**Concurrent coupling between a particle simulation and a continuum description: case study of a polymer blend** MARCUS MUELLER, Institut fuer Theoretische Physik, Georg-August-Universitaet — We introduce a numerical scheme that concurrently couples a particle simulation of a multi-component polymer melt to a continuum description. We use a soft, coarse-grained model in the particle simulation and a time-dependent Ginzburg-Landau approach for the continuum description. The coupling between the particle coordinates and the order-parameter field, $m$, (e.g., composition) allows us to estimate the parameters the free-energy functional, $\mathcal{F}_{GL}[m]$, and the non-local Onsager coefficient of the Ginzburg-Landau approach. It makes the particle model follow the time-evolution of the order-parameter field and can be exploited to speed-up the particle simulation. The algorithm is based on the separation between the strong bonded interactions, which dictate the dynamics of the particle simulation, and the weak non-bonded interactions, which control the kinetics of the order-parameter field. A detailed analysis is presented for the spinodal decomposition of a binary polymer blend based on the Random-Phase Approximation and Monte-Carlo simulations. Generalizations to other systems will be discussed.

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