In this section we consider the numerical discretization of the equations of motion.

The lectures will be based closely on the text

Atmospheric Modeling, Data Assimilation and Predictability
by Eugenia Kalnay

Numerical Methods (Kalnay, Ch. 3)

• NWP is an initial/boundary value problem

• Given
  – an estimate of the present state of the atmosphere (initial conditions)
  – appropriate surface and lateral boundary conditions
the model simulates or forecasts the evolution of the atmosphere.

• The more accurate the estimate of the initial conditions, the better the quality of the forecasts.

• Similarly, the more accurate the solution method, the better the quality of the forecasts.

We now consider methods of solving PDEs numerically.

Partial Differential Equations

We begin by looking at the classification of partial differential equations (PDEs).

The general second order linear PDE in 2D may be written

\[ A \frac{\partial^2 u}{\partial x^2} + 2B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + D \frac{\partial u}{\partial x} + E \frac{\partial u}{\partial y} + Fu = 0 \]

Second order linear partial differential equations are classified into three types depending on the sign of \( B^2 - AC \):

• **Hyperbolic**: \( B^2 - AC > 0 \)
• **Parabolic**: \( B^2 - AC = 0 \)
• **Elliptic**: \( B^2 - AC < 0 \)

Recall the equations of the conic sections

\[
\begin{align*}
\frac{x^2}{a^2} - \frac{y^2}{b^2} &= 1 & \text{Hyperbola} \\
\frac{x^2}{a^2} &= y & \text{Parabola} \\
\frac{x^2}{a^2} + \frac{y^2}{b^2} &= 1 & \text{Ellipse}
\end{align*}
\]
The simplest (canonical) examples of these equations are

(a) \( \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \)

Wave equation (hyperbolic).

(b) \( \frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2} \)

Diffusion equation (parabolic).

(c) \( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \)

Poisson’s equation (elliptic).

Example of hyperbolic equation:
- Vibrating String.
- Water Waves.

Example of parabolic equation:
- Heated Rod.
- Viscous Damping.

The behaviour of the solutions, the proper initial and/or boundary conditions, and the numerical methods that can be used to find the solutions depend essentially on the type of PDE that we are dealing with.

Thus, we need to study the canonical PDEs to develop an understanding of their properties, and then apply similar methods to the more complicated NWP equations.

A fourth canonical equation, of central importance in atmospheric science, is

(d) \( \frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \)

Advection equation.

The advection equation has the solution \( u(x, t) = u(x - ct, 0) \).

The advection equation is a first order PDE, but it can also be classified as hyperbolic, since its solutions satisfy the wave equation:

\[
\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = \left( \frac{\partial}{\partial t} + c \frac{\partial}{\partial x} \right) \left( \frac{\partial}{\partial t} - c \frac{\partial}{\partial x} \right) u = 0
\]

Obviously, if \( \partial u/\partial t + c \partial u/\partial x = 0 \), then \( u \) is a solution of the wave equation.

We note that if the elliptic Laplace equation is split up like this, the component operators are complex:

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) u = 0
\]

We cannot split this equation into two real first-order factors.

Examples of Elliptic Equation:
- Shape of a drum.
- Streamfunction/vorticity relationship.

Note: The following standard elliptic equations arise repeatedly in a multitude of contexts throughout science:

- Poisson’s Equation: \( \nabla^2 u = f \).
- Laplace’s Equation: \( \nabla^2 u = 0 \).
Example: Solve the Wave Equation

We will derive the solution of the wave equation by transformation of variables.

Define the new variables $\xi = x - ct$ and $\eta = x + ct$.

Then

$$
\begin{align*}
    u_x &= \xi u_\xi + \eta u_\eta = u_\xi + u_\eta \\
    u_t &= \xi u_\xi + \eta u_\eta = -cu_\xi + cu_\eta \\
    u_{xx} &= [u_{\xi\xi} + 2u_{\xi\eta} + u_{\eta\eta}] \\
    u_{tt} &= c^2[u_{\xi\xi} - 2u_{\xi\eta} + u_{\eta\eta}]
\end{align*}
$$

Therefore

$$
[u_{tt} - c^2u_{xx}] = -4c^2u_{\xi\eta} = 0 \quad \text{which means} \quad \frac{\partial^2 u}{\partial \xi \partial \eta} = 0.
$$

The solution of this equation may be expressed as a sum of a function of $\xi$ and another of $\eta$: $u = f(x - ct) + g(x + ct)$.

In any of the above cases we have an ill-posed problem. We can never find a numerical solution of a problem that is ill posed: the computation will react by blowing up.

* * *

Example: Solve the hyperbolic equation

$$
\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0
$$

subject to the following conditions:

$$
\begin{align*}
    u(x, 0) &= a_0(x) \\
    u(x, 1) &= a_1(x) \\
    u(0, t) &= b_0(t) \\
    u(1, t) &= b_1(t)
\end{align*}
$$

Example: Solve the advection equation

$$
\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0
$$

on $0 \leq x \leq 1$ and $t \geq 0$ with the initial/boundary conditions

$$
\begin{align*}
    u(x, 0) &= u_0(x) \\
    u(0, t) &= u_L(t) \\
    u(1, t) &= u_R(t)
\end{align*}
$$

Well-posedness

A well-posed initial/boundary condition problem has a unique solution that depends continuously on the initial/boundary conditions.

The specification of proper initial conditions and boundary conditions for a PDE is essential in order to have a well-posed problem.

