Numerical Simulations of 3D Fluid-Structure interacion

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Computational Methods with Applications
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Thermo-mechanical Institute CAS

Outline

Motivation

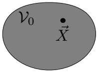
Biological problem: Blood flow in vessels

- Solid and Fluid parts (2 domains)
- Interaction of materials
- Various kind of materials
  (Easy to change Constitutive relations)
- Full 3D setting

Usual assumptions

- Incompressibility, Isotermicity

The ALE



- $\mathcal{V}_0$ Material volume
  initial configuration
- $\mathcal{V}_{(t)}$ Material volume
  actual state
- $x^i = \vec{x}(X^i, t)$ deform.
- $V_{(t)}$ Control volume
  $y^i = \vec{y}(X^i, t)$ deform.

Position and velocity in coordinate system y^i

$$\vec{y}(\vec{X}, t) = \vec{x}(\vec{X}, t) - \vec{w}(\vec{X}, t)$$

$$\left.\frac{\partial \vec{y}}{\partial t}\right|_X = \vec{v}_{V_{(t)}} = \vec{v} - \left.\frac{\partial \vec{w}}{\partial t}\right|_X$$

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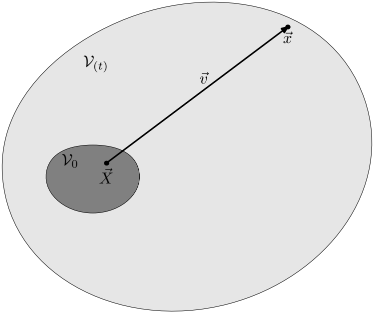

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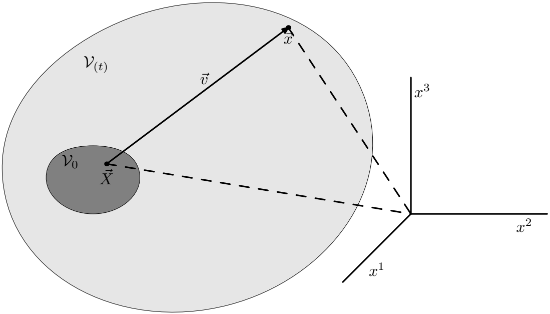

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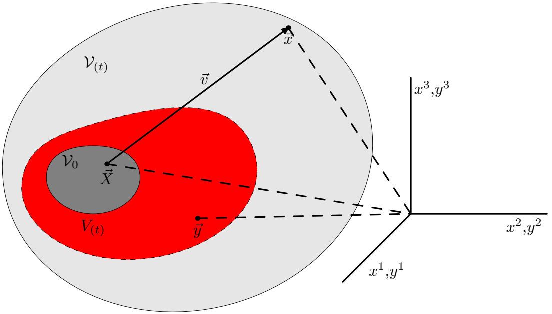

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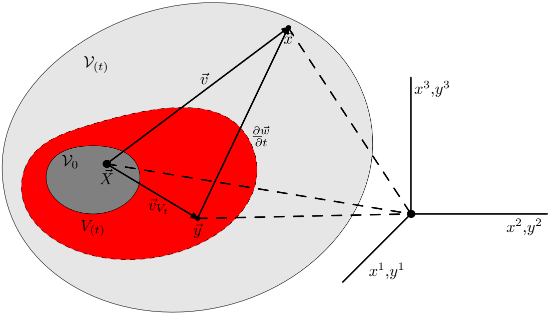

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Balance laws in the ALE

Extensive quantity

$$\Phi(t) = \int_{\mathcal{V}_0} \Phi(\vec{X}, t) d\mathcal{V} = \int_{\mathcal{V}_{(t)}} \varphi(\vec{x}, t) dv = \int_{V_{(t)}} \varphi(\vec{y}, t) dv_y$$

