

APS March Meeting 2021 (Online)

Updates in Scientific Research during Pandemic Times

by Vianney Gimenez-Pinto, PhD

While the ongoing global pandemic continues to affect our everyday lives, researchers in Science, Technology, Engineering and Math found a way to come together at the American Physical Society (APS) March Meeting 2021. The conference was online-only and had more than 11,000 registered attendants who actively participated in the program during March 14- 19, 2021.

DSOFT Short Course

Conference programming started with technical workshops sponsored by different Research Divisions within the American Physical Society. I had the opportunity to attend the DSOFT (Division of Soft Matter) short course on “*Topological Data Analysis*”, which introduced Topology to interested (and/or curious) students, postdoctoral researchers, and early career faculty members). In this program, I learned about Topological Data Analysis (TDA) techniques, such as Persistent Homology which monitors the appearance/disappearance (birth/death) of features in a data set. The workshop included a *TDA Software Tutorial Session for Python* presented by Abigail Hickok (UCLA). It also featured research reports by other experts in the field, such as Eleni Kafitori (University of Pennsylvania). Her scientific research applies persistent homology (a *mathematical* technique) to the study of *functional networks*, including those in *biological systems*. Mason Porter (UCLA), Giovanni Petri (ISI Foundation) and Konstantin Mischaikow (Rutgers University) also taught in this short course.

This workshop provided me with priceless information and resources for research projects and for mentoring undergraduate students interested in related research. Mason Porter’s talk provided great bibliographic recommendations on articles suitable for general audiences (including teens and pre-teens), less-gentle reading material for researchers, as well as lecture notes + books. Most of our student population pursues an undergraduate degree (our younger students are still in their teen years). Thus, reading materials for general audiences would allow them to learn about these complex topics earlier in their studies. Interested students in their senior undergraduate year or graduate studies can dive into the less-gentle reading materials and books.

Porter's general-audience recommended readings include:

- *"Topological Data Analysis, One Applied Mathematician's Heartwarming Story of Struggle, Triumph, and (Ultimately) More Struggle"* by Chad Topaz [1]
- *"Connecting the Dots: Discovering the Shape of Data"* by Michelle Feng, Abigail Hickok, Yacoub Kureh, Mason Porter and Chad Topaz [2]

Listing the full list of resources and references is beyond the scope of this report. However, if interested in the complete list of reading materials, please feel free to contact me gimenez-pintov@lincolnu.edu. I would be happy to share useful information and resources.

Research Updates

In the conference, I presented the talk *"Custom made actuation driven by smooth yet complex liquid crystal director microstructures."* This work was carried out in collaboration with Hillel Aharoni (previously a Postdoctoral Researcher at University of Pennsylvania, now faculty at Weizmann Institute of Science) during my time as a Visiting Researcher at University of Pennsylvania. We conducted finite-element elastodynamics simulations for the actuation of a liquid crystal polymer network with a director configuration that encodes a specific target shape: a Volkswagen Beetle. Abstract can be found in the Bulletin of the American Physical Society [3]. Presentation slides are given as an appendix of this report.

My talk was part of the Thursday session *"Liquid Crystals I,"* which included authors from all career levels: undergraduate students, graduate students, early career researchers, junior and senior faculty members. Presenting in the same session was Keith Hedlund, an undergraduate student at University of Colorado - Boulder. His work *"Interactions and dynamics of oil and ferromagnetic droplets on 2D Smectic Films"* [4] was carried out in the laboratory of Noel Clark. It investigated droplets of paraffin oil doped with barium hexaferrite colloidal particles and suspended on films of liquid crystal smectic A and C. In the study, he monitored the response and motion of these droplets under applied AC Electric and Magnetic fields. I am always excited to listen undergraduate students conducting liquid crystal research. They motivate me to craft undergraduate-suitable projects for interested LU students. Also, they serve as a reference point on the depth and scope that can be pursued by undergrads.

