Extending continuum conservation laws

May 8, 2014

Overview

These notes cover the following:

- Conservation of energy
- Internal energy density, production rate density
- advective and conductive flux

Conservation of energy

Previously, we discussed the transport of mass, and how to represent mathematically the fact that mass is conserved. Fundamental physics tells us that there are other conserved quantities,such as momentum, angular momentum and energy. Like mass in a contunuum, these are in general not concentrated in point particles, but are distributed in space. We would like to extend the concept of density, of transport through a flux to these quantities, and formulate a conservation law mathematically.

Momentum is harder to deal with because it is a vector quantity, and the same is true of angular momentum. Energy, on the other hand, is a scalar, and can be dealt with similarly to mass. The energy content of a sample of material can be composed of a number of different forms of energy. The material may be moving at some velocity $\mathbf{v}$ (which could be a function of time and position), and the material may therefore have kinetic energy. There may also be potential energy arising from work done against an external force such as gravity. In addition, there may be potential energy due to the chemical composition of the material, for instance if there is a combustible or other reactive material. This potential energy therefore depends on the composition of the material, or more specifically, on the amounts of different chemical species. In addition, there is a 'thermal' component: the energy content of a sample of material will change as its temperature changes.

To make our job easier, we assume here that energy content of a sample of material can be separated additively into a macroscopic kinetic energy E_K, macroscopic potential energy E_P, chemical potential energy E_C and thermal energy E_T,

$$E = E_K + E_P + E_C + E_T, \tag{1}$$

and, somewhat simplistically, that only E_T depends on temperature. In what follows, we will concern ourselves only with the thermal energy content E_T of the material.

Note 1 *If you are familiar with thermodynamics, you will know that separating chemical potential and 'thermal' energy is not necesarily possible. In reality, the material has an* internal energy *that covers both, the chemical potential and 'thermal' components, but that these two cannot necessarily be separated neatly. The situation we have in mind here is that only a small fraction of the material is reactive but the amount of chemical potential energy it can realease is significant. In that case, we can treat the reactive material as having only chemical potential energy, and the non-reactive remainder as having only 'thermal energy', and the sum of the two makes up the total internal energy. 'Thermal energy' is then really the internal energy of the non-reactive component. The separation into a chemical and thermal component is a useful simplification later.*

To define the thermal energy content of a continuum, we need to define thermal energy density ε. As with mass density, we will define this density as a field by considering the thermal energy δe contained in a small volume δV surrounding the point (x, y, z) at time t, and put

$$\varepsilon(x, y, z, t) = \frac{\delta e}{\delta V};$$

the internal energy content δE is proportional to volume δV provided that volume is small, and the thermnal energy density is the constant of proportionality.

The thermal energy content of an extended volume V is then computed by splitting V up into small volume δV, finding their thermal energy content $\delta e = \varepsilon \delta V$ and summing. In other words

$$E_T = \int_V \varepsilon \, \mathrm{d}V.$$

To construct a conservation law, we need to know how the thermal energy content of a fixed volume V changes over time. As in the case of transfer of mass, one way in which the thermal energy content can change is that material leaves or enters the volume V, carrying thermal energy with it. Quantifying this is perfectly analogous to the case of mass. We take the boundary S of the volume V and split it into surface elements δS. We then compute the volume of material δV that passes *out* of the volume V through each δS in δt.

$$\delta V = \delta S \mathbf{v} \cdot \hat{\mathbf{n}} \delta t. \tag{2}$$

Exercise 1 *Give a careful derivation of the result* (2)*, making sure to explain why the dot product* $\mathbf{v} \cdot \hat{\mathbf{n}}$ *appears. Which way does* $\hat{\mathbf{n}}$ *need to point? What happens if* $\mathbf{v}$ *and* $\hat{\mathbf{n}}$ *are at an obtuse angle to each other?*

Next, we compute the amount of thermal energy carried out of V through each δS,

$$\delta e = \varepsilon \mathbf{v} \cdot \hat{\mathbf{n}} \delta S \delta t$$

and the total thermal energy carried out by summing over the δS,

$$\delta E = \int_S \varepsilon \mathbf{v} \cdot \hat{\mathbf{n}} \, \mathrm{d}S \delta t$$

The *rate* at which internal energy is carried out of the volume is then, explicitly taking the limit of $\delta t \to 0$

$$Q = \lim_{\delta t \to 0} \frac{\delta E}{\delta t} = \int_S \varepsilon \mathbf{v} \cdot \hat{\mathbf{n}} \, \mathrm{d}S, \tag{3}$$

where we deliberately use the same symbol Q for the rate of transfer of energy as we did for the rate of transfer of mass; similarly, we can identify $\mathbf{q} = \varepsilon \mathbf{v}$ as a thermal energy flux.