- If too many initial/boundary conditions are specified, there will be no solution.
- If too few are specified, the solution will not be unique.
- If the number of initial/boundary conditions is right, but they are specified at the wrong place or time, the solution will be unique, but it will not depend smoothly on initial/boundary conditions.

For ill-posed problems, small errors in the initial/boundary conditions may produce huge errors in the solution.

The Elliptic Case

Second order elliptic equations require one boundary condition at each point of the spatial boundary.

These are pure boundary value, time-independent problems. The boundary conditions may be:

- The value of the function (Dirichlet problem), as when we specify the temperature on the edge of a plate.
- The normal derivative (Neumann problem), as when we specify the heat flux.
- A mixed boundary condition, involving a linear combination of the function and its derivative (Robin problem).
The Parabolic Case

Linear parabolic equations require one initial condition at the initial time and one boundary condition at each point of the spatial boundaries.

For example, for a heated rod, we need the initial temperature at each point $T(x,0)$ and the temperature at each end, $T(0,t)$ and $T(L,t)$ as a function of time.

In atmospheric science, the parabolic case arises mainly when we consider diffusive processes: internal viscosity; boundary layer friction; etc.

To give an example, consider the highlighted terms of the Navier-Stokes Equations

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} + 2\Omega \times \mathbf{V} + \frac{1}{\rho} \nabla p = \nu \nabla^2 \mathbf{V}$$

The Hyperbolic Case

Linear hyperbolic equations require as many initial conditions as the number of characteristics that come out of every point in the surface $t = 0$, and as many boundary conditions as the number of characteristics that cross a point in the (space) boundary pointing inwards.

For example: Solve $\partial u / \partial t + c \partial u / \partial x = 0$ for $x > 0, t > 0$.

The characteristics are the solutions of $dx/dt = c$.

The space boundary is $x = 0$.

If $c > 0$, we need the initial condition $u(x,0) = f(x)$ and the boundary condition $u(0,t) = g(t)$.

If $c < 0$, we need the initial condition $u(x,0) = f(x)$ but no boundary conditions.

For nonlinear equations, no general statements can be made, but physical insight and local linearization can help to determine proper initial/boundary conditions.

For example, in the nonlinear advection equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$$

the characteristics are $dx/dt = u$.

We don’t know a priori the sign of $u$ at the boundary, and whether the characteristics will point inwards or outwards.

One method of solving simple PDEs is the method of separation of variables. Unfortunately in most cases it is not possible to use it.

Nevertheless, it is instructive to solve some simple PDE’s analytically, using the method of separation of variables.
Example 1: An Elliptic Equation.

Solve, by the method of separation of variables, the PDE:

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad 0 \leq x \leq 1 \quad 0 \leq y \leq 1$$

subject to the boundary conditions

$$u(x, 0) = 0 \quad u(0, y) = 0 \quad u(1, y) = 0 \quad u(x, 1) = A \sin m\pi x,$$

Assume the solution is a product of a function of $x$ and a function of $y$:

$$u(x, y) = X(x) \cdot Y(y)$$

The equation becomes

$$Y \frac{d^2 X}{dx^2} + X \frac{d^2 Y}{dy^2} = 0 \quad \text{or} \quad \frac{1}{X} \frac{d^2 X}{dx^2} = -\frac{1}{Y} \frac{d^2 Y}{dy^2}$$

The left side is a function of $x$, the right a function of $y$.

Thus, $C_1 C_3 = A / \sinh m\pi$, and the solution is

$$u(x, y) = \left( \frac{A}{\sinh m\pi} \right) \sin m\pi x \sinh m\pi y$$

More general BCs

Suppose the solution on the “northern” side is now

$$u(x, 1) = f(x)$$

Find the solution.

We note that the equation is linear and homogeneous, so that, given two solutions, a linear combination of them is also a solution of the equation.

We assume that we can Fourier-analyse the function $f(x)$:

$$f(x) = \sum_{k=1}^{\infty} a_k \sin k\pi x \quad \text{with} \quad \sum_{k=1}^{\infty} k^2 |a_k| < \infty$$

Then the solution may be expressed as:

$$u(x, y) = \sum_{k=1}^{\infty} \left( \frac{a_k}{\sinh k\pi} \right) \sin k\pi x \sinh k\pi y$$

In the same way, we can find solutions for non-vanishing boundary values on the other three edges.

Thus, the more general problem on a rectangular domain:

$$\nabla^2 u(x, y) = 0, \quad u(x, y) = F(x, y) \quad \text{on the boundary}$$

may be solved.
Another Example: A Parabolic Equation.

\[
\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2} \quad 0 \leq x \leq 1 \quad t \geq 0
\]

Boundary conditions:
\[u(0, t) = 0 \quad u(1, t) = 0\]

Initial condition:
\[u(x, 0) = f(x) = \sum_{k=1}^{\infty} a_k \sin k\pi x\]

Find the solution:
\[u(x, t) = \sum_{k=1}^{\infty} a_k e^{-\sigma k^2 \pi^2 t} \sin k\pi x\]

Note that the higher the wavenumber, the faster it goes to zero, i.e., the solution is smoothed as time goes on.

Conclusion: Before trying to solve a problem numerically, we must make sure that it is well posed: it has a unique solution that depends continuously on the data that define the problem.

Food for Thought

Lorenz showed that the atmosphere has a finite limit of predictability:

Even if the models and the observations are perfect, the flapping of a butterfly in Brazil will result in a completely different forecast for Texas.

Does this mean that the problem of NWP is not well posed?

If not, why not?

Consider again the definition of an ill-posed problem.