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LOW-RANK UPDATING ALGORITHMS FOR DISORDERED MATERIALS SYSTEMS

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ABSTRACT

Many of statistical physics based models used in computational materials science applications involve problems in which a basic linear algebra sub-problem is repetitively solved during each of the simulation steps. For example, investigation of material fracture of disordered systems using discrete lattice systems involves repetitively solving a new, large system of equations each time a lattice bond fails. Failure of a bond is equivalent to a low-rank downdating of the original system of equations. Similarly, Monte Carlo (MC) simulation of a strongly correlated electron or spin-fermion systems involves repetitive computation of eigenvalues of a new Hamiltonian matrix each time a local change is accepted. Each of these local changes in MC simulation is equivalent to a low-rank updating of the Hamiltonian matrix. Thus, an important feature of such problems is that successive matrices differ by a low-rank update/downdate.

Traditional algorithms employ repetitive computation techniques wherein the linear algebra sub-problem is repetitively solved during each of the simulation steps. This poses a significant computational challenge even for modern supercomputers since a large number of MC steps are required to solve the problem. Furthermore, the linear algebra sub-problem involved in each of these MC steps does not scale well and the computational complexity of these sub-problems increases as $\mathcal{O}(N^3)$, where N is the size of the matrix. On the other hand, since successive matrices differ by a low-rank update, an updating scheme of some kind is likely to be more efficient than employing a repetitive computational technique during each of the MC steps.

This work presents algorithms based on low-rank updates, namely, a multiple-rank sparse Cholesky algorithm for efficiently computing the successive solutions of linear systems, and an algorithm for recomputing eigenvalues when successive Hamiltonian matrices differ by a low-rank update.

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