Optimized Implementation for Calculation and Fast-Update of Pfaffians Installed to the Open-Source Fermionic Variational Solver mVMC

RuQing G. Xu\textsuperscript{a}, Tsuyoshi Okubo\textsuperscript{b,c}, Synge Todo\textsuperscript{a,b,d}, Masatoshi Imada\textsuperscript{e,f}

\textsuperscript{a}Department of Physics, University of Tokyo, Hongo 7-3-1, Bunkyo, Tokyo, 113-0033, Japan
\textsuperscript{b}Institute for Physics of Intelligence, University of Tokyo, Hongo 7-3-1, Bunkyo, Tokyo, 113-0033, Japan
\textsuperscript{c}JST, PRESTO, Honcho 4-1-8, Kawaguchi, Saitama, 332-0012, Japan
\textsuperscript{d}Institute for Solid State Physics, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa, Chiba, 277-8581, Japan
\textsuperscript{e}Department of Applied Physics, Waseda University, Okubo 3-4-1, Shinjuku, Tokyo, 169-8555, Japan
\textsuperscript{f}Toyota RIKEN, Yokomichi 41-1, Nagakute, Aichi, 480-1118, Japan

Abstract

In this article, we present a high performance, portable and well templated implementation for computing and fast-updating Pfaffian and inverse of an even-ranked skew-symmetric (antisymmetric) matrix. It is achieved with a skew-symmetric, blocked variant of the Parlett-Reid algorithm and a blocked update scheme based on the Woodbury matrix identity. Installation of this framework into the geminal-wavefunction-based many-variable Variational Monte Carlo (mVMC) code boosts sampling performance to up to more than 6 times without changing Markov chain’s behavior. The implementation is based on an extension of the BLAS-like instantiation software (BLIS) framework which has optimized kernel for many state-of-the-art processors including Intel Skylake-X, AMD EPYC Rome and Fujitsu A64FX.

Keywords: Variational Monte Carlo, Ground-state Method, Quantum Lattice Model, Skew-symmetric Matrix, Pfaffian, Blocked Algorithm, LAPACK, BLAS

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\textsuperscript{*}Intro for software package Pfaffine and its installation to mVMC with additional fast-update techniques.

Email address: ruqing.xu@phys.s.u-tokyo.ac.jp (RuQing G. Xu)
1. Program Summary

**Program title:** Pfaffine and PfUpdates library for mVMC[1]

**CPC Library link to program:** TBA

**Developer’s repository link:** https://github.com/issp-center-dev/mVMC/tree/master/src/pfupdates
https://github.com/xrq-phys/Pfaffine

**Code Ocean capsule:** TBA

**Licensing provisions:** MPL-2.0 (for new Library part)

**Programming language:** C++14 (for new Library part)

**Nature of problem:** Finding a method for computing and updating Pfaffian and inverse of a skew-symmetric matrix that yields a high performance on modern processor architectures.

**Solution method:** Deploying a blocked version of the Parlett-Reid algorithm with BLIS serving as assembly-level backend. Updating is approached using a modified Woodbury matrix identity.

2. Introduction

Numerical variational methods for correlated many-body systems have played an important role in studies of novel condensed-matter phenomena such as high-temperature superconductivity and spin liquids[2, 3, 4, 5, 6, 7, 8, 9]. Compared to exponentially expensive methods like exact diagonalization[10], variational methods retain advantage that it demands polynomial computational complexity, yet is able to provide results of decent accuracy. For Fermionic systems, there are several popular formulations of variational approaches. Density matrix renormalization group (DMRG)[2], which later evolved into the matrix product state (MPS)[11] ansatz, has achieved tremendous success in one-dimensional systems but suffers from lack of expressiveness in higher dimensions, while its extension for two-dimensional systems called projected entangled pair state (PEPS)[12, 13, 14] proved to be very challenging to optimize due to local minima problems[15, 16, 17]. On the contrary, the variational Monte Carlo method is easy to evaluate and optimize, while still capable to express those novel quantum states well[18, 19, 20, 21, 22].

