PDEs: Initial Value Problem

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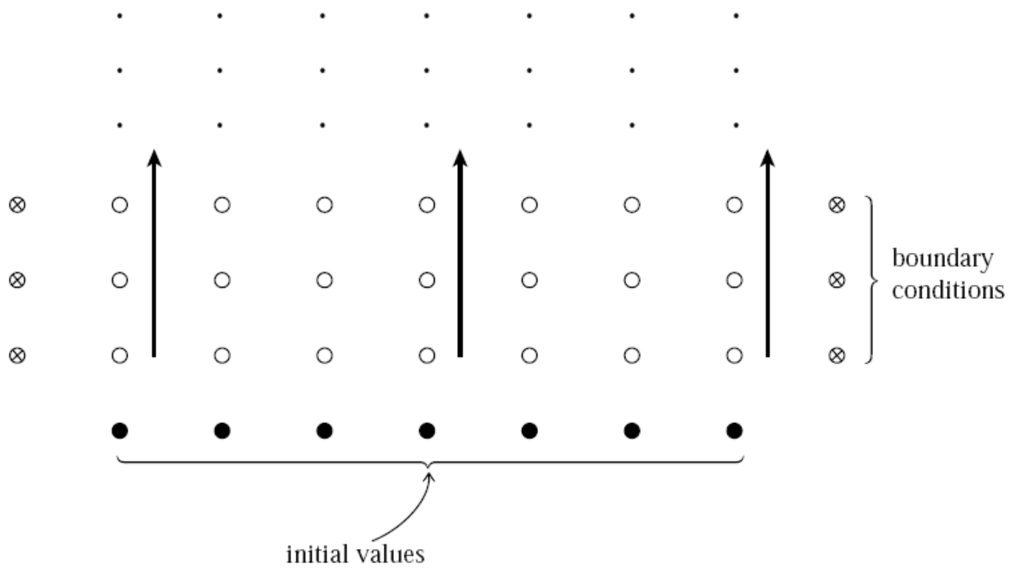
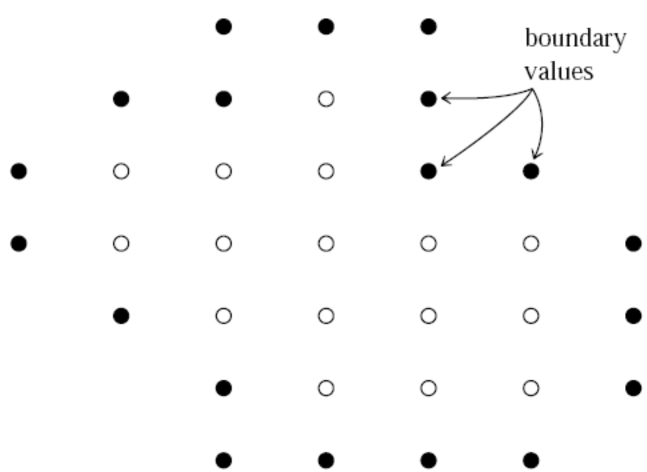


(a)

Initial Value Problem



(b)

Boundary Value Problem

One-Dimensional Wave Equation

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}$$

- How do we solve this?
- Does relaxation work? No: the values on the time boundary in the future are not specified.
- Can we make a first-order PDE out of this by introducing generalized coordinates, as we did for ODEs? Yes, we can.

First-Order Representation

Define $$r \equiv c\frac{\partial y}{\partial x}, \quad s \equiv \frac{\partial y}{\partial t}$$

The 2nd order wave equation becomes a set of two 1st order equations:

$$\frac{\partial r}{\partial t} = c\frac{\partial s}{\partial x}, \qquad \frac{\partial s}{\partial t} = c\frac{\partial r}{\partial x}$$

Generalize: *flux-conservative equation*

$$\frac{\partial \vec{u}}{\partial t} = -\frac{\partial \vec{F}(\vec{u}, \partial \vec{u}/\partial x)}{\partial x}$$

Wave: $$\vec{u} = \begin{pmatrix} r \\ s \end{pmatrix}, \quad \vec{F} = \begin{pmatrix} 0 & -c \\ -c & 0 \end{pmatrix} \vec{u}$$

Advection Equation

- The simplest nontrivial flux-conservative equation is

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}$$

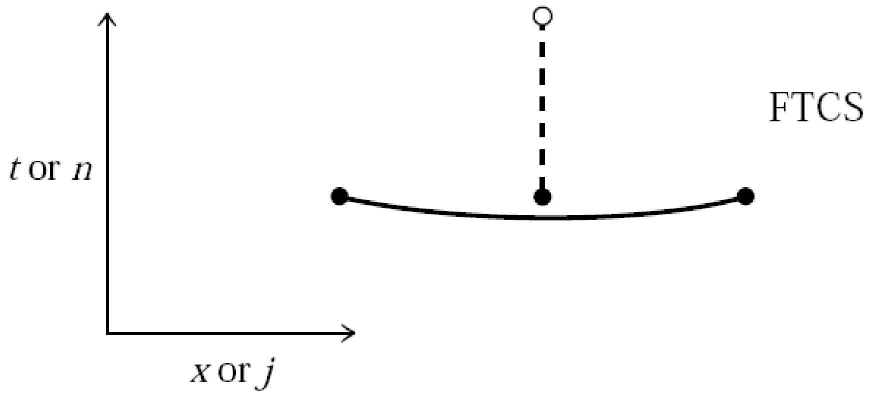
- Describes the evolution of a scalar field carried by a flow with constant velocity:

$$u(x,t) = f(x-ct)$$

  where *f* is an arbitrary function

- Let's develop a finite differencing scheme for this equation

FTCS Finite Difference Approximation



- FTCS stands for *Forward Time Centered Space*. For *t* it looks like the Euler scheme for ODEs:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -c \, \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$$

- Simple, fast, easy to program algorithm. Too bad it doesn't work!

Von Neumann Stability Analysis

- Advection equation is linear, so superposition works. Expect one of the wave components to look like

$$u(x,t) = A(t)\, e^{ikx}$$

- In discretized form, this becomes

$$u(x_j, t_n) \equiv u_j^n = A^n\, e^{ikj\Delta x}$$

- Advance by one step:

$$u_j^{n+1} = A^{n+1}\, e^{ikj\Delta x} = \xi\, A^n\, e^{ikj\Delta x}, \quad \xi \equiv A^{n+1} / A^n$$

- A differencing scheme is unstable if, for any *k*, amplification factor exceeds unity:

$$|\,\xi\,| > 1$$

FTCS Stability Analysis for Advection Equation

- Explicit FTCS updating formula is

$$u_j^{n+1} = u_j^n - \frac{c\Delta t}{2\,\Delta x}(u_{j+1}^n - u_{j-1}^n)$$

- Insert the solution:

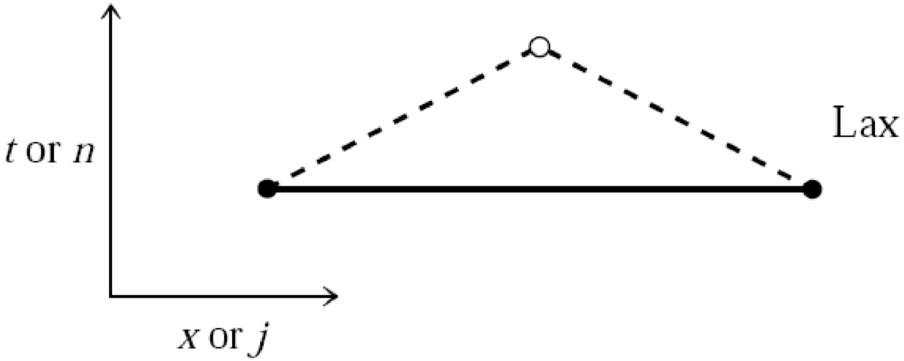
$$\xi\, A^n\, e^{ikj\Delta x} = A^n\, e^{ikj\Delta x}\left(1 - \frac{c\Delta t}{2\,\Delta x}(e^{ik\Delta x} - e^{-ik\Delta x})\right)$$

- Calculate the amplification factor:

$$\xi = 1 - i\,\frac{c\Delta t}{\Delta x}\sin(k\Delta x), \quad |\,\xi\,| = \sqrt{1 + \left(\frac{c\Delta t}{\Delta x}\right)^2 \sin^2(k\Delta x)}$$

- Conclusion: the scheme is unconditionally unstable

Lax Differencing Scheme



- Fixes FTCS by replacing

$$u_j^n \rightarrow \left(u_{j+1}^n + u_{j-1}^n\right)/\,2$$

- Averaging introduces an element of dissipation into the system (*numerical viscosity*). Lax scheme for advection equation is equivalent to FTCS scheme for

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2\Delta t}\frac{\partial^2 u}{\partial x^2}$$

Stability Analysis for the Lax Scheme

- Lax updating formula is

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n) - \frac{c\Delta t}{2\,\Delta x}(u_{j+1}^n - u_{j-1}^n)$$

- Insert the solution:

$$\xi\, A^n\, e^{ikj\Delta x} = A^n\, e^{ikj\Delta x}\left(\frac{1}{2}(e^{ik\Delta x} + e^{-ik\Delta x}) - \frac{c\Delta t}{2\,\Delta x}(e^{ik\Delta x} - e^{-ik\Delta x})\right)$$

- Calculate the amplification factor:

$$\xi = \cos(k\Delta x) - i\frac{c\Delta t}{\Delta x}\sin(k\Delta x), \quad |\,\xi\,| = \sqrt{\cos^2(k\Delta x) + \left(\frac{c\Delta t}{\Delta x}\right)^2 \sin^2(k\Delta x)}$$

