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Multiscale Simulations of Polymers with the Hybrid Capriccio Method

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Particle-based considerations take into account the specific atomistic or molecular structure of matter and may thus consider effects originating from very small time and length scales, which are usually not accessible by continuum mechanics. However, due to the huge number of particles to be captured, particle-based methods are restricted to very small amounts of material. In recent years, hybrid schemes have been proposed to benefit from advantages of both approaches. Whereas most of them have been developed for crystalline materials, our novel Capriccio method is suited for amorphous polymers: we embed a particle-based region treated by molecular dynamics (MD) at finite temperature into a larger continuum solved by the finite element method (FEM). The continuum overlaps with the particle domain in a so-called bridging domain, where an energy-based coupling together with a suitable kinematic constraint is established. Our recent publications [1, 2] demonstrate the suitability of Capriccio method to study the complex behaviour of nanoscaled filler particles embedded into a polymer. In these kind of materials, the interphases between filler particles and polymer matrix are of particular interest, but barely accessible by continuum approaches due to the lack of reliable constitutive descriptions.

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