Lecture 1

NONLINEAR
ELASTICITY

Soft-Matter Engineering: Mechanics, Design, & Modeling

Mechanics

Rigid/Hard Systems	bending or torsion (but not stretching) small strains (~0.1% metals; ~1% plastics) linearized stress-strain response; "Linear Elasticity"
Soft Systems	stretch (~10-100% strain) large deflections (including self-contact) nonlinear stress-strain response; "Finite Elasticity"

Design

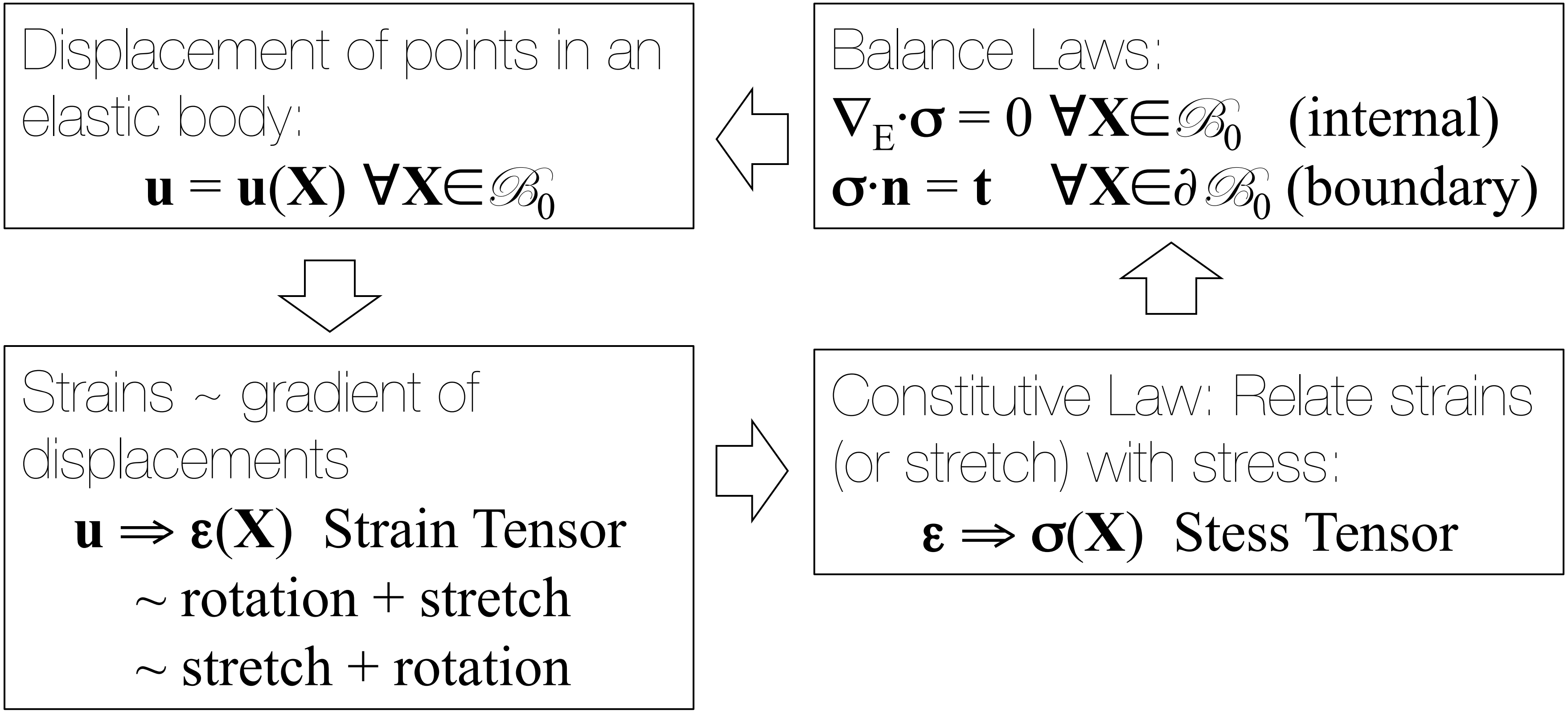
Actuators/Transducers	pneumatics, dielectrics, shape memory, IPMCs, bio-hybrid
Circuits/Sensors	flex circuits, conductive fabrics, wavy circuits, soft microfluidics

Modeling

derived from governing equations of nonlinear elasticity
Pneumatics – elastic **shell** theory
Dielectrics – elastic **membrane** theory
Shape Memory – elastic **rod** theory

THEORY OF ELASTICITY

(Displacement Formulation)



Displacement of points in an elastic body:

$$\mathbf{u} = \mathbf{u}(\mathbf{X}) \ \forall \mathbf{X} \in \mathscr{B}_0$$

Strains ~ gradient of displacements

$$\mathbf{u} \Rightarrow \boldsymbol{\varepsilon}(\mathbf{X}) \ \text{ Strain Tensor}$$

$$\sim \text{rotation} + \text{stretch}$$

$$\sim \text{stretch} + \text{rotation}$$

Constitutive Law: Relate strains (or stretch) with stress:

$$\boldsymbol{\varepsilon} \Rightarrow \boldsymbol{\sigma}(\mathbf{X}) \ \text{ Stess Tensor}$$

Balance Laws:

$$\nabla_E \cdot \boldsymbol{\sigma} = 0 \ \forall \mathbf{X} \in \mathscr{B}_0 \quad \text{(internal)}$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t} \quad \forall \mathbf{X} \in \partial \mathscr{B}_0 \ \text{(boundary)}$$

THEORY OF ELASTICITY

Choice of materials dictates the limits of stress and strain as well as the constitutive law.

