Module 2B - Constitutive Laws and Continuum Mechanics

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Contents

Objectives: Build the foundation of continuum mechanics.

Prerequisite Knowledge: Highschool Physics

Prerequisite Modules: 1A - Calculus, 1B - Linear Algebra, 1D - Differential Equations

Difficulty: Intermediate

Summary: Basic field equations were derived for many food manufacturing applications.

1 Theory

Remark: Throughout this work, boldface symbols imply vectors or tensors. For the inner product of two vectors (first order tensors) $\boldsymbol{u}$ and $\boldsymbol{v}$ we have in three dimensions, $\boldsymbol{u} \cdot \boldsymbol{v} = v_i u_i = u_1 v_1 + u_2 v_2 + u_3 v_3$, where Cartesian bases and Einstein index summation notation are used. At the risk of over simplification, we will ignore the difference between second order tensors and matrices. Furthermore, we exclusively employ a Cartesian bases. Readers that feel uncomfortable with this approach should consult the wide range of texts which point out the subtle differences, for example the texts listed in the references. Accordingly, if we consider the second order tensor $\boldsymbol{A} = A_{ik}\boldsymbol{e}_i \otimes \boldsymbol{e}_k$ with its matrix representation

$$[\boldsymbol{A}] \overset{\text{def}}{=} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \tag{1.1}$$

then a first order contraction (inner product) of two second order tensors $\boldsymbol{A} \cdot \boldsymbol{B}$ is defined by the matrix product $[\boldsymbol{A}][\boldsymbol{B}]$, with components of $A_{ij}B_{jk} = C_{ik}$. It is clear that the range of the inner index j must be the same for $[\boldsymbol{A}]$ and $[\boldsymbol{B}]$. For three dimensions we have $i, j = 1, 2, 3$. The second order inner product of two tensors or matrices is $\boldsymbol{A} : \boldsymbol{B} = A_{ij}B_{ij} = \operatorname{tr}\left([\boldsymbol{A}]^T[\boldsymbol{B}]\right)$. The divergence of a vector $\boldsymbol{u}$, which results in a contraction to a scalar, is defined by $\nabla_x \cdot \boldsymbol{u} = u_{i,i}$, whereas for a second order tensor, $\boldsymbol{A}$, $\nabla_x \cdot \boldsymbol{A}$ describes a contraction to a vector with the components $A_{ij,j}$. The gradient of a vector $\boldsymbol{u}$ (a dilation to a second order tensor) is given by $\nabla_x \boldsymbol{u}$ and has the components $u_{i,j}$, whereas for a second order tensor (a dilation to a third order tensor) $\nabla_x \boldsymbol{A}$ has components of $A_{ij,k}$. The gradient of a scalar ϕ (a dilation to a vector) is defined by $\nabla_x \phi$ and has the components $\phi_{,i}$. The scalar product of two second order tensors, for example the gradients of first order vectors, is defined as $\nabla_x \boldsymbol{v} : \nabla_x \boldsymbol{u} = \frac{\partial v_i}{\partial x_j}\frac{\partial u_i}{\partial x_j} \overset{\text{def}}{=} v_{i,j}u_{i,j}$, where $\partial u_i/\partial x_j, \partial v_i/\partial x_j$ are partial derivatives of u_i and v_i, and where u_i, v_i are the Cartesian components of $\boldsymbol{u}$ and $\boldsymbol{v}$. An example for the product of a tensor with a vector is $\nabla_x \boldsymbol{u} \cdot \boldsymbol{n}$ which has components of $u_{i,j}n_j$ in a Cartesian bases.

1.1 Kinematics of Deformation

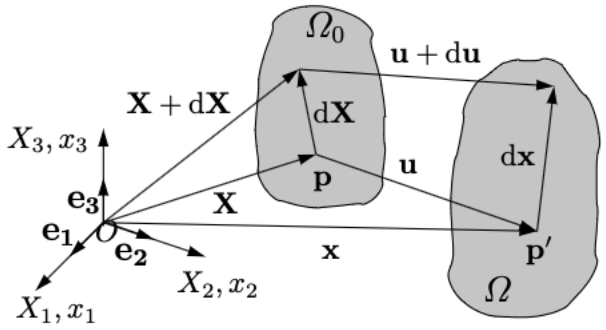

Figure 1.1: Different descriptions of a deforming body.

The term deformation refers to a change in the shape of the continuum between a reference configuration and current configuration. In the reference configuration, a representative particle of the continuum occupies a point $\mathbf{p}$ in space and has the position vector (Figure 1.1)

$$\boldsymbol{X} = X_1\boldsymbol{e}_1 + X_2\boldsymbol{e}_2 + X_3\boldsymbol{e}_3 \tag{1.2}$$

where $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ is a Cartesian reference triad, and X_1, X_2, X_3 (with center O) can be thought of as labels for a point. Sometimes the coordinates or labels (X_1, X_2, X_3, t) are called the referential coordinates. In the current configuration the particle originally located at point $\mathbf{p}$ is located at point $\mathbf{p}^0$ and can be expressed also in terms of another position vector $\boldsymbol{x}$, with the coordinates (x_1, x_2, x_3, t). These are called the current coordinates. It is obvious with this arrangement, that the displacement is $\boldsymbol{u} = \boldsymbol{x} \quad \boldsymbol{X}$ for a point originally at $\boldsymbol{X}$ and with final coordinates $\boldsymbol{x}$.

When a continuum undergoes deformation (or flow), its points move along various paths in space. This motion may be expressed by

$$\boldsymbol{x}(X_1, X_2, X_3, t) = \boldsymbol{u}(X_1, X_2, X_3, t) + \boldsymbol{X}(X_1, X_2, X_3, t) \tag{1.3}$$

which gives the present location of a point at time t, written in terms of the labels X_1, X_2, X_3. The previous position vector may be interpreted as a mapping of the initial configuration onto the current configuration. In classical approaches, it is assumed that such a mapping is a one-to-one and continuous, with continuous partial derivatives to whatever order is required. The description of motion or deformation expressed previously is known as the Lagrangian formulation. Alternatively, if the independent variables are the coordinates $\boldsymbol{x}$ and t, then $\boldsymbol{x}(x_1, x_2, x_3, t) = \boldsymbol{u}(x_1, x_2, x_3, t) + \boldsymbol{X}(x_1, x_2, x_3, t)$, and the formulation is denoted as Eulerian (Figure 1.1).

1.1.1 Deformation of line elements

Partial differentiation of the displacement vector $\boldsymbol{u} = \boldsymbol{x} \quad \boldsymbol{X}$, with respect to $\boldsymbol{x}$ and $\boldsymbol{X}$, produces the following displacement gradients:

$$\nabla_{\boldsymbol{X}}\boldsymbol{u} = \boldsymbol{F} \quad \mathbf{1} \quad \text{and} \quad \nabla_{\boldsymbol{x}}\boldsymbol{u} = \mathbf{1} \quad \overline{\boldsymbol{F}} \tag{1.4}$$

where

$$\nabla_{\boldsymbol{X}}\boldsymbol{x} \overset{\text{def}}{=} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} = \boldsymbol{F} \overset{\text{def}}{=} \begin{bmatrix} \frac{\partial x_1}{\partial X_1} & \frac{\partial x_1}{\partial X_2} & \frac{\partial x_1}{\partial X_3} \\ \frac{\partial x_2}{\partial X_1} & \frac{\partial x_2}{\partial X_2} & \frac{\partial x_2}{\partial X_3} \\ \frac{\partial x_3}{\partial X_1} & \frac{\partial x_3}{\partial X_2} & \frac{\partial x_3}{\partial X_3} \end{bmatrix} \tag{1.5}$$

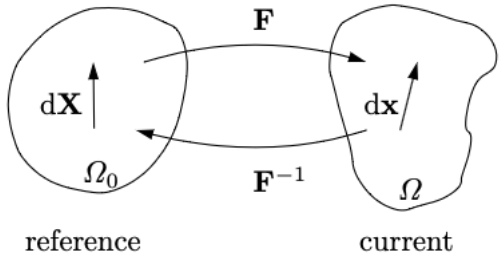

Figure 1.2: Mapping back and forth with the deformation gradient.

and

$$\nabla_{\boldsymbol{x}}\boldsymbol{X} \overset{\text{def}}{=} \frac{\partial \boldsymbol{X}}{\partial \boldsymbol{x}} = \overline{\boldsymbol{F}} \tag{1.6}$$

with the components $F_{ik} = x_{i,k}$ and $\bar{F}_{ik} = X_{i,k}$. $\boldsymbol{F}$ is known as the material deformation gradient, and $\bar{\boldsymbol{F}}$ is known as the spatial deformation gradient.

Now, consider the length of a differential element in the reference configuration $d\boldsymbol{X}$ and $d\boldsymbol{x}$ in the current configuration, $d\boldsymbol{x} = \boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{x}\ \ d\boldsymbol{X} = \boldsymbol{F}\ \ d\boldsymbol{X}$. Taking the difference in the magnitudes of these elements yields

$$\begin{aligned} d\boldsymbol{x}\ \ d\boldsymbol{x} \quad d\boldsymbol{X}\ \ d\boldsymbol{X} &= (\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{x}\ \ d\boldsymbol{X})\ \ (\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{x}\ \ d\boldsymbol{X}) \quad d\boldsymbol{X}\ \ d\boldsymbol{X} \\ &= d\boldsymbol{X}\ \ \left(\boldsymbol{F}^T\ \ \boldsymbol{F} \quad \mathbf{1}\right)\ \ d\boldsymbol{X} \overset{\text{def}}{=} 2d\boldsymbol{X}\ \ \boldsymbol{E}\ \ d\boldsymbol{X} \end{aligned} \tag{1.7}$$

Alternatively, we have with $d\boldsymbol{X} = \boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{X}\ \ d\boldsymbol{x} = \overline{\boldsymbol{F}}\ \ d\boldsymbol{x}$ and

$$\begin{aligned} d\boldsymbol{x}\ \ d\boldsymbol{x} \quad d\boldsymbol{X}\ \ d\boldsymbol{X} &= d\boldsymbol{x}\ \ d\boldsymbol{x} \quad (\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{X}\ \ d\boldsymbol{x})\ \ (\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{X}\ \ d\boldsymbol{x}) \\ &= d\boldsymbol{x}\ \ \left(\mathbf{1} \quad \overline{\boldsymbol{F}}^T\ \ \overline{\boldsymbol{F}}\right)\ \ d\boldsymbol{x} \overset{\text{def}}{=} 2d\boldsymbol{x}\ \ \boldsymbol{e}\ \ d\boldsymbol{x} \end{aligned} \tag{1.8}$$

Equation 1.7 defines the so-called Lagrangian strain tensor

$$\boldsymbol{E} \overset{\text{def}}{=} \frac{1}{2}\left(\boldsymbol{F}^T\ \ \boldsymbol{F} \quad \mathbf{1}\right) = \frac{1}{2}\left[\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u} + (\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u})^T + (\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u})^T\ \ \boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u}\right] \tag{1.9}$$

Frequently, the Lagrangian strain tensor is defined in terms of the so-called right Cauchy-Green strain, $\boldsymbol{C} = \boldsymbol{F}^T\ \ \boldsymbol{F}$ leading to $\boldsymbol{E} \overset{\text{def}}{=} \frac{1}{2}(\boldsymbol{C} \quad \mathbf{1})$. The Eulerian strain tensor is defined by Equation 1.8 as

$$\boldsymbol{e} \overset{\text{def}}{=} \frac{1}{2}\left(\mathbf{1} \quad \overline{\boldsymbol{F}}^T\ \ \overline{\boldsymbol{F}}\right) = \frac{1}{2}\left(\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u} + (\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u})^T \quad (\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u})^T\ \ \boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u}\right) \tag{1.10}$$

In a similar manner as for the Lagrangian strain tensor, the Eulerian strain tensor can be defined in terms of the so-called left Cauchy-Green strain $\boldsymbol{b} = \boldsymbol{F}\ \ \boldsymbol{F}^T$ which then yields $\boldsymbol{e} \overset{\text{def}}{=} \frac{1}{2}\left(\mathbf{1} \quad \boldsymbol{b}^{\ 1}\right)$.

Remark: It should be clear that $d\boldsymbol{x}$ can be reinterpreted as the result of a mapping $\boldsymbol{F}\ \ d\boldsymbol{X}\ \ !\ \ d\boldsymbol{x}$, or a change in configuration (reference to current), while $\overline{\boldsymbol{F}}\ \ d\boldsymbol{x}\ \ !\ \ d\boldsymbol{X}$, maps the current to the reference system. For the deformations to be invertible, and physically realizable, $\overline{\boldsymbol{F}}\ \ (\boldsymbol{F}\ \ d\boldsymbol{X}) = d\boldsymbol{X}$ and $\boldsymbol{F}\ \ (\overline{\boldsymbol{F}}\ \ d\boldsymbol{x}) = d\boldsymbol{x}$. We note that $(\det \overline{\boldsymbol{F}})(\det \boldsymbol{F}) = 1$ and have the following obvious relation $\overline{\boldsymbol{F}}\ \ \boldsymbol{F} = \mathbf{1}$. It should be clear that $\overline{\boldsymbol{F}} = \boldsymbol{F}^{\ 1}$.

1.1.2 Infinitesimal strain measures

In infinitesimal deformation theory, the displacement gradient components being "small" implies that higher order terms like $(\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u})^T\ \ \boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u}$ and $(\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u})^T\ \ \boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u}$ can be neglected in the strain measures $\boldsymbol{e}$ and $\boldsymbol{E}$ leading to $\boldsymbol{e}\quad^E \overset{\text{def}}{=} \frac{1}{2}\left[\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u} + (\boldsymbol{r}_{\boldsymbol{x}}\boldsymbol{u})^T\right]$ and $\boldsymbol{E}\quad^L \overset{\text{def}}{=} \frac{1}{2}\left[\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u} + (\boldsymbol{r}_{\boldsymbol{X}}\boldsymbol{u})^T\right]$. If the displacement gradients are small compared with unity, ^{E} and ^{L} coincide closely to $\boldsymbol{e}$ and $\boldsymbol{E}$, respectively. If we assume that, $\frac{\partial}{\partial \boldsymbol{X}} \quad \frac{\partial}{\partial \boldsymbol{x}}$, we may use ^{E} or ^{L} interchangeably. Usually $\quad$ is the symbol used for infinitesimal strains. Furthermore, to avoid confusion, when using models employing the geometrically linear infinitesimal strain assumption we use the symbol of $\boldsymbol{r}$ with no $\boldsymbol{X}$ or $\boldsymbol{x}$ subscript. Hence the infinitesimal strains are defined by

$$= \frac{1}{2}\left(\boldsymbol{r}\,\boldsymbol{u} + (\boldsymbol{r}\,\boldsymbol{u})^T\right) \tag{1.11}$$

1.1.3 The Jacobian of the Deformation Gradient

The Jacobian of the deformation gradient, $\boldsymbol{F}$, is defined as

$$J \overset{\text{def}}{=} \det \boldsymbol{F} = \begin{vmatrix} \frac{\partial x_1}{\partial X_1} & \frac{\partial x_1}{\partial X_2} & \frac{\partial x_1}{\partial X_3} \\ \frac{\partial x_2}{\partial X_1} & \frac{\partial x_2}{\partial X_2} & \frac{\partial x_2}{\partial X_3} \\ \frac{\partial x_3}{\partial X_1} & \frac{\partial x_3}{\partial X_2} & \frac{\partial x_3}{\partial X_3} \end{vmatrix} \tag{1.12}$$

To interpret the Jacobian in a physical way, consider a reference differential volume in Figure 1.3 which is given by $dS^3 = d\omega$, where $d\boldsymbol{X}^{(1)} = dS\boldsymbol{e}_1, d\boldsymbol{X}^{(2)} = dS\boldsymbol{e}_2$ and $d\boldsymbol{X}^{(3)} = dS\boldsymbol{e}_3$. The current differential element

is described by $d\boldsymbol{x}^{(1)} = \frac{\partial \boldsymbol{x}}{\partial X}\ d\boldsymbol{X}^{(1)} = \frac{\partial \boldsymbol{x}}{\partial X}\ \boldsymbol{e}_1 dS, d\boldsymbol{x}^{(2)} = \frac{\partial \boldsymbol{x}}{\partial X}\ d\boldsymbol{X}^{(2)} = \frac{\partial \boldsymbol{x}}{\partial X}\ \boldsymbol{e}_2 dS$ and $d\boldsymbol{x}^{(3)} = \frac{\partial \boldsymbol{x}}{\partial X}\ d\boldsymbol{X}^{(3)} = \frac{\partial \boldsymbol{x}}{\partial X}\ \boldsymbol{e}_3 dS$ where $\boldsymbol{e}_1 = (1,0,0)^T, \boldsymbol{e}_2 = (0,1,0)^T$ and $\boldsymbol{e}_3 = (0,0,1)^T$ are unit vectors, and

$$\underbrace{d\boldsymbol{x}^{(1)} \quad \left(d\boldsymbol{x}^{(2)} \quad d\boldsymbol{x}^{(3)}\right)}_{\stackrel{\text{def}}{=} d\omega} = \begin{vmatrix} dx_1^{(1)} dx_2^{(1)} dx_3^{(1)} \\ dx_1^{(2)} dx_2^{(2)} dx_3^{(2)} \\ dx_1^{(3)} dx_2^{(3)} dx_3^{(3)} \end{vmatrix} = \underbrace{\begin{vmatrix} \frac{\partial x_1}{\partial X_1} \frac{\partial x_2}{\partial X_1} \frac{\partial x_3}{\partial X_1} \\ \frac{\partial x_1}{\partial X_2} \frac{\partial x_2}{\partial X_2} \frac{\partial x_3}{\partial X_2} \\ \frac{\partial x_1}{\partial X_3} \frac{\partial x_2}{\partial X_3} \frac{\partial x_3}{\partial X_3} \end{vmatrix}}_{|\boldsymbol{F}^T| = |\boldsymbol{F}| \stackrel{\text{def}}{=} J} dS^3. \tag{1.13}$$

Therefore, $d\omega = J d\omega_0$. Thus, the Jacobian of the deformation gradient must remain positive definite, otherwise we obtain physically impossible "negative" volumes.

