Chapter 1. Partial Differential Equations

Reading: P1-P20 of Durran, Chapter 1 of Lapidus and Pinder (Numerical solution of Partial Differential Equations in Science and Engineering)

Before even looking at numerical methods, it is important to understand the **types of equations** we will be dealing with.

1. Differences between PDE's and ODE's

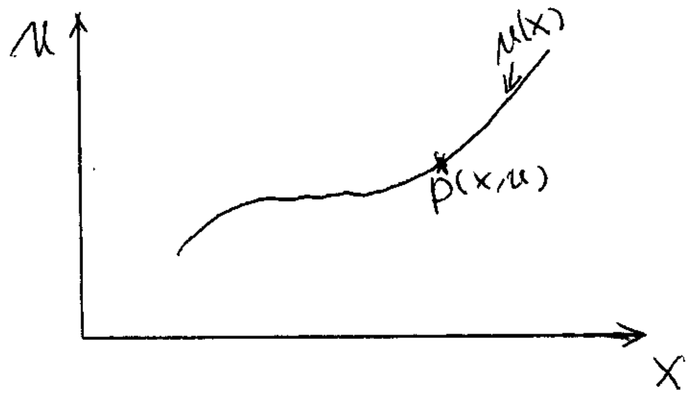
1) PDE's contain >1 <u>independent</u> variable, e.g.,

$$F(x, y, u, \partial u/\partial x, \partial^2 u/\partial x\partial y, ...) = 0$$

whereas ODE's contain 1 independent variable:

$$\frac{du}{dx} = F(x, u).$$

2) In an ODE, a specification of (x,u), for the above example, yields a unique value of du/dx, because there is only one direction (x) that one can move.



For a similar PDE, F(x, u, u_x, u_y, y)= 0, specifying (x,y,u) only relates u_x to u_y, but does not uniquely determine either

⇨ for a PDE, the solution <u>surfaces</u> pass through a <u>curve</u> in a 3-D space, rather than a curve through a point in the ODE.

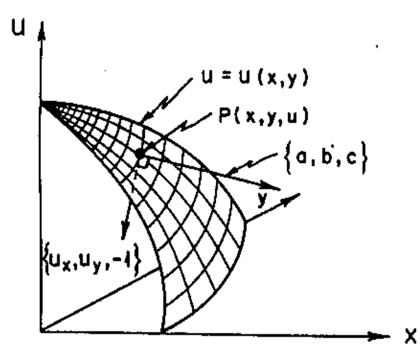


Figure 1.1. Solution surface $u = u(x,y)$ with vector $\{a, b, c\}$ tangent to u and vector $\{u_x, u_y, -1\}$ normal to u at point $P(x, y, u)$.

3) ODE's have nice convergence proofs when solved using iterative methods

4) Therefore, ODE's can be solved quickly because convergence is guaranteed. You will see a lot of black box ODE solvers in standard libs such as LINPAK, IMSL, but not so many PDE's.

2. Properties of PDE's

1) Order – the order of the highest partial derivative present,

e.g., $\frac{\partial u}{\partial t} = a \frac{\partial^3 u}{\partial^2 x \partial y}$ is 3rd order

We'll focus primarily on 1st and 2nd order equations

Note that high-order equations may often be written in terms of a low-order systems, e.g.,

$$w_{xx} + w_{yy} = w_{xz} \qquad (w_x \equiv \frac{\partial w}{\partial x})$$

can be written as

$$u_x + v_y = u_z,$$
$$u = w_x,$$
$$v = w_y.$$

Another example – the shallow water equations

$$\frac{\partial u}{\partial t} = -g \frac{\partial h}{\partial x}$$
$$\frac{\partial h}{\partial t} = -H \frac{\partial u}{\partial x} \qquad \Rightarrow \qquad \frac{\partial^2 u}{\partial t^2} = -c^2 \frac{\partial^2 u}{\partial x^2} \text{ where } c = \sqrt{gH} .$$

The order has important implications for the number of boundary conditions required and the classification of the equation in the canonical form.

2) Linearity – In simplest terms, nonlinearity implies a feedback.

Linear example: If you are a linear eater, the amount you eat does not affect your appetite.

Nonlinear example: If you are nonlinear eater, the more you eat, the more you can eat and the heavier you become (your properties change), and the more you do eat.

The linearity property is crucial for solving PDE's – it determines the techniques we use, etc. Properties of nonlinear equations are often discussed after they are linearized.

Definition: An operator L( ) is linear if

$$L(a\,u + b\,v) = a\,L(u) + b\,L(v)$$

where α and β are constant. This is a universal test!

Note that, since analytical solutions are often available to linear equations, we ten to linearize complex systems to gain a better understanding of them, at least in the vicinity where the linearization occurs.

Example: $L(u) = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}$ is linear.

Verify that $L(u) = u\dfrac{\partial^2 u}{\partial x^2}$ is not linear.

Example: $\dfrac{\partial u}{\partial t} + c\dfrac{\partial u}{\partial x} = 0$ (c>0 & constant)

is a linear equation and solution can be superimposed.

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

is nonlinear and the sum of 2 solutions does not yield a correct third one.