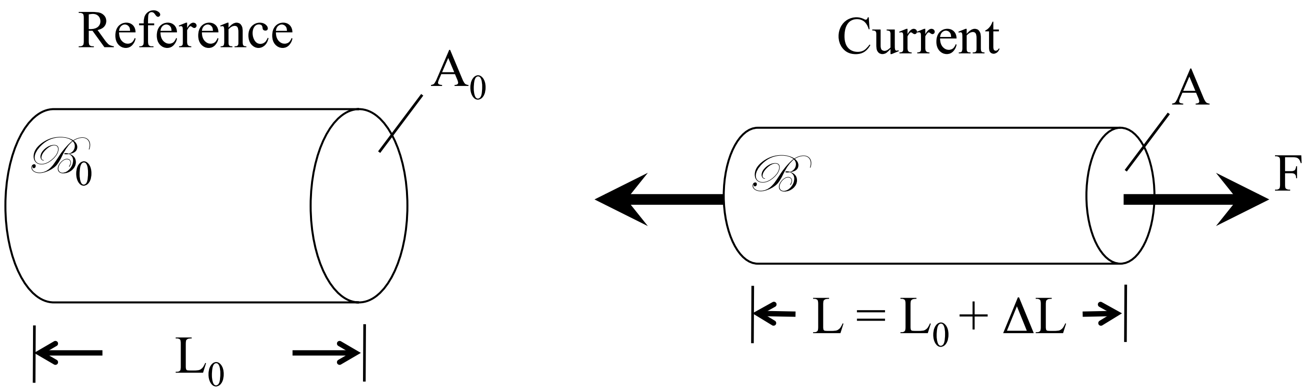
For small strains, the constitutive law can be linearized:

- for linear elastic, homogenous, isotropic solids, use Hooke's Law
- w/ Hooke's Law, elasticity can be represented by only two values:
  - Young's modulus ($\mathbf{E}$) and Poisson's ratio ($\boldsymbol{\nu}$)
  - Shear modulus ($\boldsymbol{\mu}$) and Bulk modulus ($\mathbf{K}$)
  - Lame constants $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$

For large strains, the constitutive relationships are typically nonlinear and require additional elastic coefficients.

In most cases, the constitutive law and its coefficients must be determined *experimentally* with materials testing equipment.

Uniaxial Loading



Strain: $\varepsilon = \dfrac{\Delta L}{L_0}$

Stretch: $\lambda = \dfrac{L}{L_0} = 1 + \varepsilon$

Incompressibility: $V = V_0$

$\Rightarrow AL = A_0 L_0$

$\Rightarrow A = A_0/\lambda$

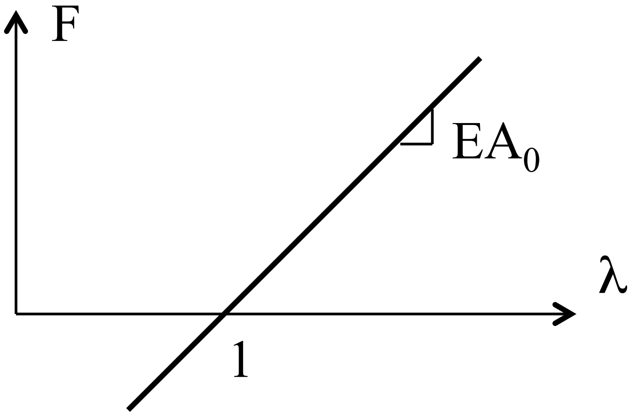
Recall the definition for engineering/nominal stress: $\sigma_e = \dfrac{F}{A_0}$

This is valid for small deformations but significantly underestimates the true (“Cauchy”) stress for moderate deformations: $\sigma = \dfrac{F}{A} = \lambda \sigma_e$

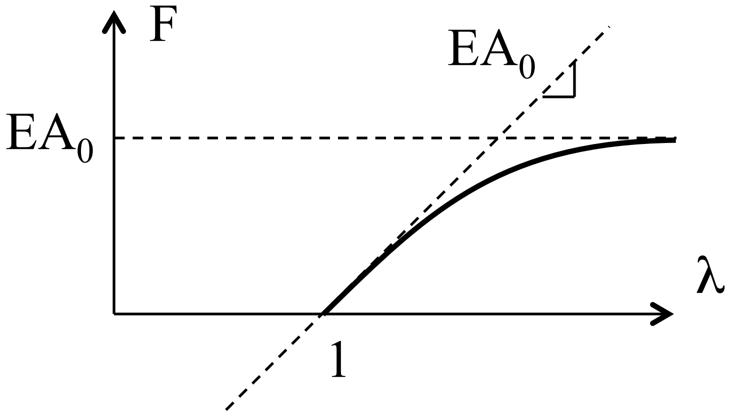
Uniaxial Loading

For uniaxial loading with small strains, σ_e and ε are related by Hooke's Law:

$$\sigma_e = E\varepsilon \Rightarrow F = EA_0\left(\lambda - 1\right)$$



What happens if we replace σ_e with σ?

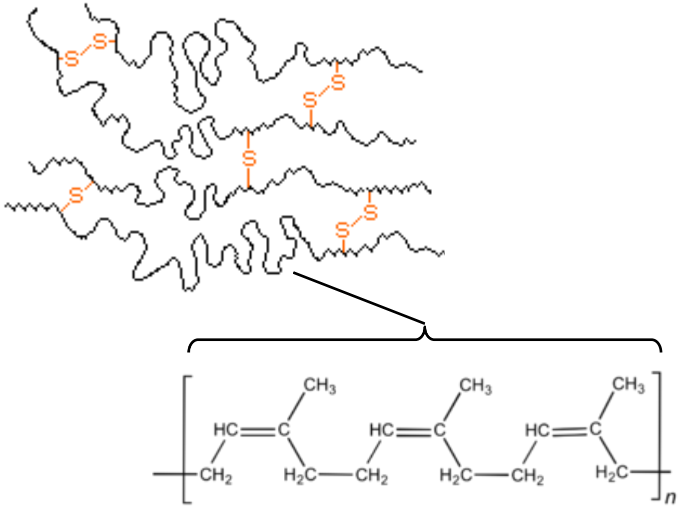


$$\sigma = E\varepsilon \Rightarrow F = EA_0\left(1 - \frac{1}{\lambda}\right)$$

$$\boxed{\lim_{\lambda \to \infty} F = EA_0}$$

These represent two distinct constitutive models, neither of which is realistic for elastomers.

Rubber Mechanics



Vulcanized natural rubber macromolecule:

- ~5000 isoprene units (C-C bonding)
- *cis*-1,4-polyisoprene
- "molecular spaghetti"
- Sulfer cross-links every ~100 units (2%)
- Between the cross-links, each isoprene unit is a freely rotating link

If monomer units are free to rotate, why is there any resistance to deformation?