I also attended the session *"Physics of Bio-Inspired Materials,"* which included the invited talk *"Counting the optical cost of disorder in biological photonic systems"* by Pete Vukusic (University of Exeter) [5]. His talk offered a thoughtful review on biological materials

with color given by order, quasi-order, and disorder within material structure. These phenomena can be observed in butterfly wings, bird's feathers, crustaceous, insects, bacteria, etc. Among the biological materials that produce structural color, we can mention: Chitin in *Insecta*, Keratin in *Aves*, Guanine in *Fish*, Cellulose in *Plants*, Amorphous Silica in *Phytoplankta*, Carbonates in *Crustacea* and Peptidoglycan in *Bacteria*. Being a Soft Matter Scientist, my research interests exist at the intersection of Physics, Chemistry, Biology, Applied Math and Engineering. Thus, attending multidisciplinary lectures is invaluable for moving forward my research duties and responsibilities as a faculty member at Lincoln.

Diversity, Inclusion, Representation and Equity

Another valuable session in the APS March meeting programing was titled: "*TEAM-UP: The Time is Now for Systemic Changes to Increase the Number of African American Bachelor's in Physics and Astronomy.*" It focused on the on-going efforts to support African Americans pursuing a Physics career. Speakers included: Philip Hammer (University of Chicago), Thomas Searles (Howard University), Tabbetha A Dobbins (Rowan University) and Elon Price (Fiske Vanderbilt Bridge Program).

Listening to Thomas Searles's talk, I learned details on the Team-UP report by the American Institute of Physics (AIP) and the five factors they identified as key to serve students from under-represented minorities in the sciences:

- 1) A sense of belonging is essential for persistence and success
- 2) Physics identity increases persistence
- 3) Effective teaching, Mentoring and Academic support
- 4) Support for financial stresses
- 5) Sustainability: academic leadership needs to prioritize supportive environments and structures to maintain their functioning for enough time to make a difference.

Having these factors clearly stated inspires me to serve as an effective mentor in STEM fields, to be vocal about being a physicist and our role within society, to advocate for the creation and/or maintenance of supportive environments for our science majors, and to pursue opportunities to provide paid research experiences for undergraduate students.

Overall, the online-held APS March Meeting 2021 was an enriching experience as an academic professional. These experiences are priceless for Lincoln University faculty as they provide us with training, information, and resources for our role as educators and scholars.

References

- [1] Topaz, C. M. 2016. *Topological data analysis: One applied mathematician's heartwarming story of struggle, triumph, and (ultimately) more struggle*. *DSWeb: The Dynamical Systems Web*. Available online at: <https://dsweb.siam.org/The-Magazine/Article/topological-data-analysis>
- [2] Feng M, Hickok A, Kureh Y, Porter M and Topaz C (2021) Connecting the Dots: Discovering the “Shape” of Data. *Front. Young Minds*. 9:551557. doi: 10.3389/frym.2021.551557. Available online at: <https://kids.frontiersin.org/articles/10.3389/frym.2021.551557>
- [3] <https://meetings.aps.org/Meeting/MAR21/Session/R05.10>
- [4] <https://meetings.aps.org/Meeting/MAR21/Session/R05.14>
- [5] <https://meetings.aps.org/Meeting/MAR21/Session/J06.4>
- [6] <http://meetings.aps.org/Meeting/MAR21/Session/L62?showAbstract>

Vianney Gimenez-Pinto, PhD is a Soft Matter scientist and an Assistant Professor of Physics and Chemistry at Lincoln University of Missouri. She is interested in multi-disciplinary scientific research suitable for undergrads, as well as reducing disparities in Science and Technology.

Custom-made actuation driven by “smooth yet complex” liquid crystal director microstructures

Copy of slides as
presented in APS
Vianney Gimenez-Pinto
March Meeting 2021
Lincoln University of Missouri

&

Hillel Aharoni
Weizmann Institute of Science



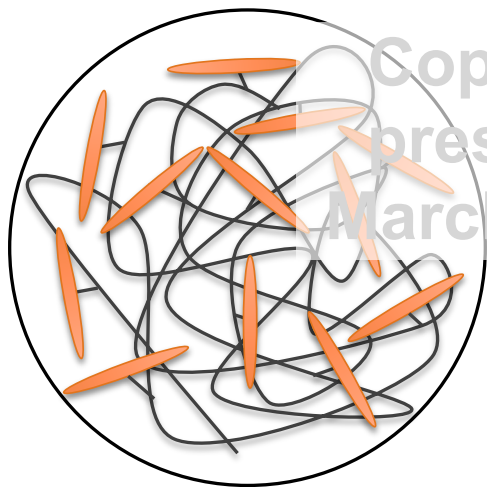
Liquid Crystal Elastomers (LCE)