During the past few years, several packages for variational Monte Carlo have been developed and opened to the public[23, 24], among them is mVMC[1] which focuses on the study of lattice-based
systems. In mVMC, the variational wavefunction with \(N_{\text{pair}}\) spin-up Fermions and the same number of spin-down Fermions is taken to be the form:

\[
|\Psi\rangle = \mathcal{L}_s \mathcal{L}_p \mathcal{P}_J \mathcal{P}_G |\phi\rangle.
\] (1)

In eq. (1), the core part \(|\phi\rangle\) is given by:

\[
|\phi\rangle = \left( \sum_{i<j} f_{ij} c_i^{\dagger} c_j^{\dagger} \right)^{N_{\text{pair}}} |0\rangle,
\] (2)

usually referred as a “pair product” (PP) or “geminal wavefunction” with \(c_i^{\dagger}\) as the Fermion creation operator on the \(i\)th spin-orbital, while \(\mathcal{P}_J, \mathcal{P}_G\) are real-space correlation operators with Jastrow and Gutzwiller factors, respectively and \(\mathcal{L}_s, \mathcal{L}_p\) are quantum-number projection operators for spin and momentum, respectively, to restore the original symmetry of the Hamiltonian. Readers interested in \(\mathcal{P}_J, \mathcal{P}_G, \mathcal{L}_s\) and \(\mathcal{L}_p\) are advised to refer to [18] and the rest sections of this article only focus on PP. With mean-field based \(|\phi\rangle\) [18] providing a very good initial state and \(\mathcal{P}_J, \mathcal{P}_G\) further considering effects introduced by interactions like Coulomb repulsion, mVMC is able to grab important features of many-body quantum mechanical systems [19, 20], providing excellent approximations to their ground states as well as low-energy excited states [25, 26].

Within the process of calculation, mVMC samples real space configurations \(\{ |x^{(k)}\rangle \}\) using a Markov chain (MC) process. The probability for some configuration \(|x\rangle\) to be sampled is proportional to its overlap with the wavefunction ansatz, i.e.:

\[
\text{Prob (} |x\rangle \text{ is sampled}) = \frac{\langle x|\Psi\rangle^2}{\langle \Psi|\Psi\rangle}.
\] (3)

According to the detailed balance condition of the Markov chain, eq. (3) yields a stochastic process dominated by:

\[
\text{Prob (} |x\rangle \rightarrow |x'\rangle) = \min \left( 1, \frac{\langle x'|\Psi\rangle^2}{\langle x|\Psi\rangle^2} \right).
\] (4)

As \(\mathcal{P}_J\) and \(\mathcal{P}_G\) are diagonal in configuration representation, while \(\mathcal{L}_p\) and \(\mathcal{L}_s\) expands to summed spatial operators, \(\langle x|\Psi\rangle\) expands to:

\[
\langle x|\Psi\rangle = \sum_{\theta} \beta_{\theta} \sum_{r} \alpha_r \langle T_r(x)|R_\theta(\phi)\rangle.
\] (5)

Here \(|R_\theta(\phi)\rangle\) is \(|\phi\rangle\) rotated by angle \(\theta\) and \(|T_r(x)\rangle\) is \(|x\rangle\) spatially translated by vector \(r\). Meshes for \((\theta, r)\) and their corresponding weights are defined so as the original symmetry of Hamiltonian can be
correctly restored. We recommended readers to refer to [18, 1] for further details of those quantities.

Equation (5) tells us that to generate samples satisfying eq. (3) we have to compute:

- \( \{ \langle T_r(x^{(0)}) | R_\theta(\phi) \rangle | r, \theta \} \) for the first sample;
- \( \{ \langle T_r(x^{(k)}) | R_\theta(\phi) \rangle | r, \theta \} \) with \( \{ \langle T_r(x^{(k-1)}) | R_\theta(\phi) \rangle | r, \theta \} \) known;

which are exactly the hotspots of the whole mVMC code.

Because \( | R_\theta(\phi) \rangle \) generates a constant set of pair products \( | R_\theta(\phi) \rangle = \left( \sum_{i<j} f_{ij}^\theta c_i^\dagger c_j^\dagger \right)^{N_{\text{pair}}} | 0 \rangle \) that does not change throughout the MC sampling process, and \( | T_r(x) \rangle \) can be viewed as from another chain of samples with a constant displacement, we omit these transformation operators in later discussion and only use \( \langle x | \phi \rangle \) which is evaluated as:

\[
\langle x | \phi \rangle = \text{Pf} \ X \quad \text{where} \quad X_{\alpha\beta} = \begin{cases} 
0 & x_\alpha = x_\beta \\
 f_{x_\alpha x_\beta} & x_\alpha < x_\beta \\
 -f_{x_\beta x_\alpha} & \text{otherwise}
\end{cases}, \tag{6}
\]

where \( x_\alpha \) denotes spin-orbital index of the \( \alpha \)-th Fermion under real-space configuration \( | x \rangle \).