General balance

$$\frac{d\Phi}{dt} = \dot{\Phi} = \mathcal{L}(\Phi) + \mathcal{P}(\Phi)$$

- $\mathcal{L}$ Total flux
- $\mathcal{P}$ Total production

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Balance laws in the ALE

The balance law in the integral form

$$\int_{\mathcal{V}_0} \frac{\partial}{\partial t}\Phi j_y d\mathcal{V} + \int_{\partial\mathcal{V}_0} \Phi(v^k - v^k_{V_t}) j_y \frac{\partial X^K}{\partial y^k} dA_K = \int_{\partial\mathcal{V}_0} I^k(\Phi) j_y \frac{\partial X^K}{\partial y^k} dA_K + \int_{\mathcal{V}_0} \sigma(\Phi) j_y d\mathcal{V}.$$

Local balance in the ALE

$$\frac{\partial}{\partial t}(j_y\phi) + \frac{\partial}{\partial X^K}\left\{\left[\phi(v^k - v^k_{V_t}) - I^k(\Phi)\right] j_y \frac{\partial X^K}{\partial y^k}\right\} - j_y\sigma(\Phi) = 0$$

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The total mass: $m(t) = \int_{\mathcal{V}_0} \varrho(\vec{X}, t) d\mathcal{V} = \int_{\mathcal{V}_{(t)}} \varrho(\vec{x}, t) dv$

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Question

Why is the ALE a generalization of the Lagrangian, Eulerian view?

Let $V_{(t)}$ be static

$\vec{y} = \vec{X}, j_y = 1$, remains:

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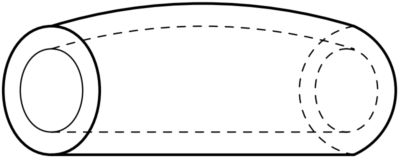

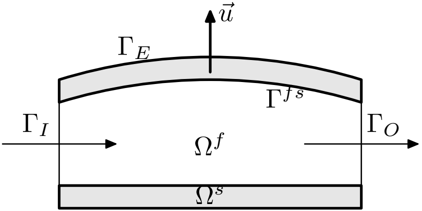

The main idea

- Ω^s solid, Ω^f fluid
- Main unknown functions :
  - displacement $\vec{u}^f$, $\vec{u}^s$
  - velocity $\vec{v}^f$, $\vec{v}^s$
- Deformation
  $\vec{u}^s(\vec{X},t) = \vec{x}^s(\vec{X},t) - \vec{X}$
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BC on $\Gamma^{fs} \times [0,T]$

- no slip condition $\vec{v}^f = \vec{v}^s$
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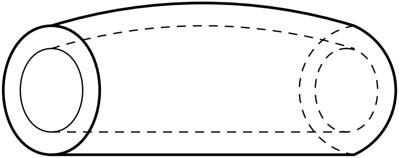

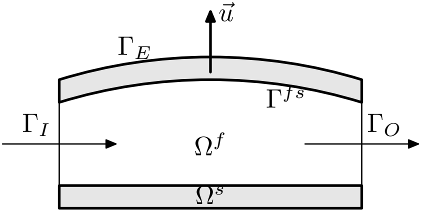

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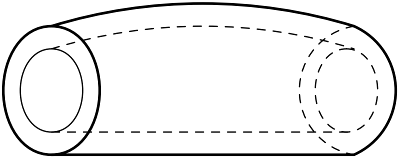

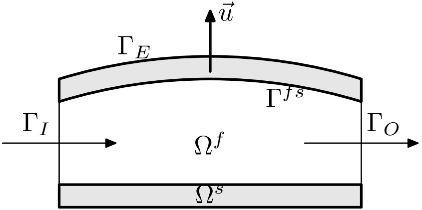

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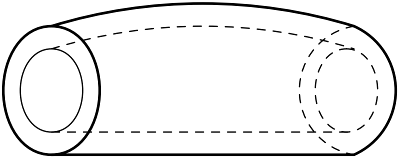

