Two

The Diffusion Equation

2.1 An Introduction to Heat Flow

A classical example of the application of ordinary differential equations is Newton's Law of Cooling which, basically, answers the question *"How does a cup of coffee cool?"* Newton hypothesized that the rate at which the temperature, $U(t)$, changes is proportional to the difference with the ambient temperature, which we call $\bar{U}$,

$$\mathbb{DE}: \qquad \frac{dU}{dt} = -\kappa(U - \bar{U}). \tag{2.1}$$

Here κ is a positive rate constant (with units of inverse time) that measures how fast heat is lost from the coffee cup to the ambient environment. If we specify the initial temperature,

$$\mathbb{IC}: \qquad U(0) = U_0, \tag{2.2}$$

we can solve for the evolution of the temperature,

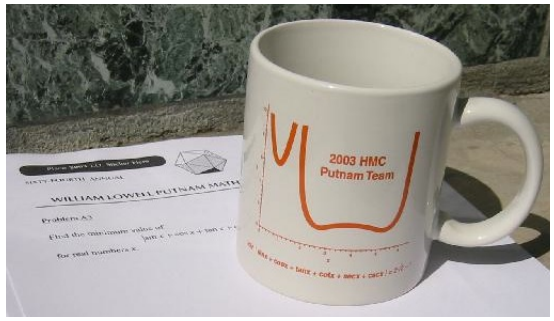
$$\boxed{U(t) = \bar{U} + (U_0 - \bar{U})e^{-\kappa t}.} \tag{2.3}$$

If we graph the temperature as a function of time, we see that it decays exponentially to the ambient temperature, $\bar{U}$, at a rate governed by κ.

When we derived Newton's Law of cooling we made several assumptions – most importantly that the temperature in the coffee cup did not vary with location. If we account for the variation of temperature with location, we can derive a PDE called the *heat equation* or, more generally, the *diffusion equation*. If the temperature, $U(x,t)$ is a function of a single spatial variable, x, we will show that it satisfies the diffusion equation,

$$U_t = DU_{xx},$$

(a)



(b)

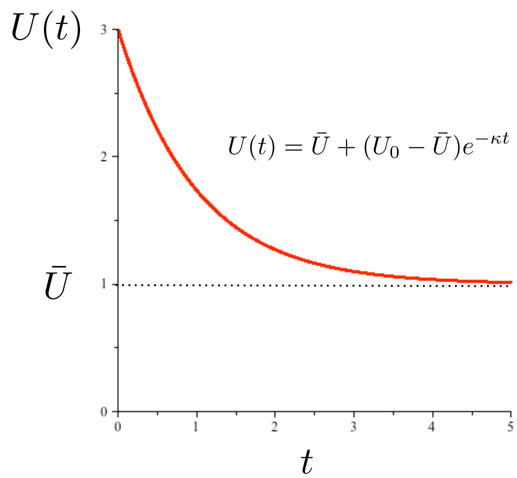


Figure 2.1: Newton's Law of Cooling. (a) A coffee cup (b) Coffee temperature as a function of time.

where D is a constant known as the thermal diffusivity. In higher dimensions, the equation can be written

$$U_t = D\nabla^2 U,$$

where ∇^2 is the *Laplacian*.

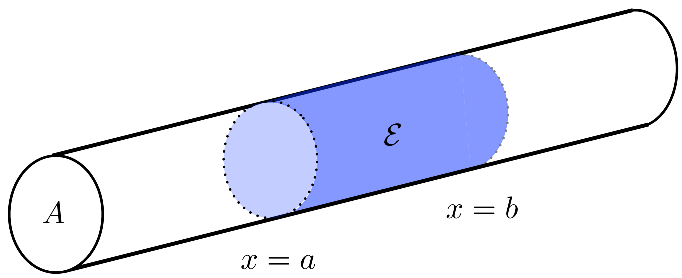


Figure 2.2: Thermal energy $\mathcal{E}$ in a metal bar of cross-sectional area A.