Isotropic phase

Disorder of LC units



Polymer Network Disordered

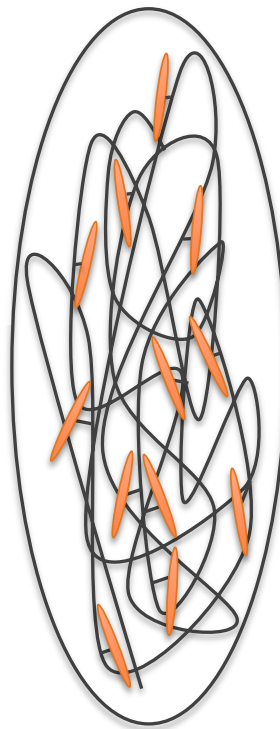


Nematic phase

Ordered LC molecules



Elongation of
Polymer Network

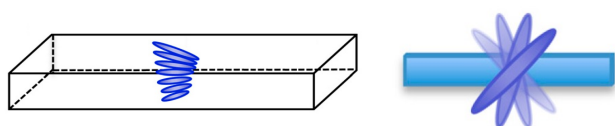


Elongated parallel to director \mathbf{n}
Contracted perpendicular to \mathbf{n}

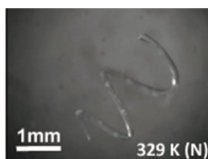
Copy of slides as
presented in APS
March Meeting 2021

Non-uniform director in LCE: Complex Shape Transformation

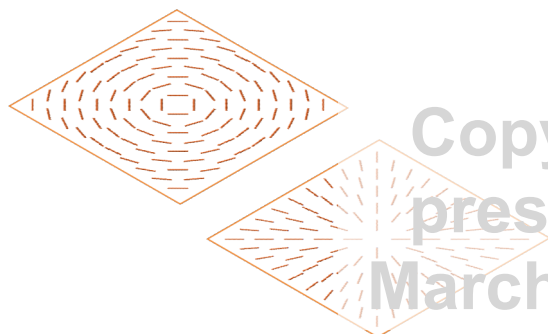
Director \mathbf{n} varies along



One direction: thickness



Sawa, et. al.
PRE. (2013)



Copy of slides as
presented in APS
March Meeting 2021

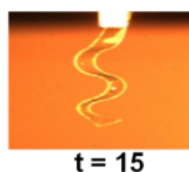
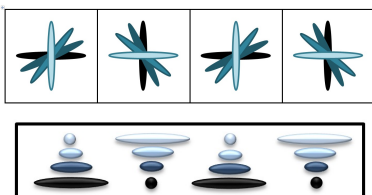


DeHaan, et. al.
Angewandte Chemie Int. Ed 2012



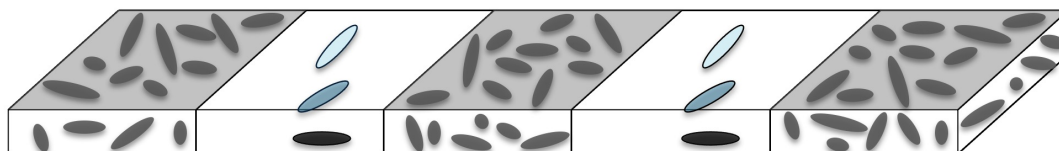
Konya, et. al.
Front. Mat.
(2016)

Two directions: length and width



DeHaan, et.al.
Adv. Funct. Mat.
(2014)

Two directions: length and thickness



Two directions: length and thickness

Copy of slides as
presented in APS
March Meeting 2021

Dual-phase accordion

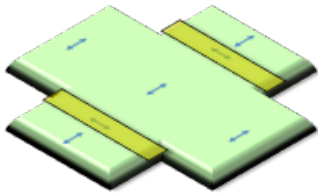


Dual-phase twist-flat ribbon

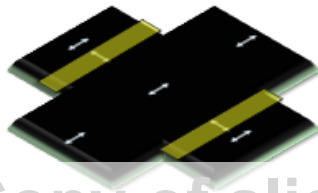
Gimenez-Pinto and Ye.
RSC Advances (2019)

Three directions: length, width and thickness
Not smooth!

