

Chapter 1. Partial Differential Equations (PDEs)

Required Readings:

Chapter 2 of Tannehill et al (text book)

Chapter 1 of Lapidus and Pinder (Numerical Solution of Partial Differential Equations in Science and Engineering – see web link)

Supplementary Reading: P1-P20 of Durran book.

Before we look 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

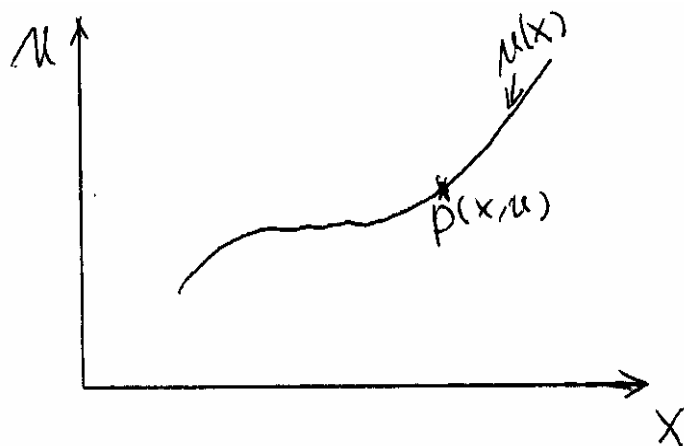
1) PDE's contain >1 independent variable, e.g.,

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

whereas ODEs (Ordinal Differential Equations) 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 (through the PDE equation), but does not uniquely determine either.

For a PDE, the solution surfaces pass through a curve in a 3-D space, rather than a curve through a point in the ODE.

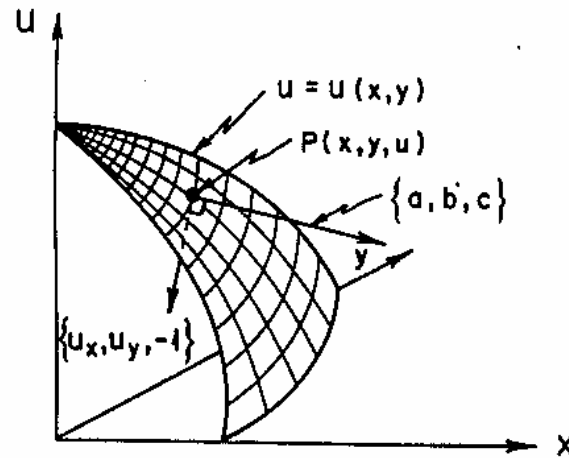


Figure 1.1. Solution surface $u = u(x, y)$ with vector $\{a, b, c\}$ tangent to u and vector $\{u_x, u_y, -1\}$ normal to u at point $P(x, y, u)$.

- 3) ODE's have nice convergence proofs when solved using iterative methods. 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.,
$$\frac{\partial u}{\partial t} = a \frac{\partial^3 u}{\partial^2 x \partial y} \quad \text{is 3rd order}$$

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 of equations, e.g.,

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

can be written as

$$u_x + v_y = u_z,$$

$$u = w_x,$$

$$v = w_y.$$

Another example – the shallow water equations

$$\begin{aligned} \frac{\partial u}{\partial t} &= -g \frac{\partial h}{\partial x} \\ \frac{\partial h}{\partial t} &= -H \frac{\partial u}{\partial x} \end{aligned} \quad \Rightarrow \quad \frac{\partial^2 u}{\partial t^2} = -c^2 \frac{\partial^2 u}{\partial x^2} \text{ where } c = \sqrt{gH}.$$

The order has important implications because of the number of boundary conditions required and the classification of the equation in the canonical or standard 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. For linear equations, the actual solution, such as the amplitude of the sine wave solution, does not affect the behavior of the equation - i.e., there is no feedback.

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 need to eat.

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

Definition: An operator $L()$ is linear if

$$L(\alpha u + \beta v) = \alpha L(u) + \beta L(v)$$

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

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

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

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

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

is a linear equation. Solutions of a linear equation can be superimposed.

Equation

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

is nonlinear. Solutions of a nonlinear equation generally can not be superimposed, i.e., the sum of 2 solutions to the equations does not yield a correct third one.

To be mathematically rigorous, we can use the following:

Consider,

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

If $a, b, c = \text{constant}$ or $\xi = \xi(x, y)$, it is Linear.

