The Diffusion Equation

Sushruth Reddy

May 1, 2015

1 Introduction

The diffusion equation is a partial differential equation modeling the diffusion of particulate matter over both space and time. When applied to heat transfer, it is often called the heat equation. Herein, we derive the form of the diffusion equation and solve it analytically in a few cases of interest.

2 Fickian Diffusion

Fickian diffusion is described by

$$\vec{J}(x, y, z) = -D\nabla f(x, y, z) \tag{1}$$

where $\vec{J}$ is the concentration flux (the net number of particles escaping a certain region per unit volume per unit time), D is the (medium- and particle-specific) diffusivity, and f is the concentration of particles at (x, y, z). Intuitively, we may explain this behavior as follows: The defining characteristic of the gradient is that it satisfies $df = \nabla f \cdot d\vec{r}$. df is thus maximized when $d\vec{r}$ points in the same direction as ∇f, implying that the gradient specifies the "direction of greatest increase". Thus, Fick's law states that particles tend to diffuse in the direction where there are fewest particles, corresponding to our intuition. The diffusivity controls the mobility of the particles.

However, Fick's law falls prey to the same shortcomings that befall other constitutive equations (such as $V = IR$ and Hooke's Law). It is important to note that the above formulation of Fick's law assumes that the medium in which the particles are suspended is *isotropic*, or that it possesses similar material properties in all directions in the vicinity of a point. The law is also *local*, in the sense that it only holds true over a small region, as in reality, the diffusion constant D may not be constant across space. Both of these assumptions can be remedied, the first by replacing D with a tensor, and the second by replacing D with a scalar function of (x, y, z), but these modifications make it extremely difficult to deal with the diffusion equation analytically.

In the context of heat flow, we have the analogue of Fick's Law, Fourier's law, with $\vec{q}$ (the heat flux density), k (thermal conductivity), and T (temperature) taking the place of $\vec{J}$, D, and f, respectively.

3 A Derivation of the Diffusion Equation

To derive the diffusion equation, we start out with the idea of a *control volume*, an imaginary, fixed region of space, which we here designate V. It is not difficult to see that the rate of change of the number of particles within V is

$$\frac{d}{dt}\iiint_V f(x, y, z)dV$$

However, this rate of change must be equal to the sum of inwards concentration fluxes over the boundary (as the only possible changes in the number of particles in V are attributable to particles crossing the boundary of V, ∂V)! Thus, switching the sign to use the outward normal, we have

$$\frac{d}{dt}\iiint_V f(x, y, z)dV + \oiint_{\partial V} \vec{J} \cdot d\vec{S} = 0$$

We could now substitute the form of the flux $\vec{J}$ stipulated by Fick's law and use the divergence theorem to derive the desired result, but this robs us of an opportunity to see why the divergence theorem is morally true. Many textbooks define the divergence of the vector field $F = P\hat{i} + Q\hat{j} + R\hat{k}$ by saying $\nabla \cdot F = \frac{\partial P}{\partial x} + \frac{\partial Q}{\partial y} + \frac{\partial R}{\partial z}$, but it then becomes annoying to derive the divergence theorem. It is much more lucrative to define the divergence as

$$\nabla \cdot F = \lim_{\Delta V \to 0} \frac{1}{\Delta V} \oiint_{\partial V} F \cdot d\vec{S}$$

It then becomes clear that the divergence measures how much flux F produces at a specific point, and the divergence theorem becomes obvious, as a sum of small changes across tiny volumes must equal the net change of a quantity across a region of space. Another advantage of this approach (and our entire treatment so far) is that it is coordinate-independent: this definition can be used to calculate the formula for the divergence in any coordinate system with equal generality. But we digress...dividing by ΔV and taking the limit as the volume goes to 0, we now have the diffusion equation:

$$\boxed{\frac{\partial f}{\partial t} = D\nabla^2 f}$$

4 Solving the Diffusion Equation in 1 dimension

So now we have the diffusion/heat equation: $f_t = Df_{xx}$. How can we use this to actually model the flow of particles in some physical situation? We have to ensure that our differential equation encapsulates all the information associated with our physical problem in order to make accurate predictions about physical phenomena. Specifically, in order for our problem to be *well-posed*, we must be able to demonstrate the existence and uniqueness of the solution to our problem (there is a third condition too, that the solution depends continuously on initial conditions, but we do not consider this difficulty here). We will demonstrate existence constructively, and uniqueness a little later on.

4.1 Finite Intervals

We consider the heat equation on the interval $[0, L]$. Our initial condition is $f(y; 0) = \phi(x)$, and we will initially make our boundary conditions $f(0; t) = f(L; t) = 0$ for all t, for simplicity. Then, we wish to solve:

$$\frac{\partial}{\partial t} f(x;t) = \alpha \frac{\partial^2}{\partial x^2} f(x;t)$$

4.1.1 A Brief Tangent

This is extremely reminiscent of the finite dimensional problem of solving the system of coupled linear equations

$$\frac{d}{dt}\bar{x}(t) = A\bar{x}(t)$$

along with some initial condition $\bar{x}(0)$, where A is some linear matrix operator. Let us first study this related problem. We may go ahead and multiply by the integrating factor e^{-At} to get:

$$e^{-At}\frac{d}{dt}\bar{x}(t) - Ae^{-At}\bar{x}(t) = \frac{d}{dt}(e^{-At}\bar{x}(t)) = 0$$

