

# Introduction to Mathematical Modeling

Class Notes

Based on the lectures and class notes of Prof. Robert Moser

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# 1. Equations

The following equation sheets were provided by TA Gopal Yalla, [http://users.oden.utexas.edu/~gopal/teaching/2019\\_CSE389C](http://users.oden.utexas.edu/~gopal/teaching/2019_CSE389C).

## Local Conservation Laws

|                      | Eulerian  | Lagrangian  |
|----------------------|---|---|
| <b>Mass</b>          | $\frac{\partial \rho}{\partial t} + \text{div}(\rho v) = 0$   | $\rho_0(X) = \rho(\varphi(X)) \det F(X)$  |
| <b>Lin. Momentum</b> | $\rho \left( \frac{\partial(\vec{v})}{\partial t} + \vec{v} \cdot \text{grad} \vec{v} \right) = \text{div} T + \vec{f}_b$                             | $\rho_0 \frac{\partial^2 u}{\partial t^2} = \text{Div} \underbrace{FS}_P + f_0$         |
| <b>Ang. Momentum</b> | $T = T^T$   | $S = S^T$   |
| <b>Energy</b>        | $\rho \left( \frac{\partial e}{\partial t} + \vec{v} \cdot \text{grad} e \right) = T : D + r - \text{div} \vec{q}$                                    | $\rho_0 \dot{e}_0 = S : \dot{E} - \text{Div} \vec{q}_0 + r_0$                           |
| <b>Entropy</b>       | $\rho \left( \frac{\partial \eta}{\partial t} + \vec{v} \cdot \text{grad} \eta \right) + \text{div} \frac{\vec{q}}{\theta} - \frac{r}{\theta} \geq 0$ | $\rho_0 \dot{\eta}_0 + \text{Div} \frac{\vec{q}_0}{\theta} - \frac{r_0}{\theta} \geq 0$ |

## Maxwell's Equations

|                      | Integral Form   | Differential Form   |
|----------------------|---|---|
| <b>Gauss's Law</b>   | $\epsilon_0 \int_{\partial\Omega} \mathbf{E} \cdot \mathbf{n} \, dA = q_\Omega = \int_\Omega \rho \, dx$  | $\epsilon_0 \nabla \cdot \mathbf{E} = \rho$   |
| <b>Faraday's Law</b> | $\int \mathbf{E} \cdot d\mathbf{s} = -\frac{d}{dt} \int_A \mathbf{B} \cdot \mathbf{n} \, dA$  | $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$                                    |
| <b>Amp.-Max. Law</b> | $\oint \mathbf{B} \cdot d\mathbf{s} = \mu_0 \int_A \mathbf{j} \cdot \mathbf{n} \, dA + \mu_0 \epsilon_0 \int_A \mathbf{n} \cdot \frac{\partial \mathbf{E}}{\partial t} \, dA$ | $\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$ |
| <b>No Mag. Mono.</b> | $\int_{\partial\Omega} \mathbf{B} \cdot \mathbf{n} \, dA = 0$   | $\nabla \cdot \mathbf{B} = 0$   |

**Kinematics of Deformable Bodies** (pg)

1.  $u = \varphi(X) - X$  (16)

2.  $F(X) = \nabla\varphi(X) = I + \nabla u(X)$  (16)

3.  $C = F^T F$  (17)

4.  $E = \frac{1}{2}(C - I)$  (17)

5.  $v = \dot{\varphi}^{-1}(x, t), t$  (21)

6.  $\frac{D\psi}{Dt} = \frac{\partial\psi}{\partial t} + v \cdot \text{grad } \psi$  (21)

7.  $L = \text{grad } v$  (22)

8.  $L = D + W$  (22)

9.  $D = \frac{1}{2}(L + L^T)$  (22)

10.  $W = \frac{1}{2}(L - L^T)$  (22)

11.  $L_m = \dot{F}F^{-1}$  (22)

12.  $\dot{F} = \text{grad } vF = L_m F$  (22)

13.  $\frac{\dot{\det F}}{\det F} = \text{det } F \text{ div } v$  (23)

14. *Piola Transform* (25)

$T_0(X) = [\text{det } F(X)] T(X) F(X)^{-T}$

15. *Polar Decomposition Theorem* (19)

$F = RU = VR$

-  $R$  orthogonal;  $U, V$  sym. P.D.

$C = F^T F = U^2$

**Divergence Theorem** (23)

$$\int_{\Omega} \text{div } \Psi \, dx = \int_{\partial\Omega} \Psi \cdot \hat{n} \, dA.$$

**Reynold's Transport Theorem** (24)

$$\begin{aligned} \frac{d}{dt} \int_{\omega_t} \Psi \, dx &= \int_{\omega_t} \frac{\partial \Psi}{\partial t} \, dx + \int_{\partial\omega_t} \Psi v \cdot \hat{n} \, dx \\ &= \int_{\omega_t} \left( \frac{\partial \Psi}{\partial t} \, dx + \text{div}(\Psi v) \right) \, dx \end{aligned}$$

**Mass**

1.  $M(\mathcal{B}) = \int_{\Omega_t} \varrho \, dx$  (32)

2.  $\int_{\Omega_0} \varrho_0(X) \, dX = \int_{\Omega_t} \varrho(x) \, dx$  (32)

3. *Material Conservation of Mass* (38)  
 $\varrho_0(X) = \varrho(x) \text{det } F(X)$

4. *Spatial Conservation of Mass* (33)  
 $\frac{\partial \varrho(x)}{\partial t} + \text{div}(\varrho(x)v) = 0$

**Linear & Angular Momentum**

1.  $\frac{dI(\mathcal{B}, t)}{dt} = \int_{\Omega_t} \varrho \frac{dv}{dt} \, dx = \vec{F}_b + \vec{F}_s$  (27)

2.  $\int_{\Omega_t} \varrho \frac{dv}{dt} \, dx = \int_{\Omega_t} f \, dx + \int_{\partial\Omega_t} \sigma(n) \, dA.$

3. *Cauchy's Theorem*  
 $\sigma(n, x, t) = T(x, t)n \quad T = T^T$

4. *Cauchy Stress*  
 $T = (\text{det } F)^{-1} P F^T = (\text{det } F)^{-1} F S F^T$

5. *First Piola-Kirchoff Stress*  
 $P = (\text{det } F) T F^{-T} = F S$

6. *Second Piola-Kirchoff Stress*  
 $S = (\text{det } F) F^{-1} T F^{-T} = F^{-1} P$

**Energy**

1. *Total Energy =  $k + U$*   
 $\rightarrow k = \text{kinetic energy}, U = \text{internal energy}.$

2. *Principle Consv. Energy*  
 $\frac{d}{dt}(k + U) = P + \dot{Q}.$   
 $\rightarrow Q = \text{internal heating}.$

3.  $\varrho \frac{de}{dt} = T : D - \text{div} q + r$

4.  $\varrho_0 \dot{e}_0 = S : \dot{E} - \text{Div} q_0 + r_0$   
 $\rightarrow r = \text{heat per unit volume}.$

**2<sup>nd</sup> Law of Thermodynamics**1. *Clausius-Duhem*

$$\rho \frac{d\eta}{dt} + \operatorname{div} \frac{q}{\theta} - \frac{r_0}{\theta}$$

$$\rho_0 \dot{\eta}_0 + \operatorname{Div} \frac{q_0}{\theta} - \frac{r_0}{\theta} > 0$$

→  $\theta$  = temp,  $\eta$  = entropy density

**Constitutive Equations**1. *Material Frame Indifference*

$$x^* = Qx + c \implies T^* = QTQ^T$$

2. *MFI Solids*

$$F^* = QF \quad \det F^* = \det F$$

3. *MFI Fluids*

$$T = -pI + 2\mu D$$

4. *Coleman-Noll (Dissipative)*

$$S = \rho_0 \frac{\partial \Psi}{\partial E}, \quad \eta_0 = -\frac{\partial \Psi}{\partial \theta}$$

$$\frac{\partial \Psi}{\partial \nabla \theta} = 0, \quad -\frac{1}{\theta} q_0 \cdot \nabla \theta \geq 0$$

5. *Coleman-Noll*  $S = F(E) + I(\dot{E})$ 

$$F(E) = \rho_0 \frac{\partial \Psi}{\partial E}, \quad I(\dot{E}) : \dot{E} - \frac{1}{\theta} q_0 \cdot \nabla \theta \geq 0$$

**Electromagnetic Waves**1. *Coulomb's Law*

$$F = k \frac{|q_1||q_2|}{r^2}, \quad k = \frac{1}{4\pi\epsilon_0}$$

2. *Gauss's Law*

$$q_\Omega = \epsilon_0 \oint_{\partial\Omega} E \cdot n \, dA = \int_\Omega \rho \, dx$$

$$\epsilon_0 \nabla \cdot E = \rho$$

→  $\rho$  = charge density

3. *Ampere's Law*

$$\oint B \cdot ds = \mu_0 i_{\text{enclosed}}, \quad i = \text{current.}$$

4. *Ampere + Maxwell Law*

$$\oint B \cdot ds = \mu_0 i + \mu_0 \epsilon_0 \frac{d}{dt} \Phi_E$$

$$\oint B \cdot ds = \mu_0 \int_A j \cdot n \, dA + \mu_0 \epsilon_0 \frac{d}{dt} \int_A E \cdot n \, dA$$

$$\nabla \times B = \mu_0 j + \mu_0 \epsilon_0 \frac{\partial E}{\partial t}$$

5. *Faraday's Law*

$$\oint E \cdot ds = -\frac{d}{dt} \int_A B \cdot n \, dA$$

$$\nabla \times E = -\frac{\partial B}{\partial t}$$

6. *No Magnetic Monopoles*

$$\int_{\partial\Omega} B \cdot n \, dA = 0$$

$$\nabla \cdot B = 0$$

**Waves**1.  $u(x, y) = \mu_0 e^{i(k \cdot x - \omega t)}$ 

→  $\mu_0$  = amplitude of wave

→  $k$  = wave number

→  $\omega$  = angular frequency

→  $\lambda = 2\pi/k$  = wave length

→  $T = 2\pi/\omega$  = period of oscillation

→  $v = \omega/k$  = wave speed

2. *General Wave Equation*

$$\frac{\partial^2 u}{\partial t^2} = \left( \frac{\omega^2}{k^2} \right) \frac{\partial^2 u}{\partial x^2}$$

3. *Electromagnetic Waves*

$$E = E_0 e^{i(k \cdot x - \omega t)}, \quad B = B_0 e^{i(k \cdot x - \omega t)}$$

→  $\omega/|k|$  = propagation speed

→  $\hat{k} = k/|k|$  = direction on propagation

→  $c = 1/\sqrt{\epsilon_0 \mu_0}$  = speed of light

4. *Electromagnetic Wave Equation*

$$\frac{\partial^2 E}{\partial t^2} = \frac{1}{\mu_0 \epsilon_0} \Delta E$$

5. *E-M Waves & Maxwell's Equations*

$$k \cdot E = 0 \implies k \cdot E_0 = 0$$

$$k \cdot B = 0 \implies k \cdot B_0 = 0$$

$$k \times E = \omega B \implies \hat{k} \times E = cB$$

$$k \times B = -\frac{1}{c^2} \omega E \implies \hat{k} \times B = -\frac{1}{c} E$$

$$E \cdot B = 0$$

$$|E_0| = c|B_0|$$

$$E \times B = \frac{k}{\omega} |E|^2 = \frac{1}{c} |E|^2 \hat{k}$$

**Quantum Mechanics**

1.  $E = \hbar\omega = h\nu$

2.  $\lambda = \frac{h}{p}$

3. *Wave Equation*

$$\Psi(x, t) = \psi_0 e^{i(px - Et)/\hbar}$$

$$\rightarrow \Psi(x, t) = \psi_0 e^{i(kx - \omega t)}$$

$$\rightarrow k = 2\pi/\lambda = p/\hbar$$

$$\rightarrow \omega = 2\pi\nu = E/\hbar$$

4.  $E\Psi = \left(-\frac{\hbar}{i} \frac{\partial}{\partial t}\right) \Psi$

5.  $p\Psi = \left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right) \Psi$

6. *Schrodinger's equation* (free particle)

$$i\hbar \frac{\partial \Psi}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = 0$$

$$\rightarrow E = p^2/2m$$

7. *Hamiltonian Operator*  $H(q, p) = E$ 

$$H(q, p) = \frac{p^2}{2m} + V(q) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

8. *Schrodinger's equation* (time independent)

$$H\psi = E\psi$$

$\rightarrow E$  constant, i.e., eigenvalue

9. *Schrodinger's equation* (general)

$$i\hbar \frac{\partial \Psi}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - V\Psi = 0$$

10.  $\Psi^* \Psi = |\Psi(x, t)|^2 = \rho(x, t)$

$$\rightarrow \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1$$

$$\rightarrow \frac{d}{dt} \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 0$$

**Dynamic Variables & Observables**1. *Dynamic Variable*

$$Q = Q(q_1, q_2, \dots, q_N; p_1, p_2, \dots, p_N)$$

$$\tilde{Q} = \tilde{Q}(q_1, \dots, q_N; -i\hbar \frac{\partial}{\partial q_1}, \dots, -i\hbar \frac{\partial}{\partial q_N})$$

2.  $\langle Q \rangle = \langle \Psi, \tilde{Q}\Psi \rangle = \int \Psi^* \tilde{Q}\Psi dq$

3. *Hermitian*

$$\langle \psi, A\phi \rangle = \langle A\psi, \phi \rangle \quad \forall \phi, \psi \in L^2$$

4.  $\sigma_Q^2 = \langle Q^2 \rangle - \langle Q \rangle^2$

5. *Uncertainty Principle*

$$\sigma_Q^2 \sigma_M^2 \geq \left( \frac{1}{2i} \langle [\tilde{Q}, \tilde{M}] \rangle \right)^2$$

**Hydrogen Atom**1. *The complete hydrogen wave functions*

$$\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \phi)$$

$n = 1, 2, \dots$  (describes energy level)

$\ell = 0, 1, \dots, n-1$  (describes shape)

$\rightarrow \ell = s, p, d, f$

$m = 0, \pm 1, \pm 2, \dots, \pm \ell$  (describes orientation)

**Ab Initio Methods**1. *Many Atom & Electron Systems*

$$H = T_e(r^N) + T_M(R^M) + V_{eM}(r^N, R^M) + V_{MM}(R^M) + V_{ee}(r^N)$$

2. *Born-Oppenheimer Approximation*

$$\psi(r^N, R^M) = \psi_e(r^N, R^M)\chi(R^M)$$

$$\bullet H_{elec}\psi_e(r^N, R^M) = E_{elec}(R^M)\psi_e(r^N, R^M)$$

$\rightarrow R^M$  treated as parameter

$$\bullet E_\chi = (T_M(R^M) + V_{MM}(R^M) + E_{elec}(R^M))\chi$$

3. *Hartree Method*

$$h(r_i)\phi_i(r_i) = e_i\phi_i(r_i)$$

$$\psi_H(r_1, \dots, r_N) = \psi_1(r_1)\psi_2(r_2) \cdots \psi_N(r_N)$$

$\rightarrow$  Solve  $\psi_i$  one at a time

$\rightarrow$  ignore elec-elec interaction

**Spin & Angular Momentum**

$$1. L = q \times p, \quad L_j = \epsilon_{rsj} q_r \frac{\hbar}{i} \frac{\partial}{\partial q_s}, \quad L^2 = L_1^2 + L_2^2 + L_3^2$$

$$2. [L_1, L_2] = i\hbar L_3, \quad [L_2, L_3] = i\hbar L_1, \quad [L_3, L_1] = i\hbar L_2$$

$$3. [L^2, L_i] = 0$$

$$4. L_{\pm} = L_1 \pm iL_2, \quad L_3(L_{\pm}\phi) = (\mu \pm \hbar)L_{\pm}\phi$$

5. Assume for spin operator  $S$

$$[S_1, S_2] = i\hbar S_3, \quad [S_2, S_3] = i\hbar S_1, \quad [S_3, S_1] = i\hbar S_2$$

$$6. S^2 q_{sm} = \hbar^2 s(1+s)q_{sm}, \quad S_3 q_{sm} = \hbar m q_{sm}$$

$$7. S_1 = \frac{\hbar}{2}\sigma_1, \quad S_2 = \frac{\hbar}{2}\sigma_2, \quad S_3 = \frac{\hbar}{2}\sigma_3$$

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

8. *Multielectron Systems*

$$\psi_{\pm}(r_1, r_2) = C (\psi_1(r_1)\psi_2(r_2) \pm \psi_2(r_1)\psi_1(r_2))$$

$$\rightarrow \psi_+(r_1, r_2) = +\psi_+(r_2, r_1) \text{ (Boson: } \mathbb{Z}\text{-spin)}$$

$$\rightarrow \psi_-(r_1, r_2) = -\psi_-(r_2, r_1) \text{ (Fermions: } \frac{1}{2}\mathbb{Z}\text{-spin)}$$

$$\implies \psi_1 \neq \psi_2 \text{ (Fermions)}$$

9. *Slater determinants*  $\rightarrow$  Simply a way to satisfy antisymmetry of wave functions.

