left(\frac{u_j^n - u_{j-1}^n}{h}\right) = 0$$

Forward time, backward space.
↑ This is differencing in the *upwind* direction.

$$u_j^{n+1} = u_j^n - \begin{cases} \nu(u_{j+1}^n - u_j^n) & a < 0 \\ \nu(u_j^n - u_{j-1}^n) & a > 0 \end{cases}$$

Essentially, we are averaging the exact solution.

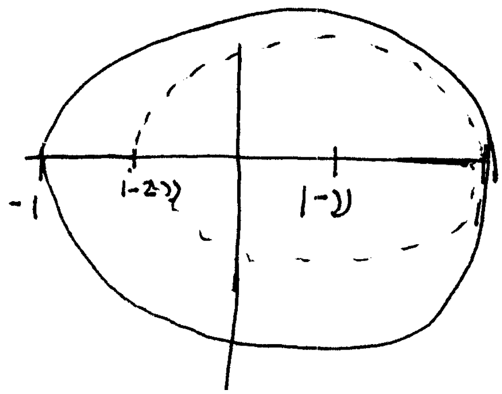
This scheme is 1st order in space and time.

We require $|\nu| \leq 1$.

Stability

Assume $a > 0$. Use von Neumann analysis:

$$\begin{aligned} g(\xi) &= 1 - \nu(1 - e^{-i\xi h}) \\ &= (1-\nu) + \nu e^{-i\xi h} \end{aligned}$$



This is stable if $\nu \leq 1$.

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11.1 Upwinding (Continued)

Assume $a > 0$.

$$\begin{aligned} u_j^{n+1} &= u_j^n - \frac{a\Delta t}{h}(u_j^n - u_{j-1}^n) \\ &= u_j^n - \nu(u_j^n - u_{j-1}^n) \\ &= (1-\nu)u_j^n + \nu u_{j-1}^n \end{aligned}$$

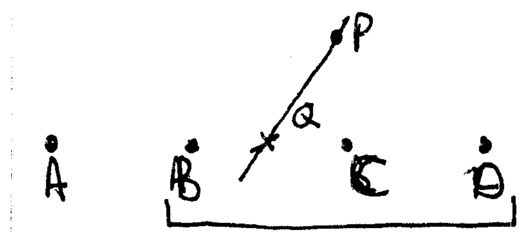
Since this scheme entails averaging of points, it does not introduce any artificial maxima (or minima).

Let

$$\begin{aligned} m^n &= \max_j |u_j^n| \\ m^{n+1} &\le m^n \\ m^{n+1} &= \max_j |u_j^{n+1}| \le \max_j \left((1-\nu)|u_j^n| + \nu|u_{j-1}^n|\right) \\ &\le m^n \end{aligned}$$

Upwinding is only first-order accurate in space and time. How do we do better?

Return to the idea of following characteristics (lines/curves where the solution is constant).



To get a second-order scheme, we could use a 3-point interpolation scheme using points B, C, D. This gives a scheme known as *Lax-Wendroff*. If we use a 3-point interpolation using A, B, C then we get the *Beam-Warming* scheme.

Note: usually Lax-Wendroff is derived using a Taylor series, which generalizes much more easily than characterisitic tracing.

Given $u(x,t)$, we want to know $u(x, t+\Delta t)$.

$$u(x, t+\Delta t) = u(x,t) + \Delta t u_t(x,t) + \frac{\Delta t^2}{2} u_{tt}(x,t) + O(\Delta t^3)$$

Use the PDE to express time derivatives in terms of space derivatives.

$$\begin{aligned} u_t + a u_x &= 0 \\ u_t &= -a u_x \\ u_{tt} &= -a u_{xt} = -a(u_t)_x = a^2 u_{xx} \\ u(x, t+\Delta t) &= u(x,t) - \Delta t a u_x(x,t) + \frac{a^2 \Delta t^2}{2} u_{xx}(x,t) + O(\Delta t)^3 \end{aligned}$$

We get the second order Lax-Wendroff scheme by ignoring the $O(\Delta t^3)$ terms and using second order differences in space.

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{2h}(u_{j+1}^n - u_{j-1}^n) + \frac{a^2\Delta t^2}{2h^2}(\underbrace{u_{j-1}^n}_{B} - 2\underbrace{u_j^n}_{C} + \underbrace{u_{j+1}^n}_{D})$$

The Local Truncation Error of this scheme is $O(h^2) + O(\Delta t^2)$.

Beam-Warming, $a > 0$, uses one-sided differences.

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{2h}(3u_j^n - 4u_j^n + u_{j-2}^n) + \frac{a^2\Delta t^2}{2h^2}\underbrace{(u_j^n - 2u_{j-1}^n + u_{j-2}^n)}_{D_- D_- u_j^n}$$

Note that we have an $O(h)$ approximation to u_{xx} at x_j.

$$\text{LTE} = O(\Delta t^2) + O(h^2) + O(h\Delta t)$$

The last term will be second order provided that $\Delta t = O(h)$.

11.2 Stability of Lax-Wendroff

$$|g(\xi)|^2 = -4\nu^2(1-\nu^2)\underbrace{\sin^4\left(\frac{\xi h}{2}\right)}_{\in[0,1]}$$

CFL constraint: $|\nu| \leq 1 \Rightarrow 0 \leq \nu^2 \leq 1$

$$|g(\xi)|^2 = 1 - B\sin^2\left(\frac{\xi h}{2}\right)$$
$$|g(\xi)| \leq 1 \quad \forall\ \xi$$

This is stable provided we meet the CFL constraint:

$$|\nu| \leq 1$$
$$\left|\frac{a\Delta t}{h}\right| \leq 1$$
$$\Delta t \leq \frac{h}{|a|}$$

- Upwinding is 1st order in space and time for smooth solutions.
- Lax-Wendroff is 2nd order in space and time for smooth solutions.

