

Abstract Submitted
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Fluctuating Field-Theoretic Polymer Simulations of Multispecies Melts and Composites KRIS DELANEY, WEI LI, DOMINIK DUECHS, GLENN FREDRICKSON, UC Santa Barbara — We discuss computational strategies for conducting efficient and stable beyond-mean-field simulations of complex multi-species block polymer melts and composites, with composition fluctuations included through complex Langevin sampling. Our framework is applicable to assemblies of polymer chains of a variety of architectures with interactions introduced through a matrix of Flory-Huggins parameters. We demonstrate the stability, efficiency, and accuracy of a multi-species exchange mapping, and apply the method to the study of fluctuation-induced microphase structures in blends and composites.

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