Highly parallel solver for multi-scale parquet quantum modeling of strongly correlated materials*

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Abstract. 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 N_f Matsubara frequencies are used for a system of size N_c, and Newton's method is used to solve the nonlinear system, the Jacobian system has $O(8N_t^3)$ variables and $O(40N_t^4)$ complex entries where $N_t = N_c N_f$. For $N_t = 1024$, the nonlinear system has over 8.5 billion degrees of freedom and the sparse Jacobian will require over 351 TBytes of memory. The Jacobian is very expensive to store but the matrix-vector products can be computed directly. We are developing a highly scalable parallel solver that uses both OpenMP and MPI to exploit the multicore nodes. We present initial scalability results on the Cray XT5 that suggests the code can be scaled to solve larger problems with $N_t \geq 1024$.

1. Introduction

The two-dimensional Hubbard model has been accepted in the community as a minimum model to study the high-temperature superconducting cuprates. An adequate solution of this model is extremely challenging, especially in the interesting parameter regime of intermediate to strong coupling, where the Coulomb repulsion between electrons is of the same order or stronger than the electronic kinetic energy. Despite some recent success, our understanding of the properties of this model in this regime is therefore still limited.

The Hubbard Hamiltonian on a square lattice is written as

$$H = \sum_{\langle i,j \rangle} (t_{i,j} - \mu) c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \tag{1}$$

where $c^{\dagger}_{i,\sigma}$ (ci,σ) creates (destroys) an electron with spin σ on site i and $n_{i,\sigma} = c^{\dagger}_{i,\sigma}\ c_{i,\sigma}$ is the corresponding occupation operator. The first term describes the hopping of electrons between sites i

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and j and the second term stands for the Coulomb repulsion U two electrons feel when residing on the same site.

Perturbation theory provides useful results only in the limits of either weak or strong coupling, but fails in the interesting regime of intermediate coupling. Methods employing resummations of Feynman diagrams to infinite order are usually biased due to the particular choice of diagrams. Exact methods such as Quantum Monte Carlo (QMC) and exact diagonalization are restricted to relatively small system size due to the computational complexity. In principle, one can imagine carrying out an analytical calculation which includes all the Feynmann diagrams. This would theoretically yield exact results on the single-particle and two-particle levels if one manages to include all relevant diagrammatic equations up to that level.

The parquet formalism is based on a two-particle self-consistent theory, where all the relevant physical conservation rules are preserved as well as the crossing symmetries at two-particle level are obeyed. It is based on the following four diagrammatic equations. To simplify the formalism, we consider systems that preserve the spin $SU(2)$ symmetry. We denote $\kappa \equiv (\mathbf{k}; i\omega_n)$ and $\nu \equiv (\mathbf{k}, i\nu_n)$ with $\omega_n = (2n+1)\,\pi T$ and $\nu_n = 2n\pi T$. In the following, r is used as a general label for $r = d, m, s, t$ which label the particle-hole density and magnetic channels (d and m), and the particle-particle singlet and triplet channels (s and t). All indexes are in modulo arithmetic so that a negative index such as $-\kappa$ is equal to mod $(N_t - \kappa, N_t)$.

– The Dyson equation

$$G^{-1}(k) = G_0^{-1}(k) + \Sigma(k) \tag{2}$$

– The Schwinger-Dyson equation

$$\Sigma(k) = -(T/N)^2 \frac{U}{2} \sum\nolimits_{k',v} G(-k'+v)\, G(k')\, G(-k+v)\, F_s(v)_{-k',-k}\,, \tag{3}$$

– The Bethe Salpeter equation

$$F_r(v)_{k,k'} = \Gamma_r(v)_{k,k'} + \sum\nolimits_{k''} F_r(v)_{k,k''}\, \chi_r^0(v)_{k''}\, \Gamma_r(v)_{k'',k'} \tag{4}$$

for $r = d, m, s, t$, and with

$$\begin{aligned} \chi_r^0(v)_{k''} &= G(k'')\, G(k''+v)\,, \quad r = d, m \\ \chi_r^0(v)_{k''} &= -\tfrac{1}{2} G(k'')\, G(k''+v)\,, \quad r = s, t \end{aligned} \tag{5}$$