If $\xi = \xi(u, \partial u / \partial x, \partial u / \partial y, u^n (n > 1))$, i.e., if one of the coefficients is a function of u , or derivatives of u , it is Nonlinear.

3. Classification of second-order PDE's

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

There are three standard types for PDE's:

Hyperbolic
Parabolic
Elliptic

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

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

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

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

We will discuss more later to see why.

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

| | | |
|-----------------|--------------------------------------|---|
| <u>Example:</u> | $u_{tt} - c^2 u_{xx} = 0$ (wave eq.) | H |
| | $u_t = c u_{xx}$ (Diffusion eq.) | P |

$$u_{xx} + u_{yy} = 0 \text{ (Laplace eq.)} \quad \text{E}$$

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

4.1. 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:

$$\begin{array}{lll} & u_{\xi\xi} - u_{\eta\eta} + \dots = 0 & \\ \text{or} & u_{\xi\eta} + \dots = 0 & \text{H} \end{array} \quad (3a)$$

$$u_{\xi\xi} + \dots = 0 \quad \text{P} \quad (3b)$$

$$u_{\xi\xi} + u_{\eta\eta} + \dots = 0 \quad \text{E} \quad (3c)$$

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 parabolic PDE has one real characteristic curve, and the elliptic PDE has no real characteristic curve.

$$\text{Examples} \quad u_{tt} - c^2 u_{xx} = 0 \text{ (wave eq.)} \quad \text{H}$$

$$\begin{array}{ll} u_t = c u_{xx} & \text{(Diffusion eq.)} \quad \text{P} \\ u_{xx} + u_{yy} = 0 & \text{(Laplace eq.)} \quad \text{E} \end{array}$$

are already in the canonical forms.

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

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

4.2. Canonical Transformation

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

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

Introduce transform

$$\xi = \xi(x, y), \quad \eta = \eta(x, y), \quad (5)$$

which essentially transforms the PDE from coordinate system (x, y) to coordinate system (ξ, η) .

Using the chain rule =>

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

$$u_x = u_\xi \xi_x + u_\eta \eta_x$$

$$u_y = u_\xi \xi_y + u_\eta \eta_y$$

$$u_{xx} = u_{\xi\xi} \xi_x^2 + 2u_{\xi\eta} \xi_x \eta_x + u_{\eta\eta} \eta_x^2 + \dots \quad (6a)$$

$$u_{xy} = u_{\xi\xi} \xi_x \xi_y + u_{\xi\eta} (\xi_x \eta_y + \xi_y \eta_x) + u_{\eta\eta} \eta_x \eta_y + \dots \quad (6b)$$

$$u_{yy} = u_{\xi\xi} \xi_y^2 + 2u_{\xi\eta} \xi_y \eta_y + u_{\eta\eta} \eta_y^2 + \dots \quad (6c)$$

The terms not including any 2nd-order derivative are not explicitly written out.

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

$$a u_{xx} + b u_{xy} + c u_{yy} = A u_{\xi\xi} + B u_{\xi\eta} + C u_{\eta\eta} + \dots, \quad (7)$$

where

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

From (8), we can obtain (show it for yourself!)

$$B^2 - 4AC = (b^2 - 4ac) (\xi_x \eta_y - \xi_y \eta_x)^2. \quad (9)$$

Note, $B^2 - 4AC$ and $b^2 - 4ac$ always have the same sign, as long as $\xi_x \eta_y - \xi_y \eta_x \neq 0$!

This is why the only the coefficients of the second order derivative terms matter, and transformations from one coordinate system to another does not change the sign of the criterion.

Therefore, nonsingular (where $\xi_x \eta_y - \xi_y \eta_x \neq 0$) coordinate transformation does not change the type of PDE.

Note that in (9), $\frac{\partial(\xi, \eta)}{\partial(x, y)} = \begin{vmatrix} \xi_x & \eta_x \\ \xi_y & \eta_y \end{vmatrix} = \xi_x \eta_y - \eta_x \xi_y$ is the Jacobian of transformation therefore it can not be zero.

Otherwise there will not be a one-to-one mapping between the two coordinate systems, in another word, the transformation becomes singular.

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 $u_{\xi\eta} + \dots = 0$.

