Nonlinear elasticity and gels

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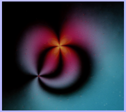

Outline

- Balance laws for gels
- Free energy: elastic plus mixing
- Constrained elasticity
- Deformable porous media
- Applications

Gels We model a gel as incompressible, immiscible mixture of polymer and solvent. ▸ immisc

Component 1: polymer; Component 2: solvent

- Ω_0 reference configuration of the gel; $\mathbf{X} \in \Omega_0$
- Ω_t domain occupied by the gel at time $t > 0$; $\mathbf{x} \in \Omega_t$

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- Ω_0 reference configuration of the gel; $\mathbf{X} \in \Omega_0$
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- ϕ_i volume fraction
- $\mathbf{v}_i$ velocity field
- $\mathcal{T}_i$ Cauchy stress tensor
- $\mathbf{i}$ friction force
- $\mathbf{\Phi}$ polymer deformation map: $\mathbf{x} = \mathbf{\Phi}(\mathbf{X}, t)$
- F polymer deformation gradient; $F = \nabla_{\mathbf{X}} \mathbf{\Phi}$, $\det F > 0$

$\phi = \phi(\mathbf{x}, t)$, $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$...

For a survey on gels, see [Tanaka, 1981]; theory of mixtures, [Truesdell, 1984]; model, [Calderer-Chabaud, 2008] and [Calderer-Zhang, 2008]

Balance laws

$$
\begin{aligned}
&\frac{\partial \rho_1}{\partial t} + (\mathbf{v}_1 \cdot \nabla)\rho_1 + \rho_1 \nabla \cdot \mathbf{v}_1 = 0 \\
&\frac{\partial \rho_2}{\partial t} + (\mathbf{v}_2 \cdot \nabla)\rho_2 + \rho_2 \nabla \cdot \mathbf{v}_2 = 0 \\
&\rho_1 \frac{\partial \mathbf{v}_1}{\partial t} + \rho_1(\mathbf{v}_1 \cdot \nabla)\mathbf{v}_1 = \nabla \cdot \mathcal{T}_1 + \mathbf{f}_1 \\
&\rho_2 \frac{\partial \mathbf{v}_2}{\partial t} + \rho_2(\mathbf{v} \cdot \nabla)\mathbf{v}_2 = \nabla \cdot \mathcal{T}_2 + \mathbf{f}_2 \\
&\phi_1 + \phi_2 = 1
\end{aligned}
$$

- Add up equations of balance of mass: $\text{div}(\phi_1 \mathbf{v}_1 + \phi_2 \mathbf{v}_2) = 0$
- Lagrangian form of balance of mass: $\phi \det F = \phi_0$

Free energy

- Elastic stored energy function (per unit reference volume) $\mu(\phi_1)W(F)$
- Flory-Huggins mixing energy (per unit deformed volume) $h(\phi_1, \phi_2)$

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Total energy:

$$\mathcal{E} = \int_{\Omega_0} \{\mu(\phi_1)W(F) + \det F\, h(\phi_1, \phi_2)\}\, d\mathbf{X}$$

$$\Psi(F, \phi) := \mu(\phi)W(F) + \det F\, h(\phi, 1 - \phi), \quad \phi := \phi_1$$

Elastic and Flory-Huggins free energies

- Prototype of Flory-Huggins energy:

$$h(\phi_1, \phi_2) = a\phi_1 \log \phi_1 + b\phi_2 \log \phi_2 + \chi\phi_1\phi_2$$

Elastic and Flory-Huggins free energies

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$$h(\phi_1, \phi_2) = a\phi_1 \log \phi_1 + b\phi_2 \log \phi_2 + \chi\phi_1\phi_2$$

- Isotropic elasticity:

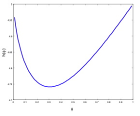
$$W(F) = \mu(\phi)w(I_1, I_2, I_3) + B(\phi)((\det F)^k - (\det F)^{-k}),\ k > 0,$$
$$\{I_1, I_2, I_3\}\,\text{principal invariants of}\ C = F^T F$$

- solid limit: $\lim_{\phi\to 1} \mu(\phi) = \mu_0$, shear modulus;
- fluid limit: $\lim_{\phi\to 0} \mu(\phi) = 0$
- $0 \le W(F) \le K|F^T F|^\beta,\ \det F > 0$

Example: neo-Heokean elasticity $W(F) = \mathrm{t}r\,(FF^T)$. Derived from statistical mechanics

