Domain Decomposition Based Solvers for the Simulation of Arteries

Kinematics, Modelling, Numerics

G. A. Holzapfel, O. Steinbach and C. M. Augustin

Institute of Computational Mathematics
Graz University of Technology

SFB: Mathematical Optimization
and Applications in Biomedical Sciences

Outline

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Arterial Histology

Arteries are vessels that transport blood from the heart to the organs.

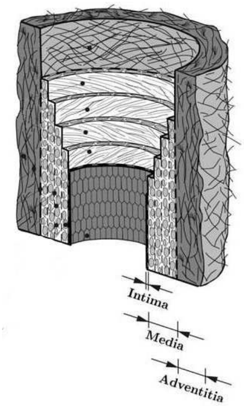

Figure: Holzapfel (2000)

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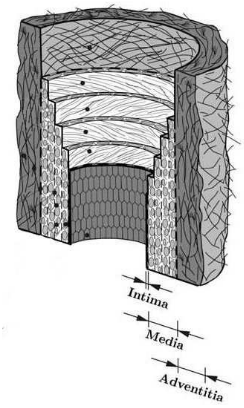

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media (middle layer)

- complex 3D network of muscle cells, and elastin and collagen fibrils
- two main fiber directions

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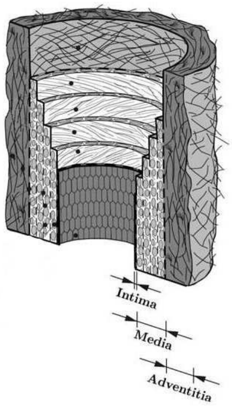

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adventitia (outermost layer)

- histological ground substance and thick bundles of collagen fibrils
- collagen fibers highly dispersed
- gets stiff at higher levels of pressure

Mechanical Behavior of Arterial Walls

Incompressibility

- no change of volume within the physiological range of deformation
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Pre-Stretches

- a segment of vessel shortens on removal from the body
  $\Rightarrow$ there exists a in vivo pre-stretch in longitudinal direction
- a load-free arterial ring contains residual stresses
  $\Rightarrow$ it opens when cut in a radial direction

Material Behavior of Arterial Walls

Material behavior

- *elastic* for proximal arteries
- *viscoelastic* (*pseudoelastic*) for distral arteries
- healthy arteries are highly deformable composite structures
- show a non-linear stress-strain response (neo-Hookean solid)

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Collagen fibers

- lead to stiffening effect at higher pressures
- lead to *anisotropic* mechanical behavior of arteries
- are not able to support compressive stresses
- active in extension and inactive in compression

Outline

Cauchy's Equation of Motion

Consider the strong formulation of the boundary value problem:
Find $u \in C^2(\Omega) \cap C^1(\Omega \cup \Gamma_N) \cap C(\overline{\Omega})$ such that

$$
\begin{aligned}
\rho \frac{\partial^2 u}{\partial t^2} - \operatorname{div} \sigma &= f(x) && \forall x \in \Omega, t > 0 \ , \\
\sigma &= p\mathbf{I} + \overline{\sigma} && \forall x \in \Omega, t > 0 \ , \\
u(x) &= u_D(x) && \forall x \in \Gamma_D, t > 0 \ , \\
\frac{\partial u}{\partial N} &= \sigma\, n = t_N(x) && \forall x \in \Gamma_N, t > 0 \ , \\
u = u_0 \, , \frac{\partial u}{\partial t} &= v_0 && \forall x \in \Omega, t = 0 \ .
\end{aligned}
$$

is satisfied with $\Gamma = \partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$.