– The Parquet equation

$$\begin{aligned} \Gamma_d^{ph}(v)_{k,k'} &= \Lambda_d^{ph}(v)_{k,k'} - \tfrac{1}{2}(\Phi_d + 3\Phi_m)(k-k')_{\tilde{k},k'} + \tfrac{1}{2}(\Psi_s + 3\Psi_t)\left(k+\tilde{k}\right)_{-k',-\tilde{k}} \\ \Gamma_m^{ph}(v)_{k,k'} &= \Lambda_m^{ph}(v)_{k,k'} - \tfrac{1}{2}(\Phi_d - \Phi_m)(k-k')_{\tilde{k},k'} - \tfrac{1}{2}(\Psi_s - \Psi_t)\left(k+\tilde{k}\right)_{-k',-\tilde{k}} \\ \Gamma_s^{pp}(v)_{k,k'} &= \Lambda_s^{pp}(v)_{k,k'} + \tfrac{1}{2}(\Phi_d - 3\Phi_m)(k-k')_{\tilde{k},-k} + \tfrac{1}{2}(\Phi_d - 3\Phi_m)\left(k+\tilde{k}\right)_{-k',-k} \\ \Gamma_t^{pp}(v)_{k,k'} &= \Lambda_t^{pp}(v)_{k,k'} + \tfrac{1}{2}(\Phi_d + \Phi_m)(k-k')_{\tilde{k},-k} - \tfrac{1}{2}(\Phi_d + \Phi_m)\left(k+\tilde{k}\right)_{-k',-k} \end{aligned} \tag{6}$$

where $\tilde{\kappa} = \kappa' + \nu$,

$$\begin{aligned} \Phi_r(v)_{k,k'} &= \sum\nolimits_{k''} F_r(v)_{k,k''}\, \chi_r^0(v)_{k''}\, \Gamma_r(v)_{k'',k'}\,, \quad r = d, m \\ \Psi_r(v)_{k,k'} &= \sum\nolimits_{k''} F_r(v)_{k,k''}\, \chi_r^0(v)_{k''}\, \Gamma_r(v)_{k'',k'}\,, \quad r = s, t \end{aligned} \tag{7}$$

and for $r = d, m$, it is labeled as Φ; while for $r = s, t$, labeled as Ψ.

The parquet equations are derived from enforcing two-particle crossing symmetries, while the other equations are necessary for a conserving approximation. The above set of equations, however, does not form a closed loop because the fully irreducible vertices, Λ_r, are not determined internally. When Λ_r is replaced by the bare interaction, one obtains the parquet approximation. One can also imagine taking the results of an exact calculation for a small system size, using e.g., exact diagonalization or QMC methods, as an input for Λ_r in the parquet equations. In this case, one obtains the full multi-scale parquet formalism, that has been discussed in [9].

2. Algorithm

The parquet equations (2) to (7) form a system of nonlinear equations. The strength and spatial range of correlations depends on the ratio between the Coulomb repulsion U and temperature T and the nonlinear system becomes increasingly difficult to solve for large U. Each entity such as $\Gamma_t^{pp}(\nu)\ \kappa, \kappa'$ or $Fr(\nu)\ \kappa_1, \kappa_2$ can be discretized and represented as three-index $N_t \times N_t \times N_t$ arrays $\Gamma_t(\kappa_1, \kappa_2, \nu)$ and $F^r(\kappa_1, \kappa_2, \nu)$. A simple algorithm is to perform fixed-point iteration by freezing some of the unknowns to solve a subset of the nonlinear equations. Starting from an initial guess, we can solve the Bethe Salpeter equation (4) to generate $F_r(\nu)\ \kappa_1, \kappa_2$. The Φ_r and Ψ_r values can be updated using the new F_r values using (7). The new $\Gamma_r(\nu)\ \kappa, \kappa'$ values are computed by the Parquet equations (6). One can iteratively solve (4) and (6) until convergence, then update the Dyson equation and self energy in (2) and (3). Although this method is efficient and simple to implement, the iterations may become unstable for large values of $U \geq 18$.

