Partial Differential Equations, lecture 2

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Derivation of the heat equation (one dimensional framework)

Recall that the one dimensional diffusion equation is the linear second order partial differential equation

$$u_t - Du_{xx} = f \tag{1}$$

where $u = u(x, t)$ is a real space variable, t is a time variable and D is a positive constant, called the diffusion coefficient. In higher dimensions, equation (1) can be extended to

$$u_t - D\Delta u = f \tag{2}$$

Although equations (1) and (2) can be used in much more general frameworks (we will get back to this when discussing Brownian motion), we will start by focusing on its use in modelling the conduction of heat in a solid.

Heat energy is caused by the agitation of molecular matter. The propagation of thermal energy can then be described by two basic processes:

- Conduction (which results from the collisions of neighboring molecules in which the energy of one molecule is transferred to its nearest neighbor. Thermal energy is thus spread by conduction even if the molecules themselves dot not move their locations appreciably.)

- In addition to conduction, if a vibrating molecule moves from one region to another, it takes its thermal energy with it. This second type of thermal propagation is called convection.
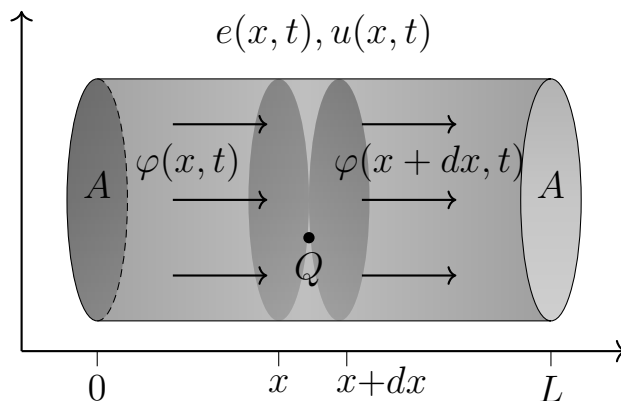
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Figure 1: Representation of the cylindrical rod, conducting heat used in the derivation of the one dimensional heat equation. We consider the conservation of thermal energy inside a thin slide (located between x and $x + dx$). The flux $\varphi(x, t)$ that enters the slice is directed along the x-axis and so is the flux $\varphi(x + dx, t)$ that leaves the slice. The total contribution of this flux to the energy in the slice is thus given by $\varphi(x, t)A - \varphi(x + dx, t)A$

In order to start with relatively simple problems, we will study heat flows in cases in which the conduction of heat energy is more significant than its convection (this is the case in solids or fluids in which the velocity is sufficiently small). To begin, let us consider a simple rod of constant cross sectional area A oriented in the x direction (from $x = 0$ to $x = L$), see figure 1 below. we consider the amount of thermal energy per unit volume and call this quantity the thermal enery density, $e(x, t)$.

We assume that all thermal quantities are constant across a section which can be achieved in part by perfectly insulating the lateral surface area of the rod.

Considering a dependence in x and t for the thermal energy density corresponds to a situation in which the rod is not uniformly heated. The thermal energy density then varies from one cross section to another. If we take our dx to be exceedingly small, $e(x, t)$ can nonetheless be approximated as a constant throughout the small volume. The total heat energy inside this volume can then read as $e(x, t)\, Adx$ and from this we can express conservation of energy through time. Generally speaking, we want the change in heat energy through time to match the heat energy flowing across the boundaries per unit time and the energy generated inside the slice per unit time, i.e.

