

Continuum Thermodynamics

Conor Rowan

March 2024

Contents

1	Introduction	2
2	Power Input	2
3	Heat Input	3
4	Path Dependence	4
5	First Law	6
6	Discussion	7
7	Second Law	8
8	Entropy in Statistical Mechanics	9
9	Entropy in Classical Thermodynamics	10
10	Equivalence of Classical and Statistical Notions of Entropy	13
11	Entropy in Continuum Mechanics	14
12	Thermodynamic Potentials	15
13	Dissipation Function	18
14	Helmholtz Energy as a Constitutive Relation	19
15	Solving Problems	20
16	An Example	21
17	Energy Formulation	25
18	Dissipative Materials and Internal Variables	26

1 Introduction

The purpose of this document is to demonstrate the connections between elasticity and thermodynamics. This involves primarily the first and second law of thermodynamics, which explain the thermal and mechanical exchanges of energy of continuum particles, and impose restrictions on the direction of such processes. These results are interesting because they connect continuum mechanics with thermodynamics, and show how they are complementary. Continuum thermodynamics is useful because it gives a better sense of how proper constitutive relations are formulated, which becomes essential for complex materials (for example, some horrifying thing like “temperature-dependent viscoelasticity at finite strains”). It is also necessary for deriving the governing equations of bodies whose thermal and mechanical responses are coupled. To the extent that thermal-mechanical coupling is a relatively familiar thing (a ductile metal repeatedly bent back and forth will heat up), sorting out the interrelations of elasticity and thermodynamics is not some pedantic exercise in obscure 20th century physics. It is the only way to tie together concepts of stress, strain, work, heat, energy, temperature, dissipation, etc. In writing these notes, I have made use of the Malvern textbook on continuum mechanics, this webpage from the University of Utah, this paper on thermoelasticity, and the Holzapfel textbook on nonlinear solid mechanics.

2 Power Input

The work done by a displacement dependent force $F(x)$ over some deformation up to position x^* is

$$W = \int_0^{x^*} F(\xi) d\xi$$

For a time dependent displacement $x(t)$, the work done is a function of time through the displacement only:

$$W(t) = \int_0^{x(t)} F(\xi) d\xi$$

By definition, power is the time derivative of the work. Work is the transfer of energy by mechanical forces, so we think of power as a rate of mechanical energy exchange. Because the time dependence of the work depends entirely on the limit of integration, we must use the Leibniz rule to compute this derivative. Notice the assumption of no explicit time dependence of the force. The following expression for power would look different if the force depended on time explicitly, rather than an implicit dependence through the displacement. The power is computed as

$$P = \frac{\partial W}{\partial t} = \frac{\partial}{\partial t} \int_0^{x(t)} F(\xi) d\xi = \frac{\partial x}{\partial t} F(x(t))$$

This is where the familiar definition of force times velocity comes from. We can now extend this to elastic systems undergoing large strains. The total power of the body comes from external forces in the form of surface tractions \underline{t} and body forces \underline{f} . The power now involves dot products of the force with the velocity:

$$P = \int t_i v_i dS + \int f_i v_i d\Omega$$

This is an extension to vector-valued forces defined over volumes and surfaces. The integral is taken over some arbitrary region of material which need not be the actual boundary of the solid. The notation dS is used to indicate surface integrals, and $d\Omega$ for volume integrals. These integrals are taken in the current configuration. The traction vector is related to the Cauchy stress with $t_i = \sigma_{ij} n_j$. Plugging this into the above expression and using the divergence theorem, the power can be written as

$$P = \int \frac{\partial}{\partial x_i} (\sigma_{ij} v_j) d\Omega + \int f_i v_i d\Omega$$

We can distribute the divergence, and use the governing equation of force equilibrium in the current configuration ($\sigma_{ij,j} + f_i = \rho Dv_i/Dt$) to arrive at

$$P = \int \rho \frac{Dv_i}{Dt} v_j + \sigma_{ij} \frac{\partial v_j}{\partial x_i} d\Omega$$

The material time derivative is used because we track the change in velocity of a particle (on which Newton's second law applies), as opposed to whatever chunk of material happens to inhabit a certain region of space. The Reynolds Transport theorem allows this time derivative to be factored out, yielding

$$P = \frac{D}{Dt} \int \frac{1}{2} \rho v_i v_i d\Omega + \int \sigma_{ij} \frac{\partial v_j}{\partial x_i} d\Omega$$

To reiterate, the material time derivative is used to indicate that we look at the time rate of change of a fixed collection of particles, as opposed to a region in space. We can now recognize the first term as the time derivative of the total kinetic energy of the region, and the second term is the power associated with deformation. This second term, called the “stress power,” is associated with an exchange of energy that does not cause macroscopic motion of the continuum. We will make use of this expression for the power of a region of a continuum soon.

3 Heat Input

Consider the same region of material as above. We showed how applied volumetric forces and elastic contact forces with the surroundings are associated with power. Power was conceptualized as a rate of energy flow. Another source of energy flow for the body arises from thermal effects—both heat sources and

conduction within the body. Because the vector normal to the region under consideration is defined as outwards, we can write the inflow of heat as

$$Q = - \int q_i n_i dS + \int r d\Omega$$

where the first term defines the inflow of heat into the body from conduction by looking at the normal component of the heat flux vector q_i . The second term is a volumetric heat source, which could model phenomena such as internal dissipative heating or thermal radiation. Power and heat are the two ways in which energy is exchanged between regions of space for most mechanical systems. Of course, this ignores phenomena such as electromagnetism or chemical reaction, which are not dominant effects in many engineering systems. Before relating heat and power, we take a brief detour to investigate the idea of exact differentials and path dependence, which is useful in understanding thermodynamic processes.

4 Path Dependence

Consider an arbitrary function f . Assume that two variables x and y influence the value of f in some way. A small change in f as a function of these coordinates can be written as

$$df = Q(x, y)dx + P(x, y)dy$$

where Q and P are arbitrary functions which quantify the sensitivity of the function f to changes in its coordinates. Say that we integrate df along some path which returns to its starting point. A path is understood as a parameterization of the position-like coordinates x and y in terms of a time-like coordinate t . This can be written as

$$\oint df = \oint Qdx + Pdy = \int_0^T \begin{bmatrix} Q \\ P \end{bmatrix} \cdot \begin{bmatrix} x'(t) \\ y'(t) \end{bmatrix} dt$$

The contour integral is meant to indicate that the path is closed. The final time T of the parameterization is such that $[x(0), y(0)]^T = [x(T), y(T)]^T$. The integral around the closed path is not equal to zero in general. Consider this situation: a particle slides around on a flat surface ($x - y$ plane) with friction. A small increment of work is given by Fds , where F is a frictional force and ds is the distance traveled in the $x - y$ plane. Note that the frictional force always opposes the velocity. The work done by friction in moving the mass in a closed loop will not be zero. Parameterizing the coordinates in terms of a time-like variable, the total work done is computed as the time integral of the instantaneous work rate, or power. Assume that the particle returns to its final state at time $t = 1$. The integral can be computed as

$$W = \int_0^1 - \frac{F}{\sqrt{x'(t)^2 + y'(t)^2}} \begin{bmatrix} x'(t) \\ y'(t) \end{bmatrix} \cdot \begin{bmatrix} x'(t) \\ y'(t) \end{bmatrix} dt \neq 0$$