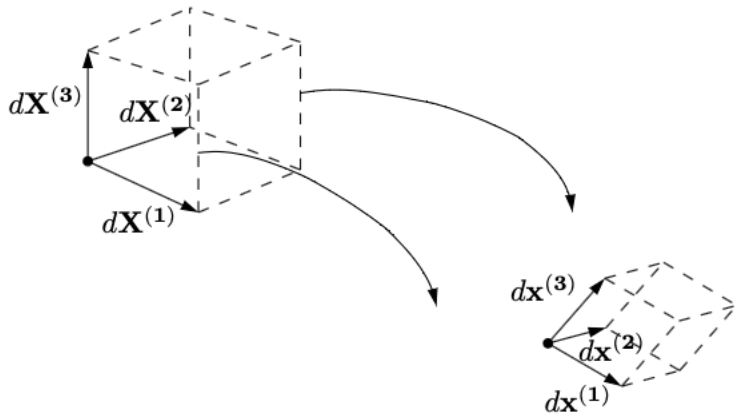

Figure 1.3: A differential volume element.

1.2 Equilibrium/kinetics of solid continua

We start with the following postulated balance law for an arbitrary part ω around a point P with boundary $\partial\omega$ of a body Ω, see Figure 1.4

$$\underbrace{\int_{\partial\omega} \boldsymbol{t}\, da}_{\text{surface forces}} + \underbrace{\int_{\omega} \boldsymbol{f}\, d\omega}_{\text{body forces}} = \underbrace{\frac{d}{dt}\int_{\omega} \rho \dot{\boldsymbol{u}}\, d\omega}_{\text{inertial forces}} \tag{1.14}$$

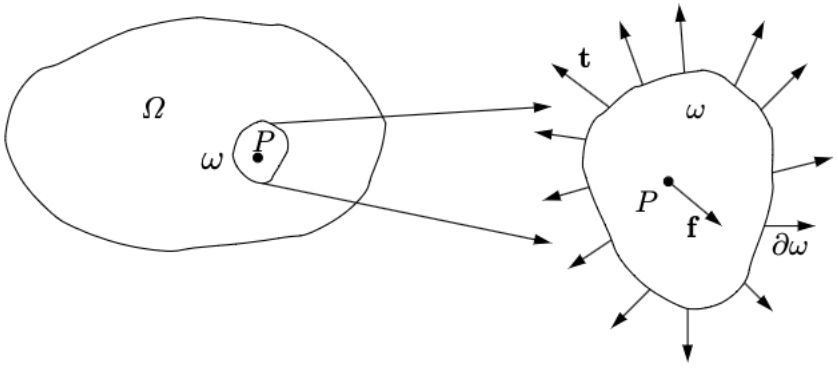

Figure 1.4: Newton's laws applied to a continuum.

where ρ is the material density, $\boldsymbol{b}$ is the body force per unit mass ($\boldsymbol{f} = \rho\boldsymbol{b}$) and $\dot{\boldsymbol{u}}$ is the time derivative of the displacement. When the actual molecular structure is considered on a sub-microscopic scale, the force densities, $\boldsymbol{t}$, which we commonly refer to as "surface forces", are taken to involve short-range intermolecular forces. Tacitly we assume that the effects of radiative forces, and others which do not require momentum transfer through a continuum, are negligible. This is a so-called local action postulate. As long as the volume element is large, our resultant body and surface forces may be interpreted as sums of these intermolecular forces. When we pass to larger scales, we can justifiably use the continuum concept.

1.2.1 Postulates on volume and surface quantities

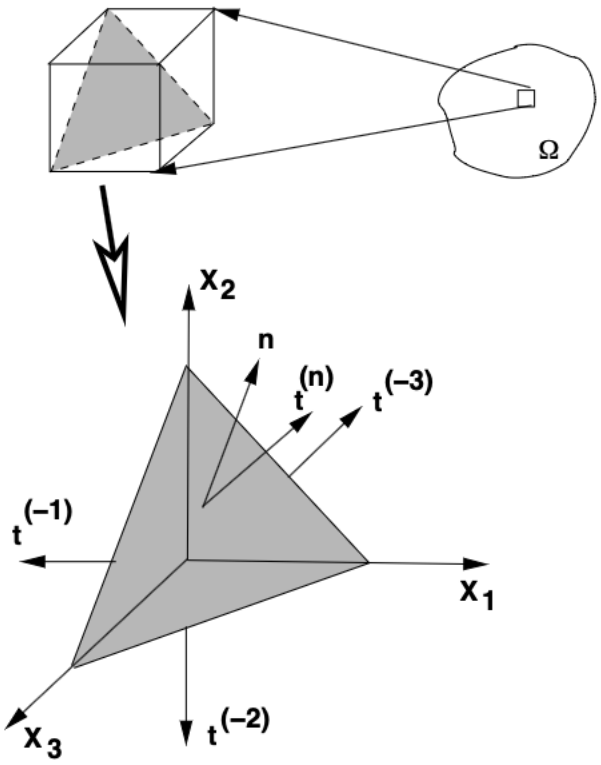

Figure 1.5: Cauchy tetrahedron: a "sectioned material point".

Now, consider a tetrahedron in equilibrium, as shown in Figure 1.5. From Newton's laws,

$$\boldsymbol{t}^{(n)}\Delta A^{(n)} + \boldsymbol{t}^{(-1)}\Delta A^{(1)} + \boldsymbol{t}^{(-2)}\Delta A^{(2)} + \boldsymbol{t}^{(-3)}\Delta A^{(3)} + \boldsymbol{f}\,\Delta V = \rho\Delta V\ddot{\boldsymbol{u}}, \tag{1.15}$$

where $\Delta A^{(n)}$ is the surface area of the face of the tetrahedron with normal $\boldsymbol{n}$, and ΔV is the tetrahedron volume. Clearly, as the distance between the tetrahedron base (located at (0,0,0)) and the surface center, denoted h, goes to zero ($h \to 0$) we have $\Delta A^{(n)} \to 0 \Rightarrow \frac{V}{A^{(n)}} \to 0$. Geometrically, we have $\frac{A^{(i)}}{A^{(n)}} = \cos(x_i, x_n) \overset{\text{def}}{=} n_i$, and therefore $\boldsymbol{t}^{(n)} + \boldsymbol{t}^{(-1)}\cos(x_1, x_n) + \boldsymbol{t}^{(-2)}\cos(x_2, x_n) + \boldsymbol{t}^{(-3)}\cos(x_3, x_n) = \boldsymbol{0}$. It is clear that forces on the surface areas could be decomposed into three linearly independent components. It is convenient to introduce the concept of stress at a point, representing the surface forces there, pictorially represented by a cube surrounding a point. The fundamental issue that must be resolved is the characterization of these surface forces. We can represent the force density vector, the so-called "traction", on a surface by the component representation:

$$\boldsymbol{t} \overset{\text{def}}{=} \left\{ \begin{array}{c} \sigma_{i1} \\ \sigma_{i2} \\ \sigma_{i3} \end{array} \right\}, \tag{1.16}$$

where the second index represents the direction of the component and the first index represents the normal to corresponding coordinate plane. From this point forth, we will drop the superscript notation of $\boldsymbol{t}^{(n)}$, where it is implicit that $\boldsymbol{t} \overset{\text{def}}{=} \boldsymbol{t}^{(n)} = \quad^{T} \boldsymbol{n}$, where

$$\overset{\text{def}}{=} \left[\begin{array}{ccc} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{array} \right], \tag{1.17}$$

or explicitly $\left(\boldsymbol{t}^{(1)} = \quad \boldsymbol{t}^{(\ 1)}, \boldsymbol{t}^{(2)} = \quad \boldsymbol{t}^{(\ 2)}, \boldsymbol{t}^{(3)} = \quad \boldsymbol{t}^{(\ 3)}\right)$

$$\boldsymbol{t} = \boldsymbol{t}^{(1)} n_1 + \boldsymbol{t}^{(2)} n_2 + \boldsymbol{t}^{(3)} n_3 = \quad^{T} \boldsymbol{n} = \left[\begin{array}{ccc} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{array} \right]^{T} \left\{ \begin{array}{c} n_1 \\ n_2 \\ n_3 \end{array} \right\}, \tag{1.18}$$

where σ is the so-called Cauchy stress tensor.[1]

1.2.2 Balance law formulations

Substitution of Equation 1.18 into Equation 1.14 yields ($\omega \quad \Omega$)

$$\underbrace{\int_{\partial\omega} \quad^{T} \boldsymbol{n} da}_{\text{surface forces}} + \underbrace{\int_{\omega} \boldsymbol{f}\, d\omega}_{\text{body forces}} = \underbrace{\frac{d}{dt} \int_{\omega} \rho \ddot{\boldsymbol{u}} d\omega}_{\text{inertial forces}} \tag{1.19}$$

A relationship can be determined between the densities in the current and reference configurations, $\int_{\omega} \rho d\omega = \int_{\omega_0} \rho J d\omega_0 = \int_{\omega_0} \rho_0 d\omega_0$. Therefore, the Jacobian can also be interpreted as the ratio of material densities at a point. Since the volume is arbitrary, we can assume that $\rho J = \rho_0$ holds at every point in the body. Therefore, we may write $\frac{d}{dt}(\rho_0) = \frac{d}{dt}(\rho J) = 0$, when the system is mass conservative over time. This leads to writing the last term in Equation 1.19 as $\frac{d}{dt}\int_{\omega} \rho \dot{\boldsymbol{u}} d\omega = \int_{\omega_0} \frac{d(\rho J)}{dt} \dot{\boldsymbol{u}} d\omega_0 + \int_{\omega_0} \rho \ddot{\boldsymbol{u}} J d\omega_0 = \int_{\omega} \rho \ddot{\boldsymbol{u}} d\omega$. From Gauss's Divergence theorem, and an implicit assumption that σ is differentiable, we have $\int_{\omega} \left(\boldsymbol{r}_x \quad \sigma^T + \boldsymbol{f} \quad \rho \ddot{\boldsymbol{u}} \right) d\omega = \boldsymbol{0}$. If the volume is argued as being arbitrary, then the relation in the integral must hold pointwise, yielding

$$\boldsymbol{r}_x \quad^{T} + \boldsymbol{f} = \rho \ddot{\boldsymbol{u}} \tag{1.20}$$

Symmetry of the stress tensor

Starting with an angular momentum balance, under the assumptions that no infinitesimal "micromoments" or so-called "couple-stresses" exist, then it can be shown that the stress tensor must be symmetric (Malvern [?]), i.e. $\int_{\partial\omega} \boldsymbol{x} \quad \boldsymbol{t} da + \int_{\omega} \boldsymbol{x} \quad \boldsymbol{f}\, d\omega = \frac{d}{dt}\int_{\omega} \boldsymbol{x} \quad \rho \dot{\boldsymbol{u}} d\omega$, which implies $\quad^{T} = \quad$ It is somewhat easier to consider a differential element, such as in Figure 1.6 and to simply sum moments about the center. Doing this one immediately obtains $\sigma_{12} = \sigma_{21}, \sigma_{23} = \sigma_{32}$ and $\sigma_{13} = \sigma_{31}$. Therefore

$$\boldsymbol{t} = \boldsymbol{t}^{(1)} n_1 + \boldsymbol{t}^{(2)} n_2 + \boldsymbol{t}^{(3)} n_3 = \quad \boldsymbol{n} = \quad^{T} \boldsymbol{n}. \tag{1.21}$$

This implies that Equation 1.19 becomes

$$\boldsymbol{r}_x \quad + \boldsymbol{f} = \rho \ddot{\boldsymbol{u}}. \tag{1.22}$$

[1] Some authors follow the notation with the rst index represents the direction of the component and the second index represents the normal to corresponding coordinate plane. This leads to $\boldsymbol{t} \overset{\text{def}}{=} \boldsymbol{t}^{(n)} = \quad \boldsymbol{n}$. In the absence of couple stresses, a balance of angular momentum implies a symmetry of stress, $\quad = \quad^{T}$, and thus the di erence in notations become immaterial.

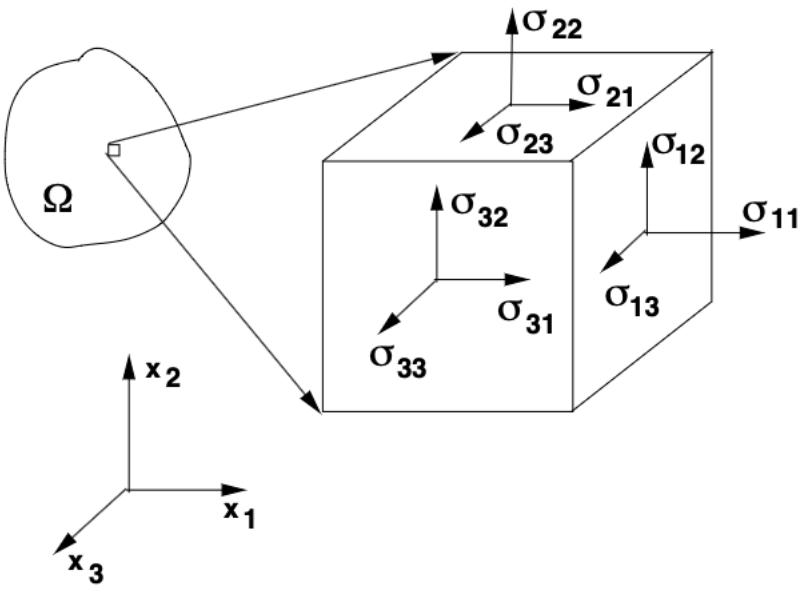

Figure 1.6: Stress at a point.