**Density Functional Theory**

$$1. n(r) = N \int |\psi(r, r_1, r_2, \dots, r_{N-1})|^2 dr$$

$\rightarrow$  pdf's are indistinguishable.

$$2. \int n(r) dr = N$$

$$3. \left\langle \psi, \sum_{i=1}^N v(r_i) \psi \right\rangle = \int v(r) n(r) dr$$

$\rightarrow$  expected value of potential in field of nuclei.

$$4. \left\langle \psi, \sum_{i=1}^N \sum_{j>i}^N U(r_i, r_j) \psi \right\rangle = \frac{c}{2} \left( 1 - \frac{1}{N} \right) \int \int \frac{n(r)n(r')}{|r-r'|} dr dr'$$

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## 2. Dimensional Analysis

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When modeling complex systems, we commonly have a set of applicable, reliable theories, which are not "closed." We then need "Closure models," often representing effects and phenomena that are not accessible by the reliable theory.

EXAMPLE: Continuum Mechanics:

Reliable Theory: Conservation laws

Closure Models: Constitutive models.

Reliable theory represents centuries of accumulated empirical knowledge, their validity is generally not questioned for the problem at hand. Constitutive models are basically "made up" to be consistent with what is known and available data. This is part of the challenge of mathematical modeling. These closure models can be formulated with the i) Empirical observations, ii) Invariance principles and dependency assumptions, iii) Established theories and principles, iv) insightful guessing.

The invariance principles can significantly constrain the closure models we formulate. Let us consider two broadly useful invariance constraints: Dimensional invariance and Coordinate invariance.

### 2.1 Dimensional Invariance (Homogeneity)

A mathematical model of a physical system is a set of relationships among mathematical descriptors of that system.

|  |
|--|
| <b>Question 1:</b> <i>Consider an object as a physical system. What descriptors might be useful?</i> |
|--|

|                                     |
|-------------------------------------|
| Dimensions, measures on properties. |
|-------------------------------------|

These descriptors (measures of properties) are defined in terms of certain arbitrary references. The principle of dimensional homogeneity is this: The validity of a model relationship cannot depend on the arbitrary references used to define the descriptors—because these descriptors are arbitrary!

Consider a relationship between two descriptors:  $A = B$  in some unit system  $U$ . In the usual way, we can express the same descriptors in terms of a second unit system  $U'$ , i.e.  $A' = C'_A A$  and  $B' = C'_B B$  where  $C'_A, C'_B$  are conversion factors. To be independent of our arbitrary unit system, we must have  $A' = B' \implies C'_A = C'_B$ . But the unit system  $U'$  is arbitrary, so it must be that  $C'_A = C'_B$  for conversion from  $U$  to any other unit system  $U'$ .

This requirement of invariance to the unit system leads to the algebra of dimensions. If two descriptors  $A$  and  $B$  have dimension (e.g. length, mass, time) denoted

$[A]$  and  $[B]$  respectively, then  $AB$  has dimensions  $[A][B]$  and  $A/B$  has dimensions  $[A]/[B]$  where having the dimension  $[A][B]$  means that the conversion factor for transforming units from  $U$  into  $U'$  is  $C'_A C'_B$

EXAMPLE: Area has dimensions of  $[length]^2$  or  $[L]^2$ . Velocity has dimensions  $\frac{[L]}{[T]}$

EXAMPLE: Newton's law implies  $F = ma$ , then dimensions of  $F$  are  $[M] \cdot \frac{[L]}{[T]^2} = \frac{[M][L]}{[T]^2}$

EXAMPLE: Kinetic energy is given by  $1/2mv^2$ , thus dimensions of kinetic energy are  $\frac{[M][L]^2}{[T]^2}$

This is of course trivial, but the requirement of dimensional homogeneity places important constraints on any model of a physical system.

Consider a model of some physical system that asserts a relationship among  $n$  descriptors of the system,  $x_1, \dots, x_n$ :

$$F(x_1, x_2, \dots, x_n) = 0$$

which satisfies the constraint of invariance to the unit system. Generally, the variables will have dimensions that can be expressed in terms of a set of  $m < n$  independent dimensions or fundamental units (e.g. mass, length, time).

We can choose  $m$  of the  $n$  variables (WLOG,  $x_1, \dots, x_m$ ) that have independent dimensions. Note that independent dimensions are analogous to linearly independent vectors in linear algebra and can indeed be represented this way by expressing each variable as a vector with coefficients equal to the power of a fundamental unit present in its units. Now we are free to choose a unit system—so let us choose the units in which  $x_1, \dots, x_m$  are all one. In these units the variables  $\tilde{x}_i$  are given by,

$$\tilde{x}_i = \begin{cases} 1 & i \leq m \\ x_i \prod_{j=1}^m x_j^{P_{ij}} & m < i \leq n \end{cases}$$

where the powers  $P_{ij}$  are chosen such that  $\tilde{x}_i$  are dimensionless. The assumptions of  $m$  independent dimensions and  $m$  variables with independent dimensions guarantees that we can find appropriate  $P_{ij}$  (Linear Algebra). Expressing the model in these units gives,

$$F(\underbrace{1, \dots, 1}_m, \tilde{x}_{m+1}, \dots, \tilde{x}_n) = 0.$$

Since the first arguments are constants we can rewrite as,

$$\tilde{F}(\tilde{x}_{m+1}, \dots, \tilde{x}_n) = 0.$$



This is a big deal as we just reduced the dimensionality of our model by  $m$ .

This result is called the Buckingham  $\Pi$  Theorem because Buckingham used  $\Pi_i$  instead of  $\tilde{x}_i$  but the result was obtained much earlier.

The variables  $x_1, \dots, x_m$  which we used to non-dimensionalize the remaining variables are referred to as *scaling* variables.

**Question 2:** *How do you choose scaling variables?*

There is no exact set of rules, but typically you want to choose variables that you believe will have the strongest or most direct impact on the phenomenon you are trying to model. This is especially important when later trying to simplify your model, if you chose an insignificant parameter it is then difficult if not impossible to remove it without going back to square one and re-picking scaling variables.

**The bottom line.** If the dependencies of a model are known or can be postulated, dimensional analysis can be used to infer simpler models and consolidate data.

## 2.2 Coordinate Invariance (Tensor Analysis)

**Cartesian tensor representation (in 3-D).** Let us define three mutually orthogonal unit vectors  $\vec{e}_i$ ,

$$(\vec{e}_i, \vec{e}_j) = \vec{e}_i \cdot \vec{e}_j = \delta_{ij} := \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

where  $(\cdot, \cdot)$  denotes the inner product. Any vector  $\vec{x} \in \mathbb{R}^3$  can be represented as a linear combination of these basis vectors,

$$\vec{x} = \sum_{i=1}^3 x_i \vec{e}_i,$$

where  $x_i \in \mathbb{R}$ . Any  $x$  that can be represented in this way is called a rank-1 tensor (scalars are rank-0 tensors).

A rank-2 tensor  $\underline{\underline{Y}}$  can be represented in terms of basis vectors by defining what we call a tensor product. The tensor product of two vectors  $\vec{a}$  and  $\vec{b}$ —denoted  $\vec{a} \otimes \vec{b}$ —is the operator that assigns for each vector  $\vec{c}$  the vector  $(\vec{b} \cdot \vec{c})\vec{a}$ ; that is,

$$\vec{a} \otimes \vec{b} := (\vec{b} \cdot \vec{c})\vec{a}.$$

Note that a tensor product is a homogeneous linear operator that maps a vector ( $\vec{c}$  in the definition) to another vector ( $\vec{a}$ ) scaled by the inner product of  $\vec{b}$  and  $\vec{c}$ .

In particular, we know that homogeneous linear operators on  $\mathbb{R}^3$  are just  $3 \times 3$  matrices, so rank-2 tensors can be represented using  $3 \times 3$  matrices. In particular,

$$\underline{\underline{Y}} = \sum_{i=1}^3 \sum_{j=1}^3 Y_{ij} \vec{e}_i \otimes \vec{e}_j.$$

Taking the product of  $\underline{\underline{Y}}$  with some vector  $\vec{x}$  gives,

$$\begin{aligned} \underline{\underline{Y}}\vec{x} &= \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 Y_{ij} (\vec{e}_i \otimes \vec{e}_j) \vec{e}_k x_k \\ &= \sum_{i=1}^3 \left( \sum_{j=1}^3 \sum_{k=1}^3 Y_{ij} \delta_{jk} \vec{e}_k \right) \vec{e}_i = \sum_{i=1}^3 \left( \sum_{j=1}^3 Y_{ij} \vec{e}_j \right) \vec{e}_i = \vec{z}, \text{ a vector.} \end{aligned}$$

But note this is a pain to carry around all the summations and unit vectors so we adopt the Einstein summation convention.

Einstein summation convention:

Tensors are represented as indexed objects, e.g.  $x_i, y_{ij}$

In any term, an index can appear at most twice

A repeated index implies summation over that index

A non-repeated index implies multiplication with unit vector with that index

EXAMPLE:

$$z_i = y_{ij}x_j = \sum_{i=1}^3 \left( \sum_{j=1}^3 y_{ij}x_j \right) \vec{e}_i.$$

**Scalars and Invariants** Invariants of vectors/tensors are just scalar functions of those vectors/tensors. They are called invariants because they are invariant to the coordinate system in which the tensors are expressed.

EXAMPLE: Which of the following are scalar invariants?

$$a_{ij}$$

$$a_{ii} \leftarrow$$

$$b_i$$

$$b_i b_i \leftarrow$$

$$a_{ij} a_{ji} \leftarrow$$

For rank-2 tensors in 3-D, two important results:

**The Cayley-Hamilton Theorem.** A matrix is a solution to its own characteristic equation. This means that  $A^n$  for  $n > 2$  is a linear combination of  $I, A, A^2$  ( $A$  is a rank-2 tensor).

The key point of this theorem is that any analytic tensor function of a tensor  $F(A)$  is a linear combination of  $I, A, A^2$ , with coefficients that are scalar functions of the invariants of  $A$ .

**There are only 3 independent invariants of a 3-D rank-2 tensor.** This implies that any scalar function of a tensor  $A$  can be expressed as a function of its eigenvalues.

A "standard set" of invariants are defined as the coefficients of the characteristic equation. That is, the eigenvalues  $\lambda$  of  $A$  are the solutions of:

$$\lambda^3 - I_1 \lambda^2 + I_2 \lambda - I_3 = 0$$

where,

$$I_1 = A_{ii}$$

$$I_2 = \frac{1}{2} (A_{ii} A_{jj} - A_{ij} A_{ji})$$

$$I_3 = \det(A)$$

Another commonly used set of invariants is:

$$\begin{aligned} I_A &= A_{ii} \\ II_A &= \frac{1}{2} (A_{ii}A_{jj} - A_{ij}A_{ji}) \\ III_A &= \det(A). \end{aligned}$$

The Cayley-Hamilton theorem, and the result on the number of independent scalar invariants allows us to write any analytic tensor function  $F$  of a tensor  $A$  as,

$$F(A) = \gamma_1(I_1, I_2, I_3)I + \gamma_2(I_1, I_2, I_3)A + \gamma_3(I_1, I_2, I_3)A^2.$$

Suppose instead that a tensor  $A$  is a function of some vector  $r$ . What can we say about the general form of this function?

Consider two arbitrary vectors  $a, r$ . Then,

$$a_i A_{ij} b_j = f(a, b, r),$$

but we know that the scalar function  $f$  must be expressed in terms of the invariants that can be formed from  $a, b, r$ . These are,

$$|a|, |b|, |r|, a_i b_i, a_i r_i, b_i r_i$$

Furthermore, the left hand side is clearly a bilinear function of  $a, b$ , thus we must choose only scalar invariants which are bilinear in  $a, b$ ; we are therefore limited to

$$a_i r_i, b_i r_i$$

Which can be multiplied by some function of  $|r|$ . This implies,

$$a_i A_{ij} b_j = g(|r|)a \cdot b + h(|r|)a \cdot r b \cdot r$$

which in turn implies that,

$$A_{ij} = g(|r|) + h(|r|)r_i r_j.$$

**Cross products and tensor consistency.** Finally, in dealing with cross products in tensor notation we introduce the "alternating tensor" or "Levi-Cevita Symbol"

$$\epsilon_{ijk} = \begin{cases} 1 & \text{if } i, j, k \text{ is an even permutation of } 1, 2, 3 \\ -1 & \text{if } i, j, k \text{ is an odd permutation of } 1, 2, 3 \\ 0 & \text{otherwise.} \end{cases} \quad (2.2.1)$$

The challenge in introducing this tensor is that if we swap any two of our basis vectors we change the sign of this tensor—meaning this tensor is not coordinate

system invariant. It is however almost coordinate system invariant, up to a sign, thus we call it a "pseudo-vector." Note however that if we were to apply the tensor again, (introduce another cross product in our term) that the result would again be a vector ( $-1^2 = 1$ ). Coordinate system invariance then imposes the restriction that models for pseudo-vectors must be expressed in terms of pseudo-vectors.

EXAMPLE: Which of the following would be a permissible/valid model?

$$a \times b = c \times d \quad \leftarrow$$

$$a = b \times d$$

$$a = b \times c \times d \quad \leftarrow$$

We conclude this section by giving the tensor representation of vector calculus differential operators:

$$\begin{aligned} \text{Gradient:} \quad (\nabla \varphi)_i &= \frac{\partial \varphi}{\partial x_i} \\ \text{Divergence:} \quad (\nabla \cdot \Psi) &= \frac{\partial \Psi_i}{\partial x_i} \\ \text{Curl:} \quad (\nabla \times \Psi)_i &= \epsilon_{ijk} \frac{\partial \Psi_j}{\partial x_k} \end{aligned} \quad (2.2.2)$$

**Bottomline.** Tensor consistency and dimensional consistency impose significant constraints on model forms.

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### 3. Kinematics of Deformable Bodies

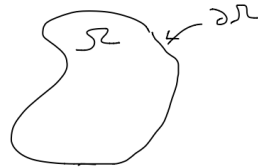
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#### 3.1 Motivation

Continuum mechanics applies a form of Newton's law to a continuum, rather than discrete masses. Instead of  $\vec{F} = m\vec{a}$  we use:

$$\frac{d\vec{M}}{dt} = \vec{F}, \quad \text{where } \vec{M} = m\vec{v}$$

Consider some domain  $\Omega$  within the material (continuum):



|  |
|--|
| <b>Question 1:</b> <i>What is the momentum of the material in <math>\Omega</math>? What forces are acting on it?</i> |
|--|

|  |
|--|
| The momentum is the sum (integral) of momentum of constituent particles.<br>Two types of forces are considered, body and surface forces. |
|--|

The analog of  $\vec{F} = m\vec{a}$  (conservation of momentum) is:

$$\frac{\partial}{\partial t} \int_{\Omega} \varrho \vec{v} dx = \int_{\Omega} \vec{f}_b dx + \int_{\partial\Omega} \vec{f}_s dA$$

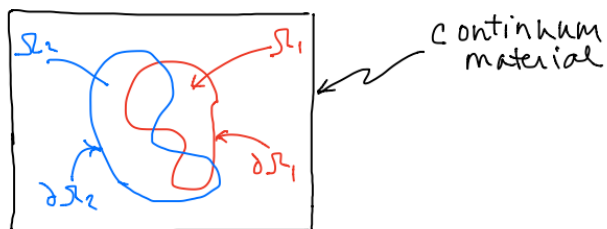
where  $\varrho$  is the mass density,  $f_b$  is the body force per unit volume acting on  $\Omega$ , and  $f_s$  is the surface force per unit area acting on  $\partial\Omega$ .

|  |
|--|
| <b>Question 2:</b> <i>What physical phenomena might <math>f_b</math> and <math>f_s</math> represent?</i> |
|--|

|   |
|---|
| $f_b$ : gravity,<br>$f_s$ : stress, pressure, |
|---|

Consider two subdomains of a continuum material,  $\Omega_1, \Omega_2$ . Neglecting body forces (their model will depend on corresponding "force fields") we can ask what the momentum of the material is on either subdomain and write the conservation of momentum for each:

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega_1} \varrho \vec{v} dx &= \int_{\partial\Omega_1} \vec{f}_{s1} dx \\ \frac{\partial}{\partial t} \int_{\Omega_2} \varrho \vec{v} dx &= \int_{\partial\Omega_2} \vec{f}_{s2} dx \end{aligned}$$



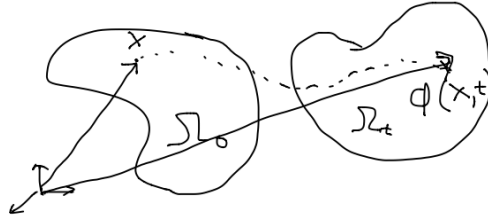
**Question 3:** *What should  $f_{s1}, f_{s2}$  depend on? How would this be different for a fluid or solid? Should  $f_{s1}, f_{s2}$  be the same at points where  $\partial\Omega_1, \partial\Omega_2$  intersect?*

The key point here is that  $f_s$  will depend on the orientation of the curve (surface)  $\partial\Omega$  (i.e. the surface normal of the boundary). For solids we care about deformation, for fluids we care about rate of deformation. The surface forces will not be the same where domains intersect since they will depend on the orientation of the boundary.