For the diffusion equation, we weren't worried about smoothness because diffusion smooths out initial conditions. This is not true for hyperbolic problems.

The solution to $u_t + au_x = 0$ is $u(x,t) = u(x - at)$.

With upwinding and Lax-Wendroff, it is not a good idea to reduce Δt by too much. Therefore, it is best to run as close to $\nu = 1$ as you can. Rather than just decreasing Δt, it is better to decrease Δt and h together.

- Upwinding smears $\Rightarrow$ better for discontinuous initial data
- Lax-Wendroff lags $\Rightarrow$ better for continuous initial data

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12.1 Discontinuous Solutions

Upwinding

- No wiggles
- Smearing of the solution
- Quality of the solution degraded when ν was reduced

Lax-Wendroff

- Wiggles $\Rightarrow$ didn't go away with refinement!
- Phase lag in the solution
- Quality of the solution degraded when ν was reduced

12.2 Modified Equations

PDE $\xrightarrow{\text{discretize}}$ Difference equations

$\downarrow$

Get a PDE to describe the behavior of the difference equations $\longleftarrow$ With Upwinding and Lax-Wendroff, the problem is that we observe behavior not exhibited by the solutions of the PDE.

Upwinding for $a > 0$, $u_t + au_x = 0$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\left(\frac{u_j^n - u_{j-1}^n}{h}\right) = 0$$

Let $v(x,t)$ be a smooth function of continuous space and time that solves the difference equations.

$$v(x_j, t_n) = u_j^n$$

Plug v into the difference equations and expand as $\Delta t, h \to 0$.

$$\frac{v(x, t+\Delta t) - v(x,t)}{\Delta t} + a\left(\frac{v(x,t) - v(x-h,t)}{h}\right) = 0$$

$$v_t + \frac{\Delta t}{2}v_{tt} + \frac{\Delta t^2}{6}v_{ttt} + O(\Delta t^3) + a\left(v_x - \frac{h}{2}v_{xx} + \frac{h^2}{6}v_{xxx} + O(h^3)\right) = 0$$

$$v_t + av_x = \underbrace{\frac{ah}{2}v_{xx} - \frac{\Delta t}{2}v_{tt}}_{\text{first order}} - \underbrace{\left(\frac{ah^2}{6}v_{xxx} + \frac{\Delta t^2}{6}v_{ttt}\right)}_{\text{second order}} + O(h^3) + O(\Delta t^3)$$

Upwinding is a first-order accurate approximation to $u_t + au_x$, but it is a second order approximation to

$$v_t + av_x = \frac{ah}{2}\left(v_{xx} - \frac{\Delta t}{ah}v_{tt}\right)$$

We can use this equation to express v_{tt} in terms of spatial derivatives.

$$v_{tt} = -av_{xt} + \frac{ah}{2}\left(v_{xxt} - \frac{\Delta t}{ah}v_{ttt}\right)$$

$$v_{tx} = -av_{xx} + \frac{ah}{2}\left(v_{xxx} - \frac{\Delta t}{ah}v_{ttx}\right) = v_{xt}$$

$$v_{tt} = a^2 v_{xx} + O(h)$$

$$v_t + av_x = \frac{ah}{2}\left(v_{xx} - \frac{\Delta t}{ah}a^2 v_{xx}\right) + O(h^2)$$

$$v_t + av_x = \frac{ah}{2}(1-\nu)v_{xx} + O(h^2)$$

Upwinding solves this equation:

$$v_t + av_x = Dv_{xx}$$

to second order accuracy, where

$$D = \frac{ah}{2}(1-\nu).$$

- As $h \to 0$ with ν fixed, $D \to 0$
- D gets smaller as $\nu \to 1$
- Reducing Δt while keeping h fixed makes $\nu \to 0$ and therefore increases D

12.3 Lax-Friedrichs Modified Equation

The modified equation to leading order for Lax-Friedrichs is

$$v_t + av_x = D_{LF}v_{xx}$$

where

$$\begin{aligned} D_{LF} &= \frac{h^2}{2\Delta t}(1-\nu^2) \\ &= \frac{h^2}{2\Delta t}(1-\nu)(1+\nu) \\ &= \frac{ah}{2}(1-\nu)\frac{h}{a\Delta t}(1+\nu) \\ &= \frac{ah}{2}(1-\nu)\left(1+\frac{1}{\nu}\right) \\ &= D_{UP}\left(1+\frac{1}{\nu}\right) \end{aligned}$$

Thus, there is at least twice as much diffusion in LF than in upwinding.

Where do the wiggles come from in Lax-Wendroff?

Lax-Wendroff is a second order approximation to $u_t + au_x = 0$, but it is a 3rd order approximation to

$$v_t + av_x = \mu v_{xxx}$$

where

$$\mu = \frac{ah^2}{6}\underbrace{(\nu^2-1)}_{<0}$$

- $a > 0 \quad \Rightarrow \quad \mu < 0$
- $a < 0 \quad \Rightarrow \quad \mu > 0$

What does the ∂_x^3 term do to the solution?

