

An Introduction to Complex Materials

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Complex Materials: Mathematical Models and Numerical Methods
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Together we span many length and time scales

User's Guide to the Workshop

Physics umbrella: Soft -Matter*

- ▶ Elasticity
- ▶ Liquid Crystals
- ▶ Biologically inspired systems

Materials classifications:

- ▶ Anisotropic fluids
- ▶ Gel membranes and biomembranes
- ▶ Poroelasticity

Mathematics:

- ▶ Finite Elements
- ▶ Calculus of Variations
- ▶ Γ -convergence
- ▶ Homogenization and dynamic metamaterials
- ▶ Peridynamics

Liquid crystals: Static configurations in domain $\Omega \subset \mathbb{R}^3$

Nematic molecules, with **head-tail symmetry** are represented by **line direction**, pair $\pm \mathbf{l}$ unit vectors, or by the tensor $\mathbf{l} \otimes \mathbf{l}$

Distribution of orientations of molecules in $B_x(\delta)$:

probability measure μ_x in $\mathbb{R}P^2$, probability measure on the unit sphere \mathcal{S}^2 such that

$$\mu(E) = \mu(-E), \quad E \subset \mathcal{S}^2$$

- ▶ First order moment $\int_{\mathcal{S}^2} \mathbf{l} d\mu(\mathbf{l}) = 0$
- ▶ Second order moment is a symmetric non-negative second order tensor

$$\mathbf{M} = \int_{\mathcal{S}^2} \mathbf{l} \otimes \mathbf{l} d\mu(\mathbf{l}) \quad \text{tr } M = 1$$

If molecules are equally distributed in all directions, distribution μ_0 is isotropic, where

$$d\mu_0(\mathbf{l}) = \frac{1}{4\pi} d\mathbf{l}, \quad \text{with } f(\mathbf{l}) = \frac{1}{4\pi}.$$

The *de Gennes* Q -tensor

$$Q = M - M_0 = \int_S (\mathbf{I} \otimes \mathbf{I} - \frac{1}{3} \mathbf{I}) d\mu(\mathbf{I})$$

measures the deviation of M from the isotropic value M_0 .
It satisfies

$$Q = Q^T, \quad \text{tr } Q = 0, \quad Q \geq -\frac{1}{3}.$$

Spectral representation

$$Q = \lambda_1 \mathbf{n}_1 \otimes \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \otimes \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \otimes \mathbf{n}_3,$$

\mathbf{n}_i orthonormal basis of eigenvectors, λ_i eigenvalues satisfying

$$\lambda_1 + \lambda_2 + \lambda_3 = 0, \text{ and } \frac{2}{3} \geq \lambda_i \geq -\frac{1}{3}.$$

Liquid crystal symmetries

Liquid crystal symmetries according to eigenvalues of Q :

- ▶ Isotropic with all eigenvalues equal to 0.
- ▶ Biaxial, in the case that $\lambda_1 \neq \lambda_2 \neq \lambda_3$,
- ▶ Uniaxial, if two eigenvalues are equal and distinct from the third one. In this case, we write

$$\lambda_1 = \lambda_2 = -\frac{s}{3}, \lambda_3 = \frac{2s}{3}, \mathbf{n}_3 := \mathbf{n}.$$

In this case,

$$Q = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}),$$

where $-\frac{1}{2} \leq s \leq 1$.

Suppose that at every $\mathbf{x} \in \Omega$ liquid crystal is described by free energy density $W(Q(\mathbf{x}), \nabla Q(\mathbf{x}))$ such that

$$E(Q) = \int_{\Omega} W(Q(\mathbf{x}), \nabla Q(\mathbf{x})) d\mathbf{x} := \int_{\Omega} W_B(Q) + W_E(Q, \nabla Q)$$

$$W_B(Q) = a \operatorname{tr} Q^2 - b \operatorname{tr} Q^3 + c \operatorname{tr} Q^4, \quad W_E(Q, \nabla Q) = \sum_{i=1}^5 L_i l_i,$$

$$l_1 = Q_{ij,j} Q_{ir,r}, \quad l_2 = Q_{ik,j} Q_{ij,k}, \quad l_3 = Q_{ij,k} Q_{ij,k},$$

$$l_4 = Q_{lk} Q_{ij,l} Q_{ij,k}, \quad l_5 = \epsilon_{ijk} Q_{ij} Q_{jl,k}$$

Coherence length $\xi = \sqrt{\frac{L}{|a|}} = 10^{-8.5} \text{ m}$ Stiff problem