Current implementation of mVMC[1] already features a nice threading behavior, making it able to run on large-scale computer clusters. However, this implementation bears defective microarchitecture usage on modern processor hardware due to the following two reasons:

- Heaviest calculation of the mVMC method involves operations on skew-symmetric (antisymmetric) matrices, which is not available via the standard BLAS interface. The alternative library, known as Pfapack77[27], is programmed without considering pipeline-level hardware efficiency hence not optimal for those state-of-the-art processors.

- To avoid recalculating Pfaffian every time for each Markov chain update, a fast-update scheme is adopted in current mVMC implementation. However, only rank-1 update scheme is implemented. The rank-1 update strategy is, by its name, mainly invoking rank-1 updates of matrices \( (X = X + uv^T) \), which is doomed to hit the memory bound and impact performance.

To get around these two severe hurdles upon mVMC’s performance, a new fast-update scheme as well as a new implementation of the skew-symmetric matrix library is necessary so that:

- All computational hotspots are effectively handled with assemblies fully optimized for the hosting hardware.
• Fast-update of Pfaffian invokes matrix-matrix operations instead of rank-1 updates.

Such are exactly what our optimization does.

This article is organized in the following fashion: Section 3 reviews and extends Wimmer’s approach in Pfapack77[27] on tridiagonalizing skew-symmetric matrices and computing Pfaffians. Section 4 presents the blocked fast-update scheme for further speeding up Pfaffian updates. Section 5 specifies programming interfaces of this acceleration framework as well as our assembly-level tuned implementation. Section 6 shows benchmarking results indicating superiority of this new implementation and finally, Sec. 7 concludes our development work.

3. Skew-symmetric Matrix and Pfaffian

Pfaffian of a size $2n \times 2n$ skew-symmetric matrix $X$ is defined as:

$$
\text{Pf} X = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) \prod_{i} X_{\sigma(2i-1), \sigma(2i)},
$$

and satisfies:

$$
(\text{Pf} X)^2 = \det X,
$$

where $S_{2n}$ is the permutation group of sets with $2n$ elements. Directly evaluating eq. (7) is of exponential complexity due to the number of elements in $S_{2n}$. However, there are linear transformations that can be applied to simplify computation just like the case of calculating determinants.

Before introducing tridiagonalization computation of Pfaffian, let us first go over definition of the Gaussian elimination matrix:

$$
M_k = I_{2n} - \alpha_k e_k^T,
$$

where $I_{2n}$ is the $2n \times 2n$ identity, $e_k$ is the $k$-th elementary vector of Euclidean space (i.e. $e_k = (0, \ldots, 0, 1, 0, \ldots, 0)^T$) and $\alpha_k$ is constructed with entries:

$$(\alpha_k)_i = \begin{cases} 0 & i \leq k \\ X_{i,k-1}/X_{k,k-1} & i > k \end{cases}$$

so that left-applying $M_k$ to $X$ eliminates all $X_{i,k-1}, i > k$ with $X_{ij}|_{i \leq k, j}$ untouched. Applying $M_k$ to both sides of a skew-symmetric matrix $X$ eliminates non-tridiagonal part of the $(k - 1)$-th column and row without changing its Pfaffian[27]. This will be the main weapon for efficient Pfaffian calculation in the formulation of this section.
**Blocked Tridiagonal Decomposition.** Blocked tridiagonal decomposition of skew-symmetric matrices (sktdf) was first formulated by Wimmer in Pfpapack77[27]. In their work a blocked and skew-symmetric variant of the Parlett-Reid algorithm[28] is adopted so that:

\[
PXP^T = LL^T, \quad (10)
\]

\[
P = P_{n-1} \cdots P_2,
\]

\[
T = M_{[n-1-r(\ell);n-1]}^\ell \cdots M_{[2;2+r(\ell)]}^\ell XM_{[2;2+r(\ell)]}^T \cdots M_{[n-1-r(\ell);n-1]}^T
\]

\[
L = \Big( M_{[n-1-r(\ell);n-1]}^\ell \cdots M_{[2;2+r(\ell)]}^\ell P^T \Big)^{-1}
\]

\[
M_{[i;i+r(\ell)]} = M_{i+r(\ell)} P_{i+r(\ell)}^T \cdots M_{i+1} P_{i+1}^T M_i P_i.
\]