For any load and configuration, we can calculate the Gibbs free energy Π of the rubber system. Changes in Π are subject to the 1st Law of Thermodynamics:

$$\delta\Pi = \delta(U - Q) \qquad 1^{st}\text{ Law: } \delta U = \delta Q \rightarrow \delta\Pi = 0$$

$U = \Gamma - TS$ = Helmholtz Free Energy

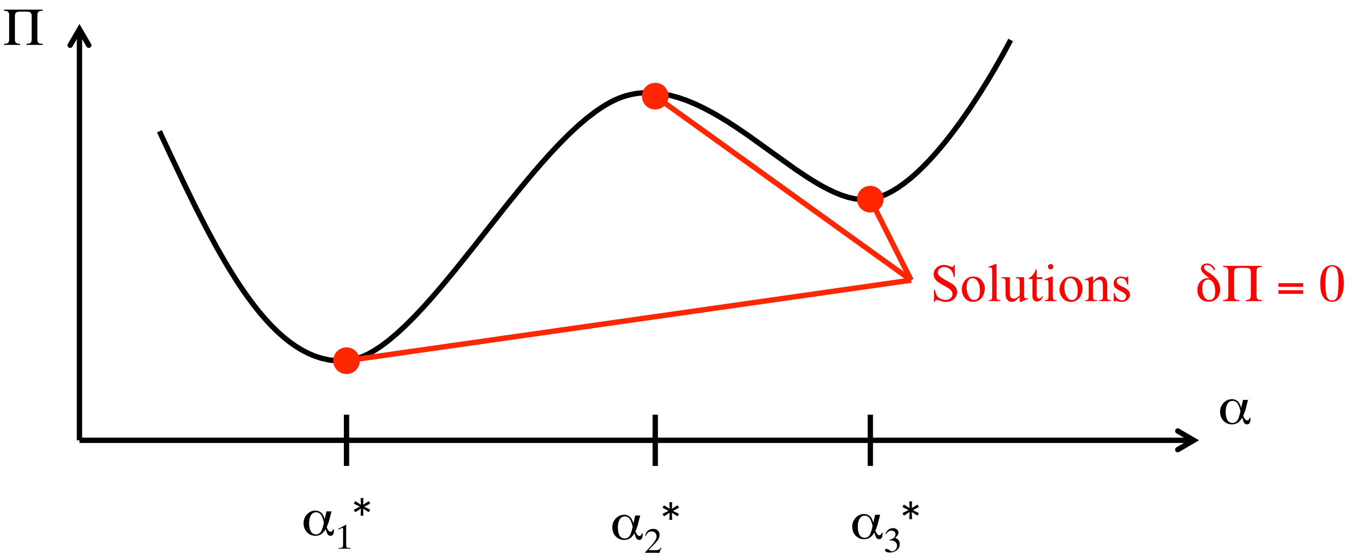
Γ = internal chemical bonding energy

S = system entropy

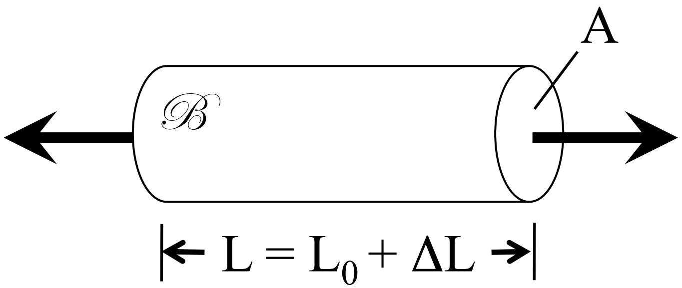
$$\delta Q = \int_{\partial B} \underline{t} \cdot \delta \underline{u} \, dS$$

= applied mechanical work

Gibbs Free Energy for a 1-DOF System



Solutions $\delta\Pi = 0$



$$\left.\begin{array}{l}\delta Q = F\delta L\\ \delta Q - \delta U = 0\end{array}\right\} \Rightarrow F = \frac{dU}{dL}$$

At *static equilibrium*, the system free (potential) energy must be “stationary” w.r.t. shape/configuration.

Principle of Stationary Potential

At static equilibrium, the total potential energy $\Pi = \Pi(\underline{u})$ must be *stationary* w.r.t. infinitesimally small changes in $\underline{u}$.

If the deformation can be parameterized so that $\Pi = \Pi(\alpha_1, \alpha_2, \ldots, \alpha_n)$, then this implies the Rayleigh-Ritz criterion for equilibrium:

$$\frac{\partial \Pi}{\partial \alpha_1} = \frac{\partial \Pi}{\partial \alpha_2} = \ldots = \frac{\partial \Pi}{\partial \alpha_n} = 0$$

Consider a 1-DOF system, i.e. $\Pi = \Pi(\alpha)$

e.g. uniaxial loading: $\alpha = \lambda$

inflating sphere: $\alpha = R$

In this case, α is the solution to the equation $d\Pi/d\alpha = 0$

2^{nd} Law of Thermodynamics

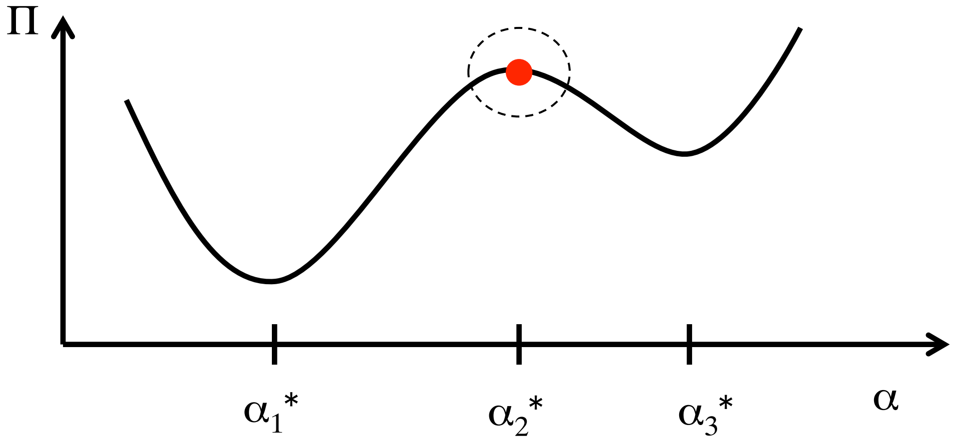
2^{nd} Law of Thermodynamics: $\Delta S_{tot} = \Delta S + \Delta S_e \geq 0$

- S and S_e are the entropy of the system and surrounding (external), respectively
- $\Delta S_e = -\Omega/T$, where Ω is the heat transferred from the surroundings
- For *fixed surface tractions* and *fixed temperature* it follows (by definition) that $\Delta\Pi = \Omega - T\Delta S$
- This implies $\Delta S_{tot} = \Delta S - \Omega/T = -\Delta\Pi/T$, i.e. total entropy decreases with increasing Gibbs free energy (potential energy)

- Now suppose that is locally Π maximized $\Rightarrow$ any perturbation will cause Π to decrease and universal entropy to increase.
- After perturbation, will the system return to its original state?
  It can't – returning to the original state requires a decrease in S_{tot}, hence violating the 2^{nd} Law.
- Therefore such equilibrium states are *unstable*.

