Simulation Studies of Liquid Crystal Elastomer Dynamics

Robin Selinger
Badel Mbanga, Jonathan Selinger

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CONTACT ROBIN@LCI.KENT.EDU FOR THE LATEST RESEARCH NEWS

http://www.e-lc.org/presentations/docs/2007_07_02_16_34_07
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Liquid Crystal Elastomer = Artificial muscle

Temperature
B. Ratna and J. Naciri
Naval Research Laboratory

Photoexcitation
M. Camacho-Lopez, H. Finkelmann, P. Palffy-Muhoray, and M. Shelley,
Nature Materials 2004

Electric Field
Chris Spillman, J. Naciri, and B. Ratna
Naval Research Laboratory

http://www.e-lc.org/presentations/2007_07_02_16_34_07
Actuation mechanisms

Nematic elastomer
- Raise Temperature
- Isotropic

Nematic+azo dye
- Photoexcitation
- Disrupts order

Smectic elastomer
- Electric field induces tilt
- Layer contraction

http://www.e-lc.org/presentations/docs/2007_07_02_16_34_07
Today’s presentation…

1. Finite Element elastodynamics:
   → Isotropic rubber
   → LC elastomers

2. Modeling devices:
   → Actuators
   → Robots
   → Pumps
   (Nematic, Smectic)

3. Director relaxation, soft elasticity
   (Badel Mbanga’s talk, Saturday)
Finite element elastodynamics: Home-made algorithm

Isotropic rubber, 3-d, tetrahedral mesh

**Potential energy density:**
\[ U^{\text{elastic}} / Vol = C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \]

**Green-Lagrange Strain:**
\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{1}{2} \frac{\partial u_k}{\partial x_i} \frac{\partial u_k}{\partial x_j} \]
Nonlinear

Strain is uniform in each element; potential energy depends on

\[ \varepsilon_{ij}, \quad U^{\text{elastic}} \]
... in body frame, invariant under rotations in target space!
**Kinetic energy:** \[ K = \sum_{\text{nodes } i} \frac{1}{2} m_i v_i^2 \]

“Lumped mass” approximation

**Hamiltonian:** \[ H_{\text{total}} = \sum_{\text{elements } j} U_{\text{elastic}} \cdot \text{Vol}_j + \sum_{\text{nodes } i} \frac{1}{2} m_i v_i^2 \]

Linear shape functions describe displacements within each element

- Assumes strain within each element is uniform

  x displacements: \[ u = a_1 + a_2 x + a_3 y + a_4 z \]
  y displacements: \[ v = b_1 + b_2 x + b_3 y + b_4 z \]
  z displacements: \[ w = c_1 + c_2 x + c_3 y + c_4 z \]

Calculate strain components explicitly, e.g.

\[ \varepsilon_{11} = \frac{\partial u}{\partial x} + \frac{1}{2} \left( \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial w}{\partial x} \right)^2 \right) = a_2 + \frac{1}{2} \left( (a_2)^2 + (b_2)^2 + (c_2)^2 \right) \]
Elastic potential energy: \[ U^{\text{elastic}} = C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \]

To calculate forces on the nodes, take derivative of \( U^{\text{elastic}} \) w.r.t. node position

For isotropic media, three elastic constants: \( C_{xxxx}, C_{xxyy}, C_{xyxy} \)

Resulting forces are calculated via the chain rule... a bit messy in 3D

\[
F_{x,i} = -2C_{xxxx} \varepsilon_{11} m_{2i} (1 + a_2) - 2C_{xxx} \varepsilon_{22} m_{3i} a_3 - 2C_{xxx} \varepsilon_{33} m_{4i} a_4 - 2C_{xyy} \varepsilon_{11} m_{3i} a_3
- 2C_{xyy} \varepsilon_{22} m_{3i} a_3 - 2C_{xyy} \varepsilon_{33} m_{4i} a_4 - 2C_{xyy} \varepsilon_{33} m_{2i} (1 + a_2)
- 2C_{xyy} \varepsilon_{11} m_{4i} a_4 - 4C_{xyy} \varepsilon_{12} m_{3i} (1 + a_2) - 4C_{xyy} \varepsilon_{12} m_{2i} a_3 - 4C_{xyy} \varepsilon_{23} m_{4i} a_3
- 4C_{xyy} \varepsilon_{23} m_{3i} a_4 - 4C_{xyy} \varepsilon_{31} m_{4i} (1 + a_2) - 4C_{xyy} \varepsilon_{31} m_{2i} a_4
\]
Move nodes via $F=ma$ (use velocity Verlet method)
Looks like molecular dynamics, but with nodes instead of atoms

Isotropic Rubber

Resulting dynamics conserves Kinetic + Potential to very high precision, even with large rotation!  Time step = $10^{-6}$ sec
Resulting dynamics conserves Kinetic + Potential to high precision, even with high amplitude oscillation, large rotation (with no dissipation included)
Adding strain –order coupling

\[ U = C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} - s \, Q_{ij} \varepsilon_{ij} \]

Potential energy per unit volume \hspace{1cm} Elastic strain energy \hspace{1cm} strain-order coupling

\[ Q_{ij} = \frac{3}{2} \left( n_i n_j - \frac{1}{3} \delta_{ij} \right) \]