2.2 Derivation of the Diffusion Equation

The diffusion equation will be our second example of a conservation law; we can derive the equation by accounting for the flow of thermal energy. Suppose we consider a metal bar, with a uniform cross-sectional area, A, whose temperature, $U(x,t)$, is a function of time, t, and the position, x, along the bar (that is we assume the temperature is uniform in every cross-section).

Let the thermal energy in the region $a < x < b$ is given by

$$\mathcal{E} = \rho_0 c_m A \int_a^b U(x,t)\, dx \tag{2.4}$$

The important term in the integral is the temperature, $U(x,t)$, measured in degrees. The remaining constants are A, the cross-sectional area (with units of [(length)^2]); ρ_0, the density [mass/(length)^3]; and c_m, the specific heat capacity per unit mass [energy/(degree $\cdot$ mass)]. Note c_m is the amount of energy needed to raise one gram of a substance one degree - it is sometimes call just the specific heat (but you need to be careful to distinguish between specific heat of an object, specific heat per unit mass and specific heat per unit volume). Note that ρ_0 and c_m are physical properties of the material, while A is determined by the geometry.

We wish to equate the change in thermal energy to the heat flux out of the bar through the planes at $x = a$ and $x = b$. To do this we use *Fourier's heat law* which states that the flux density (with units of [energy/((length)^2$\cdot$time)]

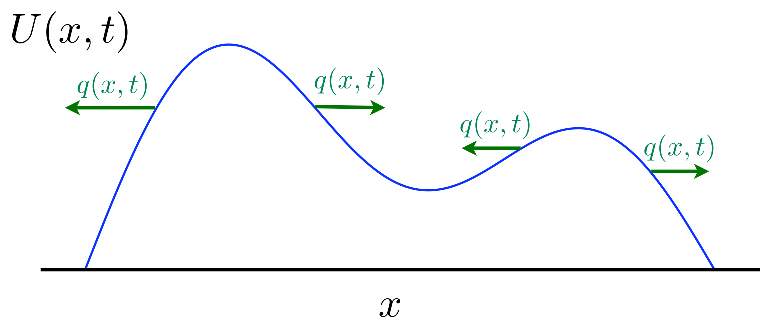


Figure 2.3: Heat flux is from hot to cold and proportional to the gradient.

of thermal energy, $q(x,t)$ is proportional to the temperature gradient,

$$q(x,t) = -kU_x, \tag{2.5}$$

where the negative sign reflects the fact that heat flows from hot to cold, just as in Newton's law of cooling, with a constant of proportionality, k, called the thermal conductivity [(energy)/(length·degrees·time)].

Now, the total flux of thermal energy into the *into* the region $a < x < b$ is given by

$$Q = A[q(a,t) - q(b,t)], \tag{2.6}$$

where we multiply by the area A to get the total flux through the cross-section.

By *conservation of energy*, the rate of change of the energy between a and b is given by the flux into the region,

$$\frac{d\mathcal{E}}{dt} = Q. \tag{2.7}$$

Once again we can rewrite the flux by a clever application of the fundamental theorem of calculus,

$$Q = A[q(a,t) - q(b,t)] = -\, Aq(x,t)|_{x=a}^{x=b} \tag{2.8}$$

$$= -A\int_a^b q_x \, dx. \tag{2.9}$$

We now rewrite the conservation of energy equation as

$$\frac{d\mathcal{E}}{dt} = \frac{d}{dt}\left[\rho c_m A \int_a^b U \, dx\right] = \int_a^b \rho c_m A U_t \, dx = Q = -A \int_a^b q_x dx, \tag{2.10}$$

or, rearranging

$$\int_a^b \rho c_m A \, U_t + A q_x \, dx = 0. \tag{2.11}$$

Since this is true for *every* interval $a < x < b$, the integrand must vanish identically. So

$$\rho c_m A U_t + A q_x = 0. \tag{2.12}$$

Substituting for the flux function $q(x,t) = -kU_x$ yields

$$\rho c_m A U_t - kA(U_x)_x = 0. \tag{2.13}$$

Rearranging the equation yields the diffusion equation,

$$\boxed{U_t = D U_{xx},} \tag{2.14}$$

where $D = k/(\rho c_m)$ is a constant with units of [(length)^2/time] called the *thermal diffusivity* which is determined by the physical properties of the metal bar.

