

NUMERICAL SIMULATION OF NANO-SCALE ELECTROMECHANICAL COUPLING BY MEANS OF AN IMMERSED BOUNDARY B-SPLINE METHOD

Onofre Marco¹, David Codony¹, Sonia Fernández-Méndez¹ and Irene Arias¹

¹ Laboratori de Càlcul Numèric (LaCàN), Universitat Politècnica de Catalunya, Campus Nord UPC-C2, E-08034 Barcelona, Spain.

e-mail: {david.codony, onofre.marco, sonia.fernandez, irene.arias}@upc.edu

Key Words: *Flexoelectricity, B-spline method, Immersed boundary, Nitsche's method.*

Continuum modeling of physical phenomena at the micron- and sub-micron scales requires high-order continuum theories in order to take into account size or length-scale effects. This is the case of flexoelectricity: a two-way electromechanical coupling between strain-gradient and electric polarization fields. In this contribution, we consider the generalized continuum model in [1], which describes the flexoelectric coupling as a fourth order partial differential equation (PDE), with displacements and electric potential as mechanical and electrical unknowns respectively.

The high-order nature of the PDE requires C^1 -continuous solutions, so the standard Finite Element Method (FEM) is not suitable, and advanced discretization methods are required such as the Meshfree Method [1] and the Mixed FEM [2]. These methods are relatively expensive, the former uses C^∞ smooth basis functions with expensive evaluation and integration whereas the latter increases the number of unknowns to circumvent the smoothness requirement.

Here, we propose an alternative numerical method based on an Immersed Boundary B-spline approach. B-spline basis functions provide high-order continuity of the original unknowns and are efficiently evaluated and integrated. Since they are defined on a Cartesian parametric space, we also consider a regular Cartesian mesh and make use of the Immersed Boundary concept to permit simulations on arbitrary domain shapes. In our approach, special high-order numerical integration is performed on cut cells [3] while boundary and interface conditions are weakly enforced by means of the Nitsche's method.

We present the particularization of the Nitsche's method to the formulation in [1] and show numerical examples of electromechanic transduction at small scales, including conductive inclusions and multi-material setups of particular engineering interest.

REFERENCES

- [1] A. Abdollahi, D. Millán, C. Peco, M. Arroyo and I. Arias, *Revisiting pyramid compression to quantify flexoelectricity: A three-dimensional simulation study*. *Phys. Rev. B.*, vol. 91(10), pp. 104103, 2015.
- [2] S. Mao, P.K. Purohit and N. Aravas, *Mixed finite-element formulations in piezoelectricity and flexoelectricity*. *Proc. Math. Phys. Eng. Sci.*, vol. 472(2190) pp. 20150879, 2016.
- [3] O. Marco, R. Sevilla, Y. Zhang, J.J. Ródenas and M. Tur, *Exact 3D boundary representation in finite element analysis based on Cartesian grids independent of the geometry*. *Int. J. Numer. Meth. Engng.*, vol. 103(6) pp. 445-468, 2015.