...where \( n \) is the nematic director

Also add: \textit{internal damping}

\[ F_{\text{drag}} = -\left[ \gamma \frac{1}{r_{12}} (\vec{v}_2 - \vec{v}_1) \cdot \hat{r}_{12} \right] \hat{r}_{12} \]

Conserves momentum and angular momentum

Simplest model: impose \( Q_{ij} \) history

... watch strain respond
Modeling devices:

1. Nematic Actuators

- Switch material between nematic/isotropic
Isotropic – nematic transition

\[ Q_{ij} = S \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix} \]

Isotropic \rightarrow Nematic

\begin{align*}
S &= 0 \\
S &= 1
\end{align*}
Response to light

Nematic film, director along x, fixed on right end
→ switch top layer ONLY to isotropic
Modeling actuators:
3-d fiber orientation control

Six “muscles” in the blue and green base
If sample has pre-existing domain structure, slightly alter model:

\[ U = C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} - S \left( Q_{ij} - Q_{ij}^{\text{init}} \right) \varepsilon_{ij} \]

Reference state is in elastic equilibrium with \( Q_{ij}^{\text{init}} \), defined in each element.
Poly-domain sample, exposed to linearly polarized light. (Every element has an initial $Q$ with randomly oriented director.)

Switch domains aligned with polarization on top surface $\rightarrow$ Induces light-controlled bending

Modeling devices:

2. Smectic Actuator

- Reorient director via applied electric field
- Assume layer structure unchanged (???)
Smectic film actuated with transverse electric field

Front/back asymmetry: gradient in strain-order coupling induces twist

Director initially points up, oscillates like a windshield wiper

Chris Spillman, NRL

6 V/μm
Modeling devices:

3. Pumps

• Modulate strength of nematic order parameter to induce propagating wave
Modeling devices: Peristaltic pump

Applications: microfluidics, “active” catheter, swimming/propulsion, clothing
Modeling devices:
Peristaltic pumping membrane
Modeling devices:

4. Self-propelled soft robots

- Add anisotropic static friction with substrate
Modeling devices: Soft Robotic Earthworm

\[ Q_{ij} = q \, e^{i(kx-\omega t)} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix} \]

Head and tail
out of phase

Sin-wave shaped substrate

(like roof of Math/CS building)
Smectic walker...

Upper and lower regions of film actuated out of phase
Soft Elasticity: Director rotates to accommodate strain

Monodomain liquid crystal elastomer
Stretch transverse to the nematic director

- Initial response is linear
- Plateau region: director rotation “soft elastic response”
- When rotation complete, again get linear response

Experiment
Warner & Terentjev p. 170
Model soft elastic response: more degrees of freedom
Allow $Q_{ij}$ in each element to evolve with local strain

$$Q_{ij} = S\left( n_i n_j - \frac{1}{3} \delta_{ij} \right)$$

Nematic order tensor: symmetric and traceless

$Q$ has five degrees of freedom:

- 2 angles… defines orientation of nematic director
- Nematic scalar order parameter
- Biaxial order strength
- 1 angle… orientation of biaxial order
Model soft elastic response: more degrees of freedom
Allow $Q_{ij}$ in each element to evolve with local strain

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Nematic order tensor: symmetric and traceless

$Q$ has five degrees of freedom:

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Relax 2 angular degrees of freedom only

$\rightarrow$ Director reorients to minimize potential energy
...aligns with local principal axis of strain

Assume: Scalar nematic order parameter = constant; no biaxial order
Time evolution of local director
3-d simulation, imaging front surface of sample only

- Sides are clamped and pulled at uniform velocity
- Plot the director at the center of each element → color by orientation
- Shown is the top layer of the sample
- Measure Force vs Displacement for different strain rates

20016 tetrahedra
Time evolution of local director
3-d simulation, imaging front surface of sample only

Striped region:

Allows rotation without macroscopic shear

Problem: Irregularities in underlying mesh may affect nucleation of tilt domains

20016 tetrahedras
Soft Elasticity: Director rotates with strain

- Noise in force-displacement curve due to small sample size
- The higher the strain rate, the later the onset of switching
- After switching complete, linear regime observed (pulling along $n$)
Soft Elasticity: Director rotates with strain

I. Kundler and H. Finkelmann

- The director rotation occurs later for higher strain rate
- Regions near clamp are constrained and do not fully rotate
  → creates defects in director field
Soft Elasticity: Director rotates with strain

- Orange regions correspond to director parallel to polarizer or analyzer
- A striped pattern can be observed near the clamps
Future research plans include…

Damped/driven torsional oscillator

...determine anisotropy of dissipation when director reorients
CONCLUSIONS

• Formulated 3-d finite element explicit dynamics simulation of a liquid crystal elastomer

• Approach 1: assume history of $Q$ and calculate resulting shape evolution → use for device design.

• Approach 2: Let director relax to align with local strain → study dynamics of soft elastic response.

• Can model complex geometries, finite strain rates

Goal: Build a bridge between basic soft matter theory and practical materials engineering/device design