Models for  $f_s, f_b$  are needed to complete the description of the motion of the continuum. We again neglect  $f_b$ , focusing only on  $f_s$  for now. In particular, we hypothesize that for solids, internal surface forces  $f_s$  will depend on deformation—or strain. For fluids, we hypothesize instead that internal surface forces  $f_s$  will depend on the *rate* of deformation—or strain-rate. The insight behind such choices will become clear eventually, but for now we build up the analytic tools necessary to define continuum motion, paying particular attention to developing representations for strain and strain-rate that we will use to model surface forces.

## 3.2 Solids

**Material configurations and motion.** Consider a deformable body  $\mathcal{B}$ . The material points within  $\mathcal{B}$  can be labeled by a vector  $X$  representing the position with respect to the origin in some "reference configuration" occupying some region  $\Omega_0 \subset \mathbb{R}^3$ .



The motion and deformation of the body can then be expressed at some time  $t$  by a function  $x = \varphi(X, t)$ .  $\varphi(X, t)$  is bijective and it cannot turn the material inside-out, thus

$$\det(\nabla\varphi(X, t)) > 0.$$

The deformation of the body is denoted

### Deformation

$$u = \varphi(X) - X \tag{3.2.1}$$

where the dependence of  $u, \varphi$  on  $t$  has been neglected. Note that  $\varphi$  is a vector field, so its gradient  $\nabla\varphi$  is a rank-2 tensor. This rank-2 tensor will be called the *deformation gradient* and denoted:

### Deformation Gradient

$$F(X) = \nabla\varphi(X) = I + \nabla u(X) \tag{3.2.2}$$

or equivalently,

$$F_{ij}(X) = \frac{\partial\varphi_i}{\partial X_j} = \delta_{ij} + \frac{\partial u_i}{\partial X_j}$$

The motion is *rigid* if the body does not deform. This requires

$$\varphi(X) = \vec{a} + Qx,$$

where  $a \in \mathbb{R}^3$  is a translation and  $Q$  is a unitary tensor—a rigid body rotation.



**Question 4:** *Should the internal surface forces be affected by rigid body motion? Why or why not?*

No they shouldn't since the continuum is not compressed or altered, just shifted and rotated.

**Deformation and Strain.** We now consider the deformation of differential line segments. Let  $dX$  denote a differential segment in the reference configuration, it will be mapped to

$$dx = FdX.$$

The deformations we are interested in (non-rigid body) will result in changes of the lengths of line segments. Considering the length of these segments,

$$\begin{aligned} dS_0^2 &= |dX|^2 = dX \cdot dX = dX_i dX_i \\ dS^2 &= |dx|^2 = (FdX) \cdot FdX = dX^\top \underbrace{F^\top F}_C dX = dX_i \underbrace{F_{ij}^\top F_{jk}}_{C_{ik}} dX_k \end{aligned}$$

Thus we define the *Cauchy-Green deformation tensor*, a rank-2 tensor  $C$  that quantifies "stretching" of continuum in different directions as

### Cauchy-Green Deformation Tensor

$$C = F^\top F. \quad (3.2.3)$$

Tensor  $C$  is symmetric positive definite. Additionally, we can define the *Green-St. Venant strain tensor*  $E$  that denotes the change in length of line segments as

### Green-St. Venant Strain Tensor

$$E = \frac{1}{2}(C - I). \quad (3.2.4)$$

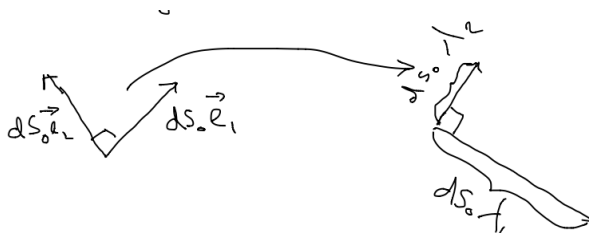
Note that tensor  $C$  can be viewed as the dilation of a line segment, while  $E$  denotes (half) the actual change in length of the segment (e.g. a segment stretched to a ratio of 1.1 times it's original size only changed .1 in length—1.1 would be value of  $C$  in this direction, .1 would be (twice) the value of  $E$  in this direction). Thus if  $\varphi$  is a rigid-body motion, then  $E = 0$ .

**Principle values and directions of deformation.** Since  $E$  is symmetric it has real eigenvalues and orthogonal eigenvectors. These eigenvectors are the *principle*

coordinates or *principle directions* of strain  $E$ . In this coordinate system,  $E = E_{ij}\vec{e}_i \otimes \vec{e}_i$  and

$$E_{ij} = \begin{cases} \frac{1}{2}(\lambda_i^2 - 1) & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad (3.2.5)$$

where  $\lambda_i^2$  are the eigenvalues of  $C$  and it is customary to write  $\lambda_i^2$  since  $C = F^T F$ . Since  $E = \frac{1}{2}(C - I)$ , eigenvectors (principle directions)  $\vec{e}_i$  are also eigenvectors of  $C$  corresponding to  $\lambda_i^2$ . Consider how the differential line segments in the principle directions transform into the current configuration:

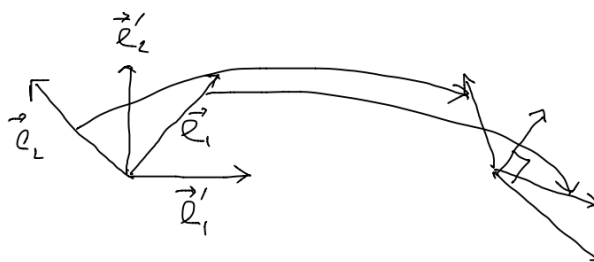


Note in particular that the images of principle directions are also mutually orthogonal.

**Question 5:** *Why are the images of vectors  $\vec{e}_i$  also mutually orthogonal?*

By the properties of SVD of  $C$ , see conditions for orthogonality of right singular vectors  $V$ .

**Shear strains (non-principle deformations).** Now consider what happens to differential segments aligned with a more general set of orthogonal bases:



The images of  $dS_0 \vec{e}_i'$ , that are not the eigenvectors to  $C$  and  $E$  are not mutually orthogonal since the projection along direction  $\vec{e}_i$  is scaled according to  $\lambda_i$  which generally are not equal.

The apparent rotation of the non-principle basis vectors is encoded in the off-diagonal elements of  $E$  when expressed in these coordinates. They are referred to as *shear strains*  $\gamma_{ij}$  and can be viewed as a consequence of anisotropic stretching.

The following equations for shear strains are not given in the notes but are included here in case they come in handy:

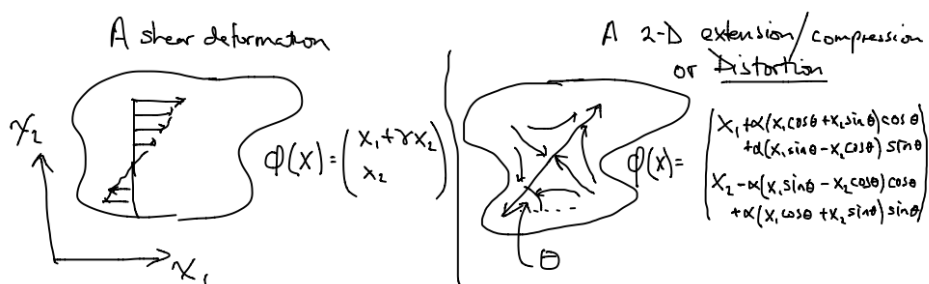
### Shear Strain

$$\sin \gamma_{ij} = \frac{2E_{ij}}{\sqrt{1 + 2E_{ii}}\sqrt{1 + 2E_{jj}}}.$$

Angle  $\gamma_{ij}$  measures the deviation of the angle between  $\vec{e}_i, \vec{e}_j$  from perpendicular.

### Relating shear and principle strain—the Polar Decomposition Theorem.

Consider two deformations:



For a given  $\gamma$  the two can be related by a scalar  $\alpha$  and rotation angle  $\theta$ . In particular, the two deformations will have the same  $C$  and  $E$ .

**Theorem 3.2.1** (Polar Decomposition Theorem). *For any invertible  $F$ ,  $\exists$  unique  $R, U, V$  s.t.*

1.  $R$  is unitary (i.e. a rotation)
2.  $U, V$  are symmetric positive definite
3.  $F = RU = VR$ .

The proof is outlined on pg. 19 of the book.

When  $F$  is the deformation gradient:

### Polar Decomposition

$$\begin{aligned} F &= RU = VR \\ C &= F^T F = U^T R^T R U = U^2 \\ B &= F F^T = R V V^T R^T = V^2 \end{aligned}$$

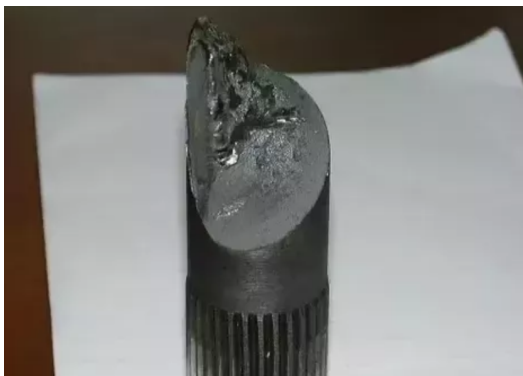
So the left and right deformation gradients do not depend on  $R$ . This is clearly the explanation for our example: in the shear case,  $R \neq I$ ; in the distortion case,  $R = I$ . Thus a pure shear in 2-D is the composition of a 2-D distortion and a rotation.

In general, the Polar Decomposition Theorem implies that any local deformation as characterized by the deformation gradient is composed of a distortion and a rotation—thus DEFORMATION TENSORS AND STRAIN TENSORS ARE INDEPENDENT OF ROTATION.

**Question 6:** *Recall—we started this discussion expecting internal forces to depend on the deformation, is the deformation tensor/strain tensor a good candidate for this dependence?*

Yes.

NOTE. This theorem has significant real-world consequences. For example, consider a rod in torsion (think a drive shaft or a bolt with a wrench applied to it). Picture a differential material element on the surface of the rod, it is in nearly pure shear. The principle stresses and directions are then a  $45^\circ$  rotation from the axis of the rod. This is often how failure occurs in shafts under torsion, note the nearly  $45^\circ$  angle of the fault in the following image.



### 3.3 Fluids

We now turn our attention to modeling internal surface forces in fluids. Note that fluids may undergo deformation without carrying residual stresses into a new reference configuration (e.g. think water bottle being shaken). Thus for fluids we consider the dependence of internal surface forces on the *rate of deformation* instead.

Consider the motion as a function of time:

$$\begin{aligned}
 \left. \begin{aligned} \dot{x} &= v(x) = \frac{\partial \varphi}{\partial t} \\ \ddot{x} &= \dot{v}(x) = \frac{\partial^2 \varphi}{\partial t^2} \end{aligned} \right\} \text{Lagrangian (material description)} \\
 \\
 \left. \begin{aligned} v(x) &= \dot{x}(\varphi^{-1}(x, t), t) \\ a(x) &= \ddot{x}(\varphi^{-1}(x, t), t) \end{aligned} \right\} \text{Eulerian (spatial description)}
 \end{aligned} \tag{3.3.1}$$

The Lagrangian frame describes the motion of a point that originated at  $X$  throughout time. The Eulerian frame describes the motion of particles passing through point  $x$  throughout time.

Now consider the material time derivative of some field quantity  $\Psi$  in each frame of reference. Elementary multivariate chain rule gives:

$$\begin{aligned}
 \text{Lagrangian: } \frac{d\Psi_m(X, t)}{dt} &= \frac{\partial \Psi_m}{\partial t} + \frac{\partial \Psi_m}{\partial x_i} \frac{\partial X_i}{\partial t} = \frac{\partial \Psi_m}{\partial t} = \frac{\partial \Psi}{\partial t} \Big|_X \\
 \text{Eulerian: } \frac{d\Psi(x, t)}{dt} \Big|_X &= \frac{\partial \Psi}{\partial t} \Big|_x + \frac{\partial \Psi_m}{\partial x_i} \frac{\partial x_i}{\partial t} \Big|_X = \frac{\partial \Psi}{\partial t} + v_i \frac{\partial \Psi}{\partial x_i} = \frac{\partial \Psi}{\partial t} + v \cdot \text{grad } \Psi
 \end{aligned}$$

We write these relations again for clarity,

$$\begin{aligned}
 \text{Lagrangian: } \frac{d\Psi_m(X, t)}{dt} &= \frac{\partial \Psi}{\partial t} \Big|_X \\
 \text{Eulerian: } \frac{d\Psi(x, t)}{dt} \Big|_X &= \frac{\partial \Psi}{\partial t} + v \cdot \text{grad } \Psi
 \end{aligned}$$

In the Eulerian description, it is convenient to have a special nomenclature for  $\frac{d}{dt} \Big|_X$ , we define:

#### Total Derivative

$$\frac{D\Psi}{Dt} := \frac{d\Psi}{dt} \Big|_X = \frac{\partial \Psi}{\partial t} + v \cdot \text{grad } \Psi, \tag{3.3.2}$$

as the so-called material time derivative, or substantial derivative.

**Quantifying rates of deformation.** In the Eulerian description we define the *velocity gradient tensor*  $L$  as

### Velocity Gradient Tensor

$$L := \text{grad } v \quad (3.3.3)$$

We can consider the rate of change of the (Lagrangian) deformation gradient  $F$  now as:

$$\begin{aligned} \dot{F} &= \frac{\partial}{\partial t} \nabla \varphi = \nabla \frac{\partial \varphi}{\partial t} = \nabla v \\ \implies \dot{F}_{ij} &= \frac{\partial v_i}{\partial X_j} = \frac{\partial v_i}{\partial x_j} \frac{\partial x_i}{\partial X_j}, \end{aligned}$$

thus

$$\dot{F} = \text{grad } v F = L_m F \quad (3.3.4)$$

where  $L_m$  is  $L$  expressed in Lagrangian frame. We can also observe the identity

$$L_m = \dot{F} F^{-1} \quad (3.3.5)$$

We note that  $L$  can be decomposed into symmetric part  $D$  and anti-symmetric part  $W$ , i.e.

$$L = D + W. \quad (3.3.6)$$

where,

$$D = \frac{1}{2} (L + L^\top) \quad (\text{strain-rate tensor}) \quad (3.3.7)$$

$$W = \frac{1}{2} (L - L^\top) \quad (\text{rotation-rate tensor}) \quad (3.3.8)$$

Note that  $Wv = \frac{1}{2}\omega \times v$  where  $\omega = \text{curl } v$  is the vorticity.

We will now illustrate the reason behind the naming of the symmetric part  $D$  (*strain-rate tensor*) and anti-symmetric part  $W$  (*rotation-rate tensor*).

Consider a the rate of change of a differential line segment  $dS$ , but first note that

$$\begin{aligned} \frac{\partial}{\partial t} (dX \cdot C dX) &= dX \cdot \frac{\partial C}{\partial t} dX = dX \cdot \frac{\partial}{\partial t} (F^\top F) dX \\ &= dX \cdot (\dot{F}^\top F + F^\top \dot{F}) dX \\ &= dX \cdot ((LF)^\top F + F^\top (LF)) dX \\ &= dX \cdot (F^\top (L + L^\top) F) dX. \end{aligned}$$

Then,

$$\begin{aligned}\frac{\partial dS^2}{\partial t} &= dX \cdot \left[ (F^\top(L + L^\top)F)dX \right] \\ &= (FdX) \cdot \left[ (L + L^\top)(FdX) \right] \\ &= (dx) \cdot \left[ (L + L^\top)(dx) \right] = 2(dx) \cdot [Ddx]\end{aligned}$$

Thus the strain-rate tensor is exactly what it claims to be, the rate that segments are stretched (strained). At the beginning of this section we hypothesized the dependence of surface forces on the rate of deformation. It can be shown (see homework) that under the assumption that the current configuration is the reference configuration (usually a good assumption for fluids as the choice of reference configuration is somewhat arbitrary),  $D = \dot{E}$ . Under these assumptions the tensor  $D$  is also rotation independent. The strain-rate tensor  $D$  could therefore be a good candidate for modeling such forces (foreshadowing).

In addition to quantifying the strain and rotation rates, we can quantify the rate of volume change as

$$\frac{\dot{\overline{\det F}}}{\overline{\det F}} = \det F \operatorname{div} v. \quad (3.3.9)$$

This identity will come in handy shortly.

