Computational Modeling of the Cardiovascular System

Finite Element Method I Mechanical Modeling of Tissues II



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Motivation and Background

Finite Element Method allows solving of physical field problems taking

- anisotropy
- inhomogeneity
- nonlinearity

of material properties into account

Applications

- Electrostatics
- (Quasi-)stationary electrical fields
- Wave propagation
- Temperature
- Structure and fluid mechanics
- ...

Commercial packages

- Ansys
- EMÁS
- ...



Finite Element Method: Overview



Finite Element Method: Element Matrix



Direct Method: Integral Equations

$$W_{e} = \int_{V} \frac{1}{2} \varepsilon E^{2} dV$$

- W_e: Electrical energy
- E: Electrical field
- ε: Permittivity

$$P_{L} = \int_{V} \sigma E^{2} dV$$

- P_L : Electrical power
- E: Electrical field
- σ : Electrical conductivity

$$W_{elast} = \int_{V} \frac{1}{2} E\epsilon^{2} dV$$

$$W_{elast}: Elastic potential energy$$

E: Young's modulus
 $\epsilon: Strain$

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Shape Functions: Motivation

- Field values are given only at some points
- Calculation of surface/volume integrals necessitates interpolation of values in domain
- Element geometry is described with some points
- Coordinate transforms Local coordinates



Global coordinates





Shape Functions

$$u(\vec{x}) = \sum_{k=0}^{K-1} u_k N_k(\vec{x})$$

- u: Interpolation function
- \vec{x} : Position vector
- u_k : Field value at node k
- N_k : Shape function

Commonly, interpolation is based on polynomial shape functions.

In general, shape functions fulfill:

$$N_k(\vec{x}) = \begin{cases} 1 & \text{at node } k \\ 0 & \text{at node } i \neq k \end{cases}$$

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Shape Functions: Barycentric Coordinates in Triangle



Shape Functions 1D: Linear Lagrangian Interpolation

$$u(x) = a + bx$$

$$N_0(\mathbf{x}) = (1 - \mathbf{x})$$
$$N_1(\mathbf{x}) = \mathbf{x}$$
$$u(\mathbf{x}) = (1 - \mathbf{x})u_0 + \mathbf{x}u_1$$

u: Field value function with parameter position

x: Position

 u_0 , u_1 : Field value at node 0 and 1, respectively





Example for Calculation of Shape Functions

General linear interpolation in 1D:

$$u(x) = a + bx$$

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Node conditions:

 $u(0) = a + bx = u_0 \implies a = u_0$ $u(1) = a + bx = u_1 \implies a + b = u_1$

Linear system of equation, inversion:

$$\mathbf{A} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}; \quad \mathbf{A} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \begin{pmatrix} \mathbf{u}_0 \\ \mathbf{u}_1 \end{pmatrix} \implies \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \mathbf{A}^{-1} \begin{pmatrix} \mathbf{u}_0 \\ \mathbf{u}_1 \end{pmatrix} \text{ mit } \mathbf{A}^{-1} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$$

Linear interpolation based on shape functions:

$$u(x) = u_0 + (-u_0 + u_1) x = (1 - x) u_0 + x u_1$$

Shape Function 1D: Quadratic Lagrangian Interpolation

$$u(x) = a + bx + cx^{2}$$

$$N_{0}(x) = (1 - x)(1 - 2x)$$

$$N_{1}(x) = 4x(1 - x)$$

$$N_{2}(x) = -x(1 - 2x)$$

$$u(x) = N_{0}(x)u_{0} + N_{1}(x)u_{1} + N_{2}(x)u_{2}$$

$$x: Position$$

$$u_{0}, u_{1}, u_{2}: Field value at node 0, 1, and 2, respectively$$

$$u(x) = V_{0}(x)u_{0} + V_{1}(x)u_{1} + V_{2}(x)u_{2}$$

$$u_{0} = U_{0}(x)u_{0} + V_{1}(x)u_{1} + V_{2}(x)u_{2}$$

$$u_{0} = U_{0}(x)u_{1} + V_{1}(x)u_{2}$$

$$u_{0} = U_{0}(x)u_{1} + V_{1}(x)u_{1} + V_{2}(x)u_{2}$$

$$u_{0} = U_{0}(x)u_{1} + V_{1}(x)u_{1} + V_{2}(x)u_{2}$$

Shape Function 1D: Cubic Hermitian Interpolation



Shape Function 2D in Quad: Bilinear Lagrangian Interpolation



Shape Function 2D in Quad: Biquadratic Lagrangian Interpolation

$$u(x,y) = a + bx + cy + dxy + ex^{2} + fy^{2} + gx^{2}y + hxy^{2}$$

$$N_{0}(x,y) = (1-x)(1-y)(1-2x-2y)$$

$$N_{1}(x,y) = -x(1-y)(1-2x+2y)$$

$$N_{2}(x,y) = xy(3-2x-2y)$$
...
$$u(x,y) = \sum_{k=0}^{7} N_{k}(x,y)u_{k}$$

$$x,y: \quad \text{Position}$$

$$u_{0} - u_{7}: \quad \text{Field value at node 0..7}$$

$$u_{0} - u_{7}(x) = \frac{1}{2} \int_{0}^{1} \frac{1}{2}$$

Shape Function 3D in Hexahedron: Trilinear Lagrangian Interpolation

$$\begin{split} u(x,y,z) &= a + bx + cy + dz + exy + fyz + gxz + hxyz \\ N_{0}(x,y,z) &= (1-x)(1-y)(1-z) \\ \vdots \\ N_{7}(x,y,z) &= xyz \\ u(x,y,z) &= \sum_{k=0}^{7} N_{k}(x,y,z)u_{k} \\ u(x,y,z) &= \sum_{k=0}^{7} N_{k}(x,y,z)u_{k} \\ u, y, z, z &= 0 \end{split}$$





Shape Function 3D in Hexahedron: Trilinear Lagrangian Interpolation



System Matrix and Vector of Stationary Problems

Transform of integral to system of linear equations

$$I = \int_{G} f(u(\vec{x})) dV \implies I = \vec{u}^{T}S \vec{u} + \vec{b}^{T}\vec{u} + C$$

- f: Energy density function
- u: Field function
- x: Position vector
- \vec{u} : Field values/derivatives at nodes
- S: System matrix
- \vec{b} : System vector
- c: Constant

Stationarity:
$$\bigvee_{k} \frac{\partial I}{\partial u_{k}} = 0 \implies S \vec{u} + \vec{b} = 0$$

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Element Matrix and Vector of Stationary Problems

Element-wise transform of integral to system of linear equations

$$I_e = \int_E f(u(\vec{x})) dV \implies I_e = \vec{u}_e^T S_e \vec{u}_e + \vec{b}_e^T \vec{u}_e + C$$

- f: Energy density function
- u: Field function
- \vec{x} : Position vector
- \vec{u}_{e} : Field values/derivatives at nodes
- S_e: System matrix
- b_e: System vector
- c: Constant



Transform of Element Function with Shape Functions

$$I_{e} = \int_{E} f(u(\vec{x})) dV \xrightarrow{=}_{k=0}^{K-1} u_{k} N_{k}(\vec{x}) = \int_{E} \sum_{k=0}^{K-1} f(u_{k} N_{k}(\vec{x})) dV$$

 U_k : Field variable at node k

 N_k : Shape function

Direct Transform of Element Function

Element Vector for Bilinear Lagrangian Quad: Example

$$I = \iint_{T_{1}} u(x,y) \, dx \, dy = \begin{pmatrix} u_{0} \\ \vdots \\ u_{3} \end{pmatrix}^{T} \begin{vmatrix} x_{0} - x_{2} & x_{1} - x_{2} \\ y_{0} - y_{2} & y_{1} - y_{2} \end{vmatrix} \begin{vmatrix} 1 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{vmatrix} dx \, dy$$
$$\begin{pmatrix} \frac{\partial I}{\partial u_{0}} \\ \frac{\partial I}{\partial u_{2}} \\ \frac{\partial I}{\partial u_{3}} \end{pmatrix} = \begin{vmatrix} x_{0} - x_{2} & x_{1} - x_{2} \\ y_{0} - y_{2} & y_{1} - y_{2} \end{vmatrix} \begin{vmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{vmatrix} = \vec{D}_{e}$$

