Heat Conduction

We have used the fundamental postulate to study experimental phenomena by following an algorithm. For a given phenomenon, we construct an isolated system with an internal variable. The isolated system has a whole set of quantum states. When the internal variable is held at a fixed value, the isolated system flips among a subset of the quantum states. The fundamental postulate implies that the internal variable evolves in time, from one value corresponding to a subset of the quantum states to another value corresponding to a subset of a larger number of quantum states. After a long time, the internal variable attains an equilibrium value, corresponding to a subset of the largest number of quantum states.

This algorithm leads to an algebraic equation to determine the internal variable in equilibrium, and an ordinary differential equation to evolve the internal variable in time. We have used this algorithm to model several phenomena:

- A half bottle of water, where the internal variable is the number of water molecules in the vapor (http://imechanica.org/node/290).
- Wine and cheese in thermal contact, where the internal variable is the amount of energy in the wine (http://imechanica.org/node/291). This model defines temperature in terms of energy and entropy.
- A more formal analysis of coexistent phases, where the internal variable is the number of molecules in one of the phases. (http://imechanica.org/node/291).

We now use the same algorithm to study phenomena in which internal variables are *time-dependent fields*. We do not change our perspective on the fundamental postulate. Rather, we change how we describe internal variables, from using numbers to using fields. This change results in a change in mathematical tools, from algebraic equations and ordinary differential equations to partial differential equations.

Such a change, however, is not as profound as it may appear. Especially in our own time, fields are routinely discretized into numbers, and the computer solves algebraic equations to determine these numbers in equilibrium, or solves ordinary differential equations to evolve these numbers in time. The computer crunches numbers; it knows no partial differential equations.

We begin with a familiar phenomenon: heat conduction. We will first recall the theory of heat conduction presented in undergraduate textbooks. Inside a body is a time-dependent field of temperature. When the field of temperature is inhomogeneous, energy will flow from a place of high temperature to a place of low temperature. When the field of temperature is homogenous, energy will cease to flow, and the body is in a state of equilibrium. This theory of heat conduction was formulated by Fourier in early 1800s, before thermodynamics was established. His formulation may be pictured by using an analogy. A fluid flows from a place of high altitude to a place of low altitude. Heat flows like a fluid, from a place of high temperature to a place of low temperature.

We will then show that Fourier's theory is consistent with the two great principles: the fundamental postulate and the conservation of energy. We would like to use this familiar phenomenon of heat conduction to describe the algorithm of modeling that will allow us to formulate theories for other phenomena.

Energy in a rigid body. A body is represented by a field of material particles. Each material particle contains a large number of molecules. The body is taken to be rigid and stationary, so that each material particle remains fixed in space. We name a material particle by its coordinate **x**.

Each material particle is regarded as a system with a single independent variable: energy. Let u be the density of energy, namely, the energy in the material particle divided by the volume of the material particle:

$$u = \frac{\text{energy}}{\text{volume}}.$$

In general, u varies from particle to particle, and also varies with time t. The time-dependent field of energy density is written as $u(\mathbf{x},t)$. The aim of the theory is to evolve the field of energy density in time.

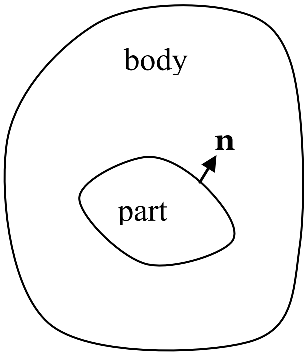
Energy flux across a plane. Energy flows from one material particle to another. Define energy flux by

$$\text{energy flux} = \frac{\text{energy across a plane}}{\text{area} \times \text{time}}.$$

Many planes pass through a material particle **x**. For a given plane, let **n** be the unit vector normal to the plane, and let J_n be the energy flux across the plane. The energy flux is time-dependent field, written as $J_n(\mathbf{x},t)$. Furthermore, its value also depends on the orientation of the plane. The flux J_n is a scalar, and is taken to be positive if energy flows from one side of the plane to the other in the direction of **n**.