Exercise 2.1. The thermal diffusivity is an example of a *diffusion constant*; verify the units of D and explain why they are consistent with the Diffusion equation 2.14. Find the value of D for an iron bar and an aluminum bar; can you explain physically the difference?

2.2.1 Initial conditions and Boundary Conditions

To complete the description of the problem, we need to supplement the diffusion equation with boundary conditions and initial conditions. Suppose we consider a bar of finite length L, occupying the region $0 < x < L$. At the boundaries of the metal bar we can specify a fixed temperature,

$$U(0,t) = U_0 \qquad U(L,t) = U_1, \tag{2.15}$$

which are usually referred to as *Dirichlet* boundary conditions. Alternatively, we could specify a heat flux,

$$q_0 = q(0,t) = -kU_x(0,t) \qquad q_1 = q(L,t) = -kU_x(L,t). \tag{2.16}$$

Specifying the gradient across the boundary is referred to as *Neumann* boundary conditions.

Finally, we also need to specify the initial temperature distribution,

$$U(x,0) = f(x) \qquad 0 < x < L. \tag{2.17}$$

We will demonstrate below that the solution to this problem (if it exists) is unique; later in this course we will solve this problem using the method of separation variables.

For completeness, we also comment here that the problem can be posed on the infinite line, $-\infty < x < \infty$ sometime called the *Cauchy* problem – in this case one usually replaces the boundary condition with the specification that the temperature remains bounded as we approach infinity,

$$\lim_{x \to \pm\infty} |U(x,t)| < C, \tag{2.18}$$

for some constant C. This condition may seem superfluous at first glance, but actually is necessary to stop heat from leaking in from infinity (speaking very, very informally an infinite source of heat infinitely far away can have a finite effect in a short amount of time). If you are interested in details, look for the examples of Tychonov in a PDEs text[1].

2.3 Examples of Solution to the Diffusion Equation

We can summarize the last section by restating a well-posed problem for the diffusion equation on the interval $0 < x < L$ with Dirichlet boundary conditions,

The Dirichlet Problem for the Diffusion Equation (Inhomogeneous Boundary Conditions)

$$\begin{array}{rccl}
\mathbb{DE}: & U_t = DU_{xx} & & 0 < x < L, t > 0 \\
\mathbb{BC}: & U(0,t) = U_0, & U(L,t) = U_1 & t > 0 \\
\mathbb{IC}: & U(x,0) = f(x) & & 0 < x < L.
\end{array}$$

Solving the general problem will have to wait, but we can find some specific solutions to the problem using the ideas of *Separation of Variables*. For the moment, we will restrict ourselves to homogeneous boundary conditions,

[1] See, for example, T. W. Körner, "Fourier Analysis," Cambridge University Press, p. 338.

THE DIRICHLET PROBLEM FOR THE DIFFUSION EQUATION
(HOMOGENEOUS BOUNDARY CONDITIONS)

$$\begin{array}{rcl} \mathbb{DE}: & U_t = DU_{xx} & 0 < x < L, t > 0 \\ \mathbb{BC}: & U(0,t) = 0, \quad U(L,t) = 0 & t > 0 \\ \mathbb{IC}: & U(x,0) = f(x) & 0 < x < L. \end{array}$$

If you want, you can skip the derivation for the moment and jump ahead to Exercise 1, if you don't mind the solution appearing *deus ex machina* (a fancy term for "out of thin air").

