A feasibility study on the acceleration and upscaling of bone ingrowth simulation

An investigation into the feasibility of applying a homogenization scheme to bone ingrowth model as well other options of accelerating the bone ingrowth model developed by A. Andreykiv.

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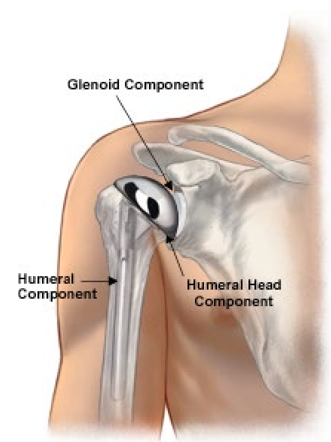
Introduction

- Uncemented Shoulder Implant

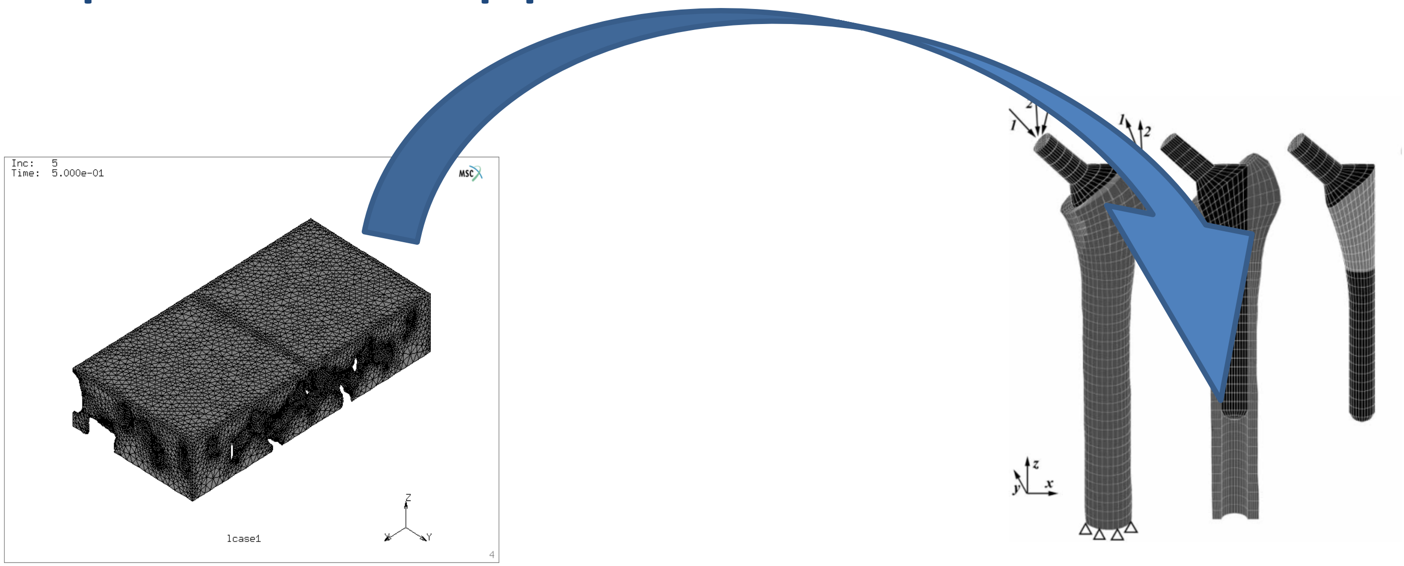
- Total Shoulder Arthroplasty
- Osteoarthritis, rheumatoid arthritis
- Porous surface in which bone can grow to ensure fixation of the implant

- Cemented implant
  - Immediate fixation
  - Tissue necrosis
  - Cement fracture



Introduction

- Finite Element Modelling of uncemented implants – 2 approaches



Andreykiv, 2006 Folgado, 2009

- How to transfer knowledge from the detailed model to the larger (macroscopic) model?

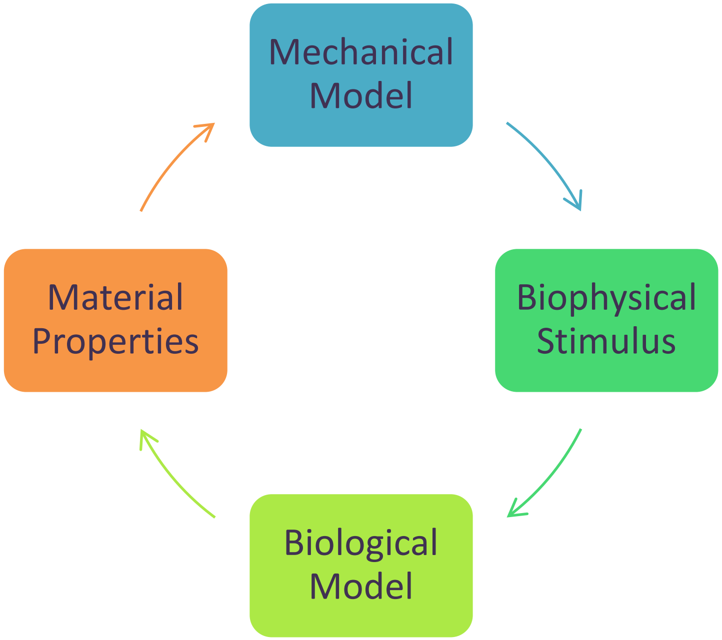
Contents

The original bone ingrowth model

The original bone ingrowth model

General Overview

- Coupled Simulation
- Prendergast tissue differentiation model for the production of bone, cartilage and fibrous tissue



The Original Bone Ingrowth Model

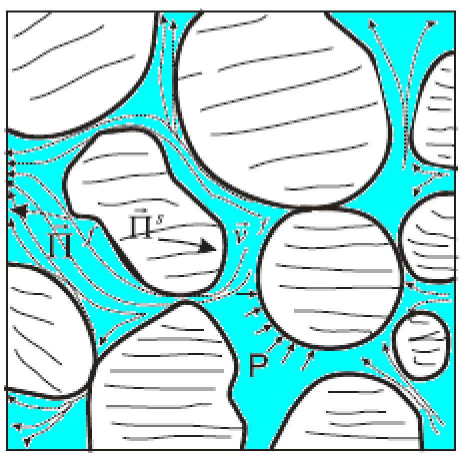
Mechanical Model

- Biological Tissue response
  - Non-linear
  - History dependent
  - Viscoelastic
- Biphasic Model
  - 80% is made up of fluid
  - Solid & Fluid component

