# ON THE DERIVATION OF PARTIAL DIFFERENTIAL EQUATIONS

ADAM BOUCHER

In this section of notes we will look over some more or less conventional approaches to deriving the classical partial differential equations of mathematical physics. We will begin with two different derivations of the heat/diffusion equation. The first derivation follows a standard argument using simple energy considerations and Fourier's law of heat conduction applied to a finite section of a uniform rod. The second derivation which is less common in mechanics and engineering, but which yields a valuable insight into the connection between the kinetic theory for molecular motion and the diffusion of heat. Here we adopt a stochastic description of a many particle system and we derive the diffusion equation by considering the probabilistic expectation of a particular continuum limit of the discrete system.

## 1. Heat Equation

Suppose we consider a finite section of some uniform material (such as a metal rod or wire), suppose further that some heat flux, $q(x,t)$, is permitted to enter and leave the material at the left and right sides.

Suppose (without any loss of generality) that we take a section centered at some point $x$, taking the section to occupy the interval $[x-\Delta x, x+\Delta x]$. If we define a positive heat-flux as left-moving, the the total flux through the ends of our section are given by:

$$Aq(x-\Delta x) - Aq(x+\Delta x)$$

(Signs are chosen to be consisten with the direction of the flux.)

Denoting the temperature of the bar $u(x,t)$ as a measure of the heat energy at a particular location we might approximate the total heat energy in our material section to be given by:

$$\rho c A 2\Delta x u(x,t)$$

where $\rho$ is the density of the material, $c$ is the heat capacity, $A$ is the cross sectional area. Assuming that the temperature lies in a restricted range so that $\rho$, $c$ and $A$ can be taken to be constant, the time rate of change of this heat energy would be given by:

$$\rho c A 2\Delta x \frac{\partial u}{\partial t}$$

In addition to the heat stored in the material, there may be additional sources or sinks of heat energy, which we will denote $Q(x,t)$ which will be a heat flux per unit volume and unit time, into (or out of) the material section. If we assume that these factors account

for all changes in heat energy, then we can set the rate of change of heat energy within the section equal to the sum of the imposed heat contributions:

$$\rho c A 2\Delta x \frac{\partial u}{\partial t} = Aq(x-\Delta x) - Aq(x+\Delta x) + 2A\Delta x Q(x,t)$$

Dividing out the $A2\Delta x$ yields a spatial difference quotient in the boundary flux:

$$\rho c \frac{\partial u}{\partial t} = -\frac{q(x+\Delta x) - q(x-\Delta x)}{2\Delta x} + Q(x,t)$$

If we assume the physical constants to be known then we still need some constitutive law which connects the boundary heat flux to the current heat levels of the neighboring section. Fourier's Law states that this heat flux is proportional to the temperature differences between adjacent sections, with some constant of proportionality:

$$q = -k\frac{\partial u}{\partial x},$$

the value of $k$ may be constant or variable, depending upon the geometry or material properties (i.e. a rod with variable cross section will have greater heat flux between sections with wide cross sectional boundaries and lower heat flux between sections with small cross sectional boundaries.) Substituting this into our heat balance yields:

$$\rho c \frac{\partial u}{\partial t} = \frac{ku_x(x+\Delta x) - ku_x(x-\Delta x)}{2\Delta x} + Q(x,t)$$

Next by assuming that $ku_x$ is sufficiently regular and taking $\Delta x \to 0$ we derive the non-homogeneous (possibly variable coefficient heat equation in one spatial dimension.

$$\rho c \frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[k\frac{\partial u}{\partial x}\right] + Q(x,t)$$

## 2. Heat Equation-Stochasic Derivation

Here I give an alternate derivation of the heat equation which does not require the leap of faith required by using Fourier's law, but does require the use of a distinguished limit.

We begin with a description of a random process (which might be though of as a statistical model for the motion of a single molecule of gas.)

