

# **Multiscale Modelling and Molecular Dynamics Characterization of Size Effects in Thin Polymer Films**

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## **ABSTRACT**

A multiscale model of thin polymeric films with size effects is constructed and characterized by molecular dynamics simulations. For this purpose, a continuum model including nonlocal elasticity is employed, whose elastic coefficients are identified by MD simulations on slab models of linear monodisperse polyethylene. Due to long-range effects in such materials, a procedure inspired from Yvonnet et al [1] is employed with different slab thickness to deduce the elastic coefficients. The continuum equations are solved by a FEM discretization and compared to the full MD model.

## **REFERENCES**

- [1] J. Yvonnet, A. Mitrushchenkov, G. Chambaud and Q.-C. He. Finite element model of ionic nanowires with size-dependent mechanical properties determined by ab initio calculations. *Computer Methods in applied Mechanics and Engineering*, Vol. **200**, pp. 614-625, (2011).