Time rate of change of heat energy	=	Heat energy flowing across boundary per unit time	+	Heat energy generated inside per unit time

To express this relation more formally, we introduce the heat flux $\varphi(x, t)$ which encodes the amount of thermal energy per unit time flowing to the right per unit area

(see figure 1). Note that from this convention, if $\varphi(x, t) < 0$, it follows that the heat energy is flowing to the left. The amount of heat energy flowing per unit time across the boundaries of the slice can then be written as

$$\varphi(x, t)A - \varphi(x + dx, t)A \tag{3}$$

In our conservation of heat energy, we also need to take into account possible heat sources which we denote generally as $Q(x, t)$. $Q(x, t)$ here encodes the heat energy per unit volume generated per unit time (arising for example, due to chemical reactions or electrical heating). Using e, φ and Q, our conservation of heat then read as

$$\frac{\partial}{\partial t}\left[e(x, t)Adx\right] = \varphi(x, t)A - \varphi(x + dx, t)A + Q(x, t)Adx \tag{4}$$

At this stage, the equation is not accurate as we assumed the various quantities to be constant. It can however be made more and more accurate by taking $dx \to 0$. In this limit, we have

$$\frac{\partial}{\partial t}e(x, t) = \lim_{dx \to 0} \frac{\varphi(x, t) - \varphi(x + dx, t)}{dx} + Q(x, t) \tag{5}$$

$$= -\frac{\partial \varphi(x, t)}{\partial x} + Q(x, t) \tag{6}$$

In our derivation of (6) we used an approximation (assuming that $e(x, t)$ was constant across the slice located between x and $x + dx$). We can actually replace our first approach with a more accurate version

$$\frac{d}{dt}\int_a^b e(x, t)\ Adx = \left(\varphi(a, t) - \varphi(b, t)\right)A + \int_a^b Q(x, t)\ Adx \tag{7}$$

which is known as the integral conservation law

- Provided that $e(x, t)$ and $\frac{\partial e(x, t)}{\partial t}$ are continuous, we can move the time derivative inside the integral

- Moreover, provided that φ is continuously differentiable, we can replace the difference $\varphi(a, t) - \varphi(b, t)$ as the integral

$$\varphi(a, t) - \varphi(b, t) = -\int_a^b \frac{\partial \varphi}{\partial x}\ dx \tag{8}$$

Together, those two steps give

$$\int_a^b \frac{\partial e(x, t)}{\partial t}\ dx = -\int_a^b \frac{\partial \varphi}{\partial x}\ dx + \int_a^b Q(x, t)\ dx \tag{9}$$

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Since the integral must be zero for arbitrary a and b and if we assume that the function $\frac{\partial e(x,t)}{\partial t} + \frac{\partial \varphi(x,t)}{\partial x} - Q(x,t)$ is continuous, this implies that the integrand

$$\frac{\partial e}{\partial t} + \frac{\partial \varphi}{\partial x} - Q(x,t) \tag{10}$$

must be zero everywhere. Indeed, by continuity, if this was not the case, there would be a value x_0 around which the sign of the integrand does not change. Hence

$$\left| \int_{x_0-\varepsilon}^{x_0+\varepsilon} \frac{\partial e}{\partial t} + \frac{\varphi}{\partial x} - Q \right| > 0 \tag{11}$$

which gives a contradiction. From the integral conservation law, we can thus derive the differential form

$$\frac{\partial e}{\partial t} = -\frac{\partial \varphi}{\partial x} + Q \tag{12}$$

In that sense, we see that the integral law is more fundamental than the differential form.

So far we have derived laws involving the thermal energy. However in general we prefer to describe materials through their temperature $u(x,t)$ and not through the termal energy density. The distinction between the two goes back to the 1700's when physicists started to realize that it might take different amounts of thermal energy to raise different materials from one temperature to another larger temperature.

The connection between thermal energy and temperature requires two additional quantities: the specific heat and the density of the material.

The specific heat c is defined as the heat energy that must be supplied to a unit mass of a substance to raise its temperature by one unit (hence $[J] \times [kg]^{-1} \times [K]^{-1}$). In general, the specific heat of a material depends on the temperature (i.e. the thermal energy needed to raise a unit mass from $0°\mathrm{C}$ to $1°\mathrm{C}$ could be different from the thermal energy needed to raise a unit mass from $85°\mathrm{C}$ to $86°\mathrm{C}$). For restricted temperature intervals, the specific heat can be considered as approximately independent of the temperature. However, experiments indicate that different materials require different amounts of thermal energy to heat up.