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

$$a \xi_x^2 + b \xi_x \xi_y + c \xi_y^2 = 0 \quad (10a)$$

$$a \eta_x^2 + b \eta_x \eta_y + c \eta_y^2 = 0 \quad (10b)$$

Let

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

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

$$a \lambda_1^2 + b \lambda_1 + c = 0 \quad (12a)$$

$$a \lambda_2^2 + b \lambda_2 + c = 0 \quad (12b)$$

Obviously, the solutions of λ_1 and λ_2 are

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

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

4.3. Characteristic Equations and Characteristic Curves

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

$$\xi_x - \lambda_1 \xi_y = 0 \quad (14a)$$

$$\eta_x - \lambda_2 \eta_y = 0 \quad (14b)$$

We will see that from them we can obtain two sets of characteristic curves.

The number of real characteristics of a PDE can actually determine its type.

Concept of Characteristics

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

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

Such lines or surfaces are related to the directions in which "information" 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 'information' 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:

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

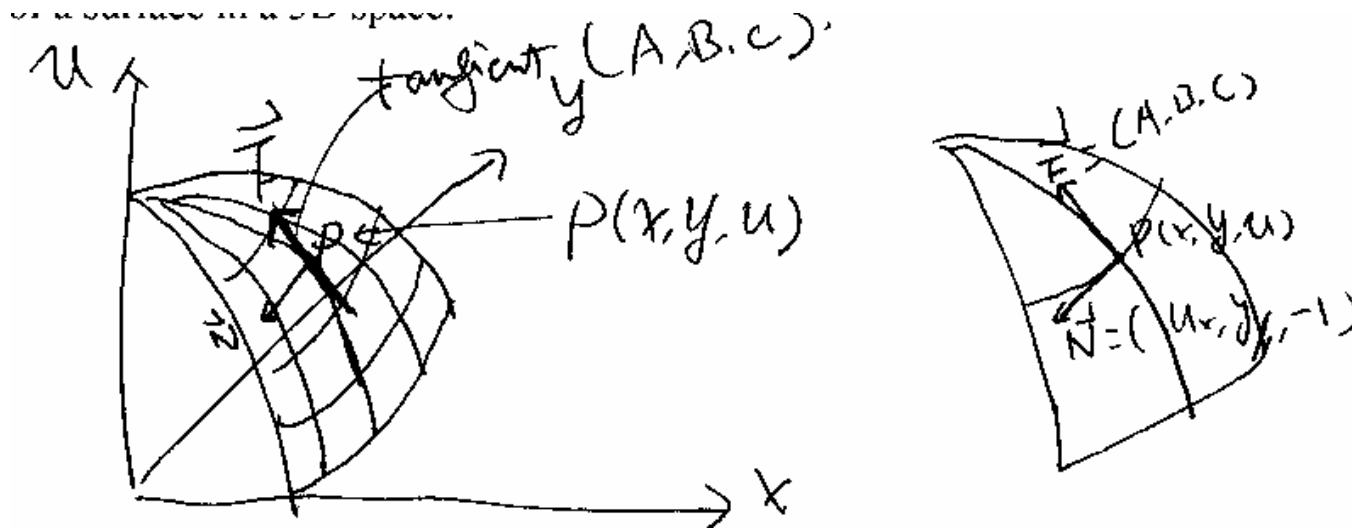
Solution u represents a curved surface in a 3D space [$u = u(x, y)$].

It can be shown that vector

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

is tangent to the surface where A , B and C are the components of vector \vec{F} .

Diagram of a surface in a 3D space:



Because the downward normal of the surface at a given point $P(x, y)$ is $\vec{N} = (u_x, u_y, -1)$ (consult your 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) .

Question: For A , B and C that are all constant, what do the solution surfaces look like?

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

$$du = u_x dx + u_y dy \quad (16)$$

In both (15) and (16), u_x and u_y can take on more than one value but still satisfy these equations.

This is because for a given vector $\vec{F} = (A, B, C)$, there can be many vector $\vec{N} = (u_x, u_y, -1)$ that is perpendicular to \vec{F} . $\vec{F} \cdot \vec{N} = 0$ is the only requirement for u to satisfy Eq.(15). Similar can be said of Eq.(16).

Therefore, u_x and u_y are non-unique (c.f., the diagram for three-D surface). This is important and we will use this property to obtain the characteristic and compatibility equations.

Using the terminology of linear algebra, we actually have two linearly dependent equations.

