# Fundamental cardiac mechanics Part 2: A glimpse of nonlinear solid mechanics

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## Modeling the complete muscle (1)

- The model of Rice et al (and similar models) gives the force development in a single cell.
- Cells are connected to form tissue, and embedded in an extracellular matrix consisting mainly of collagen
- As cells contract, they interact with the elastic response of the tissue
- Overall deformation and heart dynamics results from a combination of actively developed force and passive elastic forces
- Both types of forces are highly clinically relevant:
  - Increased stiffness leads to reduced filling and heart failure (diastoloc HF)
  - Reduced contractility leads to reduced ejection and HF (systolic HF)
- Modeling the complete muscle mechanics is based on the framework of *nonlinear solid mechanics*

## Solid mechanics (1)

- The key variables in solid mechanics problems are *stresses* and *strains*
- Stress = force per area, strain = relative deformation
- Important distinction between small and large deformations:

– Small deformation; neglect the change in area as the material deforms
– Large deformations (> ca 5% strain); need to consider change in area

- Small deformation problems are often linear, large deformations give non-linear problems

## Solid mechanics (2)

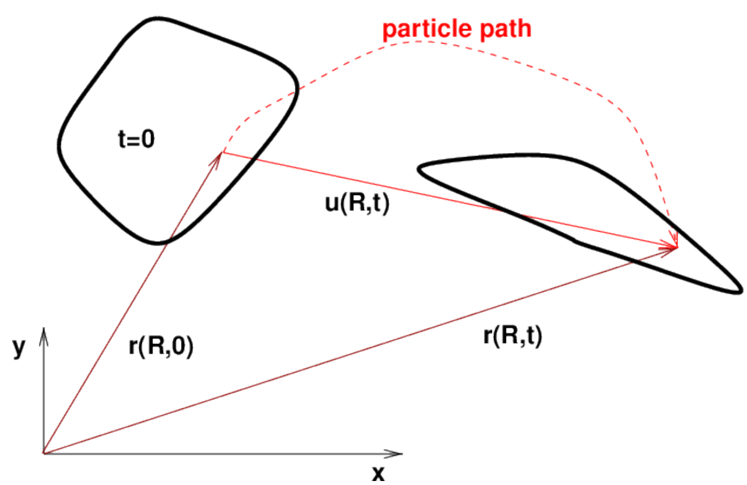
In short, the field of solid mechanics has three main parts:

- Kinematics; the description of motion and deformation of the material (i.e. strains)
- Balance laws; fundamental equations based on balance of mass and momentum, or equilibrium of forces/stresses in the static case
- Constitutive laws; experimentally derived laws that relate stresses to strains.

## Kinematics

How do we quantify deformation/change of shape?

## Deformation and displacement (1)




- The path of each particle: $x(X, t)$
- Initial position: $r(X, 0) = X$ (particle label)
- Displacement field $u$:

$$u(X, t) = x(X, t) - X$$

## Deformation and displacement (2)

- The displacement $u$ is often the primary unknown in solid mechanics
- $u$ contains everything we need to know about the deformation;
  - Change of shape ("true" deformation)
  - Rigid mody motion (rotation and translation)
- Our goal is to relate internal forces (stresses) to deformations
- Rigid body motion does not give rise to internal forces
- We need a measure of deformation that only contains *change of shape*

## The deformation gradient

We are interested in *relative* displacement between different points. It makes sense to take the derivative of the mapping:

$$F = \frac{\partial x}{\partial X} = \nabla x = I + \nabla u$$

This is the *deformation gradient*, a fundamental quantity in nonlinear solid mechanics. In particular, an infinitesimal line segment $dX$ in the reference configuration deforms according to

$$dx = F dX$$

## The right Cauchy-Green tensor

- The deformation gradient includes both rotation and change of shape.
- Rotation does not induce internal forces, and must be removed to get a measure of of pure change of shape.
- According to the Polar decomposition theorem, if $F$ is non-singular we have $F = RU$, where $R$ is an orthogonal rotation tensor, while $U$ is symmetric and contains no rotation.
- We introduce

$$C = F^T F = (RU)^T (RU) = U^T R^T R U = U^T U$$

$C$ is called the *right Cauchy-Green tensor*.