1.3 Referential descriptions of balance laws

In some cases it is quite difficult to perform a stress analysis for finite deformation solid mechanics problem, in the current configuration, primarily because it is unknown a priori. Therefore, frequently, all quantities are usually transformed ("pulled") back to the original coordinates, the referential frame. Therefore, it is preferable to think of a formulation in terms of the referential fixed coordinates $\boldsymbol{X}$, a so called Lagrangian formulation. With this in mind, there are two commonly used referential measures of stresses. We start by developing a purely mathematical result, leading to the so-called "Nanson" formula for transformation of surface elements. Consider the cross product of two differential line elements in a current configuration, $d\boldsymbol{x}^{(1)} \quad d\boldsymbol{x}^{(2)} = \left(\boldsymbol{F} \quad d\boldsymbol{X}^{(1)}\right) \quad \left(\boldsymbol{F} \quad d\boldsymbol{X}^{(2)}\right)$. The right hand side of this relation can be reformulated[2] $\left(\boldsymbol{F} \quad d\boldsymbol{X}^{(1)}\right) \quad \left(\boldsymbol{F} \quad d\boldsymbol{X}^{(2)}\right) = (\det \boldsymbol{F})\boldsymbol{F}^{\quad T} \quad \left(d\boldsymbol{X}^{(1)} \quad d\boldsymbol{X}^{(2)}\right)$. This leads to the so-called Nanson formula

$$\boldsymbol{n}da = (\det \boldsymbol{F})\boldsymbol{F}^{\quad T} \quad \boldsymbol{n}_0 da_0 = J\boldsymbol{F}^{\quad T} \quad \boldsymbol{n}_0 da_0 \tag{1.23}$$

[2] An important vector identity (see Chandriashakiah and Debnath [1]) for a tensor $\boldsymbol{T}$ and two rst order vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is $(\boldsymbol{T} \quad \boldsymbol{a}) \quad (\boldsymbol{T} \quad \boldsymbol{b}) = \boldsymbol{T}^* \quad (\boldsymbol{a} \quad \boldsymbol{b})$, where the $\boldsymbol{T}^*$ is the transpose of the adjoint de ned by $\boldsymbol{T}^* \stackrel{\text{def}}{=} (\det \boldsymbol{T})\boldsymbol{T}^{-T}$.

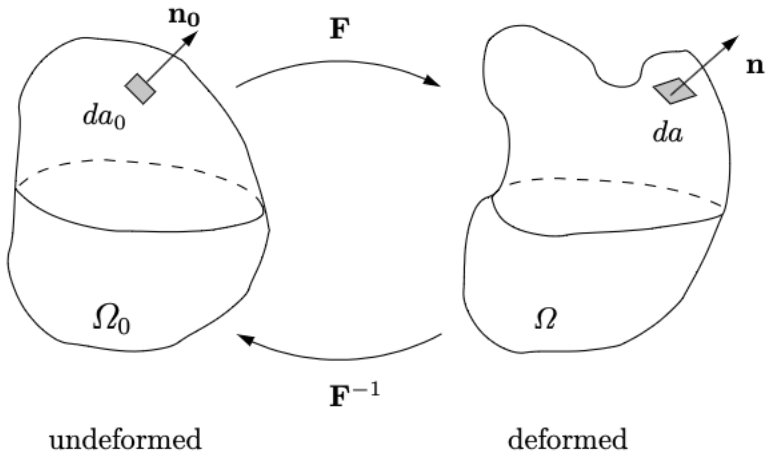

Figure 1.7: A current and reference surface element.

Knowing this, we now formulate the equations of equilibrium in the current or a reference configuration. Consider two surface elements, one on the current configuration, and one on a reference configuration. Let us form a new kind of stress tensor, call it $\boldsymbol{P}$, such that the amount of force is the same:[3] $\boldsymbol{P}^T \boldsymbol{n}_0 da_0 = {}^T \boldsymbol{n} da = {}^T \boldsymbol{F}^{-T} (\det \boldsymbol{F}) \boldsymbol{n}_0 da_0$. This implies ($J = \det \boldsymbol{F}$)

$$\boldsymbol{P}^T = J {}^T \boldsymbol{F}^{-T} \quad) \quad \boldsymbol{P} = J \boldsymbol{F}^{-1} \tag{1.24}$$

The tensor $\boldsymbol{P}$ is called the first Piola-Kirchhoff stress, and gives the actual force on the current area, but calculated per unit area of reference area. *It is is not symmetric, and this sometimes causes di culties in an analysis.* Therefore, we symmetrize it by forming a new tensor $\boldsymbol{S} \overset{\text{def}}{=} \boldsymbol{P} \boldsymbol{F}^{-T} = \boldsymbol{S}^T$. This yields the so-called second Piola-Kirchhoff stress

$$\boldsymbol{S} = \boldsymbol{P} \boldsymbol{F}^{-T} = J \boldsymbol{F}^{-1} \boldsymbol{F}^{-T} \tag{1.25}$$

By definition we have $\int_{\partial\omega_0} \boldsymbol{P}^T \boldsymbol{n}_0 da_0 = \int_{\partial\omega} {}^T \boldsymbol{n} da$, and thus

$$\underbrace{\int_{\partial\omega_0} \boldsymbol{P}^T \boldsymbol{n}_0 da_0}_{\text{surface forces}} + \underbrace{\int_{\omega_0} \boldsymbol{f} J d\omega_0}_{\text{body forces}} = \frac{d}{dt} \int_{\omega_0} \rho_0 \dot{\boldsymbol{u}} d\omega_0, \tag{1.26}$$

and therefore

$$\underbrace{\int_{\omega_0} r_X \boldsymbol{P}^T d\omega_0}_{\text{surface forces}} + \underbrace{\int_{\omega_0} \boldsymbol{f} J d\omega_0}_{\text{body forces}} = \int_{\omega_0} \rho_0 \frac{d\dot{\boldsymbol{u}}}{dt} d\omega_0. \tag{1.27}$$

With $\boldsymbol{P} = \boldsymbol{S} \boldsymbol{F}^T$ the last equation yields $\int_{\omega_0} r_X \left(\boldsymbol{S} \boldsymbol{F}^T\right)^T d\omega_0 + \int_{\omega_0} \boldsymbol{f} J d\omega_0 = \int_{\omega_0} \rho_0 \frac{d\dot{\boldsymbol{u}}}{dt} d\omega_0$ Since the control volume is arbitrary, we have

$$r_X \boldsymbol{P}^T + \boldsymbol{f} J = \rho_0 \frac{d\dot{\boldsymbol{u}}}{dt} \quad \text{or} \quad r_X (\boldsymbol{F} \boldsymbol{S}) + \boldsymbol{f} J = \rho_0 \frac{d\dot{\boldsymbol{u}}}{dt}. \tag{1.28}$$

[3] We start from the general case where the Cauchy stress is not symmetric, then enforce symmetry later.

1.4 The First Law of Thermodynamics / An energy balance

The interconversions of mechanical, thermal and chemical energy in a system are governed by the first law of thermodynamics. It states that the time rate of change of the total energy, $K + I$, is equal to the work rate, P and the net heat supplied, $H + Q$,

$$\frac{d}{dt}(K + I) = P + H + Q \tag{1.29}$$

Here the kinetic energy of a subvolume of material contained in Ω, denoted ω, is $K \stackrel{\text{def}}{=} \int_\omega \frac{1}{2}\rho \dot{\mathbf{u}} \quad \dot{\mathbf{u}} d\omega$, the rate of work or power of external forces acting on ω is given by $P \stackrel{\text{def}}{=} \int_\omega \rho \mathbf{b} \quad \dot{\mathbf{u}} d\omega + \int_{\partial\omega} \quad \mathbf{n} \quad \dot{\mathbf{u}} da$, the heat flow into the volume by conduction is $Q \stackrel{\text{def}}{=} \quad \int_{\partial\omega} \mathbf{q} \quad \mathbf{n} da = \quad \int_\omega \nabla_x \quad \mathbf{q} d\omega$, the heat generated due to sources, *such as chemical reactions*, is $H \stackrel{\text{def}}{=} \int_\omega \rho z d\omega$ and the stored energy is $I \stackrel{\text{def}}{=} \int_\omega \rho w d\omega$. If we make the assumption that the mass in the system is constant, one has,

$$\text{current mass } = \int_\omega \rho d\omega = \int_{\omega_0} \rho J d\omega_0 \quad \int_{\omega_0} \rho_0 d\omega_0 = \text{ original mass,} \tag{1.30}$$

which implies $\rho J = \rho_0 \;\;) \;\; \dot{\rho} J + \rho \dot{J} = 0$. Using this and the energy balance leads to

$$\begin{aligned} \frac{d}{dt}\int_\omega \frac{1}{2}\rho \dot{\mathbf{u}} \quad \dot{\mathbf{u}} d\omega &= \int_{\omega_0} \frac{d}{dt}\frac{1}{2}(\rho J \dot{\mathbf{u}} \quad \dot{\mathbf{u}}) d\omega_0 \\ &= \int_{\omega_0} \left(\frac{d}{dt}\rho_0\right)\frac{1}{2}\dot{\mathbf{u}} \quad \dot{\mathbf{u}} d\omega_0 + \int_\omega \rho \frac{d}{dt}\frac{1}{2}(\dot{\mathbf{u}} \quad \dot{\mathbf{u}}) d\omega \\ &= \int_\omega \rho \dot{\mathbf{u}} \quad \ddot{\mathbf{u}} d\omega \end{aligned} \tag{1.31}$$

We also have

$$\frac{d}{dt}\int_\omega \rho w d\omega = \frac{d}{dt}\int_{\omega_0} \rho J w d\omega_0 = \int_{\omega_0} \frac{d}{dt}(\rho_0)\, w d\omega_0 + \int_\omega \rho \dot{w} d\omega. \tag{1.32}$$

By using the divergence theorem, we obtain

$$\int_{\partial\omega} \quad \mathbf{n} \quad \dot{\mathbf{u}} da = \int_\omega \nabla_x \quad (\quad \dot{\mathbf{u}}) d\omega = \int_\omega (\nabla_x \quad) \quad \dot{\mathbf{u}} d\omega + \int_\omega \quad : \nabla_x \dot{\mathbf{u}} d\omega. \tag{1.33}$$

Combining the results, and enforcing balance of momentum, leads to

$$\begin{aligned} \int_\omega (\rho \dot{w} + \dot{\mathbf{u}} \quad (\rho \ddot{\mathbf{u}} \quad \nabla_x \quad \rho \mathbf{b}) \quad : \nabla_x \dot{\mathbf{u}} + \nabla_x \quad \mathbf{q} \quad \rho z)\, d\omega = \\ \int_\omega (\rho \dot{w} \quad : \nabla_x \dot{\mathbf{u}} + \nabla_x \quad \mathbf{q} \quad \rho z)\, d\omega = 0 \end{aligned} \tag{1.34}$$

Since the volume ω is arbitrary, the integrand must hold locally and we have

$$\rho \dot{w} \quad : \nabla_x \dot{\mathbf{u}} + \nabla_x \quad \mathbf{q} \quad \rho z = 0 \tag{1.35}$$

In later chapters dealing with multifield problems, this equation will be investigated more extensively.

Remark: Through similar arguments as above, one can reformulate the First Law of Thermodynamics in the reference configuration as

$$\rho_0 \dot{w} \quad \mathbf{S} : \dot{\mathbf{E}} + \nabla_X \quad \mathbf{q}_0 \quad \rho_0 z = 0, \tag{1.36}$$

where $\mathbf{q}_0 = \mathbf{q} J \quad \mathbf{F} \quad ^T$.

1.5 The Second Law of Thermodynamics/A restriction

Consider the quantity commonly known as the "entropy" of a volume $H \stackrel{\text{def}}{=} \int_\omega \rho\eta d\omega$, where η is the entropy per unit mass, or "specific" entropy[4]. The rate of entropy input is $Q \stackrel{\text{def}}{=} \int_\omega \rho\frac{z}{\theta}d\omega - \int_{\partial\omega}\frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{n}da$, where $\rho\frac{z}{\theta}$ is the entropy source and $\frac{\boldsymbol{q}}{\theta}$ is the entropy "influx". *The basic postulate of Clausius (1854)-Duhem (1901), is*

$$\dot{H} \geq Q \;\Rightarrow\; \frac{d}{dt}\int_\omega \rho\eta d\omega \geq \int_\omega \rho\frac{z}{\theta}d\omega + \int_{\partial\omega}\frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{n}da \geq 0. \tag{1.37}$$

In other words, the time rate of change of entropy in the body is no less than the entropy input into the body. The last expression can be recast in various useful forms. We have $\frac{d}{dt}\int_\omega \rho\eta d\omega = \frac{d}{dt}\int_{\omega_0}\rho J\eta d\omega_0 = \int_{\omega_0}\frac{d}{dt}(\rho_0)\,\eta d\omega_0 + \int_\omega \rho\dot{\eta}d\omega$. Furthermore, by the divergence theorem we have $\int_{\partial\omega}\frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{n}da = \int_\omega \nabla_x\cdot\frac{\boldsymbol{q}}{\theta}d\omega$. Inserting these relations, and since the volume ω is arbitrary, the integrand must hold locally and we have

$$\rho\dot{\eta} \geq \rho\frac{z}{\theta} + \nabla_x\cdot\frac{\boldsymbol{q}}{\theta} \geq 0 \tag{1.38}$$

By expanding $\nabla_x\cdot\frac{\boldsymbol{q}}{\theta} = \frac{1}{\theta}\nabla_x\cdot\boldsymbol{q} - \frac{1}{\theta^2}(\nabla_x\theta)\cdot\boldsymbol{q}$, we obtain $\rho\dot{\eta} \geq \rho\frac{z}{\theta} + \left(\frac{1}{\theta}\nabla_x\cdot\boldsymbol{q} - \frac{1}{\theta^2}(\nabla_x\theta)\cdot\boldsymbol{q}\right) \geq 0$. Employing the First Law of Thermodynamics, we obtain $\rho\theta\dot{\eta} \geq \rho\dot{w} + \mathbf{T}:\nabla_x\dot{\boldsymbol{u}} - \rho z - \frac{1}{\theta}(\nabla_x\theta)\cdot\boldsymbol{q} \geq 0$. A consistent physical observation is that, in the absence of external input, heat flows from a region of higher temperature to that of a lower temperature (hot to cold), i.e. heat never flows against the temperature gradient, $\nabla_x\theta\cdot\boldsymbol{q} \leq 0$. Thus, if Fourier's law ($\boldsymbol{q} = -\mathbf{K}\nabla_x\theta$) is used, $\nabla_x\theta\cdot\mathbf{K}\nabla_x\theta \geq 0$ implies that $\mathbf{K}$ must be positive definite. Since $\nabla_x\theta\cdot\boldsymbol{q} \leq 0$, we have $\rho\theta\dot{\eta} \geq \rho\dot{w} + \mathbf{T}:\nabla_x\dot{\boldsymbol{u}} - \frac{1}{\theta}(\nabla_x\theta)\cdot\boldsymbol{q} \geq 0$ or $\rho\theta\dot{\eta} \geq \rho z + \nabla_x\cdot\boldsymbol{q} - \frac{1}{\theta}(\nabla_x\theta)\cdot\boldsymbol{q} \geq 0$. When $\nabla_x\theta = \mathbf{0}$ then we have $\rho\theta\dot{\eta} \geq \rho\dot{w} + \mathbf{T}:\nabla_x\dot{\boldsymbol{u}} \geq 0$ or $\rho\theta\dot{\eta} \geq \rho z + \nabla_x\cdot\boldsymbol{q} \geq 0$, either of which is referred to as the Clausius (1854)-Planck (1887) inequality. Such inequalities can be used to invalidate or construct (complicated) constitutive laws, although throughout this monograph, standard models, where the Second Law of Thermodynamics is satisfied automatically, are employed.