The Original Bone Ingrowth Model

Mechanical Model

- Solid (3 displacements)
  - Neo-Hookean Hyperelastic Material model
- Fluid (pressure)
  - Mass balance



$$\dot{\vec{v}}^s \rho^s - \nabla \cdot \boldsymbol{\sigma}^s - \rho^s f^s - \Pi^s = 0$$

$$\nabla \cdot \left(\boldsymbol{\sigma}^s - p\mathbf{I}\right) = 0$$

$$\dot{\vec{v}}^f \rho^f - \nabla \cdot \boldsymbol{\sigma}^f - \rho^f f^f - \Pi^f = 0$$

$$\frac{n^f}{K^f}\frac{dp}{dt} + \nabla \cdot \vec{v}^s - \nabla \cdot \left(\frac{\kappa}{\mu}\nabla p\right) = 0$$

$$\frac{n^f}{K^f}\frac{dp}{dt} + \nabla \cdot \vec{v}^s - \nabla \cdot \left(\frac{\kappa}{\mu}\nabla p\right) = 0$$

The Original Bone Ingrowth Model

Biophysical Stimulus

- Input for the biological model
- Determines the preference of the formation of bone, cartilage of fibrous tissue
- Based on maximal shear strain and fluid velocity

$$S = \frac{\gamma}{a} + \frac{v}{b}$$

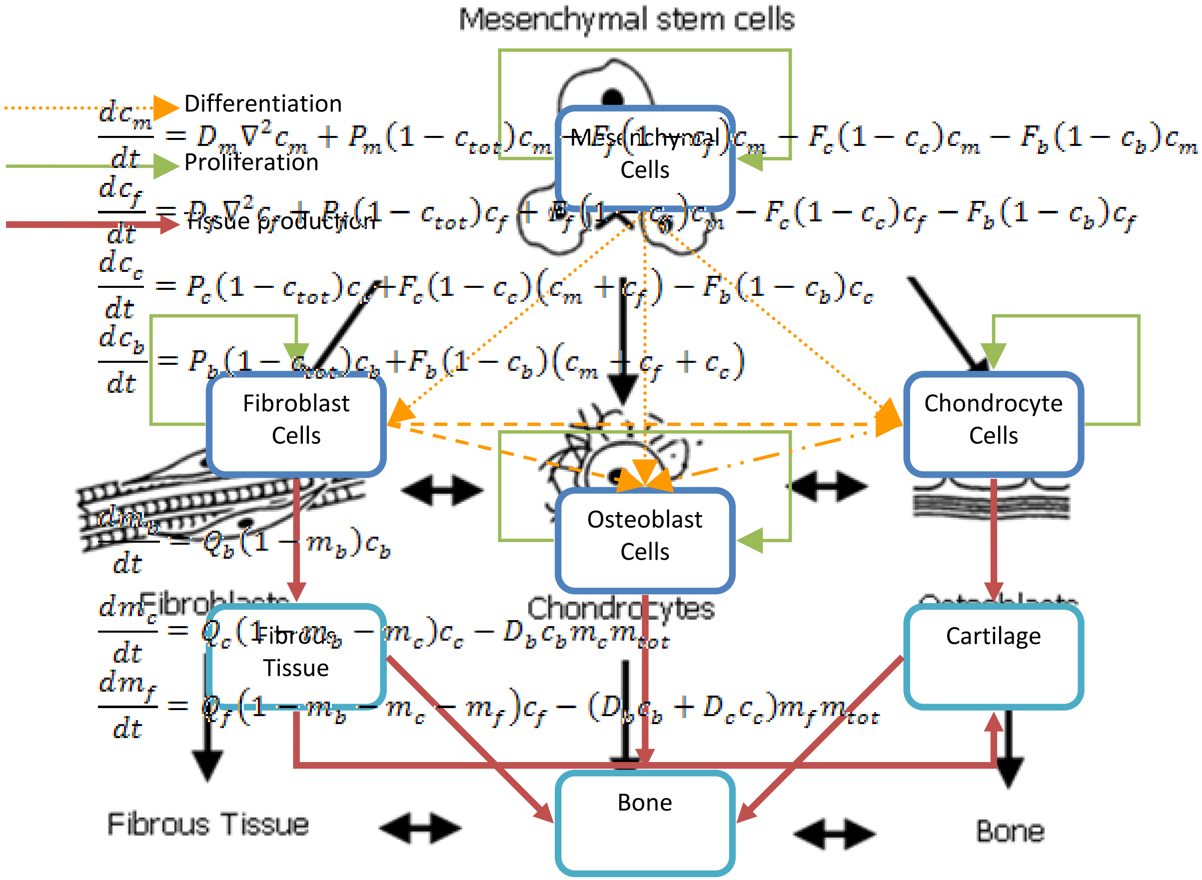
The Original Bone Ingrowth Model

Biological Model

- Diffusion
  - Mesenchymal stem cells
  - Fibroblast
- Cell Proliferation
- Cell Differentiation
- Tissue Production
- Tissue Degradation
- As a function of the biophysical stimulus

The Original Bone Ingrowth Model

Biological Model



$$\frac{dc_m}{dt} = D_m \nabla^2 c_m + P_m(1 - c_{tot})c_m - F_f(1 - c_f)c_m - F_c(1 - c_c)c_m - F_b(1 - c_b)c_m$$

$$\frac{dc_f}{dt} = D_f \nabla^2 c_f + P_f(1 - c_{tot})c_f + F_f(1 - c_f)c_m - F_c(1 - c_c)c_f - F_b(1 - c_b)c_f$$

$$\frac{dc_c}{dt} = P_c(1 - c_{tot})c_c + F_c(1 - c_c)(c_m + c_f) - F_b(1 - c_b)c_c$$

$$\frac{dc_b}{dt} = P_b(1 - c_{tot})c_b + F_b(1 - c_b)(c_m + c_f + c_c)$$

$$\frac{dm_b}{dt} = Q_b(1 - m_b)c_b$$

$$\frac{dm_c}{dt} = Q_c(1 - m_b - m_c)c_c - D_b c_b m_c m_{tot}$$

$$\frac{dm_f}{dt} = Q_f(1 - m_b - m_c - m_f)c_f - (D_b c_b + D_c c_c)m_f m_{tot}$$

