Anisotropic Non-Equilibrium thermodynamics of solids

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ABSTRACT

A summary of thermodynamics of solids is presented.

This document has not received much of my attention, so it is in an EXTREMELY disorganized very very ROUGH draft state.

This document is posted only to show a taste how much things change and get complicated in solid mechanics in comparison to simple fluid mechanics.

Bringing a document like this to a polished coherent state would be a multiyear effort working full time. Chipping at it for an hour or two each month (as I have) puts its completion date into my retirement -- don't hold your breath!

Acknowledgments

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Preface

Thermodynamics is an extrordinarily difficult subject to master. Even after achieving a reasonable compentance at it, one is still left with a nagging feeling that "there must be a better way." I still have this feeling. Nonetheless, one must proceed with the tools at hand.

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August 28, 2003 12:11 pm

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> ***Warning: this is work in progress. Some sections start or stop abruptly. Comments like this one (with the big bold italic typeface and change bar in the margin) are:***
> ***1. notes that I (Rebecca) have written to myself, or***
> ***2. questions that I cannot yet answer, or***
> ***3. warnings to you, the friendly draft reader.***
>
> ***I would appreciate reader feedback on the content (e.g., topics included, level of difficulty, mistakes). Deficiencies in grammar, spelling, and organization are being continually addressed, but you can flame me on them anyway.***

1. Introduction

Purpose of this report

This report describes summarizes classical and non-equilibrium thermodynamics in a format that is well-suited for numerical applications..

The body of this report focuses on the *physical theory* of the CKP model. Details about the numerical implementation are found in the appendices.

Problems addressed by this report

Scope of material covered in this report

Limitations of this work

Overview of main report contents

This report is organized as follows:

Overview of report appendices

This presentation of the CKP model is followed by several appendices that provide the following detailed information relating to the main text:

Notation

Throughout this report, scalars are denoted in plain italics (s, r, t). Vectors are typeset with a single under-tilde ($\underset{\sim}{v}, \underset{\sim}{w}, \underset{\sim}{x}$). Second-order tensors are shown with two under-tildes ($\underset{\approx}{\sigma}, \underset{\approx}{S}, \underset{\approx}{T}$). Likewise, the order of higher-order tensors is indicated by the number of under-tildes.

Two vectors written side-by-side are multiplied dyadically. For example, $\underset{\sim}{a}\underset{\sim}{b}$ is a second-order tensor with ij components given by $a_i b_j$. Any second-order tensor $\underset{\approx}{T}$ may be expanded in terms of basis dyads as $\underset{\approx}{T} = T_{ij}\underset{\sim}{e}_i\underset{\sim}{e}_j$. Here (and throughout this report) repeated indices imply summation from 1 to 3.

A single raised dot denotes the vector inner-product defined by

$$\underset{\sim}{u} \bullet \underset{\sim}{v} = u_1 v_1 + u_2 v_2 + u_3 v_3 = u_k v_k \quad . \tag{1.1}$$

The single raised dot continues to denote the vector inner product even when acting between higher-order tensors. For example,

$$\underset{\approx}{A} \bullet \underset{\sim}{x} = A_{ij} x_j \; \underset{\sim}{e}_i \quad . \tag{1.2}$$

Composition of two tensors is another example:

$$\underset{\approx}{A} \bullet \underset{\approx}{B} = A_{ik} B_{kj} \; \underset{\sim}{e}_i\underset{\sim}{e}_j \quad . \tag{1.3}$$

The deviatoric part of a tensor is denoted by a "prime." Hence,

$$\underset{\approx}{A}' \equiv \underset{\approx}{A} - \tfrac{1}{3}(\mathrm{tr}\underset{\approx}{A})\underset{\approx}{I} \; , \tag{1.4}$$

where $\underset{\approx}{I}$ is the identity tensor and "tr" denotes the trace. Specifically,

$$\mathrm{tr}\underset{\approx}{A} \equiv A_{11} + A_{22} + A_{33} = A_{kk} \quad . \tag{1.5}$$

The tensor inner product is denoted by " $:$ " and is defined by

$$\underset{\approx}{A}:\underset{\approx}{B} = A_{ij} B_{ij} \quad . \tag{1.6}$$

Note that

$$\underset{\approx}{A}:\underset{\approx}{B} = \underset{\approx}{B}:\underset{\approx}{A} \quad . \tag{1.7}$$

The magnitude of a second-order tensor is defined

$$\|\underset{\approx}{A}\| \equiv \sqrt{\underset{\approx}{A}:\underset{\approx}{A}} \quad . \tag{1.8}$$

The tensor inner product is allowed to operate between any two tensors of *at least* second order. For example, if $\underset{\approx}{\underset{\approx}{E}}$ is a fourth-order tensor, then

$$\underset{\approx}{\underset{\approx}{E}}:\underset{\approx}{A} = E_{ijkl} A_{kl} \; \underset{\sim}{e}_i\underset{\sim}{e}_j \quad . \tag{1.9}$$

2. Fields in time and space

Control volume (CV)

A control volume (CV) is a region in space. The nature of a control volume is typically defined by the manner in which the boundary moves through time. An Eulerian control volume is fixed in space. A Lagrangean control volume moves with the material particles *as if its boundary were an impermeable surface*. Some problems, such diffussion and turbulence involve mass fluxes at a scale below what can be captured at typical continuum level finite elements, so the notion of mass-impermeable surfaces is often generalized to permit balanced mass flux of each species forming the mixture or to permit higher-order mass oscillations due to subscale turbulence. Other kinds of control volumes, such as those sketched in Fig. 2.1, are neither Lagrangean nor Eulerian, but are selected to avoid singularities or discontinuities and optimally exploit steady-state conditions. In these cases, the boundary of the control volume is transient (it moves over time, so it is not Eulerian), but it does not move with the material particles (so it is also not Lagrangean). The control volume shown in Fig. 2.1 for the crack problem is particularly convenient when studying steady state crack growth because an observer who translates to the right with a speed exactly equal to the crack tip speed will perceive all field variables to be constants even though a Lagrangean observer (i.e., one who moves with particles will see time variation). Since crack tips move relative to the material, this control volume permits mass flux across its boundaries.
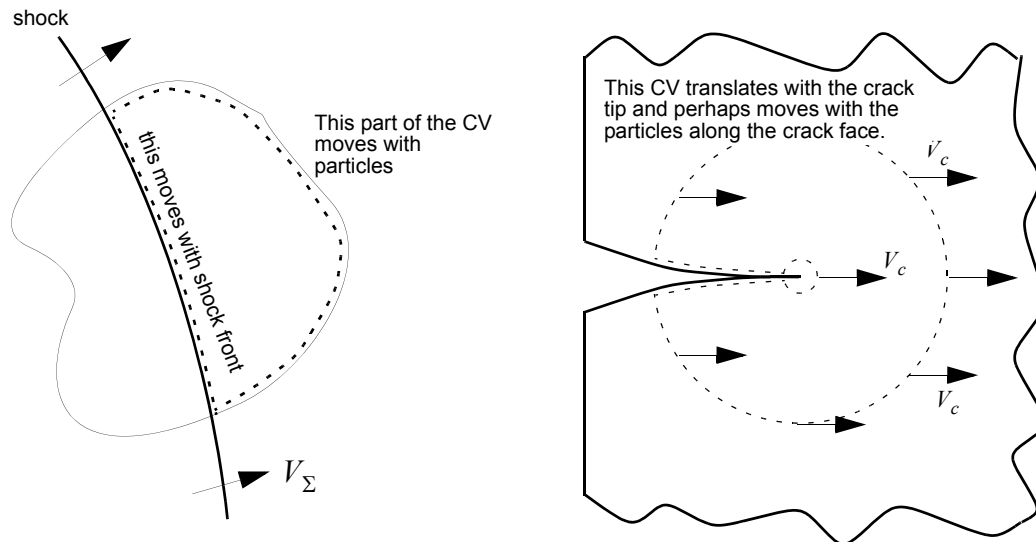
Figure 2.1.   Situations for which neither a Lagrangean nor an Eulerian control volume is appropriate. On the left is shown a special control volume (dashed) moves with the shock front on part of its boundary and with the particles on the remaining part of the boundary. On the right is shown a special control volume commonly used for steady-state crack growth; this control volume is always of the same shape, but it moves to the right with a speed equal to the velocity V_c of the crack tip.

We will use the subscripts "*L, E,* and *G*" to denote a Lagrangean, Eulerian and general control volume, respectively. Our integral equations will always presume that the control volumes are *instantaneously* coincident ($\Omega_L = \Omega_E = \Omega_G$) with each other. They will coincide only for an instant — they will be distinct from each other a moment later because their boundaries move in different ways. For most engineering applications, the choice of control volume — Lagrangean, Eulerian, or general — will be natural for the problem at hand. If, for example, the problem deals with the movement of air and exhaust fumes through a turbine engine, then it makes sense to use an Eulerian control volume in which material passes into the control volume at the inlet of the engine and out at the outlet of the engine. On the other hand, if the problem deals with the damage imposed on a baseball while it is being struck by a bat, then the natural control volume would be a Lagrangean one that surrounds *and moves with* the surface of the baseball.

We will let Ω_G denote a general control volume that might be non-Lagrangean or non-Eulerian. The transient nature of the control volume Ω_G is defined by the surface velocity of its boundary $\partial \Omega_G$. Specifically, let's define

$$\underset{\sim}{v}_G \;=\; \text{velocity of boundary } \partial \Omega_G \tag{2.1}$$

$$\underset{\sim}{n} \;=\; \text{outward unit normal of boundary } \partial \Omega_G \tag{2.2}$$

$$v_G^n \;=\; \underset{\sim}{v}_G \bullet \underset{\sim}{n} \;=\; \text{normal component of boundary velocity} \tag{2.3}$$

Only the normal component v_G^n of the boundary velocity $\underset{\sim}{v}_G$ enters into the physical laws. When the generalized control volume is specialized to Lagrangean motions, then the subscript "G" is replaced by "L" and the velocity $\underset{\sim}{v}_G$ (now denoted $\underset{\sim}{v}_L$) can be equated with the material velocity $\underset{\sim}{v}$. When the generalized control volume is specialized to Eulerian description, then the subscript "G" is replaced by "E" and the velocity $\underset{\sim}{v}_G$ (now denoted $\underset{\sim}{v}_E$) is simple the zero vector $\underset{\sim}{0}$ because the boundary of an Eulerian control volume does not move. To reiterate,

- Ω_E is an Eulerian control volume iff $\underset{\sim}{v}_E \bullet \underset{\sim}{n} = 0$ everywhere on $\partial \Omega_E$.

- Ω_L is a Lagrangean control volume iff $\underset{\sim}{v}_L \bullet \underset{\sim}{n} = \underset{\sim}{v} \bullet \underset{\sim}{n}$ everywhere on $\partial \Omega_L$.

Here, $\underset{\sim}{v}$ is the material velocity, so a Lagrangean control volume moves in such a manner that it always encloses the same set of material particles.[*]

Time derivatives of volume integrals (Leibniz rule)

Let $\Upsilon(\underset{\sim}{x}, t)$ denote a field that varies with time t and spatial position $\underset{\sim}{x}$. The Leibniz rule for differentiating a GENERAL volume integral is†

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[*] For gases, fluids, and mixtures, this statement is somewhat incorrect. We all know that the molecules of a gas move all around, so any control volume that always encloses a single set of particles would quickly become deformed into a twisted mess. Whenever subgrid scale fluxing (diffusion) occurs, the a Lagrangean boundary is defined such that *macroscopic* mass flux across the boundary is zero.

$$\frac{d}{dt} \int\limits_{\Omega_G} \underline{\Upsilon}(\pmb{x}, t) dV = \int\limits_{\Omega} \frac{\partial \underline{\Upsilon}(\pmb{x}, t)}{\partial t} dV + \int\limits_{\partial\Omega} \underline{\Upsilon}(\pmb{v}_G \bullet \pmb{n}) dS \qquad (2.4)$$

This identity is the rule that governs how to bring a time derivative inside an integral. The result depends on how the boundary itself is moving. Specifically, the last term accounts for flux of $\underline{\Upsilon}$ brought into the control volume simply because of motion of the boundary. Importantly, once the time derivative has been brought inside of the integrals, it is no longer necessary to identify the nature of the control volume with the subscript "G" (Ω_G can be written as simply Ω).

If Ω is an Eulerian control volume, then (recall) we denote it by Ω_E and $\pmb{v}_G \bullet \pmb{n} = \pmb{v}_E \bullet \pmb{n} = 0$. If Ω is a Lagrangean control volume, then we denote it by Ω_L and $\pmb{v}_G \bullet \pmb{n} = \pmb{v}_L \bullet \pmb{n} = \pmb{v} \bullet \pmb{n}$. Thus, two important special cases of the Leibniz rule are

$$\frac{d}{dt} \int\limits_{\Omega_E} \underline{\Upsilon}(\pmb{x}, t) dV = \int\limits_{\Omega} \frac{\partial \underline{\Upsilon}(\pmb{x}, t)}{\partial t} dV \qquad (2.5)$$

$$\frac{d}{dt} \int\limits_{\Omega_L} \underline{\Upsilon}(\pmb{x}, t) dV = \int\limits_{\Omega} \frac{\partial \underline{\Upsilon}(\pmb{x}, t)}{\partial t} dV + \int\limits_{\partial\Omega} \underline{\Upsilon}(\pmb{v} \bullet \pmb{n}) dS \qquad (2.6)$$

Eq. (2.6) is commonly called the **Reynolds Transport Theorem** — it is merely a particular instance of the Leibniz formula for which the boundary of the control volume moves with the particles.

Note that the "*L, E,* and *G*" subscripts have been dropped from the right-hand sides of Eqs. (2.4), (2.5), and (2.6). It is important to identify the nature of the control volume only when the d/dt operator is on the *outside* of the integral. Once the Leibniz formula has been used to bring the time derivative inside the integral, there is no distinction between integrals over Ω_L and Ω_E. Likewise, the surface integrals (over $\partial\Omega_L$ and $\partial\Omega_E$) are equal at the instant that Ω_L coincides with Ω_E. In other words, if Ω_L coincides with Ω_E *at an instant of interest*, then we know that

$$\int\limits_{\Omega_E} \Upsilon(\pmb{x}, t) dV = \int\limits_{\Omega_L} \Upsilon(\pmb{x}, t) dV \quad \text{at this instant} \qquad (2.7)$$

and
$$\int\limits_{\Omega_E} \frac{\partial \Upsilon(\pmb{x}, t)}{\partial t} dV = \int\limits_{\Omega_L} \frac{\partial \Upsilon(\pmb{x}, t)}{\partial t} dV \quad \text{at this instant} \qquad (2.8)$$

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†In 1D, the Leibniz formula is $\dfrac{d}{dt} \int\limits_{a(t)}^{b(t)} f(x, t) dx = \int\limits_{a(t)}^{b(t)} \dfrac{\partial f(x, t)}{\partial t} dx + f(b, t)\dfrac{db(t)}{dt} - f(a, t)\dfrac{da(t)}{dt}$. Here, the "outward unit normal" is +1 on the right boundary and –1 on the left boundary. The velocity of the boundary is $V = \dfrac{db(t)}{dt}$ on the right boundary and $V = \dfrac{da(t)}{dt}$ on the left boundary. Note:

Leibniz is *pronounced* as though it were spelled Leibni**t**z, but the correct spelling has no "t."

Consequently, for these integrals, there's no need to use a subscript E or L to identify the control volume. Because Ω_L does *not* coincide with Ω_E at some later time, we know that Eq. (2.7) does not hold for all time. Thus, we cannot differentiate both sides of Eq. (2.7) with respect to time without reintroducing the distinction of the boundary velocities. Thus

$$\int_{\Omega_E} \underline{\Upsilon}(\underline{x}, t)dV = \int_{\Omega_L} \underline{\Upsilon}(\underline{x}, t)dV \quad , \tag{2.9}$$

but

$$\frac{d}{dt}\int_{\Omega_E} \underline{\Upsilon}(\underline{x}, t)dV \neq \frac{d}{dt}\int_{\Omega_L} \underline{\Upsilon}(\underline{x}, t)dV \quad ! \tag{2.10}$$

Whenever there is a time derivative (or any other operation) acting on the *outside* of the integral, it is essential to identify the nature of the control volume as Lagrangean ($\underline{v}_L \bullet \underline{n} = \underline{v} \bullet \underline{n}$), Eulerian ($\underline{v}_E \bullet \underline{n} = 0$), or general ($\underline{v}_G \bullet \underline{n} = v_G^n$).

Time derivatives of Lagrangean control volumes occur so often in thermodynamics, that it becomes tiresome to always use an "L" subscript to identify the control volume to be Lagrangean. Another convention for identifying a control volume to be Lagrangean is to write the d/dt operator as D/Dt. Thus,

$$\frac{D}{Dt}\int_{\Omega} \underline{\Upsilon}(\underline{x}, t)dV \text{ is an alternative notation for } \frac{d}{dt}\int_{\Omega_L} \underline{\Upsilon}(\underline{x}, t)dV \tag{2.11}$$

In essence, using D/Dt tells the reader that the boundary moves with the particles. So, when using this notation, there is no need to add a subscript "L" to the Ω symbol.

In general, we can always convert the rate of a Lagrangean control volume to the rate of an instantaneously coincident general control volume by subtracting Eq. (2.6) from (2.4) to give

$$\frac{D}{Dt}\int_{\Omega} \underline{\Upsilon}(\underline{x}, t)dV = \frac{d}{dt}\int_{\Omega_G} \underline{\Upsilon}(\underline{x}, t)dV + \int_{\partial\Omega} \underline{\Upsilon}(\underline{v} - \underline{v}_G) \bullet \underline{n}dS \tag{2.12}$$

Generalized "divergence" theorem (jump form)

Let $\underline{f}$ denote a field (of any tensor order) defined on the surface of a control volume whose outward normal is $\underline{n}$. Let the product $\underline{f}\underline{n}$ be defined

$(fn_i)\underline{e}_i$ if $\underline{f}$ is a scalar, f

$(f_in_j)\underline{e}_i\underline{e}_j$ if $\underline{f}$ is a vector, $\underline{f}$

$(f_{ij}n_k)\underline{e}_i\underline{e}_j\underline{e}_k$ if $\underline{f}$ is a second-order tensor, $\underline{\underline{f}}$

etc.   (2.13)

The generalized divergence theorem is of the form

$$\int_{\partial\Omega} (\underline{f}\underline{\boldsymbol{n}})\,dS = \int_{\Omega} \left(\frac{d\underline{f}}{d\underline{\boldsymbol{x}}}\right)dV + \quad \text{extra jump terms} \quad , \tag{2.14}$$

where

$$\frac{d\underline{f}}{d\underline{\boldsymbol{x}}} = \left(\frac{\partial f}{\partial x_i}\right)\boldsymbol{e}_i \quad \text{if } \underline{f} \text{ is a scalar, } f$$

$$\frac{d\underline{f}}{d\underline{\boldsymbol{x}}} = \left(\frac{\partial f_i}{\partial x_j}\right)\boldsymbol{e}_i\boldsymbol{e}_j \quad \text{if } \underline{f} \text{ is a vector, } \underline{\boldsymbol{f}}$$

$$\frac{d\underline{f}}{d\underline{\boldsymbol{x}}} = \left(\frac{\partial f_{ij}}{\partial x_k}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k \quad \text{if } \underline{f} \text{ is a second-order tensor, } \underline{\underline{\boldsymbol{f}}}$$

etc. $\tag{2.15}$

The "extra jump terms" mentioned in Eq. (2.14) are zero whenever the function $\underline{f}$ is "sufficiently smooth" (i.e., continuous spatial derivatives). Our goal now is to derive the form of the jump terms when the integrand in the left-hand-side of Eq. (2.14) is smooth everywhere except across a jump surface Σ across which the function $\underline{f}$ jumps discontinuously. We will assume that the jump surface orientable with a unit normal is denoted by $\underline{\boldsymbol{n}}_\Sigma$.

The integral in Eq. (2.14) is well defined even though the integrand is discontiuous. There's nothing wrong with integrating a discontinuous function — issues arise, however, if you try to *differentiate* a discontinuous field. The divergence theorem provides a way for an integral over a surface to be converted to a volume integral, but the volume integral involves a spatial derivative. Hence, you cannot apply the divergence theorem in its classical (non-jump) form if the integrand is discontinuous. This section provides a generalized

version of the divergence theorem for use when the integrand is discontinuous. Fig. 2.2 illustrates a region of space that is cut by a surface of discontinuity in one or more field variables. That figure illustrates how the volume can be split into two volumes over which fields are smooth.
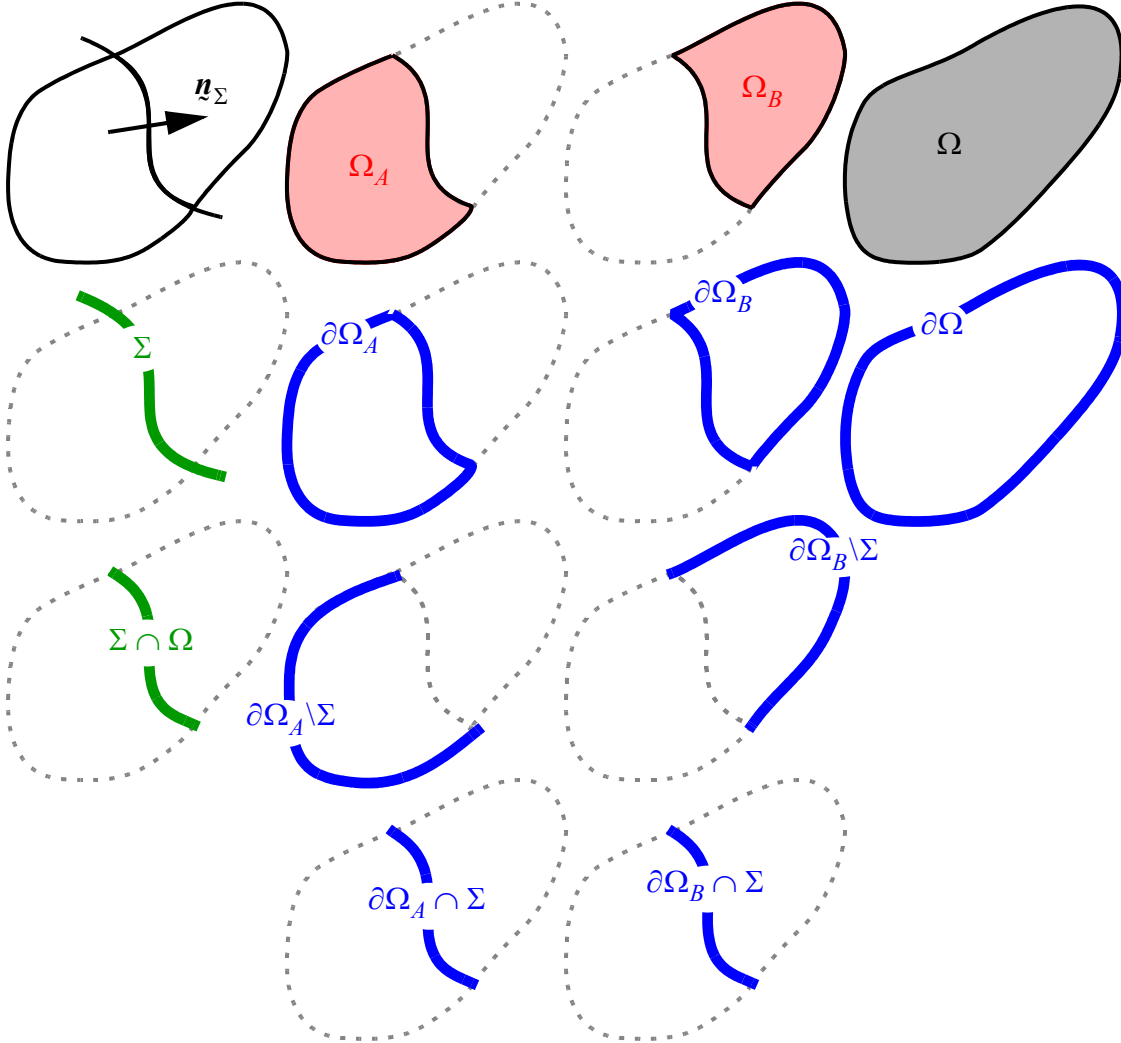
Figure 2.2.   *Set nomenclature used to identify regions and surfaces in a body that is divided by a surface of discontinuity.* The backslash denotes set subtraction (for example, $\partial\Omega_A\backslash\Sigma$ denotes the portion of the boundary of Ω_A that does *not* intersect Σ). Note that $\Omega = \Omega_A \cup \Omega_B$, but $\partial\Omega = (\partial\Omega_A \cup \partial\Omega_B) \backslash \Sigma$. Also note that $\Sigma\cap\Omega = \partial\Omega_A\cap\Sigma = \partial\Omega_B\cap\Sigma$.

We may decompose a region Ω into two parts Ω_A and Ω_B, defined such that $\underset{\sim}{n}_\Sigma$ points away from Ω_A into Ω_B. We assume that the region Ω_A is simply connected. Its boundary $\partial\Omega_A$ has two parts:

$$\partial\Omega_A\backslash\Sigma \;=\; \partial\Omega_A\cap\partial\Omega \;=\; \text{part of } \partial\Omega_A \text{ away from the jump surface} \tag{2.16}$$

$$\partial\Omega_A\cap\Sigma \;=\; \partial\Omega_A\backslash\partial\Omega \;=\; \Omega\cap\Sigma \;=\; \text{part of } \partial\Omega_A \text{ coinciding with the jump}$$
surface
$$\tag{2.17}$$

Likewise, the boundary $\partial\Omega_B$ can be similarly decomposed:

$$\partial\Omega_B\backslash\Sigma \;=\; \partial\Omega_B \cap \partial\Omega = \text{part of } \partial\Omega_B \text{ away from the shock} \tag{2.18}$$

$$\partial\Omega_B \cap \Sigma \;=\; \partial\Omega_B\backslash\partial\Omega \;=\; \Omega \cap \Sigma = \text{part of } \partial\Omega_B \text{ coinciding with the shock} \tag{2.19}$$

We can always perform the integral of Eq. (2.14) over each of the smooth parts of the domain individually:

$$\int_{\partial\Omega} (\underline{f}\underline{n})dS \;=\; \int_{(\partial\Omega_A \cap \partial\Omega)} (\underline{f}_A\underline{n}_A)dA_A + \int_{(\partial\Omega_B \cap \partial\Omega)} (\underline{f}_B\underline{n}_B)dA_B \tag{2.20}$$

where we have added the subscripts A and B to emphasize that the integrand is evaluated on the indicated part of the domain. We have also changed the surface element from dS to dA to further emphasize that the integral over dS is applied to a *closed* surface whereas the area element symbol dA is used for *open* surfaces.