## The Green-Lagrange strain tensor (1)

- We are now ready to define strain
- Look at a small line segment $dX$, which deforms to $dx$
- If $||dx|| = ||dX||$: pure rotation
- $\Rightarrow$ Suitable strain measure arises from

$$\begin{aligned}||dx||^2 - ||dX||^2 &= dx^T dx - dX^T dX \\ &= (FdX)^T (FdX) - dX^T dX \\ &= dX^T F^T F dX - dX^T dX = 2dXEdX\end{aligned}$$

$E$ is the important quantity holding strain information.

## The Green-Lagrange strain tensor (2)

The Green Lagrange strain tensor is the most commonly used strain tesnor for large elastic deformations. We have

$$E = \frac{1}{2}(C - I) = \frac{1}{2}(F^T F - I)$$

or

$$\begin{aligned}E_{ij} &= \frac{1}{2}\left(\frac{\partial x_k}{\partial X_i}\frac{\partial x_k}{\partial X_j} - \delta_{ij}\right) \\ &= \frac{1}{2}\left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} + \frac{\partial u_k}{\partial X_i}\frac{\partial u_k}{\partial X_j}\right)\end{aligned}$$

If deformations are small we can neglect higher order terms to get

$$E_{ij} \approx \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i}\right)$$

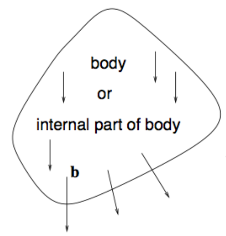
which may be recognized as the standard linear strain tensor used for small strains:

$$\varepsilon_{ij} = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

## Equilibrium of forces

Newton's second law applied to a continuous and deforming material.

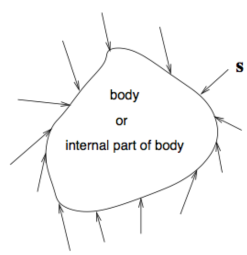
## Body forces




- Body forces $\boldsymbol{b}$ are "distant" forces acting in each point of the body
- Example: gravity $\boldsymbol{b} = \boldsymbol{g}$
- Example: centrifugal force $\boldsymbol{b} = \boldsymbol{\omega} \times \boldsymbol{\omega} \times \boldsymbol{r}$
- Total force:

$$\boldsymbol{B} = \int\limits_{\text{body}} \varrho \boldsymbol{b} dV$$

## Surface forces



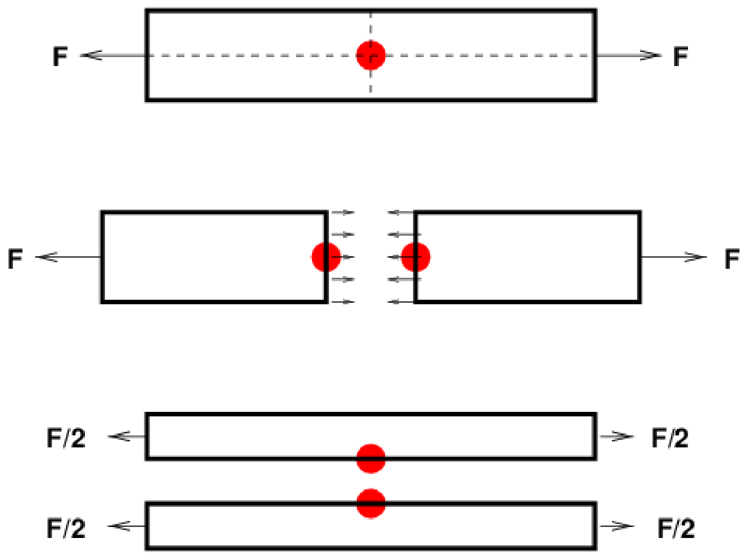

- Distributed along the surface of a body or of an internal part of a body
- Stress = force per unit area, $\boldsymbol{s}(\boldsymbol{x}, t)$
- Total force:

$$\boldsymbol{S}(\boldsymbol{x}, t) = \int\limits_{\text{surface}} \boldsymbol{s}(\boldsymbol{x}, t) dA$$