This implies that

$$e^{-At}\bar{x}(t) = \bar{c}$$

for some fixed vector $\bar{c}$. Plugging in $t = 0$, we recognize that $\bar{c} = \bar{x}(0)$, giving us:

$$\boxed{\bar{x}(t) = e^{tA}\bar{x}(0)}$$

Now, our task is to interpret the meaning of e^{tA}. The exponential is defined algebraically, via taylor series. However, more profoundly, a matrix can in general be characterized by its eigenvalues and eigenvectors (eigenvalues are λ for which there is an associated eigenvector $\bar{v}$ such that $A\bar{v} = \lambda\bar{v}$). Matrix multiplication behaves like scalar multiplication by λ in the direction of the associated eigenvector. If the eigenvectors span our space, we can consider writing an arbitrary vector as a linear combination of our eigenvectors (the eigenbasis), and then linearity allows us to easily compute the action of A on our vector. This kind of "independence" of our eigenvectors allows us to write:

$$e^{tA}(c_1\bar{v_1} + c_2\bar{v_2} + \cdots + c_n\bar{v_n}) = c_1e^{t\lambda_1}\bar{v_1} + \cdots + c_ne^{t\lambda_n}\bar{v_n}$$

where $\bar{v_i}$ are the eigenvectors associated with the eigenvalues λ_n. This solves our system problem neatly.

4.1.2 Some Wishful Thinking

Let us apply our previous mode of thinking to the operator ∂_{xx}. The difference between this and the last case is that this operator cannot be written as a matrix, as it takes functions to functions and not finite vectors to finite vectors. However, functions can be thought of infinite vectors of data, with each "entry" giving the function value at a point, and so we can think of operators as infinidimensional matrices. Let's just assume this viewpoint works. We can then write:

$$f(x;t) = e^{\alpha t\frac{d^2}{dx^2}}\phi(x)$$

As before, assuming this makes sense, it makes sense to study the eigenvectors of $e^{\alpha t \frac{d^2}{dx^2}}$, which will be identical to those of $\frac{d^2}{dx^2}$. These will satisfy the (differential) equation

$$\frac{d^2 g}{dx^2} + \lambda g = 0$$

Notice that the eigenvalue here is $-\lambda$ [1]. It is a standard calculation to show that all such g are given by $g = c_1 \sin(\sqrt{\lambda} x) + c_2 \cos(\sqrt{\lambda} x)$ where c_1 and c_2 are real constants. However, very few of these functions will be physically meaningful for us. As before, we want to express our initial condition $f(x; 0)$ as a linear combination of functions of this form. Here, we enforce our boundary conditions: $\phi(0) = \phi(L) = 0$ allows us to enforce $g(0) = g(L) = 0$. The first condition gives us $c_2 = 0$ and the second gives us $\sin(\sqrt{\lambda} L) = 0$ or $\lambda = \frac{k^2\pi^2}{L^2}$ for some integral k.

We can thus say that our eigenbasis is given by $\{\sin(\frac{k\pi x}{L})\}_{k=1}^{\infty}$. As our eigenvalue, as we noted before, was $-\lambda$, we can write our solution as:

$$\boxed{f(x;t) = \sum_{k=1}^{\infty} c_k e^{-\frac{\alpha k^2 \pi^2 t}{L^2}} \sin\left(\frac{k\pi x}{L}\right)}$$

The weights c_k, as usual with differential equations, will be determined by using our initial conditions. Specifically, we must express an arbitrary function $\phi(x)$ in our (Fourier) sine basis:

$$\phi(x) = \sum_{k=1}^{\infty} c_k \sin\left(\frac{k\pi x}{L}\right)$$

Although it's difficult to motivate, it turns out that in fact, we can find:

$$\boxed{c_k = \frac{2}{L} \int_0^L \phi(x) \sin\left(\frac{k\pi x}{L}\right) dx}$$

This follows neatly from the orthogonality of our eigenbasis with respect to an inner product over $[0, L]$:

$$\int_0^L \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}\delta_{mn}$$

which can be motivated more deeply via the study of hermitian operators. We do not have sufficient time here, so we do not go into details.

5 Problems

1. Calculate the fourier coefficients c_k for initial condition $\phi(x) = \sin(\pi x)$ over [0, 1]. What does the solution look like over time?
2. Solve the 1-dimensional heat equation with boundary conditions $f(0) = a$, $f(L) = b$. (Hint: convert this problem to one you know how to solve).
3. Solve the heat equation for with circular ring geometry. (Hint: Define f on the real line such that $f(x+1) = f(x)$)
4. How do you suppose one would extend the analytic solution to the 1-D heat equation to multiple dimensions (e.g. within the unit cube)? What is an orthogonal basis for $\mathcal{L}^2([0,1]^3)$)

[1] This was done for a reason. If the eigenvalue were positive, our boundary conditions would force $c_1 e^{L\sqrt{\lambda}} + c_2 e^{-L\sqrt{\lambda}} = 0$, implying $c_1 = c_2 = 0$