Naturally, the appearance of the unit normal induces an urge to apply the divergence theorem. However, the divergence theorem only applies to a *closed* area integrals. Hence, we are going to "close" the area integrals on the right-hand-side of Eq. (2.20) by adding and subtracting the integral over the remaining part of the surface area. Note that

$$\partial\Omega_A \text{ is the union of } \partial\Omega_A \cap \partial\Omega \text{ and } \partial\Omega_A\backslash\partial\Omega \tag{2.21}$$

In plain English, the above equation says that $\partial\Omega_A$ has two parts: the part that it has in common with $\partial\Omega$ and the part that it does not have in common with $\partial\Omega$. Therefore

$$\int_{(\partial\Omega_A \cap \partial\Omega)} (\underline{f}_A\underline{n}_A)dA_A \;\;=\; \int_{\partial\Omega_A} (\underline{f}_A\underline{n}_A)dS_A - \int_{\partial\Omega_A\backslash\partial\Omega} (\underline{f}_A\underline{n}_A)dA_A \tag{2.22}$$

Note that we have used the area element dS_A for the integral over $\partial\Omega_A$ because this surface is a closed surface. By assumption, the integrand is smooth inside $\partial\Omega_A$, so we may apply the divergence theorem for the first term on the right-hand-side of Eq. (2.22) to obtain

$$\int_{(\partial\Omega_A \cap \partial\Omega)} (\underline{f}_A\underline{n}_A)dA_A \;\;=\; \int_{\Omega_A}\left(\frac{d\underline{f}_A}{d\underline{x}}\right)dV_A - \int_{\partial\Omega_A\backslash\partial\Omega} (\underline{f}_A\underline{n}_A)dA_A \tag{2.23}$$

Recall that $\partial\Omega_A\backslash\partial\Omega = \partial\Omega_A \cap \Sigma$. The vector $\underline{n}_A$ is the *outward* unit normal to Ω_A consequently,

$$\underline{n}_A \;=\; \underline{n}_\Sigma \text{ on } \partial\Omega_A \cap \Sigma \tag{2.24}$$

Noting that $\partial\Omega_A\backslash\partial\Omega = \Omega \cap \Sigma$, we may now write Eq. (2.23) as

$$\int_{(\partial\Omega_A \cap \partial\Omega)} (\underline{f}_A\underline{n}_A)dA_A \;\;=\; \int_{\Omega_A}\left(\frac{d\underline{f}_A}{d\underline{x}}\right)dV_A - \int_{(\Omega \cap \Sigma)} (\underline{f}_A\underline{n}_\Sigma)dA \tag{2.25}$$

We can perform a similar analysis for the second term in Eq. (2.20) to obtain

$$\int\limits_{(\partial\Omega_B \cap \partial\Omega)} (\underline{f}_B \boldsymbol{n}_B)dA_B \quad = \int\limits_{\Omega_B} \left(\frac{d\underline{f}_B}{d\boldsymbol{x}}\right)dV_B + \int\limits_{(\Omega\cap\Sigma)} (\underline{f}_B\boldsymbol{n}_\Sigma)dA \tag{2.26}$$

The key difference between Eqs. (2.25) and (2.26) is that one has a minus sign before the last term while the other does not. This occurs because, on $\partial\Omega_B \cap \Sigma$, the outward normal $\boldsymbol{n}_B$ points in the *opposite direction* of the jump surface normal $\boldsymbol{n}_\Sigma$.

$$\boldsymbol{n}_B = -\boldsymbol{n}_\Sigma \text{ on } \partial\Omega_B \cap \Sigma, \tag{2.27}$$

This equation is to be contrasted with Eq. (2.24), which has no minus sign. Substituting Eqs. (2.25) and (2.26) into (2.20) gives

$$\boxed{\int\limits_{\partial\Omega} (\underline{f}\boldsymbol{n})dS = \int\limits_{\Omega}\left(\frac{d\underline{f}}{d\boldsymbol{x}}\right)dV - \int\limits_{\Omega\cap\Sigma} [[\underline{f}]]\boldsymbol{n}_\Sigma dA} \tag{2.28}$$

where

$$\int\limits_{\Omega}\left(\frac{d\underline{f}}{d\boldsymbol{x}}\right)dV = \int\limits_{\Omega_A}\left(\frac{d\underline{f}_A}{d\boldsymbol{x}}\right)dV_A + \int\limits_{\Omega_B}\left(\frac{d\underline{f}_B}{d\boldsymbol{x}}\right)dV_B \tag{2.29}$$

and

$$\int\limits_{\Omega\cap\Sigma} [[\underline{f}]]\boldsymbol{n}_\Sigma dA = \int\limits_{(\partial\Omega_A \cap \Sigma)} (\underline{f}_A\boldsymbol{n}_\Sigma)dA - \int\limits_{(\partial\Omega_B \cap \Sigma)} (\underline{f}_B\boldsymbol{n}_\Sigma)dA \tag{2.30}$$

The double brackets are a shorthand notation for the value in region A (*away from which the shock normal $\boldsymbol{n}_\Sigma$ points*) minus the value in region B. That is,

$$[[\underline{f}]] \equiv \underline{f}_A - \underline{f}_B \tag{2.31}$$

Some texts adopt the negative of this sign convention. We will find that the jump forms of the physical laws take a more intuitive form with our definition. Specifically, when the shock is propagating in the direction $\boldsymbol{n}_\Sigma$, then region B is the state of the material *before* the shock front arrives while region A is the state of the material *after* the shock passes. Thus, our definition corresponds to the jump in *time* (value after the shock arrives minus value before). Consequently, where the smooth forms of the field laws contain material time rates, we will see the appearance of our double brackets in the jump forms.

Incidentally, note that the right-hand side of Eq. (2.30) involves the regions $\partial\Omega_A \cap \Sigma$ and $\partial\Omega_B \cap \Sigma$. In writing the left-hand-side, we have noted that these surfaces are identical — they both correspond to the surface $\Omega\cap\Sigma$ where Σ intersects Ω, which is the domain indicated on the right-hand-side of Eq. (2.30).

Jump form of the Leibniz rule

Suppose that we wish to compute the derivative of an integral

$$\frac{d}{dt} \int_{\Omega_G} \underline{\Upsilon}(\pmb{x}, t) dV, \tag{2.32}$$

Suppose the integrand contains a moving shock surface Σ across which $\underline{\Upsilon}$ is discontinuous, but away from which, $\underline{\Upsilon}$ is smooth. Since integration is well defined even for discontinuous integrands, we may always write

$$\frac{d}{dt} \int_{\Omega_G} \underline{\Upsilon}(\pmb{x}, t) dV = \frac{d}{dt} \int_{\Omega_A} \underline{\Upsilon}(\pmb{x}, t) dV + \frac{d}{dt} \int_{\Omega_B} \underline{\Upsilon}(\pmb{x}, t) dV \tag{2.33}$$

Thus, we have broken up the integral of a discontinuous function into two separate integrals of smooth functions. Below, we will apply the classic Leibniz rule to both integrals separately, and then eventually combine the results back together. The key here is to identify the velocities of the individual boundaries. On $\partial\Omega_G$, the boundary velocity is $\pmb{v}_G$, which is presumably known. Thus, the boundary velocity on $\partial\Omega_A\backslash\Sigma$ and on $\partial\Omega_B\backslash\Sigma$ is $\pmb{v}_G$. However, in order to enclose the smooth regions Ω_A and Ω_B, the remaining parts of both $\partial\Omega_A$ and $\partial\Omega_B$ must move with the shock speed $\pmb{v}_\Sigma$.

Region Ω_A that lies on one side of the moving discontinuity surface will be called the "after-shocked" region. Region Ω_B that lies on the other side will be called the "before-shocked" region.

Again, the region Ω_A is assumed simply connected region, so its boundary $\partial\Omega_A$ has two parts:

$$\partial\Omega_A\backslash\Sigma = \partial\Omega_A \cap \partial\Omega = \text{part of } \partial\Omega_A \text{ away from the shock} \tag{2.34}$$

$$\partial\Omega_A \cap \Sigma = \partial\Omega_A\backslash\partial\Omega = \Omega \cap \Sigma = \text{part of } \partial\Omega_A \text{ coinciding with the shock} \tag{2.35}$$

The boundary $\partial\Omega_B$ can be similarly decomposed.

For the general Leibniz rule, recall that the boundary $\partial\Omega_G$ moves with a known velocity $\pmb{v}_G$. Therefore, the *part* of $\partial\Omega_A$ that coincides with $\partial\Omega_G$ also moves with velocity $\pmb{v}_G$. However, the remaining part of $\partial\Omega_A$ moves with the shock front, so that part has a velocity equal to the shock velocity $\pmb{v}_\Sigma$. In summary, the outward unit normal $\pmb{n}_A$ and boundary velocity $\pmb{v}_A$ on $\partial\Omega_A$ are

$$\begin{aligned} \pmb{n}_A &= \pmb{n} \text{ and } \pmb{v}_A = \pmb{v}_G \text{ on } \partial\Omega_A\backslash\Sigma \\ \pmb{n}_A &= \pmb{n}_\Sigma \text{ and } \pmb{v}_A = \pmb{v}_\Sigma \text{ on } \partial\Omega_A \cap \Sigma \end{aligned} \tag{2.36}$$

The outward unit normal $\pmb{n}_B$ and the velocity $\pmb{v}_B$ on $\partial\Omega_B$ are similar except for a change in sign on the shock surface:

$$\begin{aligned} \pmb{n}_B &= \pmb{n} \text{ and } \pmb{v}_B = \pmb{v}_G \text{ on } \partial\Omega_B\backslash\Sigma \\ \pmb{n}_B &= -\pmb{n}_\Sigma \text{ and } \pmb{v}_B = \pmb{v}_\Sigma \text{ on } \partial\Omega_B \cap \Sigma \end{aligned} \tag{2.37}$$

Note the sign distinctions in Eq. (2.37). The *outward* normal to $\partial\Omega_B$ points in the opposite direction of $\boldsymbol{n}_\Sigma$ because we arbitrarily elected to define $\boldsymbol{n}_\Sigma$ such that it points *into* region B. However, the *velocity* of the part of $\partial\Omega_B$ that intersects the shock must, by definition, move with the shock velocity. Hence, there is no negative sign on the boundary velocity.

Recall that we can always write

$$\frac{d}{dt}\int_{\Omega_G} \underline{\Upsilon}(\boldsymbol{x}, t)dV = \frac{d}{dt}\int_{\Omega_A} \underline{\Upsilon}(\boldsymbol{x}, t)dV + \frac{d}{dt}\int_{\Omega_B} \underline{\Upsilon}(\boldsymbol{x}, t)dV \qquad (2.38)$$

Each of the individual integrals on the right hand side now contain smooth integrands, and the standard Leibniz formula may be applied to them individually to give

$$\frac{d}{dt}\int_{\Omega_G} \underline{\Upsilon}(\boldsymbol{x}, t)dV = \int_{\Omega_A} \frac{\partial\underline{\Upsilon}(\boldsymbol{x}, t)}{\partial t}dV + \int_{\partial\Omega_A} \underline{\Upsilon}_A(\boldsymbol{v}_A \bullet \boldsymbol{n}_A)dS$$

$$+ \int_{\Omega_B} \frac{\partial\underline{\Upsilon}(\boldsymbol{x}, t)}{\partial t}dV + \int_{\partial\Omega_B} \underline{\Upsilon}_B(\boldsymbol{v}_B \bullet \boldsymbol{n}_B)dS \qquad (2.39)$$

Now we compute the boundary integrals *separately* over the two distinct parts of $\partial\Omega_A$:

$$\int_{\partial\Omega_A} \underline{\Upsilon}_A(\boldsymbol{v}_A \bullet \boldsymbol{n}_A)dS = \int_{\partial\Omega_A\backslash\Sigma} \underline{\Upsilon}_A(\boldsymbol{v}_A \bullet \boldsymbol{n}_A)dS + \int_{\partial\Omega_A\cap\Sigma} \underline{\Upsilon}_A(\boldsymbol{v}_A \bullet \boldsymbol{n}_A)dS \qquad (2.40)$$

or, using Eq. (2.36),

$$\int_{\partial\Omega_A} \underline{\Upsilon}_A(\boldsymbol{v}_A \bullet \boldsymbol{n})dS = \int_{\partial\Omega_A\backslash\Sigma} \underline{\Upsilon}_A(\boldsymbol{v}_G \bullet \boldsymbol{n})dA + \int_{\partial\Omega_A\cap\Sigma} \underline{\Upsilon}_A(\boldsymbol{v}_\Sigma \bullet \boldsymbol{n}_\Sigma)dA \qquad (2.41)$$

Similarly, the last term in Eq. (2.39) may be written

$$\int_{\partial\Omega_B} \underline{\Upsilon}_B(\boldsymbol{v}_B \bullet \boldsymbol{n}_B)dS = \int_{\partial\Omega_B\backslash\Sigma} \underline{\Upsilon}_B(\boldsymbol{v}_G \bullet \boldsymbol{n})dA - \int_{\partial\Omega_B\cap\Sigma} \underline{\Upsilon}_B(\boldsymbol{v}_\Sigma \bullet \boldsymbol{n}_\Sigma)dA \qquad (2.42)$$

Substituting Eqs. (2.41) and (2.42) back into Eq. (2.39) gives

$$\boxed{\frac{d}{dt}\int_{\Omega_G} \underline{\Upsilon}(\boldsymbol{x}, t)dV = \int_{\Omega} \frac{\partial\underline{\Upsilon}(\boldsymbol{x}, t)}{\partial t}dV + \int_{\partial\Omega} \underline{\Upsilon}(\boldsymbol{v}_G \bullet \boldsymbol{n})dS + \int_{\Omega\cap\Sigma} [[\underline{\Upsilon}]](\boldsymbol{v}_\Sigma \bullet \boldsymbol{n}_\Sigma)dS} \qquad (2.43)$$

This is the generalized version of the Leibniz formula when the integrand contains a moving discontinuity. The only new term is the last one involving the jump. A point of caution is in order however: the area integral in the second term of the right-hand-side involves a discontinuous integrand, so the divergence theorem may not be applied. We may, however apply the discontinuous form of the divergence theorem — Eq. (2.28) — to write

$$\int_\Omega \underline{\Upsilon}(\boldsymbol{v}_G \bullet \boldsymbol{n})dS = \int_\Omega (\underline{\Upsilon}\boldsymbol{v}_G) \bullet \underset{\sim}{\nabla}dV - \int_{\Omega\cap\Sigma} [[\underline{\Upsilon}\boldsymbol{v}_G]] \bullet \boldsymbol{n}_\Sigma dA \qquad (2.44)$$

Therefore when $\boldsymbol{v}_G$ can be regarded as a field, Eq. (2.43) becomes

$$\frac{d}{dt}\int_{\Omega_G} \underline{\Upsilon}(\pmb{x},\, t)dV \;=\; \int_{\Omega}\left[\frac{\partial\underline{\Upsilon}(\pmb{x},\, t)}{\partial t} + (\underline{\Upsilon}\pmb{v}_G)\bullet\underset{\sim}{\nabla}\right]dV + \int_{\Omega\cap\Sigma} [[\underline{\Upsilon}(\pmb{v}_\Sigma - \pmb{v}_G)]]\bullet\pmb{n}_\Sigma dS \qquad (2.45)$$

This result shows that the jump term disappears whenever the discontinuity moves with the same (normal) speed as the control volume! For example, if the control volume is Lagrangean, then the jump term disappears whenever the "shock" velocity $\pmb{v}_\Sigma$ equals the material velocity $\pmb{v}$, as might be the case at a material interface. Thus, to be non-trivial shock, the shock front must move *relative to the particles*.

3. Kinematics

The spatial time derivative

Consider a time varying field

$$f = f(\underline{x}, t) \tag{3.1}$$

The spatial derivative is defined as the rate of f as seen by a *stationary* observer (i.e., by an observer for whom $\underline{x}$ is constant). Thus, the spatial time derivative is

$$\text{spatial time derivative} \equiv \left(\frac{\partial f}{\partial t}\right)_{\underline{x}} \tag{3.2}$$

The spatial derivative occurs quite frequently in mechanics, so it is routinely abbreviated by using a special comma $(\quad)_{,t}$ notation. Namely,

$$f_{,t} \text{ is a shorthand notation for } \left(\frac{\partial f}{\partial t}\right)_{\underline{x}} \tag{3.3}$$

The act of writing $f_{,t}$ tells the reader that the f operand is expressible as a function of $\underline{x}$ and t.

The material time derivative

Consider a time varying field

$$f = f(\underline{x}, t) \tag{3.4}$$

Using the mapping function, we note that $\underline{x} = \underline{x}(\underline{X}, t)$. Thus, the field f is alternatively expressible in the reference configuration:

$$f = f(\underline{X}, t) \tag{3.5}$$

The material time derivative of a field $f(\underline{x}, t)$ is the rate of change of that field as seen by an observer *who is moving with the material particles*. If the observer is moving with the particle, then the "identity" of the particle (i.e., its location $\underline{X}$) is fixed. Thus, the material derivative of the field is given by

$$\text{material derivative} \equiv \left(\frac{\partial f}{\partial t}\right)_{\underline{X}} \tag{3.6}$$

The material time derivative occurs so often that it is often useful to denote it more compactly via superimposed dot. For lengthy expressions, the symbol $D(\quad)/Dt$ is also frequently used. Thus

$$\dot{f} \text{ is a shorthand notation for } \left(\frac{\partial f}{\partial t}\right)_{\underline{X}}, \text{ and}$$

$$\frac{Df}{Dt} \text{ is also a shorthand notation for } \left(\frac{\partial f}{\partial t}\right)_{\underline{X}} \tag{3.7}$$

The act of using the dot or "D" notation tells the reader that the operation denotes partial differentiation with respect to time when the operand is regarded as a function of $\underset{\sim}{X}$ and t.

Material differentials. In constitutive modelling, one seeks relationships between state variables. For example, the internal energy u of a gas might be considered to be a function of specific volume v and specific entropy s. Thus, one often writes

$$u = u(v, s) \tag{3.8}$$

Implicit in this expression is the assumption that the internal energy *really is* expressible as a function of v and s *only* — knowing v and s is sufficient to assign a value to u. If this is true, then we can write

$$du = \left(\frac{\partial u}{\partial v}\right)_s dv + \left(\frac{\partial u}{\partial s}\right)_v ds \tag{3.9}$$

The function $u(v, s)$ for, say, air is generally different from the function for hydrogen. Consequently, if you were to analyze a problem involving air, hydrogen, and steel, then the constitutive function for u would have to vary in *space*. In other words, for practical fluid dynamics problems, we know that Eq. (3.8) should really be written

$$u = u(v, s, \underset{\sim}{X}) \tag{3.10}$$

The increment in u is therefore

$$du = \left(\frac{\partial u}{\partial v}\right)_{s, \underset{\sim}{X}} dv + \left(\frac{\partial u}{\partial s}\right)_{v, \underset{\sim}{X}} ds + \left(\frac{\partial u}{\partial \underset{\sim}{X}}\right)_{u, v} \bullet d\underset{\sim}{X} \tag{3.11}$$

Such an expression would be useful when computing how the energy changes with respect to both time and position, such as when the observer moves across various points along an acceleration wave.

Most of the time, however, we are interested in discussing how u varies when observing a particular material particle $\underset{\sim}{X}$. Dependence on particle position $\underset{\sim}{X}$ is almost never shown explicitly in the thermodynamics literature, so one must realize that equations such as Eq. (3.9) implicitly hold particle position $\underset{\sim}{X}$ constant. The independent variables are time varying fields, so a derivative that holds $\underset{\sim}{X}$ constant is essentially a derivative with respect to time. In that case, we might write

$$Du = \left(\frac{\partial u}{\partial v}\right)_s Dv + \left(\frac{\partial u}{\partial s}\right)_v Ds \tag{3.12}$$

The act of using the "D" tells the reader that the increment is not entirely arbitrary — it must hold the particle $\underset{\sim}{X}$ constant. A more clear way to write the above equation is to simply use material rates. Namely,

$$\dot{u} = \left(\frac{\partial u}{\partial v}\right)_s \dot{v} + \left(\frac{\partial u}{\partial s}\right)_v \dot{s} \tag{3.13}$$

Incidentally, there doesn't even exist a function $u(v, s)$ for solids such as steel which require more than just v to describe the strain.

Connection between spatial and material time derivatives

We may apply the chain rule as follows

$$\left(\frac{\partial f}{\partial t}\right)_{X} = \left(\frac{\partial f}{\partial t}\right)_{x}\left(\frac{\partial t}{\partial t}\right)_{X} + \left(\frac{\partial f}{\partial x}\right)_{t} \bullet \left(\frac{\partial x}{\partial t}\right)_{X} \tag{3.14}$$

We now use our compact derivative notation to write

$$\left(\frac{\partial f}{\partial t}\right)_{X} = \dot{f} \tag{3.15}$$

$$\left(\frac{\partial f}{\partial t}\right)_{x} = f_{,t} \tag{3.16}$$

$$\left(\frac{\partial t}{\partial t}\right)_{X} = 1 \tag{3.17}$$

$$\left(\frac{\partial f}{\partial x}\right)_{t} = f\overleftarrow{\nabla} \tag{3.18}$$

$$\left(\frac{\partial x}{\partial t}\right)_{X} = \dot{x} = v \tag{3.19}$$

Thus

$$\boxed{\dot{f} = f_{,t} + f\overleftarrow{\nabla} \bullet v} , \tag{3.20}$$

which may be written in terms of a right-del as

$$\boxed{\dot{f} = f_{,t} + v \bullet \overrightarrow{\nabla} f} \tag{3.21}$$

Non-Lagrangean moving observers

Sometimes we seek the time rate of a field as seen by a moving observer. Let $y = y(t)$ denote the current position of the observer, and let $\dot{y}$ denote the observer's velocity.

The time rate of a field f as seen by the moving observer is

$$\boxed{f_{,t} + f\overleftarrow{\nabla} \bullet \dot{y}} \tag{3.22}$$

Let Y denote the *image* of the observer in the reference configuration. That is, let

$$Y \equiv \chi^{-1}(y(t), t) \tag{3.23}$$

The velocity of the image observer will be denoted by $\dot{Y}$. Written without the inverse, Eq. (3.23) implies that

$$y = \chi(Y, t) \tag{3.24}$$

Recall that

$$\underset{\approx}{F}(X, t) \;=\; \frac{\partial \chi(\underset{\sim}{X}, t)}{\partial \underset{\sim}{X}} \tag{3.25}$$

and

$$\underset{\sim}{v}(\underset{\sim}{X}, t) \;=\; \frac{\partial \chi(\underset{\sim}{X}, t)}{\partial t} \tag{3.26}$$

Thus, taking rates of Eq. (3.24) gives

$$\dot{\underset{\sim}{y}} \;=\; \underset{\approx}{F}(\underset{\sim}{Y}, t) \bullet \dot{\underset{\sim}{Y}} + \underset{\sim}{v}(\underset{\sim}{Y}, t) \tag{3.27}$$

This is usually written without explicitly showing the function arguments:

$$\boxed{\dot{\underset{\sim}{y}} \;=\; \underset{\approx}{F} \bullet \dot{\underset{\sim}{Y}} + \underset{\sim}{v}} \tag{3.28}$$

Here, it must be understood that $\underset{\approx}{F}$ and $\underset{\sim}{v}$ are the deformation gradient and the material velocity *evaluated at the current location of the observer.* Knowing this is important if you seek to find the *acceleration* of the observer.

The time rate of a field f as seen by a moving observer can be expressed in terms of the reference configuration by

$$\boxed{\dot{f} + f\overset{\leftarrow}{\nabla}_o \bullet \dot{\underset{\sim}{Y}}} , \tag{3.29}$$

where

$$\boxed{\dot{\underset{\sim}{Y}} \;=\; \underset{\approx}{F}^{-1} \bullet (\dot{\underset{\sim}{y}} - \underset{\sim}{v})} \tag{3.30}$$

4. The "laws" of physics

Conservation of mass

The law* of conservation of mass states that the total mass of the universe never changes. This means that whatever flows into a system must have flowed *out* of the environment. When using control volumes, the law of conservation of mass may be stated in a loose sense as

"What comes in must go out . . . or stay there!"

To cast this statement into a mathematically precise form, we slightly rephrase the above statement to instead read

"Net rate of influx of mass equals the rate of collection of mass"

This statement must be true regardless of the nature of the control volume. Then we introduce an arbitrary region of space (i.e., a general control volume) Ω_G bounded by a closed surface $\partial\Omega$. If the normal component v_G^n of the boundary velocity $\mathbf{v}_G$ is outpacing the normal component of material velocity $\mathbf{v}$, then the control volume must be gaining mass. If the boundary velocity exactly matches the material velocity, then mass is neither entering nor leaving the control volume. If the boundary velocity lags behind the material velocity, then the control volume is losing mass, which is simply identified as a *negative* mass influx.

We define a field variable denoted ρ called "density" that equals the mass per unit volume. During a small increment in time, Δt, an area element dA on the boundary moves a distance $\Delta t(\mathbf{v}_G - \mathbf{v}) \bullet \mathbf{n}$ relative to the material. Thus, the small amount of mass fluxed through the control volume equals $\rho\Delta t(\mathbf{v}_G - \mathbf{v}) \bullet \mathbf{n}dA$. Dividing by Δt gives the *rate* of mass influx, and integrating over the entire surface gives the total rate of mass influx caused by motion of the boundary relative to the material particles:

$$\text{Net RATE of influx of mass = } -\int_{\partial B} \rho(\mathbf{v} - \mathbf{v}_G) \bullet \mathbf{n}dS \qquad (4.1)$$

Again, $\mathbf{v}$ is the velocity of the material, $\mathbf{v}_G$ is the velocity of the surface $\partial\Omega$, $\mathbf{n}$ is the outward unit normal to the surface, and dS is the element of surface area. If $(\mathbf{v} - \mathbf{v}_G) \bullet \mathbf{n} > 0$, then the material is *exiting* the body, representing an *outflow*. That's

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* The term "law" is used in physics in a very sloppy way. So-called laws are frequently "violated" whenever they are applied outside their intended regime of applicability. For example, Hooke's "law" of elasticity is an idealization that is intended to be applied only at small strains. The law of mass conservation applies for situations in which there is no nuclear conversion of mass into energy. The **jurisdiction** of a law is defined by the broadness of its regime of applicability. In this sense, Hooke's law has a small jurisdiction (since materials quite often behave nonlinearly). The conservation of mass has a very large jurisdiction (since it applies to *any* non-nuclear situation). To date, the first law of thermodynamics has an "infinite" jurisdiction since there has never been *any* process found for which it does not apply.

why we have the negative sign in front of the above integral to obtain an expression for *inflow*. If the control volume happens to be Lagrangean, then $(\underline{v} - \underline{v}_G) \bullet \underline{n} = 0$, meaning that mass neither enters nor exits a Lagrangean control volume. If the control volume is Eulerian, then $\underline{v}_G = \underline{0}$. Hence, for an Eulerian control volume, $(\underline{v} - \underline{v}_G) \bullet \underline{n} = \underline{v} \bullet \underline{n}$, meaning that mass flux is caused entirely by material convection. We will continue with the analysis using a general control volume to illustrate that the final expression for the conservation of mass is independent of the choice of control volume.