Shape of free energy function with respect to χ

(1) Swollen ($\phi \approx 0.3$)



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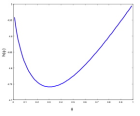

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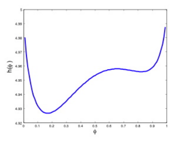

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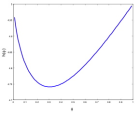

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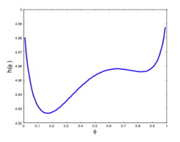

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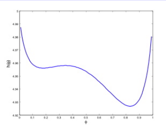

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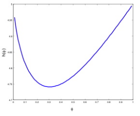

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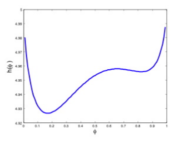

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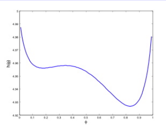
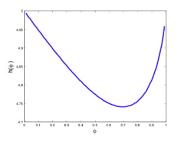


(4) Collapsed ($\phi \approx 0.7$)



Boundary conditions Let

$$\partial\Omega = \Gamma_1 \cup \Gamma_2,\ \Gamma_1 \cap \Gamma_2 = \mathbf{0}$$

- Elasticity
  1. Displacement: $\mathbf{\Phi} = \mathbf{\Phi}_0$, on Γ_1
  2. Traction: $(\mathcal{T}_1 + \mathcal{T}_2)\boldsymbol{\nu} = \mathbf{t}_0$, on Γ_2
- Permeability of membrane
  1. impermeable: $\frac{\partial \phi}{\partial \boldsymbol{\nu}} = 0$ on $\partial\Omega$ (or part of it)
  2. fully permeable: $-\phi_2 p + \Pi_2(\phi_1, \phi_2) = P_0$,
     - P_0 pressure of surrounding solvent
     - Π_2 osmotic pressure of in-gel solvent
  3. semi-permeable: $P - \big(p + \Pi_2(\mathbf{x}, t)\big) = \kappa(\mathbf{v}_2 - \mathbf{v}_1) \cdot \boldsymbol{\nu}$, $\kappa > 0$ permeability constant

Equilibrium states: convex mixing energy

$$
\begin{aligned}
\mathcal{X}_0 = &\quad \{u : u \in u_0 + W_0^{1,2\beta},\ \det F > 0\,\text{a.e.}\} \\
\mathcal{X}_\Gamma = &\quad \{u : u \in u_0 + W_\Gamma^{1,2\beta},\ \det F > 0\,\text{a.e.}\} \\
W_\Gamma^{1,2\beta} = &\quad \{u \in W^{1,2\beta},\ u = 0\,\text{on}\,\Gamma \subset \partial\Omega_0\}
\end{aligned}
$$

$$
\text{Minimize}\,\mathcal{E} = \int_{\Omega_0} \{\mu(\phi_1) W(F) + \det F\, h(\phi_1, \phi_2)\}\, dX
$$

$$
\text{subject to } \phi \det F = \phi_0,\ 0 < \phi_0 < 1,\ u \in \mathcal{X}_0 \cup \mathcal{X}_\Gamma
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$$\text{subject to } \phi \det F = \phi_0,\ 0 < \phi_0 < 1,\ u \in \mathcal{X}_0 \cup \mathcal{X}_\Gamma$$

Theorem (Zhang-2007)

Let Ω_0 be bounded and with Lipschitz boundary. Let $\beta > \frac{3}{2}$. Suppose that $g(s) = sh(\frac{1}{s}, 1 - \frac{1}{s})$ is a convex monotonically decreasing function of s. Assume that $W(F)$ is polyconvex. Then there exists at least one minimizer of $\mathcal{E}$ in X_0 and in X_Γ.

Existence theorems in nonlinear elasticity, see [Ball, 1977] and [Ciarlet, 1987]

Nonconvex free energy

Suppose that h is nonconvex with respect to ϕ.