Write these two equations in a matrix form:

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

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.,

$$\begin{vmatrix} A & B \\ dx & dy \end{vmatrix} = 0. \Rightarrow \frac{dx}{A} = \frac{dy}{B} \quad (18)$$

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 also vanish (c.f., the Cramer's rule for solving linear systems of equations). Therefore we have

$$\begin{vmatrix} C & B \\ du & dy \end{vmatrix} = 0 \Rightarrow \frac{du}{C} = \frac{dy}{B} \quad (20)$$

$$\begin{vmatrix} A & C \\ dx & du \end{vmatrix} = 0 \Rightarrow \frac{du}{C} = \frac{dx}{A} \quad (21)$$

or $\frac{dx}{A} = \frac{dy}{B} = \frac{du}{C} \quad (22)$

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

$$\frac{dy}{dx} = \frac{B}{A} \quad (23)$$

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

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

$$\frac{\partial u}{\partial t} + \beta \frac{\partial u}{\partial x} = 0, \quad \beta > 0 \text{ and const.} \quad (24)$$

The characteristic equation is

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

The solution represents a family of parallel lines in x - t space.

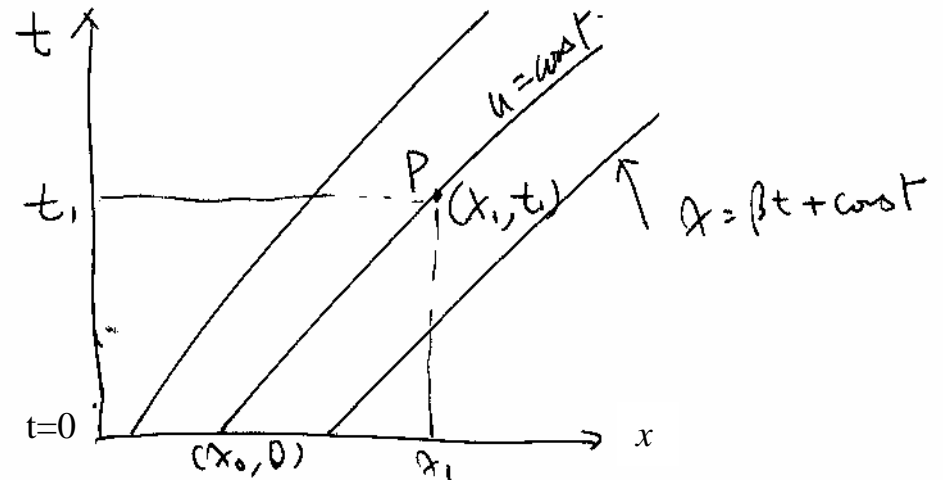
From (20) or (21), we have

$$du = 0 \text{ - which is called the } \underline{\text{Compatibility Equation}}. \quad (26)$$

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 along the characteristics.**

Diagram:



4.4. Method of Characteristics (MOC)

Reading: Section 6.2 of Textbook.

For the previous problem, 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.

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

Since $x_I - \beta t_I = x_0 + \beta 0 \rightarrow x_0 = x_I - \beta t_I$, the general solution is

$$u(x_I, t_I) = u(x_0, 0) = f(x_I - \beta t_I) \quad (27)$$

where the functional form of f is specified by the I.C.

There general solution is therefore

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

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

In the above example, $du = 0$, $u = \text{const}$ 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.

Still the integration of this equation is usually much easier than that of the original PDE (the procedure to obtain the characteristic and compatibility 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:

$$\xi_x - \lambda_I \xi_y = 0 \quad (29)$$

Compared to Eq.(15), $A = 1$, $B = -\lambda_1$, $C = 0$, therefore according to (22), we have

$$\frac{dx}{1} = \frac{dy}{-\lambda_1} = \frac{d\xi}{0}. \quad (30)$$

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

$$\frac{dx}{1} = \frac{dy}{-\lambda_2} = \frac{d\eta}{0}. \quad (31)$$

From them, we obtain the characteristics and compatibility equations:

$$\frac{dy}{dx} = -\lambda_1 \text{ and } d\xi = 0 \quad (32)$$

$$\frac{dy}{dx} = -\lambda_2 \text{ and } d\eta = 0 \quad (33)$$

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 ($\xi = \text{const}$, $\eta = \text{const}$) in the new coordinate

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

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.

We have shown that one of the two canonical form of hyperbolic equation, i.e., the form of $u_{\xi\eta} + \dots = 0$, can be obtained. To obtain the alternative canonical form,

$$u_{\bar{\xi}\bar{\xi}} - u_{\bar{\eta}\bar{\eta}} + \dots = 0 \quad (35)$$

we can use a linear combination of ξ and η :

$$\bar{\xi} = (\xi + \eta)/2 \text{ and } \bar{\eta} = (\xi - \eta)/2. \quad (36)$$

In another word, we can perform the another transform from (ξ, η) coordinate system to $(\bar{\xi}, \bar{\eta})$ and convert equation $u_{\xi\eta} + \dots = 0$ into the form Eq. (35). Of course, we can also perform a transform directly from the original equation in (x, y) coordinate, by requiring that $B = 0$ in Eq.(7).