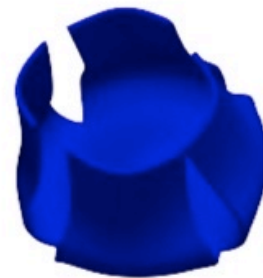
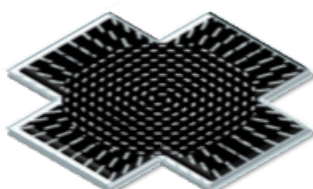
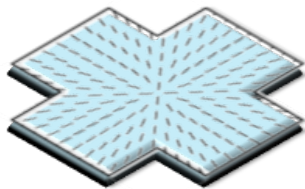
Top layer



Bottom layer



Copy of slides as
presented in APS
March Meeting 2021

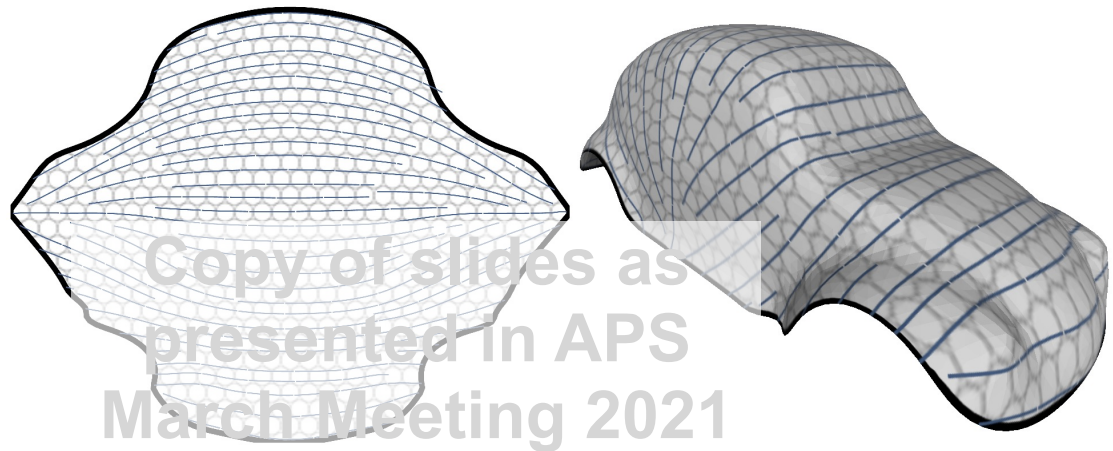


**Aiming for cost reduction
towards a Target Shape
March Meeting 2021**

Motor-sport: Volkswagen Beetle

Solution to the inverse problem for a specific target shape
Smooth yet complex

Mid-plane view



Three directions: length, width and thickness

Director configuration has two components:

Intrinsic curvature (in-plane variations of \mathbf{n})

Extrinsic curvature (along-thickness variations of \mathbf{n})

**Custom-made Director
by Hillel Aharoni**



Methodology details at
Aharoni et. al. *PRL* 2014

Finite Element Elastodynamics, R. Selinger, Kent State University

3-D sample discretized to an unstructured tetrahedral mesh



$$F = \frac{\lambda}{2} \varepsilon_{ii} \varepsilon_{jj} + \mu \left[\varepsilon_{ij} \varepsilon_{ij} - \alpha \varepsilon_{ij} (S - S^{flat}) Q_{ij}^0 \right] \quad \text{Free energy of each tetrahedra}$$

Green-Lagrange
non-linear strain tensor

$$\varepsilon_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i + \partial_i u_k \partial_j u_k)$$

Order parameter

$$Q_{ij}^0 = n_i n_j - \frac{\delta_{ij}}{3}$$

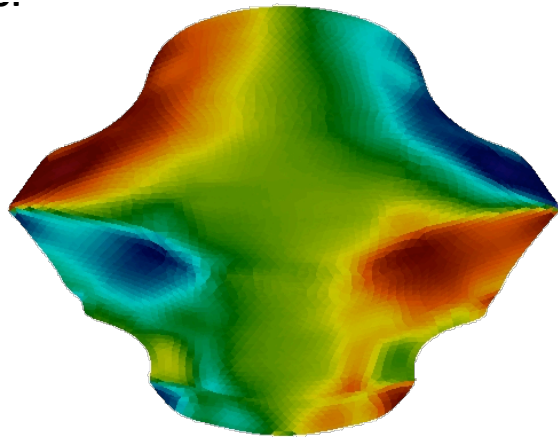
\vec{n} director configuration at cross-linking