Conservation of energy. We apply the law of the conservation of energy to any part of the body. The energy in the part is

$$\int u(\mathbf{x},t)dV .$$



The integral extends over the volume of the part.

Consider an element of the surface of the part, of area dA and with the unit normal vector $\mathbf{n}$. We adopt the sign convention that the unit normal vector points outside the part. The energy across this element per unit time is $J_n(\mathbf{x},t)dA$. The energy flowing out the part per unit time is

$$\int J_n(\mathbf{x},t)dA .$$

The integral extends over the surface of the part.

The conservation of energy requires that

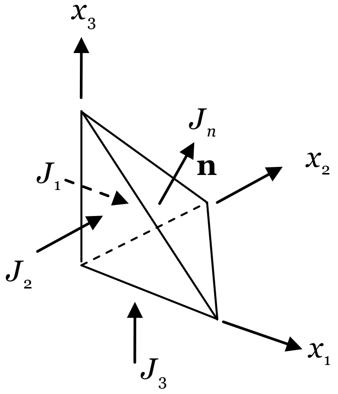
$$\frac{d}{dt}\int u(\mathbf{x},t)dV + \int J_n(\mathbf{x},t)dA = 0 .$$

The first integral extends over the volume of the part, and the second integral extends over the surface of the part.

Conservation of energy defines a field of vector. Consider a part of the body in the shape of a tetrahedron. One face of the tetrahedron is the inclined triangle of area A, with unit vector n_i normal to the area. The other three faces are triangles in the coordinate planes, of areas A_1, A_2, A_3. The areas satisfy a mathematical relation:

$$A_i = An_i .$$

Let J_n be the flux of energy across the inclined triangle. Let J_i be the flux through an element of area normal to the axis x_i. We adopt the sign convention that the flux is positive if energy flows in the positive direction of the axis.



We next apply the law of the conservation of energy to the tetrahedron. According to our sign convention, the three components J_i are fluxes of energy entering the tetrahedron, and J_n is the flux of energy exiting the tetrahedron. Let V be the volume of the tetrahedron. When the tetrahedron is small, all the quantities are homogeneous in the tetrahedron. The law of the conservation of energy is written as

$$\frac{\partial u}{dt}V + J_n A = J_1 A_1 + J_2 A_2 + J_3 A_3 .$$

Divide the above equation by A, and we obtain that

$$\frac{\partial u}{dt}\frac{V}{A} + J_n = J_1 n_1 + J_2 n_2 + J_3 n_3$$

When the tetrahedron is made very small, the volume of the tetrahedron over the area of the tetrahedron, V/A, will become very small. Consequently, we can ignore the term associated with the volume of the tetrahedron, and obtain that

$$J_i n_i = J_n .$$

We adopt the convention that a repeated index means a sum over 1,2,3.

Recall that J_n is the energy across the inclined plane per unit area per unit time. Thus, J_n is a scalar. The above equation shows that the energy flux $\{J_1, J_2, J_3\}$ maps a vector n_i to a scalar J_n. According linear algebra, the fluxes $\{J_1, J_2, J_3\}$ are the components of a vector. We write the energy flux as $\mathbf{J}(\mathbf{x}, t)$, which is a time-dependent field of vector.

Conservation of energy written as a partial differential equation. Recall that the energy flowing out a part of the body per unit time is

$$\int J_n dA .$$

The integral extends over the surface of the part. Substituting $J_n = J_i n_i$, and applying the divergence theorem, we obtain that

$$\int J_n dA = \int J_i n_i dA = \int \frac{\partial J_i(\mathbf{x}, t)}{\partial x_i} dV .$$

The last integral extends over the volume of the part. This equality transforms an integral over the surface of the part to an integral over the volume of the part. The physical basis of this transformation is the law of the conservation of energy.