## The stress vector

- Stress is force per unit area (vector)
- The stress vector depends on the orientation of the area
- That is, the stress at a point on a surface depends on the location of the point (on the surface) and on the orientation of the surface at that point

## Stress in a rod




## Observations

- The stress at the bullet point was in one case $F/A$ ($A$: area) and in another case 0!
- "Stress" means stress at a *point* on a *surface*
- The surface orientation (normal vector $\boldsymbol{n}$) is needed for stress vector computations

## Stress vector computation

- The stress vector depends on space, time and the orientation (unit outward normal vector $\boldsymbol{n}$) of the surface on which the stress vector acts
- Notation: $\boldsymbol{s}(\boldsymbol{r}, t; \boldsymbol{n})$
- Cauchy's 1. law (Cauchy's stress theorem):

$$\boldsymbol{s}(\boldsymbol{r}, t; \boldsymbol{n}) = \boldsymbol{n}(\boldsymbol{r}, t) \cdot \boldsymbol{\sigma}(\boldsymbol{r}, t)$$

($\Rightarrow$ $\boldsymbol{s}$ has a simple (linear) dependence on $\boldsymbol{n}$)

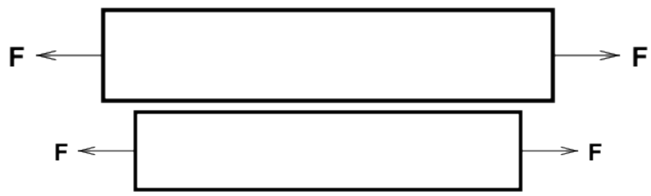
## The stress tensor

- The quantity $\boldsymbol{\sigma}$ or $\sigma_{ij}$ in Cauchy's 1. law is called the stress tensor
- $\boldsymbol{\sigma}$ contains 9 entries:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

The entries have a physical interpretation, but represent mainly ingredients in a tool (Cauchy's 1. law) for computing the stress vector at an arbitrary surface

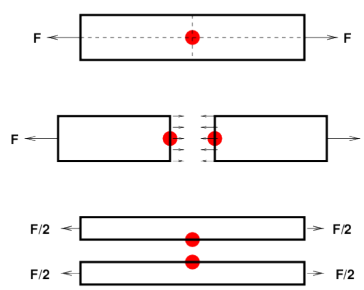
## Stress tensor in a rod (1)




- Uni-axial tension force
- How can we find the stress tensor in this case?
- General approach: solve the governing PDE with boundary conditions (possible even analytically!)
- Or: use physical reasoning to guess at a stress tensor (usually difficult, but possible in this case)

## Stress tensor in a rod (2)

- Cutting the body along coordinate planes ($x = \text{const}$, $y = \text{const}$, $z = \text{const}$)




suggests

$$\boldsymbol{\sigma} = \begin{pmatrix} F/A & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

## Stress tensor in a rod (3)

- How can we know that this guess is correct?

- Rhysical reasoning indicates such a stress tensor, but only the solution of a full model for elastic deformation can tell if our assumption of $\boldsymbol{\sigma}$ is correct
- Classically, such guesses based on physical reasoning were required to treat the problem analytically
- Today, such guesses are crucial to assess whether numerical results are reasonable

## Equilibrium of forces (1)

For an arbitrary volume inside a material, Newton's 2nd law reads

$$\frac{d\boldsymbol{I}}{dt} = \sum \boldsymbol{F}$$

where $\boldsymbol{I}$ is momentum:

$$\boldsymbol{I} = \int_V \varrho \boldsymbol{v} dV$$

and $\sum \boldsymbol{F}$ is the total external force: surface forces + body forces.