For conservation of mass, we had

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_V \rho \, \mathrm{d}V = -\int_S \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S,$$

and we might now be tempted to write

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_V \varepsilon \, \mathrm{d}V = -\int_S \varepsilon \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S. \tag{4}$$

There are however two crucial differences between mass and internal energy that mean that (4) generally does not hold:

1. Thermal energy itself is not conserved; total energy is.

2. Different bits of material can exchange thermal energy.

We will address these two points separately next.

Production rate density

Even if there is absolutely no transport of internal energy, the internal energy content of the volume V may still change because other forms of energy can be converted to internal energy. Consequently, we cannot assume that (4) holds: even if $\mathbf{v} = \mathbf{0}$, the thermal energy content $\int_V \varepsilon \,\mathrm{d}V$ may not remain constant, so there is something missing in (4).

We need a way of quantifying the rate of conversion of other forms energy into thermal energy. It should not come as a surprise that we need to do this in a way that allows for variations in conversion rate in space and time: for instance, when you look at flames in a fire, you are looking at the conversion of chemical potential energy into what we have termed 'thermal energy'. Obviously, this conversion does not happen uniformly in space or time, or else flames would not have spatial structure that changes constantly.

Consider the amount δe of other forms of energy converted to thermal energy in a volume element δV during a short time interval δt. It is natural that, so long as δV and δt remain small, δe should be proportional to δV and δt. We will denote the constant of proportionality by a, to get

$$\delta e = a \delta V \delta t$$

Obviously, a is a constant only with respect to δV and δt. It will depend on position (x, y, z) and on time t: as we have seen, thermal energy is not produced with uniform intensity. This is analogous for instance to how we defined ρ as the constant of proportionality that relates δV to δm. We have

$$a(x, y, z, t) = \frac{\text{thermal energy } \delta e \text{ produced in volume } \delta V \text{ around } (x, y, z) \text{ between } t \text{ and } t + \delta}{\delta V \delta t}$$

If we are to give a a name, the most 'natural' phrase would be be 'thermal energy production rate density'; 'density' because we have defined a as the rate of thermal energy production $\delta e / \delta t$ per volume size δV. The phrase is however a bit of a mouthful.

Exercise 2 *What are the units of a?*

Suppose we know a as a function of time and position, for instance because we know the rate at which chemical reactions are taking place. Can we compute the rate at which thermal energy is produced in the volume V as a whole? This is easy to do: we simply integrate to get

$$\int_V a \,\mathrm{d}V$$

Exercise 3 *Why do we simply integrate? Show from first principles that $\int_V a \,\mathrm{d}V$ is the rate at which thermal energy is produced by finding the total amount of energy of thermal energy produced in the volume V in time δt in terms of a. 'First principles' means you make* everything *in your derivation explicit.*

Exercise 4 *Radioactive decay releases a form of 'chemical potential energy', even though the bonds being broken and formed are not chemical bonds in the ordinary sense (between separate atoms) but are 'bonds' inside the nuclei of atoms.*

Uranium oxide, UO_2, has a density of 11000 kg m^{-3}. Suppose that the uranium in UO_2 is purely uranium-238, with a half life of 4.47×10^9 years and an atomic mass of 238 a.m.u., where 1 a.m.u. (atomic mass unit) = 1.66×10^{-27} kg. Oxygen has an atomic mass of 16 a.m.u.

1. *The rate at which the number n of radioactive nuclei in a sample decays is given by the differential equation*
$$\frac{\mathrm{d}n}{\mathrm{d}t} = -\lambda n,$$
where λ is a constant. Solve this using separation of variables, letting the number of nuclei at $t = 0$ be n_0. Determine, in terms of λ the time $t_{1/2}$ at which $n(t_{1/2}) = n_0/2$ nuclei are left.
2. *$t_{1/2}$ is called the half-life of the radionuclide. Find the decay constant λ in terms of $t_{1/2}$.*
3. *Assume you have a sample of pure uranium oxide, occupying a volume δV. In a small time interval δt, what number δn of nuclei that will decay in the sample? Keep δV and δt as variables, but express everything else in numerical terms. (There is a constant of proportionality here; compute that constant of proportionality numerically, making sure to state its units as well as its numerical value.)*
4. *If the decay of a single U-238 nucleus produces 7.61×10^{-12} J of heat, what is the amount of energy δe released in the volume δV in time δt? What is the thermal energy production rate density a?*
5. *The geothermal heat flux coming out of the Earth's surface is about 0.04 W m^{-2} on average. How thick a layer of pure uranium oxide just below the Earth's surface would be required to generate this flux?*

Conduction

Even if there was no conversion of other forms of energy into thermal energy, and no motion of material carrying thermal energy out of V, the thermal energy content of V could still change. Imagine heating a pot of water on an electric stove. There is no chemical reaction or other conversion of potential or kinetic energy inside the pot of water. There is also no movement of material into or out of the pot, especially if we assume that there is a lid on the pot. And yet we know that we can heat the pot, increasing its thermal energy content.