We will solve this equation using the Fourier transform.

$$\begin{aligned} \hat{v}_t + ai\xi\hat{v} &= -\mu i\xi^3\hat{v} \\ \hat{v}_t &= -i(a\xi + \mu\xi^3)\hat{v} \\ \hat{v}(\xi,t) &= \hat{v}(\xi,0)e^{-i(a\xi+\mu\xi^3)t} \\ |\hat{v}(\xi,t)| &= |\hat{v}(\xi,0)| \end{aligned}$$

Thus, the amplitude is preserved for each mode. By Parseval's relation, we can conclude that

$$\|v(x,t)\|_2 = \|v(x,0)\|_2$$

Transform back:

$$\begin{aligned} v(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{v}(\xi,t)e^{ix\xi}\, d\xi \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{v}(\xi,0)e^{-i(a\xi+\mu\xi^3)t+ix\xi}\, d\xi \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{v}(\xi,0)e^{i\xi(x-ct)}\, d\xi \end{aligned}$$

where

$$c = a + \mu\xi^2.$$

The mode with wavenumber ξ travels at speed $a + \mu\xi^2$. For small values of ξ, $c = a + O(\xi)^2$.

For Lax-Wendroff, this property means that high spatial frequencies travel more slowly than the low spatial frequencies. Wave velocity depends on the wave number; this is called *dispersion*.

$$v_t + av_x = \mu v_{xxx}$$

is a dispersive equation.

Lax-Wendroff is great for smooth solutions, but has bad behavior on high frequency modes.

For C^∞ functions, $\hat{v}(\xi)$ decays exponentially in ξ as $|\xi| \to \infty$. For u discontinuous, $\hat{u}(\xi)$ decays like $1/\xi$.

The equation

$$v_t + av_x = \mu v_{xxx}$$

preserves the 2-norm of the initial data. Lax-Wendroff does not because of the higher order terms.

$$v_t + av_x = \mu v_{xxx} - \epsilon v_{xxxx}, \qquad \epsilon = O(h^3)$$

Question: what is the accuracy of these methods? After all, we are using Taylor series to represent a discontinuous function.

Answer: these methods will not converge in the max norm, but they will converge in the integral norms.

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13.1 Comments on HW2

- Problem 1: when showing that the scheme is conditionally stable, we can get a bound (not necessarily a tight bound), but we need to show that if Δt is large enough then the scheme will not converge

13.2 Wrapping Up Modified Equations

Dissipative vs. Dispersive Properties of a Scheme

- Dissipative: how do the wave numbers get damped?
  - Upwinding: at 2nd order
  - Lax Wendroff: at 4th order
- Dispersive: how faithfully do you match the right wave speeds?
  - Lax Wendroff: leading order error is dispersive (waves travel at different speeds)
  - To analyze further, plot the amplification factors for schemes as a function of wave number, see how dissipative it is
    - Leapfrog and Crank-Nicolson are non-dispersive

<u>Accuracy of using Taylor series for discontinuous initial data: Upwinding</u>

Use a modified equation and compare the solution to the solution of the original equation. Solve

$$u_t + au_x = 0$$

$$v_t + av_x = Dv_{xx}$$

on the whole real line with initial conditions

$$u(x,0) = v(x,0) = \begin{cases} 1 & x \leq 0 \\ 0 & x > 0 \end{cases}$$

The solution of the advection equation is

$$u(x,t) = u_0(x - at)$$

and the solution of the modified equation is

$$v(x,t) = 1 - \text{erf}\left(\frac{x - at}{\sqrt{4Dt}}\right)$$

where

$$\text{erf} = -\frac{2}{\sqrt{\pi}} \int_{-\infty}^{x} e^{-z^2}\, dz$$

Upwinding resembles $v(x,t)$ more than $u(x,t)$, so we can get an idea for how accurate it is by comparing the two. Let's use the 1-norm to estimate the rror of upwinding.

$$\begin{aligned}
\|u(x,t)-v(x,t)\|_1 &= \int_{-\infty}^{\infty} \left| u_0(x-at) - \left(1 - \operatorname{erf}\left(\frac{x-at}{\sqrt{4Dt}}\right)\right)\right| dx \\
&= \int_{-\infty}^{\infty} \left| u_0(z) - \left(1 - \operatorname{erf}\left(\frac{z}{\sqrt{4Dt}}\right)\right)\right| dz \qquad \text{where } z = x - at \\
&= \int_{-\infty}^{0} \left| \operatorname{erf}\left(\frac{z}{\sqrt{4Dt}}\right)\right| dz + \int_{0}^{\infty} \left| 1 - \operatorname{erf}\left(\frac{z}{\sqrt{4Dt}}\right)\right| dz \\
&= \int_{-\infty}^{0} \operatorname{erf}\left(\frac{z}{\sqrt{4Dt}}\right) dz \\
&= 2\sqrt{4Dt}\int_{-\infty}^{0} \operatorname{erf}(s)\, ds \qquad \text{where } s = \frac{z}{\sqrt{4Dt}} \\
\|u-v\|_1 &= C\sqrt{Dt}
\end{aligned}$$

where C is independent of D and t.

For upwinding,

$$D = \frac{ah}{2}(1-\nu)$$

$$\|u-v\|_1 = O(\sqrt{h})$$

*** We will verify this on HW3.

13.3 Boundary Conditions

We've been avoiding having to deal with boundary conditions by using periodic domains. What boundary conditions are required on finite domains?

$$u_t + au_x = 0 \qquad \text{on } (0,1), \qquad a > 0$$

The solution is constant along the characteristic curves $x - at = C$. The solution depends on the initial condition and the values at the left boundary, $x = 0$, a.k.a. the inflow boundary, but it does not depend on the values at $x = 1$, a.k.a. the outflow boundary (for $a > 0$). Therefore, we need to be given a boundary condition at $x = 0$: $u(0,t) = f(t)$. We cannot specify a right boundary conditions.

On a discretized domain, the first point ($j = 0$) must be given and the last point ($j = N+1$) is solved for.