Suppose that we have a particle undergoining a discrete random walk on a discrete lattice. We will make observations of this particle at discrete time-steps $\Delta t$, and we will discretize space by 'binning' the real line into bins with width $\Delta x$. Without any loss of generality we assuming that whenever our particle starts in a bin centered at some point $x_n = n\Delta x$, the particle moves around according to an imposed probability distribution, which is linked to our time steps in the following way:

Let $X[t_n]$ be a discrete random variable denoting the location of our particle at time $t_n$. Then we suppose:

$$X[t_{n+1}] = \begin{cases} X[t_n] + 1, & \text{with probability } \frac{1}{4}, \\ X[t_n], & \text{with probability } \frac{1}{2}, \\ X[t_n] - 1, & \text{with probability } \frac{1}{4}, \end{cases}$$

This means that during a single time step our particle might stay still, move left, or move right. We assume that it moves half of the time, and has no bias either way. Notice that when we look at a single particle we see that at each time-step the expected position of that particle remains the same, so on average a particle should remain in the same position. Next if we consider a large finite collection of different particles, and we assume their motions are all independent, we can use this base model to derive a difference equation for the **average** number of particles to expect in a given position based upon the distribution of particle during the previous time-step.

Skipping the details, and defining $w(x_n, t_n)$ as the number of particles in bin $x_n$ at time $t_n$ we obtain the following difference equation:

$$w(x_n, t_{n+1}) = \frac{1}{4}w(x_{n-1}, t_n) + \frac{1}{2}w(x_n, t_n) + \frac{1}{4}w(x_n, t_n)$$

Note that this is a deterministic difference equation, this describes the evolution of averages which removes all of the stochastic nature of the original model. If the number of particles is very large, then we might study this equation to understand the normal or expected behavior of these particles in an ensemble. Furthermore, if $\Delta t$ and $\Delta x$ are sufficiently small, we may further wish to look at this problem in the continuum limit. This will allow us to pass from a difference equation on a large lattice to a partial differential equation. If we suppose that $w(x,t)$ is sufficiently smooth, then we might try to expand each of the terms in our difference equation using a Taylor series for either small $\Delta t$ or small $\Delta x$. The first few terms of each of the relevant series are given by:

$$\begin{aligned} w(x, t + \Delta t) &\approx w(x,t) + \Delta t w_t(x,t) + O(\Delta t^2) \\ w(x + \Delta x, t) &\approx w(x,t) + \Delta t w_x(x,t) + \frac{\Delta x^2}{2} w_{xx}(x,t) + O(\Delta x^3) \\ w(x - \Delta x, t) &\approx w(x,t) - \Delta t w_x(x,t) + \frac{\Delta x^2}{2} w_{xx}(x,t) + O(\Delta x^3) \end{aligned}$$

Substituting these expansions into our difference equation yields the following:

$$\begin{aligned} w(x,t) + \Delta t w_t(x,t) + O(\Delta t^2) = &\frac{1}{4}\left( w(x,t) - \Delta t w_x(x,t) + \frac{\Delta x^2}{2} w_{xx}(x,t) \right) + \frac{1}{2} w(x,t) \\ &+ \frac{1}{4}\left( w(x,t) + \Delta t w_x(x,t) + \frac{\Delta x^2}{2} w_{xx}(x,t) \right) + O(\Delta x^3) \end{aligned}$$

Summing like terms and canceling the opposite sign terms on the right we have:

$$\Delta t w_t(x,t) + O(\Delta t^2) = \frac{1}{2}\frac{\Delta x^2}{2} w_{xx}(x,t) + O(\Delta x^3)$$

Next we divide by $\Delta t$, and collect our error terms on the right hand side:

$$w_t(x,t) = \frac{1}{2}\frac{\Delta x^2}{2\Delta t} w_{xx}(x,t) + \frac{O(\Delta x^3)}{\Delta t} - O(\Delta t)$$

If we take a distinguished limit so that:

$$\lim_{\Delta x \to 0} \lim_{\Delta t \to 0} \frac{\Delta x^2}{2\Delta t} = k \in \mathbb{R}$$

Then we obtain the diffusion equation at leading order.

$$w_t(x,t) = k w_{xx}(x,t) + O(\Delta x) + O(\Delta t)$$

Thus, we can use the heat equation to describe the evolution of the average concentration of a large number of particles undergoing unbiased, independent random motion...this is why the equation is described as both the heat and the diffusion equation. Additional deep connections between diffusion and random walks may also be derived. Lin and Segel gives a brief overview.

## 3. Wave Equation

My derivation of the wave equation will follow a pretty standard application of force balances, and will follow the same pattern as the derivation of most models in solid-mechanics. We begin by finding the kinematic equations of equilibrium, then we pass to a dynamic problem by using some type of minimization principle or energy consideration. For the one dimensional wave equation, we can just attempt to use Newton's second law at each material point.

