PARTITIONED-DOMAIN PARTICLE-CONTINUUM COUPLING METHODS FOR SIMULATIONS OF INELASTIC AMORPHOUS POLYMER-BASED NANOCOMPOSITES

Wuyang Zhao*, **Sebastian Pfaller**

Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
* wuyang.zhao@fau.de

Partitioned-domain particle-continuum coupling methods can find a compromise between accuracy and computational cost by only treating regions of specific interest at atomistic resolution while considering the remaining region at continuum resolution. Most partitioned-domain methods are designed for crystalline materials and cannot be applied to polymer-based nanocomposites (PNCs) due to their amorphous structures and inelastic mechanical behavior. We present the Capriccio method as a particle-continuum coupling technique for PNCs based on [1], which introduces artificial anchor points in the bridging domain to communicate between the particle domain and the continuum. The Capriccio method was initially limited to small deformations within the elastic regime and has been recently extended to inelastic deformation by employing a viscoelastic-viscoplastic constitutive model for the continuum [2]. This extended Capriccio method is validated by comparing its averaged stress-strain curves to coarse-grained molecular dynamics simulations of glassy polystyrene under different loading conditions. In this presentation, we further investigate the advantages and limitations of the Capriccio method in multiscale simulations of glassy silica-polystyrene nanocomposites. In addition to averaged mechanical properties, the local stress and deformation in the vicinity of silica particles are also taken into account and compared to pure coarse-grained molecular dynamics simulations.

References

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

[2] W. Zhao, P. Steinmann and S. Pfaller. A particle-continuum coupling method for multiscale simulations of viscoelastic-viscoplastic amorphous glassy polymers. *Submitted.*