Modelling and simulations of polymers across scales and methods

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Abstract

Considering the atomistic or molecular structure of complex materials like polymers is still a challenge since these kinds of materials typically exhibit multiple hierarchical levels spanning a large range of length and time scales. In addition, the formation of entanglements and/or crosslinks of the chain-like macromolecules demand for simulation techniques that can appropriately capture these peculiarities. This, in turn, means that established strategies specifically developed for crystalline materials are usually not sufficient. This contribution discusses briefly the foundations of continuum mechanical and molecular approaches for polymers and introduces the Capriccio method as a means to link molecular dynamics and the finite element method to consider molecular processes for typical engineering applications at the macroscale. By design, the Capriccio method is a multiscale domain-decomposition strategy that employs the fine-scale, discrete atomistic or molecular description only in regions of a specimen exposed to high loads or exhibiting, e.g., material or geometric discontinuities. Some examples from recent research activities in the context of fracture of amorphous materials highlight the capabilities of the Capriccio method.

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