This expression looks a little messy, but simply says that the frictional force is opposite the velocity and has magnitude F . Note that the frictional force is typically related to the weight and a friction coefficient, but this is not important to us. Because the integrand never changes sign, this integral is guaranteed to be nonzero. When the path integral is zero, we say that df is an “exact differential,” implying that

$$Q = \frac{\partial f}{\partial x}, \quad P = \frac{\partial f}{\partial y}$$

When df is an exact differential, we can measure its change by looking at end states alone. Mathematically, this means that

$$\Delta f = f(x_2, y_2) - f(x_1, y_1)$$

An example of this is the gravitational potential. Considering a particle moving in the $x - y$ plane where y is the vertical height, and x the horizontal position. The gravitational potential is

$$V = Fy(t)$$

In this case, the force of gravity is computed with the gradient of the potential. The work done by traveling is a closed loop (same parameterized path) is given by

$$W = \int_0^1 \nabla V \cdot \begin{bmatrix} x'(t) \\ y'(t) \end{bmatrix} dt = 0$$

See this interactive plot for a comparison of the path dependent frictional process, and the path independent process involving the force of gravity. A process involving a potential is guaranteed to be path independent. It is also often called a “state variable,” meaning that its value is uniquely determined by its “state” (x, y) . There is notion of the “state” of the work of friction, because looking at the position (x, y) tells you nothing about how much work has been done. Naturally, it is called path-independent because we can understand the change in its value by looking only at the initial and final points, without considering the path that connects them. In contrast, a path dependent process depends on the details of how the process was carried out. When the position is parameterized in terms of a time-like variable, this means that for a path dependent process

$$\int_1^2 df = \begin{bmatrix} Q \\ P \end{bmatrix} \cdot \begin{bmatrix} x'(t) \\ y'(t) \end{bmatrix} dt \neq \int_1^2 df' = \int \begin{bmatrix} Q \\ P \end{bmatrix} \cdot \begin{bmatrix} q'(t) \\ s'(t) \end{bmatrix} dt$$

where this means that the change in the function f depends on the path taken between the end points. It is helpful to think of functions which are path independent as quantifying the “storage” of something, usually energy of some sort.

5 First Law

It can be shown empirically that the total mechanical energy exchanged throughout a time-dependent process is path dependent. This means that

$$\oint P dt \neq 0$$

There is no “stored mechanical energy” for which the power is the rate of change. Power only gives the instantaneous rate of change of the mechanical energy, but cannot be computed as a time derivative of a total mechanical energy function. The same can be said for the heat transfer. It has been proven empirically that

$$\oint Q dt \neq 0$$

meaning that there is no “stored thermal energy” function for which the heat flux is the time rate of change. A cyclic process can occur which generates or absorbs heat. Heat flux gives the instantaneous rate of change of thermal energy, but is not the rate of change of some heat function. What can be said, however, is the following:

$$\oint (P + Q) dt = 0$$

This is also an empirical statement. It says that the sum of heat flux and power is a path independent quantity. We call this the total energy of the system. Because it is path independent, the change in the energy depends only on the initial and final points of a process. We think of “points” in a process as defined by state variables such as strain, temperature, etc. Because the energy depends on states and not the specifics of the path between states, it is called a function of state. Denoting the total energy by E , the differential form of the above statement says that

$$\dot{E} = P + Q$$

Let’s say that we have two state variables x and y . They are used for the purpose of demonstration, so their meaning is not important. The above tells us that

$$dE = (P + Q)dt$$

As we have remarked, the energy E is a function of state, so it can be integrated without reference to the path a process takes. This is not true for the power and heat flux individually, only their sum. We parameterize the path in terms of time with $x(t)$ and $y(t)$. The change in energy is then

$$\Delta E = \int_1^2 dE = E(x(t_2), y(t_2)) - E(x(t_1), y(t_1)) = \int_1^2 (P(x(t), y(t)) + Q(x(t), y(t))) dt$$

That the energy is a function of state alone says that for any two paths with the same endpoints, the integral involving heat and power shown above will yield the same value. What we have shown is that the energy changes in time due to power and heat inputs. This is the first law of thermodynamics.

Returning to the continuum body considered in deriving the power and heat input expressions, we apply the first law to an arbitrary volume of material. The total energy E is split up into a kinetic energy term, which quantifies the energy associated with macroscopic motion, and an internal energy term, which quantifies the energy associated with microscopic motion (temperature) and deformation. Using the expressions we derived for the power and heat inputs, the first law applied to a continuum reads

$$\frac{D}{Dt} \int \frac{1}{2} \rho v_i v_i d\Omega + \frac{D}{Dt} \int \rho e d\Omega = \frac{D}{Dt} \int \frac{1}{2} \rho v_i v_i d\Omega + \int \sigma_{ij} \frac{\partial v_j}{\partial x_i} d\Omega - \int q_i n_i dS + \int r d\Omega$$

The left side is the time rate of the change of the energy written for a collection of particles found at the current instant of time in the region defined by the volume integrals. We introduce the notation e as the specific internal energy of the solid (energy per mass). The kinetic energy terms cancel out, and the divergence theorem can be used to convert the surface integral for heat flux into a volume integral. The integral expression of the first law for a continuum then reads

$$\frac{D}{Dt} \int \rho e d\Omega = \int \sigma_{ij} \frac{\partial v_j}{\partial x_i} d\Omega - \int \frac{\partial q_i}{\partial x_i} d\Omega + \int r d\Omega$$

The volume over which this expression holds has been chosen arbitrarily. For this to hold in general, it should be satisfied in a pointwise sense. Localizing the integrals, we have the strong form of the first law:

$$\rho \frac{De}{Dt} = \sigma_{ij} \frac{\partial v_j}{\partial x_i} - \frac{\partial q_i}{\partial x_i} + r$$

The Reynolds Transport theorem is used to pass the material time derivative inside the integral. This explains why there is no time derivative on density, even without assuming that it is constant.

6 Discussion

So far, we haven't done anything too crazy. The first law of thermodynamics says that heat and work come together to change the total energy of a system. This is a statement that mechanical and thermal energy can be converted into one another. From Newton's second law, we can derive the governing equations of an elastic body in the current configuration:

$$\rho \frac{Dv_i}{Dt} = \frac{\partial \sigma_{ij}}{\partial x_j} + f_i$$

This is the balance of linear momentum, a fundamental mechanical principle which we have already made use of in deriving the expression for the power. The reader is assumed to be familiar with this. We have introduced an additional principle of mechanics, which is the first law of thermodynamics for a continuum:

$$\rho \frac{De}{Dt} = \sigma_{ij} \frac{\partial v_j}{\partial x_i} - \frac{\partial q_i}{\partial x_i} + r$$

Note that all of these expressions could be converted to the reference configuration if desired—this is shown in many texts. We operate in the current configuration for simplicity. When there are no thermal effects incorporated into the analysis of an elastic body, the balance of momentum (along with a constitutive relation between stress and strain) is sufficient to find the displacement. However, when a thermodynamic variable like temperature is introduced as an additional unknown, we need to appeal to the first law in order to close the system. The balance of linear momentum and the balance of energy are thus coupled. At least they might be, for example in the case of a dissipative material. A dissipative material is one for which mechanical energy is converted into heat, thus introducing a connection between the elastic and thermal response. If the stress-strain relation is dependent on the temperature, there is additional coupling. It is not clear at this point how to actually solve a problem of this sort. The reason is that we do not know what the specific internal energy e is. Presumably, it depends on the deformation and thermal response of the material in some way. *The crux of understanding and solving a thermoelastic problem is understanding the specific internal energy.* It should be thought of as a constitutive relation which does more than simply connect stress and strain. The internal energy quantifies how a material stores energy both in terms of the mechanical and thermodynamic aspects of the body’s response. It turns out this is quite a complex thing. Unfortunately, we will have to defer discussion on computational aspects of thermoelasticity to later. We first need to explore additional restrictions imposed by the thermodynamics of continua before solution techniques can be discussed.