Defects

Defects are points, lines or surfaces with $Q = 0$

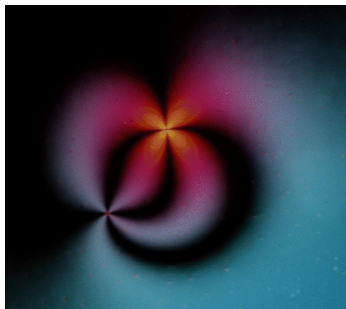


Figure: O.Lavrentovich. Liquid crystal under crossed polarizers. Point defects and surrounding brushes

For a typical liquid crystal (5CB):¹

$$L_i = 4.0 \times 10^{-11} \text{ N}, \quad a = -.172 \times 10^6 \frac{\text{N}}{\text{m}^2}$$

Coherence length $\xi = \sqrt{\frac{L}{|a|}} = 10^{-8.5} \text{ m}$ Stiff problem

¹I. Bajc, F.Hecht, S.Zumer, arXiv-sbumit/1263139, May 26-2015

Frank-Oseen theory

$$E(\mathbf{n}, s) = \int_{\Omega} [K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n})|^2 \\ + (K_2 + K_4)(\text{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2)] d\mathbf{x} \\ K_1 = 2L_1s^2 + L_2s^2 + L_3s^2 - \frac{2}{3}L_4s^3, K_2 = \dots$$

s is constant in Frank-Oseen model.

For $Q = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I)$ (and equal K 's) yields **Ericksen model**:

$$E(\mathbf{n}, s) = \int_{\Omega} [K(|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2) + f(s)] d\mathbf{x}$$

- ▶ Are Frank-Oseen and Landau (uniaxial case, s constant) equivalent ? (D.Golovaty, J. Robbins, P.Dassbach)
- ▶ Defects in each theory; non-orientability issue
- ▶ Computation with Ericksen's model: S. Walker
- ▶ Surface anchoring energy
- ▶ Flow theories

Ericksen-Leslie Equations of Liquid Crystal Flow

Postulate generalized velocities and generalized forces ²

	fields	vel.	stress vec.	stress tensor	body force
mechanic	φ	\mathbf{v}	\mathbf{t}	\mathbf{T}	\mathbf{F}
optic	\mathbf{n}	$\dot{\mathbf{n}}$	\mathbf{s}	\mathbf{S}	\mathbf{G}

Dependent fields $\mathbf{v} = \mathbf{v}(\mathbf{y}, t)$, $\mathbf{n} = \mathbf{n}(\mathbf{y}, t)$, $\mathbf{t} = \mathbf{t}(\mathbf{y}, t)$

$\mathbf{y} \in \Omega_t := \varphi(\Omega)$, l.c. domain at time t ; $\mathbf{y} = \varphi(\mathbf{x})$, $\mathbf{x} \in \Omega$, def. map

- ▶ \mathbf{t} contact force (per unit area); \mathbf{s} contact torque (per u.area)
- ▶ \mathbf{F} body force (per u. vol); \mathbf{G} body torque (per u. vol)
- ▶ \mathbf{T} Cauchy stress tensor ($\mathbf{T} \neq \mathbf{T}^T$); \mathbf{S} generalized stress tensor

$$\mathbf{t} = \mathbf{T}\boldsymbol{\nu}, \quad \mathbf{s} = \mathbf{S}\boldsymbol{\nu}, \quad \boldsymbol{\nu} \text{ unit normal vector to the contact surface}$$

²Theory of Flow Phenomena in Liquid Crystals, F.M. Leslie, Advances in Liquid Crystals, Vol 4, 1979, 1-88

Balance of energy

Postulate equation of balance of energy:

$$\frac{d}{dt} \int_{\Omega_t} \left(\frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \frac{1}{2} \sigma \dot{\mathbf{n}} \cdot \dot{\mathbf{n}} + W(\mathbf{n}, \nabla \mathbf{n}) \right) d\mathbf{x} = \int_{\Omega_t} (\mathbf{F} \cdot \mathbf{v} + \mathbf{G} \cdot \dot{\mathbf{n}}) d\mathbf{x} + \int_{\partial\Omega_t} (\mathbf{t} \cdot \mathbf{v} + \mathbf{s} \cdot \dot{\mathbf{n}}) da.$$