In this derivation, we will assume that the specific heat depends on x so that $c = c(x)$. We can now relate the thermal energy and the temperature more precisely. The thermal energy is in fact also defined as the energy it takes to raise the temperature of a material from a reference temperature (e.g. $0°\mathrm{C}$) to the actual temperature $u(x,t)$. From the description of the specific heat, we also know that we can write the amount of energy stored in the material (per unit mass) as $c(x,t)u(x,t)$. From this, we can then derive the relation

$$e(x,t)\ Adx = c(x)u(x,t)\rho(x)\ Adx \tag{13}$$

where we introduced the density ρ (mass per unit volume). Going back to (12), we get

$$c(x)\frac{\partial u(x,t)}{\partial t}\rho(x) = -\frac{\partial \varphi}{\partial x} + Q \tag{14}$$

When looking at equation (14), this equation is often regarded as an equation in two unknowns. Quite logically we would like to eliminate one of these unknowns (the source of heat Q being usually given). On our way to achieve this objective, it seems natural to wonder what φ really means in this case.

The definition of the heat flux is based on the following properties

(i) If temperature is constant, no heat flux flows

(ii) If there are temperature differences, heat energy flows from the hotter region to the colder region

(iii) The greater the temperature differences, the greater the flow of energy

(iv) The flow of energy will vary for different materials even with the same temperature differences

Fourier (1768-1830) recognized those properties and summarized them by the formula

$$\varphi(x,t) = -k_0 \frac{\partial u}{\partial x} \tag{15}$$

known as Fourier's law of heat conduction.

In this equation, k_0 measures the ability of the material to conduct heat and is called thermal conductivity

Experiments show that k_0 depends on the material. In the general case, k_0 will be a function of x and even depend on the temperature.

However, the dependence on the temperature is usually less important and we will thus assume that $k_0 = k_0(x)$ only, or more simply, that k_0 is a constant. If we substitute Fourier's law into the conservation of heat energy (14), we get the equation

$$c(x)\rho(x)\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(k_0 \frac{\partial u}{\partial x}\right) + Q \tag{16}$$

In the special case of a uniform rod with constant c, ρ and k_0, the equation (16) becomes

$$c\rho \frac{\partial u}{\partial t} = k_0 \frac{\partial^2 u}{\partial x^2} + Q \tag{17}$$

and if we assume $Q = 0$ we recover our original heat/diffusion equation

$$\frac{\partial u}{\partial t} = \frac{k_0}{c\rho} \frac{\partial^2 u}{\partial x^2} \tag{18}$$

$$= D\frac{\partial^2 u}{\partial x^2} \tag{19}$$

in the second line above, we introduced the constant D known as the thermal diffusivity (or diffusion constant).

Derivation of the heat equation (multi-dimensional framework)

We now consider the general multi-dimensional framework. we consider a general sub-region $\mathcal{R}$ for which we will write down the conservation of energy as before. Extending the one dimensional framework, we can write the amount of heat energy inside the sub-region as

$$\text{Total heat energy} = \int_{\mathcal{R}} c\rho u \, dV \tag{20}$$

We then need an expression for the flow of heat energy. In dimension one, we define the flux to be oriented along the x direction. In the multi-dimensional framework, the heat flux is a vector $\boldsymbol{\varphi}$ whose magnitude is the amount of heat energy flowing per unit time per unit surface.

When considering the conservation of energy within the region $\mathcal{R}$, we are only interested in the heat that flows across the boundary. When the heat flow is parallel to the boundary, there will be not heat energy crossing the surface. It is in fact only the normal component to the surface that will contribute to a change in the heat energy. At any point on the surface, there are two normal vectors, an inward and an outward normal $\boldsymbol{n}$. We will take the convention of only utilizing the unit outward normal vector $\boldsymbol{n}$.