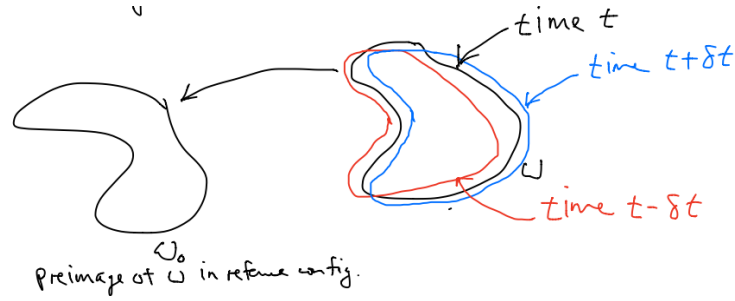
**Divergence theorem.** Before continuing we briefly note the Divergence Theorem, which will allow us to transition between volume and flux integrals. Let  $\Psi$  represent some vector field, then

#### Divergence Theorem

$$\int_{\Omega} \operatorname{div} \Psi \, dx = \int_{\partial\Omega} \Psi \cdot \hat{n} \, dA. \quad (3.3.10)$$

**Reynold's Transport Theorem.** Conserved quantities like mass, momentum, and energy are carried by the material. In writing conservation laws for continua in an Eulerian description it will be convenient to determine the material derivative of an intensive quantity integrated over some volume. Let  $\Psi$  be the quantity of interest. We want to know  $\frac{\partial}{\partial t} \int_{\omega_t} \Psi \, dx$  in some subdomain  $\omega_t$  corresponding to a subdomain  $\omega_0$  in the reference configuration. In particular we note that the preceding integral is difficult to evaluate because the domain of integration is changing with time. The following identity provides the multivariate analogue of the Leibniz rule (for 1D integrals with varying bounds of integration).

The material occupying  $\omega_t$  at time  $t$  was in some region  $\omega_0 \in \Omega_0$  in the reference configuration—and the region occupied by this material evolves continually in time as shown.



The time derivative we want is of the material occupying  $\omega_t$  at time  $t$ , but following the material. So we can write,

$$\begin{aligned} \frac{d}{dt} \int_{\omega_t} \Psi dx &= \frac{d}{dt} \int_{\omega_0} \Psi_m \det F dX = \int_{\omega_0} \frac{d}{dt} (\Psi_m \det F) dX \\ &= \int_{\omega_0} \left( \frac{\partial \Psi_m}{\partial t} + v \cdot \text{grad } \Psi_m \right) \det F dX + \int_{\omega_0} \Psi_m \overline{\det F} dX \end{aligned}$$

The term inside the first integral is obtained for the time derivative of  $\Psi_m$  using the multivariate chain rule, as  $\Psi_m$  is dependant on variables  $(x(t), t)$ . Switching back to the Eulerian integral,

$$\begin{aligned} &= \int_{\omega_t} \left( \frac{\partial \Psi}{\partial t} + v \cdot \text{grad } \Psi \right) \det F dx + \int_{\omega_t} \Psi \text{div } v dx \\ &= \int_{\omega_t} \left( \frac{\partial \Psi}{\partial t} + \text{div}(\Psi v) \right) \det F dx \end{aligned}$$

Finally, applying the divergence theorem we get,

### Reynold's Transport Equation

$$\begin{aligned} \frac{d}{dt} \int_{\omega_t} \Psi dx &= \int_{\omega_t} \frac{\partial \Psi}{\partial t} dx + \int_{\partial \omega_t} \Psi v \cdot n dx \\ &= \int_{\omega_t} \left( \frac{\partial \Psi}{\partial t} dx + \text{div}(\Psi v) \right) dx \end{aligned} \quad (3.3.11)$$

This result is known as Reynold's Transport Theorem. The surface integral can be interpreted as the net flux of the  $\Psi$  quantity carried by the material across the boundary of  $\omega$ .

**The Piola Transformation.** The Piola transform is detailed on pg. 17 of the book and will be considered in more detail later. While we do not go into detail here, we note the main equality and the resulting transformation for surface normals that will allow us to internal surface forces between reference and current configurations.



The following identity holds for tensor fields defined at two times,  $T_0$  at  $t_0$  and  $T$  at  $t$ :

$$\int_{\partial\Omega_0} T_0(X)\hat{n}_0(X) dA_0 = \int_{\partial\Omega} T(x)\hat{n}(x) dA \quad (3.3.12)$$

if the following equality is satisfied:

$$T_0(X) = [\det F(X)] T(X) F(X)^{-T}.$$

This result can be used to establish the following correspondence between surface normals at different times:

$$\hat{n} = \frac{\text{Cof}F \hat{n}_o}{\|\text{Cof}F \hat{n}_o\|}. \quad (3.3.13)$$

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## 4. Eulerian Conservation (Fluids)

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As we return to conservation laws for continua we could proceed in various ways. In particular, each of the conservation laws we derive will have both Eulerian and Lagrangian forms. While it may in some sense be natural to develop these two representations simultaneously, our focus here is on constructing a model for continuum mechanics. For fluid mechanics the choice of reference domain is somewhat arbitrary so we often prefer an Eulerian or spatial representation. For solid mechanics however, material largely maintains the same spatial relation (locally) as some reference configuration and a Lagrangian approach is often desired. For this reason we have decided to present Eulerian conservation laws in this chapter, and defer Lagrangian conservation for the next. Note however that the derivations in this chapter are not necessarily limited to fluids until we begin constructing models and assume dependencies.

This chapter proceeds as follows: We begin by developing Eulerian conservation of momentum to derive overarching fluid mechanical equations. In defining momentum conservation we introduce the concept of surface stresses  $\sigma$ , and we deviate slightly from rigorous derivation of conservation to define a model for surface stresses that will lead to the famous Navier-Stokes equations for Newtonian fluids. We then return to conservation to develop Eulerian representations of mass conservation and energy conservation. These later conservation laws lead to equations commonly studied under the guise of thermodynamics in engineering fields. In particular we hope to emphasize the inextricable connection between these fields through conservation laws.

## 4.1 Momentum

**Question 1:** *What is momentum?*

Recalling our formulation of Newton's law in a continuum however we can instead write  $\frac{dm\vec{v}}{dt} = \vec{F}$ , thus it can also be seen as the integral of force. In particular when no force is applied momentum remains constant—Newton's first law. It is this relation that we seek to conserve when we speak of momentum conservation.

Conservation of momentum is the fundamental relationship that describes motion of a body under the action of force. The momentum of a body, denoted  $I(\mathcal{B}, t)$ , is given by

$$I(\mathcal{B}, t) = \int_{\Omega_t} \rho v \, dx.$$

From Newton's law,

$$\frac{dI(\mathcal{B}, t)}{dt} = \frac{d}{dt} \int_{\Omega_t} \rho v \, dx = \int_{\Omega_t} \rho \frac{dv}{dt} \, dx = F_{net}, \quad (4.1.1)$$

where  $F_{net}$  are the net forces on body  $\mathcal{B}$ . As described in the beginning of the previous chapter, these forces are *body forces* ( $F_b$ )—exerted volumetrically, and *surface forces* ( $F_s$ )—exerted on the boundary of a region. Writing this relationship as before (in the previous chapter) we have,

$$\frac{\partial}{\partial t} \int_{\Omega_t} \rho \vec{v} \, dx = \vec{F}_b + \vec{F}_s = \int_{\Omega_t} \vec{f}_b \, dx + \int_{\partial\Omega_t} \vec{f}_s \, dA \quad (4.1.2)$$

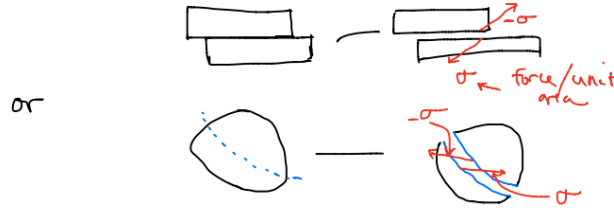
**Body Forces.** Let  $f(x, t)$  be the force per unit volume, then the body force  $F_b$  is

$$\vec{F}_b = \int_{\Omega_t} f_b(x, t) \, dx.$$

EXAMPLE: for gravity,  $f = \rho g$ .

**Surface Forces.** Forces exerted on external surfaces may have different origins but they enter the formulation in the same way. Let  $\sigma$  be the force per unit area acting on the body occupying  $\Omega_t$ .

For external forces, we can consider this to be imposed at the surface of an actual body. Momentum must be conserved everywhere, so (4.1.2) must hold for any subdomain  $\Omega$  of the material, not just for those domains whose boundaries align with physical boundaries. Thus in addition to imposed forces, we will have internal forces—that can be imposed on the many surfaces passing through any material



point. Note in particular that these internal forces depend not only on the point at which a surface passes through, but the orientation of the surface passing through that point (as can be reasoned by considering material anisotropy and the varying force responses obtained in different orientations).

The following hypothesis and theorem identify a model (dependencies) for surface stresses  $\sigma$ .

**Cauchy Hypothesis:** There is a vector field  $\sigma(\vec{x}, t, \hat{n})$  that defines the force/area (stress) at point  $x$  in the current configuration, which depends on the normal (outward pointing)  $\hat{n}$  to the surface  $\partial\Omega$ . Newton's laws imply that

$$\sigma = \sigma(\vec{x}, t, \hat{n}) = -\sigma(\vec{x}, t, -\hat{n}).$$

---

**Theorem 4.1.1** (Cauchy Stress Theorem). *Assume the following conditions:*

1. *body forces  $f_b$  continuous on  $\Omega$*
2.  *$\sigma(\vec{x}, t, \hat{n})$  is continuously differentiable w.r.t.  $\hat{n}$  at constant  $x$*
3.  *$\sigma(\vec{x}, t, \hat{n})$  is continuously differentiable w.r.t.  $x$  at constant  $\hat{n}$*

*Then  $\exists$  a tensor field  $T(x, t) \ni \sigma(\vec{x}, t, \hat{n}) = T(x, t)n$ , and  $T(x, t) = T(x, t)^T$  where  $T(x, t)n$  is a rank-2 tensor that maps normal vector to force per unit area on surface of  $\Omega$ .*

---

The proof of the Cauchy Stress Theorem can be found on pages 37-38 of the book, but the basic idea is to consider a differential tetrahedron and apply conservation of momentum and conservation of angular momentum.

In short, this theorem allows us to represent the surface stress  $\sigma$  as the product of a (rank-2) tensor  $T(x, t)$  and surface normal  $\hat{n}$ . Surface forces  $F_s$  then take the form

$$\vec{F}_s = \int_{\partial\Omega_t} T(x, t) \cdot \hat{n} dA_t.$$

While we yet lack a model for the tensor  $T$ , in terms of the displacements and displacement rates that were the subject of the previous chapter we begin to have some idea of the form such a model might take. We will develop this model in time—for fluids in this chapter and for solids in the next—but first we further develop momentum conservation (4.1.2).

**Eulerian (*Spatial*) Conservation of Momentum.** Substituting the Cauchy stress tensor  $T$  representation of surface forces and applying the Divergence Theorem equation (4.1.2) can now be written,

$$\frac{d}{dt} \int_{\Omega} \rho \vec{v} \, dx = \int_{\Omega} \vec{f}_b \, dx + \int_{\Omega} \operatorname{div} T \, dx.$$

We wish to derive a differential form of this relationship, thus aim to combine each of these integrands under a single integral. We can achieve this by applying Reynold's transport theorem to the term on the right hand side yielding:

$$\int_{\Omega} \frac{\partial(\rho \vec{v})}{\partial t} + \operatorname{div}(\rho \vec{v} \otimes \vec{v}) \, dx = \int_{\Omega} \vec{f}_b \, dx + \int_{\Omega} \operatorname{div} T \, dx$$

and combining integrands,

#### Momentum Conservation (Eulerian)

$$\int_{\Omega} \left[ \frac{\partial(\rho \vec{v})}{\partial t} + \operatorname{div}(\rho \vec{v} \otimes \vec{v}) - \vec{f}_b - \operatorname{div} T \right] dx = 0. \quad (4.1.3)$$

Since  $\Omega$  was arbitrary, this immediately implies the differential form,

#### Differential Momentum Conservation (Eulerian)

$$\frac{\partial(\rho \vec{v})}{\partial t} + \operatorname{div}(\rho \vec{v} \otimes \vec{v}) - \vec{f}_b - \operatorname{div} T = 0. \quad (4.1.4)$$

This is the Eulerian representation (since  $\Omega$  was the current configuration domain). As tensor  $\rho \vec{v} \otimes \vec{v}$  is not symmetric however there is some ambiguity to how the divergence operator should be applied. Writing this relationship instead in Cartesian tensor notation removes the ambiguity:

#### Differential Momentum Conservation (Eulerian)

$$\frac{\partial \rho \vec{v}_i}{\partial t} + \frac{\partial \rho \vec{v}_i \vec{v}_j}{\partial x_j} - \vec{f}_i - \frac{\partial T_{ij}}{\partial x_j} = 0. \quad (4.1.5)$$

We still lack a model for  $T$ . However, once we have developed such a model we will see that under certain assumptions (4.1.5) will take the form of the famous Navier-Stokes equations. We turn our attention to developing such a model.

**Modeling the Cauchy Stress Tensor  $T$ .** In Chapter 3 we hypothesized that the internal surface forces in fluids are dependent on the rate of deformation or strain. The reasoning for this hypothesis is that fluids can be deformed from a starting configuration and will again settle in a different configuration with no tendency to return to the starting configuration. Also in Chapter 3 we derived a relationship for the so-called *strain-rate* tensor  $D$ . Such a tensor is independent of rotations of the underlying coordinate system and is a good candidate to model surface stresses  $\sigma$  in the context of fluids. We assume therefore the dependence of  $T$  on  $D$ ,

$$T = T(D).$$

Thus we have a rank-2 tensor  $T$  as a function of another rank-2 tensor  $D$ . Without assuming anything about the structure of either quantity we can apply the Cayley-Hamilton Theorem (discussed in Chapter 2) to get a general form of the relationship as:

$$T = aI + bD + cD^2$$

where  $a, b, c$  are scalar functions of the three scalar invariants of  $D$ . It would be difficult to quantify all these functions experimentally or otherwise, so we make the following assumption:

ASSUME:  $T$  is a linear function in  $D$ .

This assumption leads to the definition of *Newtonian Fluids*, fluids where internal stresses depend linearly on strain-rate. This is a fair assumption for a wide class of fluids including water, oil, and others, but is a poor assumption for others including some important fluids including blood. However, models for these non-Newtonian fluids often rely on very similar assumptions, we will point out where one might modify this assumption to include a broader class of fluids.

From the assumption of linearity, we can immediately remove the dependence of  $T$  on  $c$ , as the  $D^2$  term is not linear. Similarly, since scalar invariants of  $D$  depend on  $D$ , the scalar function  $b$  must necessarily be constant. Finally, only one scalar invariant of  $D$  is linear in  $D$ , i.e.  $\text{tr}[D]$ , so function  $a$  must be a scalar multiple of  $\text{tr}[D]$ , possibly plus some constant. This gives the form,

$$T = \alpha + \beta \text{tr}[D] + \gamma D$$

where  $\alpha, \beta, \gamma$  are constants (in  $D$ ). We can rewrite this expression in the form

$$T = P + \kappa \text{tr}[D]I + 2\mu \left( D - \frac{\text{tr}[D]}{3}I \right)$$

where constants are now given the names,

$P$ — Hydrodynamic pressure

$\kappa$ — Bulk viscosity

$\mu$ — Shear viscosity

The bulk viscosity  $\kappa$  is commonly assumed to be zero. This is the standard model for internal stresses of Newtonian fluids; substituting this model for  $T$  into (4.1.5) gives the Navier-Stokes equations as promised. To modify this model for non-Newtonian fluids, a common practice is to make  $\mu$  a function of an invariant of  $D$ . The class of fluids that this extends to are known as shear-thinning or shear-thickening fluids, since the shear-viscosity is a function of shear-rate.

If we were to substitute  $T$  into (4.1.5) note that we would have three equations, one for each component of velocity (plus three equations imposing the symmetry of  $T$ )—but we have a number of unknowns including:  $v_i$ ,  $\rho$ ,  $P$ ,  $\kappa$ ,  $\mu$ . It turns out that parameters  $\mu$  will depend on additional variables like temperature  $T$ , but this will be dealt with later when we consider energy conservation. The point here is that our system is severely under-determined. We now derive additional equations for conservation of mass and conservation of energy but note that this pattern of under-determined-ness will persist, necessitating constitutive equations (the topic of Chapter 6).

## 4.2 Mass

We consider the conservation of mass first as it is fairly straight-forward to derive.

|   |
|---|
| <b>Question 2:</b> <i>What is mass? How is it measured?</i> |
|---|

|  |
|--|
| A measure of how much stuff is in an area. It can be measured as density times volume. |
|--|

Consider a body  $\mathcal{B}$  occupying a domain  $\Omega_0$  in the reference configuration. Its mass is given by

$$M_0(\mathcal{B}) = \int_{\Omega_0} \varrho_0 dX,$$

where  $\varrho_0$  is the mass density field in the reference configuration. At some time  $t$  the same body occupies  $\Omega_t$  and has mass density  $\varrho(x, t)$ . At time  $t$ , the mass is

$$M(\mathcal{B}) = \int_{\Omega_t} \varrho(x, t) dx. \quad (4.2.1)$$

|   |
|---|
| <b>Question 3:</b> <i>How are <math>M_0</math> and <math>M_t</math> related? Why?</i> |
|---|

|  |
|--|
| They are the same since the mass of particles does not change and $\Omega_t$ tracks particles through space. |
|--|

We then have that

$$\int_{\Omega_0} \varrho_0(X) dX = \int_{\Omega_t} \varrho(x) dx \quad (4.2.2)$$

Until now we have not limited ourselves to a Lagrangian or Eulerian frame and the preceding analysis holds for both. We again defer the Lagrangian formulation for now, as the Eulerian formulation is often desired for fluids.

