GELS IN BIOMEDICAL APPLICATIONS: MODELING AND FINITE ELEMENT METHODS

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What is a Gel?

A gel is a viscoelastic material. It consists of elastic polymer chains chemically bonded together to form a network than contains a liquid solvent within its pores. The chemical bonds enable the gel to flow like a viscous fluid.

A Mathematical Model of Gel Equilibrium Problems

A wide variety of gel models have been proposed since the early 1970s. The model we use is a continuum model that was developed in [1].

1. Free Energy. Let $\Omega \subset \mathbb{R}^n$ $(n = 1, 2, 3)$ be a reference domain with coordinates X and boundary $\partial\Omega$. Let $\mathrm{x} : \Omega \to \mathrm{X}(\boldsymbol{\Omega})$ denote a smooth deformation map satisfying $\det \nabla \mathrm{x}(\mathrm{X}) > 0$. The free energy $\mathcal{E}$ of the gel, the energy available for thermodynamic processes, is given as

$$\mathcal{E}(F, \phi) = \int_\Omega \mathcal{W}_E(F) + (\det F)\mathcal{W}_{FH}(\phi)\, d\mathrm{X}$$

where the variables are

- $F = \nabla \mathrm{x}(\mathrm{X})$, the deformation gradient of the network
- ϕ, the volume fraction of the polymer.

The local balance of mass constraint stipulates that

$$\phi_I = \det F \phi$$

where ϕ_I denotes the (constant) initial volume fraction of the polymer. Using this constraint allows us to eliminate the variable ϕ and treat the problem as a purely elastic one. The terms in the free energy account for different physical properties of the gel:

- $\mathcal{W}_E(F)$ accounts for the isotropic, rubber elasticity of the polymer network
- $\mathcal{W}_{FH}(\phi)$ accounts for the mixing of the polymer and solvent

2. The Equilibrium Problem. We assume that the gel is hyperelastic, and this allows us to derive the stress from the free energy by differentiating with respect to F :

$$\mathcal{S}(F; \phi_I) = \frac{d}{dF}\left[\mathcal{W}_E(F) + (\det F)\mathcal{W}_{FH}\left(\frac{\phi_I}{\det F}\right)\right].$$

The resulting nonlinear tensor is the First Piola-Kirchoff Stress, and a calculation shows us that it is a of the form

$$\mathcal{S}(F; \phi_I) = \nu(F; \phi_I)F - \kappa(F; \phi_I)F^{-T}$$

where $\nu(F; \phi_I)$ and $\kappa(F; \phi_I)$ are scalar functions. We thus can state the strong form of the general equilibrium problem:

Find a deformation $\mathrm{x} : \Omega \to \mathrm{X}(\boldsymbol{\Omega})$ and the associated stress tensor $\mathcal{S}$ such that

$$\nabla \cdot \mathcal{S} = g, \quad \text{in } \Omega, \tag{1a}$$
$$\mathrm{x} = \mathrm{x}_0 \quad \text{on } \Omega_D, \quad \mathcal{S} \cdot n = s_0 \text{ on } \Omega_N \tag{1b}$$

where $\partial\Omega = \Omega_D \bigcup \Omega_N$ and n denotes the outward oriented normal of the boundary. Both x_0 and s_0 are prescribed, as well as g.

A Numerical Method for Gel Equilibrium Problems

There are a variety of issues to consider when formulating the numerics for the equilibrium equation. Below is a summary of some of these issues (cf. [4] for a more thorough discussion).

1. Qualitative Swelling Effects. In our model, the gel swelling depends on environmental factors such as temperature. Let T denote the temperature. The expression for $\mathcal{W}_{FH}(\phi)$ depends on this parameter:

$$\mathcal{W}_{FH}(\phi) = a(T)\phi \log\phi + b(T)(1-\phi)\log(1-\phi) + c(T)\phi(1-\phi) + c_{FH}(T)$$

If we consider small fluctuations in temperature, we obtain an approximate idea of temperature change effects by looking at perturbations about an initial temperature, T_0. We can consider this to be the forcing term f in the equilibrium equation.

2. The Linearized Problem. The linear regime is a reasonable assumption for many biomedical applications, so we fix a constant ϕ_I and consider linearizations of $\mathcal{S}$ about two parameters:

- $F_0 = f_0 I$ with $f_0 > 0$, a homogeneous bulk state deformation
- T_0, an initial environmental parameter,

and this results in the approximation

$$\mathcal{S}(F, T; \phi_I) \approx \mathcal{S}(F_0, T_0; \phi_I) + \frac{\partial\mathcal{S}}{\partial F}(F_0, T_0; \phi_I)[\nabla u] + \frac{\partial\mathcal{S}}{\partial T}(F_0, T_0; \phi_I)[\Delta T]. \tag{2}$$

These term represent the following forces:

- $\mathcal{S}(F, T; \phi_I)$, the force induced by residual stress. We must choose our parameters such that this term vanishes. By linearizing about a general bulk deformation, we can prescribe ϕ_I and find the corresponding F_0 such that the residual stress vanishes.
- $\frac{\partial\mathcal{S}}{\partial F}(F_0, T_0; \phi_I)[\nabla u]$, the linearized elasticity tensor. Here ∇u is the displacement gradient.
- $\frac{\partial\mathcal{S}}{\partial T}(F_0, T_0; \phi_I)[\Delta T]$, the force induced by the change in temperature. The physical origin of this force depends on the application of interest.