To be mathematically rigorous, we can use the following:

Consider,

$$a(x)\frac{\partial u}{\partial x} + b(x)\frac{\partial u}{\partial y} = c(x)\,.$$

If a, b, c = cost. or $\xi=\xi(x,y)$, it is Linear.
If $\xi=\xi(u)$, then eq. is Quasi-Linear
If $\xi=\xi(u, \partial u/\partial x, \partial u/\partial y, u^n (n>1))$, it is Nonlinear.

3. Classification of PDE's

(Reading Assignment: Sections 1.1.1, 1.2.1, 1.2.2 in Lapridus and Pinder).

There are three standard types for PED's:

Hyperbolic
Parabolic
Elliptic

Consider a linear second-order PDE with 2 independent variables
(can be generalized to >2 cases):

$$A\frac{\partial^2 u}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}+ D\frac{\partial u}{\partial x}+ E\frac{\partial u}{\partial y}+Fu+G=0, \qquad (1)$$

where A, B, …, G are constants or functions of (x,y). It turned out that this equation is

$$\begin{array}{ll} \text{Hyperbolic} & \text{if } B^2 - 4AC > 0, \\ \text{Parabolic} & \text{if } B^2 - 4AC = 0, \\ \text{Elliptic} & \text{if } B^2 - 4AC < 0. \end{array} \qquad (2)$$

We will discuss more later to see why.

Note the definition depends on only the highest-order derivatives in each independent variable.

Example:	$u_{tt} - c^2 u_{xx} = 0$	(wave eq.)	H
	$u_t = c\, u_{xx}$	(Diffusion eq.)	P
	$u_{xx} + u_{yy} = 0$	(Laplace eq.)	E

In order to understand this classification, we need to look into a certain aspect of PDE's known as the characteristics.

4. Canonical or standard forms of PDE's

1) Three Canonical or Standard Forms of PDE's

Every linear 2nd-order PDE in 2 independent variables, i.e., Eq.(1)) can be converted into one of three canonical or standard forms, which we call hyperbolic, parabolic or elliptic.

Written in new variables ξ and η, the three forms are:

$u_{\xi\xi} - u_{\eta\eta} + \ldots. = 0$

or $u_{\xi\eta} + \ldots = 0$ H (3a)

$u_{\xi\xi} + \ldots = 0$ P (3b)

$u_{\xi\xi} + u_{\eta\eta} + \ldots. = 0$ E (3c)

In this canonical form, at least one of the second order terms is not present.

We will see that hyperbolic PDE has two real characteristic curves, the P PDE has one real characteristic curve, and the elliptic PDE has no real characteristic curve.

Examples	$u_{tt} - c^2 u_{xx} = 0$	(wave eq.)	H
	$u_t = c\, u_{xx}$	(Diffusion eq.)	P
	$u_{xx} + u_{yy} = 0$	(Laplace eq.)	E

are already in the canonical forms. The classification of some may depend on the value of the coefficients – need to use criteria in (2) to determine. E.g.,

$y\, u_{xx} + u_{yy} = 0$ Elliptic for $y > 0$ and hyperbolic for $y < 0$.

2) Canonical Transformation

Consider again the general linear second-order PDE with 2 independent variables:

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu + g = 0, \tag{4}$$

Introduce transform

$$\xi = \xi\,(x,y), \qquad \eta = \eta(x,y) \tag{5}$$

Using the chain rule =>

[since $u(x,y) = u(\xi(x,y),\ \eta(x,y))$]

$$\begin{aligned}
u_x &= u_\xi\, \xi_x + u_\eta\, \eta_x \\
u_y &= u_\xi\, \xi_y + u_\eta\, \eta_y \\
u_{xx} &= u_{\xi\xi}\, \xi_x^2 + 2u_{\xi\eta}\xi_x\eta_x + u_{\eta\eta}\, \eta_x^2 + \ldots \\
u_{xy} &= u_{\xi\xi}\, \xi_x\xi_y + u_{\xi\eta}(\xi_x\eta_y + \xi_y\eta_x) + u_{\eta\eta}\, \eta_x\eta_y + \ldots \\
u_{yy} &= u_{\xi\xi}\, \xi_y^2 + 2u_{\xi\eta}\xi_y\eta_y + u_{\eta\eta}\, \eta_y^2 + \ldots
\end{aligned} \tag{6}$$

The terms not including any 2nd-order derivative are omitted.

Substituting the derivatives in (6) for those in (4) yields

$$a\, u_{xx} + b\, u_{xy} + c\, u_{yy} = A\, u_{\xi\xi} + B\, u_{\xi\eta} + C\, u_{\eta\eta} + \ldots, \tag{7}$$

where

$$\begin{aligned} A &= a\, \xi_x^2 + b\, \xi_x \xi_y + c\, \xi_y^2 \\ B &= 2a\xi_x\eta_x + b(\xi_x\eta_y + \xi_y\eta_x) + 2c\xi_y\eta_y \\ C &= a\, \eta_x^2 + b\, \eta_x\eta_y + c\, \eta_y^2 \end{aligned} \tag{8}$$

From (8), we can obtain

$$B^2 - 4AC = (b^2 - 4ac)\, (\xi_x\eta_y - \xi_y\eta_x)^2. \tag{9}$$

Note, $B^2 - 4AC$ and $b^2 - 4ac$ always have the <u>same sign</u>!

> This is why the only the coefficients of the second order derivative terms matter.
> $\therefore$ Nonsingular coordinate transformation does not change the type of PDE.

