Forward Difference Equation

- From last time:
  - a mathematical model for simple advection (1D motion of fluid):
    \[
    \frac{\partial \phi(x,t)}{\partial t} + u \frac{\partial \phi(x,t)}{\partial x} = 0
    \]
  - use Taylor series expansion to derive a discrete form of the PDE:
    \[
    \frac{\phi_{j,n+1} - \phi_{j,n}}{\Delta t} + u \frac{\phi_{j+1,n} - \phi_{j,n}}{\Delta x} = 0
    \]
  - the discrete form defines a 2D grid
    - rows are time steps, columns are spatial positions
    - \( \phi_{j,n} \) is density of particles at position \( x = j \) at time \( t = n \)

Stencils

- The pattern of relationships between terms used to compute the value at a grid point is called a stencil
- For the forward difference equation:
  \[
  \phi_{j,n+1} = \phi_{j,n} - u \frac{\Delta t}{\Delta x} (\phi_{j+1,n} - \phi_{j,n})
  \]
  Convenient graphical notation to compare different discrete forms
  Illustrates why this is “forward difference”
Characteristics

- In the exact solution of the advection equation it would be possible to plot the progress of any point in the initial density distribution
  - a curve that follows the path of a single value from the initial function is a characteristic
    - "curve of information propagation"
  - in this model the characteristic is a line, with a slope that depends on \( u \)

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0
\]

Solution Region

- Plotting the characteristics of each point in the initial distribution defines a region where we have information for a solution
  - a large region to the left of the characteristic for \( x_0 \) is undefined

Periodic Boundary Conditions

- To provide information for this undefined region use periodic boundary conditions
  - the stencil for the forward difference equation uses values from the right
  - copy the corresponding information from the right edge to the left
- May not be realistic
  - particles from Pasadena don't just reappear in Santa Monica
- For abstract models (e.g. general groundwater flow) it may be OK
  - useful for evaluating models and solutions

Evaluating the Forward Difference Equation

- This plot shows an initial distribution and expected vs computed values after one time step
  - Not too good....
  - After a few time steps the distribution is unrecognizable (see Fosdick chapter)
Backward Differences

- In deriving the forward difference equation we started with an estimate for a value of $\phi(x + \Delta x, t)$:
  \[ \phi(x + \Delta x, t) = \phi(x, t) + \phi_x(x, t)\Delta x + O((\Delta x)^2) \]
- We could have asked for a prediction of $\phi(x - \Delta x, t)$:
  \[ \phi(x - \Delta x, t) = \phi(x, t) - \phi_x(x, t)\Delta x + O((\Delta x)^2) \]
- Solve for $\phi(x, t)$, and combine with the old equation for $\phi(x, t)$

Backward Differences (cont’d)

- The new equation is slightly different, but has a big effect on accuracy:
  \[ \phi_{j,n+1} = \phi_{j,n} - \mu \frac{\Delta t}{\Delta x}(\phi_{j,n} - \phi_{j-1,n}) \]

Accuracy of Backward Difference Equation

- Much better after one time step
- But why?

Backward Difference and Characteristic

- Short answer to why backward is better:
  - when $u > 0$ the distribution is moving right
  - getting information from the left (direction of flow) is more accurate
- (Slightly) more technical answer:
  - the characteristic that goes through a point also passes over paths used to compute the value for the point
With periodic boundary conditions the initial distribution will wrap around and overlay the original. Comparing the two can provide a measure of accuracy:
- backward difference looked OK after a few time steps
- not as good after a full cycle

Why does the triangular distribution flatten out?
Ans: dispersion
- Fourier transform of shapes with sharp edges (this triangle, square wave, ...) show lots of high frequencies
- Numeric waves with higher frequencies disperse more slowly

See Fosdick for details

One of the difficulties in building computational models is testing:
- For PDE solvers:
  - verify the PDE is a correct model of the system
  - evaluate the discretization
  - debug the software implementing the discretization

This process is hard enough, but now we see a new complication:
- pick a test distribution that has similar characteristics to system being modeled
- smog won’t likely be distributed as a square wave or other distribution with sharp edges
- test with a Gaussian or other smooth pattern

Different applications of Taylor series expansion lead to other methods for numerically solving the equations:
- Centered difference equation (aka “forward time centered space”, or FTCS):
Other Difference Equations (cont’d)

- Leapfrog
  - evaluation of a row requires two previous rows
  - use one of previous methods for \( n = 1 \)
  - much better accuracy for triangle distribution (see Fosdick)

\[
\Phi_{j,n+1} = \Phi_{j,n-1} + \frac{\Delta t}{\Delta x} (\Phi_{j+1,n} - \Phi_{j-1,n})
\]

Implicit Methods

- A difference equation that is useful in diffusion problems (next topic) compares values from the same time step
  - \( u \) is the quantity being modeled
  - \( D \) is a diffusion coefficient
  - this is a second-order equation, which is why there is a \((\Delta x)^2\) term

\[
u_{j,n+1} = u_{j,n} + \frac{D \Delta t}{(\Delta x)^2} (u_{j-1,n+1} - 2u_{j,n+1} + u_{j+1,n+1})
\]

Implicit Methods (cont’d)

- It may seem there isn’t any way to compute \( u_{j,n+1} \)
  - values in one column depend on values from both neighboring columns
  - The equation for an interior grid point is a linear equation
  - For the entire grid there are \( t \times n \) equations but fewer than that many unknowns
  - we have initial values for boundary cells
  - Gaussian elimination or other methods to solve systems of linear equations can find values of grid points

Diffusion Problems

- Mathematicians classify PDEs according to the shape of the characteristics

\[
\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}
\]

hyperbolic (“wave equation”)

\[
\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial u}{\partial x} \right)
\]

parabolic (“diffusion equation”)

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y)
\]

elliptic (Poisson, Laplace)
Initial Value Problems

- Our advection equation is a special case of a parabolic equation
  - no diffusion, i.e. wave keeps its shape as it moves
- From a computational point of view, hyperbolic and parabolic equations are very similar
  - both are derivatives with respect to time
  - used to describe systems that evolve over time
- Computational science term: initial value problem
- An important consideration for numeric solution:
  - presence or absence of diffusion
  - FTCS usually a poor choice for advection problems, but can be stable for diffusion problems

Boundary Value Problems

- Elliptic PDEs describe a different type of problem
  \[
  \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y)
  \]
  - Note time is not represented in this equation
- These equations describe the spatial distribution of some quantity, e.g. heat
- The goal is to describe the steady-state distribution of the quantity
- In computational science, these are boundary value problems
  - values at boundaries are known
  - goal is to compute values at internal points

To Learn More

- Numeric solution of PDEs is a huge area
- From Press, et al, Numerical Recipes:
  - an art as much as a science (e.g. using "upstream" vs "downstream" differences)
  - many techniques work well on some types of equations, poorly on others
  - could devote an entire second volume of NR to PDEs alone
- For more information:
  - Heath, Scientific Computing (2e), 2002
  - many other books on numeric methods