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Abstract for an Invited Paper for the MAR12 Meeting of the American Physical Society

Simulations of Strongly Correlated Systems¹

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The field of strongly correlated systems is one of the most active areas in condensed matter physics. This interest is motivated, in part, by a variety of complex emergent phenomena, including high-temperature superconductivity, quantum criticality and complex phases induced by electron-phonon couplings. The recent very rapid development of high performance heterogeneous computer platforms together with a similar emergence of highly accurate many-body algorithms allow the treatment and modeling of complex correlated material systems which were intractable just a few years ago. Important progress has been made by the development of finite size methods, including exact diagonalization and Quantum Monte Carlo techniques. However, due to the minus sign problem, these methods are limited to small lattice sizes. Another successful approach is the dynamical mean field approximation and its cluster extensions, which treat the local or short-ranged dynamical correlations exactly and non-local or long-ranged correlations in a mean field approximation. Due to the effective medium, the Fermion minus sign problem is much milder than that found in finite sized simulations. However, it is still the primary limitation of these methods. To address this problem, multiscale approaches are used which treat only the correlations at the shortest length scales with exact cluster solvers, intermediate length scales are treated using a diagrammatic approach, such as the parquet equations or the dual-fermion formalism and, the longest length scales are captured by the mean field. I will discuss how these new algorithms impact a few model systems including our understanding of quantum criticality in the Hubbard and Anderson model, new phases in ultracold quantum gases, spintronics materials and the role of electronphonon interaction. I will conclude discussing recent algorithm redesign motivated by the evolution towards hybrid multicore architectures employing graphical processing unit (GPU).

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