## Equilibrium of forces

In solid mechanics, it is common to neglect inertia effects:

$$\frac{d\boldsymbol{I}}{dt} \approx 0$$

Newton's second law reduces to a force equilibrium: $\sum \boldsymbol{F} = 0$

## Two types of forces

Surface forces:

$$\int\limits_{\partial V} \boldsymbol{\sigma} \cdot \boldsymbol{n} dS$$

Body forces (e.g. gravity)

$$\int\limits_{V} \varrho \boldsymbol{b} dV$$

## The equilibrium equation (1)

We have

$$\int\limits_{\partial V} \boldsymbol{\sigma} \cdot \boldsymbol{n} dS + \int\limits_{V} \varrho \boldsymbol{b} dV = 0$$

Applying Gauss' theorem to the first term gives

$$\int\limits_{V} \nabla \cdot \boldsymbol{\sigma} dV + \int\limits_{V} \varrho \boldsymbol{b} dV = 0$$

## The equilibrium equation (2)

Since the volume is arbitrary we must have

$$\nabla \cdot \boldsymbol{\sigma} + \varrho \boldsymbol{b} = 0.$$

- This is the static (equilibrium) version of Cauchy's equation of motion.
- In heart mechanics the effects of gravity are negligible, and we are left with

$$\nabla \cdot \boldsymbol{\sigma} = 0$$

## The equilibrium equation (3)

- The equilibrium equation derived above is completely valid for all materials in equilibrium
- Inconvenient to use for large deformations, since Cauchy stress $\sigma$ is defined relative to the undeformed area, which is unknown
- Differentiation (the divergence operator) is also performed relative to the deformed coordinates of the material, which are not known
- A so-called Lagrangian approach is common:
  - Map all quantities and operations back to the undeformed geometry of the material
  - Introduce alternative stress tensors that are computed on the undeformed geometry

## The Piola-Kirchoff stress tensors

The first Piola-Kirchoff stress tensor

$$\boldsymbol{P} = J\boldsymbol{\sigma}\boldsymbol{F}^{-T}$$

gives the actual force referred to the undeformed surface area.

The second Piola-Kirchoff stress tensor

$$\boldsymbol{S} = J\boldsymbol{F}^{-1}\boldsymbol{\sigma}\boldsymbol{F}^{-T}$$

is derived by mapping the force back to the undeformed geometry.

These stress tensors are only used as tools in computations. The relevant physical quantity is the Cauchy stress $\boldsymbol{\sigma}$.

## The equilibrium equation for large deformations

In terms of the Piola-Kirchoff stresses, the equilibrium equation reads

$$\nabla \cdot \boldsymbol{P} = 0,$$

or

$$\nabla \cdot \boldsymbol{F}\boldsymbol{S} = 0$$

These are the versions we will use for modeling heart muscle mechanics.

## Constitutive equations

How are stresses in the material related to the strains?

## Relating stress and strain

We have introduced several important concepts:

- Strain; a precise measure of change of shape in a material
- Stress; force/area, a useful measure of forces acting on internal and external surfaces
- The fundamental equation that describes equilibrium of forces in the material

What is missing is a description of material behavior:

- Equation of motion is valid for any solid (rubber, steel, soft tissues...)
- Has six unknowns (components of the symmetric stress tensor), but only three equations (divergence of a tensor is a vector)
- We need *constitutive equations* to close the system