$(\xi_x\eta_y - \xi_y\eta_x)$ is the <u>Jacobian</u> of transformation therefore it <u>can not be zero</u>. Otherwise there will be no one-to-one mapping between the two coordinate systems, in another word, the transformation becomes <u>singular</u>.

$$[\frac{\partial(x,h)}{\partial(x,y)} = \begin{vmatrix} x_x & h_x \\ x_y & h_y \end{vmatrix} = x_x h_y - h_x x_y\ ].$$

Consider the case of $b^2 - 4ac > 0$, i.e., the hyperbolic case, let's show that Eq.(4) can be reduced to a canonical form as in (3a). Let consider the case of $u_{\xi\eta} + \ldots = 0$.

To achieve this form, we require that A and B given in (8) vanish, i.e.,

$$a\, \xi_x^2 + b\, \xi_x\xi_y + c\, \xi_y^2 = 0 \tag{10a}$$
$$a\, \eta_x^2 + b\, \eta_x\eta_y + c\, \eta_y^2 = 0 \tag{10b}$$

Let

$$\lambda_1 = \xi_x/\xi_y \text{ and } \lambda_2 = \eta_x/\eta_y, \tag{11}$$

We find Eqs.(10a,b) can be satisfied when

$$a\, \lambda_1^2 + b\, \lambda_1 + c = 0 \tag{12a}$$
$$a\, \lambda_2^2 + b\, \lambda_2 + c = 0 \tag{12b}$$

Obviously, the solutions of λ_1 and λ_2 are

$$l_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad (13)$$

Therefore, we see that if $b^2 - 4ac > 0$, we can find 2 real solutions of λ so that (10) is satisfied and the general 2nd-order PDE (4) can be transformed into the standard form like $u_{\xi\eta} + \ldots = 0$ which is hyperbolic.

3) Characteristic Equations and Characteristic Curves

Notice that equations in (11) are two 1st-order PDE's. They can be re-written as

$$\xi_x - \lambda_1 \xi_y = 0 \qquad (14a)$$
$$\eta_x - \lambda_2 \eta_y = 0 \qquad (14b)$$

We will see that from them we can obtain two sets of characteristic curves.
The number of real characteristics a PDE can have actually determines its type.

Concept of Characteristics

Classification of PDE's is actually based on the mathematical concept of characteristics.

Characteristics are lines (in 2D, in terms of the number of independent variables) or surfaces (in 3D) along which certain properties remain constant or certain derivatives may be discontinuous.

Such lines or surfaces are related to the directions in which "info" can be transmitted in physical problems governed by PDE's.

Because of this property, many methods developed before the digital computers for solving PDE's are based on the characteristics and compatibility equations. The latter describes the conservation property of the 'info' along the characteristics.

- Equations (single or system) that admit wave-like solutions are known as hyperbolic.
- Those admitting solutions for damped waves are called parabolic.
- If the solutions are not wave-like, they are called elliptic.

It is important to know which type we are dealing with in order to choose the numerical method, the boundary conditions, etc. Further, different physical interpretations are attached to different types, as we can see from the above discussion.

Characteristic Equations of 1st-order PDE's

Let's go back and look at 1st-order PDE's in the following general form:

$$A\, u_x + B\, u_y = C \qquad (15)$$

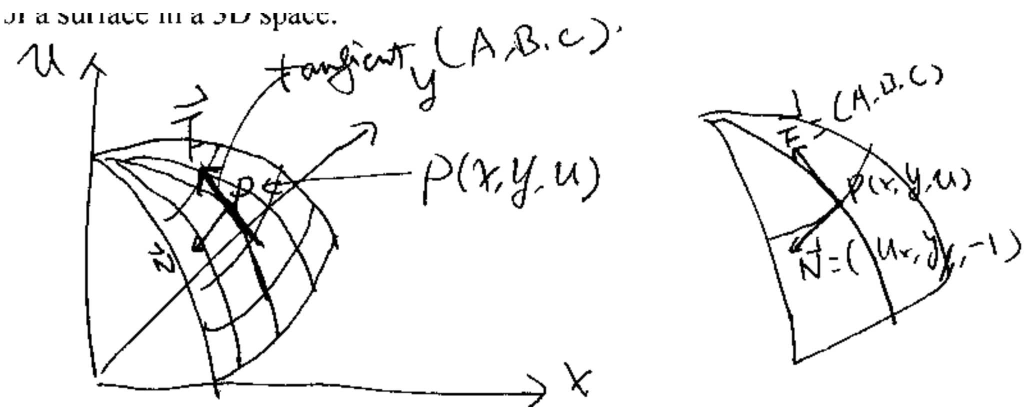
Solution u represents a curved surface in a 3D space.

It can be shown that vector

$$\vec{F} = (A, B, C)$$

is tangent to the surface.

Diagram of a surface in a 3D space:



Because the downward normal of the surface at a given point (x,y) is $\vec{N} = (u_x, u_y, -1)$ (consult advanced calculus text book) and $\vec{F} \cdot \vec{N} = Au_x + Bu_y - C = 0$.
Therefore, the PDE can be geometrically interpreted as the requirement that any solution surface through point P must be tangent to the coefficient vector (A, B, C).

We also know, from u=u(x,y),

$$du = u_x dx + u_y dy \tag{16}$$

In both (15) and (16), u_x and u_y can take on more than one values but still satisfy these equations, i.e., u_x and u_y are non-unique (c.f., the diagram for three surface). This important and we will use this property to obtain the char. and comp. equations. Using the terminology of linear algebra, we actually have two <u>linearly dependent</u> equations.