Upwinding with $a > 0$:

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{h}(u_j^n - u_{j-1}^n)$$

This is no problem because it uses only one point to the left.

$$u_0^n = f(n\Delta t)$$

<u>Lax-Wendroff</u>
↑ Depends on spatial points to the left and right. So what do we doe at the last point, $j = N+1$?

<u>Beam-Warming</u>
↑ This is one-sided, so there is no problem at $x = 1$. The problem is at $j = 1$ because we need the data at $j = 0$ and $j = 1$.

What to do at outflow boundaries?

- Switch to a one-sided scheme
- Use a numerical boundary condition
  - Add a $j = N + 2$ point
    - Constant extrapolation: Let $u_{N+2} = u_{N+1}$
    - Linear extrapolation: $u_{N+2} = 2u_{N+1} - u_N$
    - Extrapolation using the PDE: $u^n_{N+2} = u^{n-1}_{N+2} - \frac{a\Delta t}{h}(u^{n-1}_{N+2} - u^{n-1}_{N+1})$

13.4 Linear Systems

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

$$u_{tt} = c^2 u_{xx} \qquad \text{equivalent to} \qquad \mathbf{q} + \begin{pmatrix} 0 & c^2 \\ 1 & 0 \end{pmatrix} \mathbf{q}_x = 0, \quad \mathbf{q} = \begin{pmatrix} u_t \\ u_x \end{pmatrix}$$

Acoustic Waves
p is pressure, u is velocity,

$$\begin{aligned} \rho_t &= -ku_x \\ \rho u_t &= -\rho x \rho u_{tt} & = Ku_{xx} \\ c^2 &= \frac{k}{\rho} \end{aligned}$$

Schemes like Lax-Wendroff, Lax-Friedrichs, etc. are no different for systems.

$$\mathbf{u}^{n+1}_j = \mathbf{u}^n_j - \frac{\Delta t}{2h} A(u_{j+1} - u^n_{j-1}) + \frac{\Delta t^2}{2h} A^2(\mathbf{u}^n_{j-1} - 2\mathbf{u}^n_j + \mathbf{u}^n_{j+1})$$

This is stable provided that

$$\left| \frac{\Delta t \lambda}{h} \right| \leq 1 \quad \forall\ \lambda$$

where the λ are the eigenvalues of A.

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Wave equation:

$$u_{tt} = c^2 u_{xx}$$
$$q_t + \begin{pmatrix} 0 & c^2 \\ 1 & 0 \end{pmatrix} q_x = 0$$

Upwinding:
We take the *upwind* direction for our difference scheme.
Question: How do we define the upwind direction?

The eigenvalues of the wave equation matrix are

$$\lambda_\pm = \pm c$$

Thus, we have information going to the right and to the left.

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

Assume that A is constant,i.e. independent of space and time. (This is not a requirement, but it makes the analysis easier.) Diagonalize A:

$$A = R\Lambda R^{-1}, \qquad \Lambda \text{ diagonal}$$

$$u_t + R\Lambda R^{-1} u_x = 0$$
$$(R^{-1}u)_t + \Lambda(R^{-1}u)_x = 0$$

$$\text{Let} \qquad \mathbf{w} = R^{-1}\mathbf{u} \quad \leftarrow \quad \text{changing to eigen-coordinates}$$
$$\mathbf{u} = \sum_j w_j \mathbf{r}_j$$
$$\mathbf{w}_t + \Lambda \mathbf{w}_x = 0$$

The equations for each w_j are decoupled.

$$A = \begin{pmatrix} 0 & c^2 \\ 1 & 0 \end{pmatrix}, \qquad \Lambda = \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix}$$

$$\frac{\partial}{\partial t} w_1 + c\frac{\partial}{\partial x} w_1 = 0$$
$$\frac{\partial}{\partial t} w_2 - c\frac{\partial}{\partial x} w_2 = 0$$

$$\Lambda = \Lambda^+ + \Lambda^-$$
$$\Lambda^+ = \frac{\Lambda + |\Lambda|}{2}$$
$$\Lambda^- = \frac{\Lambda - |\Lambda|}{2}$$
$$w_j^{n+1} = w_j^n - \underbrace{\Delta t \Lambda^+ \left(\frac{w_j^n - w_{j-1}^n}{h} \right)}_{\text{right moving waves}} - \underbrace{\Delta t \Lambda^- \left(\frac{w_{j-1}^n - w_j^n}{h} \right)}_{\text{left moving waves}}$$

To be clear,

$$\mathbf{w}_j^n \approx \mathbf{w}(x_j, t_n)$$

Now transform back to the original variables:

$$\mathbf{u}_j^{n+1} = \mathbf{u}_j^n - \frac{\Delta t}{h} A^+ (\mathbf{u}_j^n - \mathbf{u}_{j-1}^n) - \frac{\Delta t}{h} A^- (\mathbf{u}_{j+1}^n - \mathbf{u}_j^n)$$

Where

$$A^+ = R\Lambda^+ R^{-1}, \qquad A^- = R\Lambda^- R^{-1}$$

We can do these compositions locally when A is non-constant.

14.1 Finite Volume Methods & Conservation Laws

1-D conservation law:

$$u_t + (f(u))_x = 0$$

where u is the conserved quantity. The advection equation is a simple example of a conservation law, with $f(u) = au$.

Assume that u and f are smooth.

$$u_t + f'(u) u_x = 0$$

This looks like a nonlinear or variable coefficient advection equation.

Next quarter we will study the Inviscid Burgers equation:

$$u_t + u u_x = 0$$

The equation $u_t + (f(u))_x = 0$ comes from the integral law

$$\frac{d}{dt} \int_{x_1}^{x_2} u(x,t)\, dx = f(u(x_1,t)) - f(u(x_2,t))$$

The amount of u in the intervale $[x_1, x_2]$ changes only by flux of u across the boundary.

