Spotlights in Computational Physics and Engineering (SCoPE)

Invited lectures on:

Mathematical and computational modeling of flexoelectric materials

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Abstract

Flexoelectricity is an electromechanical coupling between polarization and strain gradients, as well as strain and electric field gradients. It is a small-scale effect, prominent in the nanoscale, and unlike piezoelectricity, it is present in all dielectric solids, regardless of the atomic structure of the constituent. Therefore, it is a promising mechanism for electromechanical transduction to be exploited in new-generation engineered devices in a wide range of applications, including sensing, actuacting and energy harvesting. However, the mathematical and computational modeling of this effect is not straightforward, mainly due to the high-order nature of the governing equations. The validation of the models via experimental measurements is also hindered by both the intrinsic difficulty of accurately measuring quantities of interest at the nanoscale, and also the correct interpretation of these measurements within a continuum model.

In these lectures, the mathematical and numerical modeling of flexoelectricity will be adressed. In particular, the constitutive laws and variational problems for flexoelectric materials at both infinitessimal and finite deformations will be formulated and studied. Numerical strategies to solve the resulting high-order boundary value problems will be proposed, including immersed boundary B-Spline frameworks and the C0-IPM method, along with a variety of illustrative examples. The correct use of continuum models within quantum mechanical frameworks to properly extract ab-initio measurements of the flexoelectric constants will also be addressed. Finally, the mathematical and computational framework for the design and optimization of apparently piezoelectric metamaterials made of non-piezoelectric, flexoelectric constituents, will also be discussed.

The lectures are structured as follows:

1. Introduction to flexoelectricity: Motivation, manifestations, technologies and challenges. Basics on the continuum modeling of flexoelectricity: Constrained and unconstrained variational problems for high-order electromechanics, Legendre transform of the flexoelectric energy density, treatment of the null-Lagrangian, formulation of the weak and strong forms, and the corresponding boundary conditions.
2. Numerical modeling of flexoelectricity. Challenges and approaches in the literature. B-Spline based methods for body-fitted and unfitted meshes. Overview of alternative C0-Interior penalty method. Illustrative examples featuring sensing electrode conditions and multimaterial designs. Introduction to numerical instabilities and weak form stabilization.
3. Flexoelectricity at finite deformations. Constitutive laws, energy density, weak and strong forms with corresponding boundary conditions. Computational aspects: modified-step Newton-Raphson and treatment of mechanical instabilities (i.e. buckling). Illustrative examples. Application to quantum mechanics: Correct measurement of flexoelectric constant in 2D-electronic systems under bending.
4. Flexoelectric metamaterials. Reduction to representative volume element using high-order generalized periodicity conditions. Multiscale variational problem, weak and strong forms. Numerical approach using high-order generalized periodic B-spline approximation spaces. Illustrative examples for apparently piezoelectric metamaterials. Level-set based geometry description for topology optimization using genetic algorithms.

When and Where?

- 13.05.2024, 10:00-12:00,
- 14.05.2024, 10:00-12:00,

Invitee: David Codony*

DAVID CODONY is an assistant professor at Universitat Politècnica de Catalunya - BarcelonaTech (UPC), Barcelona, Spain, since 2023. He is interested in material science and the design of smart materials. He is collaborating with the FLEXOCOMP (UPC) and MP&M (GeorgiaTech) research groups on the mathematical and computational modelling of flexoelectricity using both continuum and quantum mechanics.

Selected Publications

- D. Codony, A. Mocci, J. Barceló-Mercader, I. Arias, Mathematical and computational modeling of flexoelectricity, Journal of Applied Physics, 130, 231102, (2021)
- D. Codony, P. Gupta, O. Marco, I. Arias, Modeling flexoelectricity in soft dielectrics at finite deformation, Journal of the mechanics and physics of solids, 146, 104182, (2020)
- D. Codony, I. Arias, P. Suryanarayana, Transversal flexoelectric coefficient for nanostructures at finite deformations from first principles, Physical Review Materials, 5, 3, L030801, (2021)
- J. Barceló-Mercader, D. Codony, A. Mocci, I. Arias, Computational homogenization of higher-order electromechanical materials with built-in generalized periodicity conditions, Computer Methods in Applied Mechanics and Engineering, 423, 11686, (2024)
- F. Greco, D. Codony, H. Mohammadi, S. Fernández-Méndez, I. Arias, Topology optimization of flexoelectric metamaterials with apparent piezoelectricity, Journal of the Mechanics and Physics of Solids, 183: 105477, (2024)