Write these two equations in a matrix form:

$$\begin{pmatrix} A & B \\ dx & dy \end{pmatrix} \begin{pmatrix} u_x \\ u_y \end{pmatrix} = \begin{pmatrix} C \\ du \end{pmatrix} \tag{17}$$

For $\begin{pmatrix} u_x \\ u_y \end{pmatrix}$ to have more than one possible solution, the determinant of the coefficient matrix needs to be zero, i.e.,

$$\begin{vmatrix} A & B \\ dx & dy \end{vmatrix} = 0. \Rightarrow \qquad \frac{dx}{A} = \frac{dy}{B} \tag{18}$$

Recall from linear algebra that, if a square coefficient matrix for a set of n linear equations has a vanishing determinant, then a necessary condition for finite solutions to exist is that when the RHS is substituted for any column of the coefficient matrix, the resulting determinant must also vanish (c.f., the Cramer's rule for solving linear systems of equations). Therefore we have

$$\begin{vmatrix} C & B \\ du & dy \end{vmatrix} = 0 \Rightarrow \qquad \frac{du}{C} = \frac{dy}{B} \tag{20}$$

$$\begin{vmatrix} A & C \\ dx & du \end{vmatrix} = 0 \Rightarrow \qquad \frac{du}{C} = \frac{dx}{A} \tag{21}$$

or

$$\frac{dx}{A} = \frac{dy}{B} = \frac{du}{C} \tag{22}$$

They actually represent two independent ODE's. They fully determine our system apart from B.C. and I.C. conditions, and they can be solved much more easily than the original PDE.

The equation

$$\frac{dy}{dx} = \frac{B}{A} \tag{23}$$

is called the characteristic equation, and if A and B = const., we have a family of parallel lines. Given the initial and boundary conditions, we can obtain the solution to our equation.

For example, when A=1, B=β, C=0 (remember at least one of them has to be zero in one of the canonical forms), and let x->t, y->x, we have

$$\frac{\partial u}{\partial t} + b\frac{\partial u}{\partial x} = 0, \qquad \beta > 0 \text{ and const.} \tag{24}$$

The characteristic equation is

$$\frac{dx}{dt} = b \quad \Rightarrow \quad x = \beta t + \text{const.} \quad \text{(const. to be determined from I.C.)} \qquad (25)$$

The solution represents a family of parallel lines.

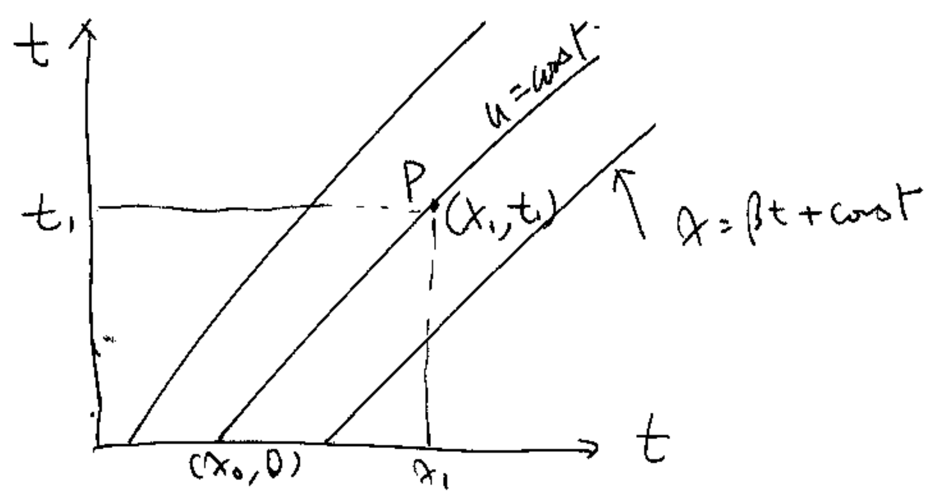
From (20) or (21), we have

du = 0 - which is called the Compatibility Equation. (26)

It says that u is conserved along the characteristic lines (c.f., earlier discussion of the properties of characteristics).

Note that for general cases, the compatibility equation can only be obtained with the aid of the characteristic equation. It is therefore said to be only valid alone the characteristics.

Diagram:



If we know the I.C. and B.C., we can use the Method of Characteristics (MOC) to find the exact solution at any point (x,t) in the solution space.

$$u(x_1, t_1) = u(x_0, 0) = f(x_0) = \text{I.C.} \qquad (26)$$

Since $x_1 - \beta\, t_1 = x_0 + \beta\, 0 \rightarrow x_0 = x_1 - \beta\, t_1$, the general solution is

$$u(x_1, t_1) = u(x_0, 0) = f(x_1 - \beta\, t_1) \qquad (27)$$

where the functional form of f is specified by the I.C. There general solution is therefore

$$u(x, t) = u(x_0, 0) = f(x - \beta\, t) \qquad (28)$$

– it says that the solution of u at x and time t is equal to the value of initial function at location x-βt.

In the above example, du = 0, u=const along the characteristic lines, it's a case of pure advection. In general cases, the characteristic lines are not straight lines and du$\neq$0 so it may have to be integrated numerically along the characteristic lines. But, still the integration of this equation is usually much easier than the original PDE (the procedure to obtain the char. and comp. equations can be non-trivial however).