Finite Difference Method: discretize the domain into a set of points

$$u_j \approx u(x_j)$$

Finite Volume Method: divide the domain into a set of volumes and represent a function by its average value over each volume.

In 2-D, divide the domain into cells

$$C_j = \left[x_{j-1/2}, x_{j+1/2}\right]$$

Let u_j represent the average value of $u(x)$ over volume j:

$$u_j \approx \frac{1}{h_j} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x)\, dx, \qquad h_j = x_{j+1/2} - x_{j-1/2}$$

$$\frac{1}{h_j} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x)\, dx = u(x_j) + O(h^2)$$

This is a midpoint approximation of that integral, and x_j is the center/centroid of the volume. This leads to a cell-centered grid (see HW2).

Conservation law on the jth cell:

$$\frac{d}{dt} \int_{C_j} u(x,t)\, dx = f(u(x_{j-1/2},t)) - f(u(x_{j+1/2},t))$$

Integrate this from time t_n to time t_{n+1}:

$$\int_{C_j} u(x,t_{n+1})\,dx - \int_{C_j} u(x,t_n)\,dx = -\int_{t_n}^{t_{n+1}} f(u(x_{j+1/2},t)) - f(u(x_{j-1/2},t))\,dt$$

Divide through by the volume of the jth grid cell, $h_j = h$ and use that

$$u_j(t) = \frac{1}{h}\int_{C_j} u(x,t)\,dx$$

to get that

$$u_j(t_{n+1}) = u_j(t_n) - \frac{\Delta t}{h}\int_{t_n}^{t_{n+1}} \frac{f(u(x_{j+1/2},t)) - f(u(x_{j-1/2},t))}{\Delta t}\,dt$$

So far we have made no approximations. Let

$$F^n_{j+1/2} \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(u(x_{j+1/2},t))\,dt$$

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{h}(F^n_{j+1/2} - F^n_{j-1/2})$$

This is equivalent to

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{F^n_{j+1/2} - F^n_{j-1/2}}{h} = 0$$

This looks like a finite difference discretization of $u_t + (f(u))_x = 0$.

Note that this scheme satisfies a discrete conservation law:

$$\begin{aligned} h\sum_{j=j_1}^{j_2} u_j^{n+1} &= h\sum_{j=j_1}^{j_2} u_j^n - \Delta t\sum_{j=j_1}^{j_2}(F_{j+1/2} - F_{j-1/2}) \\ &= h\sum_{j=j_1}^{j_2} u_j^n - \Delta t(F_{j_2+1/2} - F_{j_1-1/2}) \end{aligned}$$

14.2 Numerical Flux Function: Advection Equation

$$f(u) = au$$

How to pick $F^n_{j+1/2}$?
Attempt 1: Average

$$\begin{aligned} F^n_{j+1/2} &= \frac{f(u_j^n) + f(u_{j+1}^n)}{2} \\ &= \frac{au_j^n + au_{j+1}^n}{2} \\ u_j^{n+1} &= u_j^n - \frac{\Delta t}{h}\left(a\left(\frac{u_j^n + u_{j+1}^n}{2}\right) - a\left(\frac{a_{j-1}^n + u_j^n}{2}\right)\right) \\ u_j^{n+1} &= u_j^n - \frac{a\Delta t}{2h}\left(u_{j+1}^n - u_{j-1}^n\right) \end{aligned}$$

But this is forward time, centered difference $\Rightarrow$ unstable.

Attempt 2: Upwind
The upwind flux is

$$F^n_{j+1/2} = \begin{cases} au_{j+1} & a < 0 \\ au_j & a > 0 \end{cases}$$

Assume $a > 0$.

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{h}(au_j - au_{j-1})$$

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15.1 Finite Volume Methods (Continued)

$$u_j = \frac{1}{h}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t)\,dx$$

$$u_t + (f(u))_x = 0$$

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{h}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$$

$$F_{j+1/2}^n \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(u(x_{j+1/2},t))\,dt$$

We choose

$$F_{j+1/2} = \begin{cases} au_j^n & a > 0 \\ au_{j+1}^n & a < 0 \end{cases}$$

This results in upwinding. Upwinding is OK. It is diffusive, but it has low order accuracy.

If we replace $F_{j+1/2}^n$ with $F_{j+1/2}^{n+1/2}$ then we get a scheme centered in time and space that should give us a second order method.

Two-Step Lax-Wendroff

1. $u_{j+1/2}^{n+1/2} = \frac{1}{2}(u_j^n + u_{j+1}^n) - \frac{\Delta t}{2h}\left(f(u_{j+1}^n) - f(u_j^n)\right)$
   This looks like a half time step of Lax-Friedrichs to predict the edge value.
2. $u_j^{n+1} = u_j^n - \frac{\Delta t}{h}\left(f(u_{j+1/2}^{n+1/2}) - f(u_{j-1/2}^{n+1/2})\right)$

In the first step we are using values at cell centers to evaluate fluxes at edges. In the second step we use the fluxes at edges to evaluate the fluxes at centers.

This two step method is equivalent to Lax-Wendroff for the linear advection equation.