Let (\mathbf{v}, \mathbf{n}) satisfy balance of energy. Assume

- Balance of energy holds for $\mathbf{v}^s = \mathbf{v} + \mathbf{c}$ and $\dot{\mathbf{n}}^s = \dot{\mathbf{n}}$, \mathbf{c} arb.
- Balance of energy holds for second motion

$$\mathbf{v}^s = \mathbf{v} + \boldsymbol{\xi} \times \mathbf{y}, \quad \dot{\mathbf{n}}^s = \dot{\mathbf{n}} + \boldsymbol{\xi} \times \mathbf{n}, \text{ and}$$

$$\mathbf{F}^s - \rho \dot{\mathbf{v}}^s = \mathbf{F} - \rho \dot{\mathbf{v}}, \quad \mathbf{G}^s - \sigma \dot{\mathbf{N}}^s = \mathbf{G} - \sigma \dot{\mathbf{N}}, \quad \mathbf{N} := \dot{\mathbf{n}}$$

$\boldsymbol{\xi}$ is an arbitrary, constant, angular velocity., then eqns of balance of linear momentum and angular momentum follow

Leslie-Ericksen equations

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \mathbf{F}$$

$$0 = \nabla \cdot \mathbf{S} + \mathbf{G} + \mathbf{g}$$

$$\mathbf{n} \cdot \dot{\mathbf{n}} = 0, \quad \nabla \cdot \mathbf{v} = 0$$

$$\mathbf{T} = \frac{\partial W}{\partial (\nabla \mathbf{n})} (\nabla \mathbf{n})^T + \tilde{\mathbf{T}}$$

$$\mathbf{S} = \frac{\partial W}{\partial (\nabla \mathbf{n})} + \mathbf{n} \otimes \boldsymbol{\beta},$$

$$\mathbf{g} = -\frac{\partial W}{\partial \mathbf{n}} - \nabla \cdot (\mathbf{n} \otimes \boldsymbol{\beta}) + \gamma \mathbf{n} + (\boldsymbol{\epsilon} \times \tilde{\mathbf{T}}) \times \mathbf{n}$$

$$\begin{aligned} \tilde{\mathbf{T}} = & \alpha_1 (A \mathbf{n} \cdot \mathbf{n}) \mathbf{n} \otimes \mathbf{n} + \alpha_2 (\tilde{\mathbf{N}} \otimes \mathbf{n}) + \alpha_3 (\mathbf{n} \otimes \tilde{\mathbf{N}}) + \alpha_4 A \\ & + \alpha_5 A \mathbf{n} \otimes \mathbf{n} + \alpha_6 \mathbf{n} \otimes A \mathbf{n} \end{aligned}$$

$$A := \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T), \quad \tilde{\mathbf{N}} = \dot{\mathbf{n}} - \frac{1}{2} (\nabla \mathbf{v} - \nabla \mathbf{v}^T) \mathbf{n}.$$

Numerical Schemes for Materials with Fine Scale Structure: Noel J. Walkington

Many material models consist of the momentum equation coupled to an equation modelling the structure of the material. Examples include liquid crystals, polymers, and crystalline solids undergoing plastic deformation. These systems possess a Hamiltonian structure which reveals the subtle structure of the terms coupling of the equations, and a delicate balance between inertia, transport, and dissipation. This talk will focus on the development and analysis of numerical schemes which inherit the Hamiltonian structure, and hence stability, of the continuous problem. Examples of schemes to approximate the Ericksen Leslie equations, Oldroyd-B fluids, and problems in plasticity, will be presented to illustrate the mathematical and numerical properties of this class of materials.