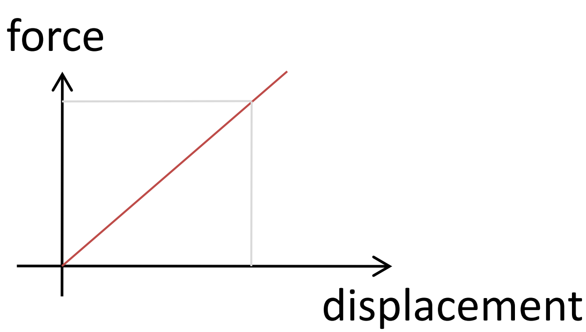
The Original Bone Ingrowth Model

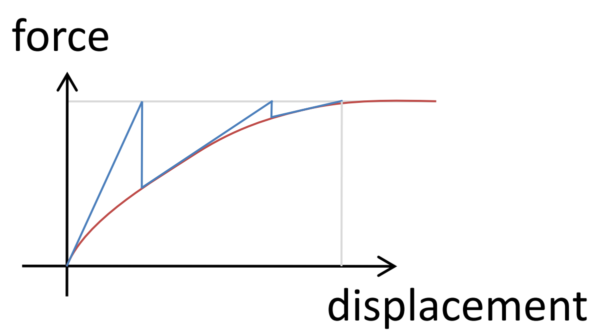
Numerical Implementation

- Implemented in subroutines of MSC Marc
- Non Linear equations requires an iterative solver

$$\begin{bmatrix} \mathbf{K}_T & -\mathbf{Q} \\ -\mathbf{Q}^T & -(\mathbf{S} + \Delta t \mathbf{H}) \end{bmatrix}_{k,n+1} \begin{bmatrix} \Delta \vec{u}^s \\ \Delta \vec{p} \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{f}^u_{n+1} \\ -\Delta t \mathbf{f}^p_{n+1} \end{bmatrix} - \begin{bmatrix} \mathbf{P}_{I_{n+1}} - \mathbf{Q}\vec{p}_{n+1} \\ -(\mathbf{S}\Delta\vec{p} + \mathbf{Q}^T \Delta \vec{u}^s + \Delta t \mathbf{H} \vec{p}_{n+1}) \end{bmatrix},$$

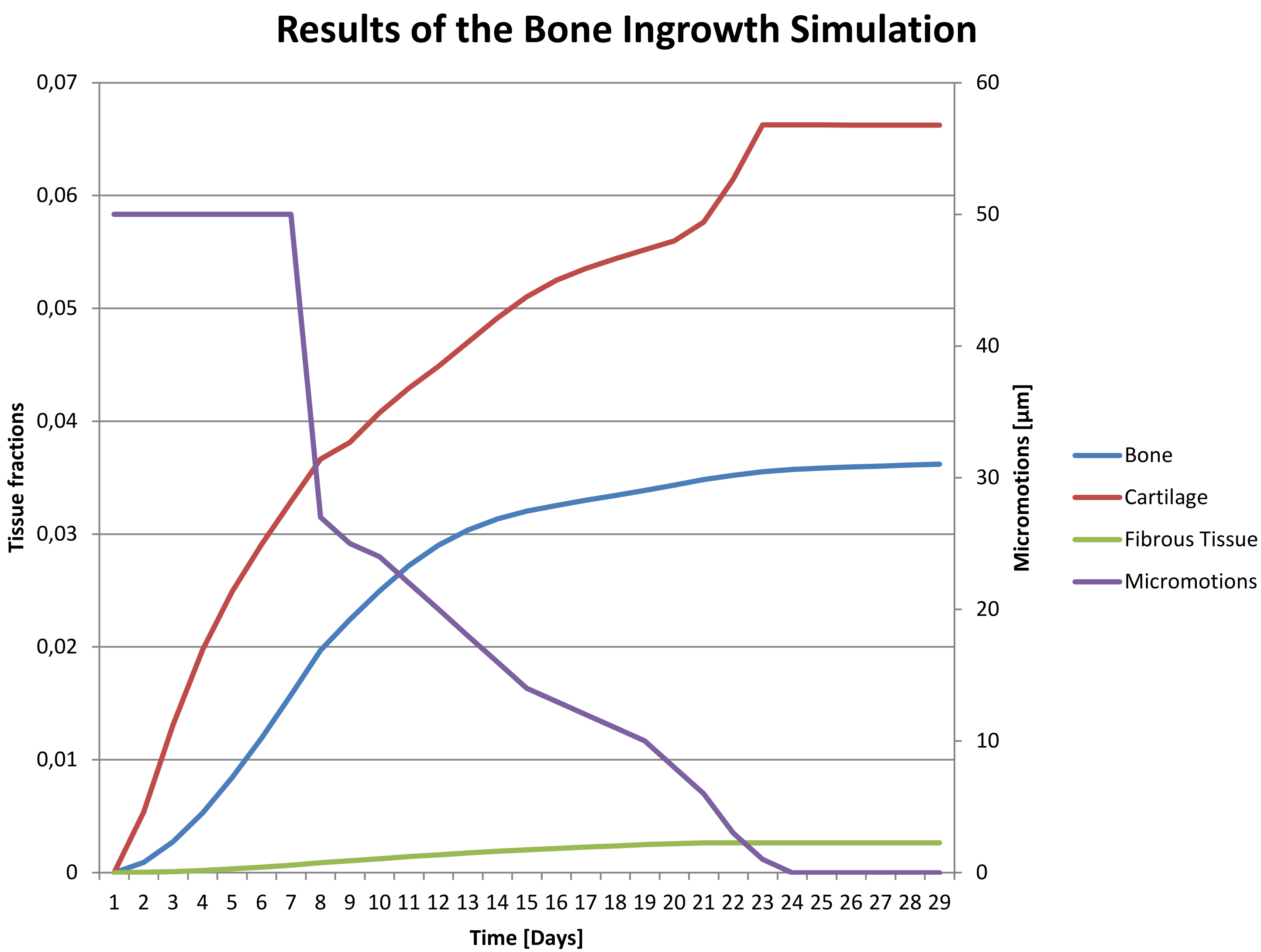
$$\begin{bmatrix} \boldsymbol{K}_{m_{stiff}} & 0 \\ 0 & \boldsymbol{K}_{f_{stiff}} \end{bmatrix} \begin{bmatrix} \Delta \vec{c}_{m_{n+1}} \\ \Delta \vec{c}_{f_{n+1}} \end{bmatrix} = \begin{bmatrix} -\vec{F}_{I_m} \\ -\vec{F}_{I_f} \end{bmatrix}$$





The Original Bone Ingrowth Model

Numerical Implementation & Results



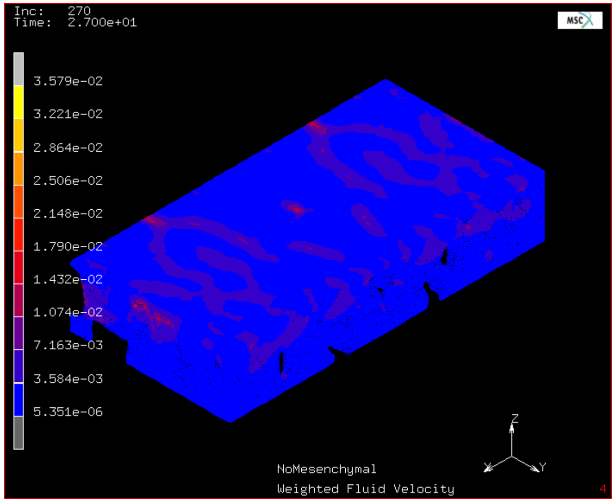
Model Optimization

Model Optimization

Possibilities for model simplification (1)