We next apply the law of the conservation of energy to a small part of the body of an arbitrary shape. The conservation of energy requires that

$$\frac{d}{dt}\int u(\mathbf{x}, t) dV + \int J_n(\mathbf{x}, t) dA = 0 .$$

The first integral extends over the volume of the part, and the second integral extends over the surface of the part.

Because the body is stationary, we can pass the time derivative into the integral. We can also change the integral over the surface of the part to the integral over the volume of the part. We obtain that

$$\int \left[\frac{\partial u(\mathbf{x},t)}{\partial t} + \frac{\partial J_i(\mathbf{x},t)}{\partial x_i} \right] dV = 0 .$$

This equation holds for any part of the body. Consequently, the integrand itself must vanish, giving that

$$\frac{\partial u(\mathbf{x},t)}{\partial t} + \frac{\partial J_i(\mathbf{x},t)}{\partial x_i} = 0 .$$

This partial differential equation is a consequence of the conservation of energy. This equation connects the scalar field $u(\mathbf{x},t)$ to a vector field $J_i(\mathbf{x},t)$. To evolve these fields, we need more equations.

Heat capacity. Each material particle is modeled as a system of single independent variable, energy. Consequently, all other variables of the system depend on energy. In particular, the temperature T of a material particle is a function of energy. We will not be concerned with phase transition here, so that the temperature and the energy have a 1-to-1 relation. We can write energy as a function of temperature, $u(T)$. This function is material-specific. The heat capacity is defined by

$$c = \frac{\partial u(T)}{\partial T} .$$

The heat capacity defined this way has the unit $\mathrm{JK^{-1}m^{-3}}$. The heat capacity is material-specific and in general varies with temperature, $c(T)$. This function has been measured for many materials.

Fourier's law. In the body the temperature varies from one material particle to another material particle, and varies from time to time. That is, the temperature in the body is a time-dependent field, $T(\mathbf{x},t)$. Energy flows from a particle of a high temperature to a particle of a low temperature. This everyday experience is embodied in Fourier's law: the heat flux is proportional to the gradient of the temperature, namely,

$$J_i = -\kappa \frac{\partial T(\mathbf{x},t)}{\partial x_i} ,$$

where κ, a positive quantity, is called thermal conductivity. Thermal conductivity is material-specific and in general varies with temperature, $\kappa(T)$. This function has also been measured for many materials.

Diffusion equation. A combination of the above three equations gives

$$c(T)\frac{\partial T(\mathbf{x},t)}{\partial t} = \frac{\partial}{\partial x_i}\left[\kappa(T)\frac{\partial T(\mathbf{x},t)}{\partial x_i}\right].$$

This partial differential equation evolves the field of temperature, $T(\mathbf{x},t)$, subject to initial and boundary conditions. The equation is known as the *diffusion equation*.

The two functions $c(T)$ and $\kappa(T)$ make the diffusion equation nonlinear. For many applications, the variation of temperature is small, so that the variations of the heat capacity and thermal conductivity are small. Consequently, we may regard the heat capacity and thermal conductivity as constants, and write the diffusion equation as

$$\frac{\partial T(\mathbf{x},t)}{\partial t} = D\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right)T(\mathbf{x},t),$$

where

$$D = \frac{\kappa}{c}.$$

The diffusivity D is material specific, and has the unit

$$D = \frac{(\text{length})^2}{\text{time}}.$$

You can estimate the order of magnitude of the diffusivity of a stick by placing one end of the stick above a flame, and use your fingers to feel the temperature at the other end of the stick. The length of the stick, along with the time for the stick to conduct the heat of the flame to your fingers, gives you an estimate the diffusivity. A representative value of the diffusivity for metals is $D \sim 10^{-4}\,\mathrm{m^2/s}$.

You must have solved some partial differential equations before, and may not wish to spend time on such activities here. But we should recall salient features of such solutions.

State of equilibrium. When the field of temperature is homogenous, the heat flux vanishes, and the body is said to be in a *state of equilibrium*.