We begin by assuming that we have a thin string under tension. The assumption of 'thinness' asserts that the position of the string can be adequately described by a one-dimension function (or space curve if we permit two dimesional deflections). We permit the string to move upward and downward with respect to a uniform gravitational field, but we neglect and transverse or longitudinal displacements. These assumptions make the physical domain two dimensional. If we assume that the tensioned string is in static equilibrium, this imposes a balance of horizontal forces and a balance of vertical forces.

If the tension in the string is given by a function $T(x)$, then the horizontal component of tension must be constant. Using the angular deflection of the string at each point to split the tension into component parts we have:

$$T(x)\cos(\theta(x)) = T_o$$

Assuming that the string has some finite mass distribution $\rho$, we can balance the vertical component of the tension with the gravitational forces acting on each segment of string:

$$T(x+\Delta x)\sin(\theta(x+\Delta x)-T(x)\sin(\theta(x))=\rho(x)g\Delta s$$

where $\Delta s$ is the arclength of the string contained within the segment of interest. Using the constant horizontal tension, and considering the ratio with the width of the segment.

$$T_o\frac{\tan(\theta(x+\Delta x)-\tan(\theta(x))}{\Delta x}=\rho(x)g\frac{\Delta s}{\Delta x}$$

Now the tangent of the angular deflection is exactly the slope of the vertical displacement, $\tan(\theta(x))=\frac{du}{dx}$. so we obtain:

$$T_o\frac{d^2u}{dx^2}=\rho(x)g\frac{ds}{dx}$$

If we linearize the arclength, which is equivalent to assuming the squared slope is negligible with respect to unity, we end up with a non-homogeneous ordinary differential equation for the equilibrium position of the string.

$$T_0\frac{d^2u}{dx^2}=\rho(x)g$$

This equation yields the force balance between the string tension and gravity. To pass to a dynamic version of the equation, we need an appropriate notion of how the configuration of the string influences it's behavior. To derive the dynamic version of the problem we assume that the internal energy of a string under tension is due completely to longitudinal stretching of the string. This leads us to the following measure of the internal energy of the string:

$$U=\mu\int_0^L\sqrt{1+\frac{\partial u}{\partial x}^2}-1dx$$

This described the internal energy due to the system's current configuration. We append a measure of the strings kinetic energy over the same section to find:

$$KE=\int_0^L\frac{1}{2}\rho\left|\frac{\partial u}{\partial t}\right|^2dx$$

From here we can apply Hamilton's principle to deduce that the actual trajectory of the motion is a minimizer of the action functional:

$$J=KE-U$$

$$J=\int_0^T\int_0^L\frac{1}{2}\rho\left|\frac{\partial u}{\partial t}\right|^2-\mu\left(\sqrt{1+\frac{\partial u}{\partial x}^2}-1\right)dxdt$$

To extract a partial differential equation from this problem we apply a beautiful argument from the Calculus of variations. The basic idea of the argument is to extract a necessary

condition for the trajectory of the string (which becomes the governing PDE) by introducing a perturbation to the argument of this functional which depends upon a scalar parameter. With the minimizer and the perturbation function fixed, the action functional becomes a real valued function subject to the techniques and theorems of single variable calculus.

Suppose that $u$ is a minimizer for the functional $J$. Then

$$J(u(x,t)) \leq J(u(x,t) + \epsilon\eta(x,t)),$$

for any appropriate choice of perturbation function $\epsilon\eta$. Substituting this argument into our functional yields:

$$J(u+\epsilon\eta) = \int_0^T \int_0^L \frac{1}{2}\rho \left|u_t + \epsilon\eta_t\right|^2 - \mu\left(\sqrt{1+\left(u_x+\epsilon\eta_x\right)^2} - 1\right) dxdt$$

Now if $u$ is actually a minimizer (even just a local minimizer) then if $u$ and $\eta$ are taken to be fixed, then $\epsilon = 0$ must be a critical point if we view this thing as a function of $\epsilon$. From calculus 1, we deduce that the $\epsilon$-derivative of this expression must be zero when we evaluate at $\epsilon = 0$. Differentiating this integral yields:

$$\frac{dj}{d\epsilon} = \int_0^T \int_0^L \rho\left(u_t + \epsilon\eta_t\right)\eta_t - \mu\frac{u_x+\epsilon\eta_x}{\sqrt{1+\left(u_x+\epsilon\eta_x\right)^2}}\eta_x dxdt$$

