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Field-Theoretic Polymer Simulations: At the Frontier

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I will review our recent work on the development of a theoretical framework and numerical strategies for conducting computer simulations of polymer field theory models. We invoke Hubbard-Stratonovich and related auxiliary field transforms to convert "particle-based" models of polymeric fluids into statistical field theories. This transformation has the effect of replacing polymer-polymer interactions with polymer-field interactions, and renders the action complex. We have developed efficient numerical techniques for computing saddle point field configurations (mean-field or SCFT solutions), as well as for sampling field fluctuations near or away from saddle points ("field-theoretic simulations"). This talk will focus on a number of contemporary topics including: high resolution and variable cell shape SCFT, geometrically complex domains, hybrid particle-field simulations, and strategies for avoiding the sign problem. Examples of applications to polymer alloys, block copolymers, and copolymer nanocomposites will be presented.