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Optimization of Large Scale Matrix Computations for Multi-length Scale Structured Matrices[1]

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Quantum monte carlo simulation of interacting electron systems is an increasingly powerful tool in investigating many of the most fundamental properties of materials, such as their magnetic and optical response, and conductivity. However, the simulations are currently limited to a few hundred particles. The primary bottleneck is the calculation of the inverse of a multi-length and highly structured matrix. In this talk, we will report our recent progress on this problem. We first present a semi-direct solver which is numerically stable and robust by a novel self-adapting block cyclic reduction technique depending on the parameters of the problem. The new solver is more than an order of magnitude faster than existing techniques. Then we will present robust preconditioning techniques in iterative solvers which can effectively precondition the matrices at much stronger coupling and lower temperatures than had hitherto been possible.

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[2]Joint work with Wenbin Chen, Richard Scalettar and Ichitaro Yamazaki