The flux for Lax-Wendroff is

$$F_{j+1/2}^{\text{LW}} = \frac{a}{2}(u_j^n u_{j+1}^n) - \frac{a^2\Delta t}{2h}\left(u_{j+1}^n - u_j^n\right)$$

Assume $a > 0$. Add and subtract the upwind flux, which is:

$$F_{j+1/2}^{\text{Up}} = au_j^n$$

$$\begin{aligned} F_{j+1/2}^{\text{LW}} &= au_j^n - au_j^n + \frac{a}{2}\left(u_j^n + u_{j+1}^n\right) - \frac{a^2\Delta t}{2h}\left(u_{j+1}^n - u_j^n\right) \\ &= au_j^n + \left(\frac{a}{2} - \frac{a^2\Delta t}{2h}\right)\left(u_{j+1}^n - u_j^n\right) \\ &= F_{j+1/2}^{\text{Up}} + \underbrace{\frac{a}{2}(1-\nu)\left(u_{j+1}^n - u_j^n\right)} \end{aligned}$$

The selected term is a second-order correction to upwinding. $F_{j+1/2}^{\text{LW}} - F_{j+1/2}^{\text{Up}}$

15.2 Idea behind high-resolution methods

$$F^{\text{HR}} = F^{\text{Up}} + (F^{\text{LW}} - F^{\text{Up}})\phi$$

The idea is to adjust ϕ locoally based on the steepness of the numerical solution. When ϕ is near zero, we get upwinding. When ϕ is near 1, we get Lax-Wendroff. ϕ is called the *flux limiter function*.

15.3 REA Algorithms

Reconstruct: from cell averages, reconstruct an approximation to the original function.
Evolve: solve the PDE exactly for one time step with the reconstruction as the initial data.
Average: compute new averages

R Step
Godunov's method (for reconstruction) is based on piecewise constant reconstruction.

E Step
Evolve the system by $a\Delta t$.

A Step

$$u_j^{n+1} = \frac{a\Delta t u_{j-1}^n + (h - a\Delta t)u^n}{h}$$
$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{h}\left(u_j^n - u_{j-1}^n\right)$$

This scheme is just upwinding.

Note that the PDE is only used in the E Step.

This idea leads to a generalization of upwinding for nonlinear PDEs.

$$u_t + (f(u))_x = 0$$
$$u_t + \underbrace{f'(u)}_{\text{speed}} u_x = 0 \qquad \text{for } f \text{ smooth}$$

This is easy to solve away from the discontinuities.

We need to know how to solve Riemann problems in order to apply the scheme. The Riemann problem is

$$u_t + (f(u))_x = 0$$

$$u(x,0) = \begin{cases} u_l & x < 0 \\ u_r & x > 0 \end{cases}$$

How to get higher-order accuracy?
We need to work on the R step $\Rightarrow$ use a more accurate reconstruction.

e.g. piecewise linear (not worrying about continuity)

$$\tilde{u}(x,t) = u_j^n + \sigma_j^n(x - x_j), \qquad x_{j-1/2} < x < x_{j+1/2}$$

$$\frac{1}{h}\int_{C_j} \tilde{u}(x,t)\,dx = u_j^n + 0$$

Thus, the average is independent of the slope.

How do we choose the slopes?

- $\sigma_j = 0 \Rightarrow$ Godunov (upwinding)

- Centered difference: $\sigma_j = \frac{u_{j+1}-u_{j-1}}{2h} \Rightarrow$ Fromm's method
- Assume $a > 0$
  - Upwind: $\sigma_j = \frac{u_j - u_{j-1}}{h} \Rightarrow$ Beam-Warming
  - Downwind: $\sigma_j = \frac{u_{j+1}-u_j}{h} \Rightarrow$ Lax-Wendroff

Any one of these results in a second-order accurate scheme.

Consider $a > 0$, downwind slope, discontinuous solution.

$$u_j^n = \begin{cases} 1 & j \le J \\ 0 & j > J \end{cases}$$

Due to the "tilting" of the piecewise linear pieces, this will overshoot (new maximum) behind the discontinuity.

With an upstream slope, we get undershoot (new minimum) in front of the discontinuity.

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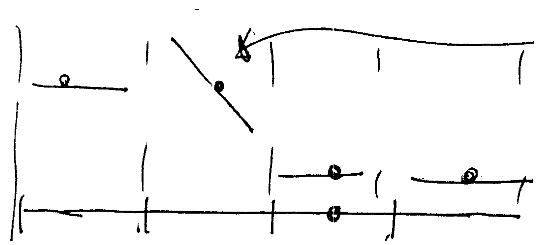
16.1 REA Algorithms (Continued)



Using upwinding/downwinding to get the slopes for reconstruction can introduce maxima and minima.

One way to remove the oscillation from the numerical scheme is to use a slope limiter to avoid over- and under-shoots.

e.g. minmod slope

$$\sigma_j = \text{minmod}\left(\frac{u_j - u_{j-1}}{h}, \frac{u_{j+1} - u_j}{h}\right)$$

$$\text{minmod}(a, b) = \begin{cases} a & |a| < |b|,\ ab > 0 \\ b & |b| < |a|,\ ab > 0 \\ 0 & ab \leq 0 \end{cases}$$

This does not introduce any new maxima/minima. This reconstruction will not give any oscillations. Essentially, we are selecting between upwinding, Lax-Wendroff, and Beam-Warming at each point.

This scheme is still very diffusive (in comparison to the ones we'll develop later). We could allow for steeper slopes.

A good "multi-purpose" choice of slope limiter is the monotonized center difference, aka MC-limiter.

$$\sigma_j = \text{minmod}\left(\frac{u_{j+1} - u_{j-1}}{2h}, 2\ \text{minmod}\left(\frac{u_j - u_{j-1}}{h}, \frac{u_{j+1} - u_j}{h}\right)\right)$$

Why do we have the factor of 2? Let $\tilde{u}_j(x, t_n)$ be the reconstruction in cell j. Suppose it is monotone: $u_{j-1} \leq u_j \leq u_{j+1}$. We want

$$\tilde{u}_j(x_{j-1/2}) \geq u_{j-1}$$
$$\tilde{u}_j(x_{j+1/2} \leq u_{j+1}$$
$$\tilde{u}_j = u_j + \sigma_j(x - x_j)$$
$$\tilde{u}_j(x_{j-1/2}) = u_j + \sigma_j\left(-\frac{h}{2}\right) \geq u_{j-1}$$
$$\sigma_j \leq 2\left(\frac{u_j - u_{j-1}}{h}\right)$$

Slope limiters and flux limiters are related. Let's compute the effective flux for an REA-type method for the advection equation using piecewise linear reconstruction.