Evaluating at $\epsilon = 0$ yields a somewhat simplified expression:

$$\int_0^T \int_0^L \rho\left(u_t\right)\eta_t - \mu\frac{u_x}{\sqrt{1+\left(u_x\right)^2}}\eta_x dxdt = 0$$

Next, we assume that these integrals are both uniformly convergent so that the order of integration may be switched. Then integrating by parts in time for the first term, and integrating by parts in space for the second term we obtain:

$$\int_0^T \int_0^L -\frac{\partial}{\partial t}\left[\rho u_t\right]\eta + \mu\frac{\partial}{\partial x}\left[\frac{u_x}{\sqrt{1+\left(u_x\right)^2}}\right]\eta dxdt + B.T. = 0$$

Now if we select $\eta \in C_0^\infty(0,L)$ so that it is zero at both boundaries, then the boundary terms from integration by parts vanish.

$$\int_0^T \int_0^L \left[-\frac{\partial}{\partial t}\left[\rho u_t\right] + \mu\frac{\partial}{\partial x}\left[\frac{u_x}{\sqrt{1+\left(u_x+\epsilon\eta_x\right)^2}}\right]\right]\eta dxdt = 0$$

Since $C_0^\infty(a,b)$ is dense in $L^2(a,b)$, and nothing in this argument depended upon $\eta$ specifically, we can conclude by the standard variational lemma, that:

$$-\frac{\partial}{\partial t}\left[\rho u_t\right] + \mu \frac{\partial}{\partial x}\left[\frac{u_x}{\sqrt{1+(u_x)^2}}\right] = 0, \qquad a.e. in (a,b)$$

Linearizing for small slope, we obtain the wave equation in one dimension.

## 4. Deriving Weak Solution Formulation

Normally when we think of partial differential equations, the partial differential equation is the central object of study. In the derivations above the partial differential equation is derived by passing from the laws of physics (often conservation principles) over regions of space to point-wise descriptions of appropriate force or energy balances. In the case of Hamilton's principle, we assert that the solution is a minimizer of an appropriate action functional. In a great deal of modern theory for partial differential equations, we find that classical solutions satisfying the PDE at every point in the domain do not exist, and we must weaken our expectations accordingly. The concept of a weak or variational solution (these terms are used almost interchangably) is central to understanding modern analytical theory of PDE's and to understanding the Galerkin method which provides the theoretical framework for understanding the method of finite elements.

Suppose we have the Poisson equation:

$$-u_{xx} - u_{yy} = f(x,y)$$

Requiring this equation be satisfied at every point in space and time may be too restrictive (for example if our initial conditions do not satisfy our boundary conditions, we cannot expect both to be true simultaneously). So in order to weaken this restriction, we might only require that this equation hold in an average sense. The technicality comes in when we try to characterize what we mean by average, we might consider a spatial average, a temporal average, or a combination of both. In order to capture different averages we introduce the idea of a test function $v(x,t)$. The $v(x,t)$ could be an indicator function whose value is 1 in the region we wish to average over, however because of the difficulty introduced by having jumps in the test function, it turns out to be much easier to assume that $v(x,t)$ is smooth. So to enforce a weaker version of this problem we might only require:

$$\int_\Omega (-u_{xx} - u_{yy}) v dx dt = \int_\Omega f v dx$$

for all suitable test functions. When starting out we typically require that $v(x,t)$ are drawn from $C_0^\infty(\Omega)$, that is the set of infinitely differentiable functions with support (non-zero values) contained within the spatial domain. This ensures that we only begin by requiring that interior averages hold. As written this formulation looks more complicated than the original differential equation, but in many cases it is much easier to analyze.

Now if $v$ is smooth, we might be tempted to manipulate this integral equation by integrating by parts. Since $v$ has compact support, the boundary terms from integration by parts will be identically zero giving:

$$\int_\Omega u_x v_x + u_y v_y dx = \int_\Omega f v dx$$

Now suppose that $u$ is actually a viable test function (it won't generally be in the class $C_0^\infty(\Omega)$, but it will often be in the closure of this class under certain norms). Then the equation reads:

$$\int_\Omega u_x^2 + u_y^2 dx = \int_\Omega f u dx$$

There are three interesting things about this equation, the first is that the left hand-side looks an awful lot like the Euclidean norms we studied, with the addition of some derivatives. The second thing is that this equation only refers to the first derivative of $u$ and doesn't contain any second derivatives. The third interesting thing is that the right hand side looks like an inner product.