- *The Courant condition*: this scheme is stable if

$$\left| c\Delta t / \Delta x \right| \le 1$$

Matrix Stability Analysis

- Works for any type/order linear PDE, not just the wave equation, as long as the differencing scheme can be written as

$$\vec{x}^{\,n+1} = L\,\vec{x}^{\,n}$$

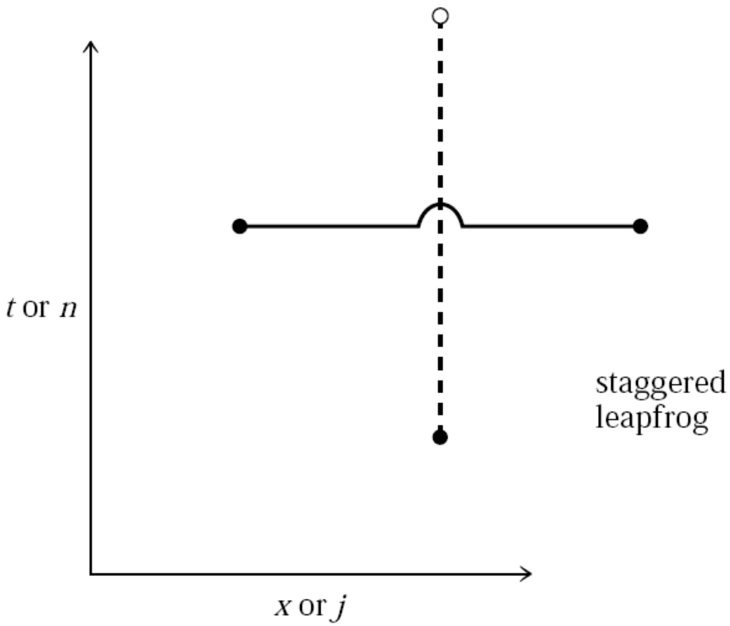
- As in QM propagator: decompose the initial condition in terms of *L* eigenvectors. Eigenvector ***v*** at step *n* evolves into

$$\vec{v}^{\,n} = L^n\,\vec{v} = \lambda^n\,\vec{v}$$

- The scheme is stable if all eigenvalues

$$|\lambda_i| \le 1$$

Second-Order Scheme in Time



- Advection equation

$$\frac{u_j^{n+1} - u_j^{n-1}}{\Delta t} = -c\,\frac{u_{j+1}^n - u_{j-1}^n}{\Delta x}$$

- Von Neumann stability analysis gives quadratic equation for ξ. Solution is

$$\xi = -i\frac{c\Delta t}{\Delta x}\sin(k\Delta x) \pm \sqrt{1-\left(\frac{c\Delta t}{\Delta x}\sin(k\Delta x)\right)^2}$$

Note that $|\xi|^2 = 1$ for any $c\Delta t \leq \Delta x$: no amplitude dissipation!

Leapfrog for the Wave Equation

Think of the mesh on which *r* and *s* are defined as being twice as fine as the mesh on which *y* is defined (purely for notational convenience). Then

$$\frac{r_{j+1/2}^{n+1} - r_{j+1/2}^{n}}{\Delta t} = c\,\frac{s_{j+1}^{n+1/2} - s_{j}^{n+1/2}}{\Delta x}, \qquad \frac{s_{j}^{n+1/2} - s_{j}^{n-1/2}}{\Delta t} = c\,\frac{r_{j+1/2}^{n} - r_{j-1/2}^{n}}{\Delta x}$$

If we discretize the original equations:

$$r_{j+1/2}^{n} = c\left.\frac{\partial y}{\partial x}\right|_{j+1/2}^{n} = c\,\frac{y_{j+1}^{n} - y_{j}^{n}}{\Delta x}, \qquad s_{j}^{n+1/2} = \left.\frac{\partial y}{\partial t}\right|_{j}^{n+1/2} = \frac{y_{j}^{n+1} - y_{j}^{n}}{\Delta t}$$

substitution of the second set of equations into the first gives:

$$\frac{y_{j}^{n+1} - 2y_{j}^{n} + y_{j}^{n-1}}{(\Delta t)^2} = c^2\,\frac{y_{j+1}^{n} - 2y_{j}^{n} + y_{j-1}^{n}}{(\Delta x)^2}$$

Stability Analysis of the Leapfrog Scheme

$$\frac{\partial}{\partial t}\begin{pmatrix} r \\ s \end{pmatrix} = \frac{\partial}{\partial x}\begin{pmatrix} cs \\ cr \end{pmatrix}$$

- Assume that eigenmode is of the following form

$$\begin{pmatrix} r_j^n \\ s_j^n \end{pmatrix} = \xi^n e^{ikj\Delta x}\begin{pmatrix} r^0 \\ s^0 \end{pmatrix}$$

- Upon substituting this into the scheme, one finds again that the Courant condition is required for stability and that there is no amplitude dissipation when it is satisfied

Diffusion Equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

- This time the FTCS scheme works

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

$$\xi = 1 - \frac{4D\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right)$$

as long as $|\xi| \le 1 \;\; \Rightarrow \;\; \dfrac{2D\Delta t}{(\Delta x)^2} \le 1$