1.6 Linearly elastic constitutive equations

The fundamental mechanism that produces forces in elastic deformation is the stretching of atomic bonds. In Figure 1.8, a force/atom-separation curve is depicted. If the deformations are small, then one can argue that we are dealing with only the linear portion of the curve. Ultimately, this allows us to usually use linear relationships for models relating forces to deformations. Atoms in materials are held together by electronic forces, or bonds, whose behavior resembles that of little springs. The stiffness of an atomic bond force between two atoms is shown in Figure 1.8. If we compute simple expressions for the force versus strain, we have $F = \frac{K(1.25-1)r}{r} = 0.25K \Rightarrow F = \frac{K}{4}$. Some materials, mainly ceramics, truly exhibit this theoretical stiffness. Most materials do not exactly exhibit this stiffness, however, the relationships are approximately *linear* between the atomic force and atom separation, for small deformations.

[4] Loosely speaking, the entropy is a measure of the disorder in a system.

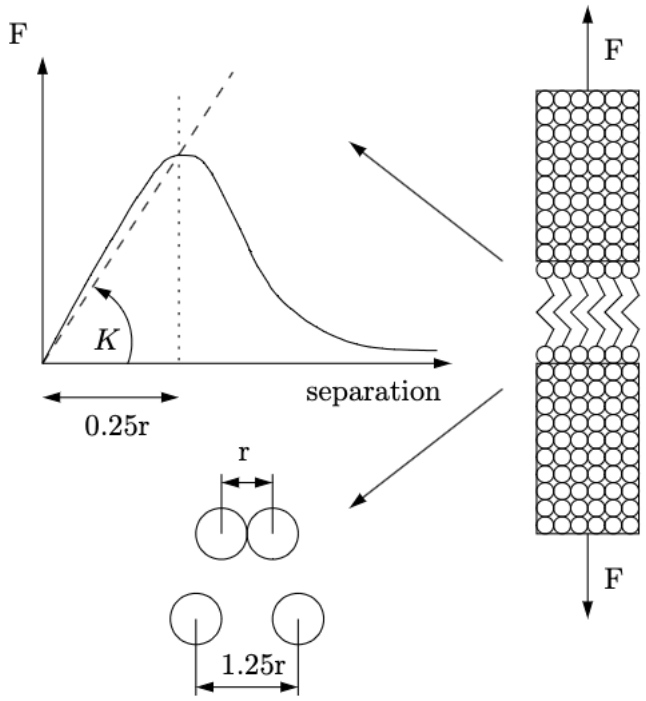

Figure 1.8: The atomic bond force as a function of atom separation.

In order to determine the material properties of structural materials, engineers usually resort to a macroscopic tension test for material data. The usual procedure to determine tensile properties of materials is to place samples of material in testing machines, apply the loads, and then to measure the resulting deformations, such as lengths and changes in diameter in a portion of the specimen, of circular cross-section, called the gage length. The location of the gage length is away from the attachments to the testing machine (Figure 1.9). The ends where the samples are attached to the machine are larger so that failure will not occur there first, which would ruin the experimental measurements. Slow rates of deformation are applied, and the response is usually measured with strain gauges or extensometers. For a metal, samples are usually 1.25 cm in diameter and 5 cm in length. Compression tests are usually on cubes (5 cm × 5 cm × 5 cm) or cylinders (2.5 cm in diameter and 2.5 cm in length). Here both the load applied by the machine, and the shortening of the specimen, should be measured over the gage length. For concrete, a material that is expected to carry compressive loads, the specimens are usually on the order of 15 cm in diameter and 30 cm long.[5]

The immediate result of a tension test is the axial force (F) divided by the original area (A_0) denoted, loosely speaking, as the "stress", and change in length $\left(\Delta L \overset{\text{def}}{=} L \quad L_0\right)$ per unit length (ϵ_0) or "engineering strain", which is typically measured by strain gauges. As a first approximation we define the tensile stiffness of the material, known as Young's Modulus, denoted E, by $\sigma_0 \overset{\text{def}}{=} \frac{F}{A_0} = E\frac{L}{L} \overset{\text{def}}{=} E\epsilon_0$. As we know, the terms σ_0 and ϵ_0 are, strictly speaking, not the true stress and strain, but simply serve our presentation purposes. Clearly, what we have presented is somewhat ad hoc, therefore, next we present the classical theory of linearly elastic material responses for three dimensional states of stress and strain.

[5] Concrete is usually aged 28 days before testing.

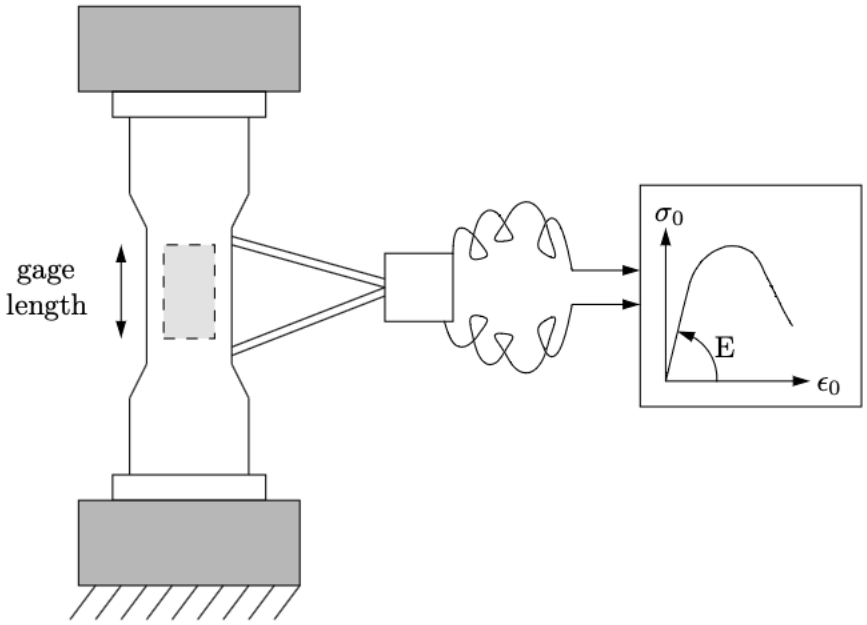

Figure 1.9: A standard metals testing machine.

1.6.1 The infinitesimal strain case

Initially we discuss relationships between the stress and strain, so-called "material laws" or " constitutive relations" for geometrically linear problems (infinitesimal deformations). Accordingly, if we neglect thermal effects, Equation 1.27 implies $\rho\dot{w} =$: $r_x\dot{\boldsymbol{u}}$, which in the infinitesimal strain linearly elastic case is $\rho\dot{w} =$: $\dot{}$. From the chain rule of differentiation we have

$$\rho\dot{w} = \rho\frac{\partial w}{\partial} : \frac{d}{dt} = \quad : \dot{} \quad = \rho\frac{\partial w}{\partial} \tag{1.39}$$

The starting point to develop a constitutive theory is to assume a stored elastic energy function exists, a function denoted $W \overset{\text{def}}{=} \rho w$, which depends only on the mechanical deformation. The simplest function that fulfills $= \rho\frac{\partial w}{\partial}$ is $W = \frac{1}{2}$: E : . Such a function satisfies the intuitive physical requirement that, for any small strain from an undeformed state, energy must be stored in the material. Alternatively, a small strain material law can be derived from $= \frac{\partial W}{\partial}$ and $W \quad c_0 + \mathbf{c}_1 : \quad + \frac{1}{2}$: I : $\quad + \ldots$ which implies $\mathbf{c}_1 + E : \quad + \ldots$. We are free to set $c_0 = 0$ is arbitrary) in order to have zero strain energy at zero strain and, furthermore, we assume that no stresses exist in the reference state ($\mathbf{c}_1 = \mathbf{0}$). With these assumptions, we obtain the familiar relation

$$\mathsf{E} : \tag{1.40}$$

This is a linear (tensorial) relation between stresses and strains. The existence of a strictly positive stored energy function in the reference configuration implies that the linear elasticity tensor must have positive eigenvalues at every point in the body. Typically, different materials are classified according to the number of independent constants in E. A general material has 81 independent constants, since it is a fourth order tensor relating 9 components of stress to strain. However, the number of constants can be reduced to 36 since the stress and strain tensors are symmetric. This is easily seen from the matrix representation[6] of E:

[6] The symbol [.] is used to indicate the matrix notation equivalent to a tensor form, while $f\,g$ is used to indicate the vector representation.

$$\underbrace{\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{Bmatrix}}_{\stackrel{\text{def}}{=} f\ g} = \underbrace{\begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1112} & E_{1123} & E_{1113} \\ E_{2211} & E_{2222} & E_{2233} & E_{2212} & E_{2223} & E_{2213} \\ E_{3311} & E_{3322} & E_{3333} & E_{3312} & E_{3323} & E_{3313} \\ E_{1211} & E_{1222} & E_{1233} & E_{1212} & E_{1223} & E_{1213} \\ E_{2311} & E_{2322} & E_{2333} & E_{2312} & E_{2323} & E_{2313} \\ E_{1311} & E_{1322} & E_{1333} & E_{1312} & E_{1323} & E_{1313} \end{bmatrix}}_{\stackrel{\text{def}}{=} [\mathsf{E}]} \underbrace{\begin{Bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{12} \\ 2\epsilon_{23} \\ 2\epsilon_{31} \end{Bmatrix}}_{\stackrel{\text{def}}{=} f\ g} \tag{1.41}$$

The existence of a scalar energy function forces E to be symmetric since the strains are symmetric, in other words $W = \frac{1}{2}\ :\mathsf{E}:\ = \frac{1}{2}(\ :\mathsf{E}:\ )^T = \frac{1}{2}\ ^T : \mathsf{E}^T :\ ^T = \frac{1}{2}\ :\mathsf{E}^T:$ which implies $\mathsf{E}^T = \mathsf{E}$. Consequently, E has only 21 free constants. The nonnegativity of W imposes the restriction that E remains positive definite. At this point, based on many factors that depend on the material microstructure, it can be shown that the components of E may be written in terms of anywhere between 21 and 2 independent parameters. We explore such concepts further via the ideas of elastic symmetry.

1.6.2 Material symmetry

Transformation matrices are used in determining the elastic symmetries. Consider a plane of symmetry, the $x_2\ \ x_3$ plane (Figure 1.10). A plane of symmetry implies that the material has the same properties with respect to that plane. Therefore, we should be able to flip the axes with respect to that plane, and have no change in the constitutive law. By definition, a plane of elastic symmetry exists at a point where the elastic constants have the same value for a pair of coordinate systems. The axes are referred to as "equivalent elastic directions". Also by definition, an axis of symmetry of order K exists at a point when there are sets of equivalent elastic directions which can be superposed by a rotation through an angle $K/2\pi$ about an axis. The way to determine elastic symmetry is as follows: first one forms $[\hat{}\,] = [\mathsf{Q}][\ ][\mathsf{Q}]^{\ 1}$ implying $f\hat{}\,g = [\mathsf{T}]f\ g = [\hat{\mathsf{E}}][\mathsf{T}]f\ g = [\hat{\mathsf{E}}]f\hat{}\,g$ which implies $f\ g = \left[\mathsf{T}^{\ 1}\right][\hat{\mathsf{E}}][\mathsf{T}]f\ g$, where $[\mathsf{Q}]$ is a rotational (or reflectional) transformation matrix. Imposing elastic symmetry means the components are invariant with respect to the transformation, hence $[\mathsf{E}] = \left[\mathsf{T}^{\ 1}\right][\hat{\mathsf{E}}][\mathsf{T}]$. Therefore, all components that are not identical must be zero if the material has the assumed elastic symmetry. In this fashion one can "carve" away components from a general anisotropic material tensor. The central point of such symmetries is that in a new transformed state, E should not change.

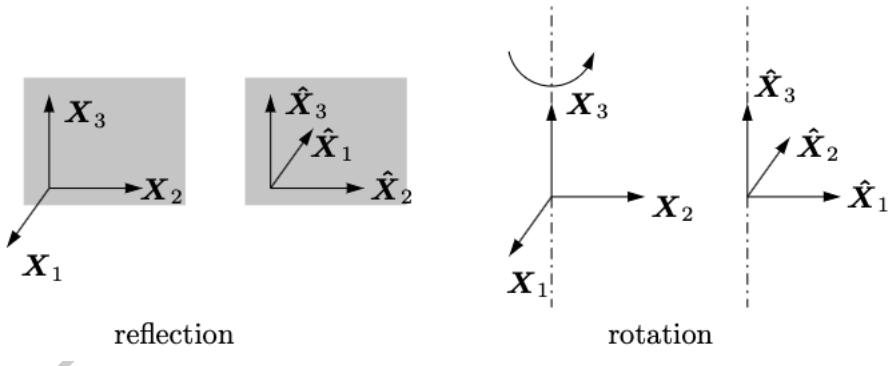

Figure 1.10: Left: reflection with respect to the x_2-x_3 plane. Right: rotation with respect to the x_3 axis.

Examples of elastic symmetry

To make things clear, consider the following steps for one plane of symmetry starting with an originally Triclinic material with 21 free constants (Equation 1.41), defined by E:

- STEP 1: Reflect the x_1 axis

$$R(x_1) \stackrel{\text{def}}{=} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \end{Bmatrix} = \begin{Bmatrix} x_1 \\ x_2 \\ \hat{x}_3 \end{Bmatrix}. \tag{1.42}$$

- STEP 2: Transform the stress and strain tensors with the same transformation, but for second order tensor rules:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \hat{\sigma}_{11} & \hat{\sigma}_{12} & \hat{\sigma}_{13} \\ \hat{\sigma}_{21} & \hat{\sigma}_{22} & \hat{\sigma}_{23} \\ \hat{\sigma}_{31} & \hat{\sigma}_{32} & \hat{\sigma}_{33} \end{bmatrix}, \tag{1.43}$$

and thus

$$\begin{bmatrix} \hat{\sigma}_{11} & \hat{\sigma}_{12} & \hat{\sigma}_{13} \\ \hat{\sigma}_{21} & \hat{\sigma}_{22} & \hat{\sigma}_{23} \\ \hat{\sigma}_{31} & \hat{\sigma}_{32} & \hat{\sigma}_{33} \end{bmatrix} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}. \tag{1.44}$$

Also,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{1.45}$$

and also

$$\begin{bmatrix} \hat{\epsilon}_{11} & \hat{\epsilon}_{12} & \hat{\epsilon}_{13} \\ \hat{\epsilon}_{21} & \hat{\epsilon}_{22} & \hat{\epsilon}_{23} \\ \hat{\epsilon}_{31} & \hat{\epsilon}_{32} & \hat{\epsilon}_{33} \end{bmatrix} = \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix}. \tag{1.46}$$

- STEP 3: Form the constitutive law in the primed frame:

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{Bmatrix} = \begin{Bmatrix} \hat{\sigma}_{11} \\ \hat{\sigma}_{22} \\ \hat{\sigma}_{33} \\ \hat{\sigma}_{12} \\ \hat{\sigma}_{23} \\ \hat{\sigma}_{31} \end{Bmatrix}, \tag{1.47}$$

and

$$\begin{Bmatrix} \hat{\sigma}_{11} \\ \hat{\sigma}_{22} \\ \hat{\sigma}_{33} \\ \hat{\sigma}_{12} \\ \hat{\sigma}_{23} \\ \hat{\sigma}_{31} \end{Bmatrix} = \begin{bmatrix} \hat{E}_{1111} & \hat{E}_{1122} & \hat{E}_{1133} & \hat{E}_{1112} & \hat{E}_{1123} & \hat{E}_{1113} \\ \hat{E}_{2211} & \hat{E}_{2222} & \hat{E}_{2233} & \hat{E}_{2212} & \hat{E}_{2223} & \hat{E}_{2213} \\ \hat{E}_{3311} & \hat{E}_{3322} & \hat{E}_{3333} & \hat{E}_{3312} & \hat{E}_{3323} & \hat{E}_{3313} \\ \hat{E}_{1211} & \hat{E}_{1222} & \hat{E}_{1233} & \hat{E}_{1212} & \hat{E}_{1223} & \hat{E}_{1213} \\ \hat{E}_{2311} & \hat{E}_{2322} & \hat{E}_{2333} & \hat{E}_{2312} & \hat{E}_{2323} & \hat{E}_{2313} \\ \hat{E}_{1311} & \hat{E}_{1322} & \hat{E}_{1333} & \hat{E}_{1312} & \hat{E}_{1323} & \hat{E}_{1313} \end{bmatrix} \begin{Bmatrix} \hat{\epsilon}_{11} \\ \hat{\epsilon}_{22} \\ \hat{\epsilon}_{33} \\ 2\hat{\epsilon}_{12} \\ 2\hat{\epsilon}_{23} \\ 2\hat{\epsilon}_{31} \end{Bmatrix}. \tag{1.48}$$

