Chapter 3: Numerical discretization of the equations of motion

3.1 Classification of Partial Differential Equations – Well-Posedness – Initial and boundary conditions

Reminder about partial differential equations:

Second order linear partial differential equation (PDE)

$$\alpha \frac{\partial^2 u}{\partial x^2} + 2\beta \frac{\partial^2 u}{\partial x \partial y} + \gamma \frac{\partial^2 u}{\partial y^2} + \delta \frac{\partial u}{\partial x} + \varepsilon \frac{\partial u}{\partial y} + \varphi u = 0$$

Second order linear partial differential equations are classified into 3 types depending on the sign of $\beta^2 - \alpha\gamma$:

$\beta^2 - \alpha\gamma > 0$ Hyperbolic

$\beta^2 - \alpha\gamma = 0$ Parabolic

$\beta^2 - \alpha\gamma < 0$ Elliptic

The simplest (canonical) examples of these equations are

a) $\dfrac{\partial^2 u}{\partial t^2} = c^2 \dfrac{\partial^2 u}{\partial x^2}$ Wave equation (hyperbolic).

Examples: vibrating string, water waves.

b) $\dfrac{\partial u}{\partial t} = \sigma \dfrac{\partial^2 u}{\partial x^2}$ Diffusion equation (parabolic).

Examples: heated rod, viscous damping.

c) $\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = 0$ Laplace's equation

(elliptic)

or $\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = f(x,y)$ Poisson's equation

Examples: temperature of a plate, streamfunction/vorticity relationship.

The behavior 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.

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

Another canonical equation very important in atmospheric science is:

d) $\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}$ advection equation (also hyperbolic)

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 a hyperbolic, since its solutions satisfy the wave equation

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

Conversely, a) can be written as a first order system

$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{A}\frac{\partial \mathbf{u}}{\partial x}$ where $\mathbf{u} = \begin{pmatrix} \frac{\partial u}{\partial t} \\ c\frac{\partial u}{\partial x} \end{pmatrix}$, and $\mathbf{A} = \begin{bmatrix} 0 & c \\ c & 0 \end{bmatrix}$

Example: solve the hyperbolic equation a) $u_{tt} - c^2 u_{xx} = 0$ by transformation of variables.

Define new variables:

$$\xi = x - ct$$
$$\eta = x + ct$$

These are the characteristics of a this hyperbolic equation along which signals are transmitted.

$$u_x = u_\xi \xi_x + u_\eta \eta_x = u_\xi + u_\eta$$
$$u_t = u_\xi \xi_t + u_\eta \eta_t = -u_\xi c + u_\eta c$$

so that

$$u_{xx} = \left[u_{\xi\xi} + 2u_{\xi\eta} + u_{\eta\eta} \right]$$
$$u_{tt} = c^2 \left[u_{\xi\xi} - 2u_{\xi\eta} + u_{\eta\eta} \right]$$

Therefore

$$u_{tt} - c^2 u_{xx} = -4c^2 u_{\xi\eta} = 0$$

which means $u_{\xi\eta} = \dfrac{\partial^2 u}{\partial\xi\partial\eta} = 0$

So, the solution of this equation may be expressed as a sum of a function of $\xi = x - ct$ and another function of $\eta = x + ct$:

$$u = f(x - ct) + g(x + ct)$$

In the atmosphere we have waves (gravity waves, sound waves, even Rossby waves, propagating along characteristics with their own characteristic speed c).

Parabolic and elliptic equations don’t have characteristics

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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 (IC) and boundary conditions (BC) for a PDE is essential in order to have a well-posed problem.

- If too many IC/BC are specified, there will be no solution.
- If too few IC/BC are specified, the solution will not be unique.
- If the number of IC/BC is right, but they are specified at the wrong place or time, the solution will be unique, but it will not depend smoothly on the IC/BC.
- This means that small errors in the IC/BC will produce huge errors in the solution.
- In any of these cases we have an *ill-posed problem*.