Here \( P_k \) are permutation matrices that swap the \( k \)-th and \( (p(k) > k) \)-th columns (rows) of \( X \) when multiplied on the right (left) side. We call linear transformation \( M_{[i;i+r(\ell)]} \) a rank-\( r(\ell) \) pivoted Gaussian elimination where \( r(\ell) \in \mathbb{Z}^+ \) is a parameter for performance tuning. It is constructed by merging multiple Gaussian elimination matrices:

\[
M_{[k:k+1]} = M_{k+1} P_{k+1} M_k
\]

\[
= \left( I_{2n} - \alpha_{k+1} e_{k+1}^T \right) P_{k+1} \left( I_{2n} - \alpha_k e_k^T \right)
\]

\[
= \begin{pmatrix} I_{2n} - \alpha_{k+1} \\ \alpha_k \end{pmatrix} \begin{pmatrix} e_{k+1}^T \\ -e_k^T \end{pmatrix} P_{k+1}
\]

\[
M_{[k-r:k+1]} = M_{k+1} P_{k+1} M_{[k-r:k]}
\]

\[
= \left( I_{2n} - \alpha_{k+1} e_{k+1}^T \right) P_{k+1} \left( I_{2n} - V_{[k-r:k]}^T E_{[k-r:k]}^T \right) P_k \cdots P_{k-r}
\]

\[
= \begin{pmatrix} I_{2n} - \alpha_{k+1} \\ V_{[k-r:k]} \end{pmatrix} \begin{pmatrix} e_{k+1}^T \\ E_{[k-r:k]}^T \end{pmatrix} P_{k+1} P_k \cdots P_{k-r}, \quad (12)
\]

where \( \alpha_k^{(p)} \) and \( \alpha_k^{(p)} \) denote a matrix and column vector with \( k \)-th and \( p(k) \)-th rows swapped. Note also that in derivation of eqs. (11) and (12) we used \( e_{k+1}^T \alpha_k = 0 \) and \( e_k = P_{k+r} e_k \) implied by eq. (8). We refer to [27] for further details of this algorithm.
Once factorization (10) is done, with the fact that neither $\mathbf{P}_k$ or $\mathbf{M}_k$ affects the matrix’s Pfaffian, $\text{Pf} \mathbf{X}$ can be computed as:

$$\text{Pf} \mathbf{X} = \text{Pf} \mathbf{T} = \prod_{i=1}^{n} T_{2i-1,2i}. \quad (13)$$

**Inversion from Tridiagonalization.** With eq. (13) completes Wimmer’s derivation in [27], but mVMC requires computation of $\mathbf{X}^{-1}$ in addition to $\text{Pf} \mathbf{X}$. Current version of the implementation is initializing another $\text{GETRF}/\text{GETRI}$ call to invert $\mathbf{X}$ as a non-symmetric matrix. This treatment requires $\sim (2n)^3$ multiply-accumulate operations (MACs). However, one might notice that by inverting eq. (10), $\mathbf{X}^{-1}$ can be expressed as:

$$\mathbf{P} \mathbf{X}^{-1} \mathbf{P}^T = (\mathbf{L}^{-1})^T \mathbf{T}^{-1} \mathbf{L}^{-1}$$

$$= \mathbf{P} \mathbf{M}_{[2::2+r(1)]}^T \cdots \mathbf{M}_{[n-1-r(r);n-1]}^T \mathbf{T}^{-1} \mathbf{M}_{[n-1-r(r);n-1]} \cdots \mathbf{M}_{[2::2+r(1)]} \mathbf{P}^T$$

$$\Rightarrow \mathbf{X}^{-1} = \mathbf{M}_{[2::2+r(1)]}^T \cdots \mathbf{M}_{[n-1-r(r);n-1]}^T \mathbf{T}^{-1} \mathbf{M}_{[n-1-r(r);n-1]} \cdots \mathbf{M}_{[2::2+r(1)]}, \quad (15)$$

so that one can either invert $\mathbf{X}$ by expanding eq. (15) from the center or by directly evaluating eq. (14) since $\mathbf{L}$ is obtainable by properly merging and swapping all $\mathbf{V}$ entries of $\mathbf{M}[27]$.

**Quantitative Cost of Computation.** Evaluation of $\mathbf{M}_{[k-r::k]} \mathbf{X}^{(k-r-1)} \mathbf{M}_{[k-r::k]}^T$ can be done as:

$$\mathbf{M}_{[k-r::k]} \mathbf{X}^{(k-r-1)} \mathbf{M}_{[k-r::k]}^T = \left( \mathbf{I} - \mathbf{V}_{[k-r::k]} \mathbf{E}_{[k-r::k]}^T \right) \mathbf{X}^{(k-r-1,p)} \left( \mathbf{I} - \mathbf{V}_{[k-r::k]} \mathbf{E}_{[k-r::k]}^T \right)^T$$