The way this works is that electrical potential energy is converted to thermal energy in the heating element in the stove, outside the pot. That thermal energy is then transferred to the pot, but without there being a simultaneous transfer of material. As a result, the transfer of thermal energy cannot be described by (3) as $\mathbf{v} = \mathbf{0}$ at the boundaries of the pot.

Instead of material moving and taking energy with it, the thermal energy moves by *conduction*: it is simply transferred from the hotter heating element to the cooler pot. It turns out that conduction can also be described by a flux $\mathbf{q}_c$. However, we already have a flux $\mathbf{q} = \varepsilon\mathbf{v}$: if there is motion of material, that material will still carry thermal energy with it, with an associated flux $\varepsilon\mathbf{v}$. To distinguish transport by motion of material from transport by conduction, we call $\mathbf{q} = \varepsilon\mathbf{v}$ the *advective flux*, and the flux $\mathbf{q}_c$ that describes transport by conduction the *conductive flux*.

Note 2 *You may be tempted to call transport by motion of material 'convection' because you have probably come acress convection before, but not heard the word 'advection'. Convection is however not quite the same as advection. It is a special case of advection that occurs when the motion of material carrying heat is driven by the fact that the material is hot and therefore less dense, so it rises buoyantly. This is a common effect: try opening the door of a hot oven. However, there are plenty of cases where advection occurs but not convection. If you stand under a hot shower, the water coming out of the shower advects thermal energy towards you, but it certainly is not rising buoyantly as it does so.*

We can define a conductive flux $\mathbf{q}_c(x, y, z, t)$ analogously to how we defined mass flux in the notes on surface integrals. Pick a surface element δS that is tied to the location (x, y, z) but whose orientation, defined through its normal $\hat{\mathbf{n}}$, can be changed. Let δe be the amount of thermal energy that passes through δS due to conduction in a short time interval from t to $t + \delta t$; naturally we expect δe to be proportional to the size of δS and δt, but the constant of proportionality may depend not only on location (x, y, z) and instant in time t, but also on the orientation of the surface element δS. We can define the magnitude of flux $\mathbf{q}_c$ by maximimizing δe with respect to the orientation of δS:

$$|\mathbf{q}_c| = \frac{\text{maximum } \delta e \text{ transferred through } \delta S \text{ in } \delta t \text{ as } \delta S \text{ is rotated through all orientations}}{\delta S \delta t}, \tag{5}$$

and define the direction of $\mathbf{q}_c$ to be the direction of $\hat{\mathbf{n}}$ when that maximum is reached.

It turns out that all the necessary information about conduction is contained in the vector field $\mathbf{q}_c$ defined in this way. When we have a surface at an oblique angle to $\mathbf{q}_c$, it is the component of $\mathbf{q}_c$ normal to δS that carries thermal energy across it. The amount of thermal energy δe that passes through δS in δt is proportional to δS and δt, the constant of proportionality being the normal component $\mathbf{q}_c \cdot \hat{\mathbf{n}}$:

$$\delta e = \mathbf{q}_c \cdot \hat{\mathbf{n}} \delta S \delta t. \tag{6}$$

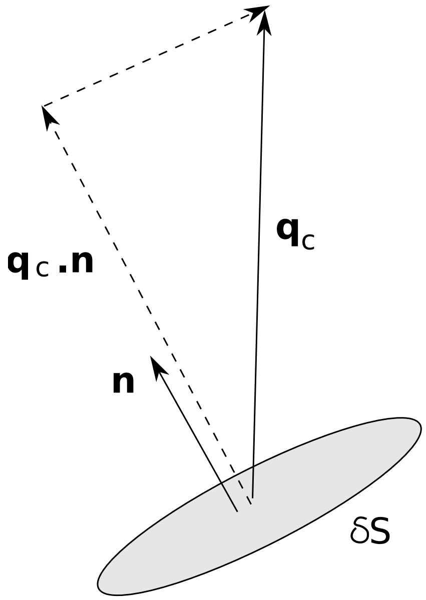

Figure 1: $\mathbf{q}_c \cdot \hat{\mathbf{n}}$ is the component of $\mathbf{q}_c$ that is parallel to $\hat{\mathbf{n}}$, and therefore perpendicular to δS. $\mathbf{q}$ can be decomposed into a part $(\mathbf{q} \cdot \hat{\mathbf{n}})\hat{\mathbf{n}}$ that is normal to δS, and a remainder that is parallel to δS.