## Hooke's generalized law

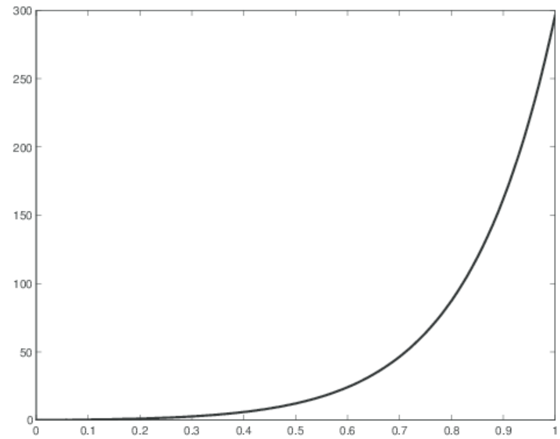
Elongation of a rod: Hooke's experiments showed that

$$\frac{F}{A} = E\frac{\Delta L}{L}$$

- Stress (force) is linearly related to strain (relative displacement)
- The general form: $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$
- $C_{ijkl}$ is a fourth-order tensor (81 components) which describes the stiffness of the material

## Non-linear (hyper)elastic materials

For materials undergoing large elastic deformations, the stress-strain relation is normally non-linear:




## The strain energy function (1)

- For all hyperelastic materials we can define a strain energy function

$W$, normally defined in terms of the Green-Lagrange strain or its invariants

- For an elastic material following Hookes law, the strain energy function

can be written as

$$W = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl}$$

(Recall that in the small deformation case $\varepsilon_{ij} \approx E_{ij}$)

## The strain energy function (2)

The stress is obtained by taking the first derivative of the strain energy function with respect to the strain

$$\sigma_{ij} = \frac{\partial W}{\partial \varepsilon_{ij}}$$

The second derivative of the strain energy function gives the stiffness tensor

$$C_{ijkl} = \frac{\partial^2 W}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

## The strain energy function (3)

Similar principles apply for non-linear hyperelastic materials:

- The first derivative of $W$ with respect to the Green-Lagrange strain

gives the 2nd Piola-Kirchoff stress; $S_{ij} = \frac{\partial W}{\partial E_{ij}}$

- Differentiating twice gives the tangential stiffness, often

referred to as the *second elasticity tensor*:

$$C_{ijkl} = \frac{\partial^2 W}{\partial E_{ij} \partial E_{kl}}$$

It is important to note that in the non-linear case this tensor is not constant, but depends on the deformation state. The tangential stiffness is used in computational techniques (Newton's method).

## The strain energy function (4)

Similar relations hold for the PK1 stress

- The first derivative of $W$ with respect to the deformation gradient

gives the 1st Piola-Kirchoff stress $P_{ij} = \frac{\partial W}{\partial F_{ij}}$

- Differentiating twice gives an alternative stiffness tensor, known as the *first elasticity tensor*

$$A_{ijkl} = \frac{\partial^2 W}{\partial F_{ij} \partial F_{kl}}$$

## Examples of strain energy functions (1)

St. Venant-Kirchoff:

$$W(E) = \frac{\lambda}{2}(\mathrm{tr}E)^2 + \mu \mathrm{tr}E^2$$

Neo-Hookean:

$$W = \frac{\mu}{2}(I_1 - 3) - \mu \log J + \frac{\lambda}{2}(\log J)^2$$

where $I_1$ is the *first invariant* of the right Cauchy-Green tensor

## Example of strain energy functions (2)

Orthotropic exponential model, Guccione et al (1995), 8 material parameters:

$$W = \frac{1}{2}K(e^Q - 1) + C_{compr}(J \ln J - J + 1),$$

with

$$\begin{aligned} Q = {} & b_{ff}E_{ff}^2 + b_{ss}E_{ss}^2 + b_{nn}E_{nn}^2 + b_{fs}(E_{fs}^2 + E_{sf}^2) \\ & + b_{fn}(E_{fn}^2 + E_{nf}^2) + b_{ns}(E_{ns}^2 + E_{sn}^2) \end{aligned}$$