7 Second Law

The first law states that mechanical work and heat can be converted into one another. At a given total energy level of a system, the first law does not differentiate between the conversion of mechanical energy into thermal energy, and thermal energy into mechanical energy. But we know from experience that thermal and mechanical energy behave differently. The kinetic energy of a car is converted into thermal energy by using the brakes. But once the brake pads heat up, we cannot recover the kinetic energy of the car. Mechanical energy naturally is converted into heat, but heat does not spontaneously transition to mechanical energy. In some sense, we can think of motion as a “battery” for thermal energy (we could heat something up with friction), but temperature is not a “battery” for motion (more effort and thought is required to extract

mechanical work from a hot object). This asymmetry between heat and work is not reflected in the first law of thermodynamics. These questions are addressed by the Second Law of Thermodynamics. This will involve trying to wrap our heads around entropy. Inevitably, this is where things go off the rails.

8 Entropy in Statistical Mechanics

This section and the following are included for some background on entropy and can be skipped if desired. Entropy in statistical mechanics is all about counting the number of microstates that a system could be in while being consistent with macroscopic variables such as energy or volume. These thought experiments are typically conducted for the canonical “gas in a box” system. What is a microstate? A microstate is thought of as a vector of observations of the position and momenta of all the particles in the box. If there is one particle in a 3D box, one microstate might be $\underline{s}_1 = [x, y, z, p_x, p_y, p_z]^T = [1, 2, 3, 4, 5, 6]^T$. Another microstate is $\underline{s}_2 = [6, 5, 4, 3, 2, 1]^T$. It is not possible to directly count the number of microstates gas particles can take on because the position and momentum take on continuous values. However, what we can do is say that the number of microstates available to a gas is proportional to the volume in state space defining position/momenta for all of the particles. If there are no constraints imposed on the gas, meaning that it could have any energy, volume, etc., there are an infinite number of microstates available to the system. This is because we integrate over the entirety of state space in finding the volume of possible states. However, if we impose a constraint, such as that the total kinetic energy of the collection of particles is equal to some constant E , we limit ourselves to a subset of state space with finite volume. We know that the energy of a single particle is $p^2/2m$. This means that a collection of N particle has a given energy when

$$\sum_{i=1}^N \sum_{j=1}^3 \frac{1}{2m} p_{ij}^2 = E$$

where p_{ij} is the j component of momentum for particle i . This equation defines a hypersphere in state space. The number of microstates available to a system with given energy is thus proportional to the area of this hypersphere, whose radius is \sqrt{E} . Using the notation $\Omega(E)$ to mean “the number of states with total energy E ,” we can write that

$$\Omega(E) \propto E^{3(N-1)/2}$$

Thus, we see that increasing the total energy of the system increases the number of microstates which are consistent with that energy. Similarly, increasing the number of particles increases the number of available microstates. We can see a similar influence of the volume of the box of gas on the number of states available to the system. The volume V imposes restrictions on the possible positions that particles can occupy, unlike the energy which imposed

requirements on the momenta. If we double the volume of a box occupied by a single particle, we double the volume of state space it can occupy. If there are two particles, the whole system can occupy four times as much volume in state space. Thus in general, we see that that

$$\Omega(V) \propto V^N$$

In statistical mechanics, the definition of entropy is

$$S = k \ln(\Omega)$$

where k is Boltzmann's constant and Ω is the number of microstates, which we have been counting by measuring volumes in state space. The effect of changing the energy and volume on the number of states is multiplicative, meaning that for a system whose volume and total energy changes, we have that the entropy is

$$S \propto k \ln \left(E^{3(N-1)/2} V^N \right) \approx kN \left(\ln V + \frac{3}{2} \ln E \right)$$

We do not have all of the details carefully sorted out here. It can be shown from statistical mechanics that the temperature (θ) is proportional to the average kinetic energy of particles in the box. Thus $E \propto \theta$. This is explored in “Equilibrium and Statistical Mechanics” notes. It suffices for our purposes to say that

$$S \propto \ln V + \ln \theta$$

where θ is the temperature. The idea is that from the perspective of statistical mechanics, entropy quantifies how many different versions of the system can be consistent with the macroscopic variables. There are many ways to distribute momentum between two particles such that they have the same total kinetic energy. Entropy quantifies this multiplicity of microstates. High entropy systems are ones for which many configurations, defined in terms of the position and momenta of the constituent particles, lead to the same macrostates of energy, volume, pressure, and so on. Counting microstates gives some insight into how this multiplicity is influenced by these macroscopic variables.

9 Entropy in Classical Thermodynamics

The classical and statistical definitions of entropy seem completely different, but are ultimately shown to be equivalent. One motivation for the classical conception of entropy is the Carnot cycle, shown in Figure 1. See the Figure and caption for a brief description of the cycle. The reader is assumed to have some familiarity with this, as this presentation is very brief. In the Carnot cycle, heat is not a conserved quantity around the cycle because it is a function of path. In doing a full loop through the cycle, the change in heat is non-zero. But if we define a new variable $S = Q/T$, we can see that over the whole process

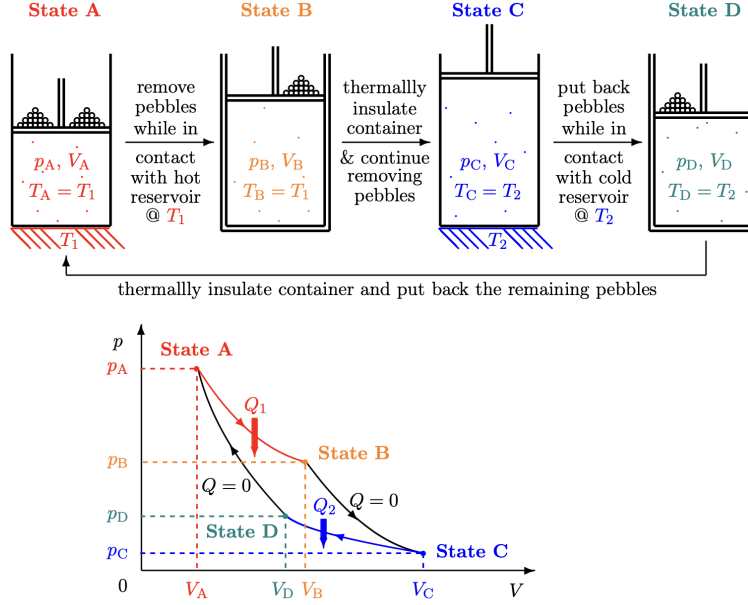


Figure 1: The Carnot cycle requires heat input in AB for the gas to stay at the same temperature as it expands. The internal energy does not change in this system because for an ideal gas the internal energy is only a function of temperature. The work done equals the heat absorbed. In BC, the piston is insulated so there is no heat transfer, but because the gas does work, the internal energy changes so it cools down. In CD, the gas is attached to a cool reservoir so that it can stay at the same temperature while being compressed. It thus dumps heat into the cool reservoir but stays at constant temperature. Finally, the piston is insulated again and the gas continues to be compressed and heats up until it returns to its original temperature. The total work that the system does is $W_{AB} + W_{BC} + W_{CD} + W_{DA} = Q_1 + Q_2$. The efficiency of the engine is work done divided by heat absorbed $\eta = |W_{tot}|/Q_1$. The fact that this value is less than 1 indicates that thermal energy cannot be perfectly transformed into mechanical energy.

$$\Delta S = \frac{Q_1}{T_1} + 0 + \frac{Q_2}{T_2} + 0$$

The two zeros are from the adiabatic (insulated and reversible) legs of the cycle. We know that in the isothermal legs, the internal energy of the ideal gas does not change, so the heat exchanged is equal to the work done. Using $W = \int p dV$ and the ideal gas law, it can be shown that

$$\Delta S = 0$$

This implies that our new variable S is a function of state, given that its net change is zero around a closed loop. It can be shown that this is only true for reversible processes. This quantity is interesting by virtue of being a state variable, but its definition in terms of heat exchanged at given temperatures does not clarify its physical interpretation. Given that the entropy S is a function of state, we can write it as an exact differential

$$dS = \frac{\delta Q}{T} \implies S_2 - S_1 = \int_1^2 \frac{\delta Q}{T}$$

The notation “ δ ” is used to indicate a small, instantaneous quantity which is not the differential of some state function.