**Eulerian (*Spatial*) Conservation of Mass.** The *Eulerian* (spatial) conservation of mass can be obtained by observing that (4.2.2) implies that

$$\frac{d}{dt} \int_{\Omega_t} \varrho(x) dx = 0$$

Recalling Reynold's transport theorem for a general field  $\Psi$ ,

$$\frac{\partial}{\partial t} \int_{\omega} \Psi dx = \int_{\omega} \frac{\partial \Psi}{\partial t} dx + \int_{\partial \omega} \Psi v \cdot n dx$$

and applying it to the density field  $\varrho(x)$  we get the spatial description of conservation of mass,

$$\int_{\Omega_t} \left[ \frac{\partial \varrho(x)}{\partial t} + \operatorname{div}(\varrho(x)v) \right] dx = 0,$$

and since  $\Omega_t$  is arbitrary we get,



**Mass Conservation (Eulerian)**

$$\frac{\partial \rho(x)}{\partial t} + \operatorname{div}(\rho(x)v) = 0. \quad (4.2.3)$$

To better understand the meaning of this expression, we can re-express it using the divergence theorem on some spatial region  $\omega$ .

$$\underbrace{\int_{\omega} \frac{\partial \rho(x)}{\partial t} dx}_{\text{rate of change of mass in } \omega} = \underbrace{- \int_{\partial \omega} \rho v \cdot \hat{n} dA}_{\text{rate at which mass leaves } \omega}$$

### 4.3 Energy

Another conserved quantity of interest is the energy. Let  $\epsilon$  be the total energy per unit volume. Then energy conservation will follow the general outline of :

$$\frac{d}{dt} \int_{\Omega_t} \epsilon dx = \text{Sources.}$$

**Question 4:** *What constitutes the energy of a continuum? What are the possible sources?*

The energy consists of kinetic energy  $\kappa$  and internal energy  $U$ . Possible sources include power, or rate of work denoted  $\mathcal{P}$  and heating rate  $\dot{Q}$ .

Thus we have simply that

$$\frac{d}{dt} \int_{\Omega_t} (\kappa + U) = \mathcal{P} + \dot{Q}.$$

Writing out this relationship in a concrete form we get,

$$\frac{d}{dt} \int_{\Omega_t} \overbrace{\left( \frac{\rho \vec{v} \cdot \vec{v}}{2} + \rho e \right)}^{\epsilon} dx = \overbrace{\int_{\Omega_t} \vec{f} \cdot \vec{v} dx + \int_{\partial \Omega_t} \vec{\sigma} \cdot \vec{v} dA}^{\mathcal{P}} + \overbrace{\int_{\Omega_t} r dx - \int_{\partial \Omega_t} \vec{q} \cdot \hat{n}}^{\dot{Q}},$$

where,  $e$  is the internal energy per unit volume,  $r$  is the volumetric heating rate, and  $q$  is the heat flux (with  $\vec{q}$  pointing into the volume, or opposing  $\hat{n}$ ). We begin to analyze this by expanding the stress term in  $\mathcal{P}$ :

$$\begin{aligned} \int_{\partial \Omega_t} \vec{\sigma} \cdot \vec{v} dA &= \int_{\partial \Omega_t} T \hat{n} \cdot \vec{v} dA = \int_{\partial \Omega_t} v_i T_{ij} n_j dA \\ &= \int_{\Omega_t} \frac{\partial v_i T_{ij}}{\partial x_j} dx = \int_{\Omega_t} \left( v_i \frac{\partial T_{ij}}{\partial x_j} + T_{ij} \frac{\partial v_i}{\partial x_j} \right) dx \\ &= \int_{\Omega_t} (v \cdot \text{div } T + T : \text{grad } v) dx \\ &= \int_{\Omega_t} (v \cdot \text{div } T + T : D) dx, \end{aligned}$$

Where  $T : D$  denotes the contraction of  $T$  and  $D$ , or the trace of their product. so,

$$\mathcal{P} = \int_{\Omega_t} \vec{v} \cdot (\text{div } T + \vec{f}) dx + \int_{\Omega_t} T : D dx.$$

But, from momentum conservation,

$$\text{div } T + \vec{f} = \rho \frac{d\vec{v}}{dt} + \text{div}(\rho \vec{v} \otimes \vec{v})$$

so,

$$\mathcal{P} = \int_{\Omega_t} \vec{v} \cdot \left( \rho \frac{d\vec{v}}{dt} + \text{div}(\rho \vec{v} \otimes \vec{v}) \right) dx + \int_{\Omega_t} T : D dx$$

which, by expanding terms, adding the Eulerian conservation of mass equation, refactoring gives, and finally applying Reynold's transport theorem to the field  $\Psi = \frac{\rho \vec{v} \cdot \vec{v}}{2}$

$$\mathcal{P} = \frac{d}{dt} \int_{\Omega_t} \frac{\rho \vec{v} \cdot \vec{v}}{2} dx + \int_{\Omega_t} T : D dx.$$

Note now that the left hand side in this term is equal to the kinetic energy term in  $\varepsilon$ . The equality between these terms is known as the conservation of kinetic energy, or the kinetic energy equation and is redundant with momentum conservation, so we can cancel these terms. To get  $\dot{Q}$  into a form amenable to our analysis we simply apply the divergence theorem to the right most term, giving

$$\dot{Q} = \int_{\Omega_t} r - \operatorname{div} \vec{q} dx.$$

Combining now all these terms into the conservation of energy equation, and cancelling the kinetic energy terms as noted we arrive at the internal energy equation,

#### Internal Energy Equation (Eulerian)

$$\frac{d}{dt} \int_{\Omega_t} \rho e dx = \int_{\Omega_t} (T : D + r - \operatorname{div} \vec{q}) dx \quad (4.3.1)$$

which enforces the first law of thermodynamics. Applying Reynolds transport theorem on the left we arrive at the differential form of (Eulerian) internal energy conservation,

#### Differential form of Internal Energy Conservation (Eulerian)

$$\frac{\partial \rho e}{\partial t} + \operatorname{div}(\rho e \vec{v}) = T : D + r - \operatorname{div} \vec{q} \quad (4.3.2)$$

**Thermodynamics and Entropy.** As any student of thermodynamics will know however, there is also a second law of thermodynamics which must be satisfied. This law—that the entropy of a closed system cannot not decrease—is not a conservation equation, but rather a constraint on the internal energy equation. Entropy, a measure of the microscale randomness in a system, is a somewhat non-intuitive concept compared to other quantities we have thus far encountered. We neglect a rigorous definition here, however a simple explanation of this law is that things do not become more ordered absent some input of energy. Physical manifestations of this law are everywhere: gas fills a room on its own, liquids mix, and heat flows from

hot to cold regions. Here we are particularly interested in entropy in constraining the direction of heat flow.

From thermodynamics we have the notion of "Thermodynamic state variables"

Temperature (absolute) –  $\theta$

Entropy –  $S$

If we denote  $Q$  as the heat added to a system at a constant temperature  $\theta$ , between times  $t_2 > t_1$  then the second law of thermodynamics implies,

$$S(t_2) - S(t_1) - \frac{Q}{\theta} \geq 0.$$

When equality holds a process is *reversible*. The concept of reversibility is key in determining theoretical limits of performance and underlies measures of efficiency in engineering. For the time evolution we have,

### 2<sup>nd</sup> Law of Thermodynamics (Entropy Equation)

$$\frac{dS}{dt} - \frac{\dot{Q}}{\theta} \geq 0 \quad (4.3.3)$$

For a continuum, we define the variable  $\eta$  as the entropy per unit mass, thus

$$S = \int_{\Omega_t} \varrho \eta \, dx$$

and,

$$\frac{d}{dt} \int_{\Omega_t} \varrho \eta \, dx + \int_{\partial\Omega_t} \frac{\vec{q} \cdot \hat{n}}{\theta} \, dA - \int_{\Omega_t} \frac{r}{\theta} \, dx \geq 0.$$

Finally, applying the divergence theorem to the surface integral, and applying Reynold's transport theorem we have,

### Entropy Equation (Continuum, Eulerian)

$$\int_{\Omega_t} \left[ \frac{\partial \varrho \eta}{\partial t} + \text{div}(\varrho \eta \vec{v}) + \text{div} \left( \frac{\vec{q}}{\theta} - \frac{r}{\theta} \right) \right] dx \geq 0. \quad (4.3.4)$$

and, since the domain  $\Omega_t$  is arbitrary we get,

### Clausius Duhem Inequality (Eulerian)

$$\frac{\partial \varrho \eta}{\partial t} + \text{div}(\varrho \eta \vec{v}) + \text{div} \left( \frac{\vec{q}}{\theta} - \frac{r}{\theta} \right) \geq 0. \quad (4.3.5)$$

---

Note that in defining our system of conservation equations we have introduced many more unknowns than equations. We will eventually remedy this in Chapter 6 where we develop constitutive or closure equations for our system. Note that up until this point we have made very few assumptions, only in defining our model for surface stresses  $\sigma$  and in defining our model for the resulting Cauchy stress tensor  $T$ . Thus, while we noted this representation is especially useful for fluids, it is valid for any continuum material.

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## 5. Lagrangian Conservation (Solids)

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We have up to now defined conservation equations for momentum, mass, and energy in an Eulerian frame. We now turn to defining similar conservation laws for a Lagrangian frame that are more convenient in dealing with solids.

### 5.1 Mass

We begin with conservation of mass due to its simplicity. We start with relationship (4.2.2), given here for reference

$$\int_{\Omega_0} \varrho_0(X) dX = \int_{\Omega_t} \varrho(x) dx.$$

The integral in  $x$  can be transformed into an integral in  $X$  since  $x = \varphi(X)$  and  $dx = \det F dX$ . The factor  $\det F$  can be understood as the ratio of differential volume  $dx$  to  $dX$ . We thus have that

$$\int_{\Omega_0} (\varrho_0(X) - \varrho(\varphi(X)) \det F) dX = 0$$

From which we can conclude (since  $\Omega_t$  is arbitrary) that

#### Mass Conservation (Lagrangian)

$$\varrho_0(X) = \varrho(\varphi(X)) \det F(X). \tag{5.1.1}$$

This is the Lagrangian or *material* description of the conservation of mass.

## 5.2 Momentum

We give the Eulerian conservation equation again here for reference,

$$\int_{\Omega} \frac{\partial(\rho \vec{v})}{\partial t} + \operatorname{div}(\rho \vec{v} \otimes \vec{v}) - \vec{f}_b - \operatorname{div} T \, dx = 0.$$

To obtain a Lagrangian representation of momentum conservation equivalent to (4.1.3), we can perform a change of variable, i.e. "transform" from  $x$  to  $X$ . For the first three terms of (4.1.3) this is a straight forward process, again multiplying by a factor  $\det F$  to transform differential volumes  $dx$  to differential volumes  $dX$ . However, for the last term in (4.1.3) we need a way to relate the changing orientation and size (stretching) of differential areas. The goal is to find a tensor field  $T_0(X) \ni \operatorname{Div} T_0 = \det F \operatorname{div} T$ . The Piola transform presented briefly at the end of Chapter 3 provides the appropriate tool to accomplish this objective.

**Piola Transform.** The derivation of the Piola transform is given on pages 16-18 of the book. The result is, if

$$T_0(X) = [\det F(X)] T(X) F(X)^{-T},$$

then

### Piola Transform

$$\operatorname{Div} T_0 = \operatorname{div} T \det F.$$

Observe,

$$\int_{\Omega_0} \operatorname{Div} T_0 \, dX = \int_{\Omega_0} \operatorname{div} T \det F \, dX = \int_{\Omega} \operatorname{div} T \, dx.$$

and by the divergence theorem,

$$\int_{\partial \Omega_0} T_0 \hat{n}_0 \, dA_0 = \int_{\partial \Omega} T \hat{n} \, dA$$

Tensor  $T$  is a linear transformation from  $\hat{n}$  (CC) to a CC force/CC area. Tensor  $T_0$  is a linear transformation of a normal  $\hat{n}_0$  (RC) to a CC force/RC area. Since  $T_0 = \operatorname{Cof} F$ ,  $\|\operatorname{Cof} F\|$  is the area scaling from the reference configuration to the current configuration. The direction of  $\operatorname{Cof} F \hat{n}_0$  is then in the direction of  $\hat{n}$ , and

$$\hat{n} = \frac{\operatorname{Cof} F \hat{n}_0}{\|\operatorname{Cof} F \hat{n}_0\|}.$$

Tensor  $T_0$  is given the symbol  $P(X)$ , the first Piola-Kirchhoff Stress Tensor,

**1<sup>st</sup> Piola-Kirchhoff Stress Tensor**

$$P = \det F T F^{-\top} = T \text{Cof } F \quad (5.2.1)$$

We can now have the tools to rewrite the conservation of momentum equation (4.1.3) in Lagrangian form,

**Momentum Conservation (Lagrangian)**

$$\varrho_0 \frac{\partial^2 u}{\partial t^2} = \text{Div } P + f_0 \quad (5.2.2)$$

where,

$$\begin{aligned} \varrho_0 &= \varrho(\varphi(X)) \det F \\ f_0 &= f(\varphi(X)) \det F. \end{aligned}$$

But note, tensor  $P$  is not symmetric (since  $F$  and therefore its cofactor are not symmetric). But, since  $P = \det F T F^{-\top}$ , it follows that  $P F^{\top} = \det F T$  is symmetric (since  $\det F$  is a scalar and  $T$  is symmetric). A symmetric tensor is also recovered if we map the CC force/RC area to an RC force/RC area. This is accomplished by pre-multiplication of  $F^{-1}$ , and we define the second Piola-Kirchhoff Stress Tensor  $S$  in this way.

**2<sup>nd</sup> Piola-Kirchhoff Stress Tensor**

$$S = F^{-1} P = \det F F^{-1} T F^{-\top} \quad (5.2.3)$$

In terms of  $S$  momentum conservation becomes,

**Momentum Conservation (in terms of  $S$ )**

$$\varrho_0 \frac{\partial^2 u}{\partial t^2} = \text{Div } \underbrace{F S}_P + f_0 \quad (5.2.4)$$

The tensor  $S$  is a linear transformation of a normal  $\hat{n}_0$  (RC) to an RC force/RC area (fully RC map).



### 5.3 Energy

We conclude with the derivation of Lagrangian energy conservation (and entropy equation). We proceed by treating each of the following terms in order.

$$\int_{\Omega_t} \underbrace{\frac{\partial \varrho e}{\partial t} + \operatorname{div}(\varrho e \vec{v})}_{(i)} dx = \int_{\Omega_t} \underbrace{T : D}_{(ii)} + \underbrace{r}_{(iii)} - \underbrace{\operatorname{div} \vec{q}}_{(iv)} dx$$

(i) Observe,

$$\begin{aligned} \frac{\partial \varrho e}{\partial t} + \operatorname{div}(\varrho e \vec{v}) &= \varrho \left( \frac{\partial e}{\partial t} + \operatorname{div}(e \vec{v}) \right) \\ &= \varrho \left( \frac{\partial e}{\partial t} + \vec{v} \cdot \operatorname{grad} e \right) \\ &= \varrho \frac{De}{dt} = \varrho \dot{e} \\ &= \varrho_0 \dot{e}_0 \end{aligned}$$

where the integrals have been neglected and,

$$\begin{aligned} \varrho_0 &= \varrho(\varphi(X)) \det F \\ e_0 &= e(\varphi(X)). \end{aligned}$$

Note that  $e_0$  is not scaled by the volume ratio  $\det F$  as it is measured per unit mass not per unit volume.

(ii)

$$\begin{aligned} \int_{\Omega_t} T : D dx &= \int_{\Omega_0} T : \operatorname{grad} v \det F dX \\ &= T_{ij} \frac{\partial^2 \varphi_i}{\partial X_k \partial t} \frac{\partial X_k}{\partial x_j} \det F \\ &= T_{ij} \dot{F}_{ik} F_{kj}^{-1} \det F \\ &= \dot{F}_{ik} \left( T_{ij} F_{jk}^{-\top} \det F \right) \\ &= \dot{F}_{ik} P_{ik} = \dot{F}_{ik} F_{ij} S_{jk} \\ &= \left( F^\top \dot{F} \right) : S \\ &= \dot{E} : S = S : \dot{E} \end{aligned}$$

where the integrals have again been neglected after the first line.