For example, when heat is added at one part of the body, the temperature is nearly homogenous in the body if the heat is added over a time scale larger than the time needed for the heat to diffuse across the body. The time needed for the heat to diffuse across the body increases with the size of the body:

$$t \sim \frac{L^2}{D},$$

where L is a characteristic length of the body. A representative value of the diffusivity for metals is $D \sim 10^{-4}\,\mathrm{m^2/s}$. For a body of size 1 m, the above time scale is 10^4 s. In this example, to add heat and maintain homogenous temperature, heat must be added over a time scale of hours.

Steady state. When the field of temperature is inhomogeneous, but is independent of time, the body is said to be in a *steady state*.

For example, a blade of a gas turbine is made of a superalloy, covered with a thermal barrier coating. The coating is made of zirconia, of thickness 200 $\mu\mathrm{m}$ and conductivity $\kappa = 2\,\mathrm{WK^{-1}m^{-1}}$. The coating maintains a drop in temperature 100 K. In this example, the heat flux is

$$J = \kappa \frac{\text{temperature drop}}{\text{thickness}} = 10^6\,\mathrm{W/m^2}.$$

The energy is produced by combustion of the fuel, and is taken away by a fluid flowing inside the superalloy. The thermal barrier coating maintain the temperature drop, so that the fuel burns at a high temperature to gain a high efficiency, while the superalloy is maintained at a allowable temperature to sustain mechanical loads.

Transient state. When the field of temperature varies from one material particle to another, and from time to time, the body is said to be in a *transient state*.

For example, the field of temperature around us is transient. While the temperature on the surface of the earth suffers a seasonal change, the change in temperature underground is negligible. You can solve a boundary-initial-value problem to show that the cyclic change in temperature decays with the depth into the ground. However, the essential result can be obtained by a dimensional consideration. The characteristic length for decay is

$$d \sim \sqrt{Dt_{period}}.$$

A representative value of diffusivity for soil is $D \sim 10^{-6}\,\mathrm{m^2/s}$. The time period of one year is $t_{period} \sim 10^8\,\mathrm{s}$. Consequently, the depth is about $d \sim 10\,\mathrm{m}$. Cavemen living underground below this level would feel no seasonal change of temperature.

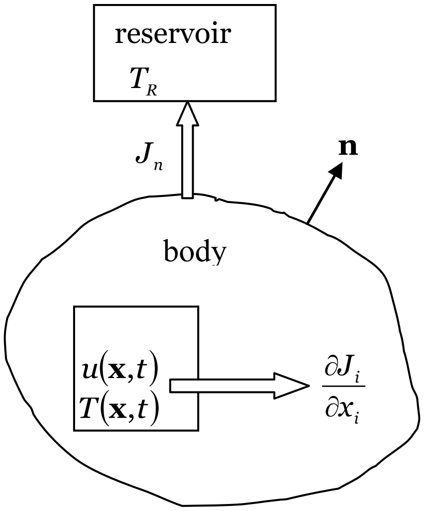
Thermodynamic model of a material. We now wish to reformulate Fourier's theory of heat conduction, starting from the fundamental postulate. So far as heat conduction is concerned, this alternative formulation will add nothing new to the theory. This lack of novelty need not disappoint us. The alternative formulation will aid us in formulating theories for more complex phenomena. Besides, it is always good to link theoretical ideas.

Let u be the energy per unit volume, and s the entropy per unit volume. A thermodynamic model of the material is specified by a function

$$s = s(u).$$

For a given material, this function is usually determined experimentally (http://imechanica.org/node/291). The temperature of the material particle, T, is given by

$$\frac{1}{T} = \frac{\partial s(u)}{\partial u}.$$



The body is taken to be rigid and stationary. We label each material particle by its coordinate $\mathbf{x}$. The energy density varies from particle to particle, and from time to time. That is, the energy density is a time-dependent field, $u(\mathbf{x},t)$. So are the entropy density $s(\mathbf{x},t)$ and temperature $T(\mathbf{x},t)$.