Having discussed the characteristic equations for 1st-order PDE, let's go back to section 2). Write down Eq.(14a) again here:

$$\xi_x - \lambda_1 \xi_y = 0 \tag{29}$$

Compared to Eq.(15), A =1, B= -λ_1, C=0, therefore according to (22), we have

$$\frac{dx}{1} = \frac{dy}{-l_1} = \frac{dx}{0}. \tag{30}$$

From $\eta_x - \lambda_2 \eta_y = 0$, we get

$$\frac{dx}{1} = \frac{dy}{-l_2} = \frac{dh}{0}. \tag{31}$$

From the, we obtain the characteristics and compatibility equations:

$$\frac{dy}{dx} = -l_1 \quad \text{and} \quad dx = 0 \tag{32}$$

$$\frac{dy}{dx} = -l_2 \quad \text{and} \quad dh = 0 \tag{33}$$

Therefore we see that when $b^2 - 4ac > 0$, 2 real roots can be found so that Eqs.(10) are satisfied, the original 2nd-order PDE can be converted to its canonical form, at the same time, two sets of characteristic curves exist.

When λ_1 and λ_2 are constant, these characteristics are straight lines which correspond to constant coordinate lines (ξ=const, η=const) in the new coordinate

$$\begin{aligned} &\xi = \text{const along } y = \lambda_1 x + C_1 \\ &\eta = \text{const along } y = \lambda_2 x + C_2 \end{aligned} \tag{34}$$

One can see the coordinate transformation from (x,y) to (ξ, η) not only simplifies the original 2nd-order PDE, but also simplify the characteristics. In a sense, the compatibility equations are the corresponding characteristic equations in the new coordinate.

In order to obtain the alternative canonical form of a hyperbolic equation,

$$u_{\bar{x}\bar{x}} - u_{\bar{h}\bar{h}} + ... = 0 \qquad (35)$$

we can use a linear combination of ξ and η:

$$\bar{x} = (x + h)/2 \text{ and } \bar{h} = (x - h)/2. \qquad (36)$$

In another word, we can perform the above transform from $(x,\ h)$ coordinate system to $(\bar{x}, \bar{h})$ and convert equation $u_{\xi\eta}$ + … = 0 into Eq.(35). Of course, we can also perform a transform directly from the original equation in (x, y) coordinate.

Similar analysis can be performed for the parabolic and elliptic cases, where, respectively, one and zero characteristic curve exists.

Recommended Reading: Sections 1.1 and 1.2 of Papidus and Pinder, *Numerical Solutions of Partial Differential Equations in Science and Engineering.*
Section 1.1.2 of Durran.

4) Domain of Dependence for second-order PDE's

Reading: Page 45, Durran.

Consider 2nd-order wave equation

$$u_{tt} - c^2 u_{yy} = 0, \qquad (37)$$

on the interval $-\infty < x < \infty$ with initial condition

$$u(x, 0) = f(x) \text{ and } u_t(x,0) = g(x) \qquad (38)$$

With coordination transform discussed earlier, (37) can be converted to

$$u_{xh} = 0 \qquad (39)$$

where ξ = x + ct and η= x – ct.

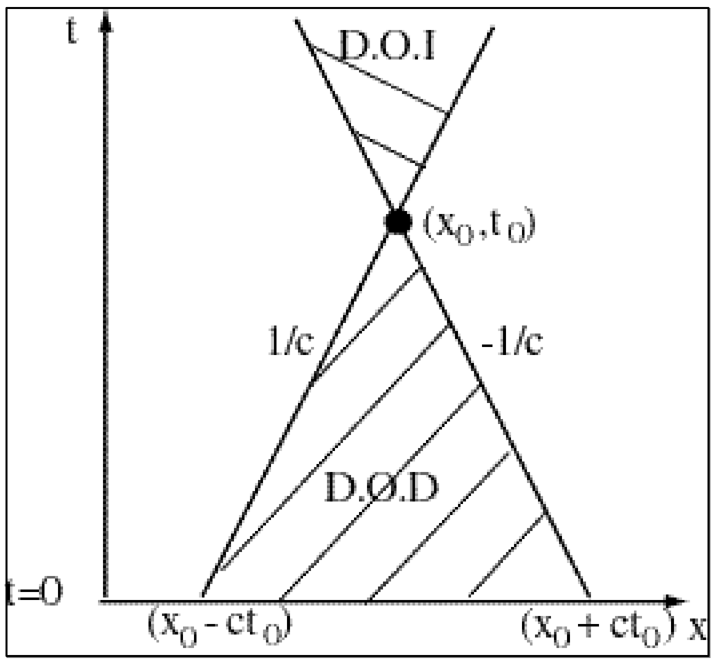
(39) can be easily integrated twice, with respect to each of the new independent variables, to obtain solution

$$u(x,t) = F_1(x+ct) + F_2(x-ct).$$

This is called the D'Alembert (see handout). The functional form of F_1 and F_2 are determined from the I.C. The resulting solution is

$$u(x,t) = \frac{f(x+ct) + f(x-ct)}{2} + \frac{1}{2c}\int_{x-ct}^{x+ct} g(x')dx' \qquad (40)$$

Diagram of Domain of Dependence.