And we can *never* find a numerical solution of a problem that is ill posed: the computer will show its disgust by "blowing up".

We briefly discuss well posed initial / boundary conditions:

1) Elliptic equations, e.g.: $\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = f(x, y)$

2nd order elliptic equations require one boundary condition on each point of the spatial boundary.

These are “boundary value”, time-independent problems, and the methods used to solve them are introduced in Section 3.4.

The boundary conditions for elliptic equations may be:

- on the value of the function (Dirichlet problem), as when we specify the temperature $u = T$ at the borders of a plate, or
- on its normal derivative (Neumann problem), as when we specify the heat flux, e.g., no flux $\frac{\partial u}{\partial x} = 0$.
- We could also have a mixed “Robin” boundary condition, involving a linear combination of the function and its derivative, as when we specify the flux depending on the temperature $\frac{\partial u}{\partial x} = C(u - T)$:.

2) Linear parabolic equations ($\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2}$) require one initial condition at the initial time and one boundary condition at each point of the spatial boundaries (if they exist). The spatial BC are similar as for elliptic equations but they depend on time.

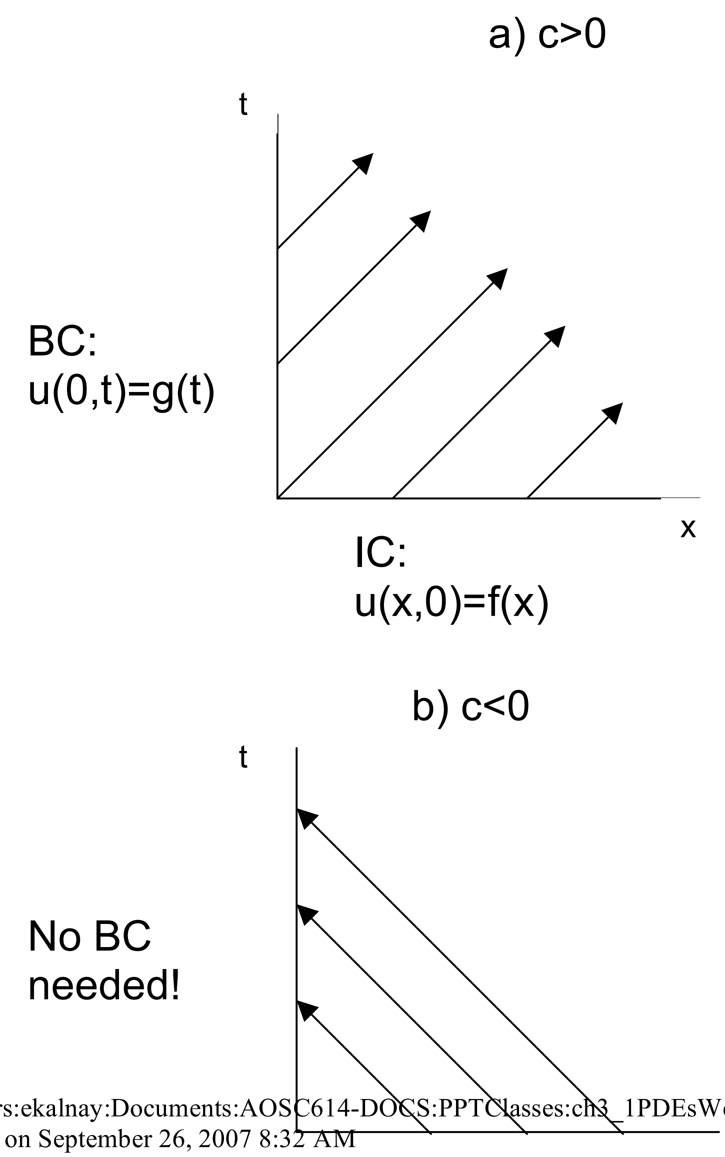
For example, for a heated rod, we need the initial temperature T(x,0) and the temperature at each end T(0,t), TL,t) as a function of time.