A careful examination of the system shows that the Bethe Salpeter equations can be written as

$$\begin{aligned} F_r(v)_{k,k'} &= \Gamma_r(v)_{k,k'} + \Phi_r(v)_{k,k'}, \quad r = d, m \\ F_r(v)_{k,k'} &= \Gamma_r(v)_{k,k'} + \Psi_r(v)_{k,k'}, \quad r = s, t \end{aligned} \tag{8}$$

so that the Bethe Salpeter equations and the Parquet equations can be written as linear expressions in F_r, Γ_r, Φ_r, and Ψ_r. The nonlinearity comes mainly from the Φ_r and Ψ_r variables that are products of just $F_r(\nu)$ and $\Gamma_r(\nu)$; therefore (4) to (7) form a complex system of affine quadratic equations.

The literature is sparse on methods for solving a general system of quadratic equations. The solution of a system of quadratic equations using Newton's method has been analyzed in [6]. It shows that multiple solutions are possible and the Jacobian matrix may be exactly singular if it is evaluated at a midpoint of two solutions. Cohen and Tomasi [3] have considered the solution of a special case of a system of homogeneous bilinear equations. Their results show the problem is related to solving the generalized eigenvalue problem. Bouaricha and Schnabel [7,1,2] have considered an extension of the Newton's method to solve $F(x) = 0$ by including a low rank tensor approximation of higher derivatives

$$M(x_c + d) = F(x_c) + F'(x_c)d + \frac{1}{2}T_c dd, \quad F : \mathbb{R}^n \to \mathbb{R}^m\,, \tag{9}$$

where T_c is a three index tensor object formed by interpolation of past Newton steps. The tensor T_c is not the second derivative of $F(x)$ but is chosen to be a sum of p rank-one tensor objects. Equation (9) may be viewed as a particular system of quadratic equations. Ultimately, Newton's method or Levenberg-Marquardt method is used to solve (9) in a least squares sense as a smaller system of p

quadratic equations. The analysis of quadratic matrix equation $AX^2 + BX + C = 0$ in $n \times n$ matrices and the connection to quadratic eigenvalue problem $(\lambda^2 A + \lambda B + C)x = 0$ have been considered by Higham and Kim [4]. The authors used Newton's method with exact line searches [5] to solve the quadratic matrix equations.

We have developed a parallel solver using Newton's method with line search to solve the complex system of biaffine quadratic equations. The unknowns are eight $N_t \times N_t \times N_t$ arrays for F_d, F_m, F_s, F_t, Γd, Γ_m, Γ_s, and Γ_t. The complicated vertex rotations to enforce crossing symmetries in the Parquet equations (6) can be viewed as permutation operations on a long vector of length N_t^3. The permutation is implemented using the Message Passing Interface (MPI) all-to-all communication primitive. This operation places high demands on the communication network and is one of the most time consuming kernels. The sparse Jacobian matrix of the bilinear quadratic equations can be analytically computed but it has $O(40N_t^4)$ nonzeros. For problems of interest $N_t \geq 256$, the sparse Jacobian matrix is very costly to store in memory. For example, if $N_t = 1024$ then there are nearly 8.6 billion degrees of freedom and explicit storage of the sparse Jacobian still requires over 351 TBytes of memory and for a larger case of $N_t = 1280$, there are over 16.7 billion degrees of freedom and storage of the Jacobian requires over 858 TBytes of memory! For this application, we have found that computing the matrix-vector operation by finite differences introduces an unacceptably high error due to numerical cancellation. Instead the action of matrix-vector multiply is computed analytically without explicit formation of the Jacobian. The Φ and Ψ expressions in (7) are simple products of F_r and Γ_r. The interaction of derivatives of Φ_r or Ψ_r with respect to F_r or Γ_r can be computed as *dense complex* matrix products of N_t by N_t matrices. The entries in the Jacobian matrix consist of terms [derived from (7)] such as

$$\frac{\partial \Phi_r(v)_{k,k'}}{\partial \Gamma_r(v)_{k,k''}} = \chi_r^0(v)_{k''}\Gamma_r(v)_{k'',k'} \text{ or } \frac{\partial \Phi_r(v)_{k,k'}}{\partial \Gamma_r(v)_{k'',k'}} = F_r(v)_{k,k''}\chi_r^0(v)_{k''} \ . \tag{10}$$