- Investigate the necessity of the biphasic model

$$S = \frac{\gamma}{a} + \frac{v}{b}$$



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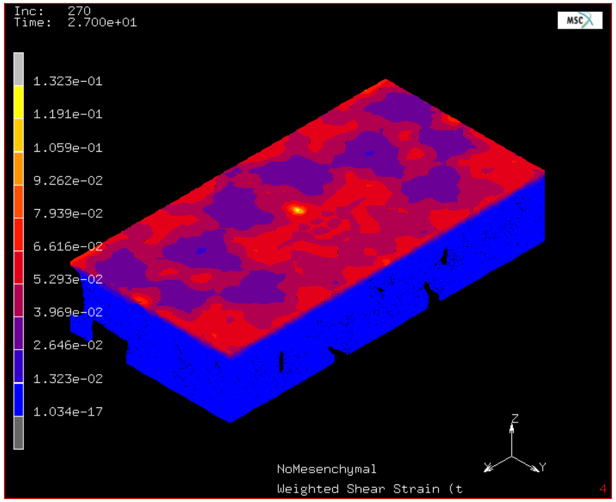


Weighted Fluid Velocity Weighted Shear Strain

Model Optimization

Possibilities for model simplification (2)

- Linearization of the biological model

$$\frac{dc_f}{dt} = D_f \nabla^2 c_f + \left(P_f(1-c_c-c_b) - F_c(1-c_c) - F_b(1-c_b)\right)c_f + F_f c_m - (F_f \ldots)c_m c_f$$

$$P \ldots c_f$$

$$\frac{dc_m}{dt} = D_m \nabla^2 c_m + \left(P_m(1-c_c-c_b) - F_f - F_c(1-c_c) + F_b(1-c_b)\right)c_m + (F_f \ldots)c_f c_m$$

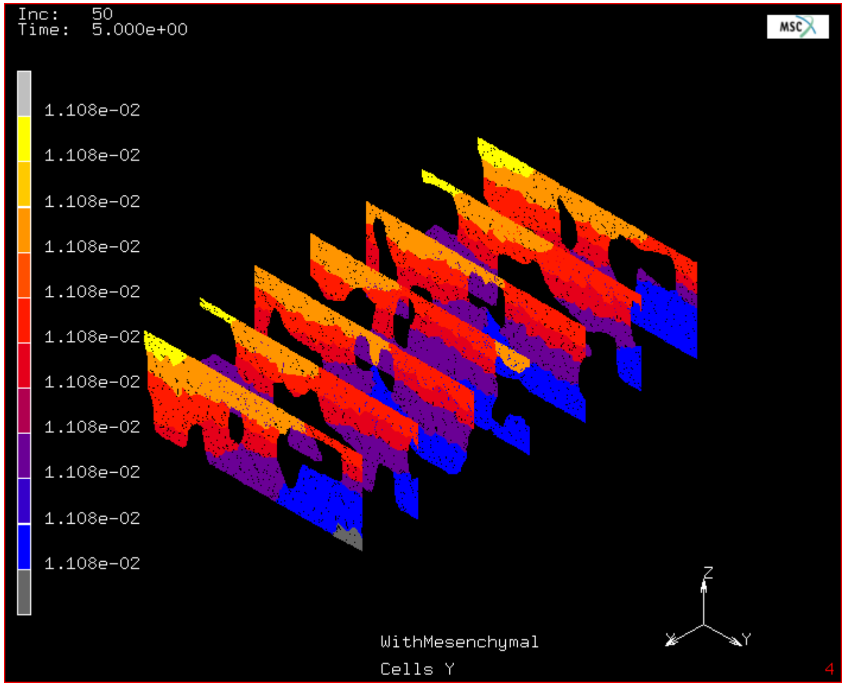
$$P \ldots_m c_m$$

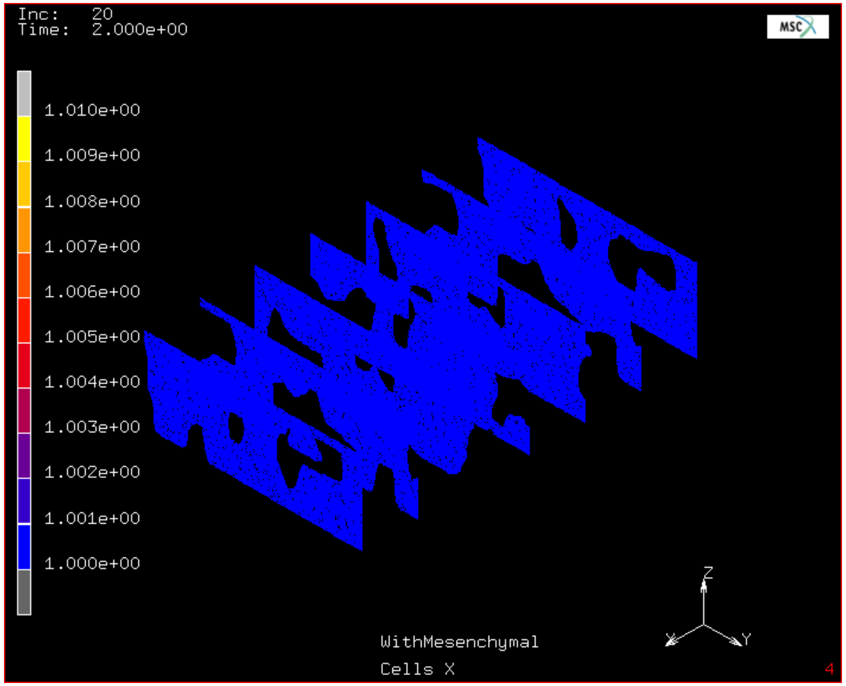
- Acceptable approximation?