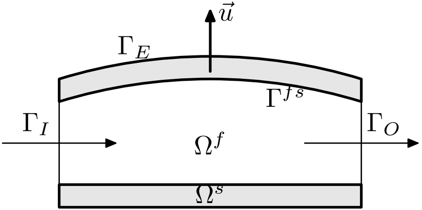

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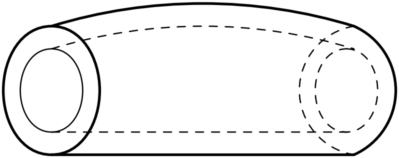

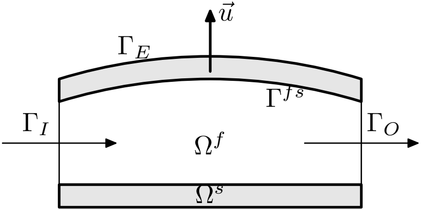

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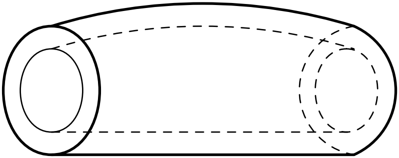

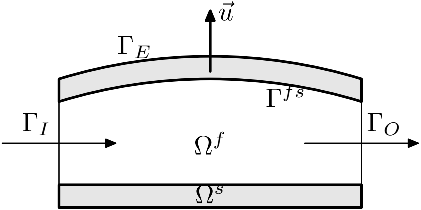

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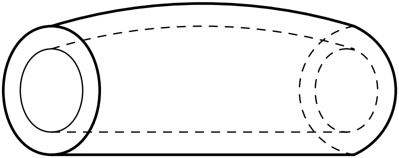

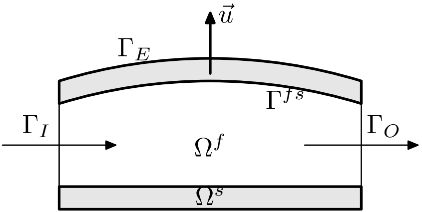

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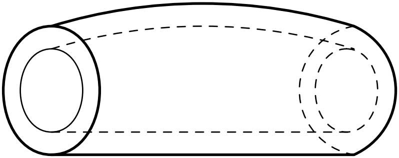

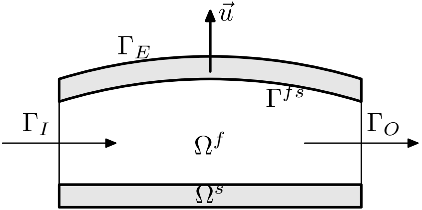

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We can define unknowns:

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When we denote $\Omega = \Omega^s \cup \Omega^f$ our new fields are

$$\vec{u} : \Omega \times [0, T] \to \mathbb{R}^3$$

$$\vec{v} : \Omega \times [0, T] \to \mathbb{R}^3.$$

The deformation gradient and its determinant

$$\mathbf{F} = \mathbf{I} + \nabla \vec{u}$$

$$j = \det \mathbf{F}$$

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Model equations

How to build model equations? (i.e. mass)

Solid: $$\frac{d}{dt}(\rho^s j) = 0$$

Fluid: $$\frac{\partial}{\partial t}\left(\rho^f j\right) + \frac{\partial}{\partial X^K}\left\{\left[\rho^f\left(v_k - \frac{\partial u^k}{\partial t}\right)\right] j \frac{\partial X^K}{\partial x^k}\right\} = 0$$

Grid deformation - equation for $\vec{u}$

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Grid deformation - equation for $\vec{u}$

Model equations

How to build model equations? (i.e. mass)

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Model equations

Momentum equation

$$\frac{\partial v^i}{\partial t} = \frac{1}{j\varrho^s}\frac{\partial \mathbf{P}^{Ki}}{\partial X^K}$$

$$\frac{\partial v^i}{\partial t} = \frac{\partial}{\partial X^K}\left\{\left[v^i(v^k - \frac{\partial u^k}{\partial t}) - \tau^{ki}\right]\frac{\partial X^K}{\partial x^k}\right\}$$