- In the absence of external tractions (e.g. fixed kinematic constraints/ displacements), a separate analysis is performed using Helmholtz (U) instead of Gibbs (Π) free energy.

Principle of *Minimum* Potential



Solutions that maximize Π are *unstable* (i.e. α_2^*)

Solutions that minimize Π are *stable* (i.e. α_1^* and α_3^*)

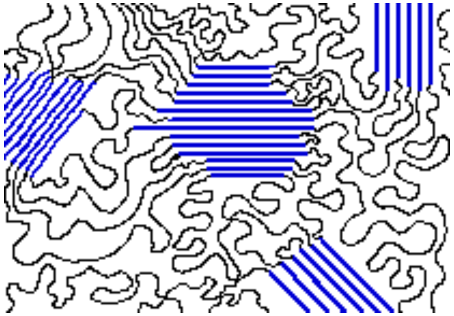
Consider the solution $\alpha = \alpha_2^*$

- Changing α results in a *decrease* in Gibbs Free Energy
- For fixed surface tractions, this corresponds to an *increase* in universal Entropy S_{tot}
- This implies that returning to the extremizing value $\alpha = \alpha_2^*$ will *decrease* S_{tot}
- Therefore, $\alpha = \alpha_2^*$ is a solution that *violates* the 2nd Law of Thermodynamics

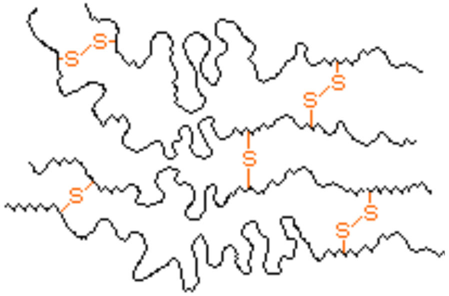
In contrast, for $\alpha = \alpha_1^*$ or $\alpha = \alpha_3^*$

- Changing α increases Π and hence reduces total entropy
- The system will *spontaneously* return to the equilibrium state in order to increase universal Entropy.

Polymers



Semi-Crystaline
e.g. HDPE
Relatively rigid



Completely Amorphous
e.g. Vulcanized Rubber
Soft & Stretchable

Crystalline, semi-crystalline, and glassy materials deform through lengthening/shortening of interatomic bonds ⇒ change in internal energy (Γ)

Elastomers deform through changes in macromolecular configuration (“morphology”) ⇒ change in entropy (S)

“Partial straightening” is an ordering processes that decreases entropy and thus requires mechanical work input.

In the case of uniaxial loading, recall that $F = dU/dL$. Noting that $U = \Gamma - TS$ and $\delta\Gamma \approx 0$, it follows that

$$\boxed{F \approx -T\left(\frac{dS}{dL}\right)_T}$$

What is the entropy of rubber and how does it scale with stretch?

Entropy of of Rubber

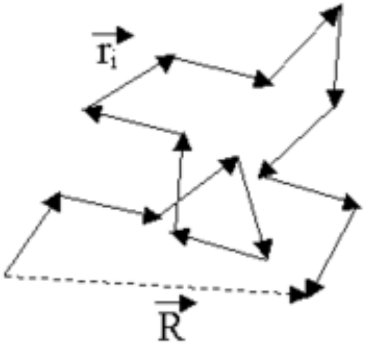
Ref: "Entropy and Rubber Elasticity" by Leonard Nash
J. Chemical Education, 56 (6) 363-368 (1979)

The configurational entropy is defined as S = k ln(M), where

- k = Boltzmann's constant
- M = discrete number of configurations that the macromolecular chains can adopt to fill a prescribed volume.

Simplifying assumptions:

- N chains each with n links of uniform length ℓ
- This ignores the stochasticity of chain lengths and cross-linking
- For random shapes, there exists a root-mean-square average end-to-end length $r_u \sim \ell n^{1/2}$



For an end-to-end vector **R** = x**i** + y**j** + z**k**,

$$M = M_0^N \exp\left\{-\frac{3N\left(x^2+y^2+z^2\right)}{2r_u^2}\right\}$$

Here, M0 is the number of possible configurations for a single chain when **R** = 0 (i.e. chain loops around)

Entropy of of Rubber

$$S = Nk \ln M_0 - \frac{3Nk}{2r_u^2}\left(x^2 + y^2 + z^2\right)$$

Now consider the following deformation:

$$x = \lambda_x x_0 \qquad y = \lambda_y y_0 \qquad z = \lambda_z z_0$$

where $x_0^2 = y_0^2 = z_0^2 = r_u^2/3$, and define S_u as the initial entropy (i.e. prior to deformation).

$$\Rightarrow \Delta S = S - S_u = -\frac{Nk}{2}\left(\lambda_x^2 + \lambda_y^2 + \lambda_z^2 - 3\right)$$

For incompressible deformation and uniaxial loading, $\lambda_x = \lambda$, $\lambda_y = \lambda_z = \lambda^{-1/2}$

$$\Delta S = -\frac{Nk}{2}\left(\lambda^2 + \frac{1}{\lambda} - 3\right) \qquad \left(\frac{dS}{d\lambda}\right)_T = -Nk\left(\lambda - \frac{1}{\lambda^2}\right)$$

Entropy of Rubber

$$F = -T\left(\frac{dS}{dL}\right)_T = -T\left(\frac{dS}{d\lambda}\right)_T \frac{d\lambda}{dL}$$