2.3.1 A Solution to the Homogeneous Dirichlet Problem

Let us look for solutions to the homogeneous Dirichlet problem of the form

$$U(x,t) = X(x)T(t) \tag{2.19}$$

we find from the differential equation ($\mathbb{DE}$) that

$$XT_t = DX_{xx}T \tag{2.20}$$

and dividing by XT we find

$$\frac{T_t}{DT} = \frac{X_{xx}}{X} = -\lambda. \tag{2.21}$$

where λ is to be determined. Now because T_t/DT is *only* a function of t and X_{xx}/X is *only* a function of x we know that λ must be independent of x and t respectively, and therefore must be a constant – consequently it is known as the *separation constant*. We can now solve the resulting ODE for $T(t)$

$$T_t = -\lambda DT \quad \Rightarrow \quad T(t) = e^{-\lambda Dt}, \tag{2.22}$$

or some constant multiple of it.

We now look for a solution for the $X(x)$ equation that also satisfies the homogeneous boundary conditions. From the boundary conditions (BC), we know that

$$U(0,t) = X(0)T(t) = 0 \quad \Rightarrow \quad X(0) = 0 \tag{2.23}$$

$$U(L,t) = X(L)T(t) = 0 \quad \Rightarrow \quad X(L) = 0 \tag{2.24}$$

So finally we conclude that we are looking for solutions to the *Boundary Value Problem* for $X(x)$,

$$\boxed{X_{xx} + \lambda X = 0, \qquad X(0) = 0 \quad X(L) = 0.} \tag{2.25}$$

Solving the DE, we find that

$$X(x) = B\cos(\sqrt{\lambda}x) + C\sin(\sqrt{\lambda}x) \tag{2.26}$$

and applying the boundary conditions we see that $X(0) = 0$ implies that $B = 0$, and that

$$C\sin(\sqrt{\lambda}L) = 0. \tag{2.27}$$

Consequently, a non-trivial solution (that is a solution for which $X(x) \neq 0$) for $X(x)$ can be found if and only if

$$\boxed{\lambda = \lambda_n \equiv \left(\frac{n\pi}{L}\right)^2 \quad for \quad n = 1, 2, 3\ldots} \tag{2.28}$$

for which we find

$$\boxed{X(x) = X_n(x) \equiv \sin\left(\frac{n\pi x}{L}\right) \quad for \quad n = 1, 2, 3\ldots,} \tag{2.29}$$

or some constant multiple of it. These special values of λ are called *eigenvalues* and the associated functions, $X_n(x)$, are known as *eigenfunctions*.

Multiplying the solution for $X_n(x)$ and $T(t)$ together finally yields a solution for $U_n(x,t)$,

$$\boxed{U(x,t) = U_n(x,t) \equiv \sin\left(\frac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 Dt} \; for \; n = 1, 2, 3\ldots.} \tag{2.30}$$

The method of separation of variables is very powerful – it will be one of our primary tools for finding solutions to PDE's in the coming lectures.

Exercise 2.2. Verify that

$$U_n(x,t) \equiv \sin\left(\frac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 t} \quad for \quad n = 1, 2, 3\ldots,$$

satisfies the diffusion equation $U_t = DU_{xx}$ and the homogeneous boundary conditions $U(0,t) = U(L,t) = 0$. Explain why any linear combination of U_n,

$$U(x,t) = \sum_{n=1}^{\infty} a_n U_n(x,t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 Dt}$$

also satisfies the diffusion equation and the homogeneous boundary condition. Does it worry you that this is an infinite sum? What initial condition, $U(x,0)$, does this correspond to?

2.3.2 A Solution to the Cauchy Problem

We can also consider a solution to the Cauchy problem for the diffusion equation, which you hopefully remember is the problem posed on the entire real line,

THE CAUCHY PROBLEM FOR THE DIFFUSION EQUATION

$$\begin{aligned}
\mathbb{DE}: &\quad U_t = DU_{xx} && -\infty < x < \infty, t > 0 \\
\mathbb{BC}: &\quad \lim_{x\to\pm\infty} |U(x,t)| < C && t > 0 \\
\mathbb{IC}: &\quad U(x,0) = f(x) && -\infty < x < \infty.
\end{aligned}$$

While there are many clever derivation for the solution to this problem, for the moment I will simply give you the most important solution, usually called the *fundamental solution* or the *diffusion kernel*,

$$U(x,t) = G(x,t+\tau) \equiv \frac{1}{\sqrt{4\pi D(t+\tau)}} e^{-\frac{x^2}{4D(t+\tau)}}. \tag{2.31}$$

where τ is a constant (which we will assume is positive). This solution can be used to construct a general solution of the diffusion equation for an arbitrary initial condition, $f(x)$.

