Delayed Slater determinant update algorithms for high efficiency quantum Monte Carlo

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Abstract

Within ab initio Quantum Monte Carlo simulations, the leading numerical cost for large systems is the computation of the values of the Slater determinants in the trial wavefunction. Each Monte Carlo step requires finding the determinant of a dense matrix. This is most commonly iteratively evaluated using a rank-1 Sherman-Morrison updating scheme to avoid repeated explicit calculation of the inverse. The overall computational cost is therefore formally cubic in the number of electrons or matrix size. To improve the numerical efficiency of this procedure, we propose a novel multiple rank delayed update scheme. This strategy enables probability evaluation with application of accepted moves to the matrices delayed until after a predetermined number of moves, $K$. The accepted events are then applied to the matrices en bloc with enhanced arithmetic intensity and computational efficiency via matrix-matrix operations instead of matrix-vector operations. This procedure does not change the underlying Monte Carlo sampling or its statistical efficiency. For calculations on large systems and algorithms such as diffusion Monte Carlo where the acceptance ratio is high, order of magnitude improvements in the update time can be obtained on both multicore CPUs and GPUs.

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I. INTRODUCTION

Ab initio Quantum Monte Carlo (QMC) techniques encompass a large class of related methods and algorithms for many-body electronic structure calculations \[1\]. The variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) algorithms in particular have found wide application where the potential accuracy of a full many-body calculation is preferred over mean field methods \[2,3\]. Improvements in computational power as well as important technical improvements to the methods are enabling calculations on more complex systems, recently including cerium metal \[4\], copper oxide based superconductors \[5,6\], and numerous binary transition metal oxides \[7–14\].

Central to all QMC algorithms is the procedure for proposing and accepting Monte Carlo moves. Each Monte Carlo step generally requires proposing a move of a single electron, evaluating the probability of the move, and updating the system state if the move is accepted. For ab initio QMC calculations, Slater-Jastrow trial wave functions are most commonly utilized, consisting of one or more Slater determinants multiplied by a Jastrow correlation factor. In molecular calculations it is now common to use large multideterminant wavefunctions \[15–17\] for small molecules with relatively low electron counts. Great improvement in the evaluation of multideterminant wavefunctions has been made recently by evaluating the changes with respect to only a single reference determinant \[17–19\], as opposed to individually updating all the determinants, thereby enabling the routine use of large multideterminant expansions in QMC. However, today, solid state calculations most commonly use a single determinant and much larger electron counts than molecular calculations due to the requirements of periodic boundary conditions and need to perform finite size scaling. Evaluating these larger determinants can occupy a significant fraction of overall computational time, e.g. 30-50% with electron counts in the thousands, indicating that improved algorithms are desirable, particularly as larger solid state calculations are performed and heavier elements with more valence electrons are studied.

A Slater determinant for a system of $N$ electrons can be represented by:

$$
\Psi(r_1, r_2, \cdots, r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix}
\phi_1(r_1) & \phi_1(r_2) & \cdots & \phi_1(r_N)
\phi_2(r_1) & \phi_2(r_2) & \cdots & \phi_2(r_N)
\vdots & \vdots & \ddots & \vdots \\
\phi_N(r_1) & \phi_N(r_2) & \cdots & \phi_N(r_N)
\end{vmatrix}
$$
where $\phi_{1,2\ldots n}$ represent single-particle wave functions and $r_{1,2\ldots N}$ represent particle coordinates. Evaluating the ratios of this determinant as single particle moves are proposed is key to efficient and affordable QMC simulations. Explicit recalculation of the determinant is an $O(N^3)$ operation which is infeasible to perform at every Monte Carlo step and for large $N$.

If $A$ is the Slater matrix and $A_{\text{new}}$ is the matrix after the proposed particle move for particle at position $r_k$ to $\tilde{r}_k$, the probability $p$ of accepting this move is related to the ratio of determinants, $p \propto \det(A_{\text{new}})/\det(A)$, where $A_{\text{new}} = A + u v'_k$, $v_k$ is $k$-th column of identity matrix, and column vector $u$, where the $i$-th entry $u_i = [\phi_i(\tilde{r}_k) - \phi_i(r_k)]$, $1 \leq i \leq N$ is the change in the $k$-th column of matrix $A$. This probability $p$ can be found via the Matrix Determinant Formula,

$$\det(A + uv'_k) = \det(1 + v'_k A^{-1} u) \det(A).$$

Dividing this equation on both sides by $\det(A)$, the existing determinant, yields the Slater change ratio on the right-hand side.