Constitutive relations

Solid

$$\mathbf{P}^s = -jp^s\mathbf{F}^{-T} + j\varrho^s \frac{\partial \Psi}{\partial \mathbf{F}}$$

$$\text{(Neo-Hook)} \quad \hat{\Psi} = c_1 (I_C - 3)$$

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Classical formulation

Find $\vec{u}, \vec{v}, p^s, p^f$ to satisfy

$$\frac{\partial \vec{u}}{\partial t} = \begin{cases} \vec{v} & \text{in } \Omega^s \\ \triangle \vec{u} & \text{in } \Omega^f \end{cases}$$

$$0 = \begin{cases} \frac{d}{dt}(\rho^s j) & \text{in } \Omega^s \\ \frac{\partial}{\partial t}(\rho^f j) + \operatorname{Div}\left(\rho^f j(\vec{v} - \frac{\partial \vec{u}}{\partial t})\mathbf{F}^{-T}\right) & \text{in } \Omega^f \end{cases}$$

$$\frac{\partial \vec{v}}{\partial t} = \begin{cases} \frac{1}{j\rho^s} \operatorname{Div} \mathbf{P}^{s\,T} & \text{in } \Omega^s \\ -(\nabla \vec{v})(\vec{v} - \frac{\partial \vec{u}}{\partial t})\mathbf{F}^{-T} + \frac{1}{j\rho^f} \operatorname{Div}(j\mathbf{t}^f \mathbf{F}^{-T}) & \text{in } \Omega^f \end{cases}$$

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Classical formulation

with initial conditions

$$\vec{u}(0) = \vec{0} \qquad \text{in } \Omega,$$
$$\vec{v}(0) = \vec{v}_0 \qquad \text{in } \Omega,$$

with constitutive relations

$$\mathbf{t}^f = -p^f \mathbf{I} + \mu \left(\nabla \vec{v} + \nabla^T \vec{v} \right),$$
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and boundary conditions

$$\vec{v} = \vec{v}_I \qquad \text{on } \Gamma_I^f,$$
$$\vec{u} = \vec{0} \qquad \text{on } \Gamma_I, \Gamma_O,$$
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$$\frac{\partial \vec{v}}{\partial \vec{n}} = \vec{0} \qquad \text{on } \Gamma_O^f,$$
$$\mathbf{t}^s \vec{n} = \vec{0} \qquad \text{on } \Gamma_E$$

The Time discretization

The time interval $(0, T)$

- divide it into n subintervals $I_n = [t^n, t^{n+1}]$
- time step $k_n = t^{n+1} - t^n$.

For time interval $[t^n, t^{n+1}]$ approximate $\frac{\partial f}{\partial t}$ by central differences

$$\frac{\partial f}{\partial t} \approx \frac{f^{n+1} - f^n}{k_n}$$

We approximate time integrals by using the Newton-Cotes formulas, especially by the trapezoidal rule $(\theta = \frac{1}{2})$

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The nonlinear problem

Nonlinear problem on each time level

$$\vec{\mathcal{R}}(\vec{\mathcal{X}}) = \vec{0}$$

Newton method with Quadratic Line search

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Implementation issue

- Computation of $\nabla\vec{\mathcal{R}}(\vec{\mathcal{X}})$ by finite differences

$$\nabla\vec{\mathcal{R}}(\vec{\mathcal{X}})e_i \approx \frac{\vec{\mathcal{R}}(\vec{\mathcal{X}} + \delta e_i) - \vec{\mathcal{R}}(\vec{\mathcal{X}} - \delta e_i)}{2\delta}$$

- Solution of linear problem $\left[\nabla\mathcal{R}(\vec{\mathcal{X}}^n)\right]\vec{s}_k = \vec{\mathcal{R}}\left(\vec{\mathcal{X}}^n\right)$ by DirectSolver (UMFPACK)