As a final note on the classical conception of entropy, we can motivate the equivalent of classical and statistical mechanical definitions with a simple example. Consider an ideal gas which undergoes reversible processes. For this situation, we have the ideal gas law and the differential form of the definition of entropy:

$$pV = R\theta, \quad \delta Q = \theta dS$$

Assuming that the energy is only a function of temperature ($E = E(\theta)$), we can write the interval energy in terms of the specific heat:

$$dE = c_v d\theta$$

From the first law for an ideal gas, where mechanical work is associated with the variables of pressure and volume, we have that

$$dE = \delta Q - p dV = c_v d\theta$$

Plugging in the ideal gas law expression of the pressure and dividing by temperature, we obtain

$$\frac{\delta Q}{\theta} = \frac{c_v}{\theta} d\theta + R \frac{1}{V} dV$$

The change in entropy is then

$$\int_1^2 dS = \int_1^2 \frac{\delta Q}{\theta} = \int \frac{c_v}{\theta} d\theta + \int \frac{R}{V} dV \propto \ln \theta + \ln V$$

This is the same dependence we had in the case of statistical mechanics for a box containing gas particles. Working out the details more carefully can demonstrate that the equivalence is more exact than this proportionality. In the next section, we can try to demystify the fact that counting microstates is related to heat exchanged at given temperatures.

10 Equivalence of Classical and Statistical Notions of Entropy

At first, it may be puzzling to look for a connection between heat exchange and the number of microstates available to a gas. But that there is *some* connection need not be mysterious. We showed already that the larger the total energy, the larger the number of microstates that are consistent with that energy. When dealing with continuous particle velocities, we use the volume in phase space as a proxy for the count of microstates. Heat is just an exchange of energy after all, so exchanging heat should increase the total energy of the gas, thus increasing the number of available microstates. The appearance of temperature scale factor in the classical definition of entropy indicates that the rate of increase of microstates with exchanged energy depends on the current energy of the gas. At low temperatures, a fixed quantity of heat increase the order of magnitude of the number of microstates available to the gas more quickly than at high temperatures. Perhaps this makes sense. Going further, we can demonstrate in a simple case the equivalence of the two notions of entropy. We will consider heating a gas with fixed volume. We are able to compute the entropy change according to the two definitions of entropy and show that they agree with one another!

First, we need to relate the total energy of the gas to its temperature. For a gas in 3D with N particles, we have that the total energy is

$$E = \frac{3}{2} N k \theta$$

which says that the temperature θ gives the average kinetic energy of each degree of freedom of each gas particle (with constant of proportionality $k/2$). We might think of this as a definition of temperature. When adding heat at constant volume, all heat goes into increasing the internal energy of the system as no work is done through volume changes. Thus we have that

$$dQ = \frac{3}{2} N k d\theta$$

Using the classical definition of entropy, we can compute the change in entropy in going from an initial temperature θ_1 to a final temperature θ_2 . This is given by

$$dS = \int_{\theta_1}^{\theta_2} \frac{3}{2} N k \frac{d\theta}{\theta} = \frac{3}{2} N k \ln \left(\frac{\theta_2}{\theta_1} \right)$$

Now, turning to the statistical definition of entropy, we have that the change is given by

$$\Delta S = k \ln \Omega_2 - k \ln \Omega_1$$

where Ω_2 is the volume of phase space consistent with a total system energy dictated by T_2 and similar for Ω_1 . How do we compute this volume? For particles with density m , the total energy is given by

$$\frac{m}{2} \sum_{i=1}^N \sum_{j=1}^3 \dot{x}_{ij}^2 = E \implies \sum_{i=1}^N \sum_{j=1}^3 \dot{x}_{ij}^2 = \frac{3}{m} N k \theta$$

This is the equation of a sphere in $3N$ dimensions with radius $\sqrt{3Nk\theta/m}$. The measure of phase space is then

$$\Omega = C(3Nk\theta/m)^{(3N-1)/2}$$

Using this relation, we can compute the change in entropy as

$$\Delta S = k \ln \left(\frac{\theta_2}{\theta_1} \right)^{(3N-1)/2} = \frac{3}{2} N k \ln \left(\frac{\theta_2}{\theta_1} \right) - \frac{1}{2} k \ln \left(\frac{\theta_2}{\theta_1} \right)$$

This is equivalent to the classical definition up to the second term in the above equation, which is very, very small when N is large. Why does this show up though?

11 Entropy in Continuum Mechanics

None of this really makes much sense, and it seems that repeated attempts to change this are futile. Please, if you have a good sense of the equivalence between classical and statistical definitions of entropy, or a nice physical interpretation of this quantity, let's talk. Let's just take this entropy business as a given, and generalize it to the case of a continuum. The real sticking points are the basics of entropy. The generalization to points in a continuum may seem a bit strange, but this is no different than what we do with forces. Note that it is not self-evident what statistical mechanics even has to say about entropy for points in a solid. How do we count states of position and momenta for molecules that are no longer free to move, as they are in the case of gas? These are tough questions, so we forget them for now. Analogous to the classical thermodynamic definition, the entropy input rate is computed by taking a heat flux and dividing it by temperature. For the continuum, this is done for both the volumetric heat input r and the heat transfer across the boundary. For an arbitrary region of solid, the entropy input rate is

$$S_{in} = \int \frac{r}{\theta} d\Omega - \int \frac{q_i n_i}{\theta} dS$$

The specific entropy is now defined as s . The second law of thermodynamics states that the rate of entropy increase for a collection of particles is greater than or equal to the entropy input from heat transfer. For the continuum, this reads:

$$\frac{D}{Dt} \int \rho s d\Omega \geq \int \frac{r}{\theta} d\Omega - \int \frac{q_i n_i}{\theta} dS$$

The divergence theorem, the Reynolds Transport theorem, and localizing the integral allow us to write the local form of the second law

$$\rho \frac{Ds}{Dt} \geq \frac{r}{\theta} - \frac{1}{\theta} \frac{\partial q_i}{\partial x_i} + \frac{1}{\theta^2} q_i \frac{\partial \theta}{\partial x_i}$$

Note that this inequality should hold in all situations, including those for which there is no volumetric heat source ($r = 0$), and when there is no spatial gradient in the heat flux ($q_{i,i} = 0$). Because the temperature is on an absolute scale, it is never negative, which implies that

$$q_i \frac{\partial \theta}{\partial x_i} \leq 0$$

which means that heat flows against temperature gradients. Because a gradient points from low to high values, this means that heat flows opposite of this, from high temperatures to low. This demonstrates that the negative sign in Fourier's Law of heat conduction is a physical requirement imposed by the second law:

$$q_i = -\kappa \frac{\partial \theta}{\partial x_i}$$

for $\kappa > 0$. For a reversible process, we obtain the equality in the second law. Multiplying through by temperature, this reads

$$\rho \theta \dot{s} = r - \frac{\partial q_i}{\partial x_i} + \frac{1}{\theta} q_i \frac{\partial \theta}{\partial x_i}$$