Note that $A^{-1} u$ is needed in the computation of determinant in Equation (1). The standard technique used in QMC [1, 20] is to construct and maintain an explicit copy of the matrix inverse $A^{-1}$. If the proposed move is accepted, the matrix inverse can be updated using a rank-1 update using the Sherman-Morrison formula [21],

$$(A + uv')^{-1} = A^{-1} - A^{-1} u (1 + v' A^{-1} u)^{-1} v' A^{-1}.$$  

The above procedure works well, but the performance of the rank-1 updating is usually limited by the performance of the matrix-vector operations and memory bandwidth. Therefore it does not run very efficiently on current computer architectures. A more compute intensive algorithm is desirable, particularly as these operations grow in relative cost with increasing $N$.

In this paper we propose a novel algorithm for computing updates to the Slater determinant inverses. The underlying Monte Carlo algorithm remains unchanged, but the numerical efficiency is significantly higher than the traditional algorithm for large matrices. The new algorithm works by delaying the updates until a large block update is eventually performed, allowing the use of matrix-matrix algebra. Although the new algorithm can be used for any QMC algorithm, the efficiency is highest where the acceptance ratio is high, such as in the DMC calculations. These are usually the most computationally expensive to perform.
Although use of rank-1 updates is standard in QMC, we note that blocking of these operations in rank-k like schemes has been used to obtain significant performance gains in other fields [22, 23].

II. ALGORITHM

We begin by observing that in many QMC calculations, the probability \( p \) for accepting a move is high, where \( p \geq 0.99 \). This is the case in projection algorithms such as DMC where a short time step is required to accurately sample the Green’s function. Since the expected average length of a contiguous sequence of accepted moves is \( p/(1-p) \), it is likely that at least \( K \) (where \( K = 32 \), or \( K = 64 \)) consecutive moves will mostly be accepted.

One approach then proposes a sequence of up to \( K \) moves and computes the determinant ratio probability at each step using a generalization of the Matrix Determinant Formula (1)

\[
\det(A + UV') = \det(I_k + V'A^{-1}U) \det(A),
\]

where \( I_k \) is the \( k \) by \( k \) identity matrix, \( U \) is \( N \) by \( k \), and \( V \) is \( N \) by \( k \).

This algorithm requires that after a particle move is proposed and accepted, the move’s application to the Slater matrix is delayed. We advance instead to finding the ratio for the next proposed move. A group of accepted changes is queued in this manner until a preset limit of unapplied moves \( K \) is reached. The sequence of accepted moves is then applied to the Slater matrix together as a rank-k update (for \( k \) accepted moves) using the Sherman-Morrison-Woodbury formula

\[
(A + UV')^{-1} = A^{-1} - A^{-1}U(I_k + V'A^{-1}U)^{-1}V'A^{-1}.
\]

The rank-k update operation can be performed very efficiently as a matrix-matrix multiplication operation using linear algebra libraries such as the Basic Linear Algebra Subroutine Library (BLAS). These are significantly more computationally intensive and less memory bandwidth limited than conventional rank-1 updates, which are matrix-vector operations. The number of moves to delay by, \( K \), can be chosen to optimize performance on a specific computational architecture and for a specific problem size.

Note that the matrix \( I_k + V'A^{-1}U \) is, at most, \( K \times K \), and the calculation of its determinant is much less burdensome than recomputing \( \det(A) \). Up to \( K \) of these smaller
determinants are computed prior to each update to $A$; we term this process look-ahead. Since the $I_k + V'A^{-1}U$ matrices are relatively small (for low values of $K$), note that in our initial testing the determinant look-ahead work is performed on CPU, even for our GPU-accelerated implementations.

It is important to see that since every move has a distinct, individual acceptance probability, our delayed update approach is entirely equivalent to the classical method of performing each particle move one move at a time, and this algorithm should not be interpreted as a multiple-particle algorithm. The Monte Carlo algorithm is unchanged at the simulation level. Only the numerical implementation is changed.