Constitutive Equation

Preliminaries

- Deformation gradient $\mathbf{F} = D_x\varphi$ and the Jacobian $J = \det \mathbf{F}$
- Strain Tensors $\mathbf{C}, \mathbf{b}, \mathbf{E}, \varepsilon$ are constructed by $\mathbf{F}$, e.g. $\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$
- Stress Tensors $\sigma, \mathbf{S}$ follow a specific constitutive law
- Elasticity Tensor $\mathbb{C}$ is a tensor of 4th order

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Constitutive Equation

from the Laws of Thermodynamics the following constitutive equations may be derived:

$$\sigma = 2J^{-1}\mathbf{F}\frac{\partial\Psi(\mathbf{C})}{\partial\mathbf{C}}\mathbf{F}^{\mathrm{T}}, \quad \mathbf{S} = 2\frac{\partial\Psi(\mathbf{C})}{\partial\mathbf{C}}, \quad \mathbb{C} = \frac{\partial\mathbf{S}}{\partial\mathbf{C}}$$

with the Helmholtz free-energy function Ψ.

Helmholtz free-energy Function

- used to describe the hyperelastic stress response of arterial walls
- it is splitted into a volumetric, an isotropic and an anisotropic part:

$$\Psi = U(J) + \overline{\Psi}_{\mathrm{iso}} + \overline{\Psi}_{\mathrm{aniso}}$$

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Neo-Hookean Model, isotropic response

$$\overline{\Psi}_{\mathrm{iso}}(\overline{I}_1) = \frac{c}{2}(\overline{I}_1 - 3) \ , \quad \overline{I}_1 = \mathrm{tr}(\overline{\mathbf{C}}) \ .$$

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Holzapfel Model (Holzapfel 2000), anisotropic response

$$\overline{\Psi}_{\mathrm{aniso}}(\overline{I}_4, \overline{I}_6) = \frac{k_1}{2k_2} \sum_{i=4,6} \left\{ \exp[k_2(\overline{I}_i - 1)^2] - 1 \right\} \ , \quad \overline{I}_i = \mathrm{tr}(\overline{\mathbf{C}}^{\mathrm{T}} \mathbf{A}_i) \ ,$$

where $\mathbf{A}_i$ represent the two fiber directions in the anisotropic material.

Summary of the Model

From $\Psi = U(J) + \overline{\Psi}_{\text{iso}} + \overline{\Psi}_{\text{aniso}}$ and the constitutive equation

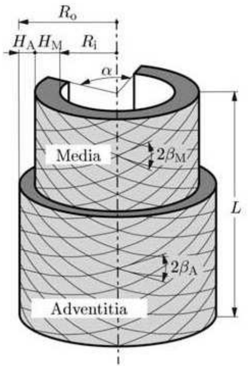


Figure: Holzapfel (2003)

$$\sigma = 2J^{-1}\mathbf{F}\frac{\partial\Psi(\mathbf{C})}{\partial\mathbf{C}}\mathbf{F}^{\mathrm{T}}$$

we may calculate the specific form of σ:

$$\sigma = p\mathbf{I} + \underbrace{c\,\mathrm{dev}(\overline{\mathbf{b}}) + \frac{k_1}{2k_2}\psi(\overline{I}_4, \overline{I}_6)}_{\overline{\sigma}}$$

$$p = \frac{\partial U(J)}{\partial J} \text{ with e.g. } U(J) = \frac{\kappa}{2}(J-1)^2$$

where the parameters have to satisfy

$$\kappa, c, k_1, k_2 > 0 \ .$$

Outline

Variational Formulation

From the Cauchy's equation of motion

$$\rho \frac{\partial^2 u}{\partial t^2} - \operatorname{div}(p\mathbf{I} + \overline{\sigma}) = f(x) \ , \quad p = \kappa(J(u) - 1) \ , \quad J = \det D_x u$$

we obtain the following variational problem: Find u such that

$$\int_\Omega \rho \frac{\partial^2 u}{\partial t^2} \cdot v \,\mathrm{d}x + \int_\Omega p \operatorname{div} v \,\mathrm{d}x + \int_\Omega \overline{\sigma}(u) : \varepsilon(v) \,\mathrm{d}x = \langle F, v \rangle$$

$$- \int_\Omega \kappa(J(u)) - 1)\, q \,\mathrm{d}x + \int_\Omega p \cdot q \,\mathrm{d}x = 0$$

for $u, v \in H^1(\Omega)$, $p, q \in L_2(\Omega)$ and $\varepsilon = 1/2\,(\operatorname{grad} v + (\operatorname{grad} v)^{\mathrm{T}})$.

