3 Conservation Laws, Constitutive Relations, and Some Classical PDEs

As a topic between the introduction of PDEs and starting to consider ways to solve them, this section introduces conservation of mass and its differential form. For specific physical situations, constitutive relations must be introduced. We give here the basic advection, diffusion, and combined advection-diffusion cases that we will be working with throughout these Notes.

We have also included a brief discussion of shock conditions and boundary conditions, which we will cycle back to later in the course. On page 8 we give a summary of what you should try to get out of this section.

3.1 Background on Classical Models Involving PDEs: One Space Dimension

Most of the classical models come from the use of conservation principles and constitutive relations relevant to a physical situation being investigated. Assuming various limits hold, differential form of the principles lead to PDEs from which analysis can be done on them, and numerical approximations can be developed. It all boils down to the power of calculus in the end. We will illustrate some of these in the context of one space dimension.

Consider a single quantity (mass, energy, bugs, vehicles, a chemical in some non-moving fluid, or simply think of it as "stuff"), and let

$\rho = \rho(x,t)$ be the *density* of this quantity (mass per unit volume)

so the amount of this quantity at location x at time t is $\rho(x,t)Adx$, where we think of a thin tube of uniform cross-section of cross-sectional area A (see Figure 1).

Remark: We assume there is a large enough amount of our 'stuff' around to consider continuum ideas, that is, the quantities defined here exist, are continuous in its variables, and any limits employed are assumed to exist.

Next consider

$\phi = \phi(x,t)$ is the *flux* of our quantity at location x at time t.

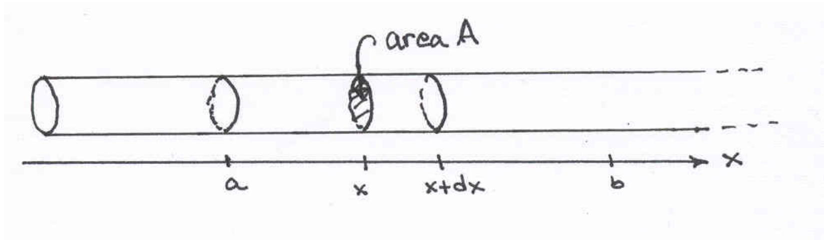

Figure 1: Domain image for the conservation argument

That is, it measures the amount of quantity crossing a unit section at x at time t per unit time. Thus, $A\phi(x,t)$ is the amount of our stuff crossing section of tube at x at time t. Let

$S = S(x,t)$=rate our stuff is being created at x per unit area at time t.

Now consider an arbitrary interval $[a,b]$. The conservation of mass law states that the rate of change of total amount of the quantity in a segment $[a,b]$ must equal the net rate at which it flows out of the interval, plus the rate at which it is being created/destroyed within the segment $[a,b]$. In symbols, since we assume A is constant,

$$\frac{d}{dt}\int_a^b \rho(x,t)Adx = A\phi(a,t) - A\phi(b,t) + \int_a^b S(x,t)Adx \tag{1}$$

or

$$\int_a^b \frac{\partial \rho}{\partial t}(x,t)dx = -\int_a^b \frac{\partial \phi}{\partial x}(x,t)dx + \int_a^b S(x,t)dx$$

or

$$\int_a^b \{\frac{\partial \rho}{\partial t}(x,t) + \frac{\partial \phi}{\partial x}(x,t) - S(x,t)\}dx = 0 \tag{2}$$

Lemma: Let f be a continuous function defined on an interval $[A,B]$. If, for every subinterval $(a,b) \subset [A,B]$, $\int_a^b f(x)dx = 0$, then $f \equiv 0$ in $[A,B]$.

Proof is left as an exercise.