Element Matrices From Grundmatrizen

Integrals:

$$\int_{0}^{1} u^{2}(x) dx, \quad \int_{0}^{1} u'(x)^{2} dx, \quad \int_{0}^{1} u''(x)^{2} dx, \quad \int_{0}^{1} u(x) dx$$

- I: Length
- u: Field function

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Transform to unit interval [0,1] by
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$$\mathbf{X} = \mathbf{I} \boldsymbol{\xi}$$

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gives Grundmatrizen with geometry factor

$$u^{2}(\xi)d\xi, \frac{1}{1}\int_{0}^{1}u'(\xi)^{2}d\xi, \frac{1}{1^{2}}\int_{0}^{1}u''(\xi)^{2}d\xi, \int_{0}^{1}u(\xi)d\xi$$

Group Work

The finite element method allows to solve field problems based on a discretization of the spatial domain and interpolation of field values.

How will

shape functions

• element types influence the accuracy of a solution?



Numerical Integration of Element Functions

Calculation of element matrices and vectors can be complicated!

Instead: Numerical integration, e.g. with Gaussian quadrature

$$\int_{V} f(\vec{x}) d\vec{x} = \sum_{i=0}^{l-1} W_i f(x_i) + E$$

- W_i: Integration weights
- E: Approximation error
- \vec{x} : Position
- x_i: Integration points
- u_k: Node points





Gaussian Quadrature: 1D Example

Approximation of integrals i with cubic function f

$$f(x) = a + bx + cx^{2} + dx^{3}$$

$$I = \int_{0}^{1} f(x) dx = a \int_{0}^{1} dx + b \int_{0}^{1} x dx + c \int_{0}^{1} x^{2} dx + d \int_{0}^{1} x^{3} dx$$

$$\mathbf{I} = \mathbf{W}_{0} \mathbf{f} (\mathbf{x}_{0}) + \mathbf{W}_{1} \mathbf{f} (\mathbf{x}_{1})$$

Calculation of weights and points by selecting appropriate parameters a, b, c, and d.



Gaussian Quadrature: Parameters

Gaussian Quadrature: Examples

$$f(x) = a + b x + c x^{2} + dx^{3} + e x^{4} + f x^{5}$$

$$\Rightarrow W_{0} = W_{2} = \frac{5}{18}, \quad W_{1} = \frac{4}{9}$$

$$x_{0/2} = \frac{1}{2} \pm \frac{1}{2} \sqrt{\frac{3}{5}}, \quad x_{1} = \frac{1}{2}$$

$$f(x, y) = a + b x + c y + dxy$$

$$\Rightarrow W_{0} = W_{1} = W_{2} = W_{3} = \frac{1}{4}$$

$$x_{0/1} = y_{0/1} = \frac{1}{2} \pm \frac{1}{2\sqrt{3}}$$

$$Computational Modeling of the Cardiovascular System - Page 29$$

Order of Gaussian Quadrature and Degree of Approximation

Dimension	Domain	Points	Approximation
1	Curve	1	1st order polynomial
1	Curve	2	3rd order polynomial
1	Curve	3	5th order polynomial
1	Curve	n	2n-1. order polynomial
2	Quad	1 x 1	
2	Quad	2 x 2	
2	Quad	n x n	
3	Hexahedron	1 x 1 x 1	
3	Hexahedron	2 x 2 x 2	
3	Hexahedron	n x n x n	