Discretization

The current domain Ω is subdivided in isoparametric finite elements (tetrahedra, quadrilaterals)

$$\overline{\Omega}_h = \bigcup_{r \in \tau_h} \overline{T}^{(r)}$$

where τ_h is the set containing the element numbers.

$$u_h = \sum_{j \in \omega_h} u_j(t)\varphi_j(x)\ , \quad p_h = \sum_{k \in \tau_h} p_k(t)\psi_k(x)$$

with

- ω_h: the set of node numbers
- $\varphi_j(\xi_1, \xi_2, \xi_3)$: the isoparametric shape function associated with node j assumed to be trilinear
- ψ_k piecewise constant

Discretization of Cauchy's Equation

The discretized version of the leading equations reads

$$-\int_\Omega \rho \frac{\partial^2 u_h}{\partial t^2} \cdot v_h \,\mathrm{d}x + \int_\Omega p_h \operatorname{div} v_h \,\mathrm{d}x + \int_\Omega \overline{\sigma}(u_h) : \varepsilon(v_h) \,\mathrm{d}x = \langle F, v_h \rangle$$

$$-\int_\Omega \kappa(J(u_h)) - 1)\, q_h \,\mathrm{d}x + \int_\Omega p_h\, q_h \,\mathrm{d}x = 0$$

This leads to a system of the form

$$\mathbf{M}\ddot{u}(t) + \mathbf{A}(u,p,t) = F^{\mathrm{ext}}(t)\ , \quad p = \kappa(J(u_h) - 1)$$

The term $\mathbf{A}(u,p,t)$ is highly nonlinear in u.

Discretization of the pressure equation

- use the same constant interpolation function over a given element
- do not have to satisfy continuity across the element boundaries

Discretization of J

$$J = det(F), \; J = J(u)$$

The variational formulation in the reference configuration yields:

$$\int_{\Omega_0} (J - J(u))\, q \,\mathrm{d}X = 0$$

for all test functions q. J is discretized by

$$J_h = \sum_{k \in \tau_h} J_k \psi_k \;, \quad \psi_k(x) = \begin{cases} 1 & \text{if } x \in T^{(k)} \\ 0 & \text{else} \end{cases} \;,$$

and $q(x) = \psi_i(x)$ piecewise constant.

Discretization of the pressure equation

Inserting the discretized version of J, considering just one element $T_0^{(k)}$, yields:

$$\int_{T_0^{(k)}} (J_k - J(u))\,\mathrm{d}X = 0$$

Since J_k does not depend on X this leads to

$$J_k = \frac{1}{V^{(k)}} \int_{T_0^{(k)}} J(u)\,\mathrm{d}X = \frac{1}{V^{(k)}} \int_{T^{(k)}} \mathrm{d}x = \frac{v^{(k)}}{V^{(k)}} .$$

where $v^{(k)}$ is the volume of the element in the current configuration and $V^{(k)}$ the volume in the reference configuration.

Discretization of the pressure equation

The discretized version of the pressure equation

$$-\int_{\Omega} \kappa(J(u)) - 1)\, q \,\mathrm{d}x + \int_{\Omega} p\, q \,\mathrm{d}x = 0$$

in just one finite element is

$$-\int_{T^{(k)}} \kappa(J_k - 1) \,\mathrm{d}x + \int_{T^{(k)}} p_k \,\mathrm{d}x = 0 \; .$$

This yields

$$p_k = \kappa(J_k - 1) = \kappa \left(\frac{v^{(k)}}{V^{(k)}} - 1 \right) \; .$$

Linearization

Nonlinear BVP

$$\mathbf{R}(u,t) = \mathbf{M}\ddot{u}(t) + \mathbf{A}(u,t) - F^{\mathrm{ext}}(t) = 0$$

Newton-Method

$$\mathbf{R}'(u^{(k)})\Delta u = r^{(k)} = -\mathbf{R}(u^{(k)}) \ , \quad u^{(k+1)} = u^{(k)} + \Delta u$$