The above expression for the net rate of mass influx takes care of the portion of mass conservation that corresponds to "what goes in *minus* what comes out." Let's now write an expression for the proviso that stuff that goes in but does *not* come out must be therefore "staying there" — it cannot simply *disappear*. The total mass inside the control volume must always be given by

$$\textbf{total mass} = \int_{\Omega_G} \rho \, dV \, , \tag{4.2}$$

where dV is the volume element. Consequently, the rate of change of mass is

$$\textbf{rate of collection of mass} = \frac{d}{dt} \int_{\Omega_G} \rho \, dV \, , \tag{4.3}$$

where t is time. Knowing that the boundary $\partial\Omega_G$ moves with a velocity $\underline{v}_G$, we may apply the generalized Leibniz formula to bring the time derivative in Eq. (4.3) to the *inside* of the integral. Specifically, if the integrand is sufficiently smooth (e.g., the control volume must not contain any singular mass sources or any discontinuities such as shock waves), then

$$\textbf{rate of collection of mass} = \int_{\Omega_G} \frac{\partial\rho}{\partial t} dV + \int_{\partial\Omega_G} \rho(\underline{v}_G \bullet \underline{n}) dS \tag{4.4}$$

Equating Eq. (4.1) with (4.4) gives

$$- \int_{\partial\Omega_G} \rho(\underline{v} - \underline{v}_G) \bullet \underline{n} \, dS = \int_{\Omega_G} \frac{\partial\rho}{\partial t} dV + \int_{\partial\Omega_G} \rho(\underline{v}_G \bullet \underline{n}) dS \tag{4.5}$$

The terms involving $\underline{v}_G$ cancel to give

$$\int_{\Omega_G} \frac{\partial\rho}{\partial t} dV + \int_{\partial\Omega_G} \rho\underline{v} \bullet \underline{n} \, dS = 0 \tag{4.6}$$

If the density field is sufficiently smooth in time and space (i.e., no shocks), then the divergence theorem on the second term gives

$$\int_{\Omega_G} \left[\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\underline{v}) \right] = 0 \tag{4.7}$$

This result holds for any system Ω_G, so the integrand must be zero. This so-called "local" form of conservation of mass is called the **continuity** equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underset{\sim}{v}) = 0 \qquad\qquad \leftarrow \text{continuity} \qquad (4.8)$$

After introducing the material time derivative ($\dot{\rho} = \frac{\partial \rho}{\partial t} + \underset{\sim}{v} \bullet \nabla \rho$) and applying the product rule to the gradient, the continuity equation becomes

$$\dot{\rho} + \rho \nabla \cdot \underset{\sim}{v} = 0 \qquad\qquad (4.9)$$

After all of the above mathematical gymnastics, it's easy to forget that our final result of Eq. (4.9) is just an obtuse way of expressing the intuitive concept that **"What comes in must go out — or stay there."**

Alternative Lagrangean analysis of mass conservation.

Under a Lagrangean viewpoint, the law of conservation of mass states that the mass contained inside any Lagrangean control volume must never change. Thus,

$$\frac{D}{Dt} \int_{\Omega} \rho \, dV = 0 \qquad\qquad (4.10)$$

The use of D/Dt tells the reader that the control volume is Lagrangean, which means that the surface $\partial\Omega$ moves with the particles.

Rather than using the Leibniz rule, we can bring the time derivative inside of the integral in the following alternative manner: We can perform a change of variables to the reference configuration. The current location $\underset{\sim}{x}$ of a particle is assumed expressible as a continuous mapping from the initial location $\underset{\sim}{X}$ of the same particle:

$$\underset{\sim}{x} = \chi(\underset{\sim}{X}, t) \qquad\qquad (4.11)$$

Thus, the integral over current space in Eq. (4.10) may be converted into an integral over the reference (initial) space though the use of the following substitutions:

$$\rho(\underset{\sim}{x}, t) \text{ is recast in the form } \rho(\underset{\sim}{X}, t)$$

$$dV = J dV_o \text{ , where } J = \det\left(\frac{\partial \underset{\sim}{x}}{\partial \underset{\sim}{X}}\right) \qquad\qquad (4.12)$$

In the initial reference space, the region Ω_o is defined to be the reference image of Ω[*]. Thus, upon this change of variables, Eq. (4.10) becomes

$$\frac{D}{Dt} \int_{\Omega_o} \rho J \, dV_o = 0 \qquad\qquad (4.13)$$

In this reference space, the region Ω_o does not move with time (it is both Lagrangean and Eulerian because $\dot{\underset{\sim}{X}} = \underset{\sim}{0}$). Thus, the time derivative may be brought directly inside the integral without the need to introduce any boundary flux terms (this is the principal advantage of switching to the reference configuration). Doing this gives

$$\int_{\Omega_o} \left(\frac{\partial(\rho J)}{\partial t}\right)_X dV_o = 0 \qquad\qquad (4.14)$$

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[*] i.e., if $\underset{\sim}{x}$ is a point on $\partial\Omega$, then $\underset{\sim}{X} = \chi^{-1}(\underset{\sim}{x}, t)$ is the corresponding point on $\partial\Omega_o$.

Recall that the partial time derivative holding X constant is the material time derivative. Hence

$$\int_{\Omega_o} \frac{D(\rho J)}{Dt} dV_o = 0 \tag{4.15}$$

or

$$\int_{\Omega_o} (\dot{\rho}J + \rho\dot{J})dV_o = 0 \tag{4.16}$$

This must hold for any control volume. Hence an alternative local form of conservation of mass is

$$\dot{\rho}J + \rho\dot{J} = 0 \tag{4.17}$$

Rearranging the terms,

$$\boxed{\frac{\dot{\rho}}{\rho} = -\frac{\dot{J}}{J}} \tag{4.18}$$

Integrating this rate equation from time zero when $\rho = \rho_o$ and $J = 1$ gives

$$\boxed{\frac{\rho}{\rho_o} = \frac{1}{J}} \tag{4.19}$$

Recalling that $dV = JdV_o$, this result shows that the spatial mass element ρdV must equal the initial reference mass element:

$$\boxed{\rho dV = \rho_o dV_o} \tag{4.20}$$

A fundamental theorem from continuum *kinematics*[*] states that

$$\boxed{\frac{\dot{J}}{J} = \nabla \cdot \underline{v}} \tag{4.21}$$

Hence, Eq. (4.18) becomes

$$\dot{\rho} + \rho(\nabla \cdot \underline{v}) = 0 \tag{4.22}$$

which agrees with our earlier result in Eq. (4.17).

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[*] Kinematics deals with the mathematics of motion (e.g., the fact that velocity is the Lagrangean time derivative of displacement), whereas mechanics deals with physical laws such as conservation of mass, momentum, etc.

Extensive and intensive quantities.

A property Ξ of a system is said to be extensive if the union of any two systems having property values equal to Ξ_1 and Ξ_2 results in a new system whose property is given by $\Xi_1 + \Xi_2$. For example, mass is an extensive property because the union of two systems having masses M_1 and M_2 results in a net system of mass $M_1 + M_2$. Likewise, volume V is an extensive property.

A property of a system is intensive if the union of two systems with *equal values* of the intensive property results in a new system that has *the same* value of the intensive property. Pressure and temperature are examples of intensive properties. Joining two systems having equal temperatures results in a new system at the same temperature.

If A and B are extensive properties, then A/B is an intensive property. For example, if N is the number of moles of material, M is mass, and V is volume, then Ξ/N, Ξ/M, and Ξ/V are all intensive properties. Thus, any extensive property has a corresponding, **molar value** Ξ/N, **specific value** Ξ/M, and **density value** Ξ/V.

Consider the extensive quantity *mass M*. Then the **molar mass** is M/N, the specific mass is $M/M = 1$, and the **mass density** is $M/V = \rho$. Consider the extensive quantity *volume V*. Then the molar volume is V/N, the **specific volume** is V/M (commonly denoted by v), and the volume density V/V is just equal to 1. Note that the specific volume v is the reciprocal of the mass density ρ.

Whenever dealing with an extensive property, it is conventional to define a *specific* property ξ to equal the value of the extensive property per unit mass. In other words, ξ is defined such that

$$\Xi = \int_\Omega \xi\rho\, dV \tag{4.23}$$

Rates of extensive quantities.

Given an extensive property Ξ, recall that we can always define an intensive specific property ξ such that

$$\Xi = \int_\Omega \xi\rho\, dV \tag{4.24}$$

By virtue of Eq. (4.20), we note that the above expression for Ξ may be alternatively computed in the reference configuration by

$$\Xi = \int_{\Omega_o} \xi\rho_o\, dV_o \tag{4.25}$$

The use of the *specific* property (rather than the density value of the property per unit volume) is especially useful when taking Lagrangean rates of Ξ. Taking the Lagrangean rate of Eq. (4.25) gives

$$\dot{\Xi} = \frac{D}{Dt}\int_{\Omega} \xi\rho dV = \frac{D}{Dt}\int_{\Omega_o} \xi\rho_o dV_o = \int_{\Omega_o} \frac{D}{Dt}(\xi\rho_o)dV_o \tag{4.26}$$

In the final step, we have invoked the Leibniz formula using the fact that the velocity of the boundary is zero in the reference configuration, which therefore permits the time derivative to be taken directly inside the integral. But the *initial* density is time independent so $\dot{\rho}_o = 0$, giving

$$\dot{\Xi} = \int_{\Omega_o} \dot{\xi}\rho_o dV_o \tag{4.27}$$

This result may be converted back to the spatial configuration by again invoking Eq. (4.20). Thus we obtain a very useful result:

$$\boxed{\frac{D}{Dt}\int_{\Omega} \xi\rho dV = \int_{\Omega} \dot{\xi}\rho dV} \qquad \text{(valid if integrand } \xi\rho \text{ is "smooth")} \tag{4.28}$$

This result is very powerful because it provides a quick way for us to immediately bring a material time derivative inside an integral without having to invoke the general Leibniz formula in the spatial configuration. This result is valid because of the law of conservation of mass. Thus, it would not apply to control volumes that contain nuclear reactions (since mass is not conserved in nuclear reactions). Even though the above result gives us a fast way to bring the time derivative inside the integral, the derivation of the result employed the classical (smooth) version of the Leibniz formula. Consequently, Eq. (4.28) is only valid for smooth integrands. If the integrand $\xi\rho$ is discontinuous, then Eq. (7.99) should be used.

Using Eq. (4.16), the result of Eq. (7.99) may be converted to a form that applies to general non-Lagrangean control volumes. Namely,

$$\int_{\Omega} \dot{\xi}\rho dV = \frac{d}{dt}\int_{\Omega_G} \xi\rho dV + \int_{\partial\Omega} \xi\rho(\underset{\sim}{v} - \underset{\sim}{v}_G) \bullet \underset{\sim}{n} dS \tag{4.29}$$

Homework: prove Eq. (4.28) in a different way by directly using the Leibniz formula to bring the derivative inside the integral. Then invoke the continuity Eq. (4.16) to cancel out appropriate terms.

Work and Power

In a very sloppy sense, the work W associated with a force $\underset{\sim}{F}$ is equal to the integral of that force dotted into the increment $d\underset{\sim}{x}$ in displacement. Thus, one often sees unsophisticated textbooks write $dW = \underset{\sim}{F} \bullet d\underset{\sim}{x}$. The problem with this notation is that it gives the impression that the force $\underset{\sim}{F}$ can be expressed as a function of position $\underset{\sim}{x}$. For conservative force fields, such as gravity and springs, the force can be expressed as a function of $\underset{\sim}{x}$ and therefore $\oint \underset{\sim}{F} \bullet d\underset{\sim}{x} = 0$ for any closed path in $\underset{\sim}{x}$. Unfortunately not all forces are conservative. Consider, for example, the force required to slide a block across a frictional surface

from a point $(a, 0, 0)$ to $(b, 0, 0)$ and then back again. On the outgoing trip, $\underset{\sim}{F} = \mu N \underset{\sim}{e}_1$, where μ is the coefficient of friction and N is the weight of the block. On the return trip, however, the force has the same magnitude, but the opposite sign. Therefore, the force must not be expressible as a function of $\underset{\sim}{x}$. Simply knowing that the position is, say, $(\frac{a+b}{2}, 0, 0)$ is not enough to know the value of the force — one must also know the direction of motion. For the frictional block, the work around this closed path is

$$\oint \underset{\sim}{F} \bullet d\underset{\sim}{x} = \int_a^b \mu N dx + \int_b^a (-\mu N) dx = 2\mu N(b-a) \quad \neq 0 \quad . \tag{4.30}$$

In thermodynamics, it is *extremely important* to carefully indicate whether quantities will integrate to zero around a closed path. The above counterexample proves that the integral of $\underset{\sim}{F} \bullet d\underset{\sim}{x}$ around a closed path is not necessarily zero. To indicate this fact, we say that $\underset{\sim}{F} \bullet d\underset{\sim}{x}$ is an *inexact* differential, and we write

$$\overline{d}W = \underset{\sim}{F} \bullet d\underset{\sim}{x} \tag{4.31}$$

The small slash through the $\overline{d}$ tells the reader that the differential is inexact and its integral around a closed path will not necessarily equal zero. This means that the quantity $\underset{\sim}{F}$ cannot generally be written as a proper function of $\underset{\sim}{x}$.

By writing $d\underset{\sim}{x} = \underset{\sim}{v}dt$, where $\underset{\sim}{v}$ is velocity, we note that

$$\overline{d}W = Pdt \text{ , where } P \equiv \underset{\sim}{F} \bullet \underset{\sim}{v} \text{ is the "power"} \tag{4.32}$$

The time variable t is sometimes called a *pseudo-time* since it does not really have to be real time — it only needs to be any scalar defined such that the path taken by the position vector $\underset{\sim}{x}$ can be parameterized as $\underset{\sim}{x} = \underset{\sim}{x}(t)$. The total work associated with the path is computed by

$$W = \int \overline{d}W = \int_{t_1}^{t_2} (\underset{\sim}{F} \bullet \underset{\sim}{v}) dt \tag{4.33}$$

The fact that $\overline{d}W$ is inexact means that the value of the integral depends on the path taken. For example, the amount of work needed to push a block from point A to point B generally depends on the path taken (a direct path requires less work than an circuitous path). If the force arises from friction between the block and the surface, then the force is not expressible as a function of position, and the work therefore is path dependent. On the other hand, if the force arises from an idealized spring and if the block is sliding on a frictionless surface, then the force is expressible as a function of position and the work in this case is path independent.

Whenever a quantity *can* be expressed as an exact differential dU, then we can write

$$dU = \dot{U}dt \tag{4.34}$$

The integral of dU over a closed path is equal to zero, and the integral of dU over an open path depends only on the end states. In this case, we call $\dot{U}$ a "true" rate because its integral over time depends *only* on the end states, not on the path connecting them.

Consider a quantity Z that *cannot* be expressed as an exact differential, it is sometimes heuristically useful to write

$$\overset{*}{Z} \equiv \frac{dZ}{dt} \tag{4.35}$$

With this notation, we may sometimes write

$$P = \overset{*}{W} \tag{4.36}$$

In general, numerous forces of different kinds can act on a system. Each force has its own associated work. The *total* work used to transform the system from state 1 at time t_1 to state 2 at time t_2 is given by

$$W_{12} = \text{work input} = \int_{t_1}^{t_2} P_M \, dt \tag{4.37}$$

Here P_M is the sum (integral over the entire system) of the forces at any point times the velocity at that point. For a continuum, we presume that there are three fundamental types of forces:

- **Body forces** such as gravity or forces from an electric field. The body force per unit mass is denoted by $\underset{\sim}{b}$. Therefore, the body force on a small mass element equals $\underset{\sim}{b}dm = \underset{\sim}{b}\rho dV = \underset{\sim}{b}\rho_o dV_o$. If the force arises from an electrical field $\underset{\sim}{E}$, then the electrical body force acting on a small mass element ρdV is given by $\underset{\sim}{b}^q = q\underset{\sim}{E}$, where q is the charge* per unit mass.

- **Surface traction** applied from the surrounding media onto the surface of the system. The force per unit area dA is denoted by $\underset{\sim}{T}$ and is conventionally called "traction." Thus, the **FORCE** on the area element is given by $\underset{\sim}{T}dA$. In the spatial configuration, the conservation of momentum equation may be used to assert the existence of a stress tensor $\underset{\approx}{\sigma}$ such that $\underset{\sim}{T} = \underset{\approx}{\sigma} \bullet \underset{\sim}{n}$, where $\underset{\sim}{n}$ is the outward unit normal to the surface area. Therefore, the **FORCE** on a small area element is $\underset{\approx}{\sigma} \bullet \underset{\sim}{n}dA$. If desired, this same elemental **FORCE** may be expressed in terms of the reference configuration as $\underset{\sim}{t} \bullet \underset{\sim}{N}dA_o$, where $\underset{\sim}{t} = J\underset{\approx}{\sigma} \bullet \underset{\approx}{F}^{-T}$. This definition of the reference stress is required in order to satisfy $\underset{\approx}{\sigma} \bullet \underset{\sim}{n}dA = \underset{\sim}{t} \bullet \underset{\sim}{N}dA_o$.

- **Extra forces.** This category for force may be regarded as all forces not included in the body force and traction force. Ordinarily, these forces are those that are idealized as singular point loads and/or externally applied surface tractions. The extra forces are usually the ones that are directly controllable by an external agent. Conversely, if

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* Whether you identify the charge to be bound charge or free charge depends on the problem. For electrically quasistatic problems, free charge must reside at the boundaries, so q is just the bound charge. The effect of the free charge then appears as a surface traction from surface charge.

one is interested in extracting work from a system, the extra forces are those that, unlike gravity, can be harnessed by an external agent.

We define three powers associated with the above three types of forces so that the total power applied to a system is expressible as

$$P_M = P_b + P_F + P_x \quad , \tag{4.38}$$

where

$$P_b = \text{power from body forces} = \int_\Omega (\underset{\sim}{b} \bullet \underset{\sim}{v}) \rho \, dV \tag{4.39}$$

$$P_F = \text{"flow" power from traction forces} = \int_{\partial\Omega} (\underset{\sim}{n} \bullet \underset{\approx}{\sigma}) \bullet \underset{\sim}{v} \, dA \tag{4.40}$$

$$P_x = \text{power from all other forces (such as point loads).} \tag{4.41}$$

Applying the divergence theorem, the flow power may be written

$$P_F = \int_\Omega \nabla \cdot (\underset{\approx}{\sigma} \bullet \underset{\sim}{v}) \, dV \tag{4.42}$$

Applying the chain rule, we note that

$$\nabla \cdot (\underset{\approx}{\sigma} \bullet \underset{\sim}{v}) = (\nabla \cdot \underset{\approx}{\sigma}) \bullet \underset{\sim}{v} + \underset{\approx}{\sigma} : \nabla \underset{\sim}{v} \tag{4.43}$$

From the momentum equation, we know that $\nabla \cdot \sigma = \rho(\underset{\sim}{a} - \underset{\sim}{b})$. Recall that acceleration is the time rate of velocity ($\underset{\sim}{a} = \dot{\underset{\sim}{v}}$). Therefore, $\tilde{\nabla} \cdot \underset{\approx}{\sigma} = \rho(\dot{\underset{\sim}{v}} - \underset{\sim}{b})$, and the first term on the right-hand side of Eq. (4.43) becomes

$$(\nabla \cdot \underset{\approx}{\sigma}) \bullet \underset{\sim}{v} = \rho(\dot{\underset{\sim}{v}} \bullet \underset{\sim}{v} - \underset{\sim}{b} \bullet \underset{\sim}{v}) \tag{4.44}$$

Substituting this result back into (4.43) and then into the integrand of Eq. (4.42) gives

$$P_F = \int_\Omega p_F \, \rho \, dV \ , \text{ where } P_F \equiv \dot{e}_k - p_b + p_s \tag{4.45}$$

Here we have defined

specific kinetic energy $= \boxed{e_k \equiv \frac{1}{2}\underset{\sim}{v} \bullet \underset{\sim}{v}}$ (Hence, $\dot{e}_k = \dot{\underset{\sim}{v}} \bullet \underset{\sim}{v}$) (4.46)

specific body force power $= \boxed{p_b \equiv \underset{\sim}{b} \bullet \underset{\sim}{v}}$ (4.47)

specific stress power $= \boxed{p_s \equiv \frac{1}{\rho}\underset{\approx}{\sigma} : \nabla \underset{\sim}{v}}$ (4.48)

Recalling Eq. (4.39), the total flow power P_F and the specific flow power p_F in Eq. (4.45) are found to be expressible in terms of three distinct parts:

$$\boxed{P_F \;=\; \dot{E}_k - P_b + P_s} \qquad \Leftrightarrow \qquad p_F \;=\; \dot{e}_k - p_b + p_s \tag{4.49}$$

where

$$\dot{E}_k \;=\; \text{the (true) rate of kinetic energy} \;=\; \int_{\Omega}\rho\dot{e}_k dV \;=\; \frac{D}{Dt}\int_{\Omega}\rho e_k dV \tag{4.50}$$

$$P_b \;=\; \text{power (inexact work ``rate'') from body forces} \;=\; \int_{\Omega}(\underline{b} \bullet \underline{v})\rho dV \tag{4.51}$$

$$P_s \;=\; \text{the so-called ``stress power''} \;=\; \int_{\Omega}\rho p_s dV \tag{4.52}$$

Importantly, note that $\dot{E}_k$ is a true rate whereas P_s and P_b are generally not true rates (their integrals over time are path dependent).

Thermal power

Early researchers in thermodynamics regarded heat as fundamentally different from mechanical work. Heat even had its own distinct units (e.g. the BTU). In hindsight, we now know from quantum mechanics that heat is merely a macroscopic manifestation of transfer of atomic vibrations. On the macroscopic scale where thermodynamics is applied, atomic velocities are decomposed into two parts: an overall bulk or drift velocity $\underline{v}$ plus large-amplitude/small-duration perturbations of the velocity resulting from atomic vibrations relative to the bulk motion. The atomic vibration speeds are very large, but they occur over such a small time frame before reversing direction that they do not result in significant macroscopic material displacement. On the macroscopic scale, atomic vibrations reveal themselves as *temperature*.

Joule's pioneering empirical observations revealed that any two thermodynamical states A and B could always be connected via a purely mechanical process. For example, one can convert ice water into boiling water by mechanically agitating it. Importantly, this statement does not imply reversibility. The existence of a connection merely says that $A \rightarrow B$ or $B \rightarrow A$ exists, but not necessarily both. For example, there does not exist any mechanical process by which boiling water may be converted into ice.

The existence of a mechanical process connecting two state does not necessarily mean that a given change in state was actually achieve via mechanical means. For example, one can also convert ice water into boiling water by adding heat. As a matter of fact, this observation is the key needed to define heat. Namely, the amount of heat generated by a device (a bunsen burner, an electric blanket, etc.) when applied to achieve a certain state change can be defined to equal the amount of *work* that connects the two states. Importantly, this definition tells us that heat and work can be expressed in the *same units*. For example, a British Thermal Unit (BTU) is equal to 9.5×10^{-4} Newton-meter.

Because heat and work have the same units, they can be added together algebraically, which leads us to the first law of thermodynamics.

The first law of thermodynamics: there exists energy

The key breakthrough towards the formulation of the first law of thermodynamics was the experimental recognition of the mechanical equivalent of heat — that is, work can be transformed to heat and heat can be transformed (at least partially) to work. Work and heat — originally thought to have different units — have the same dimensions. The *British thermal unit* (BTU) and the *calorie* can be expressed in terms of the *foot-pound* or the *Newton-meter* work unit. Most of us are so familiar with this fact that we fail to recognize its profoundness.

The same change in state can be achieved by mechanical work, by heating, or by some combination of the two. Consequently, simply knowing the beginning and ending states is insufficient to know the amount of work or heating done. Stated mathematically, this means that the mechanical work,

$$W_{12} = \text{work input} = \int_{t_1}^{t_2} P_M \, dt \tag{4.53}$$

and the heating

$$Q_{12} = \text{heat input} = \int_{t_1}^{t_2} P_T \, dt \tag{4.54}$$

depend on the path connecting the end states. For example, pushing a block across a rough surface directly from x_1 to x_2 involves a certain amount of work and it also heats up the block because of friction. The same temperature increase can be obtained by simply heating the block. An observer who only sees the initial and final states will be unable to tell whether the temperature rise came from mechanical work or from thermal heating.

We know that work and heat are *individually* path dependent. The first law of thermodynamics says that their *sum* is path-independent! Thus, there must exist a state variable*
E (hereafter called **energy**) such that

$$E_2 - E_1 = W_{12} + Q_{12} \tag{4.55}$$

where E_1 is the value of E at state 1 and E_2 is the value of E at state 2. Note that the first law does *not* tell you how to measure energy. The first law merely asserts that *energy exists*. Finding a way to assign a value to energy is the principal subject of constitutive (equation of state) modelling.

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* A state variable is any property that can be theoretically measured at any time, without needing information about the past history of the material. In practice, the values of variables are often modeled using history dependent models, but that doesn't make the variable itself history dependent. For example, the yield stress of a metal is often modeled to harden linearly with the amount of past plastic straining. However, the yield stress is still a state variable in the sense that we can always go to the lab and *measure* it without having any knowledge of the past history of the sample.

The fact that work is path dependent means that, despite being rate-like, P_M is not a *true* rate. In other words, there does not exist any state variable W such that $P_M = \dot{W}$. Likewise, there does not exist any state variable Q such that $P_T = \dot{Q}$.

Even though P_M and P_T are not true rates, the first law of thermodynamics states that *their sum* is a true rate. Thus, the first law of thermodynamics says there exists a state variable E, called **energy**, such that

$$\boxed{\dot{E} = P_T + P_M}$$

(4.56)

If, for example, you exercise a material through a closed path (i.e., a sequence of states that start and end with the same state), then the integral of $P_M + P_T$ around that closed path will always be zero. By contrast, the *individual* integrals of P_M and P_T around a closed path are not generally zero.

Substituting Eq. (4.38) into (4.56) gives

$$\dot{E} = P_T + P_b + P_F + P_x$$

(4.57)

Note that the kinetic energy rate $\dot{E}_K$ is a true rate. It's customary to define an internal energy U to equal the part of the energy not due to kinetic energy:

$$U = E - E_{\text{K.E.}}$$

(4.58)

Substituting $\dot{E} = \dot{U} + \dot{E}_{\text{K.E.}}$ permits Eq. (4.57) to be written

$$\dot{U} = P_T + P_b + P_F + P_x - \dot{E}_k$$

(4.59)

From Eq. (4.49) we recognize that $P_b + P_F - \dot{E}_k$ is just the stress power P_s. Thus, a very compact form of the first law is

$$\boxed{\dot{U} = P_T + P_s + P_x}$$

(4.60)

Thus, the internal energy of a body can be altered via three fundamental modes of stimulation:

- P_s is the mechanical work "rate" associated with material deformation.

- P_x is the mechanical work "rate" from any extra singular point and surface forces that are not already included in the boundary integral of the stress field. (Hence, these must be loads that can't be expressed as tractions or body forces without using Dirac delta functions.)

- P_T is the "rate" of heat input to the system either by body radiation or by conduction. Keep in mind that we are considering Lagrangean systems, so heat does not flow via convection (except for mixture models).