From (40), we can see that solution u at a point (x_0, t_0) depends only on the initial data contained in the interval

$$x_0 - ct_0 \leq x \leq x_0 + ct_0,$$

i.e., the solution is only <u>dependent on</u> the condition in <u>a domain bounded by the two characteristic lines</u> through point (x_0, t_0).

The 1st part of solution (40) represents propagation of signals along the characteristic lines and the 2nd part the effect of data within the closed interval at t=0.

We call this domain the Domain of Dependence (DOD).

General properties of hyperbolic PDE's:

- They have limited domain of dependence (DOD)
- Disturbances outside the DOD cannot influence the solution at a particular point
- Shows why hyperbolic equations usually describe <u>initial value</u> problems.

- I.C. cannot be specified on a characteristic line – otherwise the problem is ill-posed, i.e., a unique solution can not be found.

The characteristic lines encompass a region outside which signal at (x_0, t_0) cannot influence at a later time. Furthermore, the signal can only propagate a finite distance in a finite time. The domain defined by

$$x_0 + ct_0 \le x \le x_0 - ct_0 \quad for\ t > t_0,$$

outside which point (x_0, t_0) cannot affect is called the Domain of Influence of this particular point.

The time-matching nature of hyperbolic equations is clear.

Now consider 2nd-order diffusion (heat transfer) equation, a parabolic equation

$$T_t = K\, T_{xx} \tag{41}$$

where K is the diffusion coefficient or thermal conductivity. Note that there is only on 2nd-order derivative term in the equation – it's already in the canonical form of parabolic equations.

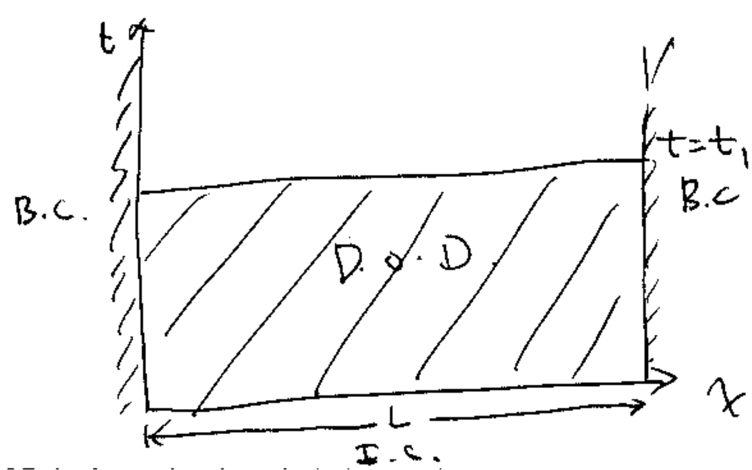
It's analytical solution is

$$T(x,t) = T(x,0) \exp(-K k^2 t) \tag{42}$$

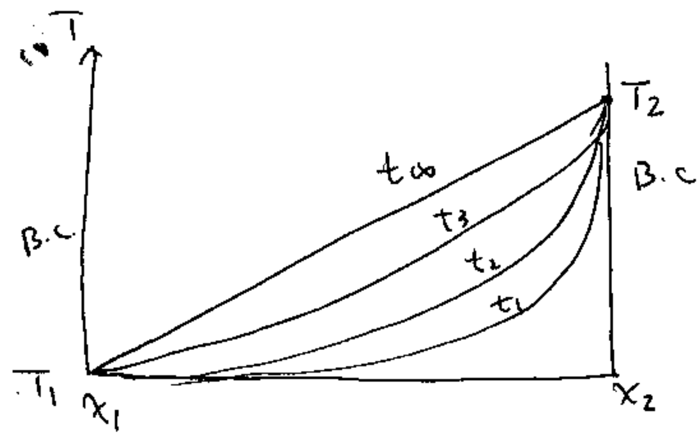
where k is wavenumber. t-> ∞ , T-> 0 for non-zero wavenumbers.

The characteristic equation for this equation is

$$\frac{dt}{dx} = 0 \tag{43}$$



=> the DOD is the entire domain below a given time t,
all points are diffused simultaneously, at a rate dependent on local gradient of T (c.f., next figure).



Comments:

- Solution depends on entire time history, is still a time matching problem but irreversible
- No MOC for diffusion equations
- Parabolic equations represent a smoothing process

Elliptic Problem

Elliptic equations have no real characteristics along which signal might propagate.
They are always boundary value problems
They involves no time matching

E.g., $u_{xx} + u_{yy} = 0$ (Laplace's Eq.)

$u_{xx}+ u_{yy} = f(x,y)$ (Possion's Eq.)

They are 'diagnostic' equations, one disturbance introduced into any part of the domain is 'felt' at all other points instantaneous.

No a suitable problem for distributed memory computers, because of the DOD is the entire domain.

Example: In a compressible fluid, pressure waves propagate at the speed of sound.

The liearized equations are

$$\frac{\partial u'}{\partial t} + U\frac{\partial u'}{\partial x} + \frac{1}{\bar{r}}\frac{\partial p'}{\partial x} = 0 \qquad (44a)$$

$$\frac{\partial p'}{\partial t} + U\frac{\partial p'}{\partial x} + \bar{r}c^2\frac{\partial u'}{\partial x} = 0 \qquad (44b)$$

Signals propagates at speed c – a finite propagation speed.