The total amount of thermal energy that conduction transfers out of S in δt is the sum over the surface elements, $\delta E = \int_S \mathbf{q}_c \cdot \hat{\mathbf{n}} \, \mathrm{d}S \delta t$, and the *rate* at which thermal energy passes out through S due to conduction is

$$Q_c = \lim_{\delta t \to 0} \frac{\delta E}{\delta t} = \int_S \mathbf{q}_c \cdot \hat{\mathbf{n}} \, \mathrm{d}S, \tag{7}$$

just as (3) gives the rate at which heat is advected out of V.

Note 3 *It is actually not trivial to show from our definition of conductive flux in* (5) *that equation* (6) *holds. The definition of* $\mathbf{q}_c$ *only tells us that* (6) *holds when* $\hat{\mathbf{n}}$ *is aligned with* $\mathbf{q}$*, so that the rate of heat flow across* δS *is maximized, in which case* $\mathbf{q}_c \cdot \hat{\mathbf{n}} = |\mathbf{q}_c|$. *The fact that* (6) *holds for surface elements oblique to* $\mathbf{q}_c$ *is demonstrated in the appendix to these notes. You do not need to know that material in order to follow the rest of the course, however.*

Conservation of energy in integral and differential form

The thermal energy content of V can change not only due to material leaving or entering V and carrying thermal energy with it, but also due to conduction into or out of V, and due to production. Summing up all these effects gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \varepsilon \,\mathrm{d}V = -\int_S \varepsilon \mathbf{v}\cdot\hat{\mathbf{n}}\,\mathrm{d}S - \int_S \mathbf{q}_c\cdot\hat{\mathbf{n}}\,\mathrm{d}S + \int_V a\,\mathrm{d}V. \tag{8}$$

As in the case of conservation of mass, we would like to turn this 'integral form' of the conservation law into a differential equation. We have seen two ways for doing this for the case of mass conservation in the notes on the divergence theorem, and we could use either. Here we opt for the second, which uses the divergence theorem.

This method has four steps. First, turn the derivative of the volume integral on the left in a volume integral over a derivative:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \varepsilon\,\mathrm{d}V = \int_V \frac{\partial \varepsilon}{\partial t}\,\mathrm{d}V.$$

Second, turn the surface integrals into volume integrals using the divergence theorem,

$$\int_S \varepsilon\mathbf{v}\cdot\hat{\mathbf{n}}\,\mathrm{d}S = \int_V \nabla\cdot(\varepsilon\mathbf{v})\,\mathrm{d}V$$
$$\int_S \mathbf{q}_c\cdot\hat{\mathbf{n}}\,\mathrm{d}S = \int_V \nabla\cdot\mathbf{q}_c\,\mathrm{d}V$$

Third, substitute and combine all the terms in (8) into a single volume integral,

$$\int_V \frac{\partial\varepsilon}{\partial t} + \nabla\cdot(\varepsilon\mathbf{v}) + \nabla\cdot\mathbf{q}_c - a\,\mathrm{d}V = 0. \tag{9}$$

Last, V is arbitrary. Recognize that if the integrand was positive in some region, we could choose the volume V to lie in that region so the integral would be positive, in contradiction to the equality in (9). If a positive integrand means the equation (9) cannot be satisfied, then the integrand cannot be positive. Similarly, if the integrand was negative in some region, the same argument would hold, So the intgerand must be zero to make sure the integral is always zero.

$$\frac{\partial\varepsilon}{\partial t} + \nabla\cdot(\varepsilon\mathbf{v}) + \nabla\cdot\mathbf{q}_c - a = 0. \tag{10}$$

Of course, if the local form (10) holds, we can reverse the steps above to show that the integral form (8) also holds, regardless of the volume V.

We can compare (10) with the equation for conservation of mass,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0. \tag{11}$$

The two are clearly very similar: if we put $a = 0$, $\mathbf{q}_c = \mathbf{0}$ and $\varepsilon = \rho$, then (10) turns into (11). This is because their construction was very similar, looking at the mass and thermal energy content of a volume V using an integral over a density, and relating changes in that content to the rate at which mass and thermal energy flow into and out of the volume. The difference between the two is that thermal enegy can be produced, represented by the thermal energy production rate density a, and that it can be transported by conduction without any movement of material, represented by the conductive flux $\mathbf{q}_c$. Neither of these processes applies to mass.