## Summary; complete large deformation elasticity problem

Static problem with no body forces:

$$
\begin{aligned}
-\nabla \cdot \boldsymbol{P} &= 0 \quad \text{in } \Omega \\
u &= g \quad \text{on } \Gamma_{\mathrm{D}} \\
P \cdot n &= T \quad \text{on } \Gamma_{\mathrm{N}}
\end{aligned}
$$

- $u$ is the displacement
- $\boldsymbol{P} = \partial W / \partial \boldsymbol{F}$ is the first Piola–Kirchoff stress tensor
- $W$ is the strain energy
- $g$ is a given boundary displacement
- $T$ is a given boundary traction (typically pressure)

## Variational form of large deformation elasticity

Multiply by a test function $v \in \hat{V}$ and integrate by parts:

$$
-\int_{\Omega} \nabla \cdot \boldsymbol{P} \cdot v dx = \int_{\Omega} \boldsymbol{P} : \nabla v dx - \int_{\partial\Omega} (\boldsymbol{P} \cdot n) \cdot v ds
$$

Note that $v = 0$ on $\Gamma_{\mathrm{D}}$ and $\boldsymbol{P} \cdot n = T$ on $\Gamma_{\mathrm{N}}$
Find $u \in V$ such that

$$
\int_{\Omega} \boldsymbol{P} : \nabla v dx = \int_{\Gamma_{\mathrm{N}}} T \cdot v ds
$$

for all $v \in \hat{V}$

## Material laws for active contraction (1)

- So far we have only considered passive mechanical behavior of the tissue
- The tissue consists of cells, which contract and develop their own force
- How can we model the actively contracting tissue?

## Material laws for active contraction (2)

The most common approach is to to an additive split of the stress tensor, the *active stress* approach:

$$
\boldsymbol{P} = \boldsymbol{P}_p + \boldsymbol{P}_a,
$$

with

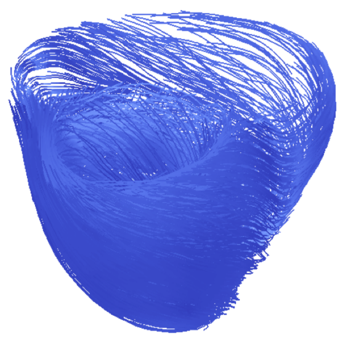
$$
\begin{aligned}
\boldsymbol{P}_p &= \frac{\partial W}{\partial \boldsymbol{F}} \\
\boldsymbol{P}_a &= \begin{pmatrix} T_a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\end{aligned}
$$

Here, $T_a$ is the output force of a cell contraction model (e.g. Rice et al 2008), typically assumed to act only in the direction of the muscle fibers.

## Boundary conditions for whole heart modeling (1)

Standard boundary conditions for whole heart modeling:

- Partly fixed ($u = 0$) at the base
- Zero pressure on the outer surface (epicardium)
- Non-zero, time-varying pressure on the inner surface (endocardium)



## Boundary conditions for whole heart modeling (2)

Endocardial pressure:

- Dynamic pressure which depends on contraction
- Depends on properties of entire circulation
- Realistic boundary conditions; couple heart model to ODE based circulation models

## Boundary conditions for whole heart modeling (2)

LV model coupled to systemic circulation:

$$\frac{dV_{lv}^{circ}}{dt} = \frac{S_{mi}(P_{sv} - P_{lv})}{R_{mi}} - \frac{S_{ao}(P_{lv} - P_{sa})}{R_{ao}},$$
$$\frac{dV_{sa}}{dt} = \frac{S_{ao}(P_{lv} - P_{sa})}{R_{ao}} - \frac{P_{sa} - P_{sv}}{R_{sys}},$$
$$\frac{dV_{sv}}{dt} = \frac{P_{sa} - P_{sv}}{R_{sys}} - \frac{S_{mi}(P_{sv} - P_{lv})}{R_{mi}}.$$

Replace the time varying elastance model for $p_{lv}$ with the constraint:

$$V_{lv}^{circ}(p_{lv}) - V_{lv}^{fem}(p_{lv}) = 0$$