Balance Laws: biphasic mixtures

Gel incompressible mixture of solid (*polymer network*) and fluid, interacting with its environment (e.g. air, fluid or another gel)

- In Ω_t (gel domain):

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}(\rho_i \mathbf{v}_i) = 0, \quad \rho_i = \phi_i \gamma_i, \quad \gamma_i = \text{constant},$$

$$\rho_i \dot{\mathbf{v}}_i = \nabla \cdot \mathcal{T}_i - \phi_i \nabla p + \mathbf{f}_i, \quad i=1, \text{ polymer}; \quad i=2, \text{ fluid}$$

$$\phi_1 + \phi_2 = 1$$

- In \mathcal{R}_t (surrounding fluid)

$$\rho_f \left(\frac{\partial \mathbf{v}_f}{\partial t} + \mathbf{v}_f \cdot \nabla \mathbf{v}_f \right) = \nabla \cdot \mathcal{T}_f - \nabla p + \mathbf{f}_f,$$

$$\nabla \cdot \mathbf{v}_f = 0$$

$$\phi = \phi(\mathbf{x}, t), \quad \mathbf{v} = \mathbf{v}(\mathbf{x}, t), \quad \mathcal{T} = \mathcal{T}(\mathbf{x}, t), \quad p = p(\mathbf{x}, t) \dots$$

Alternate derivation in the viscosity dominating regime by Onsager's principle of minimum dissipation.

Deformation and Stress

- ▶ polymer deformation map: $\mathbf{y} = \mathbf{y}(\mathbf{x}, t)$, $\mathbf{x} \in \Omega$.
- ▶ $\Omega_t = \mathbf{y}(\Omega)$: current configuration of gel.
- ▶ $\partial\Omega_t := \partial\Omega_t$: interface gel-surrounding fluid.

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- ▶ polymer volume fraction $\phi_1 \equiv \phi$; **fluid** $\phi_2 = 1 - \phi_1$.

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- ▶ polymer volume fraction $\phi_1 \equiv \phi$; **fluid** $\phi_2 = 1 - \phi_1$.
- ▶ $\Psi(F, \phi)$: free energy density.
- ▶ Cauchy stress tensors:
 \mathcal{T}_1 : polymer; \mathcal{T}_2 : solvent; \mathcal{T}_f : environmental fluid.
- ▶ p : hydrostatic pressure associated with constraint:

$$\nabla \cdot (\phi_1 \mathbf{v}_1 + \phi_2 \mathbf{v}_2) = 0.$$

Mechanical model: energy

Mechanical equilibrium ³

$$\mathcal{E} = \int_{\Omega_t} \Psi(F, \phi) := \int_{\Omega_t} \phi_1 \mathcal{W}(F) + (\det F) \mathcal{W}_{\text{FH}}(\phi_1, 1 - \phi_1).$$

- ▶ $\mathcal{W}(F)$: elastic energy density.
- ▶ \mathcal{W}_{FH} : Flory-Huggins energy of mixing

$$\mathcal{W}_{\text{FH}} = \frac{k_B T}{v_s} \left(\frac{v_s}{v_p} \phi_1 \ln \phi_1 + \phi_2 \ln \phi_2 + \chi \phi_1 \phi_2 \right),$$

v_s : volume occupied by a single molecule of solvent.

$$\mathcal{T}_1 = \phi_1 \frac{\partial \mathcal{W}}{\partial F} F^T + (\mathcal{W}_{\text{FH}}(\phi_1) - \phi_1 \frac{d}{d\phi_1} \mathcal{W}_{\text{FH}}(\phi_1)) I + \mathcal{T}_1^d(\nabla \mathbf{v}_1, \phi)$$

$$\mathcal{T}_2 = \mathcal{T}_2^d(\nabla \mathbf{v}_2, \phi)$$

³M. Rognes, M.C. Calderer and C. Micek. Mixed finite element methods for gels with biomedical applications, SIAM J. Appl.Math, Vol 70, 1305-1329, 2009

Boundary conditions at the gel-fluid interface, $\partial\Omega_t$

Interface $\partial\Omega_t$ moves with polymer: $\mathbf{v}_1 \cdot \mathbf{n} \equiv v_f$

- Balance of mass of fluid phase across $\partial\Omega_t$:

$$(\mathbf{v}_f - \mathbf{v}_1) \cdot \boldsymbol{\nu} = \phi_2(\mathbf{v}_2 - \mathbf{v}_1) \cdot \boldsymbol{\nu}$$

