

Overview of frequently encountered PDE's

1. PDE's in the natural sciences

Ordinary and partial differential equations (ODE's and PDE's henceforth) are frequently encountered in numerous areas of study. A knowledge of the basic scientific background is necessary to write down equations of interest. Perhaps one should not be surprised that the same background knowledge is useful in devising solution methods. The typical procedures by which PDE's are derived should be known to researchers working on solution methods.

1.1. Conservation laws. A large number of PDE's arise from the physical principle of *conservation*. Physicists have always been interested in describing changes in the world surrounding us. By observation, theory and experiment certain concepts have been arrived at, among which the concept that one can define physical quantities that remain the same during some process. These quantities are said to be *conserved*. Typically a quantity is conserved in a hypothesized *isolated* system. In reality no system is truly isolated and the most interesting applications come about when we study the interaction of two or more systems. This leads to the question of how one can follow the changes in physical quantities of the separate systems. An extremely useful procedure is to set up an accounting procedure. To start with a mundane example, consider the physical quantity of interest to be the quantity of currency Q in a building B . If the building is a commonplace one, it is to be expected that when completely isolated, the amount of currency in the building is fixed

$$(1.1) \quad Q = Q_0 .$$

Q_0 is some constant. Eq. (1.1) is self-evident but not particularly illuminating – of course the amount of money is constant if nothing goes in or out! Similarly in physics, statements such as “the total mass-energy of the universe is constant” are not terribly useful, though one should note this particular statement is not obviously true.

Things get more interesting when we consider a more realistic scenario in which the system is not isolated. People might be coming and going from building B and some might actually have money in their pockets. In more leisurely economic times, one might be interested just in the amount of money in the building at the end of the day. Just a bit of thought leads to

$$Q_n = Q_{n-1} + \Delta Q_{n-1,n}$$

where Q_n is the amount of money at the end of day n , Q_{n-1} that from the previous day and $\Delta Q_{n-1,n}$ the difference between money received and that paid in the

building during day n

$$\Delta Q_{n-1,n} = R_{n-1,n} - P_{n-1,n} .$$

Keeping track of $R_{n-1,n}$ and $P_{n-1,n}$ separately, for instance in two distinct columns on a ledger, seems easier to people more inclined towards addition than subtraction, and this leads to double entry accounting, an important discovery of Renaissance Italy (see http://www.acaus.org/history/hs_pac.html).

As economic activity picks up and we take building B to mean “bank” it becomes important to keep track of the money in the bank at all times, not just at the end of the day. It then makes sense to think of the rate at which money is moving in or out of the building so we can not only track the amount of currency at any given time, but also be able to make some future predictions. Since some time has passed in order for economic activity to pick, we can assume that addition and subtraction have become much more familiar and are actively taught to small children. We’ll therefore use a single quantity F to denote the amount of money leaving or entering building B during time interval Δt with the understanding that positive values of F represent incomes and negative ones expenditures. Such understandings go by the name of sign conventions. They’re not especially meaningful but it aids communication if we all stick to the same ones. The amount of currency in the building then changes in accordance to

$$(1.2) \quad Q(t + \Delta t) = Q(t) + F \Delta t .$$

By the time such equations were being written out fluid flow was a scientific frontier investigated by the Bernoullis (see http://www.maths.tcd.ie/pub/HistMath/People/Bernoullis/RouseBall/RB_Bernoullis.html) and F got to be referred to as a *flux*, the Latin term for flow.

It is readily apparent that (1.2) is a good approximation for small intervals, but probably a bad one if Δt is large since economic activity might change from hour to hour. In order to better keep track of things one might think of F as being defined at any given time t so we have $F(t)$ the instantaneous flux of currency at time t . By the time people were thinking along these lines Newton and Leibniz had introduced calculus and sufficient time has since passed that the notions of calculus are widely known at least among college students if not small children. We can therefore write

$$(1.3) \quad Q(t + \Delta t) = Q(t) + \int_t^{t+\Delta t} F(\tau) d\tau$$

and get a suitably impressive statement which, form notwithstanding, carries the same significance as (1.2).