12 Thermodynamic Potentials

Remember that the local form of the first law is

$$\rho \dot{e} = \sigma_{ij} \dot{\epsilon}_{ij} - \frac{\partial q_i}{\partial x_i} + r$$

where we have replaced the spatial gradient of the velocity with the time derivative of the strain and material derivatives with dots to ease the notation. We can solve for the heat flux in the first law and plug in to the second law for reversible processes to obtain

$$0 \geq \rho \dot{e} - \sigma_{ij} \dot{\epsilon}_{ij} - \rho \theta \dot{s} + \frac{1}{\theta} q_i \frac{\partial \theta}{\partial x_i}$$

We want to expand the time derivative of the internal energy with the chain rule, and the variables on which it depends are suggested by the terms that already have time derivatives on them. Taking the hint, this reads

$$0 \geq \left(\frac{\partial(\rho e)}{\partial \epsilon_{ij}} - \sigma_{ij} \right) \dot{\epsilon}_{ij} + \left(\frac{\partial(\rho e)}{\partial s} - \rho \theta \right) \dot{s} + \frac{1}{\theta} q_i \frac{\partial \theta}{\partial x_i}$$

This suggests that the “natural” variables used to write the internal energy are the strain and entropy. Note that this relation says that for constant entropy and zero temperature gradient, the stress is the strain derivative of the internal energy. But because the entropy and strain are independent variables, the inequality must hold for any arbitrary deformation and entropy process. This ensures that

$$\frac{\partial(\rho e)}{\partial \epsilon_{ij}} = \sigma_{ij}, \quad \frac{\partial(\rho e)}{\partial s} = \rho \theta$$

Consider a new thermodynamic quantity, called the “Helmholtz Free Energy.” It is defined as

$$\rho \Psi = \rho e - s \theta$$

This is a Legendre transformation of the internal energy used to switch dependence on entropy and strain to dependence on temperature and strain. A nice reference for further reading on the Legendre transform can be found [here](#). To illustrate this, note that

$$d(\rho e) = \frac{\partial(\rho e)}{\partial \epsilon} d\epsilon + \frac{\partial(\rho e)}{\partial s} ds = \sigma d\epsilon + \theta ds$$

See Figure 2. This is a differential form of the first law commonly seen in classical thermodynamics. The effect of the Legendre transform is observed by computing differentials of $\rho \Psi$:

$$d(\rho \Psi) = d(\rho e) - s d\theta - \theta ds = \sigma d\epsilon - s d\theta$$

The appearance of the density everywhere gets a little wild. This does not seem particularly fundamental, and there may be some errors here. The above relation says that Ψ is a path independent state variable which depends on the strain ϵ and the temperature θ , and whose differentials give the stress and negative of entropy. When we solve for the internal energy in terms of Ψ , take the time derivative, plug this into the first law, and then substitute the resulting expression into the second law, we obtain

$$0 = \rho \dot{\Psi} - \sigma_{ij} \dot{\epsilon}_{ij} + \rho s \dot{\theta} + \frac{1}{\theta} q_i \frac{\partial \theta}{\partial x_i}$$

By another route, we have shown that the natural variables of the Helmholtz energy are strain and temperature. Expanding the time derivative, this can be seen with

$$0 = \left(\frac{\partial(\rho \Psi)}{\partial \epsilon_{ij}} - \sigma_{ij} \right) \dot{\epsilon}_{ij} + \left(\frac{\partial(\rho \Psi)}{\partial \theta} + \rho s \right) \dot{\theta} + \frac{1}{\theta} q_i \frac{\partial \theta}{\partial x_i}$$

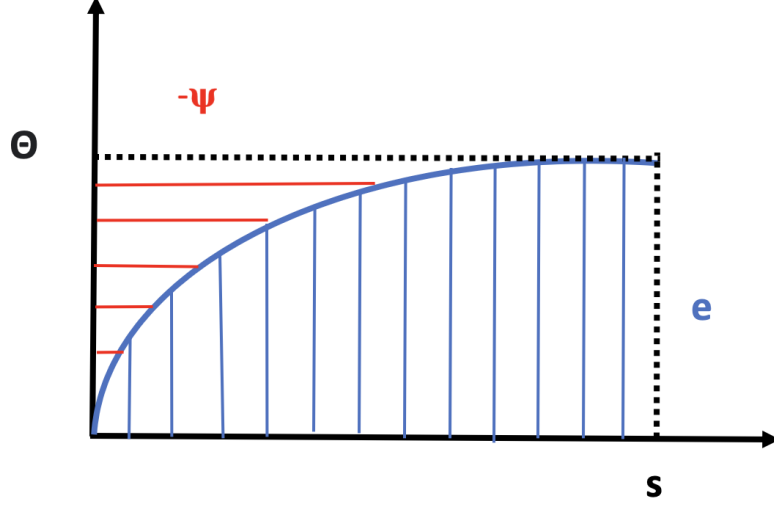


Figure 2: The area of the rectangle defined by the dotted lines is $s\theta$. Remember that $\theta = \frac{\partial(\rho e)}{\partial s}$, which implies that $\rho e = \int \theta ds$. We recognize the internal energy as the blue shaded area in the figure. We can see that $s\theta - \rho e = (-\rho\Psi)$ is the “complementary” energy, or the remainder of the area once the internal energy is subtracted off. We recognize the computation of this complementary area as the Legendre transform, yielding the Helmholtz energy in terms of the internal energy: $\rho\Psi = \rho e - s\theta$.

The Helmholtz energy is advantageous because it allows us to characterize the thermal and mechanical constitutive response of the material in terms of strain and temperature, which is more intuitive than entropy as a state variable. The dependencies of the energy function might be conceptualized as “causal” variables—when we write the strain energy in terms of strains, we implicitly state that strains cause stresses. To me, stress is a more abstract concept than strain, so it is nice to treat it as a response rather than an input. A similar thing is at play with entropy and temperature—temperature is a concept backed by fairly clear physical intuition, whereas entropy is quite nasty and abstract. It is nice to think of the problem as driven by temperature, with entropy as a kind of response and/or means to an end of computing a solution. It seems that the Helmholtz energy allows us to not think too much about entropy, while still being consistent with the thermodynamics.