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- Finite Element Method
- 3D Mesh $\mathcal{T}_h$, tetrahedrons K_i
- Element choice: Stable elements [Babuška-Brezzi]
- Our uniform formulation - the same element type for $\vec{u}$, $\vec{v}$

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What are the Stable alements? **From the NS theory**

- $P_2 P_1$
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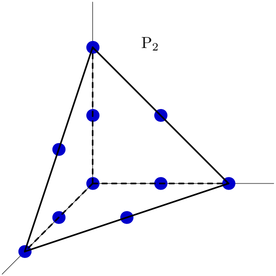

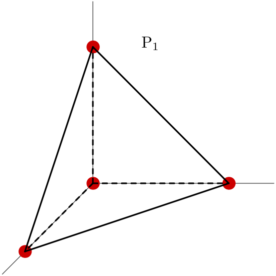

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$$R = span\{\lambda_1 \ldots \lambda_4\} \quad \lambda_i \text{ barycentric cooradinates}$$

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$$P_h = \{\underline{p}_i \in L_0^2(\Omega_h) : \underline{p}_i \lceil_{K_i} \in P_1(K_i) \quad \forall K_i \in \mathcal{T}_h\}$$
$$P_2^+ = P_2 \oplus span\{\lambda_1 \ldots \lambda_4\} \oplus span\{\lambda_i \lambda_j \lambda_k\}$$

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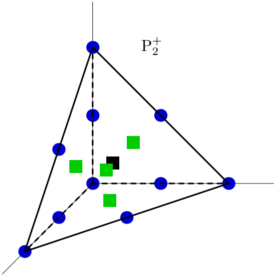

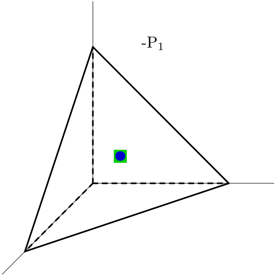

FEM Detail

Structure of $\nabla\vec{\mathcal{R}}$

- $P_2 P_1$ dofs per element $6 \times 10 + 4 = \mathbf{64}$
- $P_1^+ P_1$ (Minielement) $6 \times 5 + 4 = \mathbf{34}$
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$$\begin{pmatrix} A_{vv} & A_{vu} & B_v \\ A_{uv} & A_{uu} & B_u \\ B_v^T & B_u^T & \emptyset \end{pmatrix}$$

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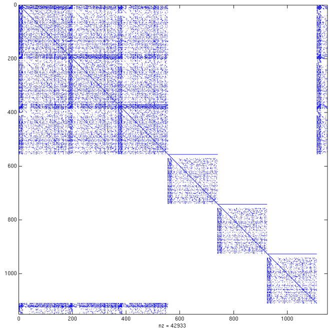
- 1158 equations



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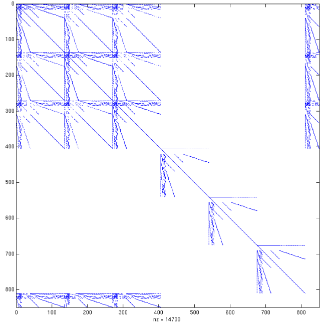

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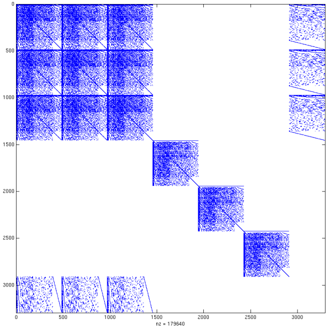

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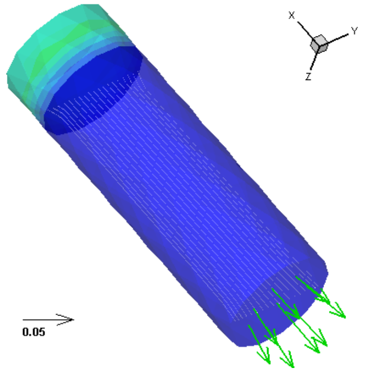