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

Reading: Section 2.3 of Text.
Section 1.1.2 of Durran.

4.5. Domain of Dependence for second-order PDE's

Reading: Section 2.3.1 of Textbook.

Consider 2nd-order wave equation

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

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

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

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

$$u_{\xi\eta} = 0 \quad (39)$$

where $\xi = x + ct$ and $\eta = x - ct$.

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

$$\begin{aligned} u_\xi &= C'(\xi) \\ u(\xi, \eta) &= \int C'(\xi) d\xi + D(\eta) = C(\xi) + D(\eta) \end{aligned}$$

which can be rewritten in terms of x and t as

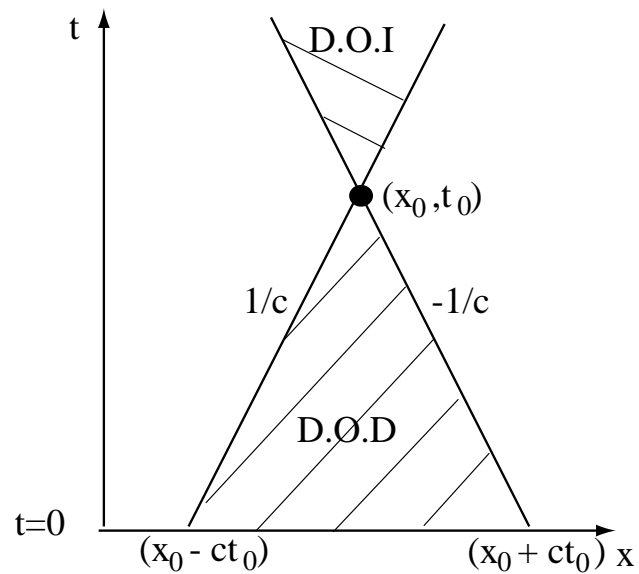
$$u(x, t) = C(x + ct) + D(x - ct) \quad (40)$$

where C and D are arbitrary functions to be determined from initial conditions. When the functional form of C and D are determined from the I.C. The resulting solution is

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

which is called the D'Alembert solution (see web link).

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 dependent on the condition in a domain bounded by the two characteristic lines 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 initial value problems.
- I.C. cannot be specified on a characteristic line (only) – otherwise the problem is ill-posed, i.e., a unique solution can not be found.

Domain of Influence

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

$$x_0 + ct_0 \leq x \leq x_0 - ct_0 \quad \text{for } t > t_0,$$

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.