On the verge of the modern era economic activity might really expand and buildings become so large that it makes sense to keep track of the amount of money in individual rooms and also track inflows and outflows through individual doors. We can identify a room or door by its spatial position denoted by $\mathbf{x} = (x_1, x_2, x_3)$ but we encounter a problem in that position vectors such as \mathbf{x} refer to a single point and no matter how small we make the currency it still has to occupy some space. This conceptual difficulty is overcome by introducing a fictitious “density of currency” at time t which we shall denote by $q(\mathbf{x}, t)$. The only real meaning we associate with this density is that if we sum up the values of $q(\mathbf{x}, t)$ in some volume

ω we obtain the amount of currency in that volume

$$Q(\omega, t) = \int_{\omega} q(\mathbf{x}, t) d\mathbf{x} .$$

On afterthought, we might observe that the same sort of question should have arisen when we defined $Q(t)$ as being defined at one instant in time. Ingrained psychological perspectives make $Q(t)$ more plausible, but were we to live our lives such that quantum fluctuations are observable, $Q(t)$ would be much more questionable.

If we have a spatial density for Q it seems natural to do the same for F and we define $\mathbf{f}(\mathbf{x}, t)$ as being the instantaneous flux of currency in a small region around (\mathbf{x}, t) . A bit of thought suggests that the flux should be a vector quantity since we have three directions along which a density can be defined. Along any given direction a scalar flux is obtained by a scalar product; in particular along the direction normal to a boundary $\mathbf{n}(\mathbf{x})$ the scalar flux is given by $\mathbf{f}(\mathbf{x}, \tau) \cdot \mathbf{n}(\mathbf{x})$. The relation between the total flux and the flux densities is given by

$$(1.4) \quad F(\tau) = \int_{\partial B} \mathbf{f}(\mathbf{x}, \tau) \cdot \mathbf{n}(\mathbf{x}) d\mathbf{x} .$$

Careful observers will notice the appearance of ∂B as defining the integration domain. By this we mean that the integration is to be taken over the boundary of the domain B , or in everyday terms, the exterior walls and doors of building B . There is a bit of inconsistency in the sciences as to what we mean by “flux”. Sometimes it means the amount of some quantity passing through a finite region such as F above. Other times it actually means “flux density” such as \mathbf{f} . This possibility of confusion shows the value of using the same conventions. Imposing such conventions is however a social activity and subject to historical iteration. In this course the convention “flux”= \mathbf{f} shall be imposed by instructor fiat. Gathering together all the above we can write a much more sophisticated-looking statement

$$(1.5) \quad Q(B, t + \Delta t) = \int_B q(\mathbf{x}, t + \Delta t) d\mathbf{x} = \underbrace{\int_B q(\mathbf{x}, t) d\mathbf{x}}_{E(B, t)} + \int_t^{t+\Delta t} \int_{\partial B} \mathbf{f}(\mathbf{x}, \tau) \cdot \mathbf{n}(\mathbf{x}) d\mathbf{x} d\tau$$

which nonetheless is essentially the same as (1.2) or (1.3).

There are some special cases in which additional events affecting the balance of Q can occur. For instance if by B we mean a reserve bank, money might be (legally) printed and destroyed in the building. Again by analogy with fluid dynamics when such an event occurs we say that there exist *sources* of E within B , much like a spring is a source of surface water. Let $\Sigma(t)$ be the total sources at time t . By now we know what to expect; $\Sigma(t)$ might actually be obtained by summing over several sources placed in a number of positions, for instance the separate printing presses and furnaces that exist in B . It is useful to introduce a spatial density of sources $\sigma(\mathbf{x}, t)$. Our conservation statement now becomes

$$(1.6) \quad \int_B q(\mathbf{x}, t + \Delta t) d\mathbf{x} - \int_B q(\mathbf{x}, t) d\mathbf{x} = \int_t^{t+\Delta t} \int_{\partial B} \mathbf{f}(\mathbf{x}, \tau) \cdot \mathbf{n}(\mathbf{x}) d\mathbf{x} d\tau + \int_t^{t+\Delta t} \int_B \sigma(\mathbf{x}, \tau) d\mathbf{x} d\tau$$

The statement above encompasses all physical conservation laws. It is however quite straightforward in interpretation:

change in money in B = net money coming in or going out of B + net money produced or destroyed in B .

It should be emphasized that the above statement has true physical meaning and is referred to as an *integral formulation of a conservation law*. The key term is “integral” and refers to the fact that we are summing over some spatial domain. Remember that the densities were artificial constructs that we introduced.

