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Free Energy Estimation in Field-Theoretic Simulations GLENN FREDRICKSON, ERIN LENNON, KIRILL KATSOV, UC Santa Barbara — A new technique is presented for computing absolute and relative free energies of polymeric fluids in the context of field-theoretic simulations. Complex Langevin sampling is combined with a thermodynamic integration scheme to provide access to free energies of homogeneous and inhomogeneous polymer phases. The scheme utilizes a harmonic crystal reference state whose free energy can be computed analytically. The method is demonstrated in the context of the order-disorder transition of diblock copolymer melts.

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