DOD of Diffusion Equations

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

$$T_t = K T_{xx} \quad (41)$$

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

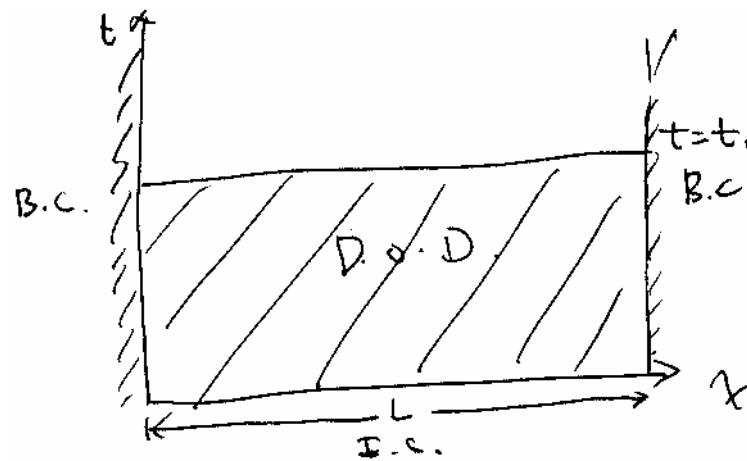
Its analytical solution is

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

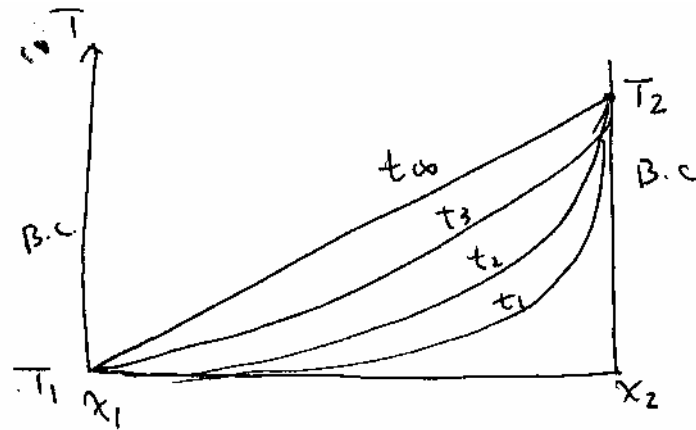
where k is wavenumber. $t \rightarrow \infty$, $T \rightarrow 0$ for non-zero wavenumbers.

The characteristic equation for this equation is

$$\frac{dt}{dx} = 0 \quad (43)$$



=> 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.)

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

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

Not 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 linearized equations are

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

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

Signals propagates at speed c – a finite propagation speed.

Now, if we make the fluid incompressible,

$$\text{i.e., } d\rho/dt = 0 \Rightarrow \frac{\partial u}{\partial x} = 0,$$

this is equivalent to setting $c = \infty$ 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 incompressible system:

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

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

Take $\nabla \cdot$ of (45a), and make use of (45b), we get

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

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: Section 2.5 of Textbook.

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.

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

$$\frac{\partial w}{\partial t} - c \frac{\partial v}{\partial x} = 0 \quad (5.1b)$$

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

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

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 obtaining characteristic and compatibility equations.

We write the system in a vector form:

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

where

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

Definition:

- If the eigenvalues of \mathbf{A} are real and distinct (n of them for n^{th} -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 that symmetric matrix has real eigenvalues. As in the above case.

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

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

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

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

$$\mathbf{T} \frac{\partial \vec{v}}{\partial t} + \mathbf{A} \mathbf{T} \frac{\partial \vec{v}}{\partial x} = 0 \Rightarrow \frac{\partial \vec{v}}{\partial t} + \mathbf{T}^{-1} \mathbf{A} \mathbf{T} \frac{\partial \vec{v}}{\partial x} = 0 \Rightarrow$$

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

which are n decoupled individual compatibility equations.

Reading: Section 2.5 of Textbook

Eigenvalues of the previous problem can be found from

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

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) Method using the auxiliary equations

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

$$dv = v_t dt + v_x dx$$

$$dw = w_t dt + w_x dx$$

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 determinant of the coefficient matrix, $| | = 0 \Rightarrow dx/dt = \pm c$ as before!

Find the compatibility equation on your own (hit: replace one of the columns 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 you know how to apply this method. The physical interpretation of this method is not as clear as the matrix method, however.

Example Problem

The 1-D linear inviscid shallow water equations can be written as

$$\frac{\partial u}{\partial t} + U \frac{\partial u}{\partial x} + g \frac{\partial h}{\partial x} = 0 \quad (1)$$

$$\frac{\partial h}{\partial t} + U \frac{\partial h}{\partial x} + H \frac{\partial u}{\partial x} = 0 \quad (2)$$

where U and H are the mean flow speed and unperturbed water depth, respectively, and u , and h are the corresponding deviations of total flow speed and water depth from U and H .

- 1) Classify the system in terms of the canonical types;
- 2) Find the characteristic equations of the system;

Equations (1) and (2) can be written as

$$u_t + U u_x + 0 h_t + g h_x = 0 \quad (3)$$

$$0 u_t + H u_x + h_t + U h_x = 0 \quad (4)$$

We make use of two auxiliary equations

$$dt u_t + dx u_x + 0 h_t + 0 h_x = du \quad (5)$$

$$0 u_t + 0 u_x + dt h_t + dx h_x = dh \quad (6)$$

Write (3)-(6) in a matrix form,

$$\begin{bmatrix} 1 & U & 0 & g \\ 0 & H & 1 & U \\ dt & dx & 0 & 0 \\ 0 & 0 & dt & dx \end{bmatrix} \begin{pmatrix} u_t \\ u_x \\ h_t \\ h_x \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ du \\ dh \end{pmatrix} \quad (7)$$