Specific energy. Energy E is extensive, so (recalling Eq. 4.23), there exists a **specific energy** e such that

$$E = \int_\Omega e\rho dV \qquad (4.61)$$

By using conservation of mass, we can invoke Eq. (4.28) to write

$$\dot{E} = \int_\Omega \dot{e}\rho dV \qquad (4.62)$$

Likewise, there exists a **specific internal energy** u such that

$$U = \int_\Omega u\rho dV \quad \text{and} \quad \dot{U} = \int_\Omega \dot{u}\rho dV \qquad (4.63)$$

Potential energy. When studying thermodynamics, determining what contributes to the energy is often very confusing, and the inconsistent approaches taken in the literature don't help this situation at all. We have already seen that *kinetic* energy arises naturally *as a part of the mechanical power*. Up to this point, we have not seen the appearance of a *potential* energy such as that associated with springs or with gravity. We will now show that potential energy arises naturally as *any part of the mechanical power from conservative forces*. As presented thus far, the mechanical power includes the power from both conservative and non-conservative forces. A conservative force is one whose associated work is always path-independent. All other forces (such as the force from friction) are non-conservative. A **conservative** force $\underset{\sim}{F}$ is one for which there exists a potential function $E_p(\underset{\sim}{x})$ called the "potential energy" such that

$$\underset{\sim}{F} = -\nabla E_p = -\frac{dE_p}{d\underset{\sim}{x}} \qquad (4.64)$$

Here, the negative sign has been introduced for convenience. As an example, let $\hat{\underset{\sim}{e}}$ denote a unit vector that points "up" away from the surface of the earth, and define $E_p = mgh$, where m is the mass of the body, g is the acceleration of gravity ($9.8 \ m/s^2$), and $h = \underset{\sim}{x} \bullet \hat{\underset{\sim}{e}}$ is the height of the body. Taking the negative gradient of E_p gives the force of gravity, $\underset{\sim}{F} = -mg\hat{\underset{\sim}{e}}$.

Of course, in continuum mechanics, we don't usually work with straight forces. We might work with forces (such as the body force) that are defined *per unit mass*. The total body force $\underset{\sim}{b}$ might contain multiple contributions. We can decompose it into a non-conservative part $\underset{\sim}{b}_{nc}$ plus a conservative part $\underset{\sim}{b}_c$ for which there exists a *specific* potential $e_p(\underset{\sim}{x})$. That is, we assume

$$\underset{\sim}{b} = \underset{\sim}{b}_{nc} + \underset{\sim}{b}_c, \quad \text{where} \quad \underset{\sim}{b}_c = -\nabla e_p \qquad (4.65)$$

We already showed that the force of gravity $\underset{\sim}{F} = -mg\hat{\underset{\sim}{e}}$ is conservative. The *specific* force of gravity is simply the acceleration of gravity $\underset{\sim}{g} = \underset{\sim}{F}/m = -g\hat{\underset{\sim}{e}}$. The *specific* potential function for gravity is $e_p = E_p/m = gh$.

Now consider the material time rate of the potential function:

$$\dot{e}_p = \frac{\partial e_p}{\partial t} + \underset{\sim}{v} \bullet \nabla e_p \tag{4.66}$$

We have already indicated that the potential function must depend only on position $\underset{\sim}{x}$, not on time t. Hence, the first term above is zero. Recalling that $\nabla e_p = -\underset{\sim}{b}_c$, Eq. (4.66) becomes

$$\dot{e}_p = -\underset{\sim}{v} \bullet \underset{\sim}{b}_c \tag{4.67}$$

This means that the mechanical power associated with conservative force fields is given by the negative rate of the potential. Importantly, $\dot{e}_p$ is a *true rate*. Its integral over time depends only on the initial and final states, not on the path connecting them. By contrast, the integral of the *non-conservative power* depends on the path.

As a result of Eq. (4.67), we may write the body force power as

$$P_b = P_{b,\,nc} - \dot{E}_p \tag{4.68}$$

Since the body force power still contains a non-conservative part, there is really no advantage to the above decomposition unless *all* body forces are known to be conservative. If the problem includes non-conservative forces, then you might as well just stick with using the total P_b that includes contributions from both types of body forces.

Potential energy can also arise from other types of forces. If, for example, one of the point loads that contribute to P_F is applied from an idealized spring, then it can be represented by a potential function. The force per unit area represented via the stress tensor might also contain conservative contributions. The stress in a viscoelastic material, for example, contains non-conservative viscous contributions and conservative elastic contributions. The potential energy associated with elastic forces appears within the material constitutive law in such a manner that the stress tensor is the derivative of the potential with respect to the elastic strain tensor.

Again we want to emphasize that potential energy E_p is *not* really part of the energy E. Potential energy is a part of the mechanical power P_M, so we can always write

$$P_M = P_{M,\,nc} + P_{M,\,c} \ , \text{where } P_{M,\,c} = -\dot{E}_p \tag{4.69}$$

If this is done, then the first law would become

$$\dot{E} = P_T + P_{M,\,nc} - \dot{E}_p \tag{4.70}$$

or

$$\dot{\xi} = P_T + P_{M,\,nc} \ , \text{where } \xi = E + E_p \tag{4.71}$$

In this viewpoint, the "apparent" energy ξ is composed of the "true" energy E plus the potential energy E_p.

We find this viewpoint horribly confusing. We mention it here for the sole purpose of helping you decipher what other researchers might be doing. Henceforth, we will *not* use the potential energy. We will assume that all mechanical powers contain contributions from all forces, both conservative and non-conservative.

Local form of the first law. Eq. (4.60) is the most general form of the first law, so we will start there:

$$\dot{U} = P_T + P_s + P_x$$

(4.72)

This equation is really an integral equation. The internal energy U is that of an entire body. The powers P_T, P_s and P_x are those applied to the entire body. Importantly, the above equation must be valid regardless of the choice of body. Hence, it must hold when the body is regarded as an infinitesimal mass. Keep in mind that the power P_x from the extra forces that are applied at singular points or along singular surfaces. Hence, this power is not well defined for a mass element unless Dirac delta functions are used. Rather than doing this, however, we will present the local form of the first law that applies only for infinitesimal bodies that do not contain any singular forces. Thus, away from the singular extra forces, the first law of Eq. (4.72) may be written on a per unit mass basis as

$$\dot{u} = p_T + p_s$$

(4.73)

As discussed in the next section, the effect of singular discontinuity surfaces is handled through the use of jump conditions. The effects of singular applied loads are handled as boundary conditions.

Physical laws in greater generality

Many laws of mechanics, thermodynamics, electricity, etc. can be written in the following generic form:

$$\frac{D}{Dt}\int_{\Omega} \underline{\xi}\rho dV \geq \int_{\Omega} \underline{\psi}\rho dV + \int_{\partial\Omega} \underset{\approx}{f} \bullet \underline{n} dS + \sum \underline{\Pi}$$

(4.74)

If equality always holds, then the law is a conservation law that basically says that the rate of collection of something must equal the net influx plus the rate of creation from internal sources. In this generic physical law, $\underline{\xi}$ is a specific value of an extensive field variable. In general, $\underline{\xi}$ can be a scalar or tensor of any order. The quantity $\underline{\psi}$ is a tensor of the same order as $\underline{\xi}$ and it is regarded as a source field. The quantity $\underset{\approx}{f}$ is a tensor of one order higher than $\underline{\xi}$ and it is regarded as a flux field. Finally, $\underline{\Pi}$ symbolically represents the set of singular sources that cannot be described in integral form without using generalized functions.

The volume integrals may be alternatively expressed in terms of the reference configuration by using conservation of mass,

$$\rho dV = \rho_o dV_o \ .$$

(4.75)

The surface integral may be converted to the reference configuration by using Nanson's relation between the spatial and reference area elements. Namely,

$$\underline{n} dS = \underset{\approx}{F}^c \bullet \underline{N} dS_o \ , \text{where } \underset{\approx}{F}^c = J\underset{\approx}{F}^{-T}$$

(4.76)

Using these relationships, the physical law of Eq. (4.74) may be written in the reference configuration as

$$\frac{D}{Dt}\int_{\Omega}\underline{\xi}\rho_o dV_o = \int_{\Omega}\underline{\psi}\rho_o dV_o + \int_{\partial\Omega}\hat{\underline{f}}\bullet\underline{N}dS_o + \sum\underline{\Pi} \quad,$$

where $\hat{\underline{f}} = \underline{f}\bullet\underline{\underline{F}}^c = J\underline{f}\bullet\underline{\underline{F}}^{-T}$ (4.77)

The equality symbol become an inequality $\geq$ in the case of the second law.

Table 4.1: Terms in the generalized integral field laws

Physical Law	$\underline{\xi}$	$\underline{\psi}$	$\underline{f}$	$\hat{\underline{f}}$	**source of** $\underline{\Pi}$
Conservation of mass (=)	1	0	$\underline{0}$	$\underline{0}$	0 in reality, but some applications permit idealized point mass sources or sinks.
Linear momentum (=)	$\underline{v}$	$\underline{b}$	$\underline{\underline{\sigma}}$	$\hat{\underline{\underline{\sigma}}}$	point loads, surface loads
Angular momentum (=)	$\underline{x}\times\underline{v}$	$\underline{x}\times\underline{b}$	$\underline{x}\times\underline{\underline{\sigma}}$	$\underline{x}\times\hat{\underline{\underline{\sigma}}}$	torques from singular loads, point moments
First Law of thermodynamics (=)	e	$r+\underline{b}\bullet\underline{v}$	$\underline{v}\bullet\underline{\underline{\sigma}}-\underline{q}$	$\underline{v}\bullet\hat{\underline{\underline{\sigma}}}-\hat{\underline{q}}$	Work from singular loads and moments. Heating from singular sources.
Second Law of thermodynamics (≥)	s	$\dfrac{r}{T}$	$-\dfrac{\underline{q}}{T}$	$-\dfrac{\hat{\underline{q}}}{T}$	entropy generated from singular heat sources.

Local forms of the physical laws. Consider the special case that *the integration domain* Ω *contains no singularities (*$\underline{\Pi} = \underline{0}$*) and no jump discontinuities, so that the integrands are all continuously differentiable.* Then so-called local forms of the governing equations are obtained by applying the Leibniz formula to bring the time derivative inside the integral on the left-hand side of Eq. (4.76) and the divergence theorem to convert the surface integral on the right-hand side into a volume integral. When the result is first analyzed for the special case of conservation of mass, then one obtains the continuity equation

$$\dot{\rho} + \rho(\underline{v}\bullet\underline{\nabla}) = 0$$ (4.78)

In the reference configuration, this becomes

$$\dot{\rho} + \rho\left(\frac{\dot{J}}{J}\right) = 0 \,,$$

where $J = \det(\underline{\underline{F}})$ (4.79)

Upon substituting the continuity equation into the generalized result, the simplified local form for the generalized physical balance law becomes

$$\dot{\underline{\xi}} - \underline{\psi} - \frac{1}{\rho}(\underline{f} \bullet \underline{\nabla}) = 0 \qquad (\geq 0 \text{ for the second law}) \tag{4.80}$$

In the reference configuration, this becomes

$$\dot{\underline{\xi}} - \underline{\psi} - \frac{1}{\rho_o}(\hat{\underline{f}} \bullet \underline{\nabla}_o) = 0 \qquad (\geq 0 \text{ for the second law}) \tag{4.81}$$

Jump forms of the physical laws.

Suppose that the integration domain contains a jump discontinuity, but no point singularities, then generalized jump forms of the Leibniz and divergence theorems may be applied to eventually obtain a relationship between jumps in the generalized field variables. When this relationship is examined for the special case of mass continuity, the result is

$$[[\rho c]] = 0$$
$$\text{where } c \equiv (\underline{v}_\Sigma - \underline{v}) \bullet \underline{n}_\Sigma \tag{4.82}$$

In the reference configuration, this becomes

$$[[\rho_o c_o]] = 0$$
$$\text{where } c_o \equiv \underline{V}_{\Sigma_o} \bullet \underline{N}_\Sigma \tag{4.83}$$

Here, Σ_o is the image of Σ in the reference configuration, and $\underline{V}_{\Sigma_o}$ is the velocity of the image surface, which (referring to Eq. (3.30) is related to the spatial velocity by

$$\underline{V}_{\Sigma_o} = \underline{F}^{-1} \bullet (\underline{v}_\Sigma - \underline{v}) \tag{4.84}$$

The normal $\underline{N}_\Sigma$ is the image of $\underline{n}_\Sigma$ and therefore

$$\underline{N}_\Sigma dA_o = \frac{1}{J}\underline{F}^T \bullet \underline{n}_\Sigma dA \tag{4.85}$$

Using these two equations in Eq. (4.83) eventually reveals that

$$\rho c dA = \rho_o c_o dA_o \tag{4.86}$$

By utilizing the mass jump condition in the general jump condition, the final expression of the jump restriction is shown in Appendix B to become

$$\rho c[[\underline{\xi}]] + [[\underline{f}]] \bullet \underline{n}_\Sigma = 0 \qquad (\geq 0 \text{ for the second law}) \tag{4.87}$$

The jump equation in the reference configuration is

$$\rho_o c_o[[\underline{\xi}]] + [[\hat{\underline{f}}]] \bullet \underline{N}_\Sigma = 0 \qquad (\geq 0 \text{ for the second law}) \tag{4.88}$$

5. Classical inviscid thermoelasticity

If a material is incapable of supporting shear stresses then the pressure P is typically regarded to be a funtion of the volume V and the temperature T. These models also depend on the amount of material contained within V, typically expressed by the number of moles n. For example, the ideal gas equation is written

$$P = nR_u T/V \ ,$$
(5.1)

where R_u is the universal ideal gas constant (a known physical quantity). In the ideal gas equation, the ratio n/V denotes the number of molecules per unit volume. Another way to quantify the amount of material contained within a unit volume is to use the mass density $\rho \equiv M/V$, where M is the total mass contained in the volume. Using density, instead of volume, the ideal gas law may be written

$$P = n\rho R_u T/M \ .$$
(5.2)

One mole of molecules has its own mass, called the molar mass m, that can be computed by knowing the atomic masses of the atoms that make up each molecule and then multiplying by Avagadro's number (i.e., one mole). Using the molar mass, the total mass M equals m times the number of moles so that $M = mn$. Thus, in terms of m, the ideal gas law may be written

$$P = \rho R_u T/m$$
(5.3)

Or simply,

$$P = \rho RT \ , \text{ where } R \equiv R_u/m \ .$$
(5.4)

The quantity R is called the gas constant. Unlike the *universal* gas constant R_u, which is the same for all materials, the presence of m in the definition of R makes it depend on the constitution of the material in question. It can be regarded as a material property.

It is very common to cast inviscid thermoelastic models in terms of the **specific volume**, defined

$$v \equiv \frac{1}{\rho}$$
(5.5)

The specific volume merely equals the volume per unit mass: $v = V/M$. In terms of the specific volume, the ideal gas law may be written compactly as

$$Pv = RT$$
(5.6)

Constitutive models implicitly are meant to apply to a given set of atoms — no material is permitted to enter or leave the representative volume to which the model will be applied. Thus, the mass of the material sample is constant. Thus, because R_u is a constant, R is also a constant. Therefore, the ideal gas law may be written as

$$\frac{Pv}{T} = \text{constant}$$
(5.7)

Quite often, to characterize the gas, a single experiment is performed at which the density ρ_o (or, equivalently, the specific volume v_o) of the gas is measured at some known pressure P_o and temperature T_o and then the ideal gas law may be written

$$\frac{Pv}{T} = \frac{P_o v_o}{T_o} \tag{5.8}$$

In this form, it becomes more clear that the ideal gas law can be regarded as a relationship governing *changes* in quantities because it involves only the ratios

$$\frac{P}{P_o}, \frac{v}{v_o}, \text{ and } \frac{T}{T_o} \tag{5.9}$$

Volumetric strain definitions. The ratio v/v_o appears so often that it has its own name in the advanced materials modeling community — the **volumetric stretch**. A volumetric strain may be defined in terms of the volumetric stretch as

$$\varepsilon_v = \frac{v - v_o}{v_o} = \left(\frac{v}{v_o}\right) - 1 \tag{5.10}$$

Of course, we could alternatively define a strain as

$$\varepsilon_v = \frac{v - v_o}{v} = 1 - \frac{1}{(v/v_o)} \tag{5.11}$$

For both choices, the strain is expressible in terms of the volumetric stretch ratio v/v_o. A more general definition of volumetric strain can be constructed through the use of a "helper" parameter, called the **Seth-Hill** parameter k so that the strain can be written

$$\varepsilon_v = \frac{1}{k}\left[\left(\frac{v}{v_o}\right) - 1\right] \tag{5.12}$$

If one chooses $k=1$, then the definition in Eq. (5.10) is recovered. With the choice $k = -1$, Eq. (5.11) is obtained. A very important choice for the Seth-Hill parameter corresponds to the limit $k \to 0$, which results in the logarithmic strain:

$$\varepsilon_v = \ln\left(\frac{v}{v_o}\right) \tag{5.13}$$

We will find this particular definition of strain quite useful because its material time rate becomes independent of the reference volume v_o:

$$\dot{\varepsilon}_v = \frac{\dot{v}}{v} \tag{5.14}$$

In incremental form

$$d\varepsilon_v = \frac{1}{v}dv \tag{5.15}$$

Consequently, when we later encounter partial derivatives of the form

$$v\frac{\partial(\quad)}{\partial v}, \tag{5.16}$$

we may mentally regard them to be derivatives with respect to *logarithmic* strain:

$$v\frac{\partial(\quad)}{\partial v} = \frac{\partial(\quad)}{\partial \varepsilon_v}, \text{ where } \varepsilon_v \equiv \ln\left(\frac{v}{v_o}\right) \tag{5.17}$$

Regardless of the choice of the Seth-Hill parameter, k, note that

$$\varepsilon_v = 0 \text{ when } v = v_o \tag{5.18}$$

$$\frac{d\varepsilon_v}{dv} = 1 \text{ when } v = v_o \tag{5.19}$$

Consequently, all definitions of the strain and its derivative are approximately equivalent whenever v differs from v_o by only a small amount. The value selected for the Seth-Hill parameter matters only for large excursions of v from v_o.

For gases, the pressure P is always compressive — the gas will always expand freely if the constriants of a container are removed. However, inviscid material models are also sometimes used to model some fluids, which won't necessarily expand to fill their containers even when those containers are subjected to a vacuum. This materials are capable of sustaining tensile pressures. Nonetheless, typical applications involve compression more often than tension. We therefore must caution the reader that, for inviscid fluid equations, the pressure P is typically taken positive in compression and the strain definition is often cited as the *negative* of what we have defined above. That way, the strain will (typically) be negative whenever P is negative.

Invisid thermoelasticity in generality. In a first course on classical thermodynamics, the student is introduced to the physical variables of internal energy u, entropy s, temperature T, specific volume v, and pressure P. In classical elementary thermodynamics, arguments are (often feebly) put forth to convince the student that these quantities are inter-related by the a set of material functions

$$u = u(v, s) \tag{5.20a}$$

$$P = -\left(\frac{\partial u}{\partial v}\right)_s \text{ (by convention, this is positive in compression)} \tag{5.20b}$$

$$T = \left(\frac{\partial u}{\partial s}\right)_v \tag{5.20c}$$

Under classical isotropic thermoelasticity, the stress power is given by

$$\Pi_s = -P\dot{v} \tag{5.21}$$

Importantly, these equations hold only if certain assumptions are valid. Specifically, the deformation must be locally reversible and the material response must be isotropic and inviscid.

In light of Eq. (5.20), we note that

$$\dot{u} = T\dot{s} - P\dot{v} \tag{5.22}$$

Using different independent variables. The following discussion might seem to dwell tediously on minor details. However, we present several "obvious" concepts here so that they may serve as examples when later discussing less obvious analogous concepts for tensor stress and tensor strain.

Note that the internal energy is written $u = u(v, s)$. Without any loss of information, the internal energy can alternatively be expressed in terms of the density

$$u = u(\rho, s) \text{ , where } \rho = \frac{1}{v} \tag{5.23}$$

The following are also legitimate alternatives:

$$u = u(\varepsilon_0, s) \text{ , where } \varepsilon_0 = \ln(v/v_o) \text{ (logarithmic strain)} \tag{5.24}$$

$$u = u(\varepsilon_1, s) \text{ , where } \varepsilon_1 = \frac{v - v_o}{v_o} \text{ (engineering strain)} \tag{5.25}$$

$$u = u(\varepsilon_2, s) \text{ , where } \varepsilon_2 = \frac{1}{2}\left[\left(\frac{v}{v_o}\right)^2 - 1\right] \text{ (Lagrange strain)} \tag{5.26}$$

In general, suppose that v^* denotes some convenient measure of volumetric deformation. It might equal v, $1/\rho$, ε_0, ε_1, or something else. As long as v^* can be expressed as a one-to-one function of v, then the fact that $u = u(v, s)$ means that $u = u(v^*, s)$. Therefore, we can always define a quantity P^* by

$$P^* = -\left(\frac{\partial u}{\partial v^*}\right)_s \tag{5.27}$$

Applying the chain rule to Eq. (5.20b) gives

$$P = -\left(\frac{\partial u}{\partial v}\right)_s = -\left(\frac{\partial u}{\partial v^*}\right)_s\left(\frac{\partial v^*}{\partial v}\right)_s = P^*\left(\frac{\partial v^*}{\partial v}\right)_s \tag{5.27b}$$

Thus

$$P^* = \frac{P}{(\partial v^*/\partial v)_s} \tag{5.28}$$

The generalized pressure P^* is said to be "conjugate" to the generalized deformation measure v^*. The key relationship that must be satisfied when selecting a deformation measure is that its conjugate generalized pressure must satisfy

$$P^*\dot{v}^* = P\dot{v} \tag{5.29}$$

Suppose, for example, that convenience suggests that v^* should be chosen to be logarithmic strain. Then

$$v^* = \ln(v/v_o) \text{ and } P^* = \frac{P}{(\partial v^*/\partial v)_s} = \frac{P}{(1/v)} = Pv = \frac{P}{\rho} \tag{5.30}$$

1

Imagine that researcher "A" is an experimentalist who discovers that a particular material happens to be inviscid with an isentropic pressure-strain relationship that is *linear* when using logarithmic volume strain $\varepsilon_A = \ln(v/v_o)$. In other words, suppose that this researcher observes that $P = -k\varepsilon_A$, where k is a constant for the given (fixed) value of entropy. Suppose that researcher "B" is a computer programmer who knows that logarithmic strain is rather expensive to compute. This programer would much rather use the so-called "Lagrangean" strain, $\varepsilon_B = \frac{1}{2}[(\frac{v}{v_o})^2 - 1]$. Recall that the measured pressure-strain relationship is linear with respect to logarithmic strain. To be consistent, the researcher "B" must use a stress strain relationship that is *nonlinear* with respect to Lagrange strain. The two pressure-strain plots must be related in a consistent manner. Specifically, if researcher "A" found the pressure-strain relationship to be $P = k\varepsilon_A$, where k is a measured constant, then researcher "B" must use a pressure strain function given by $P = \frac{k}{2}\ln(2\varepsilon_B + 1)$. As long as the two researchers use consistent material functions, then they will both obtain the same final result in their analyses regardless of their choice of strain measure.

Incidentally, in the above example, researcher "A" used pressure P, but P is not conjugate to the logarithmic strain. Does this mean that researcher "A" was somehow violating the tenets of thermodynamics? No, of course not. From Eq. (5.30), we recall that the generalized "pressure" that is conjugate to the logarithmic strain is $P^* = Pv$. Recall that Researcher "A" measured $P = k\varepsilon_A$, Also note that, for logarithmic strain, $v = v_o e^{\varepsilon_A}$. Hence, the relationship $P^* = Pv$ can be written as $P^* = (k\varepsilon_A)(v_o e^{\varepsilon_A})$. This is the stress strain relationship between logarithmic strain and its conjugate "pressure". Clearly, no sane person would prefer to use this relationship when the equivalent and far simpler equation $P = k\varepsilon_A$ is available. The point of this paragraph is that stress-strain relations do *not* have to be written in terms of conjugate stress and strain measures — mixed variables are perfectly legitimate.

We have now shown that changes of variables are certainly permissible in thermodynamics. Furthermore, if you introduce a new variable v^* as a measure of the deformation, then there exists a new variable P^* that is "conjugate" to v^* such that

$$P^*\dot{v}^* = P\dot{v} \tag{5.31}$$

Consequently,

$$\text{If} \quad P^* = -\left(\frac{\partial u}{\partial v^*}\right)_s \quad \text{then} \quad P = -\left(\frac{\partial u}{\partial v}\right)_s, \quad \text{and vice versa!} \tag{5.32}$$

The above equation implies that it is possible to express P^* as a proper function of v^* and s. For thermodynamic analyses, we usually only need to invoke the *existence* of such a function.

6. Classical *anisotropic* thermoelasticity

When a material is capable of supporting shear stresses, then the pressure P is no longer sufficient to completely characterize the physical loads on the material. Likewise, the internal energy in a material can be altered under isochoric (volume preserving) motions. Consequently, the energy depends on more than just the entropy and specific volume.

For thermostatics of solids, we presume the existence of some measure of stress $\underset{\approx}{P}$ and some measure of strain $\underset{\approx}{y}$ such that

$$u = u(\underset{\approx}{y}, s) \tag{6.1a}$$

$$\underset{\approx}{P} = +\left(\frac{\partial u}{\partial \underset{\approx}{y}}\right)_s \quad \text{(by convention, this is positive in } \textit{tension}\text{)} \tag{6.1b}$$

$$T = \left(\frac{\partial u}{\partial s}\right)_{\underset{\approx}{y}} \tag{6.1c}$$

Note the distinction between the sign conventions in Eqs. (5.20b) and (6.1b). In solid mechanics, the stress is conventionally taken to be positive in tension.

We permit the choice for $\underset{\approx}{P}$ and $\underset{\approx}{y}$ to be arbitrary except we will assume for convenience that they are "conjugate" to each other in the sense that the stress power must be expressible as

$$\Pi_s = \underset{\approx}{P} : \dot{\underset{\approx}{y}} \tag{6.2}$$

Recall that one expression for the stress power is

$$\Pi_s = \frac{1}{\rho_o} \hat{\underset{\approx}{\sigma}} : \dot{\underset{\approx}{F}}, \tag{6.3}$$

The first Piola Kirchhoff stress $\hat{\underset{\approx}{\sigma}}$ is defined so that $\hat{\underset{\approx}{\sigma}} \bullet \underset{\sim}{N} \, dA_o = \underset{\approx}{\sigma} \bullet \underset{\sim}{n} \, dA$. Specifically,

$$\hat{\underset{\approx}{\sigma}} = \underset{\approx}{\sigma} \bullet \underset{\approx}{F}^c = J\underset{\approx}{\sigma} \bullet \underset{\approx}{F}^{-T} \tag{6.4}$$

Comparing Eqs. (6.2) and (6.3). We note that we could select our conjugate stress and strain measures as:

$$\underset{\approx}{P} = \hat{\underset{\approx}{\sigma}}/\rho_o \quad \text{and} \quad \underset{\approx}{y} = \underset{\approx}{F} \tag{6.5}$$

and therefore

$$\underset{\approx}{P} = \left(\frac{\partial u}{\partial \underset{\approx}{y}}\right)_s \quad \text{becomes} \quad \frac{\underset{\approx}{\sigma}}{\rho_o} = \left(\frac{\partial u}{\partial \underset{\approx}{F}}\right)_s \tag{6.6}$$

Recall that

$$\Pi_s = \frac{1}{\rho_o} \bar{\underset{\approx}{s}} : \dot{\underset{\approx}{\varepsilon}} \tag{6.7}$$

Comparing Eqs. (6.2) and (6.7) we might therefore be inclined to choose

$$\underset{\approx}{P} = \underset{\approx}{\bar{s}}/\rho_o \quad \text{and} \quad \underset{\approx}{v} = \underset{\approx}{\bar{\varepsilon}} \tag{6.8}$$

Of course, since initial density is a constant property of a particle, we could alternatively define

$$\underset{\approx}{P} = \underset{\approx}{\bar{s}} \quad \text{and} \quad \underset{\approx}{v} = \underset{\approx}{\bar{\varepsilon}}/\rho_o \tag{6.9}$$

This choice has the appealing property that the stress $\underset{\approx}{P}$ actually has dimensions equal to stress and the strain has dimensions of specific volume. Hence, Eq. (6.9) might be a more attractive if one wishes to retain a close analog to classical isotropic inviscid thermodynamics. However, there are many instances in thermomechanics where using *specific stress* (i.e., stress divided by density) is preferable.