For a homogenous material, the function $s(u)$ is the same for all material particles and for all time. Once any one of the three fields, $u(\mathbf{x},t)$, $s(\mathbf{x},t)$ and $T(\mathbf{x},t)$, is known, the other two fields can be calculated by invoking the basic relations given above.

An isolated system with internal variables. Each material particle on the surface of the body is in thermal contact with a heat reservoir, held at temperature T_R. The temperature of the reservoir, T_R, needs not be the same as that of the material particle, T. Let J_n be the flux of energy from a particle on the surface of the body to a reservoir. The body and the field of reservoirs together constitute an isolated system. For this isolated system, we have identified six fields of internal variables:

$$u(\mathbf{x},t),\ s(\mathbf{x},t),\ T(\mathbf{x},t),\ J_i(\mathbf{x},t),\ J_n(\mathbf{x},t).$$

These six fields are subject to the constraints of the thermodynamic model of the material and conservation of energy. Consequently, only some of these fields can vary independently. For example, here is a choice of independent internal variables:

$$J_i(\mathbf{x},t),\ J_n(\mathbf{x},t).$$

The conservation of energy determines variation of the energy of the material particle, and the thermodynamic model of the material determines the entropy and the temperature of the material particle.

How entropy of the isolated system varies with the internal variables. The isolated system flips among a set of quantum states. A subset of the quantum states with given values of the internal variables constitute a macrostate of the isolated system. We need to count the number of quantum states in each of the macrostates of the composite. That is, we need to relate the entropy of the composite to the independent internal variables.

The entropy of the field of reservoirs increases per unit time by

$$\frac{\text{increase in entropy in reservoirs}}{\text{time}} = \int \frac{J_n}{T_R} dA .$$

The entropy of the body increases per unit time by

$$\begin{aligned}
\frac{\text{increase in entropy in body}}{\text{time}} &= \int \frac{\partial s(\mathbf{x},t)}{\partial t} dV \\
&= \int \frac{1}{T(\mathbf{x},t)} \frac{\partial u(\mathbf{x},t)}{\partial t} dV \\
&= -\int \frac{1}{T} \frac{\partial J_i}{\partial x_i} dV \\
&= \int \left[-\frac{\partial}{\partial x_i}\left(\frac{J_i}{T}\right) + \frac{\partial}{\partial x_i}\left(\frac{1}{T}\right) J_i \right] dV \\
&= -\int \frac{J_i n_i}{T} dA + \int \frac{\partial}{\partial x_i}\left(\frac{1}{T}\right) J_i dV \\
&= -\int \frac{J_n}{T} dA + \int \frac{\partial}{\partial x_i}\left(\frac{1}{T}\right) J_i dV
\end{aligned}$$

Pay close attention to each step of the above calculation. This is the type of calculation which we will repeat many times throughout this course. The first equality uses the thermodynamic relation $ds = T^{-1} du$. The second equality follows the conservation of energy. The third equality is a mathematical identity. The fourth equality invokes the divergence theorem. The last equality follows the conservation of energy. The above equation expresses the rate of the entropy of the body in terms of the independent internal variables.

The sum of the entropy of the body and that of the reservoirs gives the entropy of the composite. Consequently, the entropy of the composite increases per unit time by

$$\frac{dS_{composite}}{dt} = \int \left(\frac{1}{T_R} - \frac{1}{T} \right) J_n dA + \int \frac{\partial}{\partial x_i} \left(\frac{1}{T} \right) J_i dV .$$

Vary internal variables to increase the entropy of the isolated system. As the internal variables change, the macrostate also changes. The fundamental postulate implies that the internal variables evolve to increase the number of quantum states in the macrostate.