- STEP 4: Put everything in terms of the original variables, which implies that the constitutive law must be the same as before (i.e. the components of E and $\hat{\mathsf{E}}$ must be the same), if the plane was a plane of symmetry, and thus the tensor relating and is:

$$\begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1112} & E_{1123} & E_{1113} \\ E_{2211} & E_{2222} & E_{2233} & E_{2212} & E_{2223} & E_{2213} \\ E_{3311} & E_{3322} & E_{3333} & E_{3312} & E_{3323} & E_{3313} \\ E_{1211} & E_{1222} & E_{1233} & E_{1212} & E_{1223} & E_{1213} \\ E_{2311} & E_{2322} & E_{2333} & E_{2312} & E_{2323} & E_{2313} \\ E_{1311} & E_{1322} & E_{1333} & E_{1312} & E_{1323} & E_{1313} \end{bmatrix}. \tag{1.49}$$

- STEP 5 : All components that are not equal before and after the reflection of axes are zero:

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{Bmatrix} = \begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & E_{1123} & 0 \\ E_{2211} & E_{2222} & E_{2233} & 0 & E_{2223} & 0 \\ E_{3311} & E_{3322} & E_{3333} & 0 & E_{3323} & 0 \\ 0 & 0 & 0 & E_{1212} & 0 & E_{1213} \\ E_{2311} & E_{2322} & E_{2333} & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & E_{1312} & 0 & E_{1313} \end{bmatrix} \begin{Bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{12} \\ 2\epsilon_{23} \\ 2\epsilon_{31} \end{Bmatrix}. \tag{1.50}$$

The end result is a Monoclinic material, i.e, one plane of elastic symmetry ($x_2 \quad x_3$ plane) (13 free constants)

$$\mathsf{E} \overset{\text{def}}{=} \begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & E_{1123} & 0 \\ E_{2211} & E_{2222} & E_{2233} & 0 & E_{2223} & 0 \\ E_{3311} & E_{3322} & E_{3333} & 0 & E_{3323} & 0 \\ 0 & 0 & 0 & E_{1212} & 0 & E_{1213} \\ E_{2311} & E_{2322} & E_{2333} & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & E_{1312} & 0 & E_{1313} \end{bmatrix}, \tag{1.51}$$

or ($x_1 \quad x_3$ plane)(13 free constants)

$$\mathsf{E} \overset{\text{def}}{=} \begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & E_{1113} \\ E_{2211} & E_{2222} & E_{2233} & 0 & 0 & E_{2213} \\ E_{3311} & E_{3322} & E_{3333} & 0 & 0 & E_{3313} \\ 0 & 0 & 0 & E_{1212} & E_{1223} & 0 \\ 0 & 0 & 0 & E_{1223} & E_{2323} & 0 \\ E_{1311} & E_{1322} & E_{1333} & 0 & 0 & E_{1313} \end{bmatrix}. \tag{1.52}$$

The basic procedure is the same, for reflectional symmetry, rotational symmetries, etc. What follows is a catalog of commonly referred to materials of various symmetries.

- Two mutually perpendicular planes of symmetry reduce the material symmetry to nine free constants, known as an orthotropic material. It also has a third mutually perpendicular plane of symmetry, without changing the number of elastic constants. In other words, if one were to reflect a reference frame located at a material point (rotated by 180 degrees) the properties are the same. Accordingly, for an orthotropic material, there are two planes of symmetry (nine free constants)

$$\mathsf{E} \overset{\text{def}}{=} \begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & 0 \\ E_{2211} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{3311} & E_{3322} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1313} \end{bmatrix}. \tag{1.53}$$

- In addition, if there is one plane in which the material properties are equal in all directions, there are only five free constants and the material is termed transversely isotropic. Accordingly, for transversely isotropic material: two planes of symmetry and one plane of directional independence (five free constants)

$$\mathsf{E} \overset{\text{def}}{=} \begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & 0 \\ E_{2211} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{3311} & E_{3322} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1313} \end{bmatrix} \tag{1.54}$$

and $E_{1111} = E_{2222}, E_{1133} = E_{2233}, E_{1313} = E_{2323}, E_{1212} = \frac{1}{2}(E_{1111} \quad E_{1122})$

- Cubic materials have two planes of symmetry and two planes of directional independence, and can be shown to have three free constants. Accordingly, for a cubic material: two planes of symmetry and two planes of directional independence (three free constants)

$$\mathsf{E} \stackrel{\text{def}}{=} \begin{bmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & 0 \\ E_{2211} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{3311} & E_{3322} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1313} \end{bmatrix}, \tag{1.55}$$

and $E_{1111} = E_{2222} = E_{3333}, E_{1122} = E_{1133} = E_{2233}, E_{1313} = E_{2323} = E_{1212}$

- Finally, if there are an infinite number of planes where the material properties are equal (in all directions), there are two free constants, the Lamé parameters, and the material is of the familiar isotropic variety. An isotropic body has material properties that are the same in every direction at a point in the body, i.e., the properties are not a function of orientation at a point in a body. Accordingly, for isotropic materials: two planes of symmetry and an infinite number of planes of directional independence (two free constants),

$$\mathsf{E} \stackrel{\text{def}}{=} \begin{bmatrix} \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & 0 & 0 & 0 \\ 0 & & 0 & & 0 & \mu & 0 & 0 \\ 0 & & 0 & & 0 & 0 & \mu & 0 \\ 0 & & 0 & & 0 & 0 & 0 & \mu \end{bmatrix}. \tag{1.56}$$

In this case we have

$$\mathsf{E} : \quad = 3\kappa \frac{\mathrm{tr}}{3}\mathbf{1} + 2\mu \quad) \qquad : \mathsf{E} : \quad = 9\kappa \left(\frac{tr}{3}\right)^2 + 2\mu \quad : \quad , \tag{1.57}$$

where $tr \quad = \epsilon_{ii}$ and $\quad = \quad \frac{1}{3}(tr \quad)\mathbf{1}$ is the deviatoric strain. The eigenvalues of an isotropic elasticity tensor are $(3\kappa, 2\mu, 2\mu, \mu, \mu, \mu)$. Therefore, we must have $\kappa > 0$ and $\mu > 0$ to retain positive definiteness of E.

Remark: Obviously, the elasticity tensor, regardless of the degree of anisotropy, must have positive eigenvalues. By forming the similarity transform $\left[\boldsymbol{Z}^T\right][\mathsf{E}][\boldsymbol{Z}] = [\Lambda]$, where the 6 6 collection of 6 1 mutually orthonormal eigenvectors of the elasticity is denoted as $\mathbf{Z}$ and where $[\Lambda]$ is diagonalized, we have $f \quad g = [\boldsymbol{Z}][\Lambda]\left[\boldsymbol{Z}^T\right] f \quad g$, which implies $\left[\boldsymbol{Z}^T\right] f \quad g = f \hat{} g = [\Lambda]\left[\boldsymbol{Z}^T\right] f \quad g = [\Lambda] f \hat{} g$. Clearly, the constitutive law in the transformed basis has the form:

$$\begin{Bmatrix} \hat{\sigma}_{11} \\ \hat{\sigma}_{22} \\ \hat{\sigma}_{33} \\ \hat{\sigma}_{12} \\ \hat{\sigma}_{23} \\ \hat{\sigma}_{13} \end{Bmatrix} = \begin{bmatrix} \Lambda_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Lambda_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Lambda_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Lambda_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Lambda_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Lambda_6 \end{bmatrix} \begin{Bmatrix} \hat{\epsilon}_{11} \\ \hat{\epsilon}_{22} \\ \hat{\epsilon}_{33} \\ 2\hat{\epsilon}_{12} \\ 2\hat{\epsilon}_{23} \\ 2\hat{\epsilon}_{13} \end{Bmatrix}. \tag{1.58}$$

The strain energy is simply

$$W = \frac{1}{2}\left(\Lambda_1 (\hat{\epsilon}_{11})^2 + \Lambda_2 (\hat{\epsilon}_{22})^2 + \Lambda_3 (\hat{\epsilon}_{33})^2 + 4\Lambda_4 (\hat{\epsilon}_{12})^2 + 4\Lambda_5 (\hat{\epsilon}_{23})^2 + 4\Lambda_6 (\hat{\epsilon}_{13})^2\right). \tag{1.59}$$

One interpretation is that of a generalized decomposition of the energy into pieces associated with the principle directions of the the elasticity tensor in matrix form. Clearly, each eigenvalue, $\Lambda_i, i = 1, \ldots, 6$, must be positive.

1.6.3 Material constant interpretation

There are a variety of ways to write isotropic constitutive laws, each time with a physically mean- ingful pair of material constants.

Splitting the strain

It is sometimes important to split infinitesimal strains into two physically meaningful parts

$$= \frac{tr}{3}\mathbf{1} + \left(\quad \frac{tr}{3}\mathbf{1} \right) \tag{1.60}$$

The Jacobian, J, of the deformation gradient $\boldsymbol{F}$ is $\det(\mathbf{1} + \nabla_X \boldsymbol{u})$, and can be written as

$$J = \det \boldsymbol{F} = \det(\mathbf{1} + \nabla_X \boldsymbol{u}). \tag{1.61}$$

Its expansion yields $J = \det(\mathbf{1} + \nabla_X \boldsymbol{u}) \quad 1 + \operatorname{tr} \nabla_X \boldsymbol{u} + \boldsymbol{O}(\nabla_X \boldsymbol{u}) = 1 + tr \ + \ldots$. Therefore, with infinitesimal strains $(1 + tr \ )d\omega_0 = d\omega$ and we can write $tr \ = \frac{d\omega \ d\omega_0}{d\omega_0}$. Hence, $tr\epsilon$ is associated with the volumetric part of the deformation. Furthermore, since $^{\prime} \stackrel{\text{def}}{=} \quad \frac{tr}{3}\mathbf{1} = \mathbf{0}$, the so-called "strain deviator" describes distortion in the material.

Infinitesimal strain material laws

The stress σ can be split into two parts (dilatational and a deviatoric):

$$= \frac{\operatorname{tr}}{3}\mathbf{1} + \left(\quad \frac{\operatorname{tr}}{3}\mathbf{1} \right) \stackrel{\text{def}}{=} \quad p\mathbf{1} + \ ^{\prime}, \tag{1.62}$$

where we call the symbol p the hydrostatic pressure and $^{\prime}$ the stress deviator. With Equation 1.57 we write

$$p = \quad 3\kappa \left(\frac{tr}{3} \right) \quad \text{and} \quad \ ^{\prime} = 2\mu \ ^{\prime}. \tag{1.63}$$

This is one form of Hooke's Law. The resistance to change in the volume is measured by κ. We note that $\left(\frac{tr}{3}\mathbf{1}\right)^{\prime} = 0$, which indicates that this part of the stress produces no distortion.

Another fundamental form of Hooke's law is

$$= \frac{E}{1+\nu} \left(\ + \frac{\nu}{1 \quad 2\nu} \operatorname{tr} \ \mathbf{1} \right), \tag{1.64}$$

which implies the inverse form

$$= \frac{1+\nu}{E} \qquad \frac{\nu}{E} \operatorname{tr} \quad \mathbf{1}. \tag{1.65}$$

To interpret the constants, consider a uniaxial tension test (pulled in the x_1 direction) where $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0$, which implies $\epsilon_{12} = \epsilon_{13} = \epsilon_{23} = 0$. Also, we have $\sigma_{22} = \sigma_{33} = 0$. Under these conditions we have $\sigma_{11} = E\epsilon_{11}$ and $\epsilon_{22} = \epsilon_{33} = \quad \nu\epsilon_{11}$. Therefore, E, the so-called "Young's" modulus, is the ratio of the uniaxial stress to the corresponding strain component. The Poisson ratio, ν, is the ratio of the transverse strains to the uniaxial strain.

Another commonly used set of stress-strain forms are the Lamé relations,

$$= \lambda tr \ 1 + 2\mu \qquad \text{or} \qquad = \quad \frac{\lambda}{2\mu(3\lambda + 2\mu)} \operatorname{tr} \quad \mathbf{1} + \frac{}{2\mu}. \tag{1.66}$$

To interpret the constants, consider a pressure test where $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0$, and where $\sigma_{11} = \sigma_{22} = \sigma_{33}$. Under these conditions we have $\kappa = \lambda + \frac{2}{3}\mu = \frac{E}{3(1 \quad 2\nu)}, \mu = \frac{E}{2(1+\nu)}$ and $\frac{\kappa}{\mu} = \frac{2(1+\nu)}{3(1 \quad 2\nu)}$. We observe that $\frac{\kappa}{\mu} \ ! \ 1$

implies $\nu \to \frac{1}{2}$, and $\frac{\kappa}{\mu} \to 0$ implies $\Rightarrow \nu \to -1$. Therefore, since both κ and μ must be positive and finite, this implies $-1 < \nu < 1/2$ and $0 < E < \infty$. For example, some polymeric foams exhibit $\nu < 0$, steels $\nu \approx 0.3$, and some forms of rubber have $\nu \to 1/2$. We note that λ *can be positive or negative.*

1.6.4 Solid-state diffusion-reaction

Consider a structure which occupies an open bounded domain in $\Omega \subset \mathbb{R}^3$, with boundary $\partial\Omega$. The boundary consists of Γ_c and Γ_g, where the solute concentrations (c) and solute fluxes are respectively specified. The diffusive properties of the heterogeneous material are characterized by a spatially varying diffusivity $\mathbf{D}_0 \subset \mathbb{R}^{3\times 3}$, which is assumed to be a symmetric bounded positive definite tensor-valued function. The mass balance for a small diffusing species, denoted by the normalized concentration of the solute c (molecules per unit volume), in an arbitrary subvolume of material contained within Ω, denoted ω, consists of a storage term ($\dot{c}$), a reaction term ($\dot{s}$), and an inward normal flux term ($-\mathbf{G}\cdot\mathbf{n}$), leading to $\int_\omega (\dot{c}+\dot{s})d\omega = -\int_{\partial\omega} \mathbf{G}\cdot\mathbf{n}da$. It is a classical *stoichiometrically inexact* approximation to assume that the diffusing species reacts (is created or destroyed) in a manner such that the rate of production of the reactant (s) is directly proportional to the concentration of the diffusing species itself and the rate of change of the diffusing species, $\dot{s} = \tau c + \varpi\dot{c}$. Here, $\tau = \tau_0 e^{\frac{Q}{R\theta}}$ and $\varpi = \varpi_0 e^{\frac{Q}{R\theta}}$, where τ_0 and ϖ_0 are rate constants, Q and $\mathcal{Q}$ ($Q \neq \mathcal{Q}$) are activation energies per mole of diffusive species, R is the universal gas constant and θ is the temperature. Upon substitution of these relations into the conservation law for the diffusing species, and after using the divergence theorem, since the volume ω is arbitrary, one has a Fickian diffusion-reaction model in strong form, assuming $\mathbf{G} = -\mathbf{D}\nabla_x c$

$$\dot{c} = \nabla_x\cdot(\mathbf{D}\nabla_x c) - \tau c - \varpi\dot{c} \Rightarrow \dot{c}(1+\varpi) = \nabla_x\cdot(\mathbf{D}\nabla_x c) - \tau c \tag{1.67}$$

When $\tau_0 > 0$, the diffusing species is destroyed as it reacts, while $\tau_0 < 0$ means that the diffusing species is created as it reacts, i.e. an autocatalytic or "chain" reaction occurs. We will only consider the nonautocatalytic case in this work. Also, depending on the sign of ϖ_0, effectively the process will have an accelerated or decelerated diffusivity as well as accelerated or decelerated reactivity. In Equation 1.67, $\mathbf{D}$ is the diffusivity tensor (area per unit time). If we ignore reactions and time-dependency, and assume that the domain is not deforming, we then arrive at the familiar

$$\nabla_X\cdot(\mathbf{D}\nabla_X c) = 0 \tag{1.68}$$

1.6.5 Conservation law families

In summary we have the following related linearized steady-state forms (with no body forces in mechanical equilibrium)

$$\boxed{\begin{aligned} &\nabla_X\cdot(\mathbf{E} : \nabla_X \boldsymbol{u}) = \mathbf{0},\\ &\nabla_X\cdot(\mathbf{K}\nabla_X\theta) = 0,\\ &\nabla_X\cdot(\mathbf{D}\nabla_X c) = 0, \end{aligned}} \tag{1.69}$$

which stem from the following coupled, time-transient, nonlinear equations:

$$\boxed{\begin{aligned} &\nabla_x\cdot\boldsymbol{\sigma} + \rho\boldsymbol{b} = \rho\ddot{\boldsymbol{u}},\\ &\nabla_x\cdot\boldsymbol{q} - \boldsymbol{\sigma} : \nabla_x\dot{\boldsymbol{u}} - \rho z = -\rho\dot{w},\\ &\nabla_x\cdot\mathbf{G} + \tau c + \varpi\dot{c} = -\dot{c}. \end{aligned}} \tag{1.70}$$

2 Example

Consider a small volume of material where all the points are displaced according to:

$$u = A(t) \quad X, \qquad [A] = \begin{bmatrix} A_{11}(t) & A_{12}(t) & A_{13}(t) \\ A_{21}(t) & A_{22}(t) & A_{23}(t) \\ A_{31}(t) & A_{32}(t) & A_{33}(t) \end{bmatrix} \tag{2.1}$$

where $A_{ij}(t)$ are some smooth functions of time (t) only.