Discrete conservation law:

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{h}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$$

$$F^n_{j+1/2} \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(u(x_{j+1/2},t))\,dt$$

Assume $f(u) = au,\ a > 0$. In our discretization, we have

$$\begin{aligned}
F^n_{j+1/2} &= \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} a\tilde{u}(x_{j+1/2},t))\,dt \\
&= \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} a\tilde{u}_j(x_{j+1/2} - a(t-t_n), t_n)\,dt \\
\tilde{u}_j(x,t_n) &= u^n_j + \sigma(x - x_j) \\
F^n_{j+1/2} &= \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} a\big(u^n_j + \sigma(x_{j+1/2} - a(t-t_n) - x_j)\big)\,dt \qquad = \underbrace{au^n_j}_{\text{upwind flux}} + \underbrace{\frac{ah}{2}\left(1 - \frac{a\Delta t}{h}\right)\sigma^n_j}_{\text{correction to upwinding}}
\end{aligned}$$

For example, if

$$\begin{aligned}
\sigma^n_j &= \frac{u_{j+1} - u_j}{h} \\
F^n_{j+1/2} &= \underbrace{F^{\text{up}}_{j+1/2} + \frac{a}{2}(1-\nu)(u_{j+1} - u_j)}_{R^{\text{LW}}_{j+1/2}} \\
F^n_{j+1/2} &= F^{\text{up}}_{j+1/2} + (F^{\text{LW}}_{j+1/2} - F^{\text{up}}_{j+1/2})\phi
\end{aligned}$$

For a positive or negative,

$$F^n_{j+1/2} = \begin{cases} au_j + \frac{a}{2}\left(1 - \frac{a\Delta t}{h}\right)h\sigma^n_j & a \geq 0 \\ au_{k+1} - \frac{a}{2}\left(1 + \frac{a\Delta t}{h}\right)h\sigma^n_{j+1} & a < 0 \end{cases}$$

In general,

$$F^n_{j-1/2} = F^{\text{up}}_{j-1/2} + \frac{|a|}{2}\left(1 - \frac{|a|\Delta t}{h}\right)\delta^n_{j-1/2}$$

where δ is a limited version of the difference

$$\begin{aligned}
(\Delta u)_{j-1/2} &= u_j - u_{j-1} \\
\delta^n_{j-1/2} &= \phi(\theta_{j-1/2})(\Delta u)_{j-1/2}
\end{aligned}$$

where ϕ is the limiter function. If things are smooth, $\phi \approx 1$. If things aren't smooth, $\phi \approx 0$. How do we measure smoothness of data?

Define

$$\theta_{j-1/2} = \frac{\Delta u_{J,\text{up}-1/2}}{\Delta u_{j-1/2}}$$

What is J_{up}?

$$J_{\text{up}} = \begin{cases} j-1 & a > 0 \\ j+1 & a < 0 \end{cases}$$

For a smooth function, $\theta \approx 1$, except near critical points (1st derivative is zero).

Note: $\Delta u_{j-1/2} = u_j - u_{j-1}$

We want ϕ near zero when not smooth, and ϕ near one when smooth.

Upwinding: $\phi = 0$
Lax-Wendroff: $\phi = 1$
Beam Warming: $\phi = \theta$ (Identity function)

16.2 Common High-Resolution Limiters

- minmod: $\phi(\theta) = \text{minmod}\,(1, \theta)$
- MC: $\phi(\theta) = \max\left(0, \min\left(\frac{1+\theta}{2}, 2, 2\theta\right)\right)$
- Superbee: $\phi(\theta) = \max\left(0, \min(1, 2\theta), \min(2, \theta)\right)$
- van Leer: $\phi(\theta) = \frac{\theta+|\theta|}{1+|\theta|}$

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17.1 High Resolution Methods (Continued)

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{h}\left(F_{j+1/2}^n - F_{j-1/2}^n\right)$$

$$F_{j-1/2}^n = F_{j+1/2}^{\text{up}} + \left|\frac{a}{2}\right|\left(1 - \left|\frac{a\Delta t}{h}\right|\right)\delta_{j-1/2}^n$$

$$\delta_{j-1/2}^n = \phi(\theta_{j-1/2})\Delta u_{j-1/2}$$

$$\Delta u_{j-1/2} = u_j - u_{j-1}$$

$$\theta_{j-1/2} = \frac{\Delta u_{J_{\text{up}}-1/2}}{\Delta u_{j-1/2}}$$

How do I get something that stays accurate on smooth parts and doesn't introduce wiggles? In other words, how do I pick our limiter function, $\phi(\theta)$, to avoid numerical oscillations when the solution is sharp (almost discontinuous) and give 2nd order accuracy when the solution is smooth?

17.2 Total Variation

Total variation of a grid function is:

$$\text{TV}(u) = \sum_j |u_j - u_{j-1}|$$

For a differentiable function f on (a, b), the total variation of f is

$$\text{TV}(f) = \int_a^b |f'(x)|\, dx$$

f = constant has zero variation. A function with wiggles has nonzero variation. A function with more wiggles will have bigger variation.

$$|\Delta y| = |f'(x)||\Delta x|$$

Variation is a measure of how much a function goes up and down; it is somewhat related to arc length.