Eq. (1.6) is useful and often applied directly in the analysis of physical systems. From an operational point of view it does have some inconveniences though. These have mainly to do with pesky integration domains B which typically are difficult to describe and over which it is difficult to perform integrations. To avoid this, mathematicians and physicists have gone one further step and imagined $\mathbf{f}(\mathbf{x}, t)$ as being defined everywhere not only on ∂B (the doors and windows of B). These internal fluxes can be shown to have a proper physical interpretation to which we shall come back later. For now let's see the implications of this extension. If we not only assume that $\mathbf{f}(\mathbf{x}, t)$ is defined everywhere, but also that it has nice properties such like enough smoothness to ensure differentiability then we can apply the Gauss theorem and transform the integral over ∂B into one over B

$$(1.7) \quad \int_{\partial B} \mathbf{f}(\mathbf{x}, \tau) \cdot \mathbf{n}(\mathbf{x}) \, d\mathbf{x} = \int_B \nabla \cdot \mathbf{f}(\mathbf{x}, \tau) \, d\mathbf{x} .$$

Here we encounter another convention problem in that some disciplines use outward pointing normals in which case (1.7) holds while other disciplines use an inward pointing normal in which case we have

$$(1.8) \quad \int_{\partial B} \mathbf{f}(\mathbf{x}, \tau) \cdot \mathbf{n}(\mathbf{x}) \, d\mathbf{x} = - \int_B \nabla \cdot \mathbf{f}(\mathbf{x}, \tau) \, d\mathbf{x} .$$

Fluid dynamics uses the second convention which leads to (1.8) and this is the one we'll adopt since so many developments in numerical methods for PDE's initially arose from fluid dynamics problems. Applying (1.8) to (1.6) leads to

$$(1.9) \quad \int_B \left[q(\mathbf{x}, t + \Delta t) - q(\mathbf{x}, t) + \int_t^{t+\Delta t} \nabla \cdot \mathbf{f}(\mathbf{x}, \tau) \, d\tau \right] d\mathbf{x} = \int_t^{t+\Delta t} \int_{\partial B} \sigma(\mathbf{x}, \tau) d\mathbf{x} \, d\tau .$$

There was nothing special about the shape of the building B or the length of the time interval Δt that we used in deriving (1.9). We can therefore consider special, infinitesimal domains and intervals and obtain a differential form

$$(1.10) \quad \frac{\partial q}{\partial t} + \nabla \cdot \mathbf{f} = \sigma ,$$

where, as is customary, the dependence of q, \mathbf{f}, σ on space and time is understood but not written out explicitly. Eq. (1.10) is known as the *local or differential form* of the conservation law for E . It is often easier to work with since there are no complications arising from the domain shape that appear directly in the statement of conservation.

In physics the above scenario is encountered many times. Physicists have arrived at certain quantities which obey (1.6). In many situation it is permissible to speak of local quantities and use (1.10). Classical physics arrived at mass, momentum, energy and electrical charge as physical concepts that lead to quantities that satisfy conservation laws. Contemporary physics unified momentum and energy

in the theory of relativity and also gave new, microscopic quantities that satisfy conservation such as lepton number.

1.2. Special forms of conservation laws.

1.2.1. *Newton's law.* The full general form (1.10) often arises in real-world applications. But it also many times possible to carry out certain simplifications that lead to equations that are easier to solve. As a simple example, consider the classic problem of dynamics of studying the motion of a point mass m . It has no internal structure and its motion is characterized by the second law of dynamics which is a statement of conservation of momentum

$$(1.11) \quad \frac{d}{dt}(m\mathbf{v}) = \sum \mathbf{F} .$$

Here we have the correspondence $q \longleftrightarrow (m\mathbf{v})$, $\sigma \longleftrightarrow \sum \mathbf{F}$ with (1.10), hence the statement: "external forces are sources of momentum". Instead of a PDE, the lack of internal structure has led to an ODE.

1.2.2. *Advection equations.* Other special forms of (1.10) are not quite so trivial. Often \mathbf{f}, σ depend on q , that is we have $\mathbf{f}(q), \sigma(q)$. The specific form of this dependence is given by physical analysis typically. But accounting for all physical effects is so difficult that often simple approximations are used. For instance we can assume that $\mathbf{f}(e)$ is sufficiently smooth to have a Taylor expansion

$$(1.12) \quad \mathbf{f}(q) = \mathbf{f}_0 + \mathbf{f}'(q_0)(q - q_0) + \dots =$$

and consider what happens when we use various truncations of the Taylor expansion.