Nonconvex free energy

Suppose that h is nonconvex with respect to ϕ. Modify the energy to include $|\nabla\phi|^2$, and keep balance of mass constraint.

$$\begin{aligned}\mathcal{X}_\infty = \quad & \{(u,\phi) : \phi \in W_{1,2}, u \in u_0 + W_0^{1,\infty}, \phi \det F = \phi_0, \text{ a.e} \\ & 0 < \phi < 1, \|\nabla u\|_{L^\infty} < C < \infty\}\end{aligned}$$

$$\begin{aligned}\text{Minimize}_{(u,\phi)\in X_\infty} \mathcal{E} = \quad & \int_{\Omega_0} \{\mu(\phi_1) W(F) + \det F\, h(\phi_1, \phi_2\}\, dX \\ + \quad & \int_\Omega \delta |\nabla\phi|^2\, dx\end{aligned}$$

$$\int_\Omega \delta|\nabla\phi|^2\, dx = \int_{\Omega_0} \left|(\det(\nabla u))^{-\frac{1}{2}} \nabla_X \mathrm{ad}j\,(\nabla u)\right|^2$$

Existence theorem

Theorem (Zhang, 2007)

Let $\beta > 0$. Then for every $C > 0$ there exists a minimizer of the regularized energy in $\mathcal{X}_\infty$.

Proof:

1. $\|\nabla u\|_{L^\infty} < C$ implies $\det \nabla u \leq 9C^3$
2. There is a minimizing sequence $\{\phi_h, u_h\} \in X_\infty$
3. Poincare inequality allows us to extract a subsequence (same label) $u \rightharpoonup \bar{u}$ weak* in $W^{1,\infty}$
4. $0 < \phi_h < 1$, $\det \nabla u_h > 1$ and $\phi_h > \frac{1}{9C^3}$
5. Obtain bound for $\int_{\Omega_0} |\nabla_X \phi_h|^2$
6. $u_h \rightharpoonup \bar{u}$ weak* in $W^{1,\infty}$ and $\phi_h \rightharpoonup \bar{\phi}$ weakly in $W^{1,2}$
7. Show that $\{\bar{\phi}, \bar{u}\} \in X_\infty$. Use the weak continuity of determinants
8. Proof of weak lower semicontinuity of last term in energy analogous to the case of liqud crystal elastomers [Calderer-Liu-Yan, 2006; 2008]

Mechanical dissipation and constitutive equations Postulate Second Law of Thermodynamics in form of Clausius-Duhem inequality (isothermal case):

$$\sum_{a} \mathrm{tr}({\mathcal{T}_a}^T \nabla \mathbf{v}_a) - \phi_a \dot{\psi}_a - \mathbf{f}_a \cdot \mathbf{v}_a \geq 0.$$

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Reversible components of the stress

$$\mathcal{T}_1^r = \phi_1 \frac{\partial \Psi}{\partial F} F^T - \big(\phi_1 p + \pi_1\big) I$$
$$\mathcal{T}_2^r = -\big(\phi_2 p + \pi_2\big) I$$

- $\pi_i = \frac{\partial h(\phi_1,\phi_2)}{\partial \phi_i}$: osmotic pressures
- $\mathcal{T}_i = \mathcal{T}_i^r + \frac{\eta_i}{2}(\nabla \mathbf{v}_i + \nabla \mathbf{v}_i^T), \quad \mathbf{f}_1 = \phi_1 \nabla p + \beta(\mathbf{v}_1 - \mathbf{v}_2) = -\mathbf{f}_2$

$\eta_i > 0$ represents Newtonian viscosity

Energy relation

Theorem (Calderer-Zhang, 2008)

. Let $\{\phi_i, \mathbf{v}_i, p\}$ be a smooth solution of the governing equations. Then it satisfies the following equation of balance of energy:

$$\frac{d}{dt}\int_{\Omega(t)}[(\frac{\phi_1}{2}|\mathbf{v}_1|^2 + \frac{\phi_2}{2}|\mathbf{v}_2|^2) + \Psi]\, d\mathbf{x} - \int_{\partial\Omega(t)}(\mathbf{t}_1 \cdot \mathbf{v}_1 + \mathbf{t}_2 \cdot \mathbf{v}_2)\, dS \leq 0,$$

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$$-\int_{\partial\Omega(t)}(\mathbf{t}_1\cdot\mathbf{v}_1 + \mathbf{t}_2\cdot\mathbf{v}_2)\,dS \leq 0,$$

- It is a consequence of the constitutive equations satisfying the second law of thermodynamics
- Applying the divergence theorem to the terms of the surface terms, we obtain an energy inequality used in proving weak solutions

