07 - balance equations - closed and open systems

Final projects - me337 2013

- cerebral aneurysm growth: sheila
- muscle growth: katrina, jaqi
- brain tumor growth: cesare, zhuozhi
- left vs right arms of athletes: ronaldo, maria, lyndia
- airway wall remodeling: mona
- corneal growth / keratoconus: yanli
- bone adaptation in birds: jan, david
- neuronal growth in fish: andrew

Homework 01 - due thu in class

Continuum mechanics of growth

- Kinematic equations for finite growth:
  \[ \mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_g \]
- Balance equations for open systems:
  \[ D_t \rho_0 = \text{Div} (\mathbf{R}) + \mathbf{K}_0 \]
  \[ \rho_0 D_t \mathbf{v} = \text{Div} (\mathbf{P}) + \mathbf{b}_0 \]
- Constitutive equations for living tissues:
  \[ \mathbf{P} = \mathbf{P} (\rho_0, \mathbf{F}, \mathbf{F}_g) \]
- FE analyses for biological structures

Where are we???
potato - kinematics

\[
\begin{array}{c}
B_0 \\
\Rightarrow \\
F \\
\Rightarrow \\
B_t
\end{array}
\]

- nonlinear deformation map \( \varphi \)
  \[ x = \varphi(X, t) \quad \text{with} \quad \varphi : B_0 \times \mathbb{R} \to B_t \]

- spatial derivative of \( \varphi \) - deformation gradient
  \[ \frac{dx}{dX} = F \cdot dX \quad \text{with} \quad F : T(B_0 \times \mathbb{R}) \to T(B_t) \quad F = \frac{\partial \varphi}{\partial X} |_{t \text{ fixed}} \]

kinematic equations

kinematics of finite growth

\[ B_0 \xrightarrow{\varphi} \frac{\partial \varphi}{\partial X} |_{t \text{ fixed}} \]

kinematics of growth

[1] consider an elastic body \( B_0 \) at time \( t_0 \), unloaded & stressfree

[2] imagine the body is cut into infinitesimal elements each of which is allowed to undergo volumetric growth

[3] after growing the elements, \( B_g \) may be incompatible
kinematics of growth

balance equations

[1] consider an elastic body $B_0$ at time $t_0$, unloaded & stressfree
[2] imagine the body is cut into infinitesimal elements each of which is allowed to undergo volumetric growth
[3] after growing the elements, $B_g$ may be incompatible
[4] loading generates compatible current configuration $B_t$

kinematics of finite growth

potato - kinematics of finite growth

• incompatible growth configuration $B_g$ & growth tensor $F_g$
  \[ F = F_e \cdot F_g \]

rodriguez, hoger & mc culloch [1994]

balance equations

balance equations

chadwick “continuum mechanics” [1976]
[1] isolation of subset $\tilde{B}$ from $B$

[2] characterization of influence of remaining body through phenomenological quantities - contact fluxes $\tilde{v}^p, \tilde{v}^e$ & $\tilde{v}^0$

[3] definition of basic physical quantities - mass, linear and angular momentum, energy

[4] postulation of balance of these quantities
**Generic Balance Equation**

\[ \mathbf{D}_t \mathbf{A} = \text{Div}(\mathbf{B}) + \mathbf{C} + \Gamma \]

**Balance of Mass**

\[ \rho_0 \mathbf{v} \quad \text{linear momentum density} \\
\mathbf{P} \quad \text{momentum flux - stress} \\
\mathbf{b}_0 \quad \text{momentum source - force} \\
0 \quad \text{no momentum production} \\
\]

**Balance of (Linear) Momentum**

\[ \rho_0 \mathbf{v} \quad \text{linear momentum density} \\
\mathbf{P} \quad \text{momentum flux - stress} \\
\mathbf{b}_0 \quad \text{momentum source - force} \\
0 \quad \text{no momentum production} \\
\]

**Equilibrium Equation**

\[ \mathbf{D}_t (\rho_0 \mathbf{v}) = \text{Div}(\mathbf{P}) + \mathbf{b}_0 \]