3. A Mixed Finite Elements Approach: Pressure-Displacement. One approach we use is a mixed finite element method. We define a pressure defined as $p = \lambda$ div u and obtain the displacement-pressure formulation for the equilibrium problem:

$$\begin{aligned} \langle 2\mu\varepsilon(u), \varepsilon(v)\rangle + \langle p, \nabla\cdot v\rangle &= -\langle f, \nabla v\rangle - \langle g, v\rangle \quad \forall v \in H_0^1(\Omega; \mathbb{V}) \\ \langle \nabla\cdot u, q\rangle - \langle \lambda^{-1}p, q\rangle &= 0 \quad \forall q \in L^2(\Omega), \end{aligned} \tag{3}$$

where ε is the symmetrized gradient, $g = 0$, $\mathbb{V}$ is the linear space of n vectors, $\langle\cdot,\cdot\rangle$ denotes the L^2 inner product, and μ and λ are the Lame constants. The condition

$$\mu > 0, 2\mu + n\lambda > 0 \tag{4}$$

must hold for stable solutions u and p to exist. We note that here μ and λ depend on material parameters.

Motivating Application: Artificial Bone Implants

Artificial bone implants are body-implantable devices made of synthetic polymers. Upon insertion into the body, the implant may experience swelling due to temperature changes. To ensure effective implant design, it is useful to be able to predict stresses from temperature changes.

Simulations

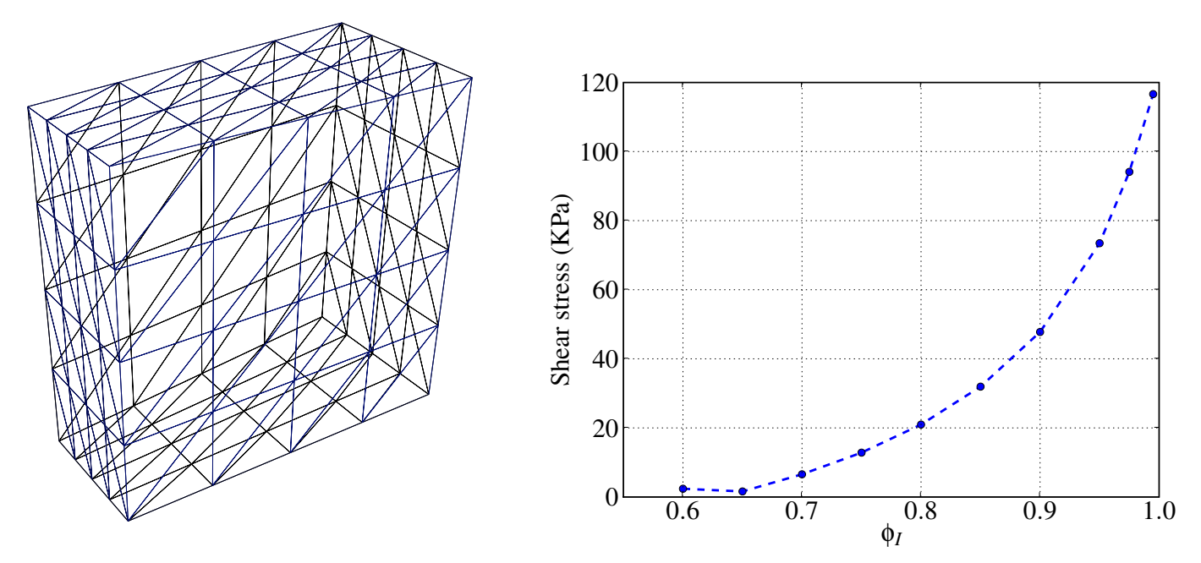
1. Choice of Finite Element Software: FEniCS. All our simulations have been performed using the DOLFIN library of the FEniCS project [2, 3].
2. Setup. We simulate the artificial bone implant using the pressure-displacement method [4]. The simulation domain is a hexahedral domain with an isosceles trapezoidal base. We consider the boundary conditions on a displacement, u, and linearized stress, σ:

$$\begin{aligned} u_0(X) &= 0,\ X \in \partial\Omega_D \\ \sigma\cdot n &= 0,\ X \in \partial\Omega_N \end{aligned}$$

where $\partial\Omega_D$ are the wedge top and bottom and $\partial\Omega_N$ are the wedge sides. The swelling force due to temperature change is derived qualitatively, with an initial temperature of $T_0 = 300$ K and $\Delta T = 1.0$. We consider ϕ_I in the range $[0.6, 1.0)$. The stresses are post-calculated by measuring the average shear stress over the top boundary, Γ:

$$S_\Gamma^2 = \frac{1}{\int_\Gamma 1\mathrm{ds}}\left(\int_\Gamma \sigma_{20}^2 + \sigma_{21}^2\mathrm{ds}\right).$$

3. Results. The stresses are shown below on the right and range from $(1.61, 117)$ KPa. These results are reasonable and support the idea that equilibrium analysis is a good approximate method of stress prediction.



Simulation Figures. *Left*: The simulation domain. *Right*: Shear stresses, in KPa, resulting from temperature changes. Average shear stress over the top boundary S_Γ versus initial volume fraction ϕ_I.

References

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