Governing system revisited

$$
\begin{aligned}
&\frac{\partial \rho_1}{\partial t} + (\mathbf{v}_1 \cdot \nabla)\rho_1 + \rho_1 \nabla \cdot \mathbf{v}_1 = 0 \\
&\frac{\partial \rho_2}{\partial t} + (\mathbf{v}_2 \cdot \nabla)\rho_2 + \rho_2 \nabla \cdot \mathbf{v}_2 = 0 \\
&\rho_1 \frac{\partial \mathbf{v}_1}{\partial t} + \rho_1 (\mathbf{v}_1 \cdot \nabla)\mathbf{v}_1 = \nabla \cdot \mathcal{T}_1 + \mathbf{f}_1 \\
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Difficulty in proving existence due to the last equation [Liu-Walkington, 2001]; it is a conservation law

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It becomes simple if $\nabla \mathbf{v}_1 = 0$, not the case here

Evolution equation for the deformation gradient Take divergence of equation:

$$F_{is,it} + v_k F_{is,ik} + v_{k,i} F_{is,k} = v_{i,ij} F_{js} + v_{i,j} F_{js,i}$$

If $\nabla \cdot \mathbf{v} = 0$, it reduces to

$$\operatorname{div}(F^T)_t + (\mathbf{v} \cdot \nabla) \operatorname{div}(F^T) = 0$$

Prescribe appropriate initial and boundary values so that $\operatorname{div}(F^T) = 0$ for all time.

Special class of problems: Linearized elasticity[1]

$$\phi_1 \mathbf{v}_{1,t} = \mathrm{div}\, \mathcal{T}^r(F,\phi) - \phi_1 \nabla p + \eta_1 \triangle \mathbf{v}_1 + \beta(\mathbf{v}_1 - \mathbf{v}_2)$$
$$\phi_2(\mathbf{v}_{2,t} + (\mathbf{v}_2 \cdot \nabla)\mathbf{v}_2) = \phi_2 \nabla(p + \pi_2)$$
$$+\eta_1 \triangle \mathbf{v}_2 + \beta(\mathbf{v}_2 - \mathbf{v}_1)$$
$$\phi_1 = \phi_0(1 - \mathrm{tr}\,(\nabla u))$$
$$\mathrm{div}(\phi_1 \mathbf{v}_1 + \phi_2 \mathbf{v}_2) = 0$$
$$F^T F = I + (\nabla u + \nabla u^T) + o(|\nabla u|), \;\; \mathbf{v}_1 = u_t$$

- u denotes displacement vector $u = \mathbf{x} - \mathbf{X}$
- Coupling of dissipative linear elasticity equations for the solid with Navier-Stokes equations for the polymer; note that the constraint is not the standard one

For experimental and modeling references on mechanics of gels, see, [Tanaka-Filmore, 1979], [Doi-Yamaue, 2004, a, b]

[1] MCC, Micek, Rognes; work in progress

Special class of problems: Deformable porous media[2] In applications $\eta_1 >> \eta_2$, polymer dissipation much larger than solvent's and also greater than elastic effects

$$\phi_0 \nabla \cdot \big((K - \frac{2}{3} G)(\nabla \cdot \mathbf{u}) I + 2GE \big) = \nabla (p + \Pi_1)$$

$$\nabla \big(\frac{K_B T}{N_2 V_m} ((1 - \phi_0) + \phi_0 \nabla \cdot \mathbf{u}) + (1 - \phi_0) p \big) = \beta (\mathbf{v}_1 - \mathbf{v}_2),$$

$$\nabla \cdot (\phi_0 \mathbf{v}_1 + (1 - \phi_0) \mathbf{v}_2) = 0,$$

$$\mathbf{v}_1 = u_t .$$

- Coupling of steady state elasticity with Stokes problem for fluids, although constraint is non-standard.
- K, G are elastic moduli
- The second equation corresponds to Darcy's law
- Mathematical analogs found in geology in dealing with soil media and clays [Bennethum-Murad-Cushman, 2000]

[2] MCC, Chabaud, Luo; work in progress

Special problems

- Application of finite element analysis to nonlinear problem (Rognes, Micek, MCC; work in progress)
- Analysis of nonlinear problem in one-dimensional geometry (Ming Chen, MCC; work in progress)

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Immiscibility and Incompressibility

- Immiscibility: the constitutive equations depend on volume fractions. It is always possible to distinguish between components
- Incompressibility: the intrinsic density is constant. Note that

$$\rho = \phi\gamma$$

$$\rho = \frac{\text{mass of component}}{\text{mixture space}}, \quad \gamma = \frac{\text{mass of component}}{\text{component space}}$$

So the incompressibility statement reduces to

$$\gamma = \text{constant}$$

◂ Back