13 Dissipation Function

The local form of the second law multiplied by temperature, and not assuming a reversible process, reads

$$\rho\theta\dot{s} - r + \frac{\partial q_i}{\partial x_i} - \frac{1}{\theta}q_i \frac{\partial \theta}{\partial x_i} \geq 0$$

From the local form of the first law, we have that

$$r = \rho\dot{e} - \sigma_{ij}\dot{\epsilon}_{ij} + \frac{\partial q_i}{\partial x_i}$$

Substituting this into the second law, we have

$$\rho\theta\dot{s} - \rho\dot{e} + \sigma_{ij}\dot{\epsilon}_{ij} - \frac{1}{\theta}q_i \frac{\partial \theta}{\partial x_i} \geq 0$$

We have already remarked that because heat flux goes against temperature gradients, the last term in the above equation is independently greater than zero. A stronger form of the second law states that

$$D := \rho\theta\dot{s} - \rho\dot{e} + \sigma_{ij}\dot{\epsilon}_{ij} \geq 0$$

It is not entirely clear what the reasoning is in eliminating the heat flux term from the full form of the second law, but perhaps it is under the assumption that the second law should be satisfied even in the absence of temperature gradients. We call this the dissipation function. If it seems odd to define a dissipation function, which intuitively would convert mechanical energy into heat, under the assumption of no temperature gradients, one might imagine a situation where a negative heat source takes away the heat generated by dissipation such that no temperature gradients result. Similarly, dissipation could be such that the change in temperature is uniform across the body. Either way, this dissipation function is non-negative independent of the heat flux term from the second law. Dissipation is zero for reversible processes and non-zero when there are irreversible effects. In terms of the Helmholtz free energy, the dissipation is

$$D := \sigma_{ij}\dot{\epsilon}_{ij} - \rho\dot{\Psi} - \rho s\dot{\theta} \geq 0$$

Note that the dissipation function is a nice way to see that stress and entropy emerge as derivatives of the Helmholtz energy for reversible deformations. When the deformation is reversible, the equality is obtained and we have

$$\left(\frac{\partial(\rho\Psi)}{\partial\epsilon_{ij}} - \sigma_{ij} \right) \dot{\epsilon} + \left(\frac{\partial(\rho\Psi)}{\partial\theta} + \rho s \right) \dot{\theta} = 0$$

14 Helmholtz Energy as a Constitutive Relation

As a brief aside, let's think about where we're at. We assumed familiarity with the balance of momentum principle, and made use of this formulating the mechanical power input to a region of material. The heat input was also derived, both of which quantify the flow of energy into a region. The first law of thermodynamics states that this flow of energy causes changes in the stored energy of the material region. The stored energy was split into a part involving macroscopic motion (kinetic energy) and an internal energy component. Internal energy measures microscopic motion (temperature), and stored energy in deformation (strain). We were not sure at this point how to think about the internal energy, though. Making use of the second law showed that the internal energy is naturally defined in terms of the strain and the entropy. As a bonus, we could demonstrate that heat flowed against temperature gradients. It makes sense that the internal energy should depend on both the deformation and the thermal response of the material, but we do not have unique choice of which mechanical and thermal variables to use in describing this stored energy. For example, it is valid to formulate a purely elastic problem (no thermal effects) purely in terms of the stress as opposed to strain and displacement. This is not common, but it is possible and there is nothing saying that it is an illegitimate approach. Similarly, the thermal variable could be either entropy or temperature. Wanting to preserve intuition about causal variables, we used the Legendre transform to define a new quantity, the Helmholtz energy, which depended on the temperature and strain, as opposed to the internal energy's dependence on entropy and strain. We saw that the stress and entropy were then "response" variables, computed by taking strain and temperature derivatives of the Helmholtz energy function. Note also that by definition, the strain derivative of the Helmholtz energy gives the stress at constant temperature, i.e.

$$\left(\frac{\partial(\rho\Psi)}{\partial\epsilon_{ij}} \right)_{\theta} = \sigma_{ij}$$

where the subscript indicates the temperature is fixed. This is another nice property of the Helmholtz energy. For example, if we are concerned that our material model respects these thermodynamic principles, but ultimately want to solve an elastic problem with no temperature effects, this property is an asset. This contrasts with the internal energy, interpreted as the constitutive relation of the material, whose strain derivative gives stress at constant entropy rather than temperature. What does constant entropy mean physically? To me, this is much less clear than keeping the temperature fixed. Thus, the Helmholtz energy is a useful quantity even when thermal effects are ultimately ignored. *The energy function, whether the internal energy, Helmholtz, or otherwise, is the constitutive relation for the material. It measures how energy storage is shared between deformation and temperature. It is quite a complex thing which we take as a given. To do otherwise is to take a deep-dive into hardcore constitutive modeling!*

15 Solving Problems

What I have found is that textbooks lack a demonstration of how continuum thermodynamics principles are used in practice. I think they also are not clear enough that the internal energy is way more complex than it seems like it should be, and that constructing these potentials is essentially a work of art. For example, an apparently simple-minded idea is that the internal energy of a linearly elastic solid is

$$e = \frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} + cT$$

where c is some constant of proportionality relating the temperature to internal thermal energy. It is difficult to appreciate all of the ways in which this errs, but the bottom line is that it's just wrong. For one, it is not a function of entropy. It is certainly not clear where or why one should insert entropy. We have to be a lot more careful than this. So that is what we'll do! Using the machinery we've developed, it is now possible to write the governing equations in the current configuration as

$$\begin{aligned} \frac{Dv_i}{Dt} &= \frac{\partial}{\partial x_j} \left(\frac{\partial(\rho\Psi)}{\partial \epsilon_{ij}} \right) + f_i \\ \rho \dot{e} &= \frac{D}{Dt}(\rho\Psi + \rho s\theta) = \left(\frac{\partial(\rho\Psi)}{\partial \epsilon_{ij}} \dot{\epsilon}_{ij} + \frac{\partial(\rho\Psi)}{\partial \theta} \dot{\theta} + \rho s \dot{\theta} + \rho \dot{s}\theta \right) = \left(\sigma_{ij} \dot{\epsilon}_{ij} - \frac{D}{Dt} \left(\frac{\partial(\rho\Psi)}{\partial \theta} \right) \theta \right) \\ &= \left(\sigma_{ij} \dot{\epsilon}_{ij} - \frac{\partial^2(\rho\Psi)}{\partial \theta^2} \theta \dot{\theta} - \frac{\partial^2(\rho\Psi)}{\partial \theta \partial \epsilon_{ij}} \theta \dot{\epsilon}_{ij} \right) = \sigma_{ij} \dot{\epsilon}_{ij} - \frac{\partial q_i}{\partial x_i} + r \end{aligned}$$

The former equation is balance of momentum and the latter equation is the first law of thermodynamics. Please be cautious of where I have put the density; we are being a little loose with this. This is a minor detail in the grand scheme of things. We have used the definition of the entropy in terms of the Helmholtz energy and the chain rule to arrive at the left-hand side of the first law. What we see is that the stress power term cancels out. This seems to be a result of having a non-dissipative stress-strain relation, where the stress is derived from the potential function. Using Fourier's law of heat conduction, the energy balance equation thus reduces to

$$-\frac{\partial^2(\rho\Psi)}{\partial \theta^2} \theta \dot{\theta} = \frac{\partial^2(\rho\Psi)}{\partial \theta \partial \epsilon_{ij}} \theta \dot{\epsilon}_{ij} + \kappa \frac{\partial^2 \theta}{\partial x_i \partial x_i} + r$$

This is a bizarre looking problem. The typical heat equation is derived from a principle of energy balance, and we would expect to see something similar to this show up from our first principles thermodynamic analysis. Of course, the heat equation doesn't consider the effect of coupling with mechanical work. So what we really expect to see is that if the strain is zero, we recover the heat equation. The right-hand side of this equation looks promising: we have the

usual second derivative of the temperature, and a volumetric heat source. The coupling term involving the Helmholtz energy drops out when the strain rate is zero. But the left hand side looks like trouble! We have a non-linearity which is at least quadratic in the temperature. We can pull a very neat trick. Remember the definition of heat capacity, in particular heat capacity at constant volume. This is rate of change of the internal energy with temperature at a fixed volume. The analogue of volumes changes from classical thermodynamics in continuum thermodynamics is strain. So when the deformation is zero, the constant volume heat capacity is the dependence of the internal energy on temperature for fixed strains. This is computed as

$$c_v(\theta) := \frac{\partial(\rho e)}{\partial\theta} = \frac{\partial(\rho e)}{\partial s} \frac{\partial s}{\partial\theta} = -\theta \frac{\partial}{\partial\theta} \left(\frac{\partial(\rho\Psi)}{\partial\theta} \right) = -\theta \frac{\partial^2(\rho\Psi)}{\partial\theta^2}$$

