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DISCRETE-TO-CONTINUUM COUPLING OF PRE-DEFORMED THERMOPLASTIC POLYMERS

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Multiscale methods coupling atomistic models with a continuum offer great potential to understand material behaviour across the scales. In [1], Pfaller et. al developed the Capriccio method to couple a continuum, which is treated by the Finite Element Method (FEM), with a region at molecular resolution. This domain-decomposition approach is specifically designed to investigate amorphous thermoplastic polymers and is able to consider the rather complex molecular dynamics (MD) procedures required to deal with this kind of material.
Embedded in our long-term research envisioning multiscale fracture simulations of polymers, the present project aims at introducing adaptivity to the Capriccio method. With such a technique at hand, simulations of cracks propagating through polymer materials with only the vicinity of the crack tip treated at molecular resolution would become possible.
An essential prerequisite is to switch between FE and MD descriptions depending on the local load level in arbitrary sub-domains. This, in turn, implies that the change of description is necessary at a certain deformation state and thus requires an appropriately pre-deformed MD domain. In a preceding study, we have shown that such an MD region can be obtained with less computational effort using a hybrid MD-CM approach that accelerates the simulation by skipping part of the MD time steps.
In this contribution, we investigate the coupling of an FE domain at a certain deformation state with an MD region that is pre-deformed in two different ways: The first option is the standard MD approach, whereas our hybrid MD-CM method is the second one. We consider polystyrene at coarse-grained (CG) resolution and use the inelastic Capriccio method [2] to study the system behaviour of the coupled MD-FE system under uniaxial loading. In view of later, our specific focus is on the appropriate choice of boundary conditions used during the MD system preparation: In case of non-affine deformations, which must be considered as the standard case for general loadings, classical periodic boundary conditions (PBC) cannot be used to pre-deform the MD region. Instead, non-periodic boundary conditions, as for instance the stochastic boundary conditions (SBC) employed in the Capriccio method, have to be chosen.

References

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