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Revised boundary conditions for FE-MD multiscale coupling of amorphous polymers

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Due to their versatility, polymer nanocomposites have become an indispensable class of materials in recent years. Classical simulation approaches like the Finite Element method (FE) often struggle to predict such composite materials' behavior since they cannot account for molecular effects taking place, particularly in the additives' vicinity. To incorporate these effects, many multiscale formulations coupling continuum mechanics with particle descriptions have been proposed. One promising candidate, focusing on amorphous polymers, is the Capriccio Method introduced by Pfaller et al. [1]. They implement a coupling of FE and molecular dynamics (MD) by introducing a handshake region, the so-called bridging domain where information is transferred via virtual particles. The method has proved its capabilities in various studies, e.g., deriving nanocomposites' interphase properties [2,3]. So far, the Capriccio method relies on stochastic boundary conditions (SBC) to confine the particles and create a thermodynamic state. However, these SBCs require cutting any protruding molecule and thus an unphysical change of the microstructure. To address this problem, we extend the SBCs by adding an outer layer of particles governed by the continuum deformation enabling us to generate coupled FE-MD samples whose density matches a periodic MD solution. Combining these new boundary conditions with the inelastic extension of the Capriccio method proposed in [4] allows us to predict amorphous polymers' stress-strain behavior under arbitrary loading accurately. This extension enhances the Capriccio method's performance and will be useful in future studies of polymer nanocomposites.

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