Each integral in the above expression involves a distinct way to transfer energy to or from material, $J_i(\mathbf{x},t)$, $J_n(\mathbf{x},t)$. The fundamental postulate implies that the entropy of the composite increases for every possible way of variation in the internal variables. Consequently, each integrand must be positive-definite:

$$\left(\frac{1}{T_R} - \frac{1}{T} \right) J_n \geq 0,$$

$$\frac{\partial}{\partial x_1} \left(\frac{1}{T} \right) J_1 + \frac{\partial}{\partial x_2} \left(\frac{1}{T} \right) J_2 + \frac{\partial}{\partial x_3} \left(\frac{1}{T} \right) J_3 \geq 0 .$$

These two inequalities are the consequences of the second law of thermodynamics. The first inequality says that, for a material particle on the surface of the body in contact with an energy reservoir, the flow of energy between the material particle and the reservoir is in the direction from high temperature to low temperature. The second inequality may be written as

$$\mathbf{J} \cdot \nabla T \leq 0 .$$

That is, at any material particle inside the body, the vector of energy flux, **J**, and the vector of the temperature gradient, ∇T, make an obtuse angle. This requirement is less restrictive than Fourier's law.

Kinetic models. Let us look at these conditions one by one. The first condition may be satisfied in several ways. For example, the surface of the body may be in thermal equilibrium with the reservoirs, so that

$$T = T_R .$$

We say that the temperature at the surface of the body is prescribed.

As a second way to satisfy the condition, the surface of the body may be insulated, $\delta q = 0$. We say that the heat flux at the surface of the body is prescribed to be zero.

As a third way to satisfy the condition, we can make the two factors of the product have the same sign. For example, we can set

$$J_n = K(T - T_R).$$

where $K > 0$ is known as the *heat transfer confident*.

The second condition is satisfied if we assume that the two factors have the same sign. We can satisfy the inequality if we assume that the heat flux is linear in the temperature gradient:

$$J_i = -\kappa(T)\frac{\partial T(\mathbf{x},t)}{\partial x_i},$$

with $\kappa(T) > 0$. This relation recovers Fourier's law.

As a generalization, we can satisfy the inequality by assuming that

$$J_i = -\kappa_{ij}\frac{\partial T(\mathbf{x},t)}{\partial x_j},$$

where κ_{ij} is a symmetric and positive-definite tensor. This model is suitable for anisotropic bodies. Further generalization is possible, but we will not pursue them here.

Summary of basic equations that govern heat conduction. The conservation of energy requires that

$$J_i n_i = J_n$$

on any plane, and that

$$\frac{\partial u(\mathbf{x},t)}{\partial t} + \frac{\partial J_i(\mathbf{x},t)}{\partial x_i} = 0$$

in the body.

The thermodynamics of the material is characterized by the function $u(T)$. The heat capacity is defined by

$$c = \frac{\partial u(T)}{\partial T}.$$

The second law of thermodynamics places certain restrictions on the direction of the energy flux. At a material particle on the surface of the body in contact with a reservoir of energy, energy exists the body if the temperature of the material particle is higher than the reservoir, but energy enters the body if the temperature of the material particle is lower than the reservoir. This requirement is satisfied by a kinetic model:

$$J_n = K(T - T_R),$$

where $K > 0$ is the heat transfer confident. At a material particle inside the body, the vector of the energy flux makes an obtuse angle with the vector of the temperature gradient. This requirement is satisfied by a kinetic model such as Fourier's law:

$$J_i = -\kappa \frac{\partial T(\mathbf{x},t)}{\partial x_i},$$

where $\kappa > 0$ is the thermal conductivity.

Appendix A: Divergence theorem. This is a theorem in calculus. Let $f(x_1,x_2,x_3)$ be a function defined in a volume in the space (x_1,x_2,x_3), and n_i be the unit vector normal to the surface enclosing the volume. The divergence theorem states that

$$\int \frac{\partial f}{\partial x_i} dV = \int f n_i dA.$$

The integral on the left-hand side extends over the volume, and the integral on the right-hand side extends over the surface enclosing the volume.