Lamé coefficients λ, μ

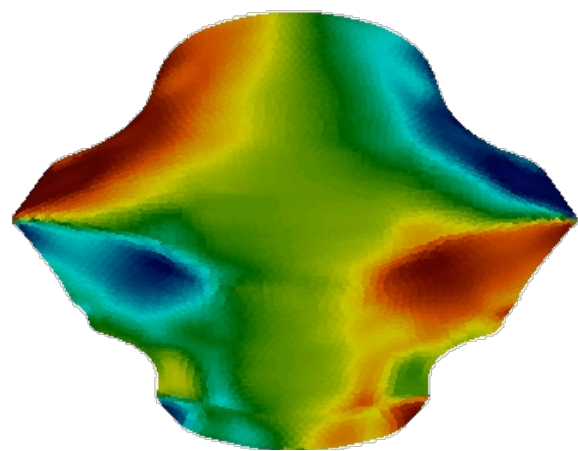
$S(T)$ Mesogens orientation relative to director

α Coupling strain and nematic order

Elastodynamics: Nodes move via $m_n \ddot{r}_n = - \frac{\partial F_n}{\partial r_n}$ Dissipation $\sim m_n \dot{r}_n$ to reach equilibrium shape

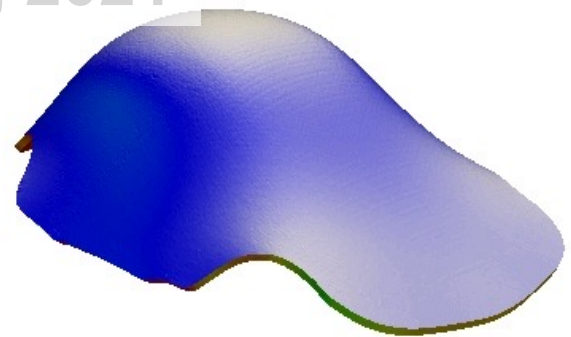
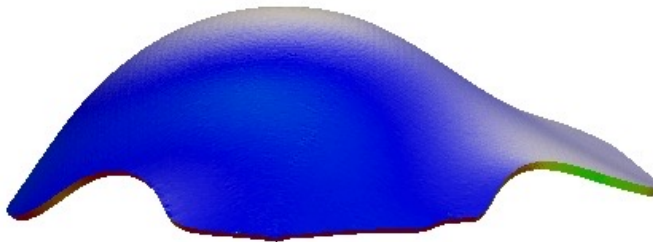


Analytical Design



*Director configuration mapped to
unstructured tetrahedral mesh for FEM
simulation*

FEM simulation



length = 346.99, width=269.449, thickness =3.00
108107 nodes and 378476 tetrahedral elements

$\alpha\delta S = -1.52$

Increasing stimulus response



Copy of slides as
presented in APS
March Meeting 2021

length = 346.99, width=269.449, thickness =3.00
108107 nodes and 378476 tetrahedral elements

$\alpha\delta S = -2.28$



Copy of slides as
presented in APS
March Meeting 2021



length = 346.99, width=269.449, thickness =3.00
108107 nodes and 378476 tetrahedral elements

$\alpha\delta S = -2.28$

Copy of slides as
presented in APS
March Meeting 2021



length = 346.99, width=269.449, thickness =3.00
108107 nodes and 378476 tetrahedral elements

$\alpha\delta S = -2.28$

Modeling 3D actuation in a 3D sample

Effect of bending energy – sample thickness:

- “Pop-up” morphing behavior
- Averaging of local curvature variations



Copy of slides as
presented in APS
March Meeting 2021



length = 346.99, width=269.449, thickness =3.00
108107 nodes and 378476 tetrahedral elements

$\alpha\delta S = -2.28$

Acknowledgements

Randall Kamien and
Penn's Soft Matter team



Robin Selinger

Copy of slides as
presented in APS
March Meeting 2021

The logo of Kent State University, featuring a yellow sunburst above the word "KENT" in a large blue serif font, with "STATE" in a smaller blue serif font to its right, and "UNIVERSITY" in a blue sans-serif font below "KENT".

Ohio Supercomputer Center
An OH-TECH Consortium Member

