Warm-up:
One-Dimensional Conservation Equation

Grétar Tryggvason
Spring 2013

Objectives:

- Introduce the basic concepts needed to solve a partial differential equation using finite difference methods.
- Discuss basic time integration methods, ordinary and partial differential equations, finite difference approximations, accuracy.
- Show the implementation of numerical algorithms into actual computer codes.

Outline

- Solving partial differential equations
  - Finite difference approximations
  - The linear advection-diffusion equation
  - Matlab code
- Accuracy and error quantification
- Stability
- Consistency
- Multidimensional problems
- Steady state

The Advection-Diffusion Equation

Model Equations

We will use the model equation:

$$\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = D \frac{\partial^2 f}{\partial x^2}$$

to demonstrate how to solve a partial equation numerically.

Although this equation is much simpler than the full Navier Stokes equations, it has both an advection term and a diffusion term.

Before attempting to solve the equation, it is useful to understand how the analytical solution behaves.

For initial conditions of the form:

$$f(x,t=0) = A \sin(2\pi kx)$$

It can be verified by direct substitution that the solution is given by:

$$f(x,t) = e^{-\frac{Dk^2}{4t}} \sin(2\pi k(x-Ut))$$

which is a decaying traveling wave.
Most physical laws are based on CONSERVATION principles: In the absence of explicit sources or sinks, \( f \) is neither created nor destroyed.

Consider a simple one-dimensional pipe of uniform diameter with a given velocity \( U(x) \).

Given \( f \) at the inlet as a function of time (as well as everywhere at time zero), how do we predict the \( f(t,x) \)?

To predict the evolution of \( f \) everywhere in the pipe, we assume that \( f \) is conserved. Thus, for any section of the pipe:

\[
\frac{df}{dt} \Delta x = F_{\text{in}} - F_{\text{out}}
\]

or:

\[
\frac{\Delta f}{\Delta t} = \frac{\Delta F}{\Delta x}
\]

Taking the limit, we get:

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

The general form of the one-dimensional conservation equation is:

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

Taking the flux to be the sum of advective and diffusive fluxes:

\[
F = Uf - F \frac{\partial f}{\partial x}
\]

Gives the advection diffusion equation

\[
\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = D \frac{\partial^2 f}{\partial x^2}
\]
Derive a numerical approximation to the governing equation, replacing a relation between the derivatives by a relation between the discrete nodal values.

\[
\Delta t \quad f(t + 2\Delta t) \\
\Delta t \quad f(t + \Delta t) \\
f(x-h) \quad f(x) \quad f(x+h) \\
h \quad h
\]

The Time Derivative

The Time Derivative is found using a FORWARD EULER method. The approximation can be found by using a Taylor series

\[
f(t + \Delta t) = f(t) + \frac{\partial f(t)}{\partial t} \Delta t + \frac{\partial^2 f(t)}{\partial t^2} \frac{\Delta t^2}{2} + \cdots
\]

Solving this equation for the time derivative gives:

\[
\frac{\partial f(t)}{\partial t} = \frac{f(t + \Delta t) - f(t)}{\Delta t} - \frac{\partial^2 f(t) \Delta t}{\partial t^2} + \cdots
\]

The Spatial First Derivative

When using FINITE DIFFERENCE approximations, the values of \( f \) are stored at discrete points.

\[
\Delta t \quad f(t + \Delta t) \\
\Delta t \quad f(t) \\
f(x-h) \quad f(x) \quad f(x+h) \\
h \quad h
\]

The derivatives of the function are approximated using a Taylor series
Start by expressing the value of $f(x+h)$ and $f(x-h)$ in terms of $f(x)$:

$$f(x+h) = f(x) + \frac{df(x)}{dx} h + \frac{d^2f(x)}{dx^2} \frac{h^2}{2} + \frac{d^3f(x)}{dx^3} \frac{h^3}{6} + \frac{d^4f(x)}{dx^4} \frac{h^4}{24} + \ldots$$

$$f(x-h) = f(x) - \frac{df(x)}{dx} h + \frac{d^2f(x)}{dx^2} \frac{h^2}{2} - \frac{d^3f(x)}{dx^3} \frac{h^3}{6} + \frac{d^4f(x)}{dx^4} \frac{h^4}{24} + \ldots$$

Subtracting the second equation from the first:

$$f(x+h) - f(x-h) = 2 \frac{df(x)}{dx} h + 2 \frac{d^2f(x)}{dx^2} \frac{h^2}{2} + \frac{d^3f(x)}{dx^3} \frac{h^3}{6} + \frac{d^4f(x)}{dx^4} \frac{h^4}{24} + \ldots$$

The result is:

$$f(x+h) - f(x-h) = 2 \frac{df(x)}{dx} h + \frac{d^2f(x)}{dx^2} \frac{h^2}{2} + \frac{d^3f(x)}{dx^3} \frac{h^3}{6} + \frac{d^4f(x)}{dx^4} \frac{h^4}{24} + \ldots$$

Rearranging this equation to isolate the first derivative:

$$\frac{df(x)}{dx} = \frac{f(x+h) - f(x-h)}{2h} - \frac{d^2f(x)}{dx^2} \frac{h^2}{12} + \frac{d^3f(x)}{dx^3} \frac{h^3}{72} - \frac{d^4f(x)}{dx^4} \frac{h^4}{576} + \ldots$$

The Spatial Second Derivative

Adding the second equation to the first:

$$f(x+h) + f(x-h) = 2f(x) + 2 \frac{d^2f(x)}{dx^2} \frac{h^2}{2} + 2 \frac{d^3f(x)}{dx^3} \frac{h^3}{6} + \frac{d^4f(x)}{dx^4} \frac{h^4}{24} + \ldots$$

