A Fractional Viscoelastic Model of the Axon in Brain White Matter

Motivation:
Viscoelasticity is a sensitive measure of the composition of brain tissue and is an important marker in predicting neurodegenerative processes.

Objective:
- We aim to develop a numerical framework of the microstructure of brain white matter that incorporates a fractional viscoelastic constitutive material model of the composite white matter comprising of axons and glia.
- Representative volume elements (RVE) of axons embedded in glia with periodic boundary conditions are developed and subjected to a relaxation displacement boundary condition.
- Homogenized orthotropic fractional material properties of axons in glia are extracted by solving the inverse problem.

Finite Element Model of the Microstructure

Hexagonally packed RVES of axons embedded in the ECM of varying volume fractions are developed with a periodic mesh using Abaqus FE. Periodic boundary conditions (PBC) are enforced between nodes of opposite faces at any coordinate, $x_j$ and periodicity vector, $p$, by

$$u_i(x_j + p_j) = u_i(x_j) + \frac{\partial u_i}{\partial x_j} p_j$$

$u_i$ is the displacement field in the $i$th direction. In Abaqus, PBC can be implemented via a set of linear constraint equations with $A_i$, number of coefficients. In the equation below, $\bar{u}$ corresponds to displacement variable of node, $p$ and degree of freedom, $i$. 

$$A_1 \bar{u}_1^j + A_2 \bar{u}_2^j + \cdots + A_n \bar{u}_n^j = 0$$

A Logistic Regression Model for Power-Law

The complex modulus of a viscoelastic model following a power-law behavior with material constants, $\kappa$ and $\beta$ can be written as

$$G(\omega) = \kappa(\omega) + iG' = \Re(G(\omega)) + i\Im(G(\omega))$$

A cost function that minimizes a logistic regression model for a power-law is defined as

$$E = \frac{1}{2N} \sum_{n=1}^{N} \left[ \ln(\kappa(x_n) + \beta h(x_n) - \Re(G(x_n))) + \beta \right]$$

A generalization of derivatives of non-integer orders can be obtained in a branch of mathematics called fractional calculus using the Liouville-Caputo derivative. The stress is thus

$$\sigma(\tau) = \frac{k}{\Gamma(1 - \beta)} \int_0^\tau \tau^\beta e(\alpha) \frac{d\alpha}{d\tau} d\tau$$

For a 3D finite element model, writing $\kappa$ in terms of the volumetric and deviatoric components, the stress equation is

$$\sigma_i = \frac{1}{\Gamma(1 - \beta)} \int_0^\tau \left[ k(\varphi) + 2\beta \frac{G'_{ij}}{1 - \beta} \right] \frac{d\alpha}{d\tau} d\tau$$

For a 3D state of stress, the Liouville-Caputo derivative can be numerically computed using the Grunwald-Letnikov operator

$$\sigma_i^{\beta} = k \int \frac{d\alpha}{d\tau} \left[ \frac{1}{\Gamma(1 - \beta)} \sum \varphi_i(\alpha + (k - 1)\Delta \alpha) + 2\beta \frac{G'_{ij}}{1 - \beta} \right] \frac{d\alpha}{d\tau} d\tau$$

$k = \frac{\text{Totaltime}}{\text{Memory Length}}$

$$\varphi_i(\alpha + (k - 1)\Delta \alpha)$$

$$\sigma_i^{\beta} = \frac{d^\beta f}{d\tau^\beta} = \frac{1}{\beta} \sum \varphi_i(\alpha + (k - 1)\Delta \alpha)$$

$$M \text{=} \min\left[ \frac{L}{\Delta \alpha} \right], L \text{=} \text{Memory Length}$$

Conclusions and Future Work

- Fractional model is phenomenologically easier to interpret in comparison to Prony series models.
- Homogenized structure becomes stiffer and more viscous with higher volume fractions. The variation, however, is not linear.
- In the corpus callosum (VF of axons $\sim$ 0.4 to 0.5), our models predict $\beta$ (0.21, 0.29) and shear modulus, $\varphi$ (11, 13.7) kPa.
- Develop RVES with random distribution of axon diameters, non periodic units cells.
- Incorporate hyperelasticity for finite strain simulations.

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