Aesthetically, we like the choice in Eq. (6.5) because *nothing* represents the deformation of a material element more completely than the deformation gradient $\underset{\approx}{F}$. It may be that the internal energy depends on only *part* of the information encrypted in $\underset{\approx}{F}$. For an inviscid fluid, for example, only the determinant of $\underset{\approx}{F}$ is really needed. We like using $\underset{\approx}{F}$ because any other measure of the deformation is readily expressible as a function of $\underset{\approx}{F}$. If we were to later favore some other deformation measure $\underset{\approx}{v}$, then we can use the chain rule to write

$$\frac{\underset{\approx}{\sigma}}{\rho_o} = \frac{\partial u}{\partial \underset{\approx}{F}} = \frac{\partial u}{\partial \underset{\approx}{v}} : \frac{d\underset{\approx}{v}}{d\underset{\approx}{F}} \tag{6.10}$$

or

$$\boxed{\frac{\underset{\approx}{\sigma}}{\rho_o} = \underset{\approx}{P} : \frac{\partial \underset{\approx}{v}}{\partial \underset{\approx}{F}}} \tag{6.11}$$

The principle of material frame indifference requires that the internal energy u must be independent of the material rotation $\underset{\approx}{R}$. Consequently, we may select our deformation measure to be the reference stretch tensor $\underset{\approx}{U}$,

$$\underset{\approx}{U} = (\underset{\approx}{F}^T \bullet \underset{\approx}{F})^{1/2} \tag{6.12}$$

Alternatively, we may select any deformation measure that is expressible as an invertible function of the reference stretch tensor. As an example, consider using Lagrangean strain $\underset{\approx}{\bar{\varepsilon}}$:

$$\underset{\approx}{v} = \underset{\approx}{\bar{\varepsilon}} = \frac{1}{2}[\underset{\approx}{F}^T \bullet \underset{\approx}{F} - \underset{\approx}{I}] \tag{6.13}$$

Note that

$$\frac{\partial v_{ij}}{\partial F_{kl}} = \frac{1}{2}\frac{\partial}{\partial F_{kl}}(F_{mi}F_{mj}) = \frac{1}{2}(\delta_{il}F_{kj} + F_{ki}\delta_{jl}) \tag{6.14}$$

Thus, for any tensor $\underset{\approx}{A}$, it is straightforward to demonstrate that

$$A : \frac{d\bar{\underset{\approx}{\varepsilon}}}{d\underset{\approx}{F}} = \underset{\approx}{F} \bullet \mathrm{sym}(\underset{\approx}{A}) \tag{6.15}$$

Therefore, if we take $\underset{\approx}{y} = \bar{\underset{\approx}{\varepsilon}}$, Eq. (6.11) becomes

$$\frac{\underset{\approx}{\sigma}}{\rho_o} = \underset{\approx}{F} \bullet \mathrm{sym}(\underset{\approx}{P}) \tag{6.16}$$

Recall that

$$\hat{\underset{\approx}{\sigma}} = \underset{\approx}{F} \bullet \bar{\underset{\approx}{s}} \tag{6.17}$$

Therefore Eq. (6.16) implies that the stress that is conjugate to Lagrange strain must satisfy

$$\mathrm{sym}(\underset{\approx}{P}) = \frac{\bar{\underset{\approx}{s}}}{\rho_o} \tag{6.18}$$

Also recall that we desire to define the conjugate stress so that

$$\underset{\approx}{P} = \left(\frac{\partial u}{\partial \underset{\approx}{y}} \right)_s \tag{6.19}$$

Hence, if $\underset{\approx}{y}$ is symmetric (as it is in this example), then $\underset{\approx}{P}$ must also be symmetric, and Eq. (6.18) becomes

$$\underset{\approx}{P} = \frac{\bar{\underset{\approx}{s}}}{\rho_o} \tag{6.20}$$

In other words, the generalized stress that is conjugate to the Lagrangean strain is the PK2 stress divided by the reference density.

We will later demonstrate that the principle of material frame indifference may be used to show that the dependence on the deformation gradient $u = u(\underset{\approx}{F})$ is not independent. If $u = \widehat{u}(\underset{\approx}{F}, s)$, then frame indifference requires that the function $\widehat{u}$ must have the property that $\widehat{u}(\underset{\approx}{Q} \bullet \underset{\approx}{F}, s) = \widehat{u}(\underset{\approx}{F}, s)$ for all rotations $\underset{\approx}{Q}$. Therefore it can be shown that $\widehat{u}(\underset{\approx}{F}, s) = \widehat{u}(\underset{\approx}{U}, s)$, where $\bar{\underset{\approx}{V}}$ is the right stretch tensor from the polar decomposition theorem. Namely,

$$\bar{\underset{\approx}{V}} = (\underset{\approx}{F}^T \bullet \underset{\approx}{F})^{1/2} \tag{6.21}$$

The square root must be taken to be the *positive definite symmetric* root.

Frame indifference is the key that permits us to regard the internal energy as a function of the right — or *reference* — stretch $\underset{\approx}{U}$. Reference strain tensors are typically defined as an invertible function of $\underset{\approx}{U}$. For example, the reference logarithmic strain tensor is

$$\bar{\underset{\approx}{\varepsilon}}^{(0)} = \ln(\underset{\approx}{U}) \tag{6.22}$$

More generally, the Seth-Hill family of strain measures is defined by

$$\bar{\underset{\approx}{\varepsilon}}^{(\kappa)} = \frac{1}{\kappa}[\bar{\underset{\approx}{V}}^{\kappa} - \underset{\approx}{I}]$$

(6.23)

The strain measure is defined by the choice for the parameter κ. Some common choices are

$\kappa = 1$	Engineering
$\kappa = 2$	Lagrange
$\kappa = -1$	"True" or Cauchy-Green
$\kappa \to 0$	Logarithmic (same as above) (6.24)

Computing $\bar{\underset{\approx}{V}}^{\kappa}$ generally requires an eigenvalue decomposition unless κ is a nonzero even number. We believe that this is the principal reason for the extreme popularity of the Lagrange strain.

The choice of stress-strain measures is inconsequential. They may be selected for convenience because of the following consistency principle

Suppose that researcher "A" uses stress-strain measures, $\{\underset{\approx}{P}^{(A)}, \underset{\approx}{v}^{(A)}\}$, (which we call the A-measures) in an analysis to obtain result-A. Suppose that researcher "B" uses a *different* stress-strain pair $\{\underset{\approx}{P}^{(B)}, \underset{\approx}{v}^{(B)}\}$, (which we call the B-measures) to performs the same analyses of the same problem to obtain result-B. By expressing $\underset{\approx}{P}^{(B)}$ and $\underset{\approx}{v}^{(B)}$ in terms of $\{\underset{\approx}{P}^{(A)}, \underset{\approx}{v}^{(A)}\}$, the final result-B can be expressed in terms A-measures. As all material functions are consistent, then result-B cast in terms of A-measures must agree *exactly* with result-A that was obtained using A-measures at the outset.

Now recall that

$$\Pi_s = \frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{D}$$

(6.25)

One might be *tempted* to heuristically say that $\dot{\underset{\approx}{v}}=\underset{\approx}{D}$, but doing that would be wrong because $\dot{\underset{\approx}{v}}$ is a true rate, but $\underset{\approx}{D}$ is not a true rate for general deformations (see Appendix _ _ for a proof). If one were interested in a specialized *subclass* of deformations for which the principal directions of the stretch tensor never change, then *for this subclass* $\underset{\approx}{D}$ would equal the true rate of logarithmic strain.

A closely related form of the stress power may be written using the *unrotated* Kirchhoff stress (J

Table __ shows some possible choices for $\underset{\approx}{P}$ and $\underset{\approx}{v}$.

It is important that all of the provisos listed above must hold for this statement to be true. The process must be reversible so that the "rate" of local heat input is given by $T\dot{s}$. The material must be inviscid so that the work "rate" is expressible as $P\dot{v}$.

"stress" $\underset{\approx}{P}$ in a material is usually expressed as a function of some measure $\underset{\approx}{v}$ of the material deformation and one other variable having to do with the thermodynamic state.

isotropic block of steel is heated while being held at constant volume, then it will be under a compressive stress despite the fact that the material undergoes no deformation.

Much of the difficulties in anistropic thermodynamics comes from mathematical diffi-culties involved in describing how the components of can change in response to a change in the volume and/or shape of the body. Many of these issues may be discussed in the sim-ple context of elasticity.

Linear thermoelasticity

Consider the energy equation:

$$u = u(\underset{\approx}{\varepsilon}, s) \tag{6.26}$$

Expanding this function in a two term series gives

$$u \approx u_o + \left(\frac{\partial u}{\partial \underset{\approx}{\varepsilon}}\right)^0_s : \Delta\underset{\approx}{\varepsilon} + \left(\frac{\partial u}{\partial s}\right)^0_{\underset{\approx}{\varepsilon}} \Delta s$$

$$+ \frac{1}{2}\Delta\underset{\approx}{\varepsilon} : \left(\frac{\partial^2 u}{\partial \underset{\approx}{\varepsilon}^2}\right)^0_s : \Delta\underset{\approx}{\varepsilon} + \left(\frac{\partial^2 u}{\partial \underset{\approx}{\varepsilon} \partial s}\right)^0 : (\Delta\underset{\approx}{\varepsilon})\Delta s + \frac{1}{2}\left(\frac{\partial^2 u}{\partial s^2}\right)^0_{\underset{\approx}{\varepsilon}} : (\Delta s)^2 + \dots \tag{6.27}$$

where all of the derivatives are evaluated at the reference state. For more compact nota-tion, define

$$\underset{\approx}{P}^0 = \left(\frac{\partial u}{\partial \underset{\approx}{\varepsilon}}\right)^0_s \tag{6.28}$$

$$T^0 = \left(\frac{\partial u}{\partial s}\right)^0_{\underset{\approx}{\varepsilon}} \tag{6.29}$$

$$\left(\frac{\partial^2 u}{\partial \underset{\approx}{\varepsilon}^2}\right)^0_s = \left(\frac{\partial \underset{\approx}{P}}{\partial \underset{\approx}{\varepsilon}}\right)^0_s = \underset{\approx}{E}_s \tag{6.30}$$

$$\left(\frac{\partial^2 u}{\partial \underset{\approx}{\varepsilon} \partial s}\right)^0 = \left(\frac{\partial \underset{\approx}{P}}{\partial s}\right)^0_{\underset{\approx}{\varepsilon}} = \left(\frac{\partial T}{\partial \underset{\approx}{\varepsilon}}\right)^0_s = -\frac{\underset{\approx}{\gamma}}{\rho_o T_o} \tag{6.31}$$

$$\left(\frac{\partial^2 u}{\partial s^2}\right)^0_{\underset{\approx}{\varepsilon}} = \frac{T_o}{c_v} \tag{6.32}$$

Then

$$u \approx u_o + \underset{\approx}{P}_0 : \Delta\underset{\approx}{\varepsilon} + T_0 \Delta s$$

$$+ \frac{1}{2}\Delta\underset{\approx}{\varepsilon} : \underset{\approx}{E}_s^0 : \Delta\underset{\approx}{\varepsilon} - \frac{\underset{\approx}{\gamma} : (\Delta\underset{\approx}{\varepsilon})\Delta s}{\rho_o T_o} + \frac{1}{2}\frac{T_o}{c_v} : (\Delta s)^2 + \dots \tag{6.33}$$

Thus

$$\underset{\approx}{P} = \left(\frac{\partial u}{\partial \underset{\approx}{\varepsilon}}\right)_s = \underset{\approx}{P}_0 + \underset{\approx}{E}_s : \Delta\underset{\approx}{\varepsilon} - \frac{\underset{\approx}{\gamma}\Delta s}{\rho_o T_o} \tag{6.34}$$

and

$$T = \left(\frac{\partial u}{\partial s}\right)_{\underset{\approx}{\gamma}} = T_0 - \frac{\underset{\approx}{\gamma} : (\Delta \underset{\approx}{\gamma})}{\rho_o T_o} + \frac{T_o}{c_v} \Delta s \qquad (6.35)$$

7. Constitutive Models

Constitutive implications of the second law

In this section, an alternative approach is used to deduce at least some conclusions about the relationship of constitutive models to the energy potential functions. This method is especially useful if your physical intuition fails to indicate how many quasi-static work modes apply for the material of interest.

Recall that the state postulate asserts that the minimum number of state variables needed to characterize the thermodynamic state of a material is equal to one plus the number of quasi-static work modes. Rather than trying to count this number, we will simply assume a larger set of independent state variables. The second law then reveals certain relationship between the dependent variables, thereby reducing the number of state functions that must be measured in the lab, as well as prescribing the general form of those constitutive functions.

Sometimes, the second law further shows that certain *dependent* variables are in fact independent of some of the chosen independent variables. After imposing the restrictions of the second law, material symmetry, and the principle of material frame indifference, we will find that the number of truly independent state variables does indeed turn out to equal one plus the number of quasistatic work modes.

Let "IV" and "DV" denote the independent an dependent variable sets respectively. For illustration purposes, let's consider a thermoplastic material whose response depends on the total deformation tensor $\underset{\sim}{F}$, some other tensor-valued internal state variable $\underset{\sim}{\xi}$ (presumably introduced for physically sensible reasons), and perhaps some additional scalar internal state variable ς. For classical plasticity, the tensor state variable $\underset{\sim}{\xi}$ might be identified as the plastic part of the deformation gradient. For porous material models, the parameter ς might be some measure of the *unloaded* porosity. For hardening materials, ς might represent a dislocation density. For damaged materials, ς might represent a damage measure of some sort. Of course, the plastic strain itself may be regarded as an internal state variable.[*] We will additionally consider the possibility that the material response depends on additional independent state variables such as the temperature T and the reference temperature gradient $\tilde{G}$. Of course, for an inhomogenous material, the material response varies with position $\underset{\sim}{X}$, but we will henceforth treat all increments to be variations holding the material particle constant and all rates will be *material* rates, so there is

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[*] For now, we are skirting the issues associated with the fact that plastic and elastic strain are difficult to define in a self-consistent manner for large deformations.

no need to show the position dependence explicitly. As our dependent variables (DV), we will be interested in deducing response functions for the Helmholtz free energy a, the right (first) Piola Kirchhoff stress $\underset{\approx}{t}$, the entropy s, and the reference heat flux vector $\tilde{q}$. Stated more succinctly,

$$\text{IV} = \left\{ \underset{\approx}{F}, \underset{\approx}{\xi}, \varsigma, T, \tilde{G} \right\} \tag{7.1}$$

$$\text{DV} = \{ a, \underset{\approx}{t}, s, \tilde{q} \} \tag{7.2}$$

Trusdell's principle of equipresence states that *unless there are specific arguments to the contrary, all constitutive relations must contain the same independent variables.* Accordingly, we write

$$a = a(\underset{\approx}{F}, \underset{\approx}{\xi}, \varsigma, T, \tilde{G}) \tag{7.3}$$

$$\underset{\approx}{t} = \underset{\approx}{t}(\underset{\approx}{F}, \underset{\approx}{\xi}, \varsigma, T, \tilde{G}) \tag{7.4}$$

$$s = s(\underset{\approx}{F}, \underset{\approx}{\xi}, \varsigma, T, \tilde{G}) \tag{7.5}$$

$$\tilde{q} = \tilde{q}(\underset{\approx}{F}, \underset{\approx}{\xi}, \varsigma, T, \tilde{G}) \tag{7.6}$$

These equations are interpreted as known or determinable constitutive functions. In the absence of such measurements, one might be tempted to postulate such constitutive functions. However, these functions cannot be given entirely by the analyst's whimsical imagination — they must not violate the second law of thermodynamics. We will now show that the second law of thermodynamics leads to two well-known conclusions:

1. Stress, specific entropy, and free energy are all independent of the temperature gradient.

2. The constitutive functions for stress and for entropy are determined wholly by the constitutive function for the free energy, provided that accurate supplemental rules are known for the evolution of the internal state variables.

The local form of the first law of thermodynamics states that the material time rate of the internal energy must equal the distortional stress power plus the heating energy supplied via external sources (radiative or conductive):

$$\dot{u} = \frac{1}{\rho_o} \underset{\approx}{t} : \dot{\underset{\approx}{F}} + P_Q \tag{7.7}$$

In mechanics, it is often convenient to introduce an alternative energy potential, called the Helmholtz free energy, defined

$$a = u + Ts \tag{7.8}$$

where T is temperature and s is entropy. In terms of the Helmholtz free energy, the first law may be written

$$\dot{a} = \frac{1}{\rho_o}\mathbf{t}:\dot{\mathbf{F}} + P_Q - (T\dot{s} + s\dot{T}) \tag{7.9}$$

In terms of our chosen set of independent state variables, the reduced dissipation inequality (RDI, which is a specialized local version of the Clausius-Duhem inequality) may be written

$$\frac{1}{\rho_o}\mathbf{t}:\dot{\mathbf{F}} - s\dot{T} - \dot{a} - \frac{1}{\rho_o T}\tilde{\mathbf{q}} \bullet \tilde{\mathbf{G}} \geq 0 \tag{7.10}$$

where P_Q is the heat input per unit mass resulting from radiation (e.g. a microwave oven) and from conduction.

Importantly, the heating power P_Q does *not* include contributions from dissipative heading of the material resulting from irreversible constitutive material response. Deducing an expression for this type of heating is a key goal of this chapter.

In light of Eq. (7.3), the chain rule gives the material time rate of the Helmholtz free energy as

$$\dot{a} = \frac{\partial a}{\partial \mathbf{F}}:\dot{\mathbf{F}} + \frac{\partial a}{\partial \xi}:\dot{\xi} + \frac{\partial a}{\partial \varsigma}:\dot{\varsigma} + \frac{\partial a}{\partial T}:\dot{T} + \frac{\partial a}{\partial \tilde{\mathbf{G}}}:\dot{\tilde{\mathbf{G}}} \tag{7.11}$$

Thus, the second law becomes

$$\left(\frac{1}{\rho_o}\mathbf{t} - \frac{\partial a}{\partial \mathbf{F}}\right):\dot{\mathbf{F}} - \left(s + \frac{\partial a}{\partial T}\right)\dot{T} - \left(\frac{\partial a}{\partial \xi}:\dot{\xi} + \frac{\partial a}{\partial \varsigma}:\dot{\varsigma} + \frac{\partial a}{\partial \tilde{\mathbf{G}}}:\dot{\tilde{\mathbf{G}}}\right)$$

$$- \frac{1}{\rho_o T}\tilde{\mathbf{q}} \bullet \tilde{\mathbf{G}} \geq 0 \tag{7.12}$$

At this point, it is essential to really think about whether or not our chosen independent variables are truly independent. We wish to invoke the following mathematical theorem

If $Aw + b \geq 0$ for all w, then $A = 0$ and $b \geq 0$. \hfill (7.13)

The key to whether or not this theorem applies to Eq. (7.12) lies in identifying which of the independent variables are truly independent in the sense that we can (in principle) vary their rates arbitrarily. Another more subtle implicit requirement for Eq. (7.12) to be true is that the coefficient A must not depend on w; for (counter) example, if $A = w - 2$ and $b = 3$, then $Aw + b$ would be positive for all choices of w without implying that $A = 0$. Thus, applying Eq. (7.13) to Eq. (7.12) is justified when we make the following assumptions:

1. The energy function $a(\mathbf{F}, \xi, \varsigma, T, \tilde{\mathbf{G}})$ really is a proper function of its arguments, not

   a functional. That way, we can rest assured that the partial derivatives of a are also functions of the same variables. Consequently, *rates* in the independent variables can be selected independently from these derivatives.

2. The rates of (at least some of) the independent variables can be selected independently from the rates of the other independent variables.

To understand the importance of the second condition, let's hypothesize that the rate of the deformation gradient can be controlled independently from the other independent variables. Then it can be selected to be so large that the first term in Eq. (7.12) "swamps" out the other terms in magnitude. Furthermore, by selecting the direction of $\dot{\underset{\approx}{F}}$, the first term can be made either positive or negative unless the coefficient of $\dot{\underset{\approx}{F}}$ is non-zero. Consequently, the only way the inequality can be satisfied for all choices of $\dot{\underset{\approx}{F}}$ is if the coefficient of $\dot{\underset{\approx}{F}}$ is zero. Similarly assuming that the temperature rate can be controlled independently (via appropriate heating processes) from the other independent variables, we may also conclude that the coefficient of $\dot{T}$ in Eq. (7.12) must also be zero. These two assumptions give us the classical relationships:

$$\underset{\approx}{t} = \rho_o \frac{\partial a}{\partial \underset{\approx}{F}} \tag{7.14}$$

and

$$s = -\frac{\partial a}{\partial T} \tag{7.15}$$

The act of writing Eqs. (7.14) and (7.15) is where we have invoked Trusdell's principle of equipresence. Specifically, we would not be able to write these results if Eqs. (7.4) through (7.6) were not true.

Following similar logic that lead to the above two equations, assuming that the temperature gradient can be controlled independently, we have

$$\frac{\partial a}{\partial \tilde{G}} = \underset{\sim}{0} \tag{7.16}$$

At this point, we will *not* go on to assume that $\dot{\underset{\approx}{\xi}}$ and ς can be varied independently. Nor will we presume that the directions of either $\dot{\underset{\approx}{\xi}}$ or ς can be selected independently of the values of $\underset{\approx}{\xi}$ or ς. To give some concrete insight into why we make these statements, consider classical small strain plasticity in which $\underset{\approx}{\xi}$ is the plastic part of the strain and ς is the dislocation density (or some other variable such as the hardening modulus which depends in some predictable way on the dislocation density). For classical plasticity, the rate of the plastic strain is taken normal to the yield surface, so the direction of this rate cannot be controlled independently. Likewise, the dislocation density cannot physically be decreased without having to alter the other state variables.

In light of the above discussion, the second law reduces to

$$D + \left[-\frac{1}{\rho_o T} \tilde{\underset{\sim}{q}} \bullet \tilde{\underset{\sim}{G}} \right] \geq 0 \ , \tag{7.17}$$

where

$$D \equiv -\left(\frac{\partial a}{\partial \underset{\approx}{\xi}} : \dot{\underset{\approx}{\xi}} + \frac{\partial a}{\partial \varsigma} : \dot{\varsigma} \right) \tag{7.18}$$

This is a very typical form for the dissipation cited in plasticity papers. Here is where it becomes clear that it is essential that you correctly identify *all* internal state variables that might have an effect on the energy — otherwise you will not be able to correctly predict the dissipation. For example, early versions of non-porous plasticity theory assumed that the free energy depended only on the elastic strain, $\varepsilon^e = \varepsilon - \varepsilon^p$, and the temperature T:

$$a = a(\varepsilon^e, T) \quad \text{for older solid plasticity models} \tag{7.19}$$

This is a special case of the general model discussed above with

$$\xi = \varepsilon^p \text{ and } \varsigma = 0 \tag{7.20}$$

Then

$$\frac{\partial a}{\partial \xi} = \left(\frac{\partial a}{\partial \varepsilon^p}\right)_{\varepsilon, T, \varsigma} = \left(\frac{\partial a}{\partial \varepsilon^e}\right)_T : \left(\frac{\partial \varepsilon^e}{\partial \varepsilon^p}\right)_{\varepsilon, T, \varsigma} = -\left(\frac{\partial a}{\partial \varepsilon^e}\right)_T = -\frac{\sigma}{\rho} \tag{7.21}$$

Consequently, the dissipation in the early versions of plastitity theory was predicted to be

$$D \equiv -\left(\frac{\partial a}{\partial \xi} : \dot{\xi} + \frac{\partial a}{\partial \varsigma} : \dot{\varsigma}\right) = \frac{1}{\rho}\sigma : \varepsilon^p \tag{7.22}$$

Experimentally, it was observed that the amount of heating caused by plastic flow was not as high as predicted by the above equation. The deficiency in the theory was not well understood, so for many years, the problem was handled in an ad hoc way allocating a fraction χD of the dissipation toward heating, the rest being presumably stored in microscale elastic domains. To match experimental observations, the reduction factor χ was typically set equal to about 0.9 at the onset of plastic flow, and was increased to 1.0 as plastic flow continued. This was obviously an unsatisfactory approach. Today, a better approach is to postulate that the free energy must depend on more than just the elastic strain and the temperature. If, for example, we presume that the free energy depends addtionally on the dislocation density Γ, then the dissipation equation becomes

$$D = \frac{1}{\rho}\sigma : \varepsilon^p - \frac{\partial a}{\partial \Gamma} : \dot{\Gamma} \tag{7.23}$$

Qualitatively, this expression has the potential to explain observed dissipation evolution. At the onset of plasticity, there are large numbers of dislocations being generated, so the second term in the above equation tends to reduce the nominal plastic dissipation. As plastic flow continues, the dislocation generation rate saturates to zero, so that the dissipation approaches 100% of the nominal dissipation.

For quasistatic motions, it is usually assumed that the two terms in Eq. (7.17) can be controlled independently, so that each of those terms are *independently* both positive. Thus, it is typically required that

$$D \geq 0 \tag{7.24}$$

$$\left[-\frac{1}{\rho_o T}\tilde{q} \bullet \tilde{G}\right] \geq 0 \tag{7.25}$$

The first of these equations states that the dissipation associated with material distortion must be positive, regardless of the presence of a local temperature gradient. The second of these equations states that heat must flow from hotter regions into colder regions.[*]

Specialization to porous plasticity

Instead of using the total deformation gradient $\underset{\approx}{F}$, alternative deformation measures are frequently used in plasticity theory. The most common choice is a strain measure $\underset{\approx}{\varepsilon}$. Whatever strain measure is selected, a conjugate stress measure is presumed to exist such that

$$\frac{1}{\rho_o}\underset{\approx}{t}:\dot{\underset{\approx}{F}} = \frac{1}{\rho^{\text{ref}}}\underset{\approx}{\sigma}:\dot{\underset{\approx}{\varepsilon}} \tag{7.26}$$

There are many important issues to be covered in this section that would only be made more difficult to understand if we were to give a fully generalized exposition that permits arbitrarily large deformations. Thus, to avoid the complications of having to carefully define the strain measure, the ensuing discussion will be limited to small deformations so that the distinctions between stress measures can be (for now) ignored. Specifically, for small deformations (and small rotations), the stress measure $\underset{\approx}{\sigma}$ may be regarded as the Cauchy stress, the strain rate $\dot{\underset{\approx}{\varepsilon}}$ may be approximated by the symmetric part of the velocity gradient[†]. Furthermore, for small deformations, the reference density may be regarded as approximately equal to the initial or current density (because, for small deformations, these densities are themselves approximately equal):

$$\rho^{\text{ref}} \approx \rho_o \approx \rho \tag{7.27}$$

For porous plasticity, the tensor internal state variable $\underset{\approx}{\xi}$ is typically identified to be equal to the plastic strain $\underset{\approx}{\varepsilon^p}$ and the scalar internal state variable ζ is identified to be the porosity ϕ (or some invertible function of the porosity). Note: it's truly a blessing that we are presently limiting our discussion to small deformations because the very definition of the plastic strain tensor becomes extremely complicated (and still controversial) when there exist large material distortions and/or large rotations. For small deformations, the *elastic* strain tensor $\underset{\approx}{\varepsilon^e}$ is defined to equal the negative of the strain that would be recovered by the material if the applied stress were to be removed. Then the plastic strain tensor is simply whatever part of the total strain is left over:

$$\underset{\approx}{\varepsilon^p} = \underset{\approx}{\varepsilon} - \underset{\approx}{\varepsilon^e} \tag{7.28}$$

With our specialized change of independent variables, Eqs. (7.3) through (7.6) become

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[*] This statement might seem very intuitive and might seem desirable to apply even in dynamic situations. However, certain dynamic shock experiments have shown instances of heat flowing from cold to warm regions in highly non-equilibrium situations [Drumheller].

