### Fundamental cardiac mechanics

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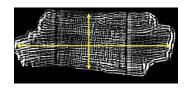
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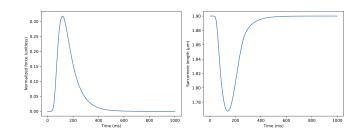
#### Outline

- From cell to tissue
  - The continuum approach
- Fundamentals of mechanics
  - Stress
  - Strain
  - Fundamental equations
- Modeling soft tissues
  - Non-linear solid mechanics
  - Material laws for the heart

### From cell to tissue (1)

We have seen how we can model the contraction of a single myocyte...

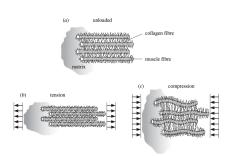




### From cell to tissue (2)

... but the heart contains around 10 billion myocytes, embedded in a complex compound of proteins, fluids, other cells, etc.





# The continuum approach

- The tissue is viewed as continuous and homogeneous, neglecting the discrete, cell-based nature
- Takes a macro-scopic, top-down view of the tissue
- The same approach is used for modeling other materials, neglecting the molecular/atomic structure
- We can apply the standard tools of continuum mechanics, which have been developed over centuries

# Some additional challenges in biomechanics

- Large deformations
- Strongly non-linear material behavior
- Active properties
- Growth and remodeling
- (The cell scale is much larger than the atomic scale, which means the continuum approach may not always be justified)

### Here, we focus on solid mechanics

#### Typical case (general):

- Apply some load (force) to a structure:
  - What are the internal forces (stresses)?
  - Will the structure hold or break?
  - How much does the structure deform?

#### Heart mechanics is similar, but with some differences:

- Load is dynamic (blood pressure)
- Material properties are dynamic (cells contract)
- What is the deformation (volume change) for a given load
- What are the internal forces (related to growth and remodeling)

### 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 nonlinear problems

## Solid mechanics (2)

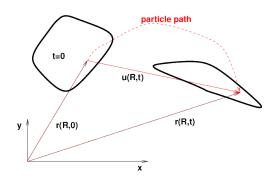
In short, the field of solid mechanics has three main parts:

- 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.



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

$$dx = FdX$$

### 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

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

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
- ⇒ Suitable strain measure arises from

$$||dx||^{2} - ||dX||^{2} = dx^{T} dx - dX^{T} dX$$
$$= (FdX)^{T} (FdX) - dX^{T} dX$$
$$= dX^{T} F^{T} F dX - dX^{T} dX = 2dXEdX$$

*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

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

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

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

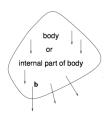
which may be recognized as the standard linear strain tensor used for small strains:

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

# Equilibrium of forces

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

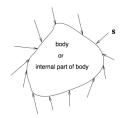
### Body forces



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

$$\mathbf{B} = \int_{\mathsf{body}} \varrho \mathbf{b} dV$$

### Surface forces



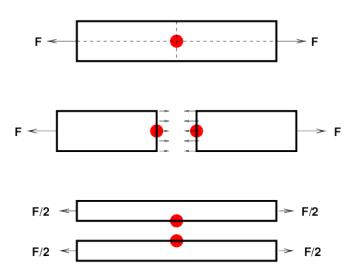
- Distributed along the surface of a body or of an internal part of a body
- Stress = force per unit area, s(x, t)
- Total force:

$$m{S}(m{x},t) = \int _{ ext{surface}} m{s}(m{x},t) dA$$

#### 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
- ullet The surface orientation (normal vector  $oldsymbol{n}$ ) is needed for stress vector computations

### Stress vector computation

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

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

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

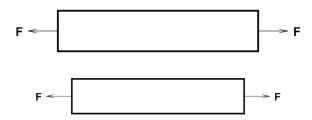
### The stress tensor

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

$$\boldsymbol{\sigma} = \left( \begin{array}{ccc} \sigma_{\mathsf{xx}} & \sigma_{\mathsf{xy}} & \sigma_{\mathsf{xz}} \\ \sigma_{\mathsf{yx}} & \sigma_{\mathsf{yy}} & \sigma_{\mathsf{yz}} \\ \sigma_{\mathsf{zx}} & \sigma_{\mathsf{zy}} & \sigma_{\mathsf{zz}} \end{array} \right)$$

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

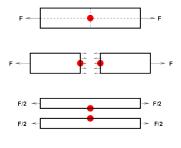
## Stress tensor in a rod (1)



- 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 = const, y = const, z = const)



suggests

$$\sigma = \left( \begin{array}{ccc} F/A & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array} \right)$$

### Stress tensor in a rod (3)

- How can we know that this guess is correct?
- ullet Rhysical reasoning indicates such a stress tensor, but only the solution of a full model for elastic deformation can tell if our assumption of  $\sigma$  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

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

where *I* is momentum:

$$I = \int_{V} \varrho \mathbf{v} dV$$

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

# Equilibrium of forces

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

$$\frac{d\mathbf{l}}{dt}\approx 0$$

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

# Two types of forces

Surface forces:

$$\int_{\partial V} \boldsymbol{\sigma} \cdot \boldsymbol{n} dS$$

Body forces (e.g. gravity)

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

# The equilibrium equation (1)

We have

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

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

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

- 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

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

gives the actual force referred to the undeformed surface area.

The second Piola-Kirchoff stress tensor

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

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  $\sigma$ .

# The equilibrium equation for large deformations

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

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

or

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

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



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

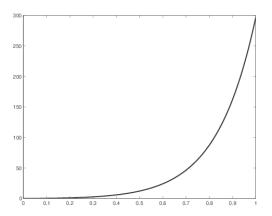
Elongation of a rod: Hooke's experiments showed that

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

- 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;  $S_{ij}=rac{\partial W}{\partial E_{ij}}$ 

• 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:

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

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

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

### Summary; complete large deformation elasticity problem

Static problem with no body forces:

$$-
abla \cdot {m P} = 0 \quad \text{in } \Omega$$
  $u = g \quad \text{on } \Gamma_{\mathrm{D}}$   $P \cdot n = T \quad \text{on } \Gamma_{\mathrm{N}}$ 

- u is the displacement
- $P = \partial W/\partial F$  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:

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

Note that  $\emph{v}=0$  on  $\Gamma_{\rm D}$  and  $\emph{\textbf{P}}\cdot\emph{n}=\emph{T}$  on  $\Gamma_{\rm N}$ 

Find  $u \in V$  such that

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

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:

$${m P} = {m P}_p + {m P}_a,$$

with

$$\mathbf{P}_{p} = \frac{\partial W}{\partial \mathbf{F}}$$

$$\mathbf{P}_{a} = \begin{pmatrix} T_{a} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

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

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)