Model Optimization

Possibilities for model simplification (3)

- 1-D Diffusion approximation

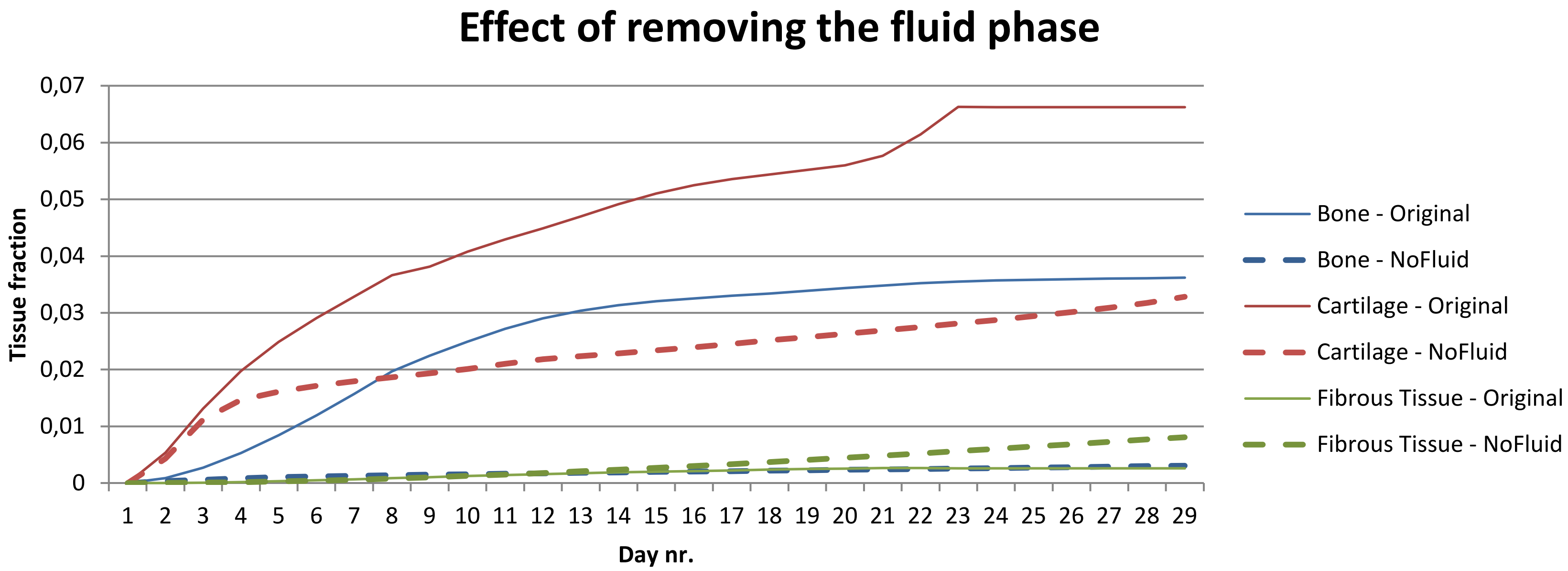




Model Optimization

Results – Removal of Fluid phase

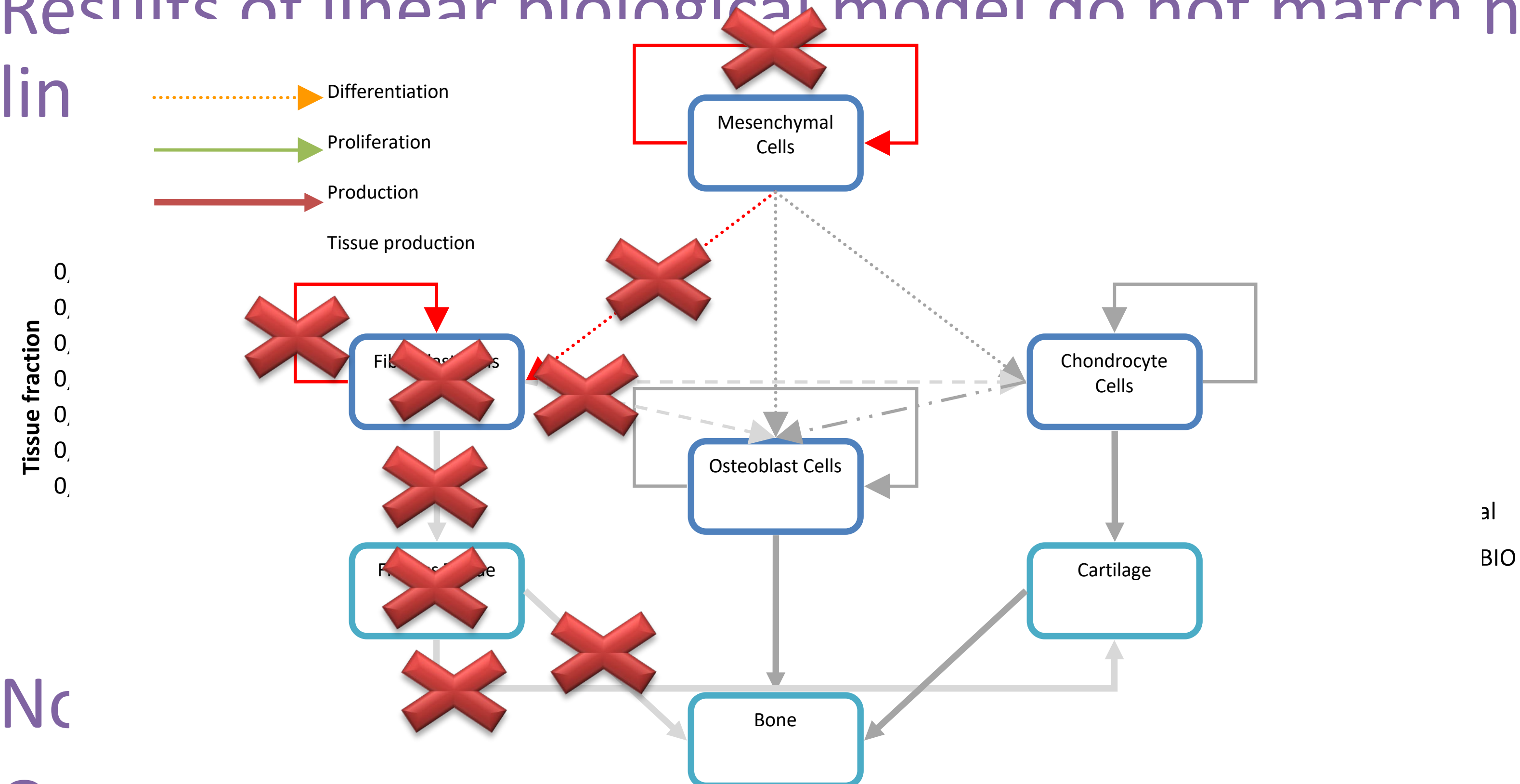
- Fluid phase is essential for correct calculations
- Increased fibrous tissue production
- Reduced bone & cartilage production