Now, if we make the fluid incompressible,

i.e., dρ/dt = 0 => $\frac{\partial u}{\partial x} = 0$,

this is equivalent to setting c = ∞ in (44b). Therefore, in incompressible fluid, disturbance is 'felt' instantaneously in the entire domain.

Let's see what equations we have to solve now..

For an impressible system:

$$\frac{\partial \vec{V}}{\partial t} + \vec{V}\cdot\nabla\vec{V} = -\frac{1}{r}\nabla p \qquad (45a)$$

$$\nabla\cdot\vec{V} = 0 \qquad (45b)$$

Take ∇· of (45a), and make use of (45b), we get

$$\nabla^2 p = -r\nabla\cdot(\vec{V}\cdot\nabla\vec{V}) \qquad (46)$$

which is an elliptic equation.

Now we see the connection between the type of equations and physical property of the fluid they describe.

5. Systems of First-order Equations

Reading: Sections 1.1.1, 1.2.2 of Durran.

In fluid dynamics, we more often deal with a system of coupled PDE's.

a) Definition and methods based on the eigenvalue of coefficient matrix

Often, high-order PDE's can be rewritten into equivalent lower-order PDE's, and vice versa.

E.g., $$\frac{\partial v}{\partial t} - c\frac{\partial w}{\partial x} = 0 \qquad (5.1a)$$
$$\frac{\partial w}{\partial t} - c\frac{\partial v}{\partial x} = 0 \qquad (5.1b)$$

$\frac{\partial}{\partial t}(5.1a) + c\frac{\partial}{\partial x}(5.1b)$ =>

$$\frac{\partial^2 u}{\partial t^2} - c^2\frac{\partial u^2}{\partial x^2} = 0 \qquad (5.2)$$

which is a 2nd-order wave equation (e.g., wave propagation along a string).

We can determine the PDE's type using the $b^2 - 4ac$ criterion and find the characteristic and compatibility equations using the method discussed earlier.

For systems of equations, we give an alternative but equivalent definition and method for obtain those equations.

We write the system in a vector form:

$$\frac{\partial \vec{u}}{\partial t} + \mathbf{A}\frac{\partial \vec{u}}{\partial x} = 0 \qquad (5.3)$$

where

$$\vec{u} = \begin{pmatrix} v \\ w \end{pmatrix} \text{ and } A = \begin{pmatrix} 0 & -c \\ -c & 0 \end{pmatrix}.$$

<u>Definition:</u>

- If the eigenvalues of **A** are real and distinct (n of them for n-order matrix), the equation is hyperbolic.
- If number of real eigenvalues is >0 but < n, it's parabolic.
- If they are all complex, it's elliptic.

Note symmetric matrix has real eigenvalues. As in the above case.

Why: If all eigenvalues are real, bounded matrix **T** and $\mathbf{T}^{-1}$ exist so that

$$\mathbf{T}^{-1}\,\mathbf{A}\,\mathbf{T} = \mathbf{D},$$

where **D** is a diagonal matrix with real eigenvalues d_{ii}. Matrix **T** actually consists of, in each column, the eigenvectors corresponding to the discrete eigenvalues.

Let $\vec{u} = \mathbf{T}\,\vec{v}$, then

$$\frac{\partial \vec{v}}{\partial t} + \mathbf{D}\frac{\partial \vec{v}}{\partial x} = 0, \quad i.e., \quad \frac{\partial v_i}{\partial t} + d_{ii}\frac{\partial v_i}{\partial x} = 0 \quad \text{for} \;\; i = 1, n$$

which is n decoupled individual characteristic equations.

Read Durran (p??-??).

Eigenvalues of the previous problem can be found from

$$|\,\mathbf{A} - \lambda\,\mathbf{I}\,| = 0 \;\;=>\;\; \begin{vmatrix} -l & -c \\ -c & -l \end{vmatrix} = 0 \;\;=>\;\; \lambda_1 = \text{c}, \lambda_2 = \text{-c}.$$

c and –c are the actual wave propagation speed of the wave equations

$$\frac{dx}{dt} = +c \text{ and } \frac{dx}{dt} = -c$$

which are actually the characteristic equations.

a) <u>Method using the auxiliary equations</u>

A more general method for obtaining characteristic and compatibility equations for problem in (5.1) is to make use of two <u>auxiliary equations</u>:

$$dv = v_t\,dt + v_x dx$$
$$dw = w_t dt + w_x dx$$

and write them in a matrix form:

$$\begin{pmatrix} 1 & 0 & 0 & -c \\ 0 & -c & 1 & 0 \\ dt & dx & 0 & 0 \\ 0 & 0 & dt & dx \end{pmatrix} \begin{pmatrix} v_t \\ v_x \\ w_t \\ w_x \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ dv \\ dw \end{pmatrix}$$

Setting | | = 0 => dx/dt = ± c as before!

<u>Find the compatibility equation</u> on your own (hit: replace on of the column of the coefficient matrix by the RHS, and set the determinant to zero).

Note: This method is more general and is most often used to find the characteristic and compatibility equations, for both single equations and equation systems. Make sure that know how to apply this method.

6. Initial and Boundary Conditions

We will devote an entire section later on to boundary conditions – for now, we will look at general conditions.

I.C. and B.C. are

- needed to obtain unique solutions
- physically and/or computationally motivated

Initial Condition - Specification of the dependent variable(s) and/or its (their) time derivative(s) at same initial time (for adjoint equations that are integrated backward, I.C. condition is specified at time T). Quite straightforward.