Given that the interval (a,b) in (2) is arbitrary, then by the Lemma we have

$$\frac{\partial \rho}{\partial t}(x,t) = -\frac{\partial \phi}{\partial x}(x,t) + S(x,t) \tag{3}$$

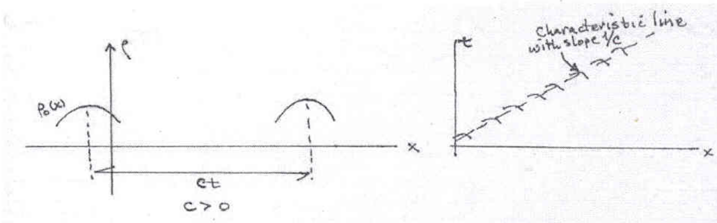

Figure 2: Pure advection is really a translating of initial data

So, at a location x the amount of stuff changes due to stuff moving around (first term on the right side) plus stuff being either created or destroyed (the second term on the right side). With $S \equiv 0$, (3) becomes the **differential form of the conservation principle**.

Remark: How is the equation changed if we assume instead that $A = A(x) \geq A_0 > 0$, i.e. A is not assumed constant?
While (1) is the codified conservation principle (when $S \equiv 0$), (3) is more restrictive form because of the continuity condition. However, it is (3) that is used in practice. Note that for the single equation (3) there are two unknowns, ρ and ϕ. This is where constitutive relations come in the modeling.

Now consider a few examples.

Example: ***pure advection*** *or* ***linear transport***: Let $S \equiv 0$ and the flux be proportional to the density: $\phi = c\rho$. (Constant c will have units of length over time so it is a *speed of propagation* of the signal.) Then (3) becomes

$$\frac{\partial \rho}{\partial t} + c\frac{\partial \rho}{\partial x} = 0. \tag{4}$$

Equation (4) is a first order, linear PDE, and represents pure advection of the initial disturbance $\rho(x, 0) = \rho_0(x)$. Hence, a solution to the equation is $\rho(x, t) = \rho_0(x - ct)$, assuming ρ_0 is a differentiable function defined on the whole real line. Such a solution is called a **traveling wave solution**, and represents a right-moving wave if $c > 0$, and a left-moving wave if $c < 0$. (See figure 2.)

Example: ***traffic flow theory***: In the most elementary version of traffic flow theory, ρ represents traffic density (the number of vehicles per unit length of highway), and ϕ is the traffic flow rate ($\phi(x,t)$ is the number of vehicles passing a given point x at time t). Here highway means a unidirectional roadway of infinite length, and with no entrances or exits (think of a very long tunnel or bridge). Then an "equation of state" (constitutive relation) might specify that flux is a function of density only, that is $\phi = \phi(\rho)$. A typical shape is given by figure 3. Now $\frac{\partial \phi}{\partial x} = \frac{d\phi}{d\rho}\,\frac{\partial \rho}{\partial x}$. Define the local wave speed as $c(\rho) := d\phi/d\rho$, then (4) becomes

$$\frac{\partial \rho}{\partial t} + c(\rho)\frac{\partial \rho}{\partial x} = 0 \quad . \tag{5}$$

This is a **nonlinear** first-order PDE for the traffic density (and is analogous to one-dimensional gas dynamics). We could consider incorporating entrances/exits by adding a source term S on the right-hand side of (5).

Example: ***Fickian diffusion***: Fick's law states that the flux is proportional to the gradient of the density. In its simplest form this implies $\phi = -D\frac{\partial \rho}{\partial x}$, where $D > 0$ is a constant *diffusivity coefficient*. So the flow, due to the sign convention, will go from places of high density to places of low density. Substituting this into (3) yields

$$\frac{\partial \rho}{\partial t} - D\frac{\partial^2 \rho}{\partial x^2} = S(x,t), \tag{6}$$

which is the (nonhomogeneous) **diffusion equation**.(See figure 4.)

Special case: the ***1D heat equation***

If one is concerned with measuring heat flow, then heat energy is measured through temperature u, in some material with material properties c, the *specific heat parameter*, and k, the *thermal conductivity*. Then ρ in (3) is replaced by $\rho c u$, here ρ notationally means a constant density of the material. Now the appropriate form of Fick's law, called Fourier's law (in one dimension), is $\phi = -k\partial u/\partial x$. Then, in the case of no heat sources, (3) becomes

$$\rho c\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left\{k\frac{\partial u}{\partial x}\right\}. \tag{7}$$

Equation (7) becomes equivalent to (6) (assuming k is a constant, and $S \equiv 0$) if we define $D := k/\rho c$. Then D is called the *thermal diffusivity*. We will