- Continuity of tangential velocity across $\partial\Omega_t$:

$$(\mathbf{v}_f - \mathbf{v}_1)_{\parallel} = (\mathbf{v}_2 - \mathbf{v}_1)_{\parallel} \equiv \mathbf{q}$$

- Balance of forces across the interface

$$(\mathcal{T}_f - \mathcal{T}_1 - \mathcal{T}_2)\boldsymbol{\nu} + [p]\boldsymbol{\nu} = 0$$

- Balance of lin moment. of fluid crossing $\partial\Omega_t$:

$$-[p] - \boldsymbol{\nu} \cdot \left(\frac{\mathcal{T}_2}{\phi_2}\right)\boldsymbol{\nu} = \eta_{\perp}\mathbf{q}, \quad (\mathcal{T}_1\boldsymbol{\nu})_{\parallel} = \eta_{\parallel}\mathbf{q}.$$

$\eta_{\perp}, \eta_{\parallel}$ interface viscosity: **fully permeable** gel at 0-limit; **impermeable** gel at ∞ -limit

Stable finite volume methods for coupled Darcy flow and deformation in geological media: Jan Nordbotten

The rise of advanced **geoengineering applications** such as enhanced geothermal systems together with energy and CO₂ storage, leads to settings where coupled **poro-mechanical systems** need to be considered. The geological complexity requires numerical methods adapting to complex grids, discontinuous material coefficients, and possibly also fractures. Herein, we explore the possibilities of using **finite volume methods as a unifying framework for solving both flow and mechanical deformation**. We illustrate the applicability using both synthetic examples as well as a preliminary comparison to field data.

Poroelastic Modelling of the Central Nervous System:

Kent-Andre Mardal

In this talk we will discuss simulations of the **central nervous system using poroelastic modelling**. We will consider the remodelling that occurs in the spinal cord under abnormal flow and pressure. Furthermore, we will discuss **sensitivity with respect to modelling choices and aspects related to simulations**. Finally, we will give a short overview of the processes that governs fluid flow within the brain and the challenges faced.

Polyelectrolyte gels and applications

In polyelectrolyte gels, ⁴. the polymer network contains fixed charge groups that dissociate and deliver counterions into the solvent, that itself may contain several species of ions. Swelling problems are free boundary problems for the swelling front ⁵. If mass inertia is included—in mimetic applications—free boundary problems are hyperbolic. ⁶

Polyelectrolyte gels form an important class of gels studied experimentally and used in applications. For device purposes, gels can be controlled by **temperature** and **pH-gradient**. ⁷

Applications to living systems often involve **slender** bodies.

Additional analysis tools of **dimensional reduction**, from classic asymptotics to Γ -convergence.

⁴A Dynamic Model of Polyelectrolyte Gels, SIAM J. Appl. Math., 2013, Vol 73, no. 7, pp. 104–123, H.Chen, C.Micek, Y. Mori, MCC

⁵Analysis and simulation of a model of polyelectrolyte gel in one spatial dimension, *Nonlinearity*, MCC, H. Chen and Y. Mori, vol 27, 2014, 1-45, 2014

⁶Long-Time Existence of Classical Solutions to a one-dimensional Swelling Gel, *Math. Models and Meth. in Appl. Sciences*, M.R. Chen and MCC, vol 25, 165-194, 2015.

⁷Rhythmomimetic drug delivery, MCC, L. Yao, Y. Mori and R.E. Siegel, in

A Membrane Theory for Swelling Polymer Gels: Alessandro Lucantonio

Stimuli-responsive materials deform in response to non-mechanical stimuli, such as temperature, pH, or humidity changes. These materials are employed, for instance, in shape-morphing applications, where the material is programmed to achieve a target shape upon activation by an external trigger, and as coating layers to alter surface properties of bulk materials, such as the characteristics of spreading and absorption of liquids. In these applications, stimuli-responsive materials are often in the form of membranes. In particular, polymer gel membranes experience swelling or shrinking when their solvent content changes and the non-homogeneous swelling field may be exploited to control their shape. Here, we develop a theory of swelling material surfaces to model polymer gel membranes and demonstrate its features by studying numerically applications in the contexts of biomedicine and micro-motility. We also specialize the theory to thermo-responsive gels, which are made of polymers that change their affinity with solvent as a function of temperature.