$$= \mathbf{X}^{(k-r-1,p)} \mathbf{V}_{[k-r::k]} \mathbf{X}^{(k-r-1,p)}{\mathbf{I} : : \mathbf{I}} - \mathbf{X}^{(k-r-1,p)}{\mathbf{I} : : \mathbf{I}} \mathbf{V}_{[k-r::k]}^T$$

where we have used during the derivation that $\mathbf{X}$ is skew-symmetric and $\mathbf{V}$’s columns are orthogonal to each other. $\mathbf{X}^{(k-r-1)}$ denotes $\mathbf{X}$ after $k - r - 1$ steps of Gaussian elimination and $\mathbf{X}^{(k-r-1,p)}$ its permuted version, i.e.:

$$\mathbf{X}^{(k-r-1)} = \mathbf{M}_{k-r-1} \mathbf{P}_{k-r-1} \cdots \mathbf{M}_2 \mathbf{P}_2 \mathbf{X}^{(k-r-1)} \mathbf{P}_2^T \mathbf{M}_2^T \cdots \mathbf{P}_{k-r-1}^T \mathbf{M}_{k-r-1}^T,$$

$$\mathbf{X}^{(k-r-1,p)} = \mathbf{P}_k \cdots \mathbf{P}_{k-r} \mathbf{X}^{(k-r-1)} \mathbf{P}_{k-r-1}^T \cdots \mathbf{P}_k^T.$$

As $\mathbf{X}^{(k-r-1,p)}$ always has the first $k - r - 1$ columns and rows tridiagonal, evaluation of eq. (16) only needs to consider the lower-right portion of size $(2n - (k - r - 1)) \times (2n - (k - r - 1))$. This fact

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1Here for ease notation, an unblock expression is used. In real computation we always adopt blocked manipulations.
together with \(X\)'s skew-symmetric property yields an evaluation cost of \((2n - (k - r - 1))^2r\). Hence the total evaluation cost to transform \(X\) to \(T\) in eq. (10) is around \(\frac{1}{4}(2n)^3\) MACs.

For extracting \(X^{-1}\), instantiation of eq. (15) requires iteratively evaluating \(M_{(k-r):(k-r-1)}^T T_{(k-r-1)}^{-1} M_{(k-r):k}\) which expands into:

\[
M_{(k-r):(k-r-1)}^T T_{(k-r-1)}^{-1} M_{(k-r):k} = P_{k-r} \cdots P_k \left( I_{2n} - V_{(k-r):k} E_{(k-r):k}^T \right) T_{(k-r-1)}^{-1} \left( I_{2n} - V_{(k-r):k} E_{(k-r):k}^T \right) P_k \cdots P_{k-r}
\]

\[
= P_{k-r} \cdots P_k \left\{ T_{(k-r-1)}^{-1} - E_{(k-r):k} \left( T_{(k-r-1)}^{-1} V_{(k-r):k} \right)^T \right\} + \left( T_{(k-r-1)}^{-1} V_{(k-r):k} \right) E_{(k-r):k} + E_{(k-r):k} V_{(k-r):k}^T T_{(k-r-1)}^{-1} V_{(k-r):k} E_{(k-r):k} \right\} P_k \cdots P_{k-r} \quad (17)
\]

Computation of matrix-matrix products in eq. (17) requires around \((2n)(2n - (k - r - 1))r + (2n)^2\) MACs. Ignoring \((2n)^2r^2\) term which is much less than \((2n)(2n - (k - r - 1))r\), total cost of eq. (15) becomes \(\approx \frac{1}{2}(2n)^3\).

The alternative approach for \(X^{-1}\), namely eq. (14) requires inverting \(L^{-1}\) first, calling a subprocedure of \textsc{getri} named \textsc{trtri} which makes \(\frac{1}{6}(2n)^3\) MACs. Since \(T\) is tridiagonal, computation of \(T^{-1}L^{-1}\) can be done by using the \(O (n^2)\)-cost procedure \textsc{gtsv} whose cost can be neglected. The final \(X^{-1} = (L^{-1})^T (T^{-1}L^{-1})\) step has triangular \(L^{-1}\) on the left hand side and only needs to write half of \(X^{-1}\) since we already know that it is skew-symmetric, resulting in \(\frac{1}{6}(2n)^3\) MACs. Hence the whole evaluation of eq. (14) totals up to \(\frac{1}{3}(2n)^3\) MACs, also lower than \textsc{getrf}/\textsc{getri} deployed by the original algorithm. Both approaches for \(X^{-1}\) are available in our implementation as different subversions.