An important question relates to the handling of rejected moves. One possibility would be to perform the matrix updates whenever a rejected move is encountered. However, this would not allow for significant delay for methods such as VMC where the acceptance ratio $p \approx 0.25 - 0.75$. As we will see numerically in Sec. III matrix update delays of tens to hundreds of moves are desirable. Instead we prefer to treat rejected moves similarly to an accepted move, only substituting the unchanged (“unmoved”) matrix columns. When the number of accepted moves has reached the preset limit $K$, then the matrix inverse is updated using the Sherman-Morrison-Woodbury formula in Equation 4 and dense matrix-matrix operations. This variant has the advantage that even if the probability of acceptance is not high, say $p = 0.5$, the rank-k operation can still maintain high performance by using effective values of $K = 32$ or $K = 64$. While the performance is therefore proportional to $p$, as we will see in Sec III the performance increase compared to rank-1 updates is great enough that the new scheme can be applied even where the acceptance is low ($p < 0.5$).

Although not explored here, we note that the above variant also simplifies the use of batched update operations across multiple walkers since each operation will be performing exactly the same amount of work in the rank-$K$ update to the matrix inverse. Batching of update operations for small $N$ is desirable on GPUs due to their greater concurrency requirements than conventional CPUs [24]. We also note that the new algorithm could be combined with that of Ref. [19] for the multideterminant case.
III. PERFORMANCE RESULTS

To test the new algorithm we developed a test application that assumes 100% acceptance probability. The performance is therefore closely representative of a DMC calculation with a small time step, and typical of production DMC calculations where the majority of compute time for QMC investigations is spent. Depending on the sophistication of the final implementation, we expect QMC simulations with lower acceptance probability to obtain proportionately lower performance.

We developed a prototype CPU implementation and also a prototype GPU implementation where the work is shared between CPU and GPU. The implementation used the current QMCPACK code [25] as a reference, which we expect is similar to other QMC codes. Vendor optimized BLAS was used for the CPU timings. Our GPU implementation performs only the final and most computationally intensive matrix updates on the GPU. These matrices are stored in the GPU memory. The CPU is used for other steps of the algorithm. For both CPU and GPU performance we therefore expect that a somewhat higher performance could be achieved with additional optimization. For example, the look ahead operations are not threaded, penalizing performance for large $K$. For small problem sizes, performance might also be sensitive to memory layout. Simultaneous updates of multiple matrices or “batching”, as is performed by the current QMCPACK GPU implementation [24], was not explored. The batching of operations reduces GPU kernel launch overhead and might also be explored on CPUs for improved memory prefetching.

Performance is measured in Monte Carlo column updates per second. Each measurement involved a complete sweep of updates through the full matrix of size $N$, with a full accounting of the look ahead cost in the delayed updating scheme. Numerical values of the determinants were checked versus direct calculation after a full update sweep. For every combination of matrix update delay and matrix size, we performed five runs to reduce any scatter from system interruptions. Limited scatter in timings was observed for the smallest $N = 256$ and $N = 512$. Scatter for larger matrices was negligible. Timings were obtained on an Intel Xeon workstation with NVIDIA K40 GPUs using the Intel 2017 compilers, Intel MKL BLAS implementation, and NVIDIA CUDA 8.0. Because our algorithm improves memory bandwidth utilization, we expect similar performance trends to be obtained on all current and upcoming architectures from ARM, AMD, IBM, Intel, and NVIDIA (etc.).
The absolute measured performance for different update delays and matrix sizes is shown in Fig. 1. The proportionate speedups relative to the conventional algorithm $K = 1$ are shown in Fig. 2. The delayed update algorithm shows performance improvements for all tested matrix sizes, with a generic shape to all of the performance curves. For $N = 256$ and $K = 2$ we obtain a limited speedup of $1.8 \times$, increasing to an optimum $5.6 \times$ for $K = 16$. Above this the speedup is reduced and is eventually lower than the conventional $K = 1$ algorithm. This is because the naive explicit calculation of as many as $K$ determinants of square matrices at most $K$ in size during the determinant look-ahead process eventually becomes a significant computational burden. A refined implementation could delay this turnover to larger $K$. For practical simulations the optimum $K$ could be chosen automatically via an autotuner.