Exercise 5 *The other method of turning an integral statement like* (8) *involved looking at a volume V that takes the form of a small cuboid $\delta x\, \delta y\, \delta z$, and computing the surface integral as the sum over flux components going into and out the six different sides of the cuboid. Follow that method (which we use at the start of the notes on the divergence theorem) to provide an alternative derivation of* (10)*.*

The need for constitutive relations

Suppose that we know how fast the material is moving and how rapidly thermal energy is produced, so $\mathbf{v}$ and a are known. Is this enough iin order to be able to use (8) to predict changes in the thermal energy density ε? Clearly, the answer must be 'no', because we have too many unknowns: ε as well as the three components of the flux $\mathbf{q}_c$. The problem is not *closed*, meaning it has too many unknowns and cannot be solved on its own.

If you recall the previous differential equation example on pressure in the atmosphere, you will see an analogous situation: we needed an equation that would link pressure and density, which we described as a constitutive relation. The fact that we need constitutive relations here, too, should not come as a surprise. (8) is very general and could describe conservation of energy in any continuum, without any particular reference to the material we are talking about or its properties. For instance, is the material a good insulator or conductor of heat? Equation (8) on its own has nothing to say about that.

The property that will link ε to $\mathbf{q}_c$ is temperature. We expect that ε goes up with temperature. We also expect that temperature will tell us about conduction: heat generally flows from high to low temperature. We deal with the relevant constitutive relations and the necessary calculus in the next set of notes.

Appendix: Conductive heat transport as a flux

We defined heat flux as a vector field in (5). That definition is all very well, but there is actually nothing in it that tells us that the thermal energy transferred across a small surface δS in δt should be related to $\mathbf{q}_c$ through

$$\delta e = \mathbf{q}_c \cdot \hat{\mathbf{n}} \delta S \delta t$$

when the surface δS is not oriented to maximimize δe. All we were really working off is that δe should be proportional to δS and δt, but that the constant of proportionality depends on the orientation of δS. Saying the constant of proportionality depends on orientation is the same as saying that it depends on the orientation of the unit normal vector $\hat{\mathbf{n}}$. We should therefore have said more generally that

$$\delta e = \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}})\delta S \delta t. \tag{12}$$

Do not be distracted by the squiggle[1] on $\tilde{q}_c$: we simply want a symbol that looks somewhat like flux (that is, like the symbol $\mathbf{q}_c$ we have been using for flux), but without the risk of confusing that symbol with the modulus of the flux vector $\mathbf{q}_c$ we have defined before. Also, do not be put off by having a function that has a vector like $\hat{\mathbf{n}}$ as an argument; this is nothing more clever than saying that it is a function of the components of the vector.

We have said that $\hat{\mathbf{n}}$ defines the orientation of δS. Obviously, δS has two possible normals that are equal and opposite to each other. As before, we take $\hat{\mathbf{n}}$ to point towards the side of δS to which δe is being transferred, and treat a negative amount of energy transferred to mean a positive amount transferred in the opposite direction. This means we immediately know that

$$\tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}) = -\tilde{q}_c(x, y, z, t, -\hat{\mathbf{n}}). \tag{13}$$

Obviously, δe, δS and δt are scalars, and therefore $\tilde{q}_c(x, y, z, t, \hat{\mathbf{n}})$ is also a scalar for given position (x, y, z), time t, and orientation $\hat{\mathbf{n}}$ of the surface element δS. What we would like to show is that

$$\tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}) = \mathbf{q}_c(x, y, z, t) \cdot \hat{\mathbf{n}}. \tag{14}$$

where $\mathbf{q}_c$ is defined in (5), as this would ensure that (6) holds. However, we cannot assume that this is the case. The only thing we know from the way we have constructed the flux is that

$$|\mathbf{q}_c(x, y, z, t)| = \max_{\hat{\mathbf{n}}} \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}),$$

where '$\max_{\hat{\mathbf{n}}}$' denotes the maximum taken as $\hat{\mathbf{n}}$ is varied over all possible orientations.

If we cannot rely on (6) but have only (12) to work with, the the rate at which thermal energy is conducted out of a volume V is therefore no longer given by (7) but by

$$Q_c = \int_S \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}})\, \mathrm{d}S \tag{15}$$

where $\hat{\mathbf{n}}$ is as before the outward-pointing normal. The conservation law then becomes

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_V \varepsilon \,\mathrm{d}V = -\int_S \varepsilon \mathbf{v} \cdot \hat{\mathbf{n}} \,\mathrm{d}S - \int_S \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}})\, \mathrm{d}S + \int_V a \,\mathrm{d}V,$$

or, after a bit of manipulation,

$$\int_S \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}})\, \mathrm{d}S + \int_V \frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{v}) - a \,\mathrm{d}V. \tag{16}$$

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[1] the squiggle ˜ is usually called a 'tilde'