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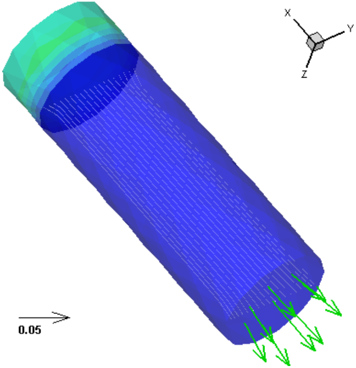

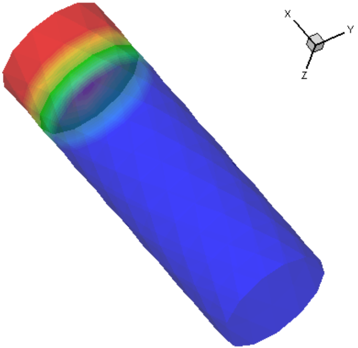

Results

To obtain numerical results we wrote our own program

Program features

- C/PETSc for possible parallel version
- Unstructured meshes (3D)
- Nonlinear-Nonstationary problems
- Any equation set
- FEM - predefined 7 element types
- Finite differences for Jacobian matrix
- up to 8^{th} order predefined Gauss. numerical quadratures
- Import modules for meshes [neutral format (Netgen)]
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Results

Lagrange deformation in solid

The deformation is in equations, no change of computational mesh. How large can be such deformation?

Pulsative flow

Pulsative flow in "artery"

- 30932 equations, 80 time iterations, 12 hours CPU time (AMD Opteron 248)

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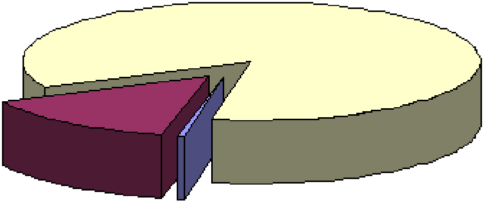
Usual Resources [39.070 equations]

CPU Time

- Computation of Residual vector $\vec{\mathcal{R}}$ 2sec
- Evaluating of $\nabla\vec{\mathcal{R}}$ 49sec
- Solution of linear problem 290sec



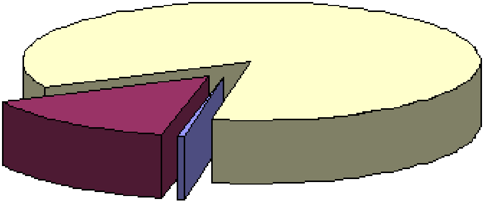
Memory

- 2.2 GB RAM

Usual Resources [39.070 equations]

CPU Time

- Computation of Residual vector $\vec{\mathcal{R}}$ 2sec
- Evaluating of $\nabla\vec{\mathcal{R}}$ 49sec
- Solution of linear problem 290sec



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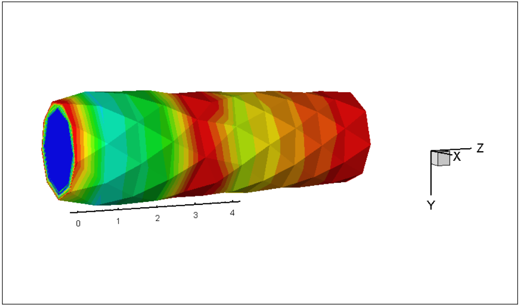
Current state

Current Work

1. Examples with real-like geometries
   - Vessel with nonuniform material property



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   - Testing our implementation, validated to serial version
   - Still not efective, the very first results

Appeal

There is a need for robust and fast parallel linear solver.

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There is a need for robust and fast parallel linear solver. Any ideas?