Typically we can take $\mathbf{f}_0 = 0$ since it doesn't affect the PDE (1.10) anyway. Choosing a system of units such that $q_0 = 0$ the simplest truncation is

$$(1.13) \quad \mathbf{f}(q) = \mathbf{f}'(0)q = \mathbf{u} q$$

and the $\sigma = 0$ form of (1.10) is

$$(1.14) \quad \frac{\partial q}{\partial t} + \nabla \cdot (\mathbf{u} q) = 0 .$$

If we consider that \mathbf{u} does not depend on the spatial coordinates we obtain

$$(1.15) \quad \frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = 0$$

which goes by the name of the *constant velocity advection equation*. The name comes from its use in modeling the transport of some substance by a flow; this process is known as *advection*. Its one-dimensional form is the basis of much development in numerical methods for PDE's

$$(1.16) \quad \frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} = 0 ,$$

and we shall study it in detail.

If \mathbf{u} does depend on \mathbf{x} we have

$$(1.17) \quad \frac{\partial q}{\partial t} + \nabla \cdot (\mathbf{u} q) = \frac{\partial q}{\partial t} + q \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla q = 0$$

or

$$(1.18) \quad \frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = -q \nabla \cdot \mathbf{u}$$

known as the *variable velocity advection equation*. In very many cases the advection velocity field \mathbf{u} is divergence free

$$(1.19) \quad \nabla \cdot \mathbf{u} = 0 ,$$

so we have the simpler form

$$(1.20) \quad \frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = 0 .$$

1.2.3. *Diffusion equations*. Another widely encountered dependence of \mathbf{f} on q is of the form

$$(1.21) \quad \mathbf{f}(q) = -\alpha \nabla q$$

and this leads to

$$(1.22) \quad \frac{\partial q}{\partial t} - \nabla \cdot (\alpha \nabla q) = \sigma(q) .$$

This is known as the *heat equation* or the *diffusion equation*. If α (the thermal diffusivity) is a constant we have

$$(1.23) \quad \frac{\partial q}{\partial t} = \alpha \nabla^2 q + \sigma(q) ,$$

a widely encountered form of the heat equation. For many problems time evolution is so slow that the $\partial q / \partial t$ derivative is negligible and (1.23) becomes

$$(1.24) \quad \nabla^2 q = -\sigma / \alpha$$

known as the *Poisson equation*. If $\sigma = 0$ we obtain the special form

$$(1.25) \quad \nabla^2 q = 0$$

known as the *Laplace or harmonic equation*.

1.2.4. *Advection-diffusion equations*. As might be expected, the physical flux dependence might combine the two forms (1.13), (1.21) encountered above

$$(1.26) \quad \mathbf{f}(q) = \mathbf{u} q - \alpha \nabla q ,$$

from which we obtain

$$(1.27) \quad \frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = \sigma(q) + \nabla \cdot (\alpha \nabla q) - q \nabla \cdot \mathbf{u} ,$$

known, naturally enough, as the *advection-diffusion equation*. Again, in most applications \mathbf{u} is divergence-free so (1.27) becomes

$$(1.28) \quad \frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = \sigma(q) + \nabla \cdot (\alpha \nabla q) .$$

1.2.5. *Vector valued conservation laws*. Up to now we have considered that the conserved quantity is a scalar q . Often it is more convenient to group scalars together as a vector, for instance when thinking of the momentum of a body. The generalization of the conservation law (1.10) is immediate

$$(1.29) \quad \frac{\partial \mathbf{q}(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{q}(\mathbf{x}, t), (\mathbf{x}, t)) = \sigma(\mathbf{q}(\mathbf{x}, t), (\mathbf{x}, t)) .$$

Here the explicit dependence on space \mathbf{x} and time t of \mathbf{q} has been pointed out, as well as the possible dependence of the fluxes \mathbf{f} and sources σ on both space and time and the conserved variables $\mathbf{q}(\mathbf{x}, t)$. Note that $\nabla \cdot \mathbf{f}$ has a different meaning in the present context. As a result of taking the divergence we should still obtain

a vector quantity for (1.29) to be consistent. This means that \mathbf{f} is now a *tensor* of dimension $n \times n$ where n is the number of components of \mathbf{e} (and σ).