4. Blocked Pfaffian Update from Modified Woodbury Matrix Identity

Theory. mVMC takes configuration samples \(\{x^{(k)}\} | k \in \mathbb{N}\) with a Markov chain (MC) process, as is shown in eq. (4). As each step \(x^{(k)} \rightarrow x^{(k+1)}\) within this MC only changes the spin-orbitals of one or two electrons of \(x^{(k)}\), we do not need to redo Sec. 3 calculations each time a new sample is generated. Instead, from the Woodbury matrix identity\cite{Woodbury1950} we have:

\[
\text{Pf} \left[ X + BCB^T \right] = \text{Pf} X \times \frac{\text{Pf} \left[ C^{-1} + B^T X^{-1} B \right]}{\text{Pf} \left[ C^{-1} \right]} \quad (18)
\]

\[
(X + BCB^T)^{-1} = X^{-1} - X^{-1}B \left( C^{-1} + B^T X^{-1} B \right)^{-1} B^T X^{-1}, \quad (19)
\]

which allows Pfaffian in eq. (6) to be updated as (To give a more intuitive image of what is happening during the MC fast-update, we also plug in here a \(4 \times 4\) exemplar matrix for \(X\):)

\[
\begin{bmatrix}
X & B \\
B^T & C
\end{bmatrix}
\]

\[
\text{Pf} \left[ X + BCB^T \right] = \text{Pf} X \times \frac{\text{Pf} \left[ C^{-1} + B^T X^{-1} B \right]}{\text{Pf} \left[ C^{-1} \right]} \quad (18)
\]

\[
(X + BCB^T)^{-1} = X^{-1} - X^{-1}B \left( C^{-1} + B^T X^{-1} B \right)^{-1} B^T X^{-1}, \quad (19)
\]
\[ |x\rangle = |j_1 j_2 j_3 j_4\rangle \quad (20) \]

\[
X = \begin{bmatrix}
0 & F_{j_2}^{j_1} & F_{j_3}^{j_1} & F_{j_4}^{j_1} \\
-F_{j_2}^{j_1} & 0 & F_{j_3}^{j_2} & F_{j_4}^{j_2} \\
-F_{j_3}^{j_1} & -F_{j_3}^{j_2} & 0 & F_{j_4}^{j_3} \\
-F_{j_4}^{j_1} & -F_{j_4}^{j_2} & -F_{j_4}^{j_3} & 0
\end{bmatrix} \quad (21) \]

\[
\langle x|\phi\rangle = \text{Pf} \ X \quad (22) \]

\[
\downarrow
\]

\[ |x^{(1)}\rangle = |i_1 j_2 j_3 j_4\rangle \quad (23) \]

\[
X^{(1)} = \begin{bmatrix}
0 & F_{i_2}^{i_1} & F_{i_3}^{i_1} & F_{i_4}^{i_1} \\
-F_{i_2}^{i_1} & 0 & F_{i_3}^{i_2} & F_{i_4}^{i_2} \\
-F_{i_3}^{i_1} & -F_{i_3}^{i_2} & 0 & F_{i_4}^{i_3} \\
-F_{i_4}^{i_1} & -F_{i_4}^{i_2} & -F_{i_4}^{i_3} & 0
\end{bmatrix} = X + B^{(1)} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} B^{(1)T} \quad (24) \]

\[
B^{(1)}_{lm} = \begin{cases} 
F_{i_l}^{j_l} - F_{j_l}^{i_l} & \text{if } l \neq 1, m = 1 \\
1 & \text{if } l = 1, m = 1 \\
0 & \text{otherwise}
\end{cases} \quad (25) \]

\[
\langle x^{(1)}|\phi\rangle = \text{Pf} \ X^{(1)} = \text{Pf} \ X \times \text{Pf} \left( C^{(1)} + B^{(1)T} X^{-1} B^{(1)} \right) / \text{Pf} \ C^{(1)} = \text{Pf} \ X \times \left( 1 - \sum_j (X^{-1})^j u_j \right) \quad (26) \]

\[
X^{(1)}^{-1} = X^{-1} - X^{-1} B^{(1)} \left( C^{(1)} + B^{(1)T} X^{-1} B^{(1)} \right)^{-1} B^{(1)T} X^{-1} \quad (27) \]