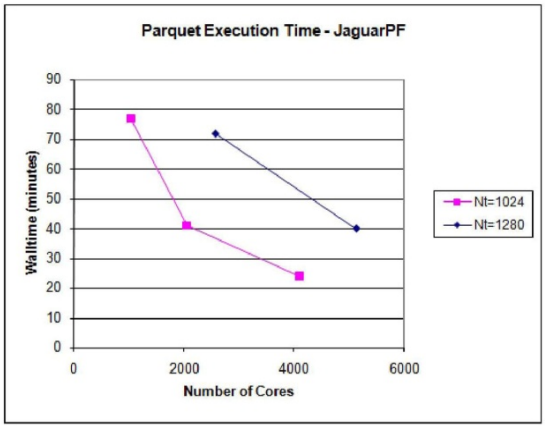
The large sparse Jacobian system is solved using the BICGSTAB(L=2) [8] Krylov iterative method† without preconditioning. Preconditioning using simple Jacobian diagonal scaling is not effective for this problem.

3. Numerical Experiments

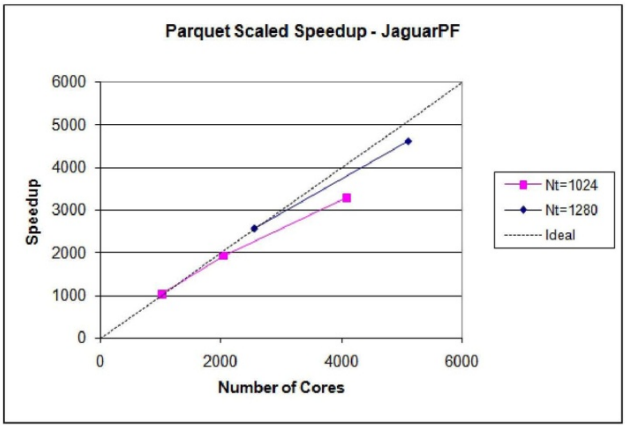
The parquet code has a robust multilevel parallel implementation and has been ported to several parallel machines, including the International Business Machine (IBM) Opteron cluster (Glenn) at the Ohio Supercomputer Center (OSC), the Sun Constellation Linux cluster (Ranger) at the Texas Advanced Computing Center (TACC), the IBM BlueGene/P (Eugene), and Cray XT4/5 (Jaguarpf) at the National Center for Computational Sciences (NCCS) at the Oak Ridge National Laboratory (ORNL).

We present performance for the 4×4 Hubbard cluster model ($N_c = 16$), with parameters, $U = 0.3$, $T = 0.05$, $t = 0.25$ for two cases, using $N_f = 64$ and $N_f = 80$ Matsubara frequencies for problem sizes $N_t = 1024$ and $N_t = 1028$ respectively. For the $N_t = 1024$ case, the number of MPI processes was varies from 256 to 1024, with 4 OpenMP threads per MPI process, using a maximum of 4096 cores. The $N_t = 1280$ case was run with 640 and 1280 MPI processes with 4 threads per process using a maximum of 5120 cores. The plots in Figure 1 show the code performs well despite the need for a large "all-to-all" exchange for tensor rotations.

† The code for bicgstab2 is available at http://www.math.uu.nl/people/vorst/zbcg2.f90



(a) Execution times



(b) Scaled speedup

Figure 1. Strong Scaling plots for the Parquet Solver base on Jaguarpf measurements (Left) Execution times for two problem sizes, on core counts from 1024 to 5120. (Right) Scaled speedup plot for the Parquet code, speedup for each problem size determined relative to measurement of lowest core count.

4. Summary

We have described the development of a parallel solver for multi-scale parquet quantum modeling of highly correlated materials. The code uses Newton's method with line search to solve the large system of affine quadratic equations. The large sparse Jacobian is too large to store and the action of matrix-vector multiply is computed analytically. Performance results on the Cray XT4/5 cluster suggest hybrid OpenMP and MPI programming technique can effectively use large numbers of cores to solve problems with several billion degrees of freedom.

Future development will focus on more sophisticated continuation method for generating good initial guesses and the exploration of effective preconditioners and iterative methods for solving the Jacobian system.

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