Bilayer Plates: Model Reduction, Discrete Gradient Flow and Gamma-Convergent Finite Element Approximation.

Ricardo H. Nochetto

The bending of bilayer plates is a mechanism which allows for large deformations via small externally induced lattice mismatches of the underlying materials. We discuss its mathematical modelling, which consists of a nonlinear fourth order problem with a pointwise isometry constraint. We devise a finite element discretization based on Kirchhoff quadrilaterals and prove its Gamma-convergence. We propose an iterative method that decreases the energy and study its convergence to stationary configurations. We explore its performance, as well as reduced model capabilities, via several insightful numerical experiments involving large (geometrically nonlinear) deformations. This work is in joint with S. Bartels (Freiburg) and A. Bonito (Texas A&M).

Active Matter Models and Their Applications in Life Science: Qi Wang

Active matter is a type of materials that energy is converted at the molecular level from chemical form to mechanical form providing energy input to the molecular motion. Active matter is abundant in nature and man-made materials. Faithfully modelling active matter is cutting-edge research. I will present a modelling framework for developing mathematical models for multiphase complex fluids that involve active matter. Then, I will discuss some basic properties of fluid flows of active matter and numerical schemes that can be used to simulate the complex fluid flows. Numerical simulations of several biological systems will be presented including cell motion, mitosis, and vesicles filled with the active matter.

⁸ ⁹ is a formulation of continuum mechanics to study deformations with discontinuities, especially fractures.

- ▶ $\mathbf{u} : \mathcal{R} \subset \mathbb{R}^3 \longrightarrow \mathbb{R}^3$, displacement field
- ▶ \mathbf{f} : particle-particle interaction force
- ▶ $\mathbf{L}_{\mathbf{u}}(\mathbf{x}, t)$: force per unit ref vol at \mathbf{x} due to interaction with other particles,

$$\mathbf{L}_{\mathbf{u}}(\mathbf{x}, t) = \int_{\mathcal{R}} \mathbf{f}(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x}) d\mathbb{V}_{\mathbf{x}}, \quad \forall \mathbf{x} \in \mathcal{R}, \quad t \geq 0.$$

peridynamic equation of motion

$$\rho \frac{d^2 \mathbf{u}}{dt^2} = \mathbf{L}_{\mathbf{u}} + \mathbf{b} \quad \text{in } \mathcal{R}, \quad t \geq 0$$

⁸Qiang Du and Robert Lipton, Peridynamics, Fracture and Nonlocal Continuum Models. From SIAM News, 47 (2014)

⁹S.A. Silling, Journal of the Mechanics and Physics of Solids, 48(2000) 175-209

Composites and Metamaterials

*By combining a compliant isotropic material that has low bulk and shear moduli with a stiff isotropic material that has high bulk and shear moduli, one can ... produce an elastically isotropic composite that effectively has the bulk modulus of the compliant phase and the shear modulus of the stiff phase.*¹⁰ Materials with negative Poisson ratio.

Metamaterials have dynamic properties that vary in space and time and so may be controlled to respond to (time and space dep.) environmental inputs. Have properties not found in standard materials: *screening* extended spatial domains from the intrusion of dynamic disturbances, storing energy in pulses of high power, compressing signals, ... Likewise, *cloaking* material from optical disturbance.¹¹

¹⁰The Theory of Composites, Graeme W. Milton, Camb. Univ. Press. 2002, online 2009.

¹¹Active Exterior Cloaking for the 2D Laplace and Helmholtz Equations, F.Guevara Vasquez, G.W. Milton and D.Onofrei, PRL 103, 073901, 2009.

Conclusions

- ▶ We presented an outlook of some of the important problems in complex materials.
- ▶ We emphasize scientific connections with other areas, especially biology.
- ▶ A common feature among many of these problems is the challenge in analyzing and computing defects.
- ▶ Continuum theories may fail at the defect length scale, requiring perhaps the use of microscopic models.
- ▶ Continuum theories need to be informed by molecular (or atomic, in some cases) theories.
- ▶ In transporting these 'ideal' theories to materials design, many other issues enter into play: polydomain structures and defects. In particular, the effect of grain boundaries has a huge effect in material properties. Statistical methods are required to evaluate these properties: Uncertainty Quantification.