[†] The symmetric part of the velocity gradient is not a "true rate" of any path independent quantity *unless* small deformations is assumed. Generalizations to large deformations will be discussed later after the introductory thermodynamical concepts are first clarified in this chapter.

$$a = a(\underset{\approx}{\varepsilon}, \underset{\approx}{\varepsilon}^p, \phi, T, \tilde{\boldsymbol{G}}) \tag{7.29}$$

$$\underset{\approx}{t} = \underset{\approx}{t}(\underset{\approx}{\varepsilon}, \underset{\approx}{\varepsilon}^p, \phi, T, \tilde{\boldsymbol{G}}) \tag{7.30}$$

$$s = s(\underset{\approx}{\varepsilon}, \underset{\approx}{\varepsilon}^p, \phi, T, \tilde{\boldsymbol{G}}) \tag{7.31}$$

$$\tilde{\boldsymbol{q}} = \tilde{\boldsymbol{q}}(\underset{\approx}{\varepsilon}, \underset{\approx}{\varepsilon}^p, \phi, T, \tilde{\boldsymbol{G}}) \tag{7.32}$$

and Eqs. (7.14) through (7.18) become

$$\underset{\approx}{\sigma} = \rho \frac{\partial a}{\partial \underset{\approx}{\varepsilon}} \tag{7.33}$$

$$s = -\frac{\partial a}{\partial T} \tag{7.34}$$

$$\frac{\partial a}{\partial \tilde{\boldsymbol{G}}} = \underset{\sim}{0} \tag{7.35}$$

$$D - \frac{1}{\rho_o T} \tilde{\boldsymbol{q}} \bullet \tilde{\boldsymbol{G}} \geq 0 \ , \tag{7.36}$$

$$D \equiv -\left(\frac{\partial a}{\partial \underset{\approx}{\varepsilon}^p} : \dot{\underset{\approx}{\varepsilon}}^p + \frac{\partial a}{\partial \phi} : \dot{\phi} \right) \tag{7.37}$$

Finally, Eqs. (7.24) remains unchanged:

$$D \geq 0 \tag{7.38}$$

In this context, it is convenient to introduce an alternative interpretation of the dissipation. A thermally isolated plastically deforming material increases its temperature even in the absence of externally supplied heating. This heating is caused by the dissipation. However, at least *part* of the mechanical energy can be regarded as *reversible*. If a deformation is reversible, then the only allowable source of entropy production is from external heating sources:

$$\text{If reversible, then } \ T\dot{s} = P_Q \ \text{ and } \ \dot{u} = \frac{1}{\rho}\underset{\approx}{\sigma}:\dot{\underset{\approx}{\varepsilon}} + T\dot{s} \tag{7.39}$$

When a deformation is irreversible, there are additional sources of entropy production. These additional sources are called the dissipation D^* and defined such that

$$\text{If } not \text{ reversible, then } \ T\dot{s} = P_Q + D \ \text{ and } \ \dot{u} = \frac{1}{\rho}\underset{\approx}{\sigma}:\dot{\underset{\approx}{\varepsilon}} + T\dot{s} + D^* \tag{7.40}$$

Under our current choice of independent variables, the first law of thermodynamics, Eq. (7.9), is written

$$\dot{a} = \frac{1}{\rho}\underset{\approx}{\sigma}:\dot{\underset{\approx}{\varepsilon}} + P_Q - (T\dot{s} + s\dot{T}) \tag{7.41}$$

Taking Eq. (7.40) to serve as an alternative definition of dissipation, this version of the first law may be written alternatively as

$$\dot{a} = \frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{\dot{\varepsilon}} - D - s\dot{T} \tag{7.42}$$

Given that the *total* mechanical power,

$$\frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{\dot{\varepsilon}},$$

is converted into a mixture of an elastically recoverable part (associated with stretching of the elastic lattice) and a non-recoverable part that manifests itself as dissipative heating, it had been conventional in the older literature to introduce either a so-called thermodynamic stress tensor $\underset{\approx}{\Sigma}$ defined such that

$$\frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{\dot{\varepsilon}} - D = \frac{1}{\rho}\underset{\approx}{\Sigma}:\underset{\approx}{\dot{\varepsilon}} \tag{7.43}$$

or a "reversible strain" tensor $\underset{\approx}{E}^{\text{rev}}$ defined such that

$$\frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{\dot{\varepsilon}} - D = \frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{\dot{E}}^{\text{rev}} \tag{7.44}$$

By defining the meaning of the "thermodynamic stress" and the "recoverable strain" we are *not* advocating their use — to the contrary, we will show below that they are probably not helpful concepts for general deformations. For isotropic inviscid fluids, the "thermodynamic pressure" is commonly used. However, whether or not conceptual "thermodynamic stress" or "recoverable strain" tensors exist for general deformations is dubious.

For the purpose of understanding older inviscid thermodynamics literature (and for assessing whether it can be generalized to present-day general shearing deformations), let's assume that either the "thermodynamic stress" or the "reversible strain" tensors really do exist. Then the first law in Eq. (7.40) takes on a form that looks more like the reversible case version of Eq. (7.39). Namely, in terms of these hypothesized stress or strain measures, the first law take the form

$$\dot{u} = \frac{1}{\rho}\underset{\approx}{\Sigma}:\underset{\approx}{\dot{\varepsilon}} + T\dot{s} \tag{7.45}$$

or

$$\dot{u} = \frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{\dot{E}}^{\text{rev}} + T\dot{s} \tag{7.46}$$

In terms of the Helmholtz free energy, these equations become

$$\dot{a} = \frac{1}{\rho}\underset{\approx}{\Sigma}:\underset{\approx}{\dot{\varepsilon}} - s\dot{T} \tag{7.47}$$

or

$$\dot{a} = \frac{1}{\rho}\underset{\approx}{\sigma}:\underset{\approx}{\dot{E}}^{\text{rev}} - s\dot{T} \tag{7.48}$$

Recalling Eq. (7.29), the time rate of the Helmholtz free energy may be written via the chain rule as

$$\dot{a} = \frac{\partial a}{\partial \underset{\approx}{\varepsilon}} : \dot{\underset{\approx}{\varepsilon}} + \frac{\partial a}{\partial \underset{\approx}{\varepsilon}^p} : \dot{\underset{\approx}{\varepsilon}}^p + \frac{\partial a}{\partial \phi} \dot{\phi} + \frac{\partial}{\partial T} \dot{T} + \frac{\partial a}{\partial \tilde{G}} \cdot \dot{\tilde{G}}$$
(7.49)

Recalling Eqs. (7.33) through (7.35), this becomes

$$\dot{a} = \frac{1}{\rho} \underset{\approx}{\sigma} : \dot{\underset{\approx}{\varepsilon}} + \frac{\partial a}{\partial \underset{\approx}{\varepsilon}^p} : \dot{\underset{\approx}{\varepsilon}}^p + \frac{\partial a}{\partial \phi} \dot{\phi} - s\dot{T}$$
(7.50)

Substituting this equation into Eqs. (7.47) and (7.48) gives

$$\frac{1}{\rho} (\underset{\approx}{\sigma} - \underset{\approx}{\Sigma}) : \dot{\underset{\approx}{\varepsilon}} + \frac{\partial a}{\partial \underset{\approx}{\varepsilon}^p} : \dot{\underset{\approx}{\varepsilon}}^p + \frac{\partial a}{\partial \phi} \dot{\phi} = 0$$
(7.51)

$$\frac{1}{\rho} \underset{\approx}{\sigma} : (\dot{\underset{\approx}{\varepsilon}} - \dot{\underset{\approx}{E}}^{\text{rev}}) + \frac{\partial a}{\partial \underset{\approx}{\varepsilon}^p} : \dot{\underset{\approx}{\varepsilon}}^p + \frac{\partial a}{\partial \phi} \dot{\phi} = 0$$
(7.52)

Note that neither the "thermodynamic stress" nor the "recoverable strain" concepts add any insight or otherwise beneficial simplification to the first law. For classical non-porous plasticity, an additional postulate is typically introduced that the energy depends on the strain $\underset{\approx}{\varepsilon}$ and the plastic strain $\underset{\approx}{\varepsilon}^p$ only through their *difference*, which is the elastic strain

$$\underset{\approx}{\varepsilon}^e = \underset{\approx}{\varepsilon} - \underset{\approx}{\varepsilon}^p$$
(7.53)

If this assumption is made, then we get

$$\frac{\underset{\approx}{\sigma}}{\rho} = \left(\frac{\partial a}{\partial \underset{\approx}{\varepsilon}} \right)_{\varepsilon^p, T, \phi} = \left(\frac{\partial a}{\partial \underset{\approx}{\varepsilon}^e} \right)_{T, \phi}$$
(7.54)

$$\frac{\partial a}{\partial \underset{\approx}{\varepsilon}^p} = -\frac{\partial a}{\partial \underset{\approx}{\varepsilon}^e} = -\frac{\underset{\approx}{\sigma}}{\rho}$$
(7.55)

and Eqs. (7.51) and (7.55) then become

$$\frac{1}{\rho} \underset{\approx}{\sigma} : \dot{\underset{\approx}{\varepsilon}}^e - \frac{1}{\rho} \underset{\approx}{\Sigma} : (\dot{\underset{\approx}{\varepsilon}}^e + \dot{\underset{\approx}{\varepsilon}}^p) + \frac{\partial a}{\partial \phi} \dot{\phi} = 0$$
(7.56)

$$\frac{1}{\rho} \underset{\approx}{\sigma} : (\dot{\underset{\approx}{\varepsilon}}^e - \dot{\underset{\approx}{E}}^{\text{rev}}) + \frac{\partial a}{\partial \phi} \dot{\phi} = 0$$
(7.57)

In the absence of porosity ($\phi = 0$), the last of these equations would become

$$\frac{1}{\rho} \underset{\approx}{\sigma} : (\dot{\underset{\approx}{\varepsilon}}^e - \dot{\underset{\approx}{E}}^{\text{rev}}) = 0$$
(7.58)

in which case, it would make sense to identify the so-called recoverable part of the strain by

$$\underset{\approx}{E}^{\text{rev}} = \underset{\approx}{\varepsilon}^e \quad \text{for non-porous}$$
(7.59)

However, for porous materials the concepts of "thermodynamic stress" and "reversible strain" don't seem to have much usefulness because there is no clear way to define them. Of course, the concept of an elastic part of the strain remains potentially useful, but it's important to realize that it no longer is the sole player in expressions for the recoverable part of the mechanical work.

Although the discussion of this section applied to the special case that the scalar internal state variable ς was identified as the porosity, similar conclusions could be made for functionally similar situations such as when the scalar ς is identified as a damage parameter or as a dislocation density.

Rate forms of constitutive laws

Realizing that there does not appear to be any well defined "recoverable strain" or "thermodynamic stress", we will revert to the equations listed at the beginning of the last section. Without any loss in generality, however, we can always introduce a change of variables so that

$$a = a(\underset{\approx}{\varepsilon}, \underset{\approx}{\varepsilon}^p, \phi, T) = a^*(\underset{\approx}{\varepsilon}^e, \underset{\approx}{\varepsilon}^p, \phi, T) \text{ , where } \underset{\approx}{\varepsilon}^e = \underset{\approx}{\varepsilon} - \underset{\approx}{\varepsilon}^p \tag{7.60}$$

Then Eqs. (7.33) and (7.34) become

$$\underset{\approx}{\tau} = \frac{\partial a^*}{\partial \underset{\approx}{\varepsilon}^e} \text{, where } \underset{\approx}{\tau} = \frac{\underset{\approx}{\sigma}}{\rho} \tag{7.61}$$

$$s = -\frac{\partial a^*}{\partial T} \tag{7.62}$$

The rate form of the stress equation is

$$\dot{\underset{\approx}{\tau}} = \frac{\partial a^*}{\partial \underset{\approx}{\varepsilon}^e \partial \underset{\approx}{\varepsilon}^e} : \dot{\underset{\approx}{\varepsilon}}^e + \frac{\partial a^*}{\partial \underset{\approx}{\varepsilon}^e \partial \underset{\approx}{\varepsilon}^p} : \dot{\underset{\approx}{\varepsilon}}^p + \frac{\partial a^*}{\partial \underset{\approx}{\varepsilon}^e \partial \phi} \dot{\phi} + \frac{\partial a^*}{\partial \underset{\approx}{\varepsilon}^e \partial T} \dot{T} \tag{7.63}$$

For large deformations, this result is typically expressed in terms of reference tensors in order to satisfy the principle of material frame indifference. In these general expressions, the density is a time independent reference density, so in the above time derivative, we have taken ρ to be constant. In general, the stress that appears in thermodynamic relations is typically a stress divided by density.

It is conventional to introduce the following notation for some of the coefficients appearing in this expression

$$\underset{\approx}{E} \equiv \rho \frac{\partial a^*}{\partial \underset{\approx}{\varepsilon}^e \partial \underset{\approx}{\varepsilon}^e} = \frac{\partial \underset{\approx}{\tau}}{\partial \underset{\approx}{\varepsilon}^e} \tag{7.64}$$

$$\underset{\approx}{B} = -\frac{\partial a^*}{\partial \underset{\approx}{\varepsilon}^e \partial T} = -\frac{\partial \underset{\approx}{\tau}}{\partial T} \tag{7.65}$$

Then the stress rate becomes

$$\dot{\underset{\sim}{\tau}} = \underset{\approx}{E} : \dot{\underset{\sim}{\varepsilon}}^e + \frac{\partial a^*}{\partial \underset{\sim}{\varepsilon}^e \partial \underset{\sim}{\varepsilon}^p} : \dot{\underset{\sim}{\varepsilon}}^p + \frac{\partial a^*}{\partial \underset{\sim}{\varepsilon}^e \partial \phi} \dot{\phi} - \underset{\sim}{B} \dot{T} \tag{7.66}$$

The forth order tensor $\underset{\approx}{E}$ is the elastic tangent stiffness and $\underset{\sim}{B}$ is the thermal stress tensor. For an isotropic material, both of these tensors are isotropic and the stress rate becomes

$$\dot{\underset{\sim}{\tau}} = 2G(\dot{\underset{\sim}{\varepsilon}}^e)^{\mathrm{dev}} + K\mathrm{tr}(\dot{\underset{\sim}{\varepsilon}}^e) + \frac{\partial a^*}{\partial \underset{\sim}{\varepsilon}^e \partial \underset{\sim}{\varepsilon}^p} : \dot{\underset{\sim}{\varepsilon}}^p + \frac{\partial a^*}{\partial \underset{\sim}{\varepsilon}^e \partial \phi} \dot{\phi} - B\underset{\sim}{I}\dot{T} \tag{7.67}$$

where G is the shear modulus and K is the bulk modulus.

As a very special case, consider a material whose stress function $\underset{\sim}{\tau}(\underset{\sim}{\varepsilon}^e, \underset{\sim}{\varepsilon}^p, \phi, T)$ is *linear* with respect to elastic strain. In other words, consider the case that the tangent stiffness is identical to the secant stiffness. In this case, the stress is expressible as

$$\underset{\sim}{\tau} = \underset{\approx}{E} : \underset{\sim}{\varepsilon}^e \tag{7.68}$$

This would imply that all dependence of the stress on the plastic strain, porosity, and temperature can be incorporated though a dependence of the elastic stiffness on these quantities. That is, for a linearly elastic material,

$$\underset{\sim}{\tau}(\underset{\sim}{\varepsilon}^e, \underset{\sim}{\varepsilon}^p, \phi, T) = \underset{\approx}{E}(\underset{\sim}{\varepsilon}^p, \phi, T) : \underset{\sim}{\varepsilon}^e \tag{7.69}$$

For this special case, the rate of stress given by

$$\dot{\underset{\sim}{\tau}} = \underset{\approx}{E} : \dot{\underset{\sim}{\varepsilon}}^e + \underset{\sim}{\varepsilon}^e : \frac{\partial \underset{\approx}{E}}{\partial \underset{\sim}{\varepsilon}^p} : \dot{\underset{\sim}{\varepsilon}}^p + \underset{\sim}{\varepsilon}^e : \frac{\partial \underset{\approx}{E}}{\partial \phi} \dot{\phi} + \underset{\sim}{\varepsilon}^e : \frac{\partial \underset{\approx}{E}}{\partial T} \dot{T} \tag{7.70}$$

Comparing this specialized result with the more general result of Eq. (7.66) gives us a more intuitive feeling for the second derivatives of the energy. Namely, for a linearly elastic material,

$$\frac{\partial a^*}{\partial \underset{\sim}{\varepsilon}^e \partial \phi} = \underset{\sim}{\varepsilon}^e : \frac{\partial \underset{\approx}{E}}{\partial \phi} \tag{7.71}$$

Thus, this mixed partial derivative is a measure of how the elastic stiffness varies with porosity.

Non-independent variables

In most plasticity models, the energy function $a^*(\underset{\sim}{\varepsilon}^e, \underset{\sim}{\varepsilon}^p, \phi, T)$ does not depend explicitly on plastic strain. Specifically, plastic strain affects the energy function only indirectly by affecting the interal state variables. Thus, a typical assumption is

$$a^*(\underset{\sim}{\varepsilon}^e, \underset{\sim}{\varepsilon}^p, \phi, T) = \hat{a}(\underset{\sim}{\varepsilon}^e, \phi(\underset{\sim}{\varepsilon}^p), T) \tag{7.72}$$

Thus, the typical evolution equation for the internal state variable is of the form:

$$\dot{\phi} = \underset{\approx}{A} : \dot{\underset{\approx}{\varepsilon}}^p \qquad (7.73)$$

for some tensor $\underset{\approx}{A}$.

In this case, the dissipation can be written

$$D \equiv \frac{1}{\rho} \underset{\approx}{\sigma} : \dot{\underset{\approx}{\varepsilon}}^p - \frac{\partial a}{\partial \phi} (\underset{\approx}{A} : \dot{\underset{\approx}{\varepsilon}}^p) \qquad (7.74)$$

$$\qquad (7.75)$$

APPENDIX A.
Specialized forms of the first law

First Law for simple inviscid fluid dynamics. We have presented the first law of thermodynamics using abstract symbols for the various kinds of powers. Now we want to unwrap the definitions and present the first law in a form that should be familiar to those readers who have worked in the past with fluid thermodynamics. For fluid dynamics problems, we make the following assumptions

- The material cannot support any shear stresses. Hence $\underset{\approx}{\sigma} = -p\underset{\approx}{I}$, where p is the pressure (which is positive in compression)
- All body forces are conservative, and the potential energy does not contain any contributions from other conservative forces (such contributions can always be incorporated as part of the regular mechanical power). Hence, we may write the body force power as $P_b = -\dot{E}_p$
- The fluid is *simple*, by which we mean that its internal energy is presumed to be expressible as a function of the entropy (to be defined later) and the specific volume v. This assumption permits us to assert the existence of enthalpy in its classical sense.

We will write Eq. (4.59) as

$$P_x + P_T = \dot{U} + \dot{E}_k - P_b - P_F \tag{7.76}$$

Applying the assumption that the body forces are all conservative, this becomes

$$P_x + P_T = \dot{U} + \dot{E}_k + \dot{E}_p - P_F \tag{7.77}$$

Now we will recall the explicit integral expression for each term:

$$\dot{U} + \dot{E}_k + \dot{E}_p = \frac{D}{Dt} \int_\Omega (u + e_k + e_p)\rho\, dV \tag{7.78}$$

Fluid materials typically deform considerably, so it is not practical to use a Lagrangean control volume. Instead, it is more natural to use an *Eulerian* control volume. Recalling Eq. (???), the right-hand side of Eq. (7.78) may be expressed in terms of an Eulerian ($\underset{\sim}{v}_E \bullet \underset{\sim}{n} = 0$) control volume as

$$\frac{D}{Dt} \int_\Omega (u + e_k + e_p)\rho\, dV = \frac{d}{dt} \int_{\Omega_E} (u + e_k + e_p)\, dV + \int_{\partial\Omega} (u + e_k + e_p)\rho\underset{\sim}{v} \bullet \underset{\sim}{n}\, dS \tag{7.79}$$

Recall from Eq. (4.40) that the flow power is defined

$$P_F = \text{``flow'' power from traction forces} = \int_{\partial\Omega} (\underset{\sim}{n} \bullet \underset{\approx}{\sigma}) \bullet \underset{\sim}{v}\, dA \tag{7.80}$$

For an inviscid fluid, the stress is isotropic, so this becomes

$$P_F = -\int_{\partial\Omega} p\underset{\sim}{n} \bullet \underset{\sim}{v}\, dA \tag{7.81}$$

Therefore the first law becomes

$$P_x + P_T$$
$$= \frac{d}{dt}\int_{\Omega_E}(u+e_k+e_p)dV + \int_{\partial\Omega}[(u+e_k+e_p)\rho+p]\underset{\sim}{n}\bullet\underset{\sim}{v}dS \qquad (7.82)$$

Let's concentrate on the quantity in the brackets. Factoring out the density gives

$$[(u+e_k+e_p)\rho+p] = \left[(u+e_k+e_p)+\frac{p}{\rho}\right]\rho \qquad (7.83)$$

We now observe that mass density (mass/volume) is the reciprocal of specific volume (volume per mass):

$$\rho = \frac{1}{v} \qquad (7.84)$$

Therefore

$$[(u+e_k+e_p)\rho+p] = [(u+e_k+e_p)+pv]\rho \qquad (7.85)$$

For simple inviscid fluids, the enthalpy h is defined

$$h = u+pv \qquad (7.86)$$

Therefore

$$[(u+e_k+e_p)\rho+p] = (h+e_k+e_p)\rho \qquad (7.87)$$

and the *specialized* first law of Eq. (7.82) becomes

$$P_x + P_T$$
$$= \frac{d}{dt}\int_{\Omega_E}(u+e_k+e_p)dV + \int_{\partial\Omega}(h+e_k+e_p)\rho\underset{\sim}{n}\bullet\underset{\sim}{v}dS \qquad (7.88)$$

This form of the first law holds if the potential energy e_k is solely that from a conservative *body* force such as gravity. Furthermore, there must be no non-conservative body forces. Finally, the material must be in a hydrostatic state so that the stress tensor will be isotropic.

   Keep in mind that P_x is the work associated with "extra" forces not accounted for in the stress field and the body force field. These extra forces are typically point loads and tractions applied across mathematically singular surfaces. If your control surface does not contain any "extra" forces, then the power from the extra forces is zero. When interested in usable work output from the system, only P_x is generally available. The flow work (hidden in the enthalpy) and the body force work are not directly controllable and are not harness-able directly.

APPENDIX B.
Jump forms of the physical laws

The most general way to express a field law is to write it in integral form, as we have done in Eq. (4.74). The integral form is usually valid even when the fields inside the integrals are discontinuous. When the fields are "smooth" (i.e., continuously differentiable), useful theorems such as the Leibniz formula and the divergence theorem apply. These theorems do not apply when the integrands are discontinuous. In this section, we will presume that the control volume Ω contains no singular sources (i.e., $\underset{\sim}{\Pi} = \underset{\sim}{0}$) but it contains exactly one "shock" surface Σ across which the field variables are discontinuous but away from which the fields are differentiable. The basic idea will be to split the integrals into the two parts that lie ahead of and behind the shock front. In this manner, the Leibniz and divergence theorems may be applied in each of the regions separately.

Jump form of the mass Leibniz formula. In this subsection, we work on the first term in Eq. (4.74). Since the integrand is discontinuous, we must derive a generalization of Eq. (4.28). First recall the generalized Leibniz formula of Eq. ( )

$$\frac{d}{dt}\int_{\Omega_G} \underline{\Upsilon}(\pmb{x}, t)dV = \int_{\Omega}\left[\frac{\partial \underline{\Upsilon}(\pmb{x}, t)}{\partial t} + (\underline{\Upsilon}\pmb{v}_G)\bullet\underset{\sim}{\nabla}\right]dV + \int_{\Omega\cap\Sigma} [[\underline{\Upsilon}(\pmb{v}_\Sigma - \pmb{v}_G)]]\bullet\pmb{n}_\Sigma dS \tag{7.89}$$

Referring to Eq. (4.74), we take the integrand to be $\underline{\Upsilon} = \underline{\xi}\rho$. Again referring to Eq. (4.74), the control volume is taken to be Lagrangean so that d/dt becomes D/Dt and $\pmb{v}_G$ becomes the material velocity $\pmb{v}$. Thus, for analyzing the left hand side of Eq. (4.74), we apply Eq. (7.89) as

$$\frac{D}{Dt}\int_{\Omega_G} \underline{\xi}\rho dV = \int_{\Omega}[(\underline{\xi}\rho)_{,t} + (\underline{\xi}\rho\pmb{v})\bullet\underset{\sim}{\nabla}]dV + \int_{\Omega\cap\Sigma} [[\underline{\xi}\rho c]]dS \quad, \tag{7.90}$$

where

$$c \equiv (\pmb{v}_\Sigma - \pmb{v})\bullet\pmb{n}_\Sigma \tag{7.91}$$

Applying the product rule for differentiation,

$$(\underline{\xi}\rho)_{,t} = \rho(\underline{\xi}_{,t}) + \underline{\xi}(\rho_{,t}) \tag{7.92}$$

and

$$(\underline{\xi}\rho\pmb{v})\bullet\underset{\sim}{\nabla} = \rho(\underline{\xi}\nabla)\bullet\pmb{v} + \underline{\xi}(\rho\underset{\sim}{\nabla}\bullet\pmb{v}) + \underline{\xi}\rho(\pmb{v}\bullet\underset{\sim}{\nabla}) \tag{7.93}$$

Thus,

$$(\underline{\xi}\rho)_{,t} + (\underline{\xi}\rho\pmb{v})\bullet\underset{\sim}{\nabla} = \rho[\underline{\xi}_{,t} + (\underline{\xi}\nabla)\bullet\pmb{v}] + \underline{\xi}[\rho_{,t} + (\rho\underset{\sim}{\nabla}\bullet\pmb{v})] + \underline{\xi}\rho(\pmb{v}\bullet\underset{\sim}{\nabla}) \tag{7.94}$$

By definition, we note that

$$\underline{\xi}_{,t} + (\underline{\xi}\nabla)\bullet\pmb{v} = \dot{\underline{\xi}} \tag{7.95}$$

and

$$\rho_{,t} + (\rho\underset{\sim}{\nabla}\bullet\pmb{v}) = \dot{\rho} \tag{7.96}$$

By mass continuity, we know that, away from the shock,

$$\dot{\rho} + \rho(\underset{\sim}{v} \bullet \nabla) = 0 \tag{7.97}$$

Therefore Eq. (7.94) is greatly simplified to

$$(\underline{\xi}\rho)_{,t} + (\underline{\xi}\rho\underset{\sim}{v}) \bullet \underset{\sim}{\nabla} = \rho\dot{\underline{\xi}} \tag{7.98}$$

and, Eq. (7.90) becomes

$$\boxed{\frac{D}{Dt}\int_{\Omega} \underline{\xi}\rho dV = \int_{\Omega} \dot{\underline{\xi}}\rho dV + \int_{\Omega\cap\Sigma} [[\underline{\xi}\rho c]]dA}$$

where $c \equiv (\underset{\sim}{v_{\Sigma}} - \underset{\sim}{v}) \bullet \underset{\sim}{n_{\Sigma}}$. $\tag{7.99}$

This is the generalization of Eq. (4.28) for the case that $\underline{\xi}\rho c$ is discontinuous. Note that c is the amount by which the shock front speed exceeds the normal component of material velocity. Thus, in order for the jump term to appear, the shock must be moving *relative to the material*.