Noting that $L = \lambda L_0$ and $d\lambda/dL = 1/L_0$,

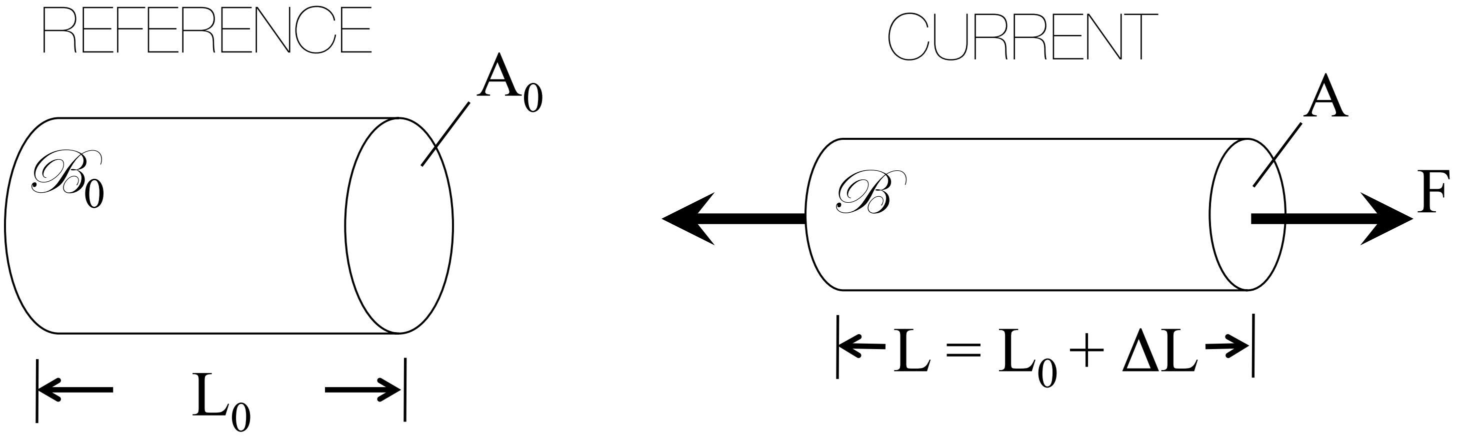
$$F = \frac{NkT}{L_0}\left(\lambda - \frac{1}{\lambda^2}\right)$$

Expressing this in terms of a nominal engineering stress $\sigma_e = F/A_0$, and noting that $A_0L_0 = V_0 = V$,

$$\sigma_e = C_1\left(\lambda - \frac{1}{\lambda^2}\right) \quad \text{where } C_1 = NkT/V$$

BALANCING FORCES

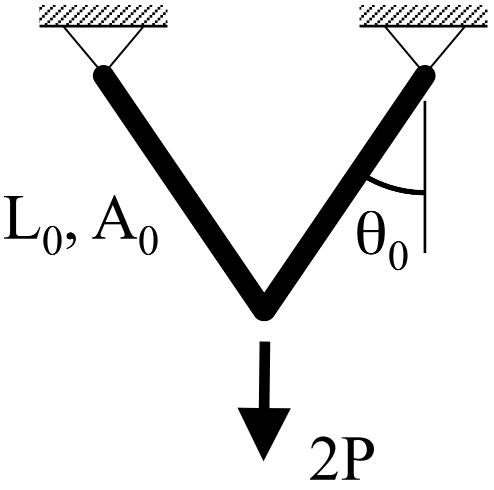
Another difference between linear and nonlinear/finite elasticity is the configuration or “placement” in which we balance forces:

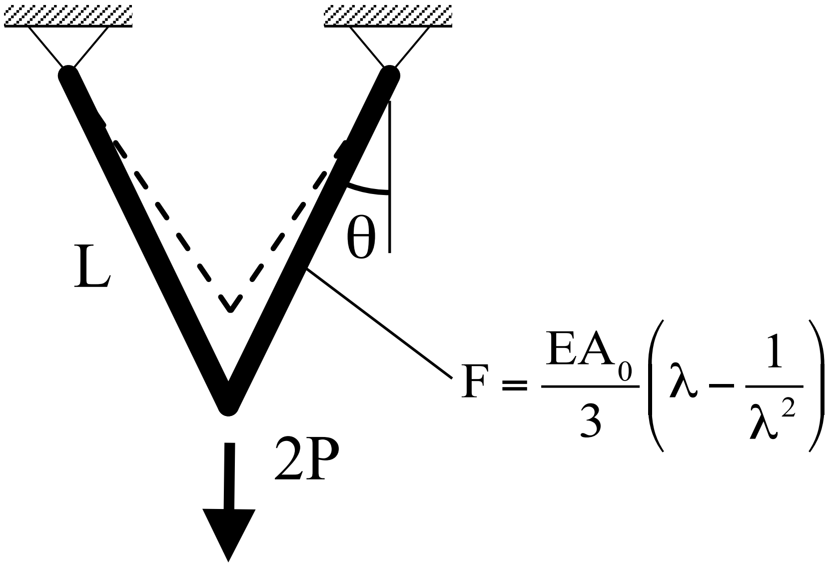


At static equilibrium, the forces acting on the body must balance.

However, for the same forces, we will calculate different stresses (and thus different strains/stretches) depending on what placement we are in.

EXAMPLE





$$F = \frac{EA_0}{3}\left(\lambda - \frac{1}{\lambda^2}\right)$$

$$P = F\cos\theta_0 = \frac{EA_0}{3}\left(\lambda - \frac{1}{\lambda^2}\right)\cos\theta_0 \quad ✗$$

$$P = F\cos\theta$$

$$L_0 \sin\theta_0 = L\sin\theta$$

$$\Rightarrow \cos\theta = \sqrt{1 - \frac{1}{\lambda^2}\left(1 - \cos^2\theta_0\right)}$$

$$\therefore P = \frac{EA_0}{3}\left(\lambda - \frac{1}{\lambda^2}\right)\sqrt{1 - \frac{1}{\lambda^2}\left(1 - \cos^2\theta_0\right)} \quad ✓$$

We must balance forces in the Current Placement!!!