Evaluation of Integration Methods

Direct method for integration

- only for element functions of low complexity
- mathematically demanding
- efficiency depends on complexity of element function

Grundmatrizen method

- only for element functions and types in library
- simple implementation
- efficient

Integration with Gaussian quadrature

- many element functions and types
- mathematically "trivial"
- efficient





Static Linear Elasticity Problems: Finite Element Method



Static Linear Elasticity Problems

$$\begin{aligned} \mathbf{u} &= \left(\mathbf{u}_{x} \quad \mathbf{u}_{y} \quad \mathbf{u}_{z}\right)^{\mathsf{T}} \\ \hat{\mathbf{\varepsilon}} &= \left(\mathbf{\varepsilon}_{x} \quad \mathbf{\varepsilon}_{y} \quad \mathbf{\varepsilon}_{z} \quad \mathbf{\varepsilon}_{xy} \quad \mathbf{\varepsilon}_{yz} \quad \mathbf{\varepsilon}_{xz}\right)^{\mathsf{T}} \\ &= \left(\frac{\partial \mathbf{u}_{x}}{\partial \mathbf{x}} \quad \frac{\partial \mathbf{u}_{y}}{\partial \mathbf{y}} \quad \frac{\partial \mathbf{u}_{z}}{\partial \mathbf{z}} \quad \frac{\partial \mathbf{u}_{x}}{\partial \mathbf{y}} + \frac{\partial \mathbf{u}_{y}}{\partial \mathbf{x}} \quad \frac{\partial \mathbf{u}_{y}}{\partial \mathbf{z}} + \frac{\partial \mathbf{u}_{z}}{\partial \mathbf{y}} \quad \frac{\partial \mathbf{u}_{x}}{\partial \mathbf{z}} + \frac{\partial \mathbf{u}_{z}}{\partial \mathbf{x}}\right)^{\mathsf{T}} \\ &= \left(\frac{1}{\mathsf{E}}\left(\sigma_{x} - \mathbf{v}\sigma_{y} - \mathbf{v}\sigma_{y}\right) \quad \cdots \cdot \quad \frac{2(1+\mathbf{v})}{\mathsf{E}}\sigma_{xy} \quad \cdots \cdots \cdot\right)^{\mathsf{T}} \\ &= \mathsf{C}^{-1}\hat{\sigma} \\ \hat{\sigma} &= \left(\sigma_{x} \quad \sigma_{y} \quad \sigma_{z} \quad \sigma_{xy} \quad \sigma_{yz} \quad \sigma_{xz}\right)^{\mathsf{T}} \\ &\mathsf{C}: \text{ Material matrix} \\ &\mathsf{E}: \text{ Young's modulus} \\ &\mathsf{v}: \text{ Poisson's ratio} \end{aligned}$$

Static Linear Elasticity Problems: Material Matrix

$$\hat{\varepsilon} = \mathbf{C}^{-1} \hat{\sigma} \xrightarrow{\text{Inversion}} \hat{\sigma} = \mathbf{C} \hat{\varepsilon}$$

$$\mathbf{C} = \frac{\mathbf{E}}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(1-2\nu) & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(1-2\nu) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1-2\nu) \end{pmatrix}$$

$$\underbrace{\text{Figure}}$$

$$\text{Computational Modeling of the Cardiovascular System - Page 35}$$

Finite Element Formulation with Shape Functions I





Lagrangian Incremental Formulation



Principal of Virtual Displacements

"The equilibrium of the body requires that any small, virtual displacement leads to identical internal and external work"



 σ : Cauchy stress tensor

 $\delta \epsilon$: Variation of infinitesimal strain tensor

 δ u: Virtual displacement

p,q: Volume and surface force vector, resp.