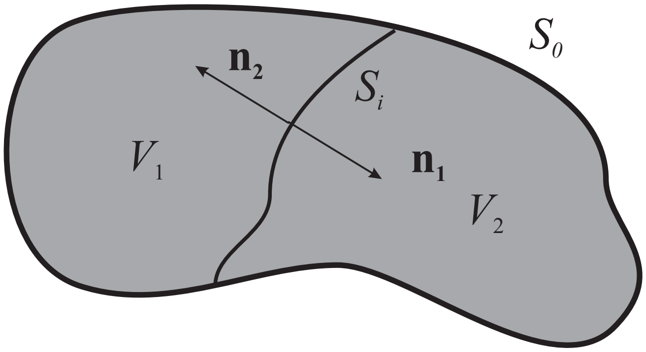

Figure 2: Energy exchange between two volumes V_1 and V_2: conductive heat flow out of V_1 has to be mass flow into V_2

Note 4 *With Q_x given by (15), we can see why (13) needs to hold. If we have two neighbouring volumes V_1 and V_2 (see figure (2), we can compute the rate of conduction out of V_1 through the shared boundary S_i as*

$$Q_1 = \int_{S_i} \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}_1) \,\mathrm{d}S,$$

and the rate of conduction out of V_2 as

$$Q_2 = \int_{S_i} \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}_2) \,\mathrm{d}S.$$

The two need to be equal and opposite — what flows out of V_1 has to flow into V_1, so $Q_1 + Q_2 = 0$ or

$$\int_{S_i} \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}_1) + \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}_2) \,\mathrm{d}S = 0.$$

With $\hat{\mathbf{n}}_2 = -\hat{\mathbf{n}}_1$,

$$\int_{S_i} \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}}_1) + \tilde{q}_c(x, y, z, t, -\hat{\mathbf{n}}_1) \,\mathrm{d}S = 0, \tag{17}$$

which is certainly the case of (13) holds. With the volumes and their contact area S_i being arbitrary, we could actually show that (17) must hold.

This must hold for arbitrary V, so let V be the triangular prism shown in figure 3, where the shaded face of the prism (labelled δS_1) is oriented at right angles to the flux vector $\mathbf{q}_c$ we defined before, with the flux $\mathbf{q}_c$ pointing *into* the volume, so in the opposite direction to the outward-pointing unit normal labelled $\hat{\mathbf{n}}_1$. This means that

$$\tilde{q}_c(x, y, z, t, -\hat{\mathbf{n}}_1) = |\mathbf{q}_c(x, y, z, t)|$$

for the normal direction $\hat{\mathbf{n}}_1$ to that face.

We assume the prism is very small, and this allows us to approximate surface and volume integrals by evaluating the integrands at $(x, y, z) = (x_0, y_0, z_0)$ (the vertex shown in figure 3 and multiplying the integrands by the relevant surface areas and volumes. When we apply this to (16), the result we get (which we demonstrate in more detail in note 5) is that

$$\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_1)\delta S_1 + \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_2)\delta S_2 + \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_3)\delta S_3 = 0. \tag{18}$$

In other words, at 'leading order' we can ignore advection, changes in thermal energy storage and thermal energy production for a very small volume (because the volume size δV gets smaller much faster than the surface area δS as we shrink the volume, so the volume integral gets smaller faster than the surface integral), as well as conduction through the bottom and top faces of the prism (because they cancel each other automatically in the limit of a small volume) and require that conduction through the three faces δS_1, δS_2 and δS_3 must cancel.

Then, knowing that $\delta S_1 = \delta S_3 \cos(\theta)$ and $\delta S_2 = \delta S_3 \sin(\theta)$. we get the simpler form of (18)

$$\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_3) + \cos(\theta)\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_1) + \sin(\theta)\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_2) = 0. \tag{19}$$

Note 5 *Here we will show that* (18) *and* (19) *must hold. The triangular face is a right-angled triangle has sides δa and an interior angle θ as shown, and the prism has height δa. The prism has a small base area $\delta^2 \sin(\theta)\cos(\theta)/2$ and therefore a small volume $\delta V = \delta a^2 \delta b \sin(\theta)\cos(\theta)/2$. The volume integral on the left-hand side of* (16) *can therefore be approximated as integrand times volume,*

$$\left(\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{v}) - a\right)\Bigg|_{(x_0, y_0, z_0)} \delta a^2 \delta b \sin(\theta)\cos(\theta)/2,$$

the integrand being evaluated at the point $(x_0 y_0, z_0)$ indicated in figure 3

