Coupling of poro-aniso-hyperelastic and solute transport finite element models in a High-Performance Computing framework, for the study of Intervertebral Disc Degeneration

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Abstract

In this work, the highly parallelizable FE solver, Alya, developed by BSC is used to perform multiscale simulations to understand the mechanisms dictating IVDD. IVDs are known to exhibit poro-aniso-hyper-elastic behavior. The anisotropic and hyperelastic behavior are accounted for by combining the Holzapfel-Gasser-Ogden and modified neo-Hookean material models in a solid mechanics solver. Coupled with the later, a porous mechanics solver whose permeability adapts to the deformation of the solid matrix, is developed. Finally, oxygen, glucose and lactate represent the key nutrients involved in IVDD. Simulations aiming to study the changes in their concentration levels are performed by coupling a solute transport solver to the poro-mechanical one.



Methods 2

The required material laws are implemented within the HPC-ready framework of **Alya**, for the purposes of this project.

For the implementation of the solution scheme, a monolithic approach is used. Each individual module is responsible for the solution of one of the three governing equations. The coupling of the individual components is facilitated using strong (Block 1) and weak (Block 2) coupling strategies within iterative block structures. This is schematically described in section 3.

The required update of the permeability and diffusion coefficients is computed using the deriving deformation gradient from the mechanical solver (Solidz). This update is necessary to maintain the validity of the model across the entire spectrum of deformation. It is proposed as an alternative to the computationally expensive remeshing strategies.

<u>Governing equations</u> $\nabla_0 (-Jp F^{-T} + P_s) + \rho_s \overrightarrow{b}_0 = \overrightarrow{0}$ $\dot{J} = \nabla_0 (\mathbf{K} \cdot \nabla_0 p)$ $\frac{\partial C_i}{\partial t} - \nabla_0 \left(\boldsymbol{D} \, \nabla_0 C_i \right) = R_i (C_{0_2})$ $D_{z,0}$ $\nabla_0 = \frac{1}{\partial \vec{X}}$ $\mathbf{K} = J\mathbf{C}^{-1}\mathbf{K}(\Delta \pi, \rho_{col})$ D_y $\boldsymbol{D}^i = J\boldsymbol{C}^{-1}\boldsymbol{D}^i$

<u>Constitutive equations</u> $\boldsymbol{P}_{s} = \boldsymbol{P}_{MNH} + \Delta \pi \boldsymbol{I} + \boldsymbol{P}_{fib}$ Fibres Donnan Osmosis Aggrecans $\Psi_{MNH} = \frac{1}{12} \mu_0 \frac{1 + \frac{0.5\phi_{s,0}}{J}}{1 - \frac{\phi_{s,0}}{J}} ln^2 (det(\mathbf{C}))$ $+\frac{1}{2}\mu_0(tr(C)-3det(C)^{1/3})$ $\Psi_{fib}(\boldsymbol{C}, \overrightarrow{a}_{0ci}) = \frac{k_1}{k_2} \sum \left(exp \left(k_2 \left(I_{0ci} - 1 \right)^2 \right) - 1 \right)$ $\Delta \pi = R\theta \left(\sqrt{(c^F)^2 + (c_b)^2} - c_b \right)$

Solution Scheme 3





8 References

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Conclusions:

- Fully coupled poromechanical & solute transport framework established
- The framework performs up to 8 times faster than equivalent implementation in commercial software
- The extension of the scheme to include system biology will be achieved using the Parallel Network [8] methodology

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