Exercise 2.3. Verify that

$$G(x,t+\tau) \equiv \frac{1}{\sqrt{4\pi D(t+\tau)}} e^{-\frac{x^2}{4D(t+\tau)}}.$$

satisfies the diffusion equation and the boundary conditions for the Cauchy problem when $\tau > 0$. Show that this solution corresponds to a Gaussian with time varying width and height. How does the Gaussian's width, height and area vary in time?

2.4 THE MAXIMUM PRINCIPLE

Looking at solutions to the heat equation, we note that they tend to average out maximums and minimums. We can develop some intuition for this by considering what the equation says. Basically, $U_t = DU_{xx}$ means: *The temperature is decreasing when the profile is convex down and the temperature is increasing when the profile is convex up.*

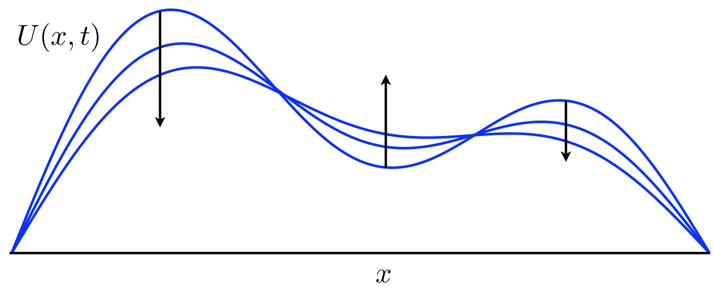


Figure 2.4: The heat equation interpreted graphically. The temperature is decreasing when the profile is convex down and the temperature is increasing when the profile is convex up.

From which we conclude that interior maximums in temperature are decreasing and interior minimums of temperature are increasing. This reasoning is not quite airtight (how to make it tighter is a good question to ponder). We can give a rigorous statement (without proof) of the maximum principle:

Theorem 2.1 (Maximum Principle for the Diffusion Equation)**.** *If $U(x,t)$ satisfies the Dirichlet problem for the diffusion equation in the semi-infinite strip $0 < x < L$, $0 < t$, then it assumes its maximum value (as a function of x and t) either initially (when $t = 0$) or on the lateral boundaries (where $x = 0$ or $x = l$).*

The same is also true of the minimum of $u(x,t)$. A proof can be found in most advanced PDE texts.

Exercise 2.4. Interpret the solutions we have found for the diffusion equation in terms of the maximum principle. Show examples where the maximum value of $u(x,t)$ occur in the initial condition and on the lateral boundaries.

2.5 Energy Dissipation and Uniqueness

By looking at what is normally known as energy for the diffusion equation, we can show that the solution for the Dirichlet problem is unique. Note this energy is a mathematical construct, not to be confused with the thermal energy discussed in the derivation of the diffusion equation.

First, suppose that $U(x,t)$ is a solution to the homogeneous Dirichlet problem,

$$\begin{array}{rccl} \mathbb{DE}: & U_t = DU_{xx} & & 0 < x < L, t > 0 \\ \mathbb{BC}: & U(0,t) = 0, & U(L,t) = 0 & t > 0 \\ \mathbb{IC}: & U(x,0) = f(x) & & 0 < x < L. \end{array}$$

Let's define, the energy,

$$W = \frac{1}{2}\int_0^L U^2 \, dx, \tag{2.32}$$

which is a function of t dependent on the particular solution $U(x,t)$ (technically it is a function of t and a *functional* of $U(x,t)$). Note that $W \geq 0$ with $W = 0$ only for the trivial solution $U(x,t) = 0$.