**Continuity Equation**

\[ \mathbf{D}_t \rho_0 = 0 \]
balance of (internal) energy

\[ \rho_0 I \quad \text{internal energy density} \]
\[ Q \quad \text{heat flux} \]
\[ Q_0 \quad \text{heat source} \]
\[ 0 \quad \text{no heat production} \]

\[ -Q \cdot n = \bar{T} \]

energy equation \( D_t(\rho_0 I) = P : D_t F - \nu \cdot b_0 + \text{Div}(-Q) + Q_0 \)

balance of entropy

\[ \rho_0 S \quad \text{entropy density} \]
\[ H \quad \text{entropy flux} \]
\[ H_0 \quad \text{entropy source} \]
\[ H_0^\text{int} \quad \text{entropy production} \]
\[ H_0^\text{int} \geq 0 \]

entropy "inequality" \( D_t(\rho_0 S) = \text{Div}(-H) + H_0 + H_0^\text{int} \)

dissipation inequality

- dissipation inequality
  \[ D_0 := \partial H_0^\text{int} = \partial \rho_0 D_t S + \partial \text{Div}(H) - \partial H_0 \geq 0 \]
- identification
  \[ H = \frac{\partial}{\partial t} S \quad H_0 = \frac{\partial}{\partial t} Q_0 \]
- with legendre-fenchel transform
  \[ \psi = I - \partial S \]
  \[ D_0 = P : D_t F - \rho_0 D_t \psi - \rho_0 S D_t \vartheta + Q \cdot \nabla_X \ln(\vartheta) \geq 0 \]
- free energy
  \[ \psi = \psi \left( F, \vartheta \right) \quad D_t \psi = D_t F + D_{\vartheta} \psi : D_t \vartheta \]
- definition of stress and entropy (e.g., neo hooke's law)
  \[ P = \rho_0 D_F \psi \quad S = -\rho_0 D_{\vartheta} \psi \]
- thermodynamic restriction (e.g., fourier's law)
  \[ Q \cdot \nabla_X \ln(\vartheta) \geq 0 \]

isolated system [also called "system"] thermodynamical system which is not allowed to have any interaction with its environment. enclosed by a rigid, adiabatic, impermeable membrane.

balance equations - closed systems
adiabatic closed system [ˈæ.dɪ.æ.bɛ.tık ˈklouzd ˈsɪst.əm] thermodynamic system which is allowed to exchange exclusively mechanical work, typically \( P = P(\nabla \varphi, ...) \), with its environment. enclosed by a deformable, adiabatic, impermeable membrane. characterized through its state of deformation \( \varphi \).

closed system [ˈklouzd ˈsɪst.əm] thermodynamic system which is allowed to exchange mechanical work and heat, typically \( P = P(\nabla \varphi, ...) \) and \( Q = Q(\nabla \theta, ...) \), with its environment. enclosed by a deformable, diathermal, impermeable membrane. characterized through its state of deformation \( \varphi \) and temperature \( \theta \).

open system [ˈou.pən ˈsɪst.əm] thermodynamic system which is allowed to exchange mechanical work, heat and mass, typically \( P = P(\nabla \varphi, ...) \), \( Q = Q(\nabla \theta, ...) \) and \( R = R(\nabla \rho, ...) \) with its environment. enclosed by a deformable, diathermal, permeable membrane. characterized through its state of deformation \( \varphi \), temperature \( \theta \) and density \( \rho \).

"...thermodynamics recognizes no special role of the biological…" bridge, the nature of thermodynamics, [1941]
why do we need open systems if we have porous media?

theory of open systems  
[ˈou.ˌpæn ˈsis.tæms]
- constituents spatially separated
- overall behavior preliminary determined by one single constituent
- exchange of mass, momentum, energy and entropy with environment

theory of porous media  
[ˈpɔːr.əs ˈmɪdɪə].a]
- local superposition of constituents
- consideration of mixture of multiple constituents
- exchange of mass, momentum, energy and entropy amongst constituents

balance of mass

\[ D_t \rho + \text{Div}(R) + \mathcal{R}_0 \]

mass flux \( R \)
- cell movement (migration)

mass source \( \mathcal{R}_0 \)
- cell growth (proliferation)
- cell division (hyperplasia)
- cell enlargement (hypertrophy)

biological equilibrium


balance equations - open systems

simulation of cell growth - cahn-hilliard equation
kuhl & schmid [2006], wels, kuhl & guricci [2006]

balance of mass

the model does not take explicitly into account that the body is growing due to the absorption of some other materials. in absence of some of the vital constituents, no growth is possible. conversely, when part of the material dies, some of the bricks contained in the cellular membrane can be re-used by other cells. in this respect, an approach using mixture theory might be useful.
balance equations - open systems

example of open systems - rocket propulsion

balance of mass
\[ D_t m = \mathbf{R} \quad \text{with} \quad \mathbf{R} \leq 0 \quad \text{ejection} \]

balance of momentum - volume specific
\[ D_t [m \mathbf{v}] = m D_t \mathbf{v} + \mathbf{D}_t m \mathbf{v} = \mathbf{f} + \mathbf{R} \mathbf{v} \]

balance of momentum - mass specific
\[ m D_t \mathbf{v} = \mathbf{f} \quad \text{with} \quad \mathbf{f} = f^\text{closed} + f^\text{open} \]

balance of momentum - rocket head-ejection
\[ D_t [m \mathbf{v}] - \mathbf{R} \mathbf{v} = f^\text{closed} \]

propulsive force
\[ f^\text{open} = [\mathbf{v} - \mathbf{v}] \mathbf{R} \quad \text{velocity of ejection} \: \mathbf{v} \]

example - rocket propulsion

A Saturn V rocket like the one that took men to the moon has a mass of 2,500,000 kg at liftoff. It goes straight up vertically and burns fuel at a uniform rate of 16,000 kg/s for a duration of 2 minutes, the exhaust speed of gas from the Saturn V is 3.0 km/s.