- The solution to the advection equation has constant variation in time, since it merely translates.
- Numerical oscillations increase the variation.
- We avoid oscillations by requiring that the total variation goes down in time (remains constant is too much to hope for).

17.3 Total Variation Diminishing (TVD)

A numerical scheme is *total variation diminishing* (TVD) if

$$\text{TV}(u^{n+1}) \leq \text{TV}(u^n)$$

TVD is a way to avoid numerical oscillations.

TVD implies *monotonicity preserving*:

$$\text{if } u_j^n \geq u_{j+1}^n \ \forall\ j, \text{ then } u_j^{n+1} \geq u_{j+1}^{n+1}$$

A monotonicity preserving scheme will not introduce new maxima/minima.

We want to choose our limiter function so that our scheme is TVD.

What about achieving 2nd order? We need

1. $\phi(1) = 1$
2. ϕ is Lipschitz continuous at $\theta = 1$
   - This is satisfied for ϕ with bounded left and right derivatives at $\theta = 1$. i.e. a corner in ϕ at $\theta = 1$ is OK, but a cusp ($\succ$, but vertical) will not work.

Scheme for $a > 0$:

$$u_j^{n+1} = u_j^n - \nu(u_j^n - u_{j-1}^n) - \frac{\nu(1-\nu)}{2}\left(\phi(\theta_{j+1/2})(u_{j+1}^n - u_j^n) - \phi(\theta_{j-1/2})(u_j^n - u_{j-1}^n)\right) \tag{17.1}$$

On HW3 we proved that a scheme of the form

$$u_j^{n+1} = u_j^n - C_{j-1}^n(u_j^n - u_{j-1}^n) + D_j^n(u_{j+1}^n - u_j^n)$$

is TVD if $C_{j-1}^n \geq 0$, $D_j^n \geq 0$, and $C_j^n + D_j^n \leq 1$ for all j.

How do we pick C and D? Try the "obvious" choice:

$$C_{j-1}^n = \nu - \frac{\nu(1-\nu)}{2}\phi(\theta_{j-1/2}, \qquad D_j^n = -\frac{\nu(1-\nu)}{2}\phi(\theta_{j+1/2}), \qquad 0 \leq \nu \leq 1 \text{ by CFL}$$

Because ϕ is positive (at least for some θ), these choices won't give TVD. The trick is to write

$$u_{j+1}^n - u_j^n = \frac{u_j^n - u_{j-1}^n}{\theta_{j+1/2}}$$

If we plug this into (17.1) then we get

$$D = 0, \qquad C_{j-1}^n = \nu + \frac{\nu(1-\nu)}{2}\left(\frac{\phi(\theta_{j+1/2})}{\theta_{j+1/2}} - \phi(\theta_{j-1/2})\right)$$

This scheme is TVD if

$$0 \leq C_{j-1}^n \leq 1$$

This will give us constraints on ϕ.

$$-\nu \leq \frac{\nu(1-\nu)}{2}\left(\frac{\phi(\theta_{j+1/2})}{\theta_{j+1/2}} - \phi(\theta_{j-1/2})\right) \leq 1 - \nu$$

$$-2 \leq -\frac{2}{1-\nu} \leq \frac{\phi(\theta_{j+1/2})}{\theta_{j+1/2}} - \phi(\theta_{j-1/2}) \leq \frac{2}{\nu} \leq 2$$

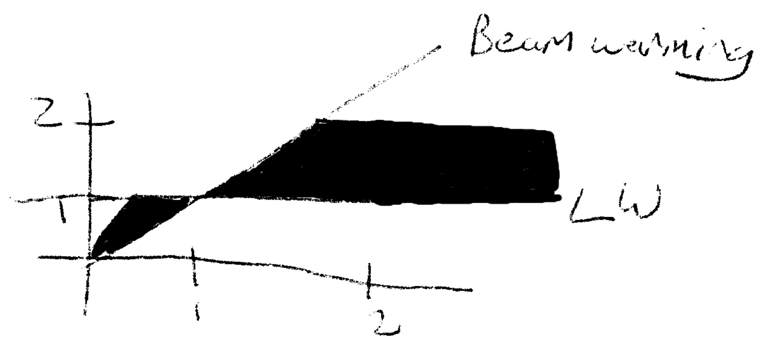
From CFL, $0 \leq \nu \leq 1$. For TVD, it is sufficient to enforce

$$\left|\frac{\phi(\theta_{j+1/2})}{\theta_{j+1/2}} - \phi(\theta_{j-1/2})\right| \leq 2$$

for all θ_1 and θ_2.

TVD Requirements

- In order to guarantee TVD, at extreme points ($\theta < 0$, meaning that the left and right slopes have different signs) we require that $\phi(\theta) = 0$ for all $\theta \leq 0$.
- We require $\phi \geq 0$ (we may reduce or accentuate slopes, but we never change directions).
- We require that $0 \leq \frac{\phi(\theta)}{\theta} \leq 2$ and $0 \leq \phi(\theta) \leq 2$
  - These last 2 imply that $0 \leq \phi(\theta) \leq \text{minmod}\ (2, 2\theta)$



A requirement to have second order is that $\phi(1) = 1$. We want $\phi(\theta)$ to be a convex combination of Beam-Warming and Lax-Wendroff. minmod is the lower bound of the Sweby region, and the superbee limiter is the upper bound of the Sweby region. minmod is as close as we can get to upwinding (diffusive). Superbee is as sharp of a reconstruction as we can get and still be TVD. MC limiter and van Leer are good all-purpose limiters. All of these methods fail to converge at discontinuities (so the max norm will not converge), but some are able to contain the lack of convergence around the discontinuity.

If θ is really big, Beam-Warming will steepen the slope, increasing it at most by a factor of 2.

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