NEO-HOOKEAN SOLID

For a Neo-Hookean Solid, recall the expression for the change in Helmholtz free energy:

$$\Delta U = -T\Delta S = \frac{NkT}{2}\left(\lambda_x^2 + \lambda_y^2 + \lambda_z^2 - 3\right)$$

This implies that strain energy density has the form

$$W = C_1\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3\right)$$

$$\Rightarrow \sigma_i = 2C_1\lambda_i^2 - p$$

Example 1: Uniaxial Loading

$$\sigma_1 = \sigma$$

$$\sigma_2 = \sigma_3 = 0$$

$$\lambda_1 = \lambda$$

$$\lambda_2 = \lambda_3$$

$$\lambda\lambda_2^2 = 1$$

$$\Rightarrow \lambda_2 = \frac{1}{\sqrt{\lambda}}$$

$$\sigma_2 = 0 \equiv \frac{2C_1}{\lambda} - p \Rightarrow p = \frac{2C_1}{\lambda}$$

$$\sigma = 2C_1\lambda^2 - p$$

$$\therefore \sigma = 2C_1\left(\lambda^2 - \frac{1}{\lambda}\right) \quad ✓$$

NEO-HOOKEAN SOLID

Example 2: Equibiaxial Loading

$$\sigma_1 = \sigma_2 = \sigma \qquad \lambda_1 = \lambda_2 = \lambda$$

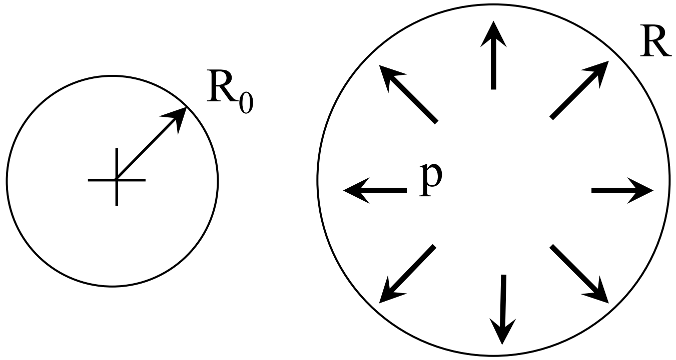
$$\sigma_3 = 0 \qquad \lambda^2\lambda_3 = 1 \Rightarrow \lambda_3 = \frac{1}{\lambda^2}$$

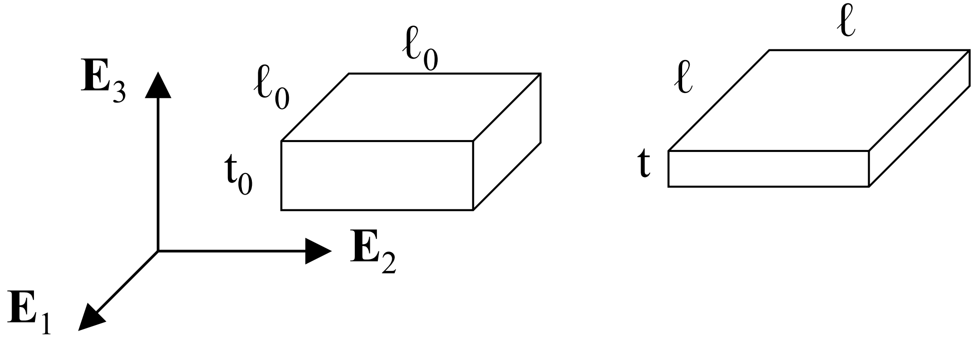
$$\sigma_3 = 0 \equiv \frac{2C_1}{\lambda^4} - p \Rightarrow p = \frac{2C_1}{\lambda^4}$$

$$\sigma = 2C_1\lambda^2 - p$$

$$\therefore \sigma = 2C_1\left(\lambda^2 - \frac{1}{\lambda^4}\right)$$

Example 3: Sphere Inflation





assume equibiaxial loading: R >> t → $\sigma_1 = \sigma_2 =: \sigma >> \sigma_2 \sim p$

BALLOON INFLATION CONT.

$$\lambda_1 = \lambda_2 = \lambda \equiv \frac{R}{R_0} \qquad \lambda_3 = \frac{1}{\lambda_1 \lambda_2} = \frac{1}{\lambda^2}$$

$$W = C_1\left(2\lambda^2 + \frac{1}{\lambda^4} - 3\right)$$

$$\Pi = WV - U_p$$

$$V = V_0 \approx 4\pi R_0^2 t_0$$

$$U_p = -pV_e$$

$$V_e = \frac{4}{3}\pi R^3$$

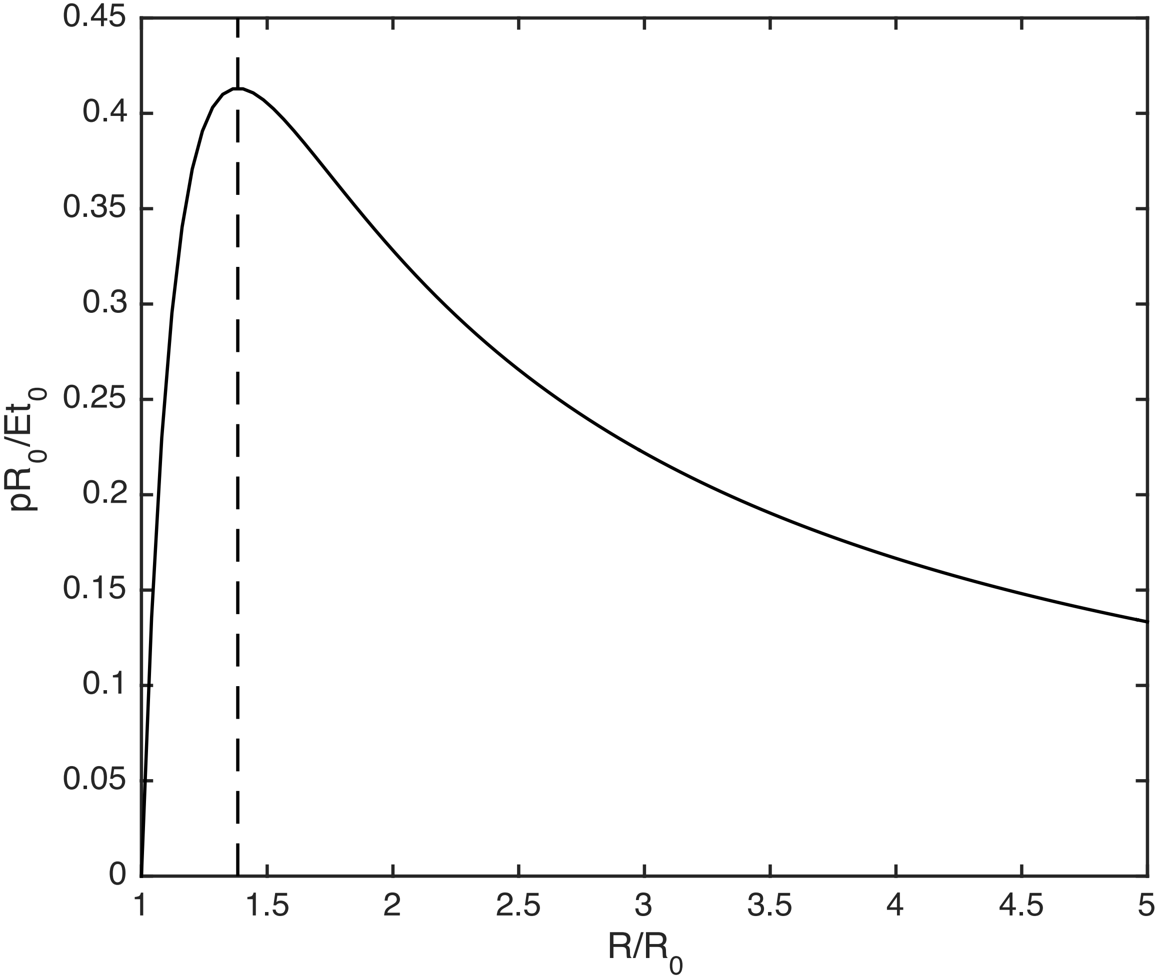
$$\Pi = 4\pi R_0^2 t_0 C_1 \left\{2\left(\frac{R}{R_0}\right)^2 + \left(\frac{R_0}{R}\right)^4 - 3\right\} - \frac{4}{3}\pi R^3 p$$