Now let's focus on the second term on the right-hand-side of Eq. (4.74). First recall Eq. (???):

$$\int_{\partial\Omega} (\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f} \otimes \underset{\sim}{n})dS = \int_{\Omega} (\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f} \otimes \overleftarrow{\nabla})dV - \int_{\Omega\cap\Sigma} [[\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f}]] \otimes \underset{\sim}{n_{\Sigma}} dA \tag{7.100}$$

By double dotting from the right by the identity tensor, this implies

$$\boxed{\int_{\partial\Omega} (\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f} \bullet \underset{\sim}{n})dS = \int_{\Omega} (\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f} \bullet \overleftarrow{\nabla})dV - \int_{\Omega\cap\Sigma} [[\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f}]] \bullet \underset{\sim}{n_{\Sigma}} dA} \tag{7.101}$$

Keep in mind that our application of the jump Leibniz formula requires us to assume that $\underline{\Pi} = \underline{0}$. Substituting Eqs. (7.99) and (7.101) into Eq. (4.74), gives

$$\int_{\Omega} \dot{\underline{\xi}}\rho dV + \int_{\Omega\cap\Sigma} [[\underline{\xi}\rho c]]dA \geq \int_{\Omega} \underline{\psi}\rho dV + \int_{\Omega} (\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f} \bullet \nabla)dV - \int_{\Omega\cap\Sigma} [[\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f}]] \bullet \underset{\sim}{n_{\Sigma}} dA \tag{7.102}$$

Rearranging gives

$$\int_{\Omega} \left[\dot{\underline{\xi}} - \underline{\psi} - \frac{1}{\rho}(\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f} \bullet \overleftarrow{\nabla})\right]\rho dV + \int_{\Omega\cap\Sigma} ([[\underline{\xi}\rho c]] + [[\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f}]] \bullet \underset{\sim}{n_{\Sigma}})dA \geq 0 \tag{7.103}$$

This must hold for any region Ω. Thus for any region that does *not* contain a singular source or jump surface, the integrand of the first term must be zero:

$$\boxed{\dot{\underline{\xi}} - \underline{\psi} - \frac{1}{\rho}(\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f} \bullet \overleftarrow{\nabla}) \geq \underline{0}} \quad \text{at any continuous neighborhood} \tag{7.104}$$

By considering a "pill-box" shaped region that collapses onto the jump surface, we obtain

$$\boxed{[[\underline{\xi}\rho c]] + [[\underset{\raise1pt\hbox{$\scriptscriptstyle\cdot$}}{f}]] \bullet \underset{\sim}{n_{\Sigma}} \geq \underline{0}} \quad \text{across jump discontinuities.} \tag{7.105}$$

Local and jump forms of conservation of mass. Recalling Table 4.1, conservation of mass corresponds to

$$\underset{\sim}{\xi} = 1, \ \underset{\sim}{\psi} = 0, \text{ and } \underset{.}{f} = \underset{\sim}{\mathbf{0}}, \tag{7.106}$$

For conservation of mass, Eqs. (7.104) and (7.105) apply with strict equality to become

$$0 = 0 \text{ at any continuous neighborhood} \tag{7.107}$$

$$[[\rho c]] \geq 0 \text{ across jump discontinuities.} \tag{7.108}$$

The reason the local equation reduced to simply 0=0 was that the local continuity equation,

$$\dot{\rho} + \rho \underset{\sim}{v} \bullet \overleftarrow{\nabla} = 0 \tag{7.109}$$

was already employed in the derivation of Eq. (7.104). However the jump form of continuity, does not reduce to a trivial relationship. Instead, Eq. (7.108) states that the *product* ρc must be continuous across a moving shock surface. Written out explicitly,

$$\rho_A c_A = \rho_B c_B \tag{7.110}$$

or, recalling the definition of c,

$$\rho_A \{ (\underset{\sim}{v}_\Sigma - \underset{\sim}{v}_A) \bullet \underset{\sim}{n}_\Sigma \} = \rho_B \{ (\underset{\sim}{v}_\Sigma - \underset{\sim}{v}_B) \bullet \underset{\sim}{n}_\Sigma \} \tag{7.111}$$

Since ρc is jumpless, we may now alternatively write Eq. (7.105) as

$$\rho c [[\underset{\sim}{\xi}]] + [[\underset{.}{f}]] \bullet \underset{\sim}{n}_\Sigma \geq \underset{\sim}{0} \tag{7.112}$$

Local and jump forms of linear momentum. Recalling Table 4.1, the law governing linear momentum corresponds to

$$\underset{\sim}{\xi} = \underset{\sim}{v}, \ \underset{\sim}{\psi} = \underset{\sim}{b}, \text{ and } \underset{.}{f} = \underset{\approx}{\sigma}, \tag{7.113}$$

so Eqs. (7.104) and (7.105) become

$$\dot{\underset{\sim}{v}} - \underset{\sim}{b} - \frac{1}{\rho} (\underset{\approx}{\sigma} \bullet \underset{\sim}{\nabla}) = \underset{\sim}{\mathbf{0}} \text{ at any continuous neighborhood} \tag{7.114}$$

$$\rho c [[\underset{\sim}{v}]] + [[\underset{\approx}{\sigma}]] \bullet \underset{\sim}{n}_\Sigma = \underset{\sim}{\mathbf{0}} \text{ across jump discontinuities.} \tag{7.115}$$

where we have invoked conservation of mass to bring ρc outside the jump brackets.

Local and jump forms of angular momentum. Recalling Table 4.1, the law governing linear momentum corresponds to

$$\underset{\sim}{\xi} = \underset{\sim}{x} \times \underset{\sim}{v}, \ \underset{\sim}{\psi} = \underset{\sim}{x} \times \underset{\sim}{b}, \text{ and } \underset{.}{f} = \underset{\sim}{x} \times \underset{\approx}{\sigma}, \tag{7.116}$$

First note that

$$\dot{\underset{\sim}{\xi}} = \dot{\underset{\sim}{x}} \times \underset{\sim}{v} + \underset{\sim}{x} \times \dot{\underset{\sim}{v}} = \underset{\sim}{v} \times \underset{\sim}{v} + \underset{\sim}{x} \times \dot{\underset{\sim}{v}} = \underset{\sim}{x} \times \dot{\underset{\sim}{v}} \tag{7.117}$$

Also note that

$$\underset{\sim}{f} \bullet \underset{\sim}{\nabla} = (\underset{\sim}{x} \times \underset{\approx}{\sigma}) \bullet \underset{\sim}{\nabla} \qquad (7.118)$$

writing this equation in component form (noting that $x_{i,j} = \delta_{ij}$) reveals that

$$\underset{\sim}{f} \bullet \underset{\sim}{\nabla} = \underset{\approx}{\varepsilon} : \underset{\approx}{\sigma} + \underset{\sim}{x} \times (\underset{\approx}{\sigma} \bullet \underset{\sim}{\nabla}) = \underset{\approx}{\varepsilon} : \underset{\approx}{\sigma} + \rho \underset{\sim}{x} \times (\underset{\sim}{\dot{v}} - \underset{\sim}{b}) \qquad (7.119)$$

where, in the last step, we used the local equation of linear momentum. With these results, Eqs. (7.104) and (7.105) become

$$\underset{\sim}{x} \times \underset{\sim}{\dot{v}} - \underset{\sim}{x} \times \underset{\sim}{b} - \left(\frac{1}{\rho}\left(\underset{\approx}{\varepsilon} : \underset{\approx}{\sigma}\right) + \underset{\sim}{x} \times (\underset{\sim}{\dot{v}} - \underset{\sim}{b})\right) = \underset{\sim}{0} \ ,$$

or, simplifying, $\underset{\approx}{\varepsilon} : \underset{\approx}{\sigma} = \underset{\sim}{0}$ \qquad (7.120)

$$\rho c[[\underset{\sim}{x} \times \underset{\sim}{v}]] + [[\underset{\sim}{x} \times \underset{\approx}{\sigma}]] \bullet \underset{\sim}{n}_\Sigma = \underset{\sim}{0} \ \text{ across jump discontinuities.} \qquad (7.121)$$

Both of these equations simplify considerably. Cancelling terms in Eq. (7.120) gives

$$\underset{\approx}{\varepsilon} : \underset{\approx}{\sigma} = \underset{\sim}{0}, \text{ which implies that } \underset{\approx}{\sigma}^T = \underset{\approx}{\sigma} \qquad (7.122)$$

Though not immediately obvious, this equation implies that the stress tensor must be symmetric:

$$\underset{\approx}{\sigma}^T = \underset{\approx}{\sigma} \qquad (7.123)$$

For Eq. (7.121), we note that the position vector $\underset{\sim}{x}$ certainly is not discontinuous. Hence, it may be taken outside of the jump brackets to give

$$\underset{\sim}{x} \times (\rho c[[\underset{\sim}{v}]] + [[\underset{\approx}{\sigma}]] \bullet \underset{\sim}{n}_\Sigma) = \underset{\sim}{0} \ \text{ across jump discontinuities.} \qquad (7.124)$$

However, by Eq. (7.115), the expression in the parentheses is zero. Hence, the jump law of angular momentum reduces to $\underset{\sim}{0}=\underset{\sim}{0}$, and therefore provides no new jump restrictions.

Local and jump forms of the first law of thermodynamics. Recalling Table 4.1, the law governing linear momentum corresponds to

$$\underset{\sim}{\xi} = e, \ \underset{\sim}{\psi} = r + \underset{\sim}{b} \bullet \underset{\sim}{v}, \text{ and } \underset{\sim}{f} = \underset{\sim}{v} \bullet \underset{\approx}{\sigma} - \underset{\sim}{q} , \qquad (7.125)$$

so Eqs. (7.104) and (7.105) become

$$\dot{e} - (r + \underset{\sim}{b} \bullet \underset{\sim}{v}) - \frac{1}{\rho}(\underset{\sim}{v} \bullet \underset{\approx}{\sigma} - \underset{\sim}{q}) \bullet \nabla = 0 \qquad \text{(local form)} \qquad (7.126)$$

$$\rho c[[e]] + [[\underset{\sim}{v} \bullet \underset{\approx}{\sigma} - \underset{\sim}{q}]] \bullet \underset{\sim}{n}_\Sigma = 0 \qquad \text{(jump form).} \qquad (7.127)$$

The local form can be written

$$\dot{e} = p_T + p_M \, ,$$

where $p_T \equiv r - \dfrac{1}{\rho} \mathbf{q} \bullet \nabla$

and $p_M = \mathbf{b} \bullet \mathbf{v} + \dfrac{1}{\rho}(\mathbf{v} \bullet \underset{\approx}{\sigma}) \bullet \nabla$ (7.128)

Applying the product rule to the last term in the above expression for p_M gives

$$\frac{1}{\rho}(\mathbf{v} \bullet \underset{\approx}{\sigma}) \bullet \nabla = \frac{1}{\rho}\{\mathbf{v} \bullet (\underset{\approx}{\sigma} \bullet \nabla)\} + \frac{1}{\rho}\underset{\approx}{\sigma}{:}(\mathbf{v}\nabla)$$ (7.129)

The local form of linear momentum may be used to write

$$\frac{1}{\rho}(\underset{\approx}{\sigma} \bullet \nabla) = \dot{\mathbf{v}} - \mathbf{b}$$ (7.130)

Hence, the specific mechanical power p_M in Eq. (7.128) becomes

$$p_M = \dot{e}_k + p_s \, ,$$

where $\dot{e}_k = \mathbf{v} \bullet \dot{\mathbf{v}} \, ,$

and $p_s = \dfrac{1}{\rho}\underset{\approx}{\sigma}{:}(\mathbf{v}\nabla)$ (7.131)

Thus, the alternative form of the local first law is

$$\dot{u} = p_T + p_s$$

where $u \equiv e - e_k$ (7.132)

This local form of the first law, expressed in terms of internal energy, was derived in an earlier section, but we have repeated it here in order to look for an analogous modification of the jump formulation. Recall the jump form of the first law:

$$\rho c[[e]] + [[\mathbf{v} \bullet \underset{\approx}{\sigma} - \mathbf{q}]] \bullet \mathbf{n}_\Sigma = 0 \qquad \text{(jump form).}$$ (7.133)

The double bracket is defined for any variable f as

$$[[f]] = f_A - f_B$$ (7.134)

Therefore, the jump of a product is

$$[[fg]] = f_A g_A - f_B g_B$$ (7.135)

we can always define

$$f^{\mathrm{avg}} \equiv \frac{1}{2}(f_A + f_B) \quad \text{and} \quad g^{\mathrm{avg}} \equiv \frac{1}{2}(g_A + g_B)$$ (7.136)

It's easy to verify that

$$[[fg]] = f^{\mathrm{avg}}[[g]] + [[f]]g^{\mathrm{avg}}$$ (7.137)

Therefore,

$$[[\mathbf{v} \bullet \underset{\approx}{\sigma}]] \bullet \mathbf{n}_\Sigma = \mathbf{v}^{\mathrm{avg}} \bullet [[\underset{\approx}{\sigma}]] \bullet \mathbf{n}_\Sigma + [[\mathbf{v}]] \bullet \underset{\approx}{\sigma}^{\mathrm{avg}} \bullet \mathbf{n}_\Sigma$$ (7.138)

Recall from the jump equation of linear momentum that

$$[[\underset{\approx}{\sigma}]] \bullet \boldsymbol{n}_\Sigma = -\rho c[[\boldsymbol{v}]] \tag{7.139}$$

Thus, Eq. (7.138) becomes

$$[[\boldsymbol{v} \bullet \underset{\approx}{\sigma}]] \bullet \boldsymbol{n}_\Sigma = -\rho c(\boldsymbol{v}^{\text{avg}} \bullet [[\boldsymbol{v}]]) + [[\boldsymbol{v}]] \bullet \underset{\approx}{\sigma}^{\text{avg}} \bullet \boldsymbol{n}_\Sigma \tag{7.140}$$

Noting that $\boldsymbol{v}^{\text{avg}} \bullet [[\boldsymbol{v}]] = [[e_k]]$ and that $e - e_k = u$, Eq. (7.133) becomes

$$\rho c[[u]] + [[\boldsymbol{v}]] \bullet \underset{\approx}{\sigma}^{\text{avg}} \bullet \boldsymbol{n}_\Sigma - [[\boldsymbol{q}]] \bullet \boldsymbol{n}_\Sigma = 0 \qquad \text{(jump form)}. \tag{7.141}$$

If the shock impedance ρc is nonzero, then the above equation may be written in the form

$$[[u]] = <<W_s>> + <<Q>> ,$$
$$\text{where} \quad <<W_s>> \equiv -\frac{\underset{\approx}{\sigma}^{\text{avg}}:([[\boldsymbol{v}]]\boldsymbol{n}_\Sigma)}{\rho c}$$
$$\text{and} \quad <<Q>> \equiv \frac{[[\boldsymbol{q}]] \bullet \boldsymbol{n}_\Sigma}{\rho c} \tag{7.142}$$

It is not clear to us that working with internal energy is necessarily advantageous in regard to the jump law. One can always work directly with the total energy using the original form of the jump law,

$$[[e]] = <<W_M>> + <<Q>>$$
$$\text{where} \quad <<W_M>> \equiv -\frac{[[\boldsymbol{v} \bullet \underset{\approx}{\sigma}]] \bullet \boldsymbol{n}_\Sigma}{\rho c}$$
$$\text{and} \quad <<Q>> \equiv \frac{[[\boldsymbol{q}]] \bullet \boldsymbol{n}_\Sigma}{\rho c} \tag{7.143}$$

Incidentally, since $[[e]] = [[u]] + [[e_k]] = [[u]] + \frac{1}{2}[[\boldsymbol{v} \bullet \boldsymbol{v}]]$, note that

$$[[u]] = <<W_s>> + <<Q>> ,$$
$$\text{where} \quad <<W_s>> = -\frac{[[\boldsymbol{v} \bullet \underset{\approx}{\sigma}]] \bullet \boldsymbol{n}_\Sigma}{\rho c} - \frac{1}{2}[[\boldsymbol{v} \bullet \boldsymbol{v}]]$$
$$\text{and} \quad <<Q>> \equiv \frac{[[\boldsymbol{q}]] \bullet \boldsymbol{n}_\Sigma}{\rho c} \tag{7.144}$$

which is an alternative form of Eq. (7.142) that does not require the use of the averaging operator.

Local and jump forms of the second law of thermodynamics. Recalling Table 4.1, the law governing linear momentum corresponds to

$$\underline{\xi} = s, \quad \underline{\psi} = \frac{r}{T}, \text{ and } \underline{f} = -\frac{\boldsymbol{q}}{T} , \tag{7.145}$$

so Eqs. (7.104) and (7.105) become

$$\dot{s} - \frac{r}{T} + \frac{1}{\rho}\left(\frac{\boldsymbol{q}}{T} \bullet \underset{\sim}{\nabla}\right) \geq \underline{0} \qquad \text{(local)} \qquad\qquad (7.146)$$

$$\rho c[[s]] \geq \left[\!\left[\frac{\boldsymbol{q}}{T}\right]\!\right] \bullet \boldsymbol{n}_{\Sigma} \qquad \text{(jump)} \qquad\qquad (7.147)$$

DRAFT!   **Text written in this large print are notes to myself or to the draft reader.**

Equations that are referenced with two underscores, for example Eq. (__), are meant to be taken from my thermomechanics write-up that I handed out when I taught the advanced Continuum Mechanics class a year and a half ago. Eventually, I'll write an "intro" section in this report deriving the needed equations. The referenced (__) equations are always repeated in this text, so the only loss here is the absence of a proof.

1. Anisotropic Mie-Grüneisen generalization

Review of traditional isotropic M-G equation of state

The traditional isotropic M-G equation of state separates the internal energy into the sum $u = u_C(\rho) + u_T(\rho, s)$ of a "cold" part that depends only on the density ρ plus a "thermal" part that depends on both density and entropy s. Then it is usually assumed that the thermal part can be multiplicatively decomposed so that $u_T(\rho, s) = A(\rho)B(s)$. With this assumption, it can be shown that $\dot{u}_T/u_T = \gamma(\rho)(\dot{\rho}/\rho) + \dot{s}/c(s)$ where the function $\gamma(\rho)$ can be shown to equal the Grüneisen parameter and the function $c(s)$ is related to the specific heat. For the generalization of the M-G formulation to include anisotropic materials, we note that $\dot{\rho}/\rho = -\dot{v}/v$, where v denotes the specific volume. In the generalization, the volumetric strain rate, $\dot{v}/v$, becomes the rate $\dot{\underset{\sim}{v}}$ of a strain tensor. In the isotropic theory, the specific work rate $-P\dot{v}$ can be written as $-(Pv)(\dot{v}/v)$, or $-(P/\rho)(\dot{v}/v)$, which generalizes to the inner product $\underset{\sim}{P}:\dot{\underset{\sim}{v}}$ where $\underset{\sim}{P}$ is the *specific* stress (i.e., stress divided by density). Throughout the development of the equations, no *particular* definition for the strain measure will be employed. It might be Lagrange strain, Euler strain, logarithmic strain, etc. The stress tensor $\underset{\sim}{P}$ is required to be work conjugate to the chosen strain measure, and it is assumed positive in tension.

Motivation for generalizing the M-G eos

REBECCA: Describe the SCM crack problem, where cracks open in a particular direction and are __not__ desired to induce a corresponding temperature drop.

Generalized derivation of the Mie-Grüneisen model.

The following analysis closely follows the isotropic analysis presented in [5 *i.e., Doug Drumheller's new book: Introduction to Wave Propagation in Nonlinear Fluids and Solids.*] and it is very instructive to follow along with that reference so that it is clear where the generalizations of the theory occur.

Warning: as is typical with thermodynamic derivations, this section is a long and tedious string of identities with no obvious thread of intent. Skip to page lxxxix for the application to cracked materials. Skip to page xc for specific application in SCRAM.

Assume that the internal energy u can be written as a function of a strain tensor $\underset{\approx}{v}$ and the entropy s and that this dependence can be decomposed into a "cold" part plus a "thermal" part:

$$u(\underset{\approx}{v}, s) = u_C(\underset{\approx}{v}) + u_T(\underset{\approx}{v}, s) \tag{1.1}$$

Further assume that the thermal part can be multiplicatively decomposed as

$$u_T(\underset{\approx}{v}, s) = A(\underset{\approx}{v})B(s) \tag{1.2}$$

Then

$$\frac{\dot{u}_T}{u_T} = \frac{\dot{A}}{A} + \frac{\dot{B}}{B} \, , \tag{1.3}$$

where

$$\frac{\dot{A}}{A} = \frac{1}{A}\frac{dA}{d\underset{\approx}{v}}:\dot{\underset{\approx}{v}} \qquad \text{(i.e., } \frac{\dot{A}}{A} = \frac{1}{A}\frac{\partial A}{\partial v_{ij}}\dot{v}_{ij} \text{)} \tag{1.4}$$

$$\frac{\dot{B}}{B} = \frac{1}{B}\frac{dB}{ds}\dot{s} \tag{1.5}$$

The functions A and B are themselves not as useful as the following alternative functions defined

$$\underset{\approx}{\gamma} \equiv -\frac{1}{A}\frac{dA}{d\underset{\approx}{v}} \qquad \text{and} \qquad c = \left[\frac{1}{B}\frac{dB}{ds}\right]^{-1} \tag{1.6}$$

Later on, the tensor $\underset{\approx}{\gamma}$ will be identified as the Grüneisen tensor and c will be related to the constant strain specific heat. At this point, however, these are merely defined as convenient functions. It is extremely important to keep in mind that

$$\underset{\approx}{\gamma} = \underset{\approx}{\gamma}(\underset{\approx}{v}) \qquad \text{and} \qquad c = c(s) \tag{1.7}$$

As a matter of fact, it is these functional dependencies that distinguish the Mie-Grüneisen model from other general models. This is so crucial to the development that, henceforth, all upcoming equations will be accompanied with reminders of the functional dependencies.

The definitions of Eq. (1.7) allow Eq. (1.3) to be written

$$\boxed{\frac{\dot{u}_T}{u_T} = -\underset{\approx}{\gamma}:\dot{\underset{\approx}{v}} + \frac{\dot{s}}{c}} \, , \qquad\qquad \text{where } \underset{\approx}{\gamma} = \underset{\approx}{\gamma}(\underset{\approx}{v}) \text{ and } c = c(s) \tag{1.8}$$

Recalling that $u_T = u_T(\underset{\approx}{v}, s)$, the chain rule implies that

$$\dot{u}_T = \left(\frac{\partial u_T}{\partial \underset{\approx}{v}}\right)_s : \dot{\underset{\approx}{v}} + \left(\frac{\partial u}{\partial s}\right)_{\underset{\approx}{v}} \dot{s} \tag{1.9}$$

Eqs. (1.8) and (1.9) both hold for all thermoelastic processes, and therefore equating coefficients of rate quantities gives

$$\boxed{\left(\frac{\partial u_T}{\partial \underset{\approx}{v}}\right)_s = -u_T \underset{\approx}{\gamma}}, \qquad\qquad \text{where } \underset{\approx}{\gamma} = \underset{\approx}{\gamma}(\underset{\approx}{v}) \tag{1.10}$$

and

$$\boxed{\left(\frac{\partial u_T}{\partial s}\right)_{\underset{\approx}{v}} = \frac{u_T}{c}}, \qquad\qquad \text{where } c = c(s) \tag{1.11}$$

Recall that the usual thermoelastic equations remain valid. In particular, temperature is still defined by Eq. (__) as

$$T = \left(\frac{\partial u}{\partial s}\right)_{\underset{\approx}{v}} \tag{1.12}$$

Recalling the decomposition of Eq. (1.2), we note that

$$\left(\frac{\partial u}{\partial s}\right)_{\underset{\approx}{v}} = \left(\frac{\partial u_T}{\partial s}\right)_{\underset{\approx}{v}} \tag{1.13}$$

and therefore Eqn. (1.11) shows that

$$T = \frac{u_T}{c}, \tag{1.14}$$

Rearranging gives an expression for u_T :

$$\boxed{u_T = cT} \qquad\qquad \text{where } T = T(\underset{\approx}{v}, s) \text{ and } c = c(s) \tag{1.15}$$

The equilibrium specific stress $\underset{\approx}{P}$ is defined to be conjugate to the strain measure $\underset{\approx}{v}$ according to Eq. (__):

$$\underset{\approx}{P} = \left(\frac{\partial u}{\partial \underset{\approx}{v}}\right)_s \tag{1.16}$$

From the decomposition of Eq. (1.2), we note that

$$\underset{\approx}{P} = \underset{\approx}{P}_C + \underset{\approx}{P}_T, \qquad\qquad \text{where } \underset{\approx}{P}_C = \underset{\approx}{P}_C(\underset{\approx}{v}) \text{ and } \underset{\approx}{P}_T = \underset{\approx}{P}_T(\underset{\approx}{v}, s) \tag{1.17}$$

Here,

$$\underset{\approx}{P}_C \equiv \frac{du_C}{d\underset{\approx}{v}} \qquad \text{and} \qquad \underset{\approx}{P}_T = \left(\frac{\partial u_T}{\partial \underset{\approx}{v}}\right)_s \tag{1.18}$$

Using Eq. (1.10) in Eq. (1.18) shows that

$$\underset{\approx}{P}_T = -u_T \underset{\approx}{\gamma} \tag{1.19}$$

and therefore Eq. (1.17) becomes

$$\boxed{\underset{\approx}{P} = \underset{\approx}{P}_C - u_T \underset{\approx}{\gamma}} \qquad\qquad \text{where } u_T = u_T(\underset{\sim}{v}, s) \;,\; \underset{\approx}{P}_C = \underset{\approx}{P}_C(\underset{\sim}{v}) \;,\text{ and } \underset{\approx}{\gamma} = \underset{\approx}{\gamma}(\underset{\sim}{v}) \tag{1.20}$$

or, using Eq. (1.15),

$$\boxed{\underset{\approx}{P} = \underset{\approx}{P}_C - cT\underset{\approx}{\gamma}} \qquad\qquad \text{where } \underset{\approx}{P}_C = \underset{\approx}{P}_C(\underset{\sim}{v}) \;,\; T = T(\underset{\sim}{v}, s) \;,\; c = c(s)\text{, and } \underset{\approx}{\gamma} = \underset{\approx}{\gamma}(\underset{\sim}{v}) \tag{1.21}$$

Taking the partial derivative of Eq. (1.20) with respect to s holding $\underset{\sim}{v}$ constant gives

$$\left(\frac{\partial \underset{\approx}{P}}{\partial s}\right)_{\underset{\sim}{v}} = -\left(\frac{\partial u_T}{\partial s}\right)_{\underset{\sim}{v}} \underset{\approx}{\gamma} \tag{1.22}$$

or, using Eqs (1.12) through (1.14),

$$\left(\frac{\partial \underset{\approx}{P}}{\partial s}\right)_{\underset{\sim}{v}} = -T \underset{\approx}{\gamma} \qquad\qquad \text{where } T = T(\underset{\sim}{v}, s) \text{ and } \underset{\approx}{\gamma} = \underset{\approx}{\gamma}(\underset{\sim}{v}) \tag{1.23}$$

Assuming the internal energy function is sufficiently smooth, the thermodynamic identity (__),

$$\left(\frac{\partial \underset{\approx}{P}}{\partial s}\right)_{\underset{\sim}{v}} = \frac{\partial^2 u}{\partial s \partial \underset{\sim}{v}} = \frac{\partial^2 u}{\partial \underset{\sim}{v} \partial s} = \left(\frac{\partial T}{\partial \underset{\sim}{v}}\right)_s \tag{1.24}$$

still holds and therefore

$$\boxed{\left(\frac{\partial T}{\partial \underset{\sim}{v}}\right)_s = -T \underset{\approx}{\gamma}} \tag{1.25}$$

This result proves that the tensor $\underset{\approx}{\gamma}$ is indeed the Grüneisen tensor defined in Eq. (__).
Now differentiate Eq. (1.14) with respect to s holding $\underset{\approx}{v}$ constant:

$$\left(\frac{\partial T}{\partial s}\right)_{\underset{\sim}{v}} = \frac{1}{c}\left(\frac{\partial u_T}{\partial s}\right)_{\underset{\sim}{v}} - \frac{u_T dc}{c^2 ds} \;, \tag{1.26}$$

Using Eq. (1.11)

$$\left(\frac{\partial T}{\partial s}\right)_{\underset{\sim}{v}} = \frac{u_T}{c^2} - \frac{u_T dc}{c^2 ds} \tag{1.27}$$

or, using Eq. (1.15), to replace u_T with cT,

$$\frac{1}{T}\left(\frac{\partial T}{\partial s}\right)_{\underset{\sim}{v}} = \frac{1 - c'(s)}{c} \tag{1.28}$$

The thermodynamic definition of specific heat at constant strain is given by Eq. (__); namely,

$$c_v = T\left(\frac{\partial s}{\partial T}\right)_{\underset{\sim}{v}} \tag{1.29}$$

Therefore

$$c_v = \frac{c}{1 - c'(s)} \qquad (1.30)$$

Elastic stiffnesses

Eq. (1.30) shows that the specific heat is a function of entropy only. It is not a function of strain, and therefore, the identity (__) shows that the isothermal elastic stiffness must be strictly a function of strain only.

