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A New Lanczos-Based Low Rank Algorithm for Inhomogeneous Dynamical Mean-Field Theory[1] PIERRE CARRIER, YOUSEF SAAD, University of Minnesota, JAMES K. FREERICKS, Georgetown University — Inhomogeneous DMFT is used to approximately solve models of ultracold atoms in optical lattices. The intensive part of the IDMFT algorithm is the solution of the Dyson equation for the local Green's function, which involves the computation of the diagonal of the inverse of a sparse matrix. Our new algorithm for finding the diagonal of the inverse of a large sparse matrix is based on domain decomposition into interior and interface points. Since the number of interface points is much less than the interior points, it is a low-rank matrix. Using this matrix allows for a much smaller number of Lanczos steps to obtain the exact solution of the diagonal of the inverse and hence reduces the need for as many re-orthogonalization steps in Lanczos. We show that the problem of finding the diagonal of the inverse is transformed into a naturally parallel GMRES solver (based on the domain decomposition) solved at each of the Lanczos iterations. We successfully implemented a coarray fortran (CAF) program code of this new algorithm for the 2D Fermionic-Bosonic Falicov-Kimball Hamiltonian (mixture of light and heavy atoms). Results of parallel performance and advantages of using a CAF implementation are discussed, in terms of a 3D implementation which is planned for the Hubbard model.

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