$\mathbf{R}'(u,t)$ is the derivative in direction of the increment Δu:

$$\mathbf{R}'(u,t) = \mathbf{A}'(u,t) = D_{\Delta u}\left(\int_\Omega (p_h \mathbf{I} + \overline{\sigma}(u_h)) : \varepsilon(v_h)\,\mathrm{d}x\right)$$

Chain rule and some tensor manipulations yield

$$\int_\Omega \big(\operatorname{grad} v_h : \operatorname{grad} \Delta u_h (p_h \mathbf{I} + \overline{\sigma}_h) + D_{\Delta u} p_h \mathbf{I} : \varepsilon_h + \varepsilon_h : [(\mathbf{I} \otimes \mathbf{I} - 2\mathbb{I}) p_h + \overline{\mathbb{C}}_h] : \Delta\varepsilon_h\big)\,\mathrm{d}x$$

Stiffness Matrix

Denoting the tensor of forth order by $\mathbb{D}_h$ yields

$$\int_\Omega \left(\operatorname{grad} v_h : \operatorname{grad} \Delta u_h(\sigma_h) + D_{\Delta u} p_h \mathbf{I} : \varepsilon_h + \varepsilon_h : \mathbb{D}_h : \Delta \varepsilon_h\right) \mathrm{d}x$$

This may be simplified to the total stiffness matrix for a typical element $T^{(r)}$

$$\mathbf{K}^{(r)} = \sum_{i,j \in \omega_h} \left(\mathbf{K}_{ij}^{\mathrm{geo}} + \mathbf{K}_{ij}^{\mathrm{pre}} + \mathbf{K}_{ij}^{\mathrm{mat}}\right).$$

The construction of the global stiffness matrix follows the standard assembly procedure of element stiffness matrices:

$$\mathbf{K}(u) = \sum_{r \in \tau_h} \mathbf{A}_r^{\mathrm{T}} \mathbf{K}^{(r)} \mathbf{A}_r$$

with $\mathbf{A}_r$ the connectivity matrices.

Summary

Nonlinear model

- one possibility: Newton method

Discretization

- large number of degrees of freedom
- fast solvers needed

Anisotropic material with different layers

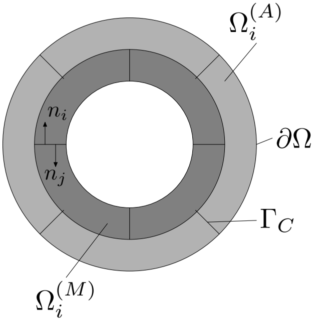
- motivates the use of domain decomposition methods
- implicates parallelization
- Idea: FETI

Outline

Domain Decomposition

Partition into non-overlapping subdomains $\{\Omega_i, 1 \leq i \leq p\}$

$$\overline{\Omega} = \bigcup_{i=1}^{p} \overline{\Omega}_i \ , \quad \Omega_i \cap \Omega_j = 0 \ , i \neq j \ , \quad \Gamma_\mathrm{C} = \bigcup_{i=1}^{p} \partial\Omega_i \setminus \partial\Omega$$



Find the displacement field **u** so that

$$\begin{aligned} \rho\ddot{u}_i - \mathrm{div}[p_i\mathbf{I} + \overline{\sigma}(u_i)] &= f && \text{in } \Omega_i \\ u_i &= u_j && \text{on } \Gamma_\mathrm{C} \\ t_i + t_j &= 0 && \text{on } \Gamma_\mathrm{C} \\ \text{with } [p_i\mathbf{I} + \overline{\sigma}(u_i)]\, n_i &= t_i. \end{aligned}$$

Outlook

Short term goals

- material model in one subdomain
- Dirichlet boundary value problem
- FE solvers (FEAP, NGsolve)

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Mid term goals

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Long term goals

- modelling of diseased arteries
  e.g. atherosclerosis
- modelling of stenting

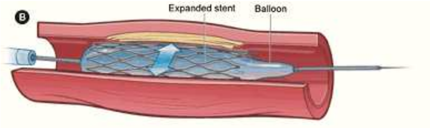

Figure: Expanding a stent

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