Because the prism is small, we can also approximate the surface integrals as integrand times surface area for each of the faces of the prism (each face having a distinct normal $\hat{\mathbf{n}}$, and therefore a distinct integrand $\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}})$). Label the faces as shown in figure 3, in which case we have $\delta S_1 = \delta a \delta b \cos(\theta)$, $\delta S_2 = \delta a \delta b \sin(\theta)$, $\delta S_3 = \delta a \delta b$ and $\delta S_4 = \delta S_5 = \delta a^2 \sin(\theta)\cos(\theta)/2$. With those, we have

$$\begin{aligned}\int_S \tilde{q}_c(x, y, z, t, \hat{\mathbf{n}})\,\mathrm{d}S \approx & \delta S_1 \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_1) + \delta S_2 \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_2) + \delta S_3 \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_3) \\ & + \delta S_4 \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_4) + \delta S_5 \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_5).\end{aligned}$$

However, the top and bottom faces have equal size, $\delta S_4 = \delta S_5$, while their outward-pointing unit normals are equal and opposite, $\hat{\mathbf{n}}_4 = -\hat{\mathbf{n}}_5$. From (13)*, we have*

$$\delta S_4 \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_4) + \delta S_5 \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_5). = \delta S_4 \left[\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_4) - \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_4)\right] = 0.$$

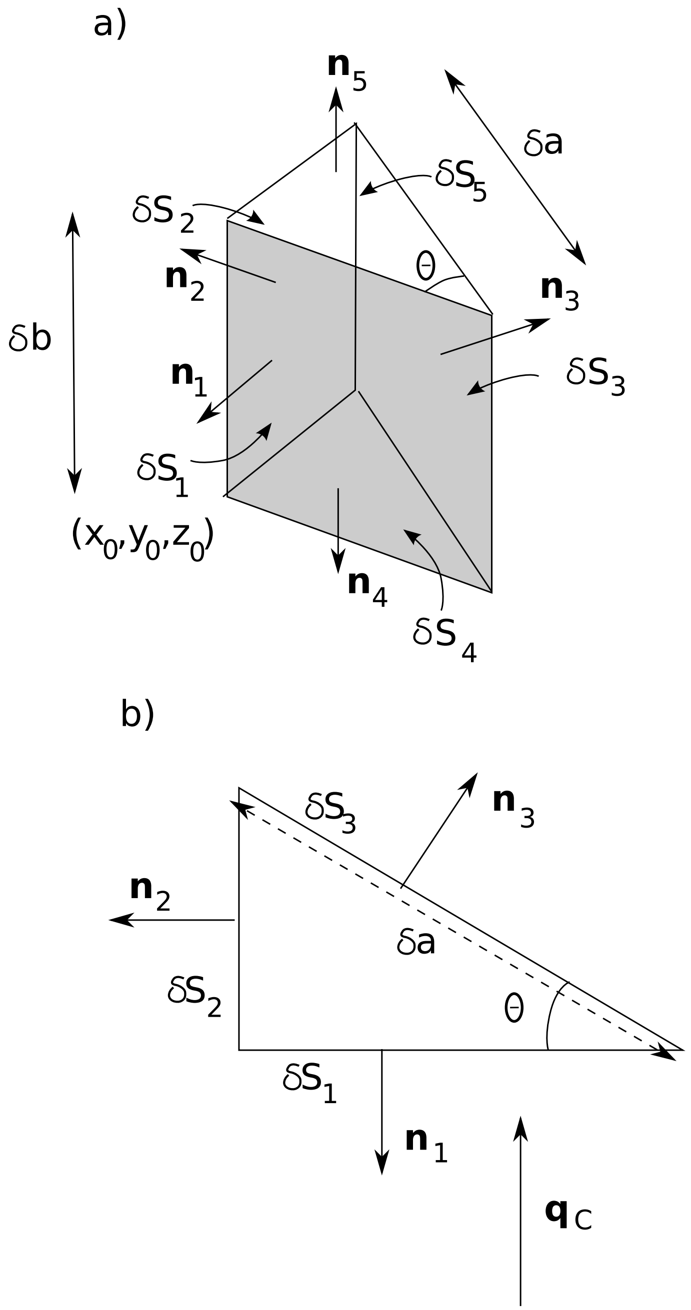

Figure 3: The prism shape of V: a) perspective view and b) top-down view. The previously defined flux vector $\mathbf{q}_c$ is perpendicular to the face δS_1, pointing inwards.