\[
\downarrow
\]
\[
\begin{align*}
\langle x^{(2)} \rangle &= |i_1i_2j_3j_4 \rangle \\
X^{(2)} &= \begin{bmatrix}
0 & F_{i_1}^{j_1} & F_{i_2}^{j_2} & F_{i_4}^{j_4} \\
-F_{i_2}^{j_1} & 0 & F_{i_3}^{j_1} & F_{i_4}^{j_3} \\
-F_{i_1}^{j_2} & -F_{i_3}^{j_1} & 0 & F_{i_4}^{j_3} \\
-F_{i_1}^{j_4} & -F_{i_2}^{j_3} & -F_{i_3}^{j_4} & 0
\end{bmatrix} = X + B^{(2)}C^{(2)}B^{(2)T} \\
\langle x^{(2)} \rangle \phi &= Pf X^{(2)} = Pf X \times Pf \left( C^{(2)} + B^{(2)T}X^{-1}B^{(2)} \right) / Pf C^{(2)} \\
X^{(2)\text{-}1} &= X^{-1} - X^{-1}B^{(2)} \left( C^{(2)} + B^{(2)T}X^{-1}B^{(2)} \right)^{-1} B^{(2)T}X^{-1} \\
\end{align*}
\]

\[
\begin{align*}
\langle x^{(3)} \rangle &= |i_1i_2i_3j_4 \rangle \\
X^{(3)} &= \begin{bmatrix}
0 & F_{i_1}^{j_1} & F_{i_2}^{j_2} & F_{i_4}^{j_4} \\
-F_{i_2}^{j_1} & 0 & F_{i_3}^{j_1} & F_{i_4}^{j_3} \\
-F_{i_1}^{j_2} & -F_{i_3}^{j_1} & 0 & F_{i_4}^{j_3} \\
-F_{i_1}^{j_4} & -F_{i_2}^{j_3} & -F_{i_3}^{j_4} & 0
\end{bmatrix} = X + B^{(3)}C^{(3)}B^{(3)T} \\
\langle x^{(3)} \rangle \phi &= Pf X^{(3)} = Pf X \times Pf \left( C^{(3)} + B^{(3)T}X^{-1}B^{(3)} \right) / Pf C^{(3)} \\
X^{(3)\text{-}1} &= X^{-1} - X^{-1}B^{(3)} \left( C^{(3)} + B^{(3)T}X^{-1}B^{(3)} \right)^{-1} B^{(2)T}X^{-1} \\
\end{align*}
\]

Matrices $B^{(r)}$ and $C^{(r)}$ appearing in eqs. (26), (27), (30), (31), (34) and (35) also have a common expression for their entries:

\[
B_{lm}^{(r)} = \begin{cases} 
F_{i_r}^{j_l} - F_{j_r}^{i_l} & l > m, m \leq r \\
F_{i_r}^{j_l} - F_{j_r}^{i_l} & l < m, m \leq r \\
1 & l = m, m > r \\
0 & \text{otherwise}
\end{cases} \\
C_{lm}^{(r)} = \begin{bmatrix}
0 & -I_r \\
I_r & 0
\end{bmatrix}.
\]
Note also that we have assumed in these equations that electrons in $|x⟩$ change their positions by order from the first one. In real implementation of mVMC where the hopping electron is selected randomly, one needs to modify $B$ accordingly to select a different set of unit vectors corresponding to that random selection.

| Table 1: Different ways for evaluating Markov Chain on $|x⟩$ with $r_{\text{max}} = 3$ |
|-----------------------------------------------|
| Configuration $|x^{(k)}⟩$                     | $j_0$ | $i_0$ | $j_0$ | $i_0$ |
| Old method evaluates:                       | eqs. (26) and (27) | eqs. (26) and (27) | eqs. (26) and (27) |
| Old method modifies:                        | Pf $X$, $X^{-1}$ | Pf $X$, $X^{-1}$ | Pf $X$, $X^{-1}$ |
| Old method calls:                            | SKPFA/SKTDI | SKMV, SKR2 | SKMV, SKR2 | SKMV, SKR2 |
| New method evaluates:                       | eq. (30) | eq. (34) and (35) |
| New method modifies:                        | Pf $X$ | Pf $X$ | Pf $X$, $X^{-1}$ |
| New method calls:                            | SKPFA/SKTDI | SKMV | SKMV | SKMV, GEMMT |

Application. With eqs. (26), (27), (30), (31), (34) and (35), mVMC is able to proceed throughout the MC without recalculating Pf $X$ upon each sample. However, in the current version of mVMC, only rank-1 update equations (i.e. eqs. (26) and (27)) are used which eventually made the program memory-bound. To get around this problem to make full use of modern CPU architectures, we extend the way of evaluating MC on $|x^{(k)}⟩$ employed in mVMC. In our new approach:

- Rank-$|r_{\in Z^+}$ (blocked) updates are used instead of just rank-1 updates;
- A tuning parameter $r_{\text{max}}$ is set to determine at which step should $X^{-1}$ be updated. Note that rank-$r$ update does not require $(X^{(l)})^{-1}$ from previous steps.