1.2.6. *Convection-diffusion equations.* In fluid flow, among other applications, the velocity field \mathbf{u} is related to the conserved quantities

$$(1.30) \quad \mathbf{u} = \mathbf{u}(\mathbf{x}, t, \mathbf{q}) .$$

This particular situation goes by the name of *convection*. Similar to (1.27) we can write a convection-diffusion equation

$$(1.31) \quad \frac{\partial q}{\partial t} + \mathbf{u}(q) \cdot \nabla q = \sigma(q) + \nabla \cdot (\alpha \nabla q) - q \nabla \cdot \mathbf{u}$$

and its vector valued generalization

$$(1.32) \quad \frac{\partial \mathbf{q}}{\partial t} + \mathbf{u}(\mathbf{q}) \cdot \nabla \mathbf{e} = \sigma(\mathbf{q}) + \nabla \cdot (\alpha \nabla \mathbf{q}) - \mathbf{q} \nabla \cdot \mathbf{u} .$$

1.3. Conservative and non-conservative forms. We have seen that a large class of differential equations are derived from conservation laws. The basic form of a conservation law is:

$$\text{time change} = -(\text{difference in outward fluxes}) + (\text{sources}).$$

In mathematical terms we have the local, differential formulation

$$(1.33) \quad \frac{\partial q}{\partial t} = -\nabla \cdot \mathbf{f}(q) + \sigma .$$

This is known as the *conservative form* of the law of conservation of q . The same principle of conservation might be stated differently if $\nabla \cdot \mathbf{f}(q)$ is expanded. For instance, when $\mathbf{f} = \mathbf{u} q$ we can derive from the conservative form

$$(1.34) \quad \frac{\partial q}{\partial t} = -\nabla \cdot (\mathbf{u} q) + \sigma$$

the mathematically equivalent form

$$(1.35) \quad \frac{\partial q}{\partial t} = -q \nabla \cdot \mathbf{u} - \mathbf{u} \cdot \nabla q + \sigma .$$

Eq. (1.35) is known as the *non-conservative form* of the conservation law for q . Though equivalent from the analytical point of view, the numerical solution procedures for the two forms show different characteristics as we shall see later on.

2. PDE's in other disciplines

Historically, most of the effort in studying PDE's has been directed at those suggested by mathematical physics and that somehow arise from a conservation law. Recently PDE's have been introduced in a number of other fields of study such as mathematical finance or ecology. For instance an important development in mathematical finance is the Black-Scholes equation describing the trading of European options

$$(2.1) \quad \frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S_t^2 \frac{\partial^2 V}{\partial s^2} + r S_t \frac{\partial V}{\partial s} - r V = 0$$

with V the value of an option, t time and s an asset allocation. Though such equations arise from different fundamental principles it is striking that they have the same form as those arising in mathematical physics. The Black-Scholes equation can be described as a mixed diffusion advection equation with a source term for example. We shall concentrate on a mathematical physics background in discussing

numerical solution of PDE's but keep in mind that the same methods are widely applicable.

3. Typical problems involving ODE's and PDE's

Now that we have arrived at the general form of PDE's which are of interest in many applications we can turn to actually finding solutions. An important first observation is that specifying the equation to be solved does not allow a unique solution. We must also specify additional *boundary* and/or *initial conditions*. Just as we have important special equations such as the advection or the Laplace equation, there are a number of important, archetypal problems involving ODE's and PDE's.

3.1. Initial value problem for ODE's. The simplest problem is the *initial value problem* for a first order system of ODE's

$$(3.1) \quad \begin{cases} \mathbf{q}' = \mathbf{f}(t, \mathbf{q}) \\ \mathbf{q}(t=0) = \mathbf{q}_0 \end{cases} .$$

This also encompasses initial value problems for ODE's of higher order since an ODE of order p can always be rewritten as a system of p ODE's of order 1. To exemplify, consider

$$(3.2) \quad q''' = g(t, q, q', q'') .$$

By introducing the auxilliary functions

$$(3.3) \quad r = q', \quad s = q''$$

we obtain the system

$$(3.4) \quad \frac{d}{dt} \begin{bmatrix} q \\ r \\ s \end{bmatrix} = \begin{bmatrix} r \\ s \\ g(t, q, r, s) \end{bmatrix}$$

which is of the form (3.1).

3.2. Boundary value problem for ODE's. For ODE's of order 2 or greater or for systems of two or more ODE's one can meaningfully impose boundary conditions at distinct points within the computational domain. The archetypal ODE boundary value problem is for a second order ODE with conditions at the end points of the computational domain

$$(3.5) \quad \begin{cases} q'' = f(t, q, q') \\ q(a) = q_1 \\ q(b) = q_2 \end{cases} .$$

Instead of the function values, its derivatives might be specified such as in

$$(3.6) \quad \begin{cases} q'' = f(t, q, q') \\ q'(a) = r_1 \\ q'(b) = r_2 \end{cases} .$$