3) Linear hyperbolic equations ($\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$) 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* (into the spatial domain).

Example: to solve $\dfrac{\partial u}{\partial t} = -c\dfrac{\partial u}{\partial x}$ for x>0, t>0.

Fig. 3.1: Schematic of the characteristics of the advection equation $\partial u / \partial t = -c \partial u / \partial x$ for positive and negative velocity c and the corresponding well posed IC/BC.



Characteristics: solutions of dx/dt=c. Space boundary: x=0. (see schematic Fig. 3.1a,b). If c>0, we need IC: u(x,0)=f(x); BC: u(0,t)=g(t) . If c<0, we need IC: u(x,0)=f(x) but *no BC*!

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

For example, in the nonlinear advection equation $\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x}$, the characteristics are dx/dt=u, and since we don't know a priori the sign of u at the boundary, and whether the characteristics will point inwards or outwards, we have to estimate the value of u from the nearby solution, and define the BC accordingly.

One method to solve simple PDE's is the method of separation of variables, but unfortunately in most cases it is not possible to use it (hence the need for numerical models!). Nevertheless, it is useful to try to solve some simple PDE's analytically.

Example 1: Solve by the method of separation of variables these prototype PDEs:

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

subject to the BCs (data on the northern boundary)

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

Separate variables: 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

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

Since a function of x can be equal to a function of y, if and only if they are both equal to the same constant $-K^2$:

$$\frac{d^2X}{dx^2} + K^2X = 0 \qquad \frac{d^2Y}{dy^2} - K^2Y = 0$$

with solutions

$$X = C_1 \sin Kx + C_2 \cos Kx \qquad Y = C_3 \sinh Ky + C_4 \cosh Ky$$

The BC $u(0,y) = 0$ forces $C_2=0$ so that $X = C_1 \sin Kx$;

the BC $u(1,y) = 0$ forces $\sin K = 0$ or $K = n\pi$; so that $X = C_1 \sin n\pi x$

The BC $u(x,0) = 0$ forces $C_4=0$ so that $Y = C_3 \sinh Kx$

The BC $u(x,1) = A \sin m\pi x$ forces n=m and $C_1C_3 \sinh m\pi = A$

Thus the solution is

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

More general BCs for the elliptic equation:

Suppose that the northern boundary is now

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

Find the solution. Assume we can Fourier analyze the function

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

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

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

$\nabla^2 u(x,y) = 0 \quad u(x,y) = F(x,y)$ on the boundary, may be solved.

Another example: a Parabolic Equation:

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2}, \qquad 0 \le x \le 1,\ t \ge 0,$$

Boundary Conditions: u(0,t)=u(1,t)=0;

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

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.

Another example: A Hyperbolic Equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \qquad 0 \le x \le 1,\ 0 \le t \le 1$$

Boundary Conditions at the two borders: u(0,t)=u(1,t)=0

Two Initial Conditions: $u(x,0) = f(x) = \sum_{k=1}^{\infty} a_k \sin k\pi x$;

$$\frac{\partial u}{\partial t}(x,0) = g(x) = \sum_{k=1}^{\infty} b_k \sin k\pi x$$

Find the solution by the method of separation of variables

Another example of a hyperbolic equation: Same as above, but now, instead of 2 initial conditions, we give an initial and a "final" condition:

BC: $u(0,t)=u(1,t)=0$

IC: $u(x,0)=f(x)$; "final condition" $u(x,1)=g(x)$.

In other words, we try to solve a hyperbolic (wave) equation as if it were a boundary value problem.

Show that the solution is unique but it does not depend smoothly on the IC/BCs, and therefore it is not a well-posed problem.

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

Question: Lorenz showed that the atmosphere has a finite limit of predictability: even if the models and the observations were perfect, "the flapping of a butterfly in Brazil (not taken into account in the model) will result in a completely different forecast over Texas after a couple of weeks".

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

Probably not, or we would not have jobs,,, Why not?