Boundary Condition – Specification of dependent variable(s) at a domain boundary. Given in a general form for 2nd-order PDE's

$$a\,u(\vec{x},t) + b\,\frac{\partial u(\vec{x},t)}{\partial n} = g$$

where $\frac{\partial u}{\partial n}$ is the gradient of u in the direction normal to the boundary. α and β are constant coefficients.

- Dirichlet or 1st B.C. β=0 => value of variable specified

- Neumann or 2nd B.C. α = 0, gradient of value specified

- Robin or 3rd B.C., neither is zero. - A linear combination of the above two.

Note for Possion's equation $\nabla^2 j = z$, if gradient boundary condition is specified at all boundaries, the solution is unique only up to an arbitrary constant – additional condition has to be used to determine this constant for a physical problem.

7. Concept of Well-posedness

The governing equations and the associated auxiliary conditions (I.C. and B.C.) are said to be well-posed mathematically if:

- the solution exists
- the solution is unique
- the solution depends continually upon the auxiliary conditions (the future state predictable – an important issue for the atmosphere).

Existence – usually there isn't a problem for CFD – it can be, however, in cases where singularities exist somewhere in the domain.

Uniqueness – this can really be a problem in fluid flow problems – We can show uniqueness for simple problems only.

Consider an example – how do we show solution is unique?

Look at the diffusion equation:

$$u_t = K\, u_{xx} \qquad (K>0,\quad 0 \le x \le L)$$

I.C. $u(x,0) = f(x)$

B.C. $u(x=0, t) = u(x=L, t) = 0$

This is a Well-posed Linear problem.

To show that a solution is unique, let's make a counter-hypothesis that 2 solutions exist:

u_1 and u_2, i.e., the solution is non-unique.

If $u_3 \equiv u_1 - u_2$, then u_3 satisfies

$$(u_3)_t = K\,(u_3)_{xx}$$

$u_3(x,0) = 0$ I.C. Note the difference from the original I.C.

$u_3(0,t)=u_3(L,0)=0$ B.C.

Let's define an "energy" or variance for this system:

$$E(t) = \int_0^L \frac{1}{2} u^2 dx \qquad u \in \text{real}$$

E is "positive definite" and is zero if and only if u=0 in the entire interval [0,L].

To derive the energy equation for our problem, multiple the PDE by u:

$$u(u_t - K\, u_{xx}) = 0$$

$$(u^2/2)_t = K\, (u\, u_x)_x - K\, (u_x)^2$$

Integrate from 0 to L gives

$$\frac{\partial E}{\partial t} = -K\int_0^L (u_x)^2 dx$$

=> energy decreases with time at a rate that can computed from u.

Now,

$$E_3(t) = \int_0^L \frac{1}{2} u_3^2 dx$$

From I.C. $u_3 = 0$ => $E_3 = 0$ at t=0. Since E_3 can not go negative, and it has an initial value of zero, <u>it has to remain zero for all t</u>. For E_3 to be zero, <u>u_3 has to be zero for all x and t.</u>

Therefore u_3=0 => u1 = u_2 => the solution is unique!

<u>Continuous Dependence on Auxiliary Conditions</u>

A small or <u>bounded</u> change in the I.C. or B.C. should lead to small or <u>bounded</u> changes in the solution.

This doesn't necessarily apply to chaotic systems, where a small change in the I.C. can lead to very large difference in the solution – in such cases, the solution can still be continuous and usually is.

<u>A Classic Example of Discontinuous Solution Near the Boundary</u>

Look at Laplace's equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad -\infty < x < \infty, \;\; y \geq 0$$

For this 2nd-order PDE, we need two boundary conditions.

We specify the conditions at y=0:

$$u(x,0) = 0$$

$$u_x(x,0) = \sin(nx)/n \quad n>0.$$

Note n here is a coefficient in the boundary condition.

Using the method of separation of variables, we can show the solution to be

$$u(x,y) = [\sin(nx) \sinh(ny)]/n^2$$

Is there continuous dependence on the B.C.?

Now, from our solution, we have

$$u_x(x,0) = \sin(nx) \cosh(0) / n = \sin(nx)/n,$$

so this works. But, does it work for all values of n?

We see that for the second B.C., there is no problem:

$$u_x(x,0) \to 0 \text{ as } n \to \propto.$$

Looking at the first B.C.,

$$u(x,y) = \frac{1}{n^2} \sin(nx) \ \frac{e^{ny} - e^{-ny}}{2}$$

As $n \to \propto$., the above $\to e^{ny}/n^2$ which <u>grows without bound even for small y!</u>

On the other hand, we have B.C. u(x,0) = 0, so the <u>continuity with the boundary data is lost</u> – the problem is ill posed.

Actually, this problem requires the solution of the PDE on an open domain.

Summary of Chapters 0 and 1 – What you should know:

Basic computer architectures
Current trend in moving toward distributed memory massively parallel systems
Vectorization and parallelization issues, Amdahl's Law
Code optimization issues

Canonical forms of second-order PDE's
Classification of first-order, second-order PDE's and systems of first-order PDE's
Methods for finding characteristic and compatibility equations and their solutions
Use method of characteristics to solve simple problems
Concept of domain of dependence and domain of influence
Basic types of I.C. and B.C.
Know something about the well-posedness of PDE systems