Consider a block of material with initial side lengths of 1 cm. We want to shape starting materials with this initial configuration into a variety of different *known* shapes as shown below.

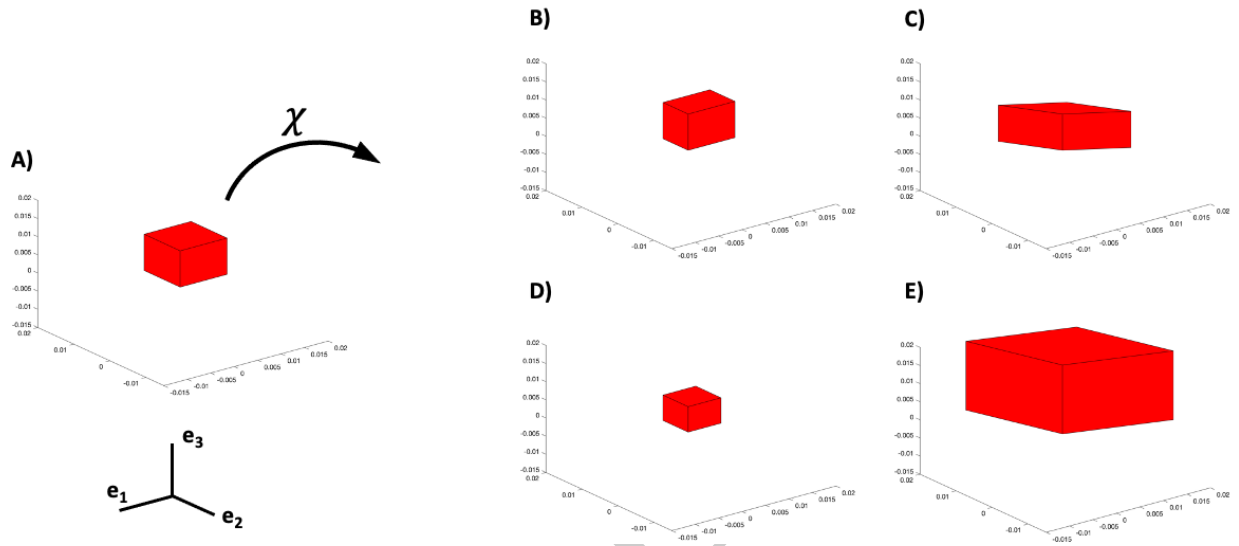

Figure 2.1: A) Initial configuration, b) unilateral compaction, c) pure shear, d) uniform compaction, e) elongation with shear.

(a) Consider a motion of the form $t[\mathbf{A}]$, where $[\mathbf{A}]$ is constant and t is time (s). Determine the non-zero elements of $[\mathbf{A}]$ required for each of the four deformations in Fig 2.1. It is important to note the directions of motion for each deformation are as follows:

- Unilateral compaction occurs in the $\mathbf{e}_2$ direction.
- Pure shear occurs in the $\mathbf{e}_1$ & $\mathbf{e}_2$ directions.
- Uniform compaction occurs equally in all directions.
- Elongation occurs uniformly in all directions, while shear occurs in the $\mathbf{e}_1$ & $\mathbf{e}_2$ directions.

(b) Plot the graphics for the (deforming) cube for frames: $t = f.5, 1.0, 2.0g$. This requires 12 plots: 3 states for each of the 4 deformation cases given. The last 4 plots should match those shown in Fig 2.1.

For the next three problems, assume $\kappa = 50GPa$ *and* $\mu = 20GPa$.

(c) Plot the Frobenius norm of the Cauchy stress $jj \quad jj_F$ over time for each deformation case. Use at least 10 points to plot each curve. Include all deformation cases in one plot.

(d) Plot the hydrostatic pressure over time for each deformation case. Use at least 10 points to plot each curve. Include all deformation cases in one plot.

(e) Plot the Frobenius norm of the deviatoric stress $jj \quad {}^0jj_F$ over time for each deformation case. Use at least 10 points to plot each curve. Include all deformation cases in one plot.

Solution

(a) The required matrix [**A**] for each case can be found by the following relation:

$$[\mathbf{A}] = u \quad X \quad ^{1} = (x \quad X) \quad X \quad ^{1}$$

- Unilateral compaction: $\mathbf{A}(t=2) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0.3 & 0 \\ 0 & 0 & 0 \end{bmatrix} \; ! \; \mathbf{A}(t) = t \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0.15 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
- Pure shear: $\mathbf{A}(t=2) = \begin{bmatrix} 0 & 0.6 & 0 \\ 0.6 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \; ! \; \mathbf{A}(t) = t \begin{bmatrix} 0 & 0.3 & 0 \\ 0.3 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
- Uniform compaction: $\mathbf{A}(t=2) = \begin{bmatrix} 0.3 & 0 & 0 \\ 0 & 0.3 & 0 \\ 0 & 0 & 0.3 \end{bmatrix} \; ! \; \mathbf{A}(t) = t \begin{bmatrix} 0.15 & 0 & 0 \\ 0 & 0.15 & 0 \\ 0 & 0 & 0.15 \end{bmatrix}$
- Elongation with shear: $\mathbf{A}(t=2) = \begin{bmatrix} 0.9 & 0.6 & 0 \\ 0.6 & 0.9 & 0 \\ 0 & 0 & 0.9 \end{bmatrix} \; ! \; \mathbf{A}(t) = t \begin{bmatrix} 0.45 & 0.3 & 0 \\ 0.3 & 0.45 & 0 \\ 0 & 0 & 0.45 \end{bmatrix}$

(b) The deformations can be plotted as the time progresses until $t = 2s$. The deformation plots are as follows:

- Unilateral compaction:

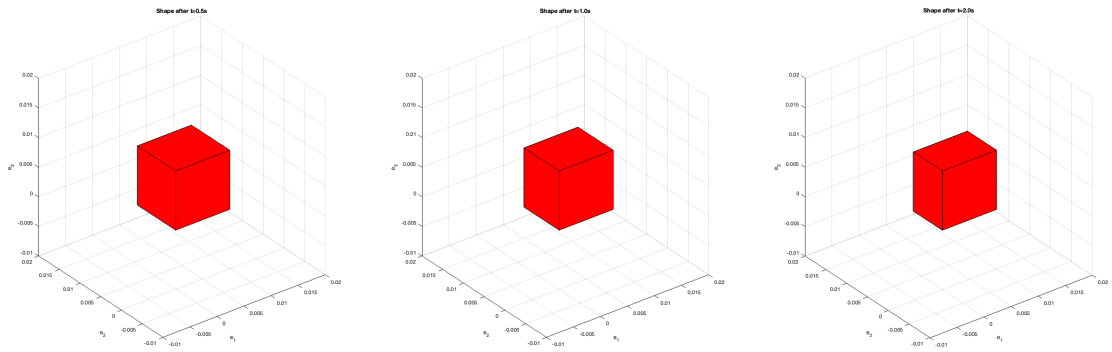

Figure 2.2: Unilateral compaction plot

- Pure shear:

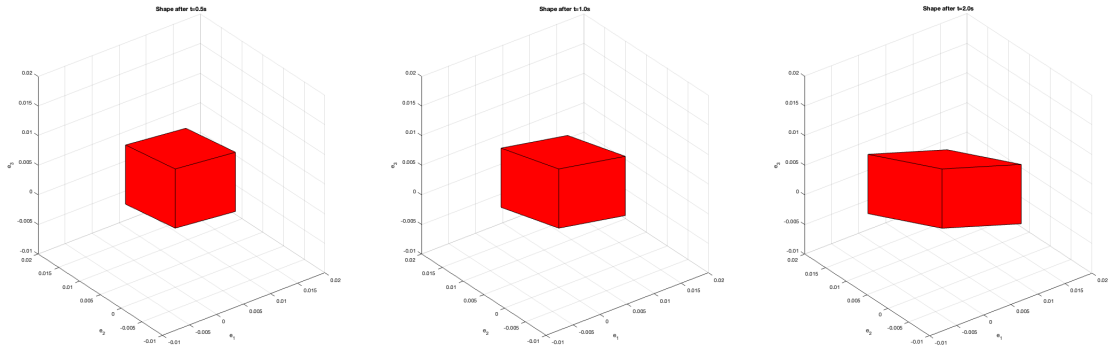

Figure 2.3: Pure shear plot

- Uniform compaction:

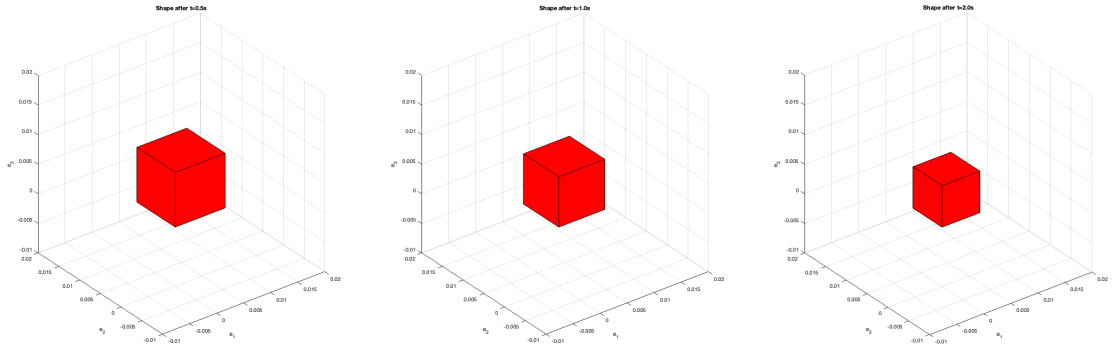

Figure 2.4: Uniform compaction plot

- Elongation with shear:

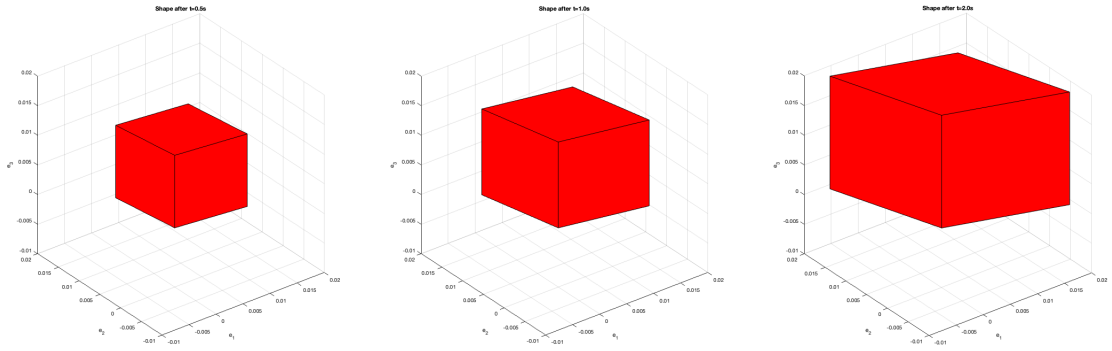

Figure 2.5: Elongation with shear plot

The last frame (t=2s) for each deformation matches the given plots.

(c) To obtain the Cauchy stress, first, the Lagrangian strain is calculated using:

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T \quad \boldsymbol{F} \quad \mathbf{1})$$

Then, the second Pilo-Kirchhoff stress is found using Venants material law:

$$\boldsymbol{S} = \underbrace{\begin{bmatrix} S_{11} \\ S_{22} \\ S_{33} \\ S_{12} \\ S_{23} \\ S_{31} \end{bmatrix}}_{\stackrel{\text{def}}{=} f S g} = \underbrace{\begin{bmatrix} c_1 & c_2 & c_2 & 0 & 0 & 0 \\ c_2 & c_1 & c_2 & 0 & 0 & 0 \\ c_2 & c_2 & c_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix}}_{\stackrel{\text{def}}{=} [\mathrm{E}]} \underbrace{\begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{12} \\ 2E_{23} \\ 2E_{31} \end{bmatrix}}_{\text{def } f E g}$$

$$\text{where } c_1 = \kappa + \frac{4}{3}\mu, c_2 = \kappa \quad \frac{2}{3}\mu.$$

Then, the Cauchy stress can be found using the following relation:

$$= \frac{1}{J} F \quad S \quad F^T$$

where the Jacobian J is the determinant of the deformation matrix F.

Finally, the Frobenius norm can be found by taking the square root of the sum of the absolute squares of its elements.[1]

$$k \quad k_F \quad \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} j \sigma_{ij} j^2}$$

MATLAB is used to calculate this quantity for each deformation case as a function of time. The resulting plot is as follows:

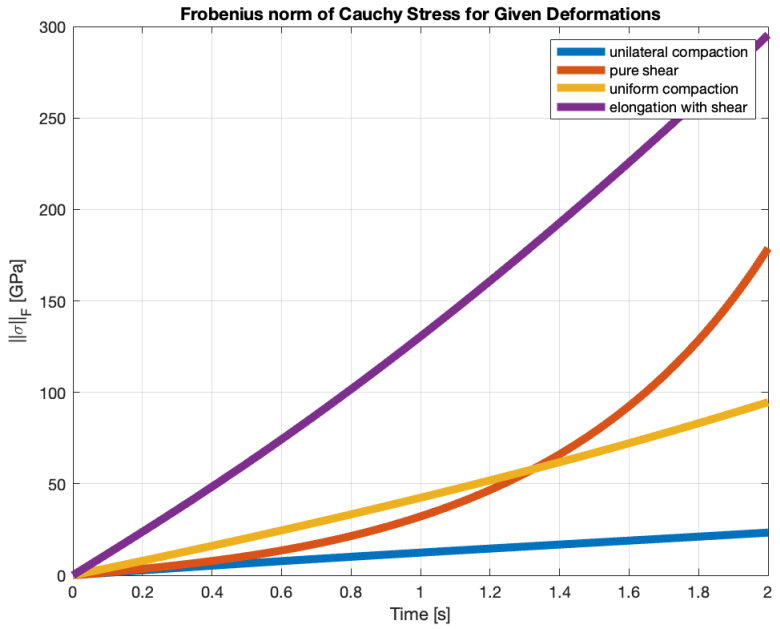

Figure 2.6: Stress for each deformation.