For the reason of linear dependence, we require the coefficient matrix [] to be zero:

$$\begin{vmatrix} 1 & U & 0 & g \\ 0 & H & 1 & U \\ dt & dx & 0 & 0 \\ 0 & 0 & dt & dx \end{vmatrix} = \begin{vmatrix} H & 1 & U \\ dx & 0 & 0 \\ 0 & dt & dx \end{vmatrix} + dt \begin{vmatrix} U & 0 & g \\ H & 1 & U \\ 0 & dt & dx \end{vmatrix} = 0$$

$$\therefore dxdtU - (dx)^2 + dtUdx + Hg(dt)^2 - U^2(dt)^2 = 0$$

Reorganize the above equations, we have

$$(dx)^2 - 2Udxdt + (U^2 - Hg)(dt)^2 = 0$$

Divide the equation by $(dt)^2$, we obtain

$$(dx/dt)^2 - 2U(dx/dt) + (U^2 - Hg) = 0,$$

which is a quadratic algebraic equations for (dx/dt) . Its solutions are

$$dx/dt = \frac{2U \pm \sqrt{4U^2 - 4(U^2 - Hg)}}{2} = U \pm \sqrt{gH} . \quad (8)$$

From (8), we obtain two families of characteristics equations:

$$x = (U + \sqrt{gH})t + C_1 \text{ and } x = (U - \sqrt{gH})t + C_2 \quad (10)$$

where C_1 and C_2 are the integration constants. Varying the values of C_1 and C_2 lead to two families of characteristics curves. We can recognize that \sqrt{gH} is the phase speed of shallow water external gravity waves, which propagate in two directions. U is the advective flow speed. $U \pm \sqrt{gH}$ are the Doppler shifted phased speeds.

Because we can find two real characteristics equations for this system of two 1st order equations, the system is hyperbolic.

3) In the case that real characteristics exist, find the corresponding compatibility equations;

To find the compatibility equations, we replace one of the columns of the coefficient matrix in (7) by the right-hand-side vector. The determinant of this matrix also has to be zero. This leads to

$$\begin{vmatrix} 1 & U & 0 & 0 \\ 0 & H & 1 & 0 \\ dt & dx & 0 & du \\ 0 & 0 & dt & dh \end{vmatrix} = \begin{vmatrix} H & 1 & 0 \\ dx & 0 & du \\ 0 & dt & dh \end{vmatrix} + dt \begin{vmatrix} U & 0 & 0 \\ H & 1 & 0 \\ 0 & dt & dh \end{vmatrix} = 0$$

$$\therefore -Hdudt - dxdh + dtUdh = 0 .$$

Divide the equation by $(-dt)$, we have

$$Hdu + (dx/dt)dh - Udh = 0.$$

Substituting for (dx/dt) using (8) yields (**note characteristics equations are used when deriving the compatibility equations**):

$$Hdu \pm \sqrt{gH} dh = 0, \text{ therefore}$$

$$d(Hu \pm \sqrt{gH} h) = 0.$$

$$Hu \pm \sqrt{gH} h = C_{3,4} \quad (11)$$

are the two compatibility equations. $Hu \pm \sqrt{gH} h$ are call the Riemann invariant that are conserved along the characteristics curves.

4) Suggest an application for characteristics and compatibility equations.

Along characteristics curves, PDE can often be reduced to ODE, which is much easier to solve. In our example, two quantities are found (from compatibility equations) to be conserved along the characteristics lines. They can be traced along the lines to the initial time and the boundary, where the known solutions are used to determine the integration constants. Therefore the solution in the interior domain can be found by solving the two conservation equations. The method of finding a solution of PDE by using characteristics and compatibility equations in combination with initial and boundary conditions is called the Method of Characteristics (MOC).

An alternative solution to this problem is given below:

Rewrite (1) and (2) in a vector-matrix form:

$$\frac{\partial V}{\partial t} + A \frac{\partial V}{\partial x} = 0, \text{ where } V = \begin{bmatrix} u \\ h \end{bmatrix} \text{ and } A = \begin{bmatrix} U & g \\ H & U \end{bmatrix}. \quad (12)$$

Find the eigenvalues of A by requiring $\begin{vmatrix} U - \lambda & g \\ H & U - \lambda \end{vmatrix} = 0$,

therefore the two eigenvalues are $\lambda_{1,2} = U \pm \sqrt{gH}$.

Because we found two (the same number as the number of 1st order equations) real eigenvalues, the system is hyperbolic.