We see that the heat capacity is a function of temperature explicitly, and implicitly through the Helmholtz energy. But it is often a good approximation to neglect this temperature dependence. Even if it is not a good assumption, which the linear dependence suggests it is not, it is what people do. Substituting this into the energy balance equation with no strains, we recover the usual heat equation

$$\rho c_v \dot{\theta} = \kappa \frac{\partial^2 \theta}{\partial x_i \partial x_i} + r$$

Finally, a familiar equation—truly a sight for sore eyes. It is exciting to see this pop out of all the abstract thermodynamic nonsense. With the assumed constant heat capacity, we can lift the assumption that the strain rate is zero and see that there is coupling between the elastic and thermal problems even when the constitutive relation is not dissipative:

$$\begin{aligned} \rho c_v \dot{\theta} &= \frac{\partial \sigma_{ij}}{\partial \theta} \theta \dot{\epsilon}_{ij} + \kappa \frac{\partial^2 \theta}{\partial x_i \partial x_i} + r \\ \frac{Dv_i}{Dt} &= \frac{\partial \sigma_{ij}}{\partial x_j} + b \end{aligned}$$

The elastic response of the body contributes to the time derivative of temperature, and the temperature influences the balance of momentum with thermal stresses/strains. What about the simple thermoelastic analysis, where the temperature field is computed independent of the deformation, but temperature contributes to thermal strains? The assumption here seems to be that the first term in the energy balance equation is very small compared to the explicit heat sources. This is an apparently reasonable assumption in many situations.

16 An Example

When a thermodynamic potential is specified, we can use all of the results we have developed above to solve the governing equations. The art of constitutive

modeling is to formulate these potentials, so it should not be clear at face value where they come from. We will use the Helmholtz free energy to write out the governing equations for a 1D linear thermoelastic bar. The thermodynamic potential for this problem is

$$\Psi = \frac{1}{2}E\epsilon^2 - k\alpha_0(\theta - \theta_0)\epsilon - \frac{c_v^0}{2\theta_0}(\theta - \theta_0)^2 - s_0\theta$$

Let's not worry too much about the exact meaning of the material constants, other than noting that they include the modulus, thermal expansion coefficient, a reference value of the specific heat at constant volume, and a reference value of entropy. There is some subtlety in making sense of what variables are held fixed in these quantities. We can take derivatives of the Helmholtz energy to obtain the thermodynamic properties of stress and entropy:

$$\sigma = \frac{\partial \Psi}{\partial \epsilon} = E\epsilon - k\alpha_0(\theta - \theta_0)$$

$$s = -\frac{\partial \Psi}{\partial \theta} = k\alpha_0\epsilon + \frac{c_v^0}{\theta_0}(\theta - \theta_0) + s_0$$

Note that the specific heat is a function of temperature as was shown above. It is computed as the rate of change of internal energy with temperature at a fixed deformation. This reads

$$\frac{\partial e}{\partial \theta} = -\theta \frac{\partial^2 \Psi}{\partial \theta^2} = \theta \frac{c_v^0}{\theta_0}$$

For this form of the Helmholtz energy, the specific heat is linear in the temperature, which means that the heat equation is technically nonlinear. We often approximate this as constant in practice, but we will keep the dependence because it makes for a more interesting problem. The balance of linear momentum with this constitutive relation is

$$\rho \ddot{u} = E \frac{\partial^2 u}{\partial x^2} - k\alpha_0 \frac{\partial \theta}{\partial x}$$

where we have assumed there is no distributed force on the bar. The balance of energy can be written as

$$\frac{\rho c_v^0}{\theta_0} \theta \dot{\theta} = -k\theta_0 \theta \frac{\partial^2 u}{\partial x \partial t} + \kappa \frac{\partial^2 \theta}{\partial x^2}$$

Let's assume that all the constants are unity because they are cumbersome. The two governing equations in this case are

$$\ddot{u} = \frac{\partial^2 u}{\partial x^2} - \frac{\partial \theta}{\partial x}$$

$$\dot{\theta} = \frac{\partial^2 u}{\partial x \partial t} + \frac{1}{\theta} \frac{\partial^2 \theta}{\partial x^2}$$

We can now give a sense of how coupled equations of this sort could be solved numerically. Discretize both the displacement and temperature with the same set of shape functions:

$$u(x, t) = \sum_i u_i(t) N_i(x), \quad \theta(x, t) = \sum_j \theta_j(t) N_j(x)$$

The governing equations are weakened by integrating against test functions coming from the same space as the solution approximations:

$$\begin{aligned} \int \ddot{u} N_k dx &= \int \left(\frac{\partial^2 u}{\partial x^2} - \frac{\partial \theta}{\partial x} \right) N_k dx \\ \int \dot{\theta} N_k dx &= \int \left(\frac{\partial^2 u}{\partial x \partial t} + \frac{1}{\theta} \frac{\partial^2 \theta}{\partial x^2} \right) N_k dx \end{aligned}$$

Plugging in this discretization of the displacement and temperature, and integrating by parts the momentum equation to expose a traction boundary condition (assuming this drives the problem), we obtain

$$\begin{aligned} \sum_i \ddot{u}_i \left(\int N_i N_k dx \right) + \sum_i u_i \left(\int \frac{\partial N_i}{\partial x} \frac{\partial N_k}{\partial x} dx \right) + \sum_i \theta_i \left(\int \frac{\partial N_i}{\partial x} N_k dx \right) &= F(t) N_k(L) \\ \sum_i \dot{\theta}_i \left(\int N_i N_k dx \right) &= \sum_i \dot{u}_i \left(\int \frac{\partial N_i}{\partial x} N_k dx \right) + Q_k(\theta) \end{aligned}$$

The notation Q for the nonlinear conduction term is used for simplicity because it cannot be written in matrix-vector form. Switching to index notation, and with matrices defined by the above relation, this can be written much more compactly as

$$M_{ij} \ddot{u}_j + K_{ij} u_j + T_{ij} \theta_j = F_j(t)$$

$$M_{ij} \dot{\theta}_j = T_{ij} \dot{u}_j + Q_j(\underline{\theta})$$

Note that the matrix \underline{T} defines the coupling between the thermal and elastic problems in both equations. The heat equation involves nonlinear heat conduction because we did not assume the specific heat is independent of temperature. A common solution approach is a staggered method, where at each time step, the deformation is first computed using the momentum equation at fixed temperature, and then temperature is computed using the energy equation at fixed deformation. This fits in nicely with the Helmholtz energy as the constitutive relation for the material. Remember that by definition, it furnishes the stress as a function of strain at fixed temperature, and the entropy at a fixed value

of strain.¹ Both the stress and entropy are used in formulating these governing equations, and when we carry out this staggered scheme, it respects the assumptions of holding variables fixed. When we solve the heat equation, it is done without varying the strain. This is in line with the entropy computed from the Helmholtz energy. Similarly, when we compute the displacement with the momentum equation, the temperature is fixed, thus respecting the fixed temperature assumption in computing the stress from the Helmholtz energy. Thus, the staggered scheme fits nicely into the thermodynamic framework.

