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AN ADAPTIVE MULTISCALE COUPLING METHOD FOR THERMOPLASTIC POLYMERS

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In order to investigate polymer fracture across the scales and thus to understand its relevant mechanics, the application of multiscale methods is of significant importance. Such techniques offer great potential since they can take into account the various processes at different levels of resolution. With the Capriccio method, Pfaller et al. [1] developed a novel partitioned-domain method, which couples a continuum treated by the finite element method (FEM) with a particle-based region employing molecular dynamics (MD). This domain-decomposition approach is specifically designed to investigate amorphous thermoplastic polymers and the associated processes occurring in these complex materials.

Our present project extends the initial Capriccio method towards adaptivity, such that the individual levels of resolution can be selected based on the current local load state a specific region is subjected to. This enables to describe only the vicinity of the crack tip at atomistic or molecular scale, which moves according to the propagating crack. In the rest of the domain, in turn, a coarser continuum treatment is sufficient and hence reduces the numerical effort for the entire system. This requires an adaptive switching between MD and FE descriptions according to the current local load level in specific subdomains. An important prerequisite for this is to provide pre-deformed MD and FE regions to substitute their associated coarser or finer counterparts depending in the individual load states.

In this contribution, we present an adaptive discrete-to-continuum coupling scheme, which provides the basis for scale bridging simulations of amorphous thermoplastic polymers. We generate the specific deformation state of the molecular system without time-consuming recalculations using a hybrid molecular dynamics-continuum mechanics (MD-CM) approach [2]. Moreover, we pass MD deformations to FE by utilizing local space averaging of microscopic quantities. We employ atactic polystyrene at coarse-grained (CG) resolution and use the Capriccio method for coupled MD-FE uniaxial deformation simulations.

REFERENCES

[1] S. Pfaller, M. Rahimi, G. Possart, P. Steinmann, F. Müller-Plathe and M. Böhm, An Arlequin-based method to couple molecular dynamics and finite element simulations of amorphous polymers and nanocomposites. *Comp. Meth. Appl. Mech. Eng.*, Vol. **260**, pp.109–129, 2013.

[2] C. Bauer, M. Ries and S. Pfaller, Accelerating molecular dynamics simulations by a hybrid molecular dynamics-continuum mechanical approach, *submitted manuscript*, 2021.