From this, the flux through a surface element dS can be obtained as $\boldsymbol{\varphi} \cdot \frac{\boldsymbol{n}}{\|\boldsymbol{n}\|} = \boldsymbol{\varphi} \cdot \hat{\boldsymbol{n}}$. In particular if $\boldsymbol{\varphi} \cdot \hat{\boldsymbol{n}} < 0$, the flux is directed inward and the outward flow of heat energy is negative.

To calculate the total heat energy flowing out of our region $\mathcal{R}$ per unit time, we must multiply $\boldsymbol{\varphi} \cdot \hat{\boldsymbol{n}}$ by the differential surface element dS and sum over the whole surface that encloses the region $\mathcal{R}$.

If we further let Q to denote the rate of heat energy generated per unit volume, we get the relation

$$\frac{d}{dt} \int_{\mathcal{R}} c\rho u \, dV = -\oint_{S} \boldsymbol{\varphi} \cdot \hat{\boldsymbol{n}} \, dS + \int_{\mathcal{R}} Q \, dV \qquad (21)$$

In the one dimensional framework, we turned our boundary expression for the flux into a volume integral by noting that $\varphi(a) - \varphi(b) = -\int_a^b \frac{\partial \varphi}{\partial x} \, dx$. We now need to turn to a more general result known as the divergence theorem. Given a vector $\boldsymbol{v} = (v_1, v_2, \ldots, v_n)$, the divergence of $\boldsymbol{v}$ is defined as

$$\nabla \cdot \boldsymbol{v} = \frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \ldots + \frac{\partial v_n}{\partial x_n} \qquad (22)$$

The divergence theorem (also known as Gauss's theorem) states that the volume integral of the divergence of any continuously differentiable vector $\boldsymbol{v}$ is the closed surface integral of the outward normal component of $\boldsymbol{v}$,

$$\int_{\mathcal{R}} \nabla \cdot \boldsymbol{v} \, dV = \oint_{S} \boldsymbol{v} \cdot \hat{\boldsymbol{n}} \, dS \qquad (23)$$

From the divergence theorem, we can thus express our conservation of heat energy as

$$\frac{d}{dt} \int_{\mathcal{R}} c\rho u \, dV = -\int_{\mathcal{R}} \boldsymbol{\nabla} \cdot \boldsymbol{\varphi} \, dV + \int_{\mathcal{R}} Q \, dV. \qquad (24)$$

As before, we can put the time derivative inside (provided that the integrand is continuous). Moreover, as for the one dimensional case, we know that the integral form implies that the integrand itself must be zero everywhere. Hence

$$c\rho \frac{\partial}{\partial t} u(\boldsymbol{x}, t) = -\boldsymbol{\nabla} \cdot \boldsymbol{\varphi} + Q \qquad (25)$$

in the one dimensional framework, we saw that the heat flux was proportional to the derivative of the temperature. I.e. $\varphi = -k_0 \frac{\partial u}{\partial x}$. This idea remains valid in higher dimensions where we can show (through empirical evidence) that the heat flux is once again proportional to the temperature gradient

$$\varphi = -k_0 \boldsymbol{\nabla} u \qquad \text{(Higher dimensional Fourier's law)} \qquad (26)$$

Substituting (26) inside (25), we get

$$c\rho \frac{\partial u}{\partial t} = \boldsymbol{\nabla} \cdot (k_0 \boldsymbol{\nabla} u) + Q \qquad (27)$$

in the case where there is no source $Q = 0$ and the thermal conductivity is constant, we recover the right-hand side of equation (2),

$$\frac{\partial u}{\partial t} = D\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} u) \qquad (28)$$

$$= D\Delta u \qquad (29)$$

References

[1] Richard Haberman, *Applied Partial Differential Equations with Fourier Series and Boundary Value Problems*, Fourth Edition, Pearson 2004.

[2] Lawrence C. Evans, *Partial Differential Equations*, Second Edition, Graduate Studies in Mathematics, Volume 19, American Mathematical Society, 2010.

[3] Sandro Salsa, *Partial Differential Equations in Action*, Third Edition, Springer 2016.