Alternatively, a monolithic time integration method could be used, where we solve for the temperature and displacement degrees of freedom simultaneously. We will briefly lay out an implicit time integration method, which is more stable than explicit time integration. For an implicit method, a system of equations will need to be solved at each time step. This contrasts with explicit formulae for updates we obtain from explicit methods. Because the heat conduction term is nonlinear, the system of equations will also be nonlinear. An implicit time integration scheme starts with writing

$$M_{ij}f_j(\underline{u}^{n+1}) + K_{ij}u_j^{n+1} + T_{ij}\theta_j^{n+1} = F_j(t^{n+1})$$

$$M_{ij}g_j(\underline{\theta}^{n+1}) = T_{ij}g_j(\underline{u}^{n+1}) + Q_j(\underline{\theta}^{n+1})$$

The functions f and g are shorthand for a generic finite difference scheme (discrete approximations of the second and first time derivatives respectively) that depend on the unknown values of the degree of freedom at the next time step (as well as known values at past time steps). The residual equations at time t^n are

$$R_i^u := M_{ij}f_j(\underline{u}^{n+1}) + K_{ij}u_j^{n+1} + T_{ij}\theta_j^{n+1} - F_j(t^{n+1}) = 0$$

$$R_i^\theta := M_{ij}g_j(\underline{\theta}^{n+1}) - T_{ij}g_j(\underline{u}^{n+1}) - Q_j(\underline{\theta}^{n+1}) = 0$$

A Newton-Raphson method can be used to solve the residual equations in terms of future displacement and temperature degrees of freedom. A linearization of these equations looks like

$$\begin{bmatrix} \underline{R}^u \\ \underline{R}^\theta \end{bmatrix} \approx \begin{bmatrix} \partial \underline{R}^u / \partial \underline{u} & \partial \underline{R}^u / \partial \underline{\theta} \\ \partial \underline{R}^\theta / \partial \underline{u} & \partial \underline{R}^\theta / \partial \underline{\theta} \end{bmatrix} \begin{bmatrix} \underline{u}^{n+1} \\ \underline{\theta}^{n+1} \end{bmatrix} = 0$$

This is solved iteratively with Newton's method. This is called a monolithic scheme because both the temperature and displacement are solved for simultaneously.

¹Thermodynamic processes are more complicated because there is more than one state variable for the system. For example, when defining the stress in terms of the strain, we need to fix temperature. The temperature does influence the stress though, because the "sensitivity" of stress to strain is dependent on temperature. This contrasts with traditional elasticity, where the stress is a function of the strain alone.

17 Energy Formulation

Transient heat transfer is not governed by a total potential energy functional. This owes to the first time derivative in the governing equations. This contrasts with elasticity, and steady state heat conduction, for which energy functionals whose minimum govern the response exist and are convenient starting points for numerical methods. If we want to formulate the thermoelastic problem energetically, we cannot model transient heat conduction. We illustrate a potential formulation of a steady-state thermoelastic problem. The relationship of this formulation to the first principle thermodynamics derivations shown above is not entirely clear. It would be nice to sort this out, but this may have to wait for the future. As will be shown, the governing equations appear to differ in some fundamental ways from the transient ones. But, this approach is taken in the literature, for example in this paper. First, note that strains in the presence temperature change can be written as

$$\tilde{\epsilon}_{ij} = \epsilon_{ij} + \alpha \delta_{ij} \theta$$

where θ is interpreted as the change in temperature from that of the reference configuration. We work in the small strain regime and with isotropic material behavior for simplicity. The total potential energy for a thermoelastic body with traction and heat flux boundary conditions is

$$\Pi(\underline{u}, \theta) = \frac{1}{2} \int \left(C_{ijkl} \tilde{\epsilon}_{ij} \tilde{\epsilon}_{kl} + a_{ij} \frac{\partial \theta}{\partial x_i} \frac{\partial \theta}{\partial x_j} \right) d\Omega - \int (t_i u_i + q_i n_i \theta) dS$$

We assume that the traction and heat flux are applied over the same region of the body's boundary to ease notation. This assumption is easily relaxed. To motivate this formulation, note that this is simply the sum of the usual variational energies from elasticity and heat conduction added up, with coupling introduced through the temperature dependence of the strain. The solution to this problem is governed by a minimum of the total potential energy in terms of both the displacement and temperature. Taking the variation with respect to the displacement first, we obtain

$$\delta_u \Pi = \int C_{ijkl} \tilde{\epsilon}_{ij} \frac{\partial \delta u_k}{\partial x_\ell} d\Omega - \int t_i \delta u_i dS = 0$$

The subscript u in the variation of the energy is meant to indicate the variation with respect to the displacement. This is the weak form of the displacement equation. We can integrate by parts the spatial derivative off the test function to obtain the strong form of the governing equation:

$$\frac{\partial}{\partial x_\ell} \left(C_{ijkl} (\epsilon_{ij} + \alpha \delta_{ij} \theta) \right) = C_{ijkl} \frac{\partial^2 u_i}{\partial x_j \partial x_\ell} + \alpha C_{iik\ell} \frac{\partial \theta}{\partial x_\ell} = 0$$

Note that for isotropic linear elasticity, the material tensor is²

²This is a nice reference on tensor forms of elastic constitutive models.

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \implies C_{iikl} = (3\lambda + 2\mu) \delta_{kl} = 3K \delta_{kl}$$

where we have extracted the bulk modulus from contracting two indices on the material tensor. It is logical that the bulk modulus would show up in computing thermal stresses, as thermal strains act entirely to change volumes with no distortion. The governing equation can be simplified to

$$C_{ijk\ell} \frac{\partial^2 u_i}{\partial x_j \partial x_\ell} + 3\alpha K \frac{\partial \theta}{\partial x_j} = 0$$

This is the Navier equation with thermal stresses. We can now turn to the variations of the total potential with respect to temperature. This reads

$$\delta_\theta \Pi = \int \left(C_{ijk\ell} \tilde{\epsilon}_{ij} \frac{\partial \tilde{\epsilon}_{kl}}{\partial \theta} \delta \theta + a_{ij} \frac{\partial \theta}{\partial x_i} \frac{\partial \delta \theta}{\partial x_j} \right) d\Omega - \int q_i n_i \delta \theta dS$$

This is the weak form of the governing equations of the thermal problem. This formulation shows that the deformation influences the thermal problem, unlike the simplest thermoelasticity where the temperature is computed independent of the displacement. The tilde indicates strains in the presence of thermal expansion. We can integrate by parts and use that $\delta \theta$ is arbitrary to obtain the strong form of the governing equations:

$$a_{ij} \frac{\partial^2 \theta}{\partial x_i \partial x_j} - C_{ijk\ell} (\epsilon_{ij} + \alpha \theta \delta_{ij}) \alpha \delta_{kl} = 0$$

This can be simplified by using the delta function to contract on the last two indices of the material tensor, which yields

$$\begin{aligned} a_{ij} \frac{\partial^2 \theta}{\partial x_i \partial x_j} - 3\alpha K \delta_{ij} (\epsilon_{ij} + \alpha \theta \delta_{ij}) &= 0 \\ \implies a_{ij} \frac{\partial^2 \theta}{\partial x_i \partial x_j} - 3\alpha K (\epsilon_{ii} + 3\alpha \theta) &= 0 \end{aligned}$$

The terms in parentheses involve local changes of volume. The trace of the strain tensor is the same as the divergence of the displacement, which measures volumetric compression and expansion of the material. Similarly, through the thermal strains, the temperature causes volume changes. As might be expected from classical thermodynamics involving compression and expansion of gases, the coupling with the strain in the thermal problem is due to volumetric effects.

18 Dissipative Materials and Internal Variables

Coming soon.