(d) Hydrostatic pressure can be calculated by using the trace of the Cauchy stress tensor:

$$\sigma_{dilatation} = \frac{1}{3} tr(\quad)$$

[1] https://mathworld.wolfram.com/FrobeniusNorm.html

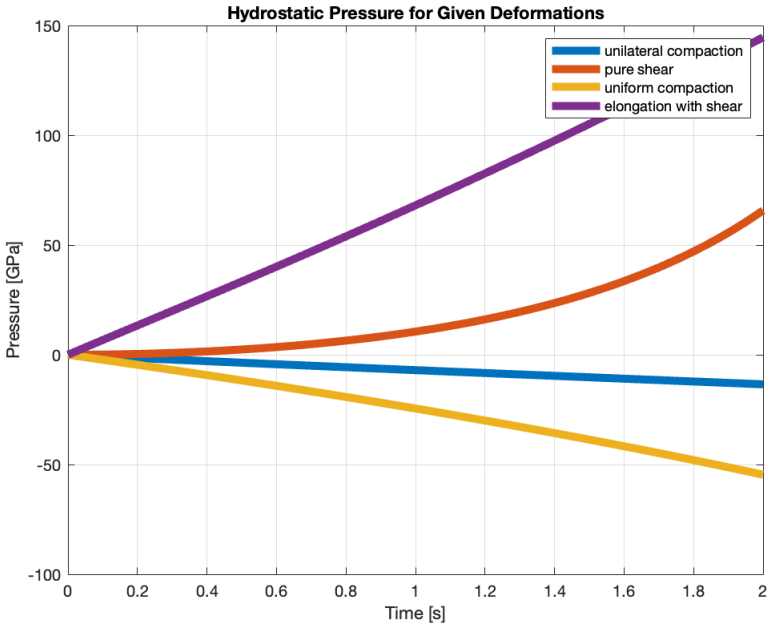

Figure 2.7: Hydrostatic pressure for each deformation.

(e) Deviatoric stress can be found by subtracting hydrostatic pressure from Cauchy stress:

$$_{deviatoric} = \quad \sigma_{dilatation} \quad I$$

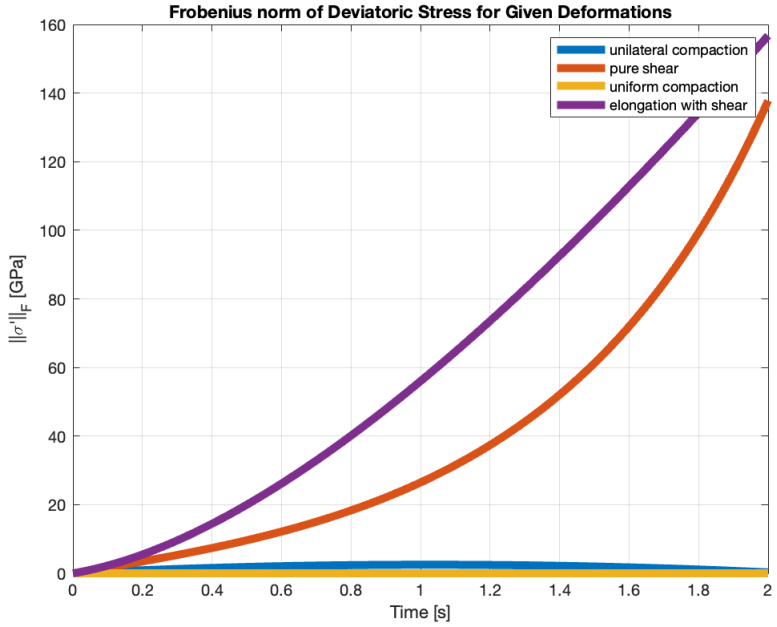

Figure 2.8: Deviatoric stress for each deformation.

3 Assignment

BASICS OF DEFORMATION AND THERMODYNAMICS (80 POINTS)

In this assignment, you will be introduced to the basics of deformation and its role in thermodynamic systems. *The typical report format will not be required for this assignment, and unless otherwise specified, either hand-written or typed information is acceptable.* If you use Matlab or another language for simplifying answers or evaluating specific numbers, clearly set up the equations before showing your numerical results. Correct answers without supporting work will be penalized, and incorrect answers without supporting work will receive zero credit.

BASICS OF DEFORMATION

3.1 Problem 1 (10 points)

Assume the material is isotropic with bulk and shear moduli κ and μ. Assume that at time $t = t_1$:

$$\boldsymbol{A}(t_1) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \tag{3.1}$$

(a) (2 points) Determine $\boldsymbol{E}$, the Green-Lagrange strain at t_1.

(b) (2 points) Determine $\boldsymbol{S}$, the second Piola-Kirchoff Stress at t_1.

(c) (2 points) Determine , the Cauchy stress at t_1.

(d) (2 points) Determine the volumetric (dilatational) component of at t_1.

(e) (2 points) Determine the deviatoric component of at t_1.

You can leave your solutions as products of matrices.

3.2 Problem 2 (5 points)

Consider the following law relating the Second Piola-Kirchhoff stress to Green-Lagrange strain:

$$\boldsymbol{S} = \mathbb{E} : \boldsymbol{E} \tag{3.2}$$

Compute $\boldsymbol{S}$ in terms $\boldsymbol{A}(t)$. It is sufficient to write your answer in terms of previously-derived expressions in terms of $\boldsymbol{A}$ as long as you are specific. The form of $\mathbb{E}$ is given on the last page.

3.3 Problem 3 (2 points)

Determine the relations that $\boldsymbol{A}(t)$ must satisfy for the balance of linear momentum to be satisfied. Express your answer entirely in terms of the referential coordinates (X_1, X_2, X_3), the function $\boldsymbol{A}(t)$.

3.4 Problem 4 (8 points)

For some other material and deformation, suppose that $\boldsymbol{F}$ and $\boldsymbol{S}$ are provided as:

$$[\boldsymbol{F}] = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix} \quad , \quad [\boldsymbol{S}] = \begin{bmatrix} d & 0 & d \\ 0 & 1 & 0 \\ d & 0 & d \end{bmatrix} \tag{3.3}$$

where $d > 1$ is a constant.

(a) (3 points) Determine all of the principal Cauchy stresses.

(b) (2 points) Determine the principal stress direction of the principal stress of largest magnitude. If the largest magnitude is not unique, report the direction of any principal stress with that magnitude.

(c) (3 points) Estimate the value of d at which yielding will occur using the von Mises criterion. Assume the yield stress from a uniaxial test is a known constant σ_y.

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Now, consider the following expression of the first law of thermodynamics:

$$\rho\dot{w} = \quad : \boldsymbol{r}_x \boldsymbol{v} \quad \boldsymbol{r}_x \quad \boldsymbol{q} + \rho z \tag{3.4}$$

3.5 Problem 5 (10 points)

Consider a point in a body undergoing deformation under stress, with no other source of energy. If the instantaneous velocity and stress are known, the rate of work can be calculated using equation 3.4. For each case below, determine the instantaneous rate of work $\rho\dot{w}$, at the point $[0, 0, 0]$.

(a) (5 points) $= \begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix}$, $\boldsymbol{v} = \begin{bmatrix} 0 & x_3 & x_2 \end{bmatrix}^T$

(b) (5 points) $= \begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix}$, $\boldsymbol{v} = \begin{bmatrix} x_1^2 + x_2^2 & x_3^4 & x_2^5 + x_3^2 \end{bmatrix}^T$

3.6 Problem 6 (15 points)

Consider the following equation for energy per unit volume of an arbitrary body:

$$W = \rho_o C\theta + \frac{1}{2}(\boldsymbol{E} \quad \boldsymbol{E}_\theta) : \boldsymbol{I}\boldsymbol{E} : (\boldsymbol{E} \quad \boldsymbol{E}_\theta) \tag{3.5}$$

Assume the body is isotropic and follows the Kirchoff-St. Venant constitutive law, that all strains are purely elastic, and that stored thermal energy is negligible.

(a) (3 points) Use the simplifying assumptions above to expand equation 3.5, in terms of the components of $\boldsymbol{E}$, and the material properties of the material. Leave your expression in terms of products of vectors and matrices.

(b) (2 points) Confirm that the SI base units of κ, μ, and W match.

(c) For each of the following deformation gradients, express the system energy per unit volume entirely in terms of the material properties of the body.

(i) (3 points) $\boldsymbol{F} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

(ii) (3 points) $\boldsymbol{F} = \begin{bmatrix} .8 & 0 & 0 \\ 0 & .8 & 0 \\ 0 & 0 & .8 \end{bmatrix}$

(iii) (3 points) $\boldsymbol{F} = \begin{bmatrix} 1.2 & 0 & 0 \\ 0 & .8 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

(d) (1 point) Explain, briefly, any notable relationships you observe between the deformation gradients and the expressions for the strain energy of that deformation. Do κ or μ entirely disappear from any of the above expressions? If so, why?

3.7 Problem 7 (5 points)

Refer again to equation 3.5. Assume that a body with mass M, density ρ, heat capacity C J/(kgK) is hit by a laser with total output power I watts for a total of t seconds. Assume that the body perfectly absorbs all incident power and stores energy exclusively as heat. Express the predicted temperature of the body at time t in terms of constants defined in this problem. Assume that the temperature is uniform over the entire body.

Hint: the total work W should be expressed in terms of I and t, possibly with other constants to adjust the units appropriately.

3.8 Problem 8 (5 points)

Refer again to equation 3.5. Assume that a body with mass M and density ρ, with heat capacity C J/(kgK) is launched sideways at velocity $\boldsymbol{v}$ m/s. Assume that the body loses no energy to its environment, and that 100% of the initial kinetic energy is converted into heat when the body collides with a rigid barrier. Express the predicted temperature of the body after impact in terms of constants defined in this problem. Assume that the temperature is uniform over the entire body.

3.9 Problem 9 (20 points)

Given the following:

- The density in the current configuration, ρ
- The stored energy is $w = C\theta$, (per unit mass)
- A heat flux of the form $\boldsymbol{q} = cos(2t)\boldsymbol{B} \quad \boldsymbol{x}$, where B is a 3 by 3 matrix of arbitrary coefficients
- A source per unit mass term, $z = aI$,

- A known initial temperature θ_o
- Assume the rate of deformation is neglible.

Provide the following:

(a) (10 points) Develop the differential equation for the temperature $\theta(\boldsymbol{x}, t)$.

(b) (5 points) Set up the solution for temperature using an explicit time stepping scheme (Forward Euler).

(c) (5 points) Given that the initial temperature is θ_0 and a time step size of Δt, write an expression for the temperature at $t = \Delta t$, $t = 2\Delta t$, and $t = 3\Delta t$. You may write the temperature at each time step in terms of the temperature at previous time steps.

Some helpful relations

$$deformation_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0.0100 & 0 & 0 \\ 0.0100 & 0.0070 & 0 \\ 0 & 0.0070 & 0 \\ 0 & 0 & 0.0100 \\ 0.0100 & 0 & 0.0100 \\ 0.0100 & 0.0070 & 0.0100 \\ 0 & 0.0070 & 0.0100 \end{bmatrix} \tag{3.6}$$

$$deformation_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0.0100 & 0.0060 & 0 \\ 0.0040 & 0.0040 & 0 \\ 0.0060 & 0.0100 & 0 \\ 0 & 0 & 0.0100 \\ 0.0100 & 0.0060 & 0.0100 \\ 0.0040 & 0.0040 & 0.0100 \\ 0.0060 & 0.0100 & 0.0100 \end{bmatrix} \tag{3.7}$$

$$deformation_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0.0070 & 0 & 0 \\ 0.0070 & 0.0070 & 0 \\ 0 & 0.0070 & 0 \\ 0 & 0 & 0.0070 \\ 0.0070 & 0 & 0.0070 \\ 0.0070 & 0.0070 & 0.0070 \\ 0 & 0.0070 & 0.0070 \end{bmatrix} \tag{3.8}$$

$$deformation_4 = \begin{bmatrix} 0 & 0 & 0 \\ 0.0190 & 0.0060 & 0 \\ 0.0130 & 0.0130 & 0 \\ 0.0060 & 0.0190 & 0 \\ 0 & 0 & 0.0190 \\ 0.0190 & 0.0060 & 0.0190 \\ 0.0130 & 0.0130 & 0.0190 \\ 0.0060 & 0.0190 & 0.0190 \end{bmatrix} \tag{3.9}$$

For isotropic materials, the Kirchoff-St. Venant material law may be written as:

$$\boldsymbol{S} = \underbrace{\begin{bmatrix} S_{11} \\ S_{22} \\ S_{33} \\ S_{12} \\ S_{23} \\ S_{31} \end{bmatrix}}_{\stackrel{def}{=} f\boldsymbol{S}g} = \underbrace{\begin{bmatrix} c_1 & c_2 & c_2 & 0 & 0 & 0 \\ c_2 & c_1 & c_2 & 0 & 0 & 0 \\ c_2 & c_2 & c_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix}}_{\stackrel{def}{=} [\boldsymbol{IE}]} \underbrace{\begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{12} \\ 2E_{23} \\ 2E_{31} \end{bmatrix}}_{\stackrel{def}{=} f\boldsymbol{E}g} \tag{3.10}$$

where $c_1 = \kappa + \frac{4}{3}\mu$, $c_2 = \kappa \quad \frac{2}{3}\mu$.