Bathe: Finite Element Procedures, Page 156



Incremental Lagrangian Formulation

$$\begin{split} & \iint_{t \neq t_{v}} t^{t + At} \sigma_{ij} \delta_{t + At} \epsilon_{ij} d^{t + At} V = \iint_{t \neq t_{v}} t^{t + At} p_{i} \delta u_{i} d^{t + At} V + \iint_{t \neq t_{v}} t^{t + At} q_{i} \delta u_{i} d^{t + At} S = t^{t + At} R \\ & \sigma: \quad \text{Cauchy stress tensor} \\ & \delta \varepsilon: \quad \text{Variation of infinitesimal strain tensor} \\ & \delta \varepsilon: \quad \text{Variation of infinitesimal strain tensor} \\ & \delta u: \quad \text{Virtual displacement} \\ & p, q: \quad \text{Volume and surface force vector, resp.} \\ & \text{R}: \quad \text{Load vector} \\ & \iint_{V_{v}} t^{t + At} S_{ij} \delta t^{t + At} E_{ij} d^{0} V = t^{t + At} R \\ & \text{S: } 2. \text{ Piola-Kirchhoff stress tensor} \\ & \delta \text{E} \quad \text{Variation of Lagrangian tensor} \\ & \text{Bathe: Finite Element Procedures, page 522} \\ & \text{Computational Modeling of the Cardiovascular System - Page 40} \end{split}$$

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Incremental Lagrangian Formulation: Given / Wanted

$$\iiint_{0} \bigcup_{i=1}^{t+\Delta t} S_{ij} \delta \overset{t+\Delta t}{}_{0} E_{ij} d^{0} V = \iiint_{0} \bigcup_{i=1}^{t+\Delta t} p_{i} \delta u_{i} d^{0} V + \iint_{0} \bigcup_{i=1}^{t+\Delta t} q_{i} \delta u_{i} d^{0} S$$

- S: 2. Piola-Kirchhoff stress tensor
- δE : Variation of Lagrangian strain tensor
- δ u: Variation of displacement
- u: Displacement
- p,q: Volume and surface force vector, resp.





Linearization of Internal Work

1

$${}^{t+\Delta t}_{0} \mathbf{S}_{ij} \delta^{t+\Delta t}_{0} \mathbf{E}_{ij} = {}^{t}_{0} \mathbf{S}_{ij} \delta^{t}_{0} \mathbf{E}_{ij} + \frac{\partial}{\partial^{t} \mathbf{u}_{k}} \Big({}^{t}_{0} \mathbf{S}_{ij} \delta^{t}_{0} \mathbf{E}_{ij} \Big) d\mathbf{u}_{k}$$

u: Displacement/node variable

Chain rule:

$$\frac{\partial}{\partial t} \left({}_{0}^{t} S_{ij} \delta_{0}^{t} E_{ij} \right) du_{k} = \frac{\partial}{\partial t} {}_{0}^{t} S_{ij} \delta_{0}^{t} E_{ij} du_{k} + {}_{0}^{t} S_{ij} \frac{\partial \left(\delta_{0}^{t} E_{ij} \right)}{\partial t} du_{k} du_{k}$$

$$= \dots$$

$$= {}_{0} C_{ijrs} \frac{\partial}{\partial t} {}_{u_{k}} \frac{\partial}{\partial t} {}_{u_{k}} \frac{\partial}{\partial t} {}_{u_{l}} \delta u_{l} du_{k} + {}_{0}^{t} S_{ij} \frac{\partial}{\partial t} {}_{u_{k}} \frac{\partial}{\partial t} {}_{u_{l}} \delta u_{l} du_{k}$$

with incremental stiffness matrix:

$$_{0}\mathbf{C}_{ijrs} = \frac{\partial_{0}^{t}\mathbf{S}_{ij}}{\partial_{0}^{t}\mathbf{E}_{rs}}$$

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Bathe: Finite Element Procedures, page 539