The result is:

$$f(x+h) + f(x-h) = 2f(x) + \frac{d^2f(x)}{dx^2} \frac{h^2}{2} + \frac{d^3f(x)}{dx^3} \frac{h^3}{6} + \frac{d^4f(x)}{dx^4} \frac{h^4}{24} + \ldots$$

Rearranging this equation to isolate the second derivative:

$$\frac{d^2f(x)}{dx^2} = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} - \frac{d^3f(x)}{dx^3} \frac{h^3}{12} + \frac{d^4f(x)}{dx^4} \frac{h^4}{576} + \ldots$$

Solving the partial differential equation
Using the shorthand notation, for space and time we will use:

\[
\begin{align*}
    f^n &= f(t, x) \\
    f^{n+1}_j &= f(t + \Delta t, x) \\
    f^{n+1}_{j+1} &= f(t, x + h) \\
    f^{n+1}_{j-1} &= f(t, x - h)
\end{align*}
\]

\[
\begin{align*}
    \frac{df^n}{dt} &= \frac{f_{j}^{n+1} - f_{j}^{n}}{\Delta t} \\
    \frac{df_{j}^{n+1}}{dx} &= \frac{f_{j+1}^{n+1} - f_{j-1}^{n+1}}{2h} + O(h^2) \\
    \frac{\partial f^{n+1}_j}{\partial x} &= \frac{f_{j+1}^{n+1} - f_{j-1}^{n+1}}{2h} + O(h^2)
\end{align*}
\]

A numerical approximation to

\[
\frac{\partial f}{\partial x} + U \frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}
\]

is found by replacing the derivatives by the following approximations

\[
\left( \frac{\partial}{\partial x} \right)^n_j \approx \frac{f_{j+1}^{n+1} - f_{j-1}^{n+1}}{2h}
\]

Substituting these approximations into:

\[
\frac{df^{n+1}_j}{dt} = \frac{U}{2h} (f_{j+1}^{n+1} - f_{j-1}^{n+1}) + \frac{D}{h} (f_{j+1}^{n+1} - 2f_{j+1}^{n+1} + f_{j-1}^{n+1}) + O(\Delta t, h^2)
\]

Thus, given \( f \) at one time (or time level), \( f \) at the next time level is given by:

\[
f^{n+1}_j = f^n_j - \frac{U\Delta t}{2h} (f^{n+1}_{j+1} - f^{n+1}_{j-1}) + \frac{D\Delta t}{h} (f^{n+1}_{j+1} - 2f^{n+1}_j + f^{n+1}_{j-1})
\]

The value of every point at level \( n+1 \) is given explicitly in terms of the values at the level \( n \).
A short MATLAB program

The evolution of a sine wave is followed as it is advected and diffused. Two waves of the infinite wave train are simulated in a domain of length 2. To model the infinite train, periodic boundary conditions are used. Compare the numerical results with the exact solution.

% one-dimensional advection-diffusion by the FTCS scheme
n=21; nstep=100; length=2.0; h=length/(n-1); dt=0.05; D=0.05;
for i=1:n, f(i)=0.5*sin(2*pi*h*(i-1)); end;
for m=1:nstep, m, time
  for i=1:n, ex(i)=exp(-4*pi*pi*D*time)*0.5*sin(2*pi*(h*(i-1)-time));
  y(i)=f(i)-0.5*dt/h*(y(i+1)-y(i-1))+D*dt/h^2*(y(i+1)-2*y(i)+y(i-1));
  f(i)=y(i);
  end;
end;

EX2

It is clear that although the numerical solution is qualitatively similar to the analytical solution, there are significant quantitative differences.

The derivation of the numerical approximations for the derivatives showed that the error depends on the size of h and Δt.

First we test for different Δt.

Number of time steps= T/Δt
Computational Fluid Dynamics

Accuracy

Repeat with a smaller time-step
\[ \Delta t = 0.025 \]
N=21

\[ \begin{align*}
\text{Exact} & \\
\text{Numerical} & 
\end{align*} \]

\[ m=21; \text{time}=0.50 \]

Repeat with a smaller time-step
\[ \Delta t = 0.0125 \]
N=21

\[ \begin{align*}
\text{Exact} & \\
\text{Numerical} & 
\end{align*} \]

\[ m=41; \text{time}=0.50 \]

How accurate solution can we obtain?

Take
\[ \Delta t = 0.0005 \]
and
N=200

\[ \begin{align*}
\text{Exact} & \\
\text{Numerical} & 
\end{align*} \]

\[ m=1001; \text{time}=0.50 \]

Very fine spatial resolution and a small time step

\[ U=1; \]
\[ D=0.05; \]
\[ k=1 \]
N=200
\[ \Delta t = 0.0005 \]

\[ \begin{align*}
\text{Exact} & \\
\text{Numerical} & 
\end{align*} \]

Quantifying the Error
Order of Accuracy

Examine the spatial accuracy by taking a very small time step, \[ \Delta t = 0.0005 \] and vary the number of grid points, N, used to resolve the spatial direction.

The grid size is \[ h = L/N \] where \( L = 1 \) for our case.
If the error is of second order:

$$E = Ch^2 = C \left( \frac{1}{h} \right)^2$$

Taking the log:

$$\ln E = \ln \left( \left( \frac{1}{h} \right)^2 \right) = \ln C - 2 \ln \left( \frac{1}{h} \right)$$

On a log-log plot, the $E$ versus ($1/h$) curve should therefore have a slope -2.