If we differentiate the energy with respect to time, we find

$$\begin{aligned} \frac{dW}{dt} &= \int_0^L UU_t \, dx, \\ &= D\int_0^L UU_{xx} \, dx, \\ &= -\int_0^L (U_x)^2 \, dx + UU_x \left.\right|_{x=0}^{x=L}, \end{aligned}$$

where we have substituted the $\mathbb{DE}$ and used integration by parts. Now, applying the $\mathbb{BC}$'s, we fine that the boundary terms from the integration by parts vanish, so,

$$\frac{dW}{dt} = -\int_0^L (U_x)^2 \, dx \leq 0$$

Now, we can conclude that W is decreasing (that is energy is dissipated!!) *unless* $U_x = 0$, that is to say that U is constant. As the only constant solution satisfying the boundary conditions is $U = 0$, we might be tempted to conclude that the solution always decays to this trivial state. This turns out to be true, although one must invest some analysis to show it rigorously.

A second conclusion one can reach is that if $f(x) = 0$, that $U(x,t) = 0$ for all $t > 0$. This follows quickly because $W = 0$ at $t = 0$, it is non-increasing and non-negative. While this seems like a trivial result, it has a very powerful consequence. Suppose we had two solutions to the non-homogeneous Dirichlet problem, call them V_1 and V_2. You should be able to convince yourself that there difference $U = V_1 - V_2$ satisfies the homogeneous Dirichlet problem with $f(x) = 0$. Consequently, we know that $U(x,t) = 0$ for all $t > 0$, which implies $V_1 = V_2$. From this we conclude that *The solution to the non-homogeneous Dirichlet problem is unique*, a powerful result indeed.

Exercise 2.5. Convince yourself the energy argument for uniqueness of solutions in the previous paragraph is correct. Show that a similar argument can be made for the Neumann problem.

2.6 Problems for Chapter 2

Problem 2.1. Consider the diffusion equation with homogeneous Neumann boundary conditions.

$$\begin{array}{rll} \mathbb{DE}: & U_t = DU_{xx} & 0 < x < L, t > 0, \\ \mathbb{BC}: & U_x(0,t) = 0 \quad U_x(L,t) = 0 & t > 0, \\ \mathbb{IC}: & U(x,0) = f(x) & 0 < x < L. \end{array}$$

(a) Explain physically why this corresponds to the diffusion of heat in a metal bar with insulated ends. Make sure you understand what each of the equations corresponds to.

(b) Show that

$$\begin{array}{ll} (i) & U_0(x,t) = 1 \\ (ii) & U_n(x,t) = \cos\left(\dfrac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 Dt} \qquad n = 1, 2, 3, \ldots \end{array}$$

satisfy both the diffusion equation (DE) and the homogeneous Neumann boundary conditions (BC).

(c) Write down a general solution as a linear combination of the solutions you found in part (b). What does this say about $f(x)$ if we assume that this solution also satisfies the initial condition (IC)?

Problem 2.2. In this problem, we will argue that for the homogeneous Neumann problem discussed in Problem 1, that the solution approaches a constant temperature, given by the average of the initial temperature.

(a) Suppose we define the total heat energy in the bar as

$$Q(t) = \int_0^L U(x,t)\, dx.$$

Show that Q is *conserved*, that is that it is independent of time (Hint: compute $\frac{dQ}{dt}$).

(b) Use the initial condition to compute Q in terms of $f(x)$.

(c) Modify the energy argument in the previous section show that the energy is decreasing unless $U(x,t)$ is constant. Use this to argue that $U(x,t)$ approaches a constant solution as $t \to \infty$.

(d) Finally, use parts (a) and (b) of the problem to show that there is only one possible constant solution for U that is consistent with the conservation of Q. Show that solution corresponds to the bar approaching the average temperature of the initial condition.