4 Solution

4.1 Problem 1

$$[\boldsymbol{A}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$[\boldsymbol{F}] = [\boldsymbol{A}] + \mathbf{1} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 2 \end{bmatrix}$$

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T \quad \boldsymbol{F} \quad \mathbf{1}) = \frac{1}{2}\left(\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 1 & 2 \end{bmatrix} \quad \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 2 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right) = \begin{bmatrix} 1.5 & 0 & 0 \\ 0 & 1.5 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

$$\boldsymbol{S} = \mathsf{E} : \boldsymbol{E}$$

$$\boldsymbol{S} = \begin{bmatrix} S_{11} \\ S_{22} \\ S_{33} \\ S_{12} \\ S_{23} \\ S_{31} \end{bmatrix} = \begin{bmatrix} \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & 0 & 0 & 0 \\ 0 & & 0 & & 0 & \mu & 0 & 0 \\ 0 & & 0 & & 0 & 0 & \mu & 0 \\ 0 & & 0 & & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} 1.5 \\ 1.5 \\ 2 \\ 0 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 5\kappa & \frac{1}{3}\mu \\ 5\kappa & \frac{1}{3}\mu \\ 5\kappa + \frac{2}{3}\mu & \\ 0 & \\ 2\mu & \\ 0 & \end{bmatrix}$$

$$\boldsymbol{S} = \begin{bmatrix} 5\kappa & \frac{1}{3}\mu & 0 & 0 \\ 0 & 5\kappa & \frac{1}{3}\mu & 2\mu \\ 0 & & 2\mu & 5\kappa + \frac{2}{3}\mu \end{bmatrix}$$

$$= \frac{1}{J}\boldsymbol{F} \quad \boldsymbol{S} \quad \boldsymbol{F}^T$$

$$J = \det(\boldsymbol{F}) = 2(2 \quad 2 \quad 0) \quad 0 + 0 = 8$$

$$= \frac{1}{8} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} 5\kappa & \frac{1}{3}\mu & 0 & 0 \\ 0 & 5\kappa & \frac{1}{3}\mu & 2\mu \\ 0 & & 2\mu & 5\kappa + \frac{2}{3}\mu \end{bmatrix} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 1 & 2 \end{bmatrix}$$

$$= \begin{bmatrix} 20\kappa & \frac{4}{3}\mu & 0 & 0 \\ 0 & & 25\kappa + \frac{22}{3}\mu & 10\kappa + \frac{28}{3}\mu \\ 0 & & 10\kappa + \frac{28}{3}\mu & 20\kappa + \frac{8}{3}\mu \end{bmatrix}$$

$$\sigma_{dilatation} = \frac{1}{3}tr(\quad) = \frac{65}{3}\kappa + \frac{26}{9}\mu$$

$$_{deviatoric} = \qquad \sigma_{dilatation} \quad \boldsymbol{I} = \begin{bmatrix} \frac{5}{3}\kappa & \frac{38}{9}\mu & 0 & 0 \\ 0 & & \frac{4}{3}\kappa + \frac{40}{9}\mu & 10\kappa + \frac{28}{3}\mu \\ 0 & & 10\kappa + \frac{28}{3}\mu & \frac{5}{3}\kappa \quad \frac{2}{9}\mu \end{bmatrix}$$

4.2 Problem 2

$$S = \mathsf{E} : E$$

$$\therefore \; E = \frac{1}{2}(F^T \; F \quad 1)$$

$$\therefore \; S = \mathsf{E} : \frac{1}{2}(F^T \; F \quad 1)$$

$$\therefore \; F = A(t) + 1$$

$$\therefore \; S = \frac{1}{2}\left[\mathsf{E} : [(A(t)+1)^T \; (A(t)+1) \quad 1]\right]$$

4.3 Problem 3

The Jacobian needs to satisfy $0 < J < 1$:

$$F = A(t) + 1$$

$$J = \det(F) = \det(A(t) + 1)$$

$$0 < \det(A(t) + 1) < 1$$

Also at $t = 0$:

$$\det(A(t=0) + 1) = 1$$

$$\therefore \; A(t=0) = 0$$

Also, using balance of linear momentum (Eqn 5.28):

$$r_X \; (F \; S) + f J = \rho_0 \frac{d\dot{u}}{dt}$$

We know that:

$$\therefore \; F = A(t) + 1$$

$$\therefore \; J = det(A(t) + 1)$$

$$\therefore \; u = A(t) \; X$$

$$\therefore \; S = \frac{1}{2}\left[\mathsf{E} : [(A(t)+1)^T \; (A(t)+1) \quad 1]\right]$$

So $A(t)$ also needs to satisfy:

$$r_X \; [(A(t)+1) \; \frac{1}{2}\left[\mathsf{E} : [(A(t)+1)^T \; (A(t)+1) \quad 1]\right]] + f \, det(A(t)+1) = \rho_0 \ddot{A}(t) \; X$$

4.4 Problem 4

$$= \frac{1}{J}\boldsymbol{F}\ \ \boldsymbol{S}\ \ \boldsymbol{F}^T = \begin{bmatrix} d & 0 & d \\ 0 & 1/9 & 0 \\ d & 0 & d \end{bmatrix}$$

To find the principal stresses:

$$\det \begin{vmatrix} d & \lambda & 0 & d \\ 0 & 1/9 & \lambda & 0 \\ d & 0 & d & \lambda \end{vmatrix} = 0$$

$$(d \quad \lambda)[(\frac{1}{9} \quad \lambda)(\ \ d \quad \lambda)] \quad d(\frac{1}{9}d \quad \lambda \ \ d) = 0$$

$$\lambda^3 \quad \frac{\lambda^2}{9} \quad 2d^2\lambda + \frac{2d^2}{9} = 0$$

$$\lambda_{1,2,3} = 1.4142d, \quad 1.4142d, 0.1111$$

There are two principal stresses that have the largest magnitude. For the eigenvalue $\lambda_1 = 1.4142d$, the direction can be found using:

$$\begin{bmatrix} d & \lambda_1 & 0 & d \\ 0 & 1/9 & \lambda_1 & 0 \\ d & 0 & d & \lambda_1 \end{bmatrix} \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$(1/9 \quad \lambda_1)n_2 = 0 \ \ \boldsymbol{)}\ \ n_2 = 0$$

$$(d \quad \lambda_1)\ \ n_1 + d \ \ n_3 = 0$$

$$n_1^2 + n_2^2 + n_3^2 = 1 \ \ \boldsymbol{)} = n_1^2 + n_3^2 = 1 \ \ \boldsymbol{)}\ \ n_3 = \sqrt{1 \quad n_1^2}$$

Plug into the previous equation:

$$(d \quad \lambda_1)\ \ n_1 + d \ \ \sqrt{1 \quad n_1^2} = 0$$

$$\boldsymbol{)}\ \ n_1 = \frac{1}{\sqrt{\frac{(d \quad \lambda_1)^2}{d^2} + 1}} = 0.9239$$

$$\boldsymbol{)}\ \ n_3 = \sqrt{1 \quad n_1^2} = 0.3827$$

The principal direction is:

$$n_{\lambda_1} = \begin{bmatrix} 0.9239 \\ 0 \\ 0.3827 \end{bmatrix}$$

For the other eigenvalue $\lambda_2 = \quad 1.4142d$, the direction can be found following the same steps:

$$n_{\lambda_2} = \begin{bmatrix} 0.3827 \\ 0 \\ 0.9239 \end{bmatrix}$$

The d value can be estimated using the definition of von Mises criterion for failure:

$$(\lambda_1 \quad \lambda_3)^2 + (\lambda_1 \quad \lambda_2)^2 + (\lambda_3 \quad \lambda_2)^2 = \sigma^0 = \sigma_y$$

Solving for d yields:

$$d = 8.33 \quad 10^{\ 36} \quad \sqrt{1.2 \quad 10^{69} \quad \sigma_y \quad 2.96 \quad 10^{67}}$$

4.5 Problem 5

$$\rho\dot{w} = \ : \mathsf{r}_x \mathsf{v} = \begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix} : \mathsf{r}_x \begin{bmatrix} 0 \\ x_3 \\ x_2 \end{bmatrix} = \begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix} : \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} = tr\left(\begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix}^T \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \right)$$

$$\rho\dot{w} = \quad b + b = 0$$

$$\rho\dot{w} = \ : \mathsf{r}_x \mathsf{v} = \begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix} : \mathsf{r}_x \begin{bmatrix} x_1^2 + x_2^2 \\ x_3^4 \\ x_2^5 + x_3^2 \end{bmatrix} = \begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix} : \begin{bmatrix} 2x_1 & 2x_2 & 0 \\ 0 & 0 & 4x_3^3 \\ 0 & 5x_2^4 & 2x_3 \end{bmatrix}$$

$$= tr\left(\begin{bmatrix} a & a & a \\ a & b & b \\ a & b & c \end{bmatrix}^T \begin{bmatrix} 2x_1 & 2x_2 & 0 \\ 0 & 0 & 4x_3^3 \\ 0 & 5x_2^4 & 2x_3 \end{bmatrix} \right) = 2ax_1 + 2ax_2 + 5bx_2^4 + 4bx_3^3 + 2cx_3$$

At point [0,0,0]:

$$\rho\dot{w} = 0$$

This conforms to expectations because the instantaneous velocity is a function of position and at the given point the velocity is zero, resulting in zero instantaneous rate of work.

4.6 Problem 6

Because stored energy is negligible, the equation takes the form:

$$W = \frac{1}{2} \boldsymbol{E} : \mathsf{E} : \boldsymbol{E}$$

$$W = \frac{1}{2} \begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{12} \\ 2E_{23} \\ 2E_{31} \end{bmatrix}^T \begin{bmatrix} \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & 0 & 0 & 0 \\ 0 & & 0 & & 0 & \mu & 0 & 0 \\ 0 & & 0 & & 0 & 0 & \mu & 0 \\ 0 & & 0 & & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{12} \\ 2E_{23} \\ 2E_{31} \end{bmatrix}$$

$$[\mathsf{E}] = GPa$$

$$[\boldsymbol{E}] = m/m$$

Then,

$$[W] = [\boldsymbol{E}][\mathsf{E}][\boldsymbol{E}]$$

$$[W] = [\mu] = [\kappa] = GPa$$

Also we can see that W has the units of energy per unit volume and stress is force per unit area:

$$[W] = \frac{J = FL}{V = L^3} = \frac{F}{L^2}$$

which matches with

$$[\mu] = [\kappa] = \frac{F}{L^2}$$

i:

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T \quad \boldsymbol{F} \quad \mathbf{1}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0.5 \end{bmatrix}$$

$$W = \frac{1}{2} \begin{bmatrix} 1 \\ 0 \\ 0.5 \\ 2 \\ 0 \\ 0 \end{bmatrix}^T \begin{bmatrix} \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0.5 \\ 2 \\ 0 \\ 0 \end{bmatrix}$$

$$W = \frac{1}{4}\kappa + \frac{13}{3}\mu$$

ii:

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T \quad \boldsymbol{F} \quad \mathbf{1}) = \begin{bmatrix} 0.68 & 0 & 0 \\ 0 & 0.68 & 0 \\ 0 & 0 & 0.68 \end{bmatrix}$$

$$W = \frac{1}{2} \begin{bmatrix} 0.68 \\ 0.68 \\ 0.68 \\ 0 \\ 0 \\ 0 \end{bmatrix}^T \begin{bmatrix} \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} 0.68 \\ 0.68 \\ 0.68 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$W = \frac{2601}{625}\kappa$$

iii:

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^T \quad \boldsymbol{F} \quad \mathbf{1}) = \begin{bmatrix} 0.28 & 0 & 0 \\ 0 & 0.68 & 0 \\ 0 & 0 & 0.5 \end{bmatrix}$$

$$W = \frac{1}{2} \begin{bmatrix} 0.28 \\ 0.68 \\ 0.5 \\ 0 \\ 0 \\ 0 \end{bmatrix}^T \begin{bmatrix} \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & \kappa & \frac{2}{3}\mu & 0 & 0 & 0 \\ \kappa & \frac{2}{3}\mu & \kappa & \frac{2}{3}\mu & \kappa + \frac{4}{3}\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} 0.28 \\ 0.68 \\ 0.5 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$W = \frac{5329}{2500}\kappa + \frac{301}{1875}\mu$$

It can be seen that for the second case, where the deformation gradient indicates a uniform compaction and no shear, the system energy per unit volume depends only on the bulk modulus of the material, which is in line with the definitions of bulk and shear modulus. The other two cases have nonzero shear contributions to the deformation, therefore include the shear modulus as well.

4.7 Problem 7

For this problem, the energy is stored exclusively as heat, meaning that the deformation term can be neglected:

$$W = \rho_0 C\Theta$$

The derivative of this equation leads to:

$$\dot{W} = \frac{d}{dt}(\rho_0 C\Theta) = \frac{\rho_0 I}{M}$$

$$\rho_0 C\frac{d\Theta}{dt} = \frac{\rho_0 I}{M}$$

$$\frac{d\Theta}{dt} = \frac{I}{MC}$$

$$\Theta(t) = \frac{I}{MC}t + \Theta_0$$

4.8 Problem 8

Similar to Problem 8, equation 7 can be reduced to the following form:

$$W = \rho_0 C\Theta = \frac{1}{2m^3}M\boldsymbol{v}^2$$

The derivative of this equation leads to:

$$\dot{W} = \frac{d}{dt}(\rho_0 C\Theta) = \frac{M}{m^3}\boldsymbol{v}\dot{\boldsymbol{v}} = \frac{\rho_0 m^3}{m^3}\boldsymbol{v}\dot{\boldsymbol{v}} = \rho_0\boldsymbol{v}\dot{\boldsymbol{v}}$$

$$C\dot{\Theta} = \boldsymbol{v}\dot{\boldsymbol{v}}$$

$$\Theta(\boldsymbol{x}, t) = \frac{1}{C}\int \boldsymbol{v}\dot{\boldsymbol{v}}dt$$

4.9 Problem 9

Given:

$$\rho\dot{w} = \quad : \boldsymbol{r}_x\boldsymbol{v} \quad \boldsymbol{r}_x \quad \boldsymbol{q} + \rho z$$

We can substitute the given variables:

$$\rho C\dot{\Theta} = \quad : \boldsymbol{r}_x\boldsymbol{v} \quad \boldsymbol{r}_x \quad (cos(2t)\boldsymbol{B} \quad \boldsymbol{x}) + \rho aI$$

The rate of deformation is negligible, so that term can be dropped:

$$\rho C\dot{\Theta} = \quad cos(2t)\,\boldsymbol{r}_x \quad (\boldsymbol{B} \quad \boldsymbol{x}) + \rho aI$$

$$\dot{\Theta} = \quad \frac{cos(2t)}{\rho C}\,\boldsymbol{r}_x \quad (\boldsymbol{B} \quad \boldsymbol{x}) + \frac{aI}{C}$$

Using Forward Euler:

$$\Theta(t + \Delta t) = \Theta(t) \quad \Delta t\left(\frac{cos(2t)}{\rho C}\,\boldsymbol{r}_x \quad (\boldsymbol{B} \quad \boldsymbol{x}) + \frac{aI}{C}\right)$$

At $t = \Delta t$:

$$\Theta(\Delta t) = \Theta_0 \quad \Delta t \left(\frac{1}{\rho C} r_x \quad (B \quad x) + \frac{aI}{C} \right)$$

At $t = 2\Delta t$:

$$\Theta(2\Delta t) = \Theta(\Delta t) \quad \Delta t \left(\frac{cos(2\Delta t)}{\rho C} r_x \quad (B \quad x) + \frac{aI}{C} \right)$$

$$) \quad \Theta(2\Delta t) = \Theta_0 \quad \Delta t \left(\frac{1 + cos(2\Delta t)}{\rho C} r_x \quad (B \quad x) + \frac{2aI}{C} \right)$$

At $t = 3\Delta t$:

$$\Theta(3\Delta t) = \Theta(2\Delta t) \quad \Delta t \left(\frac{cos(4\Delta t)}{\rho C} r_x \quad (B \quad x) + \frac{aI}{C} \right)$$

$$) \quad \Theta(3\Delta t) = \Theta_0 \quad \Delta t \left(\frac{1 + cos(2\Delta t)}{\rho C} r_x \quad (B \quad x) + \frac{2aI}{C} \right) \quad \Delta t \left(\frac{cos(4\Delta t)}{\rho C} r_x \quad (B \quad x) + \frac{aI}{C} \right)$$

$$) \quad \Theta(3\Delta t) = \Theta_0 \quad \Delta t \left(\frac{1 + cos(2\Delta t) + cos(4\Delta t)}{\rho C} r_x \quad (B \quad x) + \frac{3aI}{C} \right)$$

5 Ethical Considerations for this Project

A goal of this project is to enable advancements in science and engineering through to address critical national challenges associated with next generation food systems. There are deep ethical considerations associated with any technology, in particular for food systems. While technology has tremendous potential to identify greater efficiencies, when it is created without appropriate consideration for who will have access to and control over new resources, or how the new technologies will impact those who work in the system, the efficiencies identified may come at the cost of greater societal inequity. It is important to pursue harnessing technology to disrupt existing inequities, rather than further entrench existing power structures. The following areas should be considered:

- Labor: 1) occupational health, 2) food manufacturing, and 3) outdoor agriculture labor;
- Producers: 1) Small- to mid-size farms, 2) urban agriculture, and 3) research in farm transitions; Technology: 1) research in technology and democracy;
- Health Human Rights: 1) land rights, 2) social justice, and 3) decolonization in agriculture;

Please consider the following questions:

- What are the societal implications of the technology that you are developing?
- Can this technology be distributed fairly and equitably to a wide variety of entities in agricultural industry?
- Are there any potential unintended consequences of this technology becoming available?
- Are there any harmful "spinoffs" of this technology?
- Are there any useful "spinoffs" of this technology?

6 References

1. Chandrasekharaiah, D. S. and Debnath, L. (1994) Continuum mechanics. Academic press.