Model Optimization

Results – Linear Biological Model

- Results of linear biological model do not match non lin



- Nc
- Overestimate bone production
- Reasonable cartilage estimate

Model Optimization

Results – 1D diffusion

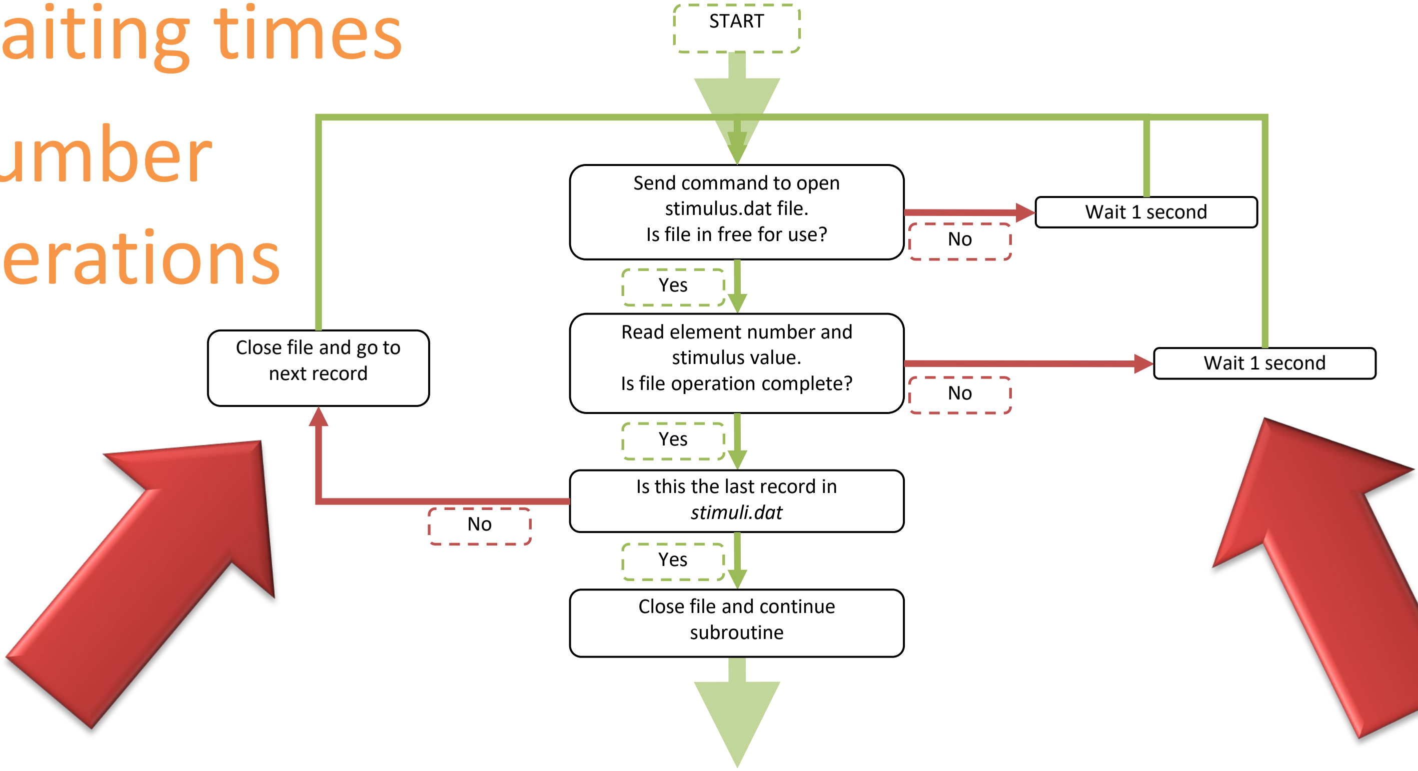
- Simulations failed
  - Non-Positive definite stiffness matrix
  - Snap back behaviour? Causing the Newton-Raphson method to fail?
  - Perhaps an arc length method can improve the results
- Potentially gained simulation time is marginal
  - A estimated decrease of 200 seconds over the complete simulations.

Code Optimizations

Code Optimizations

Potential for increasing speed

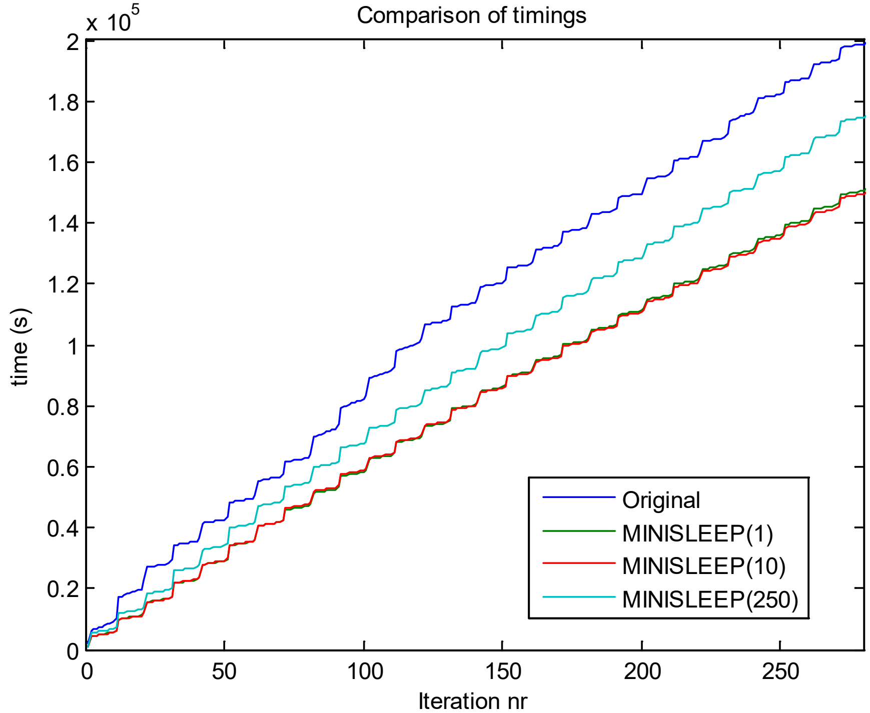
- Culprit: Disk operations
- Example: Reading the stimuli.dat file
- Reduce waiting times
- Reduce number of disk operations



Code Optimizations

Minisleep

- Reduce waiting time
- FORTRAN limits the waiting period to 1 sec
- Write the MINISLEEP



20%

Code Optimizations

Batchwrites

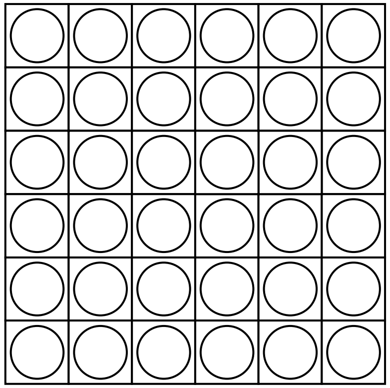
- Reduce the number of disk writes.
- Store all variables in memory and write at the end of an iteration
- Keep in mind data sharing