What is the speed of the rocket immediately after the combustion ceases? You should include the effect of gravity near the surface of the earth, but you can neglect air resistance.

Plot the burnout velocity as a function of time over the range of 0 to 120 seconds to see the increase in speed of the rocket with time.
example of open systems - rocket propulsion

\[ m \frac{D_t v}{m(0)} = f^{\text{closed}} + f^{\text{open}} \]

with \[ f^{\text{closed}} = -m g \quad \text{gravity} \]

\[ f^{\text{open}} = (\vec{v} - \vec{v}_0) \mathcal{R} = w D_t m \]

\[ m \frac{D_t v}{m(0)} = -m g - D_t m \quad || : m \]

\[ D_t v = -g - \frac{1}{m} D_t m \quad \text{integration} \]

\[ v(t) = -g t - w \int_{m(0)}^{m(t)} \frac{1}{m} \, dm \]

\[ m(t) = m(0) + \mathcal{R} t \]

velocity

\[ v(t) = -g t - w \ln \frac{m(0) + \mathcal{R} t}{m(0)} \]

\[ \text{balance of (internal) energy} \]

- volume specific version

\[ \frac{D_t}{\rho_0 I} = \mathbf{P} : D_t \mathbf{F} - \mathbf{v} \cdot \mathbf{b}_0 + \text{Div}(Q + I \mathcal{R}) + |Q_0 + I \mathcal{R}_0 - \nabla_x I \cdot \mathbf{R}| \]

- subtract weighted balance of mass

\[ I D_t \rho_0 = \text{Div} (I \mathcal{R}) + I \mathcal{R}_0 - \nabla_x I \cdot \mathbf{R} \]

- mass specific version

\[ \rho_0 D_t I = \mathbf{P} : D_t \mathbf{F} - \mathbf{v} \cdot \mathbf{b}_0 + \text{Div}(-Q) + Q_0 \]

energy equilibrium
balance of entropy

- volume specific version
  \[ H_0^{\text{int}} \geq 0 \]
  \[ D_t(\rho_0 S) = \text{Div}(\mathbf{H} + S \mathbf{R}) + [\mathcal{H}_0 + S \mathcal{R}_0 - \nabla X S \cdot \mathbf{R}] + H_0^{\text{int}} \]

- subract weighted balance of mass
  \[ S D_t \rho_0 = \text{Div}(S \mathbf{R}) + S \mathcal{R}_0 - \nabla X S \cdot \mathbf{R} \]

- mass specific version
  \[ \rho_0 D_t S = \text{Div}(\mathbf{H}) + \mathcal{H}_0 + H_0^{\text{int}} \]

entropy 'inequality'

dissipation inequality

- dissipation inequality
  \[ D_0 := \partial H_0^{\text{int}} = \rho_0 \partial D_t S + \partial \text{Div}(\mathbf{H}) - \partial \mathcal{H}_0 \geq 0 \]

- identification
  \[ \mathbf{H} = \frac{1}{\beta} \mathcal{Q} + S \]
  \[ \mathcal{H}_0 = \frac{1}{\beta} \mathcal{Q}_0 + S_0 \]

- free energy
  \[ \psi = \psi(\rho_0, \mathbf{F}, \theta) \]

- definition of stress and entropy
  \[ \mathbf{P} = \rho_0 D_F \psi \]
  \[ S = -D_\theta \psi \]

- thermodynamic restrictions
  \[ S_0 \leq \rho_0 D_{\rho_0} \psi_\beta \mathcal{R}_0 \]
  \[ S \geq \rho_0 D_{\rho_0} \psi_\beta \mathcal{R} \]
  \[ Q \cdot \nabla X \ln(\theta) \geq 0 \]

"... a living organism can only keep alive by continuously drawing from its environment negative entropy. It feeds upon negative entropy to compensate the entropy increase it produces by living."