(iii)

$$r = r_0 \det F$$

(iv) See homework,

$$\operatorname{div} \vec{q} = \operatorname{Div} \vec{q}_0$$

where,

$$\vec{q}_0 = (\operatorname{Cof} F)^{\top} \vec{q}$$

Substituting the preceding relationships we arrive at the Lagrangian conservation of internal energy,

### Energy Conservation (Lagrangian)

$$\varrho_0 \dot{e}_0 = S : \dot{E} - \operatorname{Div} \vec{q}_0 + r_0 \quad (5.3.1)$$

Finally, the entropy equation can be transformed by combining trivial analogues of the preceding transformations,

### Clausius Duhem Inequality (Lagrangian)

$$\varrho_0 \dot{\eta}_0 + \operatorname{Div} \frac{\vec{q}_0}{\theta} - \frac{r_0}{\theta} \geq 0 \quad (5.3.2)$$

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## 6. Constitutive Equations (Closure Models)

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Consider the Eulerian conservation equations (note that this form of Eulerian conservation is obtained by applying product rule and applying conservation of mass, it does not simply assume  $\rho$  is time independent as this is not generally true):

### Eulerian Conservation

|               |   |  |
|---------------|---|--|
| Mass          | $\frac{\partial \rho}{\partial t} + \text{div}(\rho v) = 0$   |  |
| Lin. Momentum | $\rho \left( \frac{\partial(\vec{v})}{\partial t} + \vec{v} \circ \text{grad} \vec{v} \right) = \text{div} T + \vec{f}_b$                             |  |
| Ang. Momentum | $T = T^T$   |  |
| Energy        | $\rho \left( \frac{\partial e}{\partial t} + \vec{v} \cdot \text{grad} e \right) = T : D + r - \text{div} \vec{q}$                                    |  |
| Entropy       | $\rho \left( \frac{\partial \eta}{\partial t} + \vec{v} \cdot \text{grad} \eta \right) + \text{div} \frac{\vec{q}}{\theta} - \frac{r}{\theta} \geq 0$ |  |

Given initial conditions, we want to solve these equations for evolution of variables describing state of the continuum (body). Note however that we have far more unknowns than equations.

Counting unknowns we have,

|        |                         |     |                                 |     |           |                           |        |          |  |                  |
|--------|-------------------------|-----|---------------------------------|-----|-----------|---------------------------|--------|----------|--|------------------|
| $\rho$ | $\vec{v}(\text{or } u)$ | $T$ | <del><math>\vec{f}</math></del> | $e$ | $\vec{q}$ | <del><math>r</math></del> | $\eta$ | $\theta$ |  | Total            |
| 1      | 3                       | 6   | <del>3</del>                    | 1   | 3         | <del>1</del>              | 1      | 1        |  | <del>20</del> 16 |

where the crossed out variables are not counted because they are determined by external data and other physical phenomenon (e.g. gravity, E&M, chemistry), and the conservation of angular momentum equation implying the symmetry of  $T$  is used to reduce the number of unknowns in  $T$  to 6.

Now counting equations we note,

|      |          |        |  |       |
|------|----------|--------|--|-------|
| Mass | Momentum | Energy |  | Total |
| 1    | 3        | 1      |  | 5     |

Thus we clearly require additional relationships. We begin by identifying quantities that characterize the state of the body (5 we hope) that we will call state variables. A convenient choice is,

Solids:  $\rho, \vec{u} (v = \dot{u}), \theta$  (or  $e$ )  
 Fluids:  $\rho, \vec{v}, \theta$  (or  $e$ )

We need to formulate relationships to determine remaining quantities from these. These relationships are:

- determined by properties of the material
- models of phenomena (atomic) not represented in the continuum approximation

We need constitutive models for:

$T$  – inner atomic forces and/or momentum diffusion

$\vec{q}$  – heat conduction

$e$  – thermodynamics and inner atomic forces

$\eta$  – thermodynamics

In addition to dimensional and coordinate invariance, we will require that our constitutive models follow these principles:

- 1.) **Determinism** – no dependence on the future state.
- 2.) **Material Frame Indifference (MFI)** – invariance to changes in the reference frame, i.e. no dependence on rigid motions (uniform velocity or rotation)
- 3.) **Physical Consistency** – cannot violate conservation laws or Clausius Duhem (2<sup>nd</sup> law)
- 4.) **Material Symmetry** – If the material is invariant to a group of "unimodular" transformations (e.g. rotations; reflections; continuous rotation group or isotropy) then constitutive model must also be invariant to these transformations
- 5.) **Local Action** – Constitutive model depends only on "local" state; essentially depends on the state and finite number of spatial derivatives at a point.
- 6.) **Dimensional Consistency** – dimensional and coordinate invariance
- 7.) **Other Considerations** – well-posedness, Equipresence

## 6.1 Application of MFI to $T$ for Solids.

Two observers can be moving or rotating differently. The motion observed by one observer,  $x(t)$  is related to the motion observed by the second observer,  $x^*(t)$  through,

$$x^*(t) = \underbrace{Q(t)}_{\text{rotation}} x(t) + \underbrace{c(t)}_{\text{translation}}$$

where  $Q$  and  $c$  do not depend on  $x$ . Since rotations are unitary transformations, it must be that

$$Q^T(t) = Q^{-1}(t).$$

We expect (hypothesize) the Cauchy stress tensor  $T$  to depend on  $x$ ,  $X$ , and  $t$  (or equivalently  $u, t$ ). But, note, to have  $T$  independent of  $c(t)$  we instead need to consider derivatives of  $u$ , i.e.  $F$  and other higher order derivatives.

**Suppose  $Q = I$ ,  $c \neq 0$ ,  $c(0) = 0$ .** Then MFI and locality principles require that

$$T = \mathcal{T}(F, \text{higher derivatives}, X)$$

and where we have assumed that  $T$  depends only on the first derivative of  $u$ ,  $F$ . Thus we have,

$$T(X, \tau) = \mathcal{T}(F(X, \tau), X) \quad \text{for } \tau \geq t$$

Now **Suppose  $Q \neq I$ .** Observe,

$$F^* = QF \quad \text{and} \quad \det F^* = \det F$$

with

$$n^* = Qn \quad \implies \quad \sigma^*(n^*) = Q\sigma(n).$$

We know that  $\sigma(n) = Tn$  and  $\sigma^*(n^*) = T^*n^*$  thus we get that

$$\sigma^*(n^*) = T^*n^* = Q\sigma(n) = QTn = QTQ^T n^*$$

which implies that,

### MFI Constraint

$$T^* = QTQ^T. \tag{6.1.1}$$

But note, this implies that the relationship

$$T = \mathcal{T}(F)$$

must have the property that

**MFI Constraint (Solids)**

$$\mathcal{T}(\underbrace{QF}_{F^*}) = Q \mathcal{T}(F) Q^\top \quad (6.1.2)$$

for all  $Q(t)$ .

Notice that for  $C = F^\top F$ ,

$$C^* = \underbrace{F^\top Q^\top}_{F^{*\top}} \underbrace{QF}_{F^*} = C.$$

We need to satisfy (6.1.2) and will thus make an educated guess that the relation takes the form,

$$\mathcal{T}(F) = F \hat{\mathcal{T}}(C) F^\top. \quad (6.1.3)$$

Then

$$\mathcal{T}(QF) = QF \hat{\mathcal{T}}(C) F^\top Q^\top = Q \mathcal{T}(F) Q^\top$$

satisfies (6.1.2) so is consistent with MFI.

Finally, because of the polar decomposition theorem,  $F = RU$  where  $R$  is orthonormal and  $U$  is symmetric and positive definite. So MFI implies,

$$\mathcal{T}(U) = \mathcal{T}(R^\top F) = R^\top \mathcal{T}(F) R \quad \implies \quad \mathcal{T}(F) = R^\top \mathcal{T}(U) R$$

Recalling that  $C = U^2$ ,  $R = FU^{-1}$ , and  $R^\top = U^{-1}F^\top$  we have that

$$\mathcal{T}(F) = F \underbrace{U^{-1} \mathcal{T}(C^{\frac{1}{2}}) U^{-1}}_{\tilde{\mathcal{T}}(C)} F^\top = F \hat{\mathcal{T}}(C) F^\top$$

where the last equality follows from (6.1.3) and since  $U = C^{\frac{1}{2}}$  we can write,

$$\hat{\mathcal{T}}(C) = \left(C^{\frac{1}{2}}\right)^{-1} \mathcal{T}\left(C^{\frac{1}{2}}\right) \left(C^{\frac{1}{2}}\right)^{-1}$$

so this is the ONLY form satisfying MFI.

In this last expression we have expressed  $U$  as  $C^{\frac{1}{2}}$  to make the dependence on  $C$  explicit as hypothesized in (6.1.3). We have finally that any constitutive relationship for  $T$  depending on  $F$  must take the form (expressed now in terms of  $U$ ) of

**MFI Solids**

$$T = \mathcal{T}(F) = FU^{-1} \mathcal{T}(U) U^{-1} F^\top \quad (6.1.4)$$

## 6.2 Restricted Classes of Constitutive Relations

**Thermo-elastic.** For this class of constitutive relations we assume that quantities  $T, \vec{q}, e, \eta$  at a point depend only on present values of the following state variables at the point:

Solids:  $F, \theta, \nabla\theta$

Fluids:  $D, \theta, \nabla\theta, \rho$

**Homogeneity.** For this class of constitutive relations we assume we have the same material everywhere (reference configuration uniform) so no explicit dependence on  $X$ .

### 6.3 Application of MFI to Fluids

A fluid is a material for which dependence of the Cauchy stress tensor  $T$  on deformation limited to dependence on  $\det F$ . As a consequence, the reference configuration becomes irrelevant. Also since  $\varrho_0 = \det F \varrho$ , the dependence on  $\det F$  is already included with dependence on  $\varrho$  in an Eulerian representation.

An **ideal fluid** (also inviscid fluid) is one in which  $T$  is isotropic, i.e.

#### Stress in Ideal Fluid

$$T = -P(x, t)I \quad (6.3.1)$$

which clearly satisfies MFI requirements since  $I$  commutes with tensor operations (note dependence of  $\varrho$ ,  $\theta$  suppressed here). From thermodynamics, a constitutive model for  $P$  in terms of  $\varrho$  at  $\theta$  is an "equation of state."

In a viscous fluid,  $T = -PI + \mathcal{F}(L)$  where  $L = \text{grad } v$  and dependence on  $\varrho, \theta$  has been suppressed.

**MFI Considerations.** Observe,

$$L = \dot{F}F^{-1} = \text{grad } v$$

and

$$L^* = \dot{F}^*(F^*)^{-1} = QLQ^T + \Omega$$

where  $\Omega = \dot{Q}Q^T$  is the *rotation rate*. But note,

$$\Omega + \Omega^T = \dot{Q}Q^T + Q\dot{Q}^T = \overline{\dot{Q}Q^T} = \dot{I} = 0$$

thus,

$$\Omega = -\Omega^T. \quad (\text{Antisymmetric})$$

Considering MFI we can see that

#### MFI Fluid

$$\mathcal{F}(\overbrace{QLQ^T + \Omega}^{L^*}) = Q\mathcal{F}(L)Q^T$$

Thus, by eliminating  $\Omega$  in the equation above and (and recalling  $D = \frac{1}{2}(L + L^T)$ ) we see (this follows because applying MFI to  $D = \frac{1}{2}(L + L^T)$  gives  $D^* = QDQ^T$ )

$$\mathcal{F}(L) = \mathcal{F}(D)$$

We then need that



**MFI Fluid (Stokes)**

$$\mathcal{F}(\overbrace{QDQ^T}^{D^*}) = Q \mathcal{F}(D) Q^T$$

for an isotropic fluid—this is a Stokes fluid.

If we further assume that  $\mathcal{F}$  is *linear* in  $D$  we obtain the general form for a Newtonian Fluid,

**Stress in Newtonian Fluid**

$$T = -PI + 2\mu \left( D - \frac{1}{3} \text{tr}[D]I \right) + \kappa \text{tr}[D]I$$

where,

$P$  – pressure

$\mu$  – viscosity (shear viscosity)

$\kappa$  – bulk viscosity (commonly assumed to be 0)

and  $P, \mu, \kappa$  can depend on  $\varrho, \theta$ . The bulk viscosity represents the irreversibility of volume change and is typically small for fluids at reasonable conditions (thus assumed to be zero).

**Special case of incompressible flow.** Valid in the limit as  $\frac{\|\vec{v}\|}{c} \rightarrow 0$  with  $c$  is the speed of sound. In this limit:

$$\text{div } \vec{v} = 0 \quad \implies \quad \text{tr}[D] = 0$$

$$\varrho = \text{constant}$$

$$T = -P_{in} + T_{\text{visc}} \quad \text{where} \quad \text{tr}[T_{\text{visc}}] = 0$$

where constitutive relation needed for  $T_{\text{visc}}$ , and  $P_{in}$  determined by  $\text{div } v = 0$ . For a Newtonian fluid,  $T_{\text{visc}} = 2\mu D$ .

## 6.4 2<sup>nd</sup> Law Consistency

We must adhere to the second law of thermodynamics, i.e. satisfy the Clausius-Duhem inequality,

$$\rho \frac{\partial \eta}{\partial t} + \operatorname{div} \frac{\vec{q}}{\theta} - \frac{r}{\theta} \geq 0$$

**For solids (Coleman-Noll).** One approach to enforce the 2<sup>nd</sup> law in solids is the so-called Coleman-Noll approach.

Consider the Helmholtz free energy

$$\Psi = e - \theta \eta.$$

We develop a relation for  $\Psi$  by subtracting the conservation equation for  $e$  from  $\theta$  times the conservation constraint (Clausius-Duhem) for  $\eta$ :

$$\begin{aligned} & - \left( \rho \frac{\partial e}{\partial t} - T : D - r + \operatorname{div} \vec{q} = 0 \right) \\ & + \left( \rho \theta \frac{\partial \eta}{\partial t} + \theta \operatorname{div} \frac{\vec{q}}{\theta} - r \geq 0 \right) \\ \hline & - \rho \frac{d\Psi}{dt} - \rho \eta \frac{d\theta}{dt} + T : D - \frac{\vec{q}}{\theta} \cdot \operatorname{grad} \theta \geq 0 \end{aligned}$$

or, in expressed in the reference configuration

$$- \rho_0 \dot{\Psi}_0 - \rho_0 \eta_0 \dot{\theta} + S : \dot{E} - \frac{\vec{q}_0}{\theta} \cdot \nabla \theta \geq 0. \quad (6.4.1)$$

Suppose,

$$\Psi_0 = \psi(E, \theta, \nabla \theta)$$

Then

$$\dot{\Psi}_0 = \frac{\partial \psi}{\partial E} : \dot{E} + \frac{\partial \psi}{\partial \theta} \dot{\theta} + \frac{\partial \psi}{\partial \nabla \theta} \cdot \nabla \dot{\theta}.$$

Substituting this into (6.4.1) we obtain that,

$$\left( S - \rho_0 \frac{\partial \psi}{\partial E} \right) : \dot{E} - \rho_0 \left( \frac{\partial \psi}{\partial \theta} + \eta_0 \right) \dot{\theta} - \rho_0 \frac{\partial \psi}{\partial \nabla \theta} \cdot \nabla \dot{\theta} - \frac{\vec{q}_0}{\theta} \cdot \nabla \theta \geq 0$$

However, notice that this must hold for arbitrary sign of  $\dot{E}, \dot{\theta}, \nabla \dot{\theta}$ , so it is convenient to let coefficient on these be zero,

$$S = \rho_0 \frac{\partial \psi}{\partial E}, \quad \eta_0 = - \frac{\partial \psi}{\partial \theta}, \quad \frac{\partial \psi}{\partial \nabla \theta} = 0.$$

Then we have simply that

$$- \frac{\vec{q}_0}{\theta} \cdot \nabla \theta \geq 0.$$

Rearranging and switching back to the current configuration we see,

$$-\vec{q} \cdot \text{grad } \theta \geq 0$$

Thus heat must flow from hot to cold.

In this case where  $S = \varrho_0 \frac{\partial \psi}{\partial E}$  the strain is non-dissipative—i.e. work done on the body to affect deformation can be recovered.

More generally  $S$  may depend also on  $\dot{E}$ , which will lead to dissipation. Then,

$$S = \mathcal{F}(E) + \mathcal{I}(\dot{E})$$

where

$$\mathcal{F}(E) = \varrho_0 \frac{\partial \psi}{\partial E}$$

and

$$\mathcal{I}(\dot{E}) : \dot{E} - \frac{\vec{q}_0}{\theta} \cdot \nabla \theta \geq 0.$$

Before considering 2<sup>nd</sup> law consistency for fluids we note that the above assumption that

$$S = \varrho_0 \frac{\partial \psi}{\partial E}$$

implies that instead of identifying a tensor function to model  $S$  we may instead be able to identify scalar function. In particular the previous equality assumes that material deformations are reversible. In the case of material deformations in the elastic regime this is fair assumption. We will return to this later.

