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Field theoretic simulations in the Gibbs ensemble ROBERT RIGGLEMAN, GLENN FREDRICKSON, University of California, Santa Barbara — Measuring the properties of phases in equilibrium and the calculation of phase diagrams is one of the most common applications of field theoretic simulations. To obtain properties of both phases from one simulation (such as the concentration of a species in each phase), it is necessary to perform simulations large enough so that the interface between the two phases does not affect the estimate of the bulk properties, which is computationally very demanding. Alternatively, one can perform a sweep through parameter space searching for multiple state points that meet the criteria for equilibrium, which is again computationally expensive. In this talk, I will describe how we have adapted the Gibbs ensemble to field theoretic simulations, where two simulation boxes are kept in chemical and mechanical equilibrium by allowing the boxes to exchange both particles and volume. By maintaining a constant total number of particles and total volume, such a simulation can efficiently simulate two bulk phases in equilibrium in the canonical ensemble, allowing a reliable estimate of the properties of the two phases. Our method will be demonstrated in both the mean-field limit and in simulations that fully sample the fluctuations of the field theory.

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