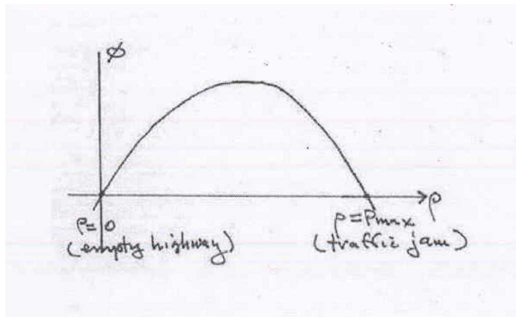

Figure 3: This is the fundamental graph of traffic theory

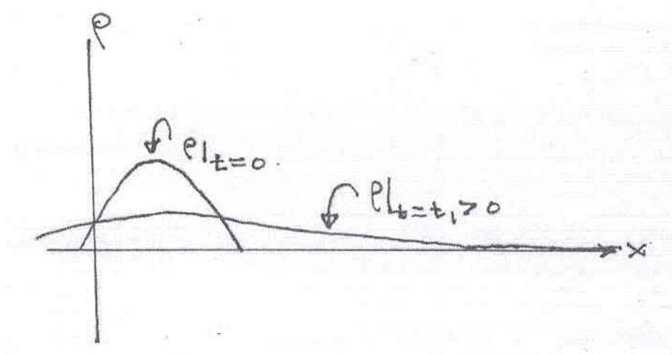

Figure 4: Diffusion spreads the data out, "forgetting" the information content in the data in the absence of source terms, i.e. $S \equiv 0$.

generally solve problem using the form of equation (6) rather than (7), but keep these definitions in mind.

Remark: There is a probabilistic approach to deriving the diffusion equation that starts with a random walk model. This leads into a notion of Brownian motion made famous by Einstein. Hence, at the microscale, diffusion is about random processes, while at the macroscale, where averaging has taken place, diffusion follows a conservation principle. The connection with random processes means there are strong connections between PDEs and probability theory (and hence application areas such as mathematical finance) that we will not have space to pursue in these Notes.

Example: ***advection-diffusion***: This case assumes we have both processes

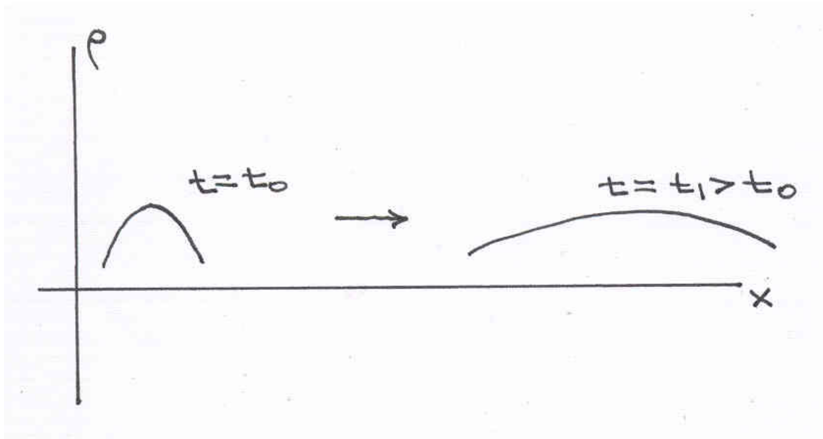

Figure 5: The combination of mechanisms tends to both translate and spread the initial data

working, so $\phi = \phi_{adv} + \phi_{diff} = u\rho - D\frac{\partial \rho}{\partial x}$, where u is a material speed parameter, D is a diffusivity. Here we might interpret the situation that a solute is being carried along (advected) with a bulk movement of fluid (solvent), say with fluid velocity $u = u(x,t)$, and ρ here means concentration. Now (3) becomes, with $S \equiv 0$,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(u\rho) = D\frac{\partial^2 \rho}{\partial x^2} \quad . \tag{8}$$