Conduction into the bottom face and out of the top face approximately cancels as the two faces are parallel to each other. This leaves only the three remaining faces, and we have

$$\begin{aligned}\int_S \tilde{q}_c(x,y,z,t,\hat{\mathbf{n}})\,\mathrm{d}S \approx& \delta S_1\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_1) + \delta S_2\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_2) + \delta S_3\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_3)\\ =& \left[\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_3) + \cos(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_1) + \sin(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_2)\right]\delta a\delta b\end{aligned}$$

Substituting in (16) *gives*

$$\begin{aligned}&\left[\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_3) + \cos(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_1) + \sin(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_2)\right]\delta a\delta b\\ &\qquad + \left(\frac{\partial\varepsilon}{\partial t} + \nabla\cdot(\varepsilon\mathbf{v}) - a\right)\Bigg|_{(x_0,y_0,z_0)}\delta a^2\delta b\sin(\theta)\cos(\theta)/2, = 0.\end{aligned}$$

If we divide both sides by $\delta a\delta b$, then we get

$$\begin{aligned}&\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_3) + \cos(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_1) + \sin(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_2)\\ &\qquad + \left(\frac{\partial\varepsilon}{\partial t} + \nabla\cdot(\varepsilon\mathbf{v}) - a\right)\Bigg|_{(x_0,y_0,z_0)}\delta a\sin(\theta)\cos(\theta)/2, = 0\end{aligned}$$

Now we can recongize that the last term is multiplied by δa while the first three terms are not, so the last term is very small compared with the first three. This means we can approximately write

$$\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_3) + \cos(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_1) + \sin(\theta)\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_2) = 0.$$

which is (19)

Next, we can show from (19) that, if the face δS_1 is perpendicular to the flux $\mathbf{q}_c$, then there cannot be any conduction into the face δS_2 at that sits at right angles to $\mathbf{q}_c$. We can do this by looking at different prisms in which the faces δS_1 and δS_2 always have the same orientation (and therefore the same normals $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_2$), but where each prism can have a different internal angle θ and therefore the face δS_3 can have a different normal $\hat{\mathbf{n}}_3$. This means that we can treat $\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_1)$ and $\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_2)$ as constant, but $\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_3)$ will be a function of θ. Putting

$$\begin{aligned}q_1 &= \tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_1)\\ q_2 &= \tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_2)\\ q_3 &= \tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}}_3)\end{aligned}$$

we treat q_1 and q_2 as constant but q_3 is a function of θ.

Now remember that the face δS_1 was chosen to be perpendicular to the flux $\mathbf{q}_c$, so $\tilde{q}_c(x_0,y_0,z_0,t,\hat{\mathbf{n}})$ should be maximized when the normal $\hat{\mathbf{n}}$ is aligned with $-\hat{\mathbf{n}}_1$.

This means that q_3 should be maximized when $\theta = 0$, in which case $\hat{\mathbf{n}}_3 = -\hat{\mathbf{n}}_1$. We therefore expect

$$\frac{\mathrm{d}q_3}{\mathrm{d}\theta} = 0 \qquad \text{when } \theta = 0.$$

But

$$q_3 = -q_1 \cos(\theta) - q_2 \sin(\theta)$$

and so

$$\frac{\mathrm{d}q_3}{\mathrm{d}\theta} = q_1 \sin(\theta) - q_2 \cos(\theta) = -q_2 = 0 \qquad \text{when } \theta = 0.$$

This implies that $q_2 = 0$.

But if $q_2 = 0$, then $q_3 = -q_1 \cos(\theta)$, or

$$\begin{aligned}\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_3) =& - \tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_1) \cos(\theta) \\ =& \tilde{q}_c(x_0, y_0, z_0, t, -\hat{\mathbf{n}}_1) \cos(\theta) \\ =& |\mathbf{q}_c(x_0, y_0, z_0, t)| \cos(\theta) \end{aligned} \tag{20}$$

because the alignment of face δS_1 was chosen so that the flux $\mathbf{q}_c$ points into the face at right angles, $\mathbf{q}_c = -|\mathbf{q}_c|\hat{\mathbf{n}}_1$. But θ is the angle between $\hat{\mathbf{n}}_3$ and $-\hat{\mathbf{n}}_1$, and therefore the angle between $\hat{\mathbf{n}}_3$ and $\mathbf{q}_c$. In other words, (20) says that

$$\tilde{q}_c(x_0, y_0, z_0, t, \hat{\mathbf{n}}_3) = \mathbf{q}_c(x_0, y_0, z_0, t) \cdot \hat{\mathbf{n}}_3.$$

But this is precisely the equation (14) we set out to derive.

The key to this derivation is that the faces δS_1 and δS_3 are related through the cosine of same angle θ that separates the normals $-\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_3$. The conductive flux $\mathbf{q}_c$ enters perpendicularly through the face δS_1. Conduction out through the oblique face δS_3, which is larger than δS_1 by a factor of $1/\cos(\theta)$ must carry out thermal energy at the same rate as $\mathbf{q}_c$ carries it in through δS_1. The rate at which heat is conducted per unit area of the face δS_3 must therefore be smaller than the flux $|\mathbf{q}_c|$ by a factor $\cos(\theta)$ to account for the larger surface area.