**For fluids.** For a viscous fluid in the Eulerian representation, we assume  $\psi$  depends on  $\theta, \text{grad } \theta$  only. That is,  $\psi(\theta, \text{grad } \theta)$ . We have,

$$T = \mathcal{I}(D)$$

where,

$$\mathcal{I}(D) : D - \frac{q}{\theta} \cdot \text{grad } \theta \geq 0.$$

Then

$$\eta = -\frac{\psi}{\theta} \qquad \frac{\partial \psi}{\partial \text{grad } \theta} = 0$$

leads to  $\mu, \kappa > 0$ .

We return to the governing equation for a Newtonian fluid. The Newtonian constitutive law for  $T$  is

$$T = -PI + 2\mu \tilde{D} + \kappa \text{tr}[D]$$

where  $\tilde{D} = D - \frac{1}{3} \text{tr}[D]I$  is the deviatoric part of  $D$  (constructed such that  $\text{tr}[\tilde{D}] = 0$ ). Most often we have the following dependencies,

$$\mu = \mu(\theta) \qquad \kappa = 0 \qquad P = P(\varrho, \theta)$$

e.g.  $P = \rho R \theta$ , (ideal gas)

We also have the Fourier heat conduction law,

#### Fourier's Law

$$\vec{q} = -k \text{grad } \theta \quad (6.4.2)$$

where  $k = k(\theta)$  is the *thermal conductivity* of the material.

For a *thermally perfect* material, we have that  $e = e(\theta)$  and

#### Specific Heat

$$\frac{de}{d\theta} = C_\nu \quad (6.4.3)$$

If we additionally assume the material is *Callorically perfect*, i.e.

$$C_\nu = \text{constant}$$

we get

$$e = C_\nu \theta.$$

Substituting these into the Eulerian equations we get the Navier-Stokes equations,

#### Navier Stokes Equations

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{v}) &= 0 \\ \rho \frac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \text{grad } \vec{v} &= -\text{grad } P + \text{div}(2\mu \tilde{D}) + \text{grad}(\kappa \text{div } \vec{v}) \\ \rho C_\nu \frac{\partial \theta}{\partial t} + \rho C_\nu \vec{v} \cdot \text{grad } \theta &= -P \text{div } \vec{v} + 2\mu \tilde{D} : D \\ &\quad + \kappa (\text{div } \vec{v})^2 + \text{div}(k \text{grad } \theta) \end{aligned} \quad (6.4.4)$$

This system is now closed if we have constitutive relations for parameters  $\mu, \kappa, k$  and an equation of state (e.g. ideal gas law) for  $P$ . The following dependencies are commonly used:  $P(\theta, \rho), \mu(\theta), k(\theta), \kappa = 0$ .

Additionally, to be able to solve this set of differential equations we need initial and boundary conditions.

**Initial Conditions** include:

$$\varrho(x, 0) = \varrho_0(x) \quad \vec{v}(x, 0) = \vec{v}_0(x) \quad \theta(x, 0) = \theta_0(x)$$

**Boundary Conditions** include:

$$\left. \begin{aligned} (PI + \kappa \operatorname{div} \vec{v}I + 2\mu\tilde{D})n &= \vec{g}(x, t) \\ \vec{v} &= \vec{v}(x, t) \end{aligned} \right\} \text{or}$$

$$\left. \begin{aligned} -\kappa\nabla\theta \cdot n &= g(x, t) \\ \theta &= \theta(x, t) \end{aligned} \right\} \text{or}$$

There are many other equivalent forms. For example:

Conservative form of momentum equation

$$\frac{\partial(\varrho\vec{v})}{\partial t} + \operatorname{div}(\varrho\vec{v} \otimes \vec{v}) = -\operatorname{grad} P + 2\operatorname{div}(\mu\tilde{D}) + \operatorname{grad}(\kappa \operatorname{div} \vec{v})$$

Conservative form of energy equation

$$\frac{\partial(\varrho E)}{\partial t} + \operatorname{div}(\varrho\vec{v}E) = -\operatorname{div}(P\vec{v}) + 2\operatorname{div}(\tilde{D}\vec{v}) + \operatorname{div}(\kappa \operatorname{grad} \theta)$$

where,  $E = \frac{1}{2}\vec{v} \cdot \vec{v}$ .

The Navier Stokes (N-S) equations describe a wide variety of observed phenomena in fluids including: turbulence, sound waves—compression waves traveling at speed  $a$ , where  $a^2 = \frac{\partial P}{\partial \varrho} \Big|_S$

If we non-dimensionalize these equations the natural scaling is,

$$\begin{aligned} \hat{x} &= \frac{x}{\delta} & \hat{v} &= \frac{\vec{v}}{v_0} & \hat{\varrho} &= \frac{\varrho}{\varrho_0} \\ \hat{P} &= \frac{P}{\varrho_0 a_0^2} & \hat{t} &= \frac{t v_0}{\delta} & \hat{\theta} &= \frac{\theta}{\theta_0} \end{aligned} \quad (6.4.5)$$

where  $a_0$  is the speed of sound at reference thermodynamic conditions.

Rewriting the momentum equation we have,

$$\hat{\varrho} \frac{\partial \hat{v}}{\partial \hat{t}} + \hat{\varrho} \hat{v} \cdot \widehat{\operatorname{grad}} \hat{v} = \frac{1}{M^2} \widehat{\operatorname{grad}} \hat{P} + \frac{1}{\operatorname{Re}} \widehat{\operatorname{div}} \hat{T}_{\text{visc}} \quad (6.4.6)$$

where  $M = \frac{v_0}{a_0}$  and  $\operatorname{Re} = \frac{\varrho_0 v_0 \delta}{\mu_0}$ . In the limit as  $M \rightarrow 0$ , for the pressure gradient term to be finite we must have

$$\hat{P} = \underbrace{\hat{P}_0(t)}_{\text{ord. 1 \& ind. of } x} + \underbrace{M^2 \hat{P}'(x, t)}_{\text{ord. 1 pressure fluctuates}}$$

from equations of state  $P = P(\rho, \theta)$  (e.g. ideal gas  $P = \rho R\theta$ ) thus, suggests that

$$\hat{\theta} = 1 + M^2\theta'(x, t)$$

$$\hat{\rho} = 1 + M^2\rho'(x, t)$$

though other behaviors are possible—leading to different equations.

Keeping terms of order 1 only in (6.4.6) gives,

$$\hat{\rho} \frac{\partial \hat{v}}{\partial \hat{t}} + \hat{\rho} \hat{v} \cdot \widehat{\text{grad}} \hat{v} = -\widehat{\text{grad}} \hat{P}' + \frac{1}{\text{Re}} \widehat{\text{div}} \hat{T}_{\text{visc}}.$$

For mass conservation,

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \hat{v} \cdot \widehat{\text{grad}} \hat{\rho} = -\hat{\rho} \widehat{\text{div}} \hat{v} \quad \implies \quad \widehat{\text{div}} \hat{v} = 0$$

Thus,

$$\begin{aligned} \hat{T}_{\text{visc}} &= 2\hat{\mu} \hat{D} + \hat{\kappa} \widehat{\text{div}} \hat{v} I \\ &= \hat{u} \left( \widehat{\text{grad}} \hat{v} + \widehat{\text{grad}} \hat{v}^\top \right) + \left( \hat{\kappa} - \frac{2}{3} \hat{\mu} \right) \widehat{\text{div}} \hat{v} I \end{aligned}$$

Further  $\hat{\mu} \rightarrow 1$  and  $\widehat{\text{div}}(\widehat{\text{grad}} \hat{v}^\top) = \widehat{\text{grad}}(\widehat{\text{div}} \hat{v}) = 0$ , therefore

$$\widehat{\text{div}} T_{\text{visc}} = \widehat{\text{div}} \widehat{\text{grad}} \hat{v} = \widehat{\Delta} \hat{v},$$

the vector Laplacian.

$$\hat{\rho} \frac{\partial \hat{v}}{\partial \hat{t}} + \hat{\rho} \hat{v} \cdot \widehat{\text{grad}} \hat{v} = -\widehat{\text{grad}} \hat{P}' + \frac{1}{\text{Re}} \widehat{\Delta} \hat{v}.$$

Note that

$$\begin{aligned} P &= P_0(t) + P'(x, t) \\ \implies \hat{P} &= \frac{P_0(t)}{\rho_0 a_0^2} + \frac{P'_0}{\rho_0 a_0^2} \\ \implies \frac{P'}{\rho a^2} &= M^2 \hat{P}' \\ \implies \hat{P}' &= \frac{P'}{\rho v_0^2} \end{aligned}$$

Expressing everything back in dimensional variables

### Incompressible Navier Stokes

$$\begin{aligned} \rho_0 \frac{\partial \vec{v}}{\partial t} + \rho_0 \vec{v} \cdot \text{grad} \vec{v} &= -\text{grad} P' + \mu_0 \Delta \vec{v} + \vec{f} \\ \text{div} \vec{v} &= 0 \end{aligned} \tag{6.4.7}$$

These are the incompressible Navier Stokes Equations—note that no constitutive relations for  $\mathbf{P}'$  are needed. We still need boundary and initial conditions however.

Initial Conditions:

$$\text{need } \vec{v}(x, 0) = \vec{v}_0(x) \quad \text{with} \quad \text{div } \vec{v}_0 = 0$$

Boundary Conditions: several types for example

1. Inflow –  $\vec{v}$  is specified
2. Walls –  $\vec{v} = 0$  (no-slip condition)
3. Free stream –  $T_{\text{visc}}n = 0$  (no stress)
4. Outflow –  $T_{\text{visc}}n = 0$

## 6.5 Heat Equation

Take what we did with energy and heat flux, i.e.

$$de = C_\nu d\theta \qquad \vec{q} = -k \operatorname{grad} \theta,$$

then if there is no deformation we get,

### Heat Equation

$$\rho C_\nu \frac{\partial \theta}{\partial t} = \operatorname{div}(\kappa \operatorname{grad} \theta) + r \tag{6.5.1}$$

with  $k > 0$  required by the 2<sup>nd</sup> law.



## 6.6 Elasticity

For a deformable body (solid) with uniform  $\theta$ , no heat flux ( $\vec{q} = 0$ ), homogeneous, and isotropic.

The free energy constitutive dependence simplifies to

$$\Psi = \psi(E).$$

We then call  $\Psi$  the *stored energy function* or *strain energy function*. This is a *hyperelastic* constitutive relation.

Since  $\psi$  is an isotropic scalar function of a tensor it must take the following form:

$$\psi = W(\overbrace{I_E, II_E, III_E}^{\text{invariants}}).$$

Then,

$$S = \frac{\partial \psi}{\partial E} = \frac{\partial W}{\partial I_E} \frac{\partial I_E}{\partial E} + \frac{\partial W}{\partial II_E} \frac{\partial II_E}{\partial E} + \frac{\partial W}{\partial III_E} \frac{\partial III_E}{\partial E}.$$

For example,  $\frac{\partial E_{ii}}{\partial E_{jk}} = \delta_{jk}$  implies that  $\frac{\partial I_E}{\partial E} = I$ .

Similarly we should get

$$\begin{aligned} \frac{\partial II_E}{\partial E} &= \text{tr}[E] I - E \\ \frac{\partial III_E}{\partial E} &= \frac{1}{2} (\text{tr}[E]^2 - \text{tr}[E^2]) I + (E^2 - \text{tr}[E]E) \end{aligned}$$

Equations then become,

### Elasticity Equations

$$\begin{aligned} \rho_0 \frac{\partial^2 u}{\partial t^2} &= \text{Div} \left( (I + \nabla u) \frac{\partial W}{\partial E} \right) + F_0 \\ E &= \frac{1}{2} \left( \nabla u + \nabla u^\top + \nabla u^\top \nabla u \right). \end{aligned} \tag{6.6.1}$$

## 6.7 Linear Elasticity

Assume all displacements are small, then non-linear terms become negligible,

$$E \approx e = \frac{1}{2} (\nabla u + \nabla u^\top).$$

What do Young's Modulus and Poisson's ratio mean? Consider a cylinder under uni-axial loading. In the central region, far from clamped ends must have,

$$S_{11} = \frac{F}{A}, \quad S_{22} = S_{33} = 0.$$

Also,

$$\frac{\partial u_2}{\partial x_2} = \frac{\partial u_3}{\partial x_3}$$

due to isotropy. Then,

$$\begin{aligned} S_{11} &= (2\mu + \lambda) \frac{\partial u_1}{\partial x_1} + 2\lambda \frac{\partial u_2}{\partial x_2} \\ S_{22} &= \lambda \frac{\partial u_1}{\partial x_1} + (2\mu + 2\lambda) \frac{\partial u_2}{\partial x_2} = 0 \\ \implies \frac{\partial u_2}{\partial x_2} &= \frac{\lambda}{2\mu + 2\lambda} \frac{\partial u_1}{\partial x_1} = -\nu \frac{\partial u_1}{\partial x_1} \end{aligned}$$

then we have,

$$S_{11} = (2\mu + \lambda(1 - 2\nu)) \frac{\partial u_1}{\partial x_1} = E \frac{\partial u_1}{\partial x_1}$$

If  $\frac{\partial^2 u}{\partial t^2}$  is zero these are the Lamé equations,

### Lamé Equations

$$(\lambda + \mu) \frac{\partial^2 u_k}{\partial x_i \partial x_k} + \mu \frac{\partial^2 u_i}{\partial x_i \partial x_k} + \vec{f}_{0i} = \rho_0 \frac{\partial^2 u_i}{\partial t^2} \quad (6.7.1)$$

These describe many important phenomena such as elastic wave propagation. Boundary conditions – no displacement, specified traction. Furthermore, if  $S$  is linear in  $E$ , in general

$$W = \frac{1}{2} E_{ijkl} e_{kl} e_{ij}$$

and

$$S_{ij} = \frac{\partial W}{\partial e_{ij}} = E_{ijkl} e_{kl}$$

and symmetry requires that,

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}$$

thus,

$$S_{ij} = E_{ijkl} \frac{\partial u_k}{\partial X_\ell}$$

So we have finally that,

### Linearized Lamé Equations

$$\varrho_0 \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial X_j} \left( E_{ijkl} \frac{\partial u_k}{\partial X_\ell} \right) + \vec{f}_{0,i} \quad (6.7.2)$$

For an isotropic material, most general form is

$$E_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$$

and  $\mu, \lambda$  and the Lamé constants

$$\lambda = \frac{\nu E}{(1 + \nu)(1 - 2\nu)} \quad \mu = \frac{E}{2(1 + \nu)}$$

$E$  is Young's Modulus,  $\nu$  is Poisson's ratio.

Then

$$S = \lambda \text{tr}[E] I + 2\mu E = \lambda \text{div } u + u \left( \nabla u + \nabla u^\top \right)$$

Finally, notice that for  $\nu \rightarrow \frac{1}{2}$ , then  $\lambda \rightarrow \infty$ ; so for  $S$  to remain finite,  $\text{tr}[E] \rightarrow 0$  and  $\text{div } u \rightarrow 0$ .

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## A. Calculus Identities

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The following reference pages were created by my good friend and mentor, Dr. Vladimir Solovjov and are available with many other engineering and math resources on his webpage, <http://www.et.byu.edu/~vps/ME505>.