Now find the eigenvectors corresponding to eigenvalues λ_1 and λ_2 by solving

$$AX = \lambda_1 X, AX = \lambda_2 X. \quad (13)$$

The solutions of (13), i.e., the two eigenvectors are

$$X_1 = \begin{bmatrix} 1 \\ \sqrt{H/g} \end{bmatrix}, X_2 = \begin{bmatrix} 1 \\ -\sqrt{H/g} \end{bmatrix}.$$

Therefore we have matrix $T = \begin{bmatrix} 1 & 1 \\ \sqrt{H/g} & -\sqrt{H/g} \end{bmatrix}$ and its inverse $T^{-1} = 1/2 \begin{bmatrix} 1 & \sqrt{g/H} \\ 1 & -\sqrt{g/H} \end{bmatrix}$ (show it for yourself) so that

$$T^{-1}AT = D \text{ where } D = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} = \begin{bmatrix} U + \sqrt{gH} & 0 \\ 0 & U - \sqrt{gH} \end{bmatrix}.$$

We multiple equation (12) by T^{-1} , so that $\frac{\partial T^{-1}V}{\partial t} + T^{-1}AT \frac{\partial T^{-1}V}{\partial x} = 0$ therefore

$$\frac{\partial \tilde{V}}{\partial t} + \begin{bmatrix} U + \sqrt{gH} & 0 \\ 0 & U - \sqrt{gH} \end{bmatrix} \frac{\partial \tilde{V}}{\partial x} = 0 \quad (14)$$

where

$$\tilde{V} = T^{-1}V = 1/2 \begin{bmatrix} 1 & \sqrt{g/H} \\ 1 & -\sqrt{g/H} \end{bmatrix} \begin{bmatrix} u \\ h \end{bmatrix} = 1/2 \begin{bmatrix} u + \sqrt{g/H}h \\ u - \sqrt{g/H}h \end{bmatrix} \quad (15)$$

We rewrite (14) into a system of equations:

$$\begin{aligned} \frac{\partial (u + \sqrt{g/H}h)}{\partial t} + (U + \sqrt{gH}) \frac{\partial (u + \sqrt{g/H}h)}{\partial x} &= 0, \\ \frac{\partial (u - \sqrt{g/H}h)}{\partial t} + (U - \sqrt{gH}) \frac{\partial (u - \sqrt{g/H}h)}{\partial x} &= 0. \end{aligned} \quad (16)$$

We know and can easily show that for (16), the compatibility equations are

$$d(u \pm \sqrt{g/H}h) = 0 \text{ or } u \pm \sqrt{g/H}h = C_{1,2} \text{ along characteristics equations } x = (U \pm \sqrt{gH})t + C_{3,4}.$$

These are the same as what we found with the first method. Mathematically it's more elegant. The two equations in (16) are now decoupled and can be solved independent of each other.

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.

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

$$\alpha u(\vec{x}, t) + \beta \frac{\partial u(\vec{x}, t)}{\partial n} = \gamma$$

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. $\beta=0 \rightarrow$ value of variable specified
- Neumann or 2nd B.C. $\alpha = 0$, gradient of value specified
- Robin or 3rd B.C., neither α nor β is zero. - A linear combination of the above two.

Note for Poisson's equation $\nabla^2 \phi = \zeta$, 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 - a small change in auxiliary conditions results in small change(s) in the solution (the future state is 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:

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

$$\text{I.C. } u(x,0) = f(x)$$

$$\text{B.C. } u(x=0, t) = u(x=L, t) = 0$$

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

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

$$u_3(x,0) = 0 \quad \text{I.C.} \quad \text{Note the difference from the original I.C.}$$

$$u_3(0,t) = u_3(L,t) = 0 \quad \text{B.C.}$$

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

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

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 be computed from u .

Now,

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

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

Therefore $u_3=0 \Rightarrow u_1 = u_2 \Rightarrow$ the solution is unique!

Continuous Dependence on Auxiliary Conditions

A small or bounded change in the I.C. or B.C. should lead to small or bounded 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.

A Classic Example of Discontinuous Solution Near the Boundary

Look at Laplace's equation:

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

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

We specify the conditions at $y=0$:

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

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

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

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

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

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

$$u_y(x,0) \rightarrow 0 \text{ as } n \rightarrow \infty.$$

Looking at the first B.C.,

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

As $n \rightarrow \infty$, the above $\rightarrow e^{ny}/n^2$ which grows without bound even for small y !

On the other hand, we have B.C. $u(x,0) = 0$, so the continuity with the boundary data is lost – 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, CPU types, memory hierarchy, common computer terminologies.

Current trend in moving toward distributed memory massively parallel systems

Superscalar, pipelining, 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