Highly Parallel Solver for Multi-scale Parquet Quantum Modeling of Strongly Correlated Materials

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The parquet formalism to calculate the two-particle Green's functions of large systems requires the solution of a large sparse complex system of quadratic equations. If Nf Matsubara frequencies are used for a system of size Nc, and Newton's method is used to solve the nonlinear system, the Jacobian system has O(Nt^3) variables and O(Nt^4) complex entries where Nt = Nc*Nf . For Nt = 256, the nonlinear system has over 134 million degrees of freedom and the sparse Jacobian will require over 2.7 TBytes of memory. The Jacobian is normally too large to store but the matrix-vector products can be computed directly. Homotopy continuation method is used to generate close initial guesses and the Jacobian linear system is solved by a Krylov iterative method. We report on the progress of developing a highly scalable parallel solver that uses both OpenMP and MPI to exploit the multicore nodes on leadership class supercomputers.