Schrödinger "What is Life?" [1944]

balance equations - open systems

open systems - dissipation inequality

\[ D_0 = \mathbf{P} : D_t \mathbf{F} - \rho_0 D_t \psi - \rho_0 S D_t \theta - s_0 \theta + \mathcal{Q} \cdot \nabla X \ln(\theta) \geq 0 \]
with definition of arguments of free energy
  \[ \psi = \psi(\rho_0, \mathbf{F}, \theta) \]
  \[ D_t \psi = D_\rho \psi D_t \rho + D_F \psi D_t \mathbf{F} + D_\theta \psi D_t \theta \]

evaluation of dissipation inequality

\[ D_0 = [\mathbf{P} - \rho_0 D_F \psi] : D_t \mathbf{F} - [\rho_0 S - \rho_0 D_\theta \psi] D_t \theta + \ldots \geq 0 \]

provides guidelines for the appropriate choice of the constitutive equations

\[ \mathbf{P} = \rho_0 D_F \psi \]
\[ S = -D_\theta \psi \]

thermodynamically conjugate pairs

\[ \mathbf{P} \Leftrightarrow \mathbf{F} \quad S \Leftrightarrow \theta \]

example of open systems - the galileo giant

...del che e manifesto, che chi volesse mantener in un vastissimo gigante le proporzioni, che hanno le membra in un huomo ordinario, bisognerebbe o trouver materia molto piu dura, e resistente per formarne l'ossa e vero ammettere, che la robustezza sua fusse a proporzione assai piu fiacca, che negli huomini de statura mediocre; altrimenti crescendogli a smisurata altezza si vedrebbono dal proprio peso opprimere, e cadere..."  

Galileo, "Discorsi e dimostrazioni matematiche", [1638]

example - the galileo giant
The tallest man in medical history is Robert Pershing Wadlow. He was born at Alton, Illinois, on February 22, 1918. He was 2.72 m / 8 ft 11.1", tall.

His weight was 222.71 kg, his shoe size was 47 cm / 18.5", and his hands measured 32.4 cm / 12.75". His arm span was 2.88 m / 9 ft 5.75", and his peak daily food consumption was 8000 calories.

Consider and compare the two cases:

Calculate the vertical displacement and the energy for a giant with a constant bone mineral density along the height.

Calculate the vertical displacement and the bone mineral density for a giant with a constant energy along the height.

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**Example of open systems - the Galileo giant**

- Balance equation closed systems
- Neo Hookean free energy
- Stress from dissipation inequality
- Quasi-static case
- Constant gravity load
- From balance eqn linear stress
- Closed system, constant density

\[ \rho_0 D_t v = \text{Div}(P) + b_0 \]
\[ \psi_0 = \frac{1}{4} E_0 \left[ F^2 - 1 - 2 \ln(F) \right] \]
\[ P = D_F \psi_0 = \frac{1}{4} E_0 \left[ 2F - 2 \frac{1}{F} \right] \]
\[ \rho_0 D_t v = 0 \]
\[ b_0 = \text{const along the height} \]
\[ P = [X - h] b_0 \]

...linear along the height \( h \)

\[ \rho = \rho_0^* \quad [\rho - \rho_0^*] / \rho_0^* = 0 \]

---

**Example of closed systems - the Galileo giant**

- Density
- Displacement
- Energy

\[ \frac{[\rho - \rho_0^*]}{\rho_0^*} = 0 \]
\[ u = \varphi - X \]
\[ \left[ \frac{\rho_0}{\rho_0^*} \right]^{-m} \psi_0 = \psi_0 \]

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**Figure 7.1: One-dimensional model problem - Closed system - Homogeneous density**
example of open systems - the galileo giant

- balance equations: open systems
  \[ D_t \rho_0 = \text{Div}(R) + \mathcal{R}_0 \]
  \[ \rho_0 \, D_t v = \text{Div}(P) + b_0 \]

- free energy: \( \psi_0 = \left[ \frac{\rho_0}{\rho_0^*} \right]^{m} \psi_0^{\text{neo}} \)
  \[ \psi_0^{\text{neo}} = \frac{1}{4} E_0 \left[ F^2 - 1 - 2 \ln(F) \right] \]
  \[ P = D_F \psi_0 = \frac{1}{4} E_0 \left[ 2F - 2 \frac{1}{F} \right] \]
  \[ \rho_0 \, D_t v = 0 \]

- stress from dissipation inequality:
  \[ b_0 = \text{const along the height } h \]

- quasi-static case
  \[ P = [X - h] b_0 \]

- constant gravity load
  \[ \text{linear along the height } h \]

- from balance eqn linear stress
  \[ D_t \rho_0 = \mathcal{R}_0 = 0 \]

- open system, varying density
  \[ \mathcal{R}_0 = \left[ \frac{\rho_0}{\rho_0^*} \right]^{m} \rho_0 - \rho_0^* \]

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Figure 7.2: One-dimensional model problem - Open system - Homogeneous stimulus