With increased matrix size $N$ we observe in Fig. 2 a general trend of greater speedups relative to $K = 1$ and a general trend to a higher delay factor $K$ being optimal. Many of recently published QMC calculations have $N \sim 512$ (for $\sim 1024$ total electrons, accounting for electron spins), and an $N = 2000$ calculation (4000 total electrons) was already published in 2012 26. For $N = 1024$ we find an optimal $K = 64$ and speedup of $7.2 \times$.

The GPU implementation displayed very similar properties to the CPU implementation in Fig. 3. Similar optimum $K$ are found as for the CPU implementation. The peak speedups are higher due the GPU numerical library’s internal use of more threads in the matrix-matrix operations, but the turnover to lower performance occurs more sharply than the CPU implementation. This is in part due to the use of a single threaded CPU-size implementation of the look-ahead process and could be further optimized.

With the aim of reducing the time per update further, we also investigated use of multithreaded BLAS in the update operations, relying solely on the vendor threaded libraries. As shown in Fig. 4 threading provides increased benefit with large $K$. For $N = 2048$, 8 threads improve the traditional $K = 1$ Sherman-Morrison performance by $32\%$ relative to the single threaded result. However, with optimum $K = 128$ and the delayed scheme, 8 threads give a speedup of $40.0 \times$ relative to the threaded $K = 1$ result, or $52.9 \times$ over the singly thread $K = 1$ case. The delayed update algorithm therefore significantly improves the utility of threads in reducing matrix update time in QMC.
IV. CONCLUSIONS

We have presented a simple and novel algorithm for improving the performance of updating the Slater determinants in QMC by using the determinant formula to delay applying updates to the explicit matrix inverse. Despite the increased cost of obtaining intermediate values, significant net speedups are obtained over the traditional Sherman-Morrison algorithm. Order of magnitude speedups are obtained with matrix sizes around 1000 on both CPU and GPU systems, with greater speedups obtained for larger matrices. These sizes are similar to those of numerous recent solid state QMC calculations. We encourage adoption in production QMC codes.

Raw data, scripts to recreate all figures in this manuscript, and additional analyses for both CPU and GPU implementations are available at [http://www.materialsdatafacility.org](http://www.materialsdatafacility.org) and [http://dx.doi.org/DATA_DOI_TO_BE_ADDED_ON_ACCEPTANCE](http://dx.doi.org/DATA_DOI_TO_BE_ADDED_ON_ACCEPTANCE).

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FIG. 1: Single thread CPU performance of the delayed matrix updating scheme as a function of delay $K$, for matrix sizes $N$ from 256 to 8192. The traditional Sherman-Morrison or rank-1 algorithm corresponds to $K = 1$. The lines pass through filled symbols indicating the average of five separate measurements at each delay and matrix size. Unfilled symbols give the individual timings, and show little variation. Speedups are found even for the smallest possible delay $K = 2$ for all shown $N$. 
FIG. 2: Relative speedup of single threaded CPU implementation of the delayed matrix updating scheme as a function of delay $K$, for matrix sizes $N$ from 256 to 8192, relative to the Sherman-Morrison or rank-1 algorithm. Highest speedups are $5.6 \times$ for $N = 256$ with $K = 16$, while for $N = 8192$ and $K = 256$ the measured speedup is $17.0 \times$ over the conventional algorithm.
FIG. 3: Relative speedup of GPU implementation of the delayed matrix updating scheme as a function of delay $K$, for matrix sizes $N$ from 256 to 8192, relative to the Sherman-Morrison or rank-1 algorithm. Highest speedups are $11.5\times$ for $N = 256$ using $K = 16$, while for $N = 8192$ and using $K = 256$ the measured speedup is $41.3\times$ over the conventional algorithm.
FIG. 4: Multiple thread performance of CPU implementation of the delayed matrix updating scheme for matrix size \( N = 2048 \). The traditional Sherman-Morrison or rank-1 algorithm corresponds to \( K = 1 \). In this unoptimized implementation, only the final update operation is threaded. While threads have limited benefit for \( K = 1 \), at optimal \( K = 128 \) the delayed scheme results in increased threading efficiency and overall faster updates.