Low-rank update algorithms for Strongly Correlated Systems

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Many of statistical physics applications involve problems in which a basic linear algebra sub-problem is repetitively solved during each of the simulation steps. For example, Monte Carlo (MC) simulation of a strongly correlated electron system involves repetitive computation of determinant of a new Greens function 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 Greens function matrix.

Traditional algorithms employ repetitive computation techniques wherein the matrix determinant is repetitively computed 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, determinant computation 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 Greens function 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 for efficiently computing the determinant of successive matrices when these successive Greens function matrices differ by a low-rank update. This algorithm significantly increases the speedup of simulation of strongly correlated systems modeled using the Hubbard model.

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