Example: ***Chemotaxis***: A large number of insects and animals rely on acute sense of smell for conveying information between members of the species, employing chemicals called pheromones. At the cellular level, motility of cells, such as in wound healing, is often controlled by specific chemical gradients. These cases lead to modeling a flux due to a chemical attractant (or repellent). In the presence of a gradient of attractant $a = a(x,t)$ (We'll stick to a one dimensional spatial description here, but the mechanism is particularly applicable in $\mathcal{R}^2$ or $\mathcal{R}^3$), gives rise to movement of cells, of density $u = u(x,t)$, up the gradient. This suggests a flux $J_{chemotaxis} = bu\ \partial a/\partial x$, where $b = b(a)$ is an affinity sensitivity coefficient that may depend on the attractant concentration. If we consider the total flux as $J = J_{diffusion} + J_{chemotaxis} = -D\partial u/\partial x + bu\partial a/\partial x$, then (3) becomes, again setting $S \equiv 0$, and letting

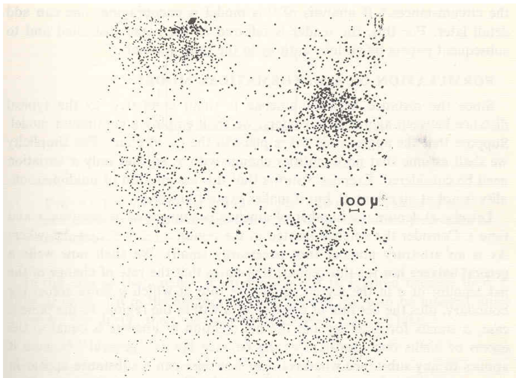

Figure 6: Population of amoebae beginning to aggregate via a chemical signal, i.e. chemotaxis. (Figure from Lin and Segel's *Mathematics Applied to Deterministic Problems in the Natural Sciences*.)

$b, D =$ constants,

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - b\frac{\partial}{\partial x}(u\frac{\partial a}{\partial x}).$$

In this case we would need an equation for the attractant, for example,

$$\frac{\partial a}{\partial t} = D\frac{\partial^2 a}{\partial x^2} + k_1 u - k_2 a.$$

Such systems lead to very interesting patterns of behavior. See a case of this in figure 6.

Example: ***1D diffusion of a population***: In population biology and other disciplines concerned with the growth and movement of "populations", there is usually a growth law (constitutive relation) under consideration. If $u(t)$ represents the population of some species at time t, a couple of dynamic law examples would be

1. Malthusian or exponential growth: $\frac{du}{dt} = ru$ (r=fixed net rate of growth)

2. Verhulst or logistic growth: $\frac{du}{dt} = ru(1 - u/u_{max})$

The second case recognizes limited resources so that unbounded growth is not possible (as in the Malthusian case). These models are further generalized to allow (random) movement of the population. The simplest cases are given by

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + ru \tag{9}$$

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + ru(1 - u/u_{max}) \tag{10}$$

Equation (9) will be easily solved by methods introduce in these Notes, partly to see what effect the ru term has on the solution behavior. Equation (10) is *Fisher's equation*, which was first investigated in the 1920's with regard to the propagation of an undesirable gene within a population. It is a nonlinear PDE, and one member of a large class of equations called **reaction-diffusion** equations that crop up in all sorts of science and engineering subdisciplines. However, techniques for analyzing such equations will not be developed in these Notes.

Summary
You should understand the basics of getting the differential form of the conservation principle. The Lemma will be used again later in the course, so you should know its statement. You should know what is meant by pure advection, diffusion, and advection-diffusion, and the character of the solutions as t increases.

Exercises

(1) In the 1D derivation of the derivative form of conservation law, (3), what would the analogous result if the cross-sectional area A is a smooth function of x, $A = A(x)$? What would the diffusion equation look like if $\phi = -k\partial\rho/\partial x$, with $k > 0$ being a constant, and $S \equiv 0$?

(2) In the pure advection case (4), if $c = 5$ and initially $\rho(x, 0) = \rho_0(x) = e^{-x^2}$, what would be the solution $\rho(x, t)$? Since $\rho_0(x)$ is a "Gaussian bump" moving out along a characteristic line, where is the top of the bump at time $t = 10$?