At equilibrium, Π must be minimized w.r.t. R. This implies $d\Pi/dR = 0$:

$$\frac{d\Pi}{dR} = 4\pi R_0^2 t_0 C_1 \left\{\frac{4R}{R_0^2} - \frac{4R_0^4}{R^5}\left(\frac{R_0}{R}\right)^4\right\} 4\pi R^2 p \equiv 0$$

BALLOON INFLATION CONT.

Solve for p: $$p = \frac{2t_0 E}{3R_0}\left\{\frac{R_0}{R} - \frac{R_0^7}{R^7}\right\}$$



WHAT ABOUT SHEAR?!

In addition to stretch, materials typically undergo shear.

However, for any elastic deformation, there is always an orientation where shear disappears.

Consider an elastic body with reference placement $\mathscr{B}_0$.

During deformation, points $\mathbf{X} \in \mathscr{B}_0$ get mapped to a final position $\mathbf{x} = \chi(\mathbf{X}) = \mathbf{X} + \mathbf{u}$, where

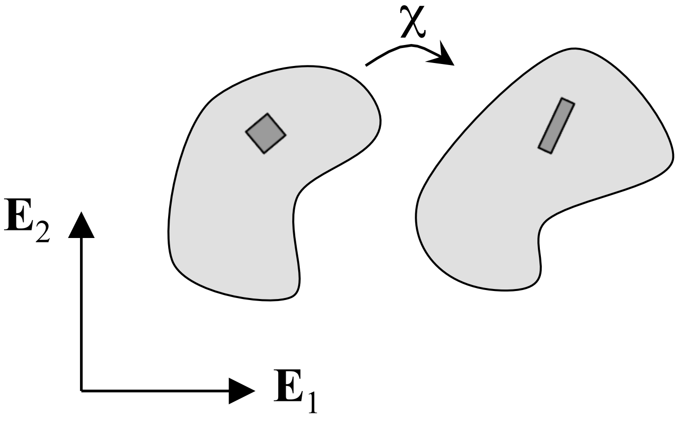
- $\mathbf{x} \in \mathscr{B}$ are the final positions
- $\mathscr{B}$ is the current placement
- $\mathbf{u} = \mathbf{u}(\mathbf{X})$ is the displacement field

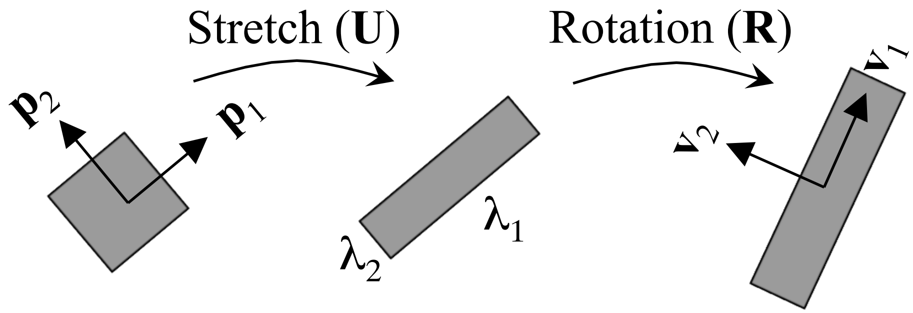
The strain tensor $\boldsymbol{\varepsilon}$ is calculated from the gradient of $\mathbf{x}$:

- $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\mathbf{F})$
- $\mathbf{F} = \nabla\chi =$ "Deformation Gradient"
- Both $\boldsymbol{\varepsilon}$ and $\mathbf{F}$ are 2nd order tensors (~3x3 matrices)

WHAT ABOUT SHEAR?!

According to the Polar Decomposition Theory, **F** can be represented as **F** = **RU**, where **R** is a rotation tensor and **U** is a tensor with only diagonal elements:



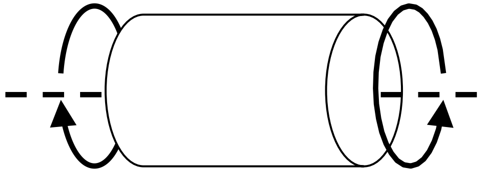


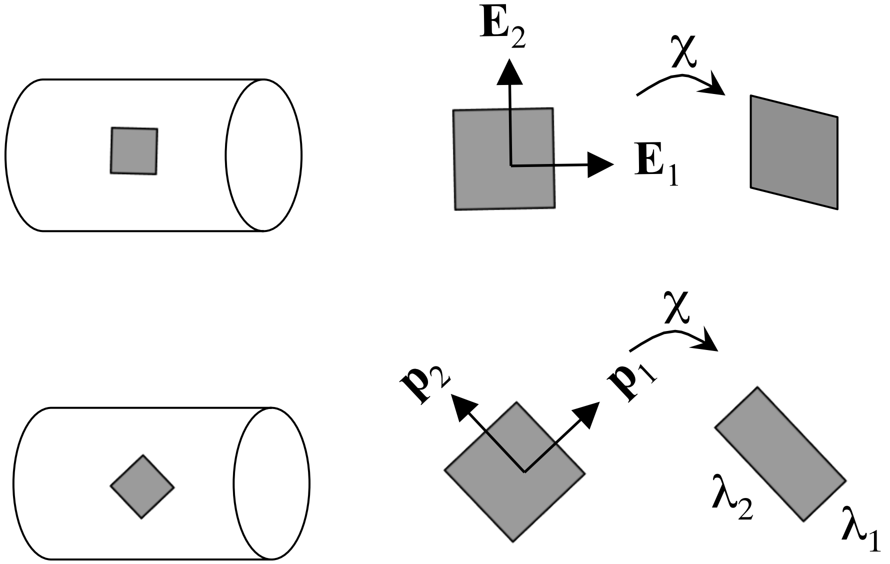
$$U \sim \begin{bmatrix} \boldsymbol{\lambda}_1 & 0 & 0 \\ 0 & \boldsymbol{\lambda}_2 & 0 \\ 0 & 0 & \boldsymbol{\lambda}_3 \end{bmatrix}$$

For any deformation, there exist principal directions ($\mathbf{p}_1$, $\mathbf{p}_2$, $\mathbf{p}_3$) along which the material undergoes only pure axial stretch.

EXAMPLE

Consider a cylinder under pure torsion. Just because it doesn’t change length or diameter, it is incorrect that it contains zero stretch:





shear w.r.t. ($\mathbf{E}_1$, $\mathbf{E}_2$)

stretch w.r.t. ($\mathbf{p}_1$, $\mathbf{p}_2$)

GENERAL LOADING CONDITIONS

In general, during virtual displacement, prescribed surface tractions $\underline{t}$ perform mechanical work on the elastic body:

$$\delta Q = \int_{\partial B} \underline{t} \cdot \delta \underline{u} \, dS$$

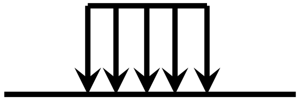
As before, this work must all be stored as elastic strain energy, i.e.

$$\delta Q \equiv \delta U \Leftrightarrow \delta U - \delta Q = 0$$

Now consider the following loading conditions:

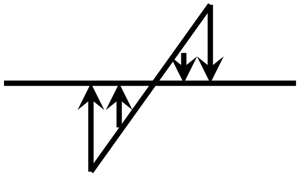
- Concentrated Traction = Point Load
- Concentrated Traction Couple = Moment
- Enclosed Air Pressure

Concentrated Traction = Point Load:



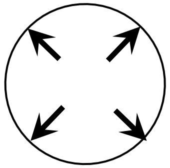
$$\int_{\partial B} \underline{t}\cdot\delta\underline{u}\,dS = \boxed{\underline{F}\cdot\delta\underline{u}}$$

Concentrated Traction Couple = Moment:



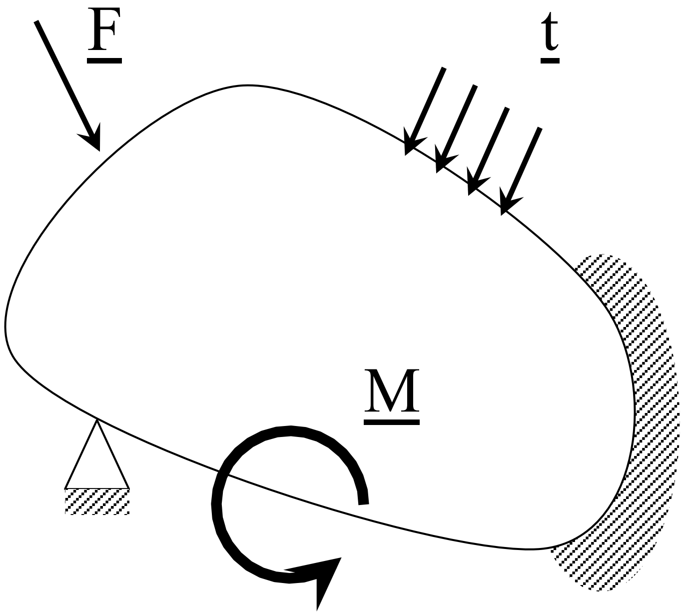
$$\int_{\partial B} \underline{t}\cdot\delta\underline{u}\,dS = \boxed{M\delta\theta}$$

Enclosed Air Pressure:



$$\int_{\partial B} \underline{t}\cdot\delta\underline{u}\,dS = \int_{\partial B} p\underline{n}\cdot\delta\underline{u}\,dS = \boxed{p\delta V_e}$$

The potential energy Π of an elastic body represents the total energy associated with both the internal elastic strain energy w and the mechanical work Q of external tractions $\underline{t}$:



$$\delta U = \delta Q$$

$$\int_{B_o} \delta W \, dV = \int_{\partial B} \underline{t} \cdot \underline{u} \, dS + \underline{F} \cdot \delta \underline{u} + M\delta\theta + p\delta V_e$$

$$\delta \left\{ \int_{B_o} W \, dV - \int_{\partial B} \underline{t} \cdot \underline{u} \, dS - \underline{F} \cdot \underline{u} - M\theta - pV_e \right\} = 0$$

$$\boxed{\therefore \delta\Pi = 0}$$

$$\Pi = \int_{B_0} W \, dV - \int_{\partial B} \underline{t} \cdot \underline{u} \, dS - \sum \underline{F} \cdot \underline{u} - \sum M\theta - pV_e$$

The condition $\delta\Pi = 0$ implies that the potential energy must be stationary at static equilibrium. Since the functional $\Pi = \Pi(\underline{u})$ is smooth and continuous, this condition is satisfied when minimized w.r.t. kinematically admissable deformations $\underline{u} \in \mathscr{K}$.

Here, $\mathscr{K}$ represents the space of all possible functions $\underline{u} = \underline{u}(\underline{X})$ that satisfy the prescribed kinematic boundary conditions.

If the deformation can be parameterized so that $\Pi = \Pi(\alpha_1, \alpha_2, \ldots, \alpha_n)$ is a function of scalars instead of a functional, then the condition $\delta\Pi = 0$ corresponds to

(Rayleigh-Ritz criterion) $\dfrac{\partial\Pi}{\partial\alpha_1} = \dfrac{\partial\Pi}{\partial\alpha_2} = \ldots = \dfrac{\partial\Pi}{\partial\alpha_n} = 0$