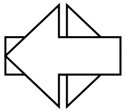
- Reduction of 65% in computation time

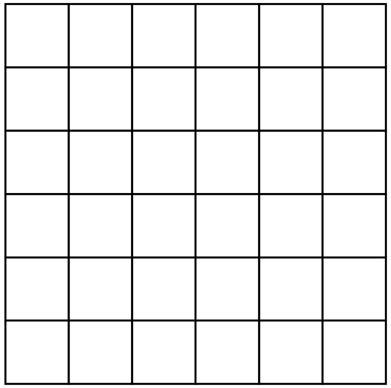
Computational Homogenization

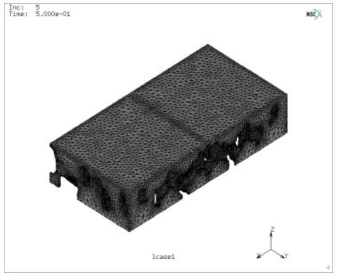
Computational Homogenization
Theory (1)

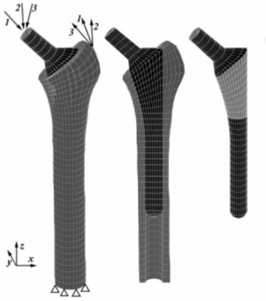
- Exploit periodicity to bridging the gap
- Microscopic level   Macroscopic level



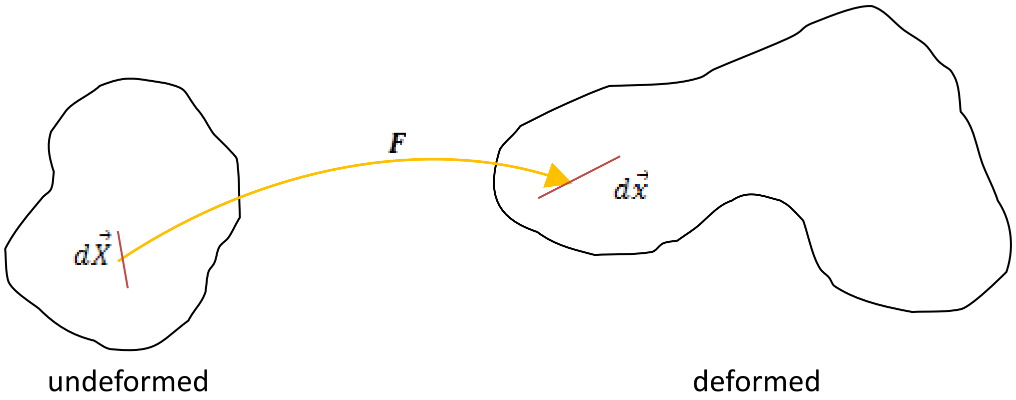








Computational Homogenization
Theory (2)



$$d\vec{X} - d\vec{x} = \Delta\vec{x} = \mathbf{F}_M \cdot \Delta\vec{X} + \vec{w}$$

- Macroscopic deformation
- Microscopic deformations / microfluctuations

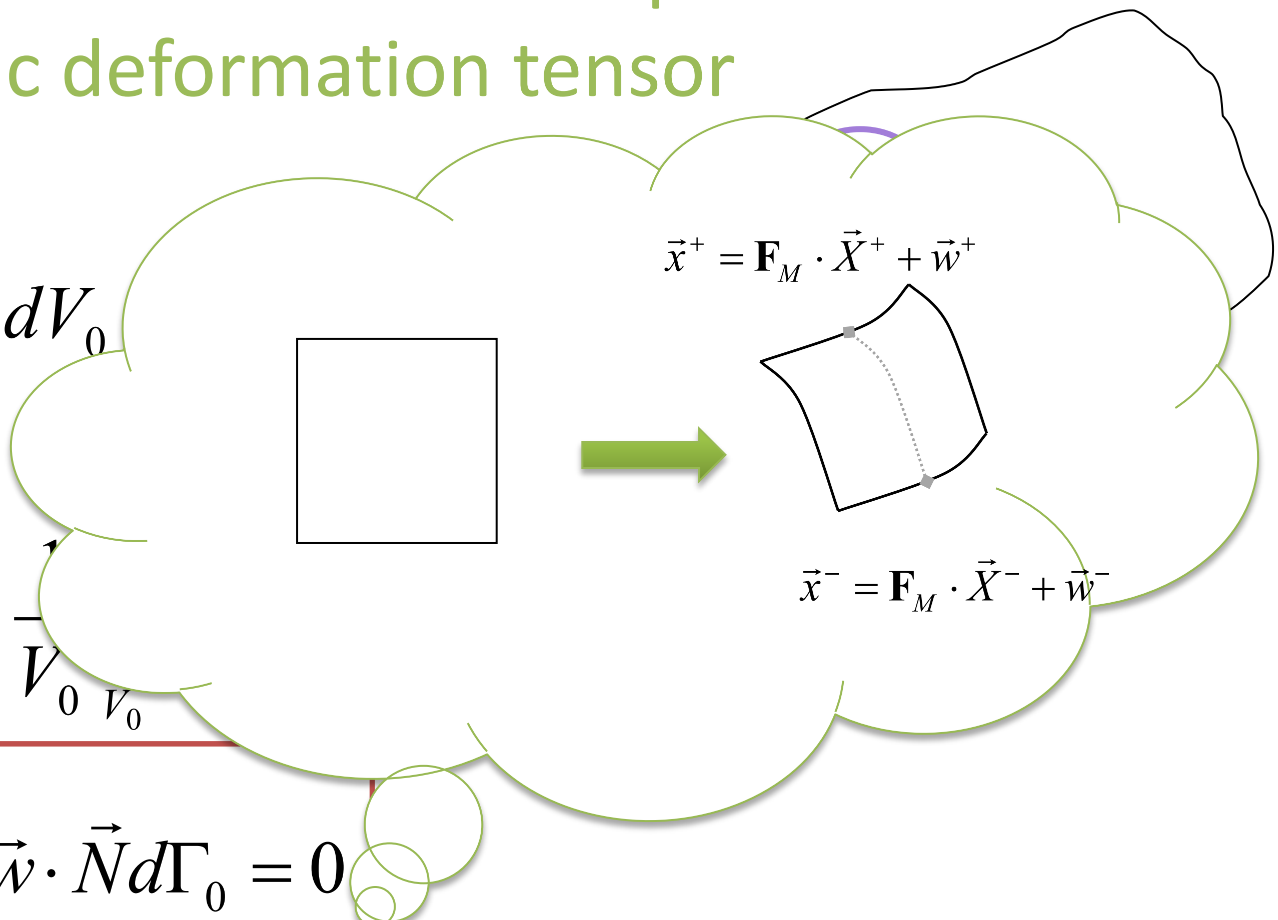
Computational Homogenization

Theory (3) - Localisation

- Translation between microscopic and macroscopic deformation tensor

$$\mathbf{F}_M = \frac{1}{V_0}\int_{V_0} \mathbf{F}_m \, dV_0$$

$$\mathbf{F}_M = \frac{1}{V_0}\int_{V_0}$$



$$\frac{1}{\Gamma_0}\int_{\Gamma_0} \vec{w}\cdot\vec{N} \, d\Gamma_0 = 0$$

Computational Homogenization

Theory (4) – Stresses

- Hill-Mandel condition $\delta W_M = \delta W_m$
- Work conjugated couple:
  - Deformation tensor & 1st Piola-Kirchhoff stress