Element Stiffness Matrix

$$\begin{split} & \iint_{V_{V}}^{t+At} S_{ij} \delta^{t+At} E_{ij} \ d^{0} V = {}^{t+At} R \\ & \iint_{V_{V}} {}^{t} S_{ij} \delta_{0}^{t} E_{ij} + \frac{\partial}{\partial^{t} u_{k}} \left({}^{t} S_{ij} \delta_{0}^{t} E_{ij} \right) du_{k} \ d^{0} V = {}^{t+At} R \\ & \iint_{V_{V}} {}^{t} S_{ij} \delta_{0}^{t} E_{ij} + {}^{t} S_{ij} \frac{\partial}{\partial^{t} u_{k}} \frac{\partial}{\partial^{t} u_{i}} \delta_{i} u_{i} du_{k} + {}^{t} S_{ij} \frac{\partial}{\partial^{t} u_{k} \partial^{t} u_{i}} \delta_{i} u_{i} du_{k} d^{0} V = {}^{t+At} R \\ & \iint_{V_{V}} {}^{t} S_{ij} \delta_{0}^{t} E_{ij} + {}^{t} S_{ij} \frac{\partial}{\partial^{t} u_{k}} \frac{\partial}{\partial^{t} u_{i}} \delta_{i} u_{i} du_{k} + {}^{t} S_{ij} \frac{\partial}{\partial^{t} u_{k} \partial^{t} u_{i}} \delta_{i} u_{i} du_{k} d^{0} V = {}^{t+At} R \\ & (\iint_{V_{V}} {}^{t} S_{ij} \frac{\partial}{\partial^{t} u_{k}} \frac{\partial}{\partial^{t} u_{i}} + {}^{t} S_{ij} \frac{\partial^{2} S_{i} E_{ij}}{\partial^{t} u_{k} \partial^{t} u_{i}} d^{0} V \right) du_{k} \delta u_{i} = {}^{t+At} R - \left(\iint_{V_{V}} {}^{t} S_{ij} \frac{\partial}{\partial^{t} u_{i}} d^{0} V \right) \delta u_{i} \\ & (K_{L} + K_{NL}) \quad \Delta U = F \\ \\ & K_{L} : \text{ Linear stiffness matrix } \\ \Delta U: \text{ Incremental displacements } K_{NL} : \text{ Nonlinear stiffness matrix } F: \text{ Force vector } \\ \end{cases}$$

Transfer Operator, Strain and Stress Vectors

Lagrangian strain vector calculated from displacements:

$$\hat{\mathbf{E}} = \begin{pmatrix} \mathbf{E}_{x} & \mathbf{E}_{y} & \mathbf{E}_{z} & \mathbf{E}_{xy} & \mathbf{E}_{yz} & \mathbf{E}_{xz} \end{pmatrix}^{\mathsf{T}} = \mathbf{B} \begin{pmatrix} \mathbf{u}_{x} & \mathbf{u}_{y} & \mathbf{u}_{z} \end{pmatrix}^{\mathsf{T}}$$

B = B(u): nonlinear transfer operator decomposition in linear and nonlinear operator

2. Piola-Kirchhoff stress vector from derivative of strain energy density function:

$$\hat{\mathbf{S}} = \begin{pmatrix} \mathbf{S}_{x} & \mathbf{S}_{y} & \mathbf{S}_{z} & \mathbf{S}_{xy} & \mathbf{S}_{yz} & \mathbf{S}_{xz} \end{pmatrix}^{\mathsf{T}} = \frac{\partial \mathbf{W}}{\partial \hat{\mathbf{E}}}$$

Incremental material matrix from derivative of stress tensor:

$$\hat{C} = \frac{\partial \hat{S}}{\partial \hat{E}}$$

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Example: Passive Cardiac Mechanics

Left ventricle model

- approximated with 3752 cubic elements
- trilinear shape functions
- 3 versions of fiber orientation
- hyperelastic material (Guccione et al. 1991)
- incompressible

Boundary condition

- tension 1 kPa in fiber direction
- homogeneous





Example: Versions of Fiber Orientation



Example: -45°, -45°, -45°



Example: -45°, 0°, 45°



Example: 0°, 0°, 0°



Group Work

Describe modules of a simulation software for cardiac electro-mechanics!

Which modules should be highly optimized?