The isentropic elastic stiffness (which governs acoustic wave speeds) is defined

$$\mathbf{E}_s \equiv \left(\frac{\partial \mathbf{P}}{\partial \mathbf{v}}\right)_s \text{, or in indicial notation, } (E_s)_{ijkl} = \left(\frac{\partial P_{ij}}{\partial v_{kl}}\right)_s \qquad (1.31)$$

Letting

$$\mathbf{E}_C \equiv \frac{d\mathbf{P}_C}{d\mathbf{v}} \qquad (1.32)$$

and applying Eq. (1.20),

$$\mathbf{E}_s = \mathbf{E}_C - \gamma\left(\frac{\partial u_T}{\partial \mathbf{v}}\right)_s - u_T\left(\frac{d\gamma}{d\mathbf{v}}\right)_s \qquad (u_T = u_T(\mathbf{v}, s) \text{ , } \mathbf{P}_C = \mathbf{P}_C(\mathbf{v}) \text{ , and } \gamma = \gamma(\mathbf{v})) \qquad (1.33)$$

Applying Eq. (1.10), the isentropic stiffness becomes

$$\mathbf{E}_s = \mathbf{E}_C + u_T\left\{\gamma\gamma - \frac{d\gamma}{d\mathbf{v}}\right\} \qquad \text{i.e., } E^s_{ijkl} = E^C_{ijkl} + u_T\left\{\gamma_{ij}\gamma_{kl} - \frac{d\gamma_{ij}}{dv_{kl}}\right\} \qquad (1.34)$$

or, with Eq. (1.15),

$$\mathbf{E}_s = \mathbf{E}_C + cT\left\{\gamma\gamma - \frac{d\gamma}{d\mathbf{v}}\right\} \qquad \text{where } T = T(\mathbf{v}, s) \text{ , } c = c(s) \text{ and } \gamma = \gamma(\mathbf{v}) \qquad (1.35)$$

The thermodynamic identity (__) still holds. Namely, we know that

$$\mathbf{E}_s = \mathbf{E}_T + c_v T\gamma\gamma \qquad (1.36)$$

where the isothermal stiffness is defined

$$\mathbf{E}_T \equiv \left(\frac{\partial \mathbf{P}}{\partial \mathbf{v}}\right)_T \qquad (1.37)$$

Eqs. (1.30) and (1.15) show that

$$c_v T = \frac{u_T}{1 - c'(s)} \qquad (1.38)$$

Hence

$$\underset{\approx}{E}_s = \underset{\approx}{E}_T + \frac{u_T}{1 - c'(s)} \underset{\approx}{\gamma\gamma} \qquad (1.39)$$

Differentiating Eq. (1.20) with respect to $\underset{\sim}{v}$ holding T constant gives

$$\underset{\approx}{E}_T \equiv \underset{\approx}{E}_C - \underset{\sim}{\gamma} \left(\frac{\partial u_T}{\partial \underset{\sim}{v}} \right)_T - u_T \frac{d\underset{\sim}{\gamma}}{d\underset{\sim}{v}} \qquad (1.40)$$

By the chain rule, we know that

$$\left(\frac{\partial u_T}{\partial \underset{\sim}{v}} \right)_T = \left(\frac{\partial u_T}{\partial \underset{\sim}{v}} \right)_s + \left(\frac{\partial u_T}{\partial s} \right)_{\underset{\sim}{v}} \left(\frac{\partial s}{\partial \underset{\sim}{v}} \right)_T \qquad (1.41)$$

or, using Eqs. (1.10) and 1.11),

$$\left(\frac{\partial u_T}{\partial \underset{\sim}{v}} \right)_T = -u_T \underset{\sim}{\gamma} + \frac{u_T}{c} \left(\frac{\partial s}{\partial \underset{\sim}{v}} \right)_T \qquad (1.42)$$

Recall the thermodynamic identity (___) that

$$\left(\frac{\partial s}{\partial \underset{\sim}{v}} \right)_T = c_v \underset{\sim}{\gamma} \qquad (1.43)$$

Therefore

$$\left(\frac{\partial u_T}{\partial \underset{\sim}{v}} \right)_T = -u_T \underset{\sim}{\gamma} + \frac{u_T}{c} c_v \underset{\sim}{\gamma} \qquad (1.44)$$

Finally, by Eq. (1.15),

$$\left(\frac{\partial u_T}{\partial \underset{\sim}{v}} \right)_T = -u_T \underset{\sim}{\gamma} + T c_v \underset{\sim}{\gamma} \qquad (1.45)$$

Substituting this result back into Eq. (1.40) gives

$$\underset{\approx}{E}_T \equiv \underset{\approx}{E}_C + (u_T - T c_v) \underset{\approx}{\gamma\gamma} - u_T \frac{d\underset{\sim}{\gamma}}{d\underset{\sim}{v}} \qquad (1.46)$$

or, using Eq. (1.38),

$$\boxed{\underset{\approx}{E}_T \equiv \underset{\approx}{E}_C - u_T \left\{ \frac{c'(s)}{1 - c'(s)} \underset{\approx}{\gamma\gamma} + \frac{d\underset{\sim}{\gamma}}{d\underset{\sim}{v}} \right\}} \qquad (1.47)$$

Note that the isothermal stiffness equals the "cold" stiffness if $c \neq c(s)$ and $\underset{\sim}{\gamma} \neq \underset{\sim}{\gamma}(\underset{\sim}{v})$.

As was derived in Section __, the governing equations are

$$\dot{s} \;=\; \underset{\approx}{\boldsymbol{B}} : \dot{\underset{\approx}{\boldsymbol{\gamma}}} + c_v \frac{\dot{T}}{T} \tag{1.48}$$

$$\dot{\underset{\approx}{\boldsymbol{P}}} \;=\; \underset{\approx}{\boldsymbol{E}}_T : \dot{\underset{\approx}{\boldsymbol{\gamma}}} - \dot{T}\underset{\approx}{\boldsymbol{B}} \tag{1.49}$$

Putting $\dot{s} = D/T$, where D is the dissipation (having a value assigned by other physical arguments), and also using the identity of Eq. (__) to write $\underset{\approx}{\boldsymbol{B}} = c_v \underset{\approx}{\boldsymbol{\gamma}}$, the governing equations become

$$\frac{\dot{T}}{T} \;=\; \frac{D}{Tc_v} - \underset{\approx}{\boldsymbol{\gamma}} : \dot{\underset{\approx}{\boldsymbol{\gamma}}} \tag{1.50a}$$

$$\dot{\underset{\approx}{\boldsymbol{P}}} \;=\; \underset{\approx}{\boldsymbol{E}}_T : \dot{\underset{\approx}{\boldsymbol{\gamma}}} - c_v \underset{\approx}{\boldsymbol{\gamma}} \dot{T} \tag{1.50b}$$

Keep in mind that here the stress is actually stress divided by density and therefore the stiffness is actually the conventional stiffness divided by density.

Specific heat for the Anisotropic Mie-Grüneisen model

All of the identities derived in the preceding section follow from the assumed functional form of the energy as defined in Eqs. (1.1) and (1.2). No other assumptions were made.

It is not uncommon for the constant strain specific heat c_v to be assumed constant. If this assumption is made, then the differential equation of Eq. (1.30) can be solved to show how the function $c(s)$ depends on s:

$$c(s) \;=\; c_v[1 - \kappa e^{-(s-s_o)/c_v}] \,, \qquad \text{where } \kappa \text{ is an integration constant} \tag{1.51}$$

DRAFT
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Grüneisen tensor for voided and/or cracked material

Consider a material for which there are numerous cracks or voids embedded in an isotropic matrix material. Recall the identity of Eq. (__) which relates the Grüneisen tensor to the linear expansion tensor $\underset{\approx}{\beta}$:

$$\underset{\approx}{\gamma} = \frac{1}{c_v}\underset{\approx}{\boldsymbol{E}}_T \cdot \underset{\approx}{\beta} \tag{1.52}$$

The linear expansion tensor represents the change in strain resulting from a unit change in temperature at fixed stress. It is well known that, upon a change in temperature, any body made strictly from a *single isotropic material* will dilate rather than generally dilatate. That is, it will expand uniformly, changing its volume in a self-similar manner without changing its shape. Our cracked/porous material falls in this category, so it seems reasonable to take the composite linear expansion tensor to equal that of the matrix material:

$$\underset{\approx}{\beta} = \beta_m \underset{\approx}{\boldsymbol{I}}, \tag{1.53}$$

where the subscript "*m*" refers to the matrix material. Recall that specific heat equals the amount of heat required per unit *mass* to raise the temperature by one degree. Thus, it seems reasonable that, for a voided/cracked composite, the specific heat for the composite must equal that of the matrix. Thus, Eq. (1.52) can be written

$$\underset{\approx}{\gamma} = \frac{\beta_m}{c_v^m}\underset{\approx}{\boldsymbol{E}}_T \cdot \underset{\approx}{\boldsymbol{I}} \tag{1.54}$$

The Grüneisen parameter for the matrix material is related to the matrix properties according to

$$\gamma_m = \frac{\beta_m}{c_v^m}3K_m^T , \tag{1.55}$$

where K_m^T is the isothermal bulk modulus of the matrix material. Note: the factor of 3 appears here because β_m is the *linear* expansion coefficient rather than the volumetric expansion coefficient.

Substituting Eq. (1.55) into Eq. (1.54) gives

$$\boxed{\underset{\approx}{\gamma} = \frac{\gamma_m}{3K_m^T}\underset{\approx}{\boldsymbol{E}}_T \cdot \underset{\approx}{\boldsymbol{I}}} \tag{1.56}$$

Note: if the material happens to be weakened by cracks in, say, the 1-direction, then the material is capable of much larger strains in that direction due to opening of cracks. Physically, this kind of volume change is not supposed to cause a temperature drop. With the above formula, a material that is weak in the 1-direction will have a correspondingly low 11 component of the Grüneisen tensor and the 11 contribution of the inner product $\underset{\approx}{\gamma} \cdot \dot{\underset{\approx}{\gamma}}$ in Eq. (1.50) will have a negligible effect on the temperature rate in comparison to other strain components in directions where the material remains stiff.

For the special case that the voids or cracks are distributed isotropically, the isothermal stiffness tensor is isotropic and the above equation becomes simply

$$\frac{\gamma}{\gamma_m} = \frac{K^T}{K_m^T} \tag{1.57}$$

For an anisotropic distribution of cracks or voids, the operation in Eq. (1.56) is most easily carried out using a Voigt or Voigt-Mandel representation in which second order tensors are stored as 6×1 arrays with the independent components ordered such that the diagonal components are listed. For example, $\{11, 22, 33, 23, 31, 12\}$ or $\{11, 22, 33, 12, 23, 31\}$. In this representation, the identity tensor is $\{1, 1, 1, 0, 0, 0\}$. The Voigt-Mandel representation of the stiffness tensor is a 6×6 matrix and the $\underset{\approx}{E}_T : \underset{\approx}{I}$ operation simply sums the first three columns of the Voigt matrix for $\underset{\approx}{E}_T$.

Application in SCRAM. Recall Eqs. (1.50):

$$\frac{\dot{T}}{T} = \frac{D}{Tc_v} - \underset{\approx}{\gamma} : \underset{\approx}{\dot{v}} \tag{1.58a}$$

$$\underset{\approx}{\dot{P}} = \underset{\approx}{E}_T : \underset{\approx}{\dot{v}} - c_v \underset{\approx}{\gamma} \dot{T} \tag{1.58b}$$

where from Eq. (1.56),

$$\underset{\approx}{\gamma} = \frac{\gamma_m}{3K_m^T} \underset{\approx}{E}_T : \underset{\approx}{I} \tag{1.59}$$

In SCRAM, the strain rate $\underset{\approx}{\dot{v}}$ in these thermodynamic relations is taken to be the elastic part of the rate of deformation. The purely mechanical phase of the model updates the anisotropic isothermal stiffness to account for crack growth and then the nominal "isothermal" stress rate is computed by

$$\boxed{\underset{\approx}{\dot{P}}_T \equiv \underset{\approx}{E}_T : \underset{\approx}{\dot{v}}} \tag{1.60}$$

With this stress rate known, the second term on the right side of Eq. (1.58a) becomes simply

$$-\underset{\approx}{\gamma} : \underset{\approx}{\dot{v}} = -\frac{\gamma_m}{3K_m^T} \underset{\approx}{\dot{v}} : \left(\underset{\approx}{E}_T : \underset{\approx}{I} \right) = -\frac{\gamma_m}{3K_m^T} (\underset{\approx}{\dot{P}}_T : \underset{\approx}{I}) = \frac{\gamma_m}{K_m^T} \dot{\Pi}_T \quad , \tag{1.61}$$

where

$$\dot{\Pi}_T \equiv -\frac{1}{3} \operatorname{tr} \underset{\approx}{\dot{P}}_T \tag{1.62}$$

Thus, also recalling that the specific heat of the cracked composite is taken to equal that of the matrix material, the governing equations become

$$\frac{\dot{T}}{T} = \frac{D}{Tc_v} + \frac{\gamma_m}{K_m^T} \dot{\Pi}_T \qquad \text{and} \qquad \underset{\approx}{\dot{P}} = \underset{\approx}{\dot{P}}_T - \frac{c_v^m \gamma_m}{3K_m^T} \left(\underset{\approx}{E}_T : \underset{\approx}{I} \right) \dot{T} \tag{1.63}$$

Recall that $\underset{\approx}{P}$ is the *specific* stress. When the strain rate is taken to be the rate of deformation, $\underset{\approx}{P}$ must be interpreted as σ/ρ, where σ is the Cauchy stress and ρ is the current density (relative to the stress free state). Equivalently,

$$\underset{\approx}{P} = \frac{\underset{\approx}{\tau}}{\rho_o}, \text{ where } \underset{\approx}{\tau} = J\underset{\approx}{\sigma} \tag{1.64}$$

Here, J is the jacobian of the deformation and $\underset{\approx}{\tau}$ is the Kirchhoff stress. With Eq. (1.64), Eqs. (1.63) give

$$\frac{\dot{T}}{T} = \frac{D}{Tc_v} + \frac{\gamma_m}{K_m^T}\dot{p}_T \tag{1.65a}$$

$$\dot{\underset{\approx}{\tau}} = \dot{\underset{\approx}{\tau}}_T - \frac{\rho_o c_v^m \gamma_m}{3K_m^T}\left(\underset{\approx}{E}_T : \underset{\approx}{I}\right)\dot{T} \tag{1.65b}$$

where the stiffnesses are now interpreted in their usual sense without factors of density. These are the final equations used to update the temperature and stress in the SCRAM coding.

It's instructive to consider the special case where the material is damaged, but in an *isotropic* manner. For this special case, the stiffness is isotropic and $\underset{\approx}{E}_T : \underset{\approx}{I} = 3K\underset{\approx}{I}$, where K is the damaged bulk modulus. Consequently, Eq. (1.63) shows that the rate of the stress deviator is simply the deviatoric part of $\dot{\underset{\approx}{P}}_T$ and the pressure rate is given by

$$\dot{p} = \dot{p}_T + \rho_o c_v^m \gamma_m \frac{K}{K_m^T}\dot{T} \tag{1.65b}$$

This equation, which holds only for *isotropic* damage, is roughly equivalent to what was coded in the original version of SCRAM and was therefore inappropriate for general anisotropic deformations.

Incidentally, for highly compressive states, nonlinear corrections (assuming a linear U_s-u_p) are imposed in the same manner as early versions of SCRAM.

Linear Hugoniot model

This section is probably too rough to make any sense. I am attempting without much luck to also generalize the linear hugoniot model to accommodate anisotropy. Fortunately, for our cracked materials, the composite is approximately isotropic whenever there is large confining pressure, so the conventional linear hugoniot model may be used in highly compressed states.

Consider a shock propagating into quiescent material. Let a subscript "o" denote the state ahead of the shock. Let U denote the absolute propagation speed of the shock. Let $\underset{\sim}{V}$ denote the particle velocity behind the shock. The component of the particle velocity in the direction of the shock normal is defined:

$$V_n = \underset{\sim}{V} \bullet \hat{\underset{\sim}{n}} , \tag{1.66}$$

where $\hat{\underset{\sim}{n}}$ is the normal to the shock surface pointing the in relative propagation direction.

The jump condition for conservation of mass requires that

$$\rho_o U = \rho(U - V_n) \tag{1.67}$$

or, solving for V_n,

$$V_n = \varepsilon U \tag{1.68}$$

where ε is the volumetric compression given by

$$\varepsilon = 1 - \frac{\rho_o}{\rho} \tag{1.69}$$

Momentum conservation across this shock results in

$$\underset{\sim}{V} = \frac{\underset{\sim}{\Pi}_n}{U\rho_o} \tag{1.70}$$

where the compressive traction vector is defined

$$\underset{\sim}{\Pi}_n \equiv -\underset{\approx}{\sigma} \bullet \hat{\underset{\sim}{n}} \tag{1.71}$$

Let Π_{nn} denote the component of traction normal to the shock surface:

$$\Pi_{nn} \equiv \underset{\sim}{\Pi} \bullet \hat{\underset{\sim}{n}} . \tag{1.72}$$

Note that Π_{nn} is not generally equal to the pressure. Eq. (1.70) implies that

$$\Pi_{nn} = \rho_o U V_n \tag{1.73}$$

Assuming zero energy ahead of the shock, with no jumps in heat flux, the jump form of conservation of energy requires that

$$U\rho_o\left(u + \frac{1}{2}\underset{\sim}{V} \bullet \underset{\sim}{V}\right) = (\underset{\sim}{V} \bullet \underset{\sim}{\Pi}_n) \tag{1.74}$$

Characteristic segment. For a shock propagating into a quiescent undeformed material, it can be shown that the deformation gradient at the back side of the shock is of the form

$$\underline{F} = \underline{I} + \lambda\hat{\underline{n}} , \tag{1.75}$$

where $\underline{\lambda}$ is called the "characteristic segment" vector. For future reference, it follows that

$$J = \det\underline{F} = 1 + \underline{\lambda} \bullet \hat{\underline{n}} \tag{1.76}$$

and

$$\underline{F}^{-1} = \underline{I} - \frac{\underline{\lambda}\underline{n}}{J} \tag{1.77}$$

With Eq. (1.76), the volumetric compression becomes

$$\varepsilon = 1 - \frac{\rho_o}{\rho} = 1 - J = -\underline{\lambda} \bullet \hat{\underline{n}} \tag{1.78}$$

Using the jump laws (specialized for a shock propagating into quiescent material), it can be shown that

$$\underline{\lambda} = (\underline{F} - \underline{I}) \bullet \hat{\underline{N}} = \frac{\underline{\sigma} \bullet \underline{n}}{\rho_o U^2} = \frac{-\underline{\Pi}_n}{\rho_o U^2} = -\frac{\underline{V}}{U} \tag{1.79}$$

Uniaxial compression waves. Now limit discussion to waves for which $\underline{\lambda}$ is coaxial with $\hat{\underline{n}}$. Then $\underline{V} = V\hat{\underline{n}}$, and therefore

$$V_n = V . \tag{1.80}$$

For this special case, Eq. (1.74) becomes

$$\Pi V = \rho_o U\left(u + \frac{1}{2}V^2\right) \tag{1.81}$$

Combining Eqs. (1.73) and (1.81) shows that the total internal energy is partitioned equally between internal and kinetic energy, so that

$$u = \frac{1}{2}V^2 \tag{1.82}$$

Recall the Mie-Grüneisen form for the specific stress given in Eq. (

$$\underline{P} = \underline{P}_C - u_T\underline{\gamma} \qquad \text{where } u_T = u_T(\underline{v}, s) , \; \underline{P}_C = \underline{P}_C(\underline{v}) , \text{ and } \underline{\gamma} = \underline{\gamma}(\underline{v}) \tag{1.83}$$

Recalling that $u_T(\underline{v}, s) = u(\underline{v}, s) - u_c(\underline{v})$,

$$\underline{P} = -\underline{\gamma}u + \frac{\underline{f}}{\rho} \qquad \text{where } \underline{f} = \underline{f}(\underline{v}) \tag{1.84}$$

Here, the function $\underline{f}(\underline{v})$ is defined

$$\frac{\underline{f}(\underline{v})}{\rho} \equiv \underline{P}_C(\underline{v}) + u_c(\underline{v})\,\underline{\gamma}(\underline{v}) \tag{1.85}$$

Recall that the tensor $\underset{\approx}{P}$ represents *specific* stress. The Cauchy representation of $\underset{\approx}{P}$ is therefore $\underset{\approx}{P} = \underset{\approx}{\sigma}/\rho$ and Eq. (1.84) becomes

$$\underset{\approx}{\sigma} = -\rho\underset{\approx}{\gamma}u + \underset{\approx}{f} \qquad\qquad \text{where } \underset{\approx}{f} = \underset{\approx}{f}(\underset{\sim}{v}) \qquad (1.86)$$

Now define

$$\bar{\gamma} \equiv \hat{\underset{\sim}{n}} \bullet \underset{\approx}{\gamma} \bullet \hat{\underset{\sim}{n}} \quad \text{and} \quad f_{nn} \equiv \hat{\underset{\sim}{n}} \bullet \underset{\approx}{f} \bullet \hat{\underset{\sim}{n}} \qquad (1.87)$$

Then dotting Eq. (1.86) from the right and left by $\hat{\underset{\sim}{n}}$ gives

$$\Pi = \rho\gamma u - f \qquad (1.88)$$

Solving this equation for f and using Eqs. (1.82) and (1.73) gives

$$f = \rho\gamma u - \Pi = \rho\gamma\frac{1}{2}V^2 - \rho_o UV \qquad (1.89)$$

Suppose it is further presumed that the shock speed is linearly related to the particle speed so that

$$U = c_o + SV \qquad (1.90)$$

or, using (1.68),

$$U = c_o + S\varepsilon U \qquad (1.91)$$

Solving for U gives

$$U = \frac{c_o}{1 - S\varepsilon} \qquad (1.92)$$

Then Eq. (1.89) becomes

$$\boxed{f = \frac{H_o\varepsilon\left(\dfrac{\rho}{\rho_o}\gamma\dfrac{\varepsilon}{2} - 1\right)}{(1 - S\varepsilon)^2}} \qquad (1.93)$$

where

$$H_o \equiv \rho_o c_o^2 \qquad (1.94)$$

If it is further assumed that $\rho\gamma$ is constant, then Eq. (1.93) becomes

$$\boxed{f = \frac{H_o\varepsilon\left(\gamma_o\dfrac{\varepsilon}{2} - 1\right)}{(1 - S\varepsilon)^2} = -F(\varepsilon)} \qquad (1.95)$$

Keep in mind that the above result assumes that the jump in velocity occurs strictly for the normal component. Such a jump might not exist for anisotropic materials. If the material symmetries are orthotropic, then a shock of this nature seems possible. In this case, there are different values of H_o, S, and γ for each of the three orthotropic directions.

Substituting Eq. (1.95) into Eq. (1.88) (again assuming that $\rho\gamma$ is constant gives

$$\Pi = \rho_o\gamma_o u + F(\varepsilon) \qquad (1.96)$$

Formally, this can be written in rate form as

$$\dot{\Pi} \;=\; \rho_o \gamma_o \dot{u} + F'(\varepsilon)\frac{\dot{\varepsilon}}{\varepsilon} \tag{1.97}$$

Where

$$F'(\varepsilon) \;=\; \frac{1+(S-\gamma)\varepsilon}{(1-S\varepsilon)^3} H_o$$

Linear Hugoniot anisotropic constitutive law.

Consider the set O* of all symmetric second order tensors having principal directions coinciding with the orthotropy directions. Any linear combination of such tensors is also in the set. Therefore the set constitutes a subspace. The projection theorem then guarantees that any general stress state, $\underset{\approx}{P}$, can be decomposed into a part that is in O* and a part that is orthogonal to O*.

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