$$\mathbf{P}_M = \frac{1}{\Gamma_0} \int_{\Gamma_0} \vec{p} \vec{X} d\Gamma_0$$

Computational Homogenization

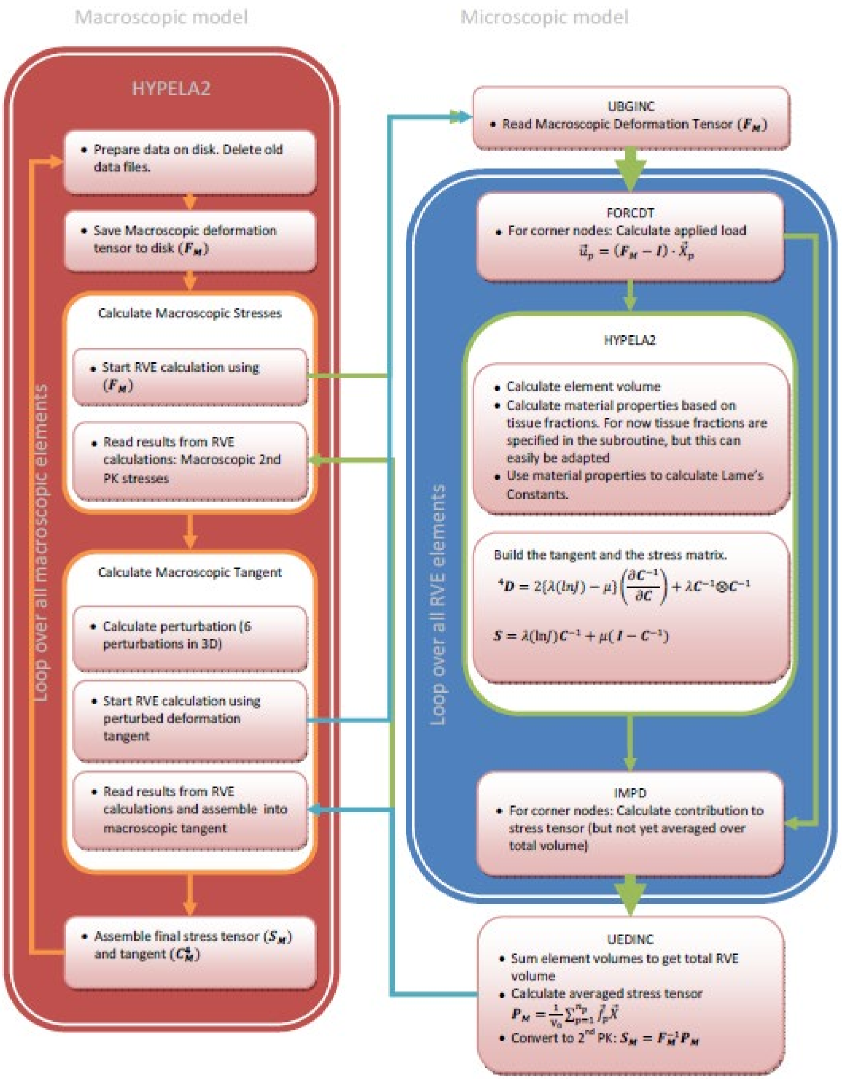
Theory (4) – Macroscopic tangent

- Tangent describes how small variations affect the stresses in the system
- Numerical differentiation
- Very cumbersome method, but Miehe (1996) developed a more efficient method.

Computational Homogenization

Implementation in MSC Marc

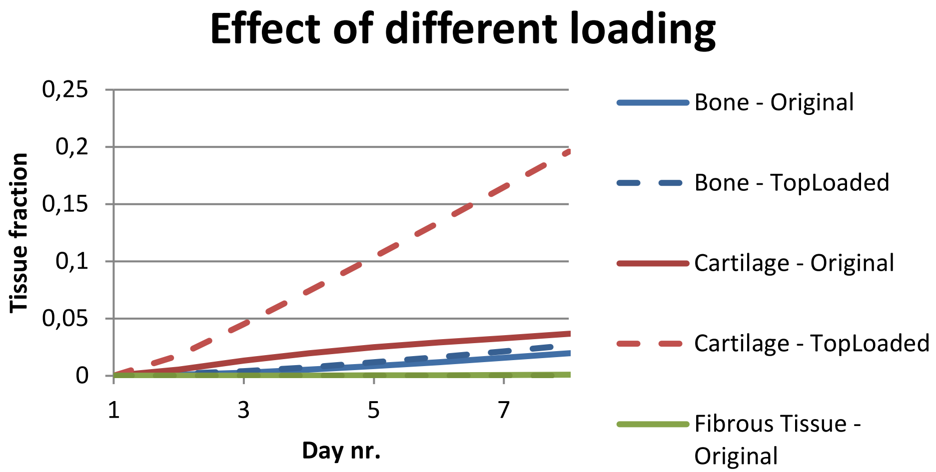
- Macroscopic Model
  - Loading
  - Deformation tensor
  - Macroscopic tangent
- Microscopic Model
  - Periodic Boundary Conditions
  - Upscale stresses

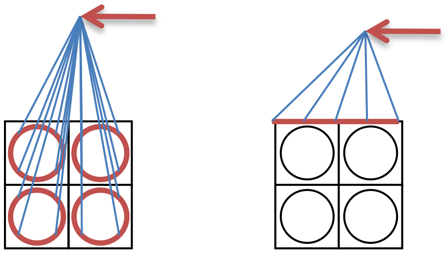


Computational Homogenization

Results / Issues

- CH implementation requires a lot a additional computing time
  - Computational overhead in the numerical differentiation scheme
- Application of loading





Summary & Conclusions

- Sections of the constitutive equations that are responsible for long calculations cannot be neglected
  - Fluid phase, non-linear biological model, diffusion
- Acceleration of the simulation was obtained by efficiently directing disk activity.
- Computational Homogenization increases simulation time and cannot account for specific loading

Recommendations

alternatives for upscaling results

- How to bridge the gap?
  - Use the model to investigate time to fixation under different loadings
  - Use a larger model to asses post-surgery micromotions
  - Develop an element that adapts the stiffness in order to ensure that at the time to fixation the micromotions are reduced to zero.

Questions?

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