Let  $\mathbf{a}(\mathbf{r}), \mathbf{b}(\mathbf{r}), \mathbf{F}(\mathbf{r}) : \mathbb{R}_3 \rightarrow \mathbb{R}_3$  be vector fields,  $\varphi(\mathbf{r}), u(\mathbf{r}) : \mathbb{R}_3 \rightarrow \mathbb{R}$  be scalar fields,  $c \in \mathbb{R}$  [see B&T, p.168]

|  |   |   |
|--|---|---|
| $\nabla \varphi$                           | $= \text{grad } \varphi$  | $\frac{\partial \varphi}{\partial x_j}$   |
| $\nabla \cdot \mathbf{a}$                  | $= \text{div } \mathbf{a}$  | $\delta_{kj} \frac{\partial a_k}{\partial x_j} = \frac{\partial a_k}{\partial x_k}$   |
| $\nabla \times \mathbf{a}$                 | $= \text{curl } \mathbf{a}$   | $\varepsilon_{ijk} \frac{\partial a_k}{\partial x_j}$   |
| $\nabla \cdot \nabla \varphi$              | $= \text{div grad } \varphi \equiv \Delta \varphi \equiv \nabla^2 \varphi$  | $\frac{\partial}{\partial x_i} \frac{\partial}{\partial x_i} \varphi = \partial_i \partial_i \varphi$ <i>Laplacian operator</i>   |
| $\nabla \times \nabla \varphi$             | $= \text{curl grad } \varphi = \mathbf{0}$  | <i>vanishes identically</i>   |
| $\nabla(\nabla \cdot \mathbf{a})$          | $= \text{grad div } \mathbf{a}$   | $\delta_{jk} \frac{\partial^2 a_j}{\partial x_i \partial x_k} = \frac{\partial}{\partial x_i} \left( \frac{\partial a_k}{\partial x_k} \right)$   |
| $\nabla \cdot (\nabla \times \mathbf{a})$  | $= \text{div curl } \mathbf{a} = 0$   | <i>vanishes identically</i>   |
| $\nabla \times (\nabla \times \mathbf{a})$ | $= \text{curl curl } \mathbf{a}$  | $\varepsilon_{ijk} \frac{\partial}{\partial x_j} \left( \varepsilon_{klm} \frac{\partial a_m}{\partial x_l} \right) = \varepsilon_{ijk} \varepsilon_{klm} \frac{\partial^2 a_m}{\partial x_j \partial x_l}$ |
| 1.   | $\Delta(\varphi + \psi) = \Delta \varphi + \Delta \psi$   |   |
| 2.   | $\nabla(\varphi + \psi) = \nabla \varphi + \nabla \psi$   | $\text{grad}(\varphi + \psi) = \text{grad } \varphi + \text{grad } \psi$  |
| 3.   | $\nabla[\nabla \cdot (\mathbf{a} + \mathbf{b})] = \nabla(\nabla \cdot \mathbf{a}) + \nabla(\nabla \cdot \mathbf{b})$  | $\text{grad div}(\mathbf{a} + \mathbf{b}) = \text{grad div } \mathbf{a} + \text{grad div } \mathbf{b}$  |
| 4.   | $\nabla \cdot (\mathbf{a} + \mathbf{b}) = \nabla \cdot \mathbf{a} + \nabla \cdot \mathbf{b}$  | $\text{div}(\mathbf{a} + \mathbf{b}) = \text{div } \mathbf{a} + \text{div } \mathbf{b}$   |
| 5.   | $\nabla \cdot (c\mathbf{a}) = c \nabla \cdot \mathbf{a}$  | $\text{div}(c\mathbf{a}) = c \text{div } \mathbf{a}$  |
| 6.   | $\nabla \times (\mathbf{a} + \mathbf{b}) = \nabla \times \mathbf{a} + \nabla \times \mathbf{b}$   | $\text{curl}(\mathbf{a} + \mathbf{b}) = \text{curl } \mathbf{a} + \text{curl } \mathbf{b}$  |
| 7.   | $\nabla \times (\nabla \times (\mathbf{a} + \mathbf{b})) = \nabla \times (\nabla \times \mathbf{a}) + \nabla \times (\nabla \times \mathbf{b})$   | $\text{curl curl}(\mathbf{a} + \mathbf{b}) = \text{curl curl } \mathbf{a} + \text{curl curl } \mathbf{b}$   |
| 8.   | $\nabla \times (\nabla \times \mathbf{a} + \nabla \varphi) = \nabla \times (\nabla \times \mathbf{a})$  | $\text{curl}(\text{curl } \mathbf{a} + \text{grad } \varphi) = \text{curl}(\text{curl } \mathbf{a})$  |
| 9.   | $\nabla(\varphi \psi) = \psi \nabla \varphi + \varphi \nabla \psi$  | $\text{grad}(\varphi \psi) = \psi \text{grad } \varphi + \varphi \text{grad } \psi$   |
| 10.  | $\nabla \cdot (\varphi \mathbf{a}) = \varphi \nabla \cdot \mathbf{a} + \mathbf{a} \cdot \nabla \varphi$   | $\text{div}(\varphi \mathbf{a}) = \varphi \text{div } \mathbf{a} + \mathbf{a} \cdot \text{grad } \varphi$   |
| 11.  | $\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b})$   | $\text{div}(\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot \text{curl } \mathbf{a} - \mathbf{a} \cdot \text{curl } \mathbf{b}$  |
| 12.  | $\nabla \times (\varphi \mathbf{a}) = \varphi (\nabla \times \mathbf{a}) + \nabla \varphi \times \mathbf{a}$  | $\text{curl}(\varphi \mathbf{a}) = \varphi \text{curl } \mathbf{a} + \text{grad } \varphi \times \mathbf{a}$  |
| 13.*                                       | $\nabla \times (\nabla \times \mathbf{a}) = \nabla(\nabla \cdot \mathbf{a}) - \overbrace{(\nabla \cdot \nabla)}^{\nabla^2 \text{ Laplacian}} \mathbf{a}$  | $\text{curl}(\text{curl } \mathbf{a}) = \text{grad}(\text{div } \mathbf{a}) - \overbrace{\Delta}^{\text{Laplacian}} \mathbf{a}$   |
| 14.  | $\nabla(\mathbf{a} \cdot \mathbf{b}) = \mathbf{a} \times (\nabla \times \mathbf{b}) + \mathbf{b} \times (\nabla \times \mathbf{a}) + (\mathbf{a} \cdot \nabla) \mathbf{b} + (\mathbf{b} \cdot \nabla) \mathbf{a}$ | $= \overbrace{\nabla}^{\text{diadic}} \mathbf{a} \mathbf{b} + \overbrace{\nabla}^{\text{diadic}} \mathbf{b} \mathbf{a}$   |
| 15.  | $\nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{a}(\nabla \cdot \mathbf{b}) - \mathbf{b}(\nabla \cdot \mathbf{a})$  | $\text{curl}(\mathbf{a} \times \mathbf{b}) = \mathbf{a} \text{div } \mathbf{b} - \mathbf{b} \text{div } \mathbf{a}$   |

For composite functions  $\varphi[f(\mathbf{r})]$  and  $\mathbf{a}[f(\mathbf{r})]$ , the chain rule is applied

|     |  |   |
|-----|--|---|
| 16. | $\nabla \varphi[f(\mathbf{r})] = \frac{d\varphi}{df} \nabla f$                       | $\text{grad } \varphi[f(\mathbf{r})] = \frac{d\varphi}{df} \text{grad } f$              |
| 17. | $\nabla \cdot \mathbf{a}[f(\mathbf{r})] = (\nabla f) \cdot \frac{d\mathbf{a}}{df}$   | $\text{div } \mathbf{a}[f(\mathbf{r})] = \text{grad } f \cdot \frac{d\mathbf{a}}{df}$   |
| 18. | $\nabla \times \mathbf{a}[f(\mathbf{r})] = (\nabla f) \times \frac{d\mathbf{a}}{df}$ | $\text{curl } \mathbf{a}[f(\mathbf{r})] = \text{grad } f \times \frac{d\mathbf{a}}{df}$ |

\*  $[\nabla \times (\nabla \times \mathbf{a})]_i = \varepsilon_{ijk} \varepsilon_{ilm} \frac{\partial}{\partial x_j} \left( \frac{\partial a_m}{\partial x_l} \right) = [\nabla(\nabla \cdot \mathbf{a})]_i - [(\nabla \cdot \nabla) \mathbf{a}]_i$  tensor notations for #13.

Laplacian of a vector field can be calculated  $(\nabla \cdot \nabla) \mathbf{a} = \nabla(\nabla \cdot \mathbf{a}) - \nabla \times (\nabla \times \mathbf{a})$  using gradient, divergence and curl operators

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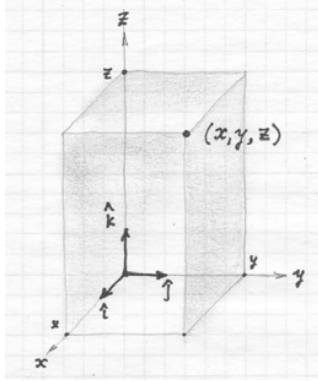
## B. Coordinate Systems

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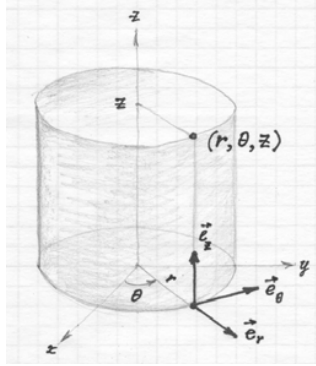
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## Coordinate Systems

Cartesian coordinates  $(x, y, z)$



Cylindrical coordinates  $(r, \theta, z)$



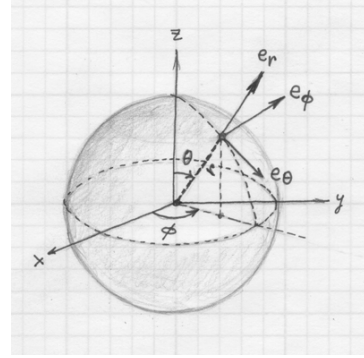
$$\begin{aligned}x &= r \cos \theta \\y &= r \sin \theta \\z &= z\end{aligned}$$

$$r^2 = x^2 + y^2$$

$$\tan \theta = \frac{y}{x}$$

$$z = z$$

Spherical coordinates  $(r, \phi, \theta)$



$$\begin{aligned}x &= r \cos \phi \sin \theta \\y &= r \sin \phi \sin \theta \\z &= r \cos \phi\end{aligned}$$

$$r^2 = x^2 + y^2 + z^2$$

$$\tan \phi = \frac{y}{x}$$

$$\tan \theta = \frac{z}{r} = \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$

Basic vectors

$$\mathbf{i} = (1, 0, 0)$$

$$\mathbf{j} = (0, 1, 0)$$

$$\mathbf{k} = (0, 0, 1)$$

$$\mathbf{e}_r = \mathbf{i} \cos \theta + \mathbf{j} \sin \theta$$

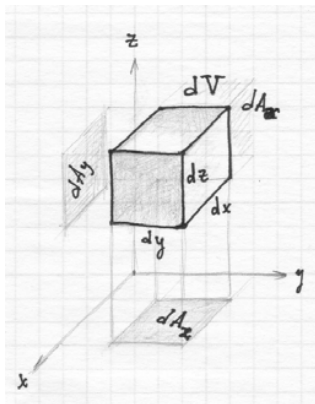
$$\mathbf{e}_\theta = -\mathbf{i} \sin \theta + \mathbf{j} \cos \theta$$

$$\mathbf{e}_z = \mathbf{k}$$

$$\mathbf{e}_r = \mathbf{i} \cos \phi \sin \theta + \mathbf{j} \sin \phi \sin \theta + \mathbf{k} \cos \phi$$

$$\mathbf{e}_\theta = -\mathbf{i} \sin \theta + \mathbf{j} \cos \theta$$

$$\mathbf{e}_\phi = \mathbf{i} \cos \phi \cos \theta + \mathbf{j} \sin \phi \cos \theta - \mathbf{k} \sin \phi$$



Line elements  $dx, dy, dz$

Differential areas

$$dA_x = dydz$$

$$dA_y = dx dz$$

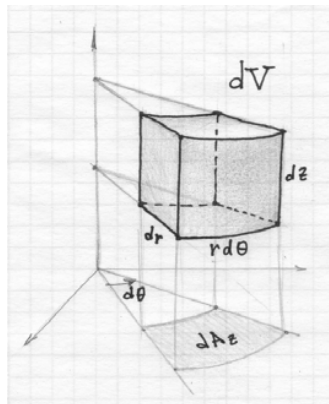
$$dA_z = dx dy$$

Differential volume

$$dV = dx dy dz$$

Arc length

$$ds^2 = dx^2 + dy^2 + dz^2$$



$dr, r d\theta, dz$

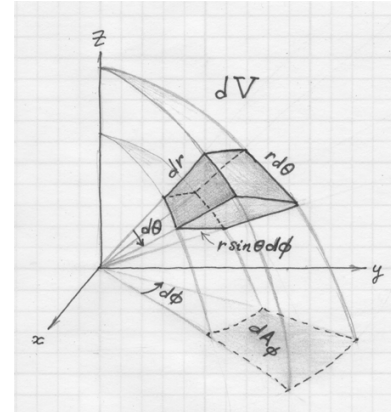
$$dA_r = r d\theta dz$$

$$dA_\theta = dr dz$$

$$dA_z = r d\theta dr$$

$$dV = r dr d\theta dz$$

$$ds^2 = dr^2 + r^2 d\theta^2 + dz^2$$



$dr, r \sin \theta d\phi, r d\theta$

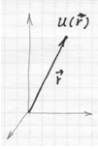
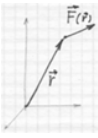
$$dA_r = r^2 \sin \theta d\phi d\theta$$

$$dA_\theta = r \sin \theta d\phi dr$$

$$dA_\phi = r d\theta dr$$

$$dV = r^2 \sin \theta d\phi d\theta dr$$

$$ds^2 = dr^2 + r^2 \sin^2 \theta d\phi^2 + r^2 d\theta^2$$

| scalar field $u(\mathbf{r})$<br><br>Gradient $\nabla u$<br>Laplacian $\nabla^2 u$  | $u(x, y, z)$<br>$\nabla u = \left( \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z} \right)$ $= \frac{\partial u}{\partial x} \mathbf{i} + \frac{\partial u}{\partial y} \mathbf{j} + \frac{\partial u}{\partial z} \mathbf{k}$ $\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$   | $u(r, \theta, z)$<br>$\nabla u = \left( \frac{\partial u}{\partial r}, \frac{1}{r} \frac{\partial u}{\partial \theta}, \frac{\partial u}{\partial z} \right)$ $= \frac{\partial u}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial u}{\partial \theta} \mathbf{e}_\theta + \frac{\partial u}{\partial z} \mathbf{e}_z$ $\nabla^2 u = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) +$ $+ \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2}$   | $u(r, \phi, \theta)$<br>$\nabla u = \left( \frac{\partial u}{\partial r}, \frac{1}{r \sin \theta} \frac{\partial u}{\partial \phi}, \frac{1}{r} \frac{\partial u}{\partial \theta} \right)$ $= \frac{\partial u}{\partial r} \mathbf{e}_r + \frac{1}{r \sin \theta} \frac{\partial u}{\partial \phi} \mathbf{e}_\phi + \frac{1}{r} \frac{\partial u}{\partial \theta} \mathbf{e}_\theta$ $\nabla^2 u = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial u}{\partial r} \right) +$ $+ \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 u}{\partial \phi^2} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial u}{\partial \theta} \right)$  |
|---|---|---|---|
| vector field $\mathbf{F}(\mathbf{r})$<br><br>Divergence $\text{div} \mathbf{F} = \nabla \cdot \mathbf{F}$<br>curl $\mathbf{F} = \nabla \times \mathbf{F}$ | $(F_x, F_y, F_z)$<br>$\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$ $\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix} =$ $\left( \frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) \mathbf{i} + \left( \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) \mathbf{j} +$ $+ \left( \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) \mathbf{k}$ | $(F_r, F_\theta, F_z)$<br>$F_r = F_x \cos \theta + F_y \sin \theta$ $F_\theta = F_x \sin \theta + F_y \cos \theta$ $F_z = F_z$ $F_x = F_r \cos \theta - F_\theta \sin \theta$ $F_y = F_r \sin \theta + F_\theta \cos \theta$ $F_z = F_z$ $\frac{1}{r} \frac{\partial}{\partial r} (r F_r) + \frac{1}{r} \frac{\partial F_\theta}{\partial \theta} + \frac{\partial F_z}{\partial z}$ $\begin{vmatrix} \mathbf{e}_r & r \mathbf{e}_\theta & \mathbf{e}_z \\ \frac{1}{r} \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial z} \\ F_r & r F_\theta & F_z \end{vmatrix} =$ $\left( \frac{1}{r} \frac{\partial F_z}{\partial \theta} - \frac{\partial F_\theta}{\partial z} \right) \mathbf{e}_r +$ $+ \left( \frac{\partial F_r}{\partial z} - \frac{\partial F_z}{\partial r} \right) \mathbf{e}_\theta +$ $\frac{1}{r} \left[ \frac{\partial (r F_\theta)}{\partial r} - \frac{\partial F_r}{\partial \theta} \right] \mathbf{e}_z$ | $(F_r, F_\phi, F_\theta)$<br>$F_r = F_x \cos \phi \sin \theta + F_y \sin \phi \sin \theta + F_z \cos \theta$ $F_\phi = -F_x \sin \phi + F_y \cos \phi$ $F_\theta = F_x \cos \phi \cos \theta + F_y \sin \phi \cos \theta - F_z \sin \theta$ $F_x = F_r \cos \phi \sin \theta - F_\phi \sin \phi + F_\theta \cos \phi \cos \theta$ $F_y = F_r \sin \phi \sin \theta + F_\phi \cos \phi + F_\theta \sin \phi \cos \theta$ $F_z = F_r \cos \theta - F_\theta \sin \theta$ $\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 F_r) + \frac{1}{r \sin \theta} \frac{\partial F_\phi}{\partial \phi} +$ $+ \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} [(\sin \theta) F_\theta]$ $\frac{1}{r^2 \sin \theta} \begin{vmatrix} \mathbf{e}_r & r \mathbf{e}_\theta & r \sin \theta \mathbf{e}_\phi \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial \phi} \\ F_r & r F_\theta & r \sin \theta F_\phi \end{vmatrix} =$ $\frac{1}{r \sin \theta} \left[ \frac{\partial (F_\phi \sin \theta)}{\partial \theta} - \frac{\partial F_\theta}{\partial \phi} \right] \mathbf{e}_r +$ $+ \frac{1}{r} \left[ \frac{\partial (r F_\theta)}{\partial r} - \frac{\partial F_r}{\partial \theta} \right] \mathbf{e}_\phi +$ $+ \frac{1}{r \sin \theta} \left[ \frac{\partial F_r}{\partial \phi} - \sin \theta \frac{\partial (r F_\phi)}{\partial r} \right] \mathbf{e}_\theta$ |