Table 1 gives an example of how this change looks like when operating on a 4-electron configuration with $r_{\text{max}} = 3$ and Fig. 1 compares the flowcharts before and after our modification. It is important to note that our optimization does not alter sampling process or acceptance ratio of the original Markov chain. What we have done is to “pack up” the heaviest computation, i.e. update of $X^{-1}$, grouping
Figure 1: Flowcharts for evaluating Markov chain on $|x\rangle$ before and after block-update optimization.
each $r_{\text{max}}$ rank-1 updates into one rank-$r_{\text{max}}$ update so that the new program becomes much faster as we will see in Sec. 6.

5. Library Interface and Accelerated Implementation

This work is basically an optimization of the open-source program mVMC. We did not make any changes on the user side interface defined in [1]. Instead, this section gives a brief specification of library routines we have made to implement procedures presented in Secs. 3 and 4.

Layered Implementation. As was stated in Sec. 2, Wimmer’s algorithm is good but their implementation Pfapack77 is not tuned to use assembly-level optimized BLAS routines as skew-symmetric operation is not part of the standard. To complete a high-performance implementation for evaluating equations appeared in Secs. 3 and 4, an extended BLAS-level implementation is needed. BLIS[30] is a fast and highly portable framework that implements BLAS-like operations with a fresh approach based on the GotoBLAS[31, 32] algorithm. It is able to instantiate multiple level-3 BLAS operations with a minimal number of assembly-based kernels[33] tuning based on an analytical model[34]. By adding a minimum amount of interface code to BLIS, skew-symmetric BLAS operations are imported with optimized kernels for AMD Zen, Intel Skylake-X and many other architectures, among them a set of
GEMM kernels designed for A64FX\(^2\) made by ourselves in another joint work with Forschungszentrum Jülich. Integrating these modules we have now built a layered approach shown in Fig. 2 for computing and block-updating Pfaffian which is fast, well-organized and runs across different CPU architectures.

Table 2: List of API handles of the Pfaffine library for Pfaffian and inverse computation. Here \(T\) refers to different floating-point data types and \(t\) their LAPACK-style prefix characters. We use “sk. matrix” as the shorthand of a skew-symmetric matrix.

| C++  | C (Simp.) | C/Fort. | Description |
|------|-----------|---------|-------------|
| sktdf\(<T>\) | N/A | N/A | Tridiagonal factorize \(X\) (eq. (10)). |
| sktdi\(<T>\) | N/A | N/A | Inverse matrix from Tridiagonal factorization (eq. (15)). |
| skpfa\(<T>\) | tskpfa\_ | cal_tskpfa\_ | Tridiagonal factorize and compute Pf \(X\) (eq. (13)), \(X^{-1}\) computed conditionally depending on input. |
| skslc\(<T>\) | N/A | N/A | Get a column from corner-stored sk. matrix. |
| skswp\(<T>\) | N/A | N/A | Swap columns and rows of corner-stored sk. matrix. |
| skr2k\(<T>\) | N/A | N/A | \(X + AB^T - BA^T\) where \(X\) is corner-stored sk. matrix. |
| skmm\(<T>\) | N/A | N/A | XB where \(X\) is corner-stored sk. matrix. |

Table 3: Method API of C++ object updated\(_{tdi}\) for rank-\(r\) update strategy.

| C++ Method | Description |
|------------|-------------|
| updated\(_{tdi}<T>\)::updated\(_{tdi}()\) | Constructor. Given \(f_{ij}\) and \(|x\rangle\), compute Pf \(X\) and \(X^{-1}\). |
| updated\(_{tdi}<T>\)::get_Pfa() | Get Pfaffian of current configuration. |
| updated\(_{tdi}<T>\)::push_update() | Push a configuration update: \(|x^{(r)}\rangle\rightarrow|x^{(r+1)}\rangle\) with one electron changed its spin-orbital position. |
| updated\(_{tdi}<T>\)::pop_update() | Revert the last push\(_{update}()\). |
| updated\(_{tdi}<T>\)::merge_updates() | Modify \(X^{-1}\) based on the last accepted configuration. |

Interface. C++ and C interfaces of our Pfaffian-inverse framework described in Fig. 2 are listed in Tab. 2, while object-based routines for Sec. 4’s blocked update are listed in Tab. 3. We recommend referring to our program distribution in [35] for more API-related information.

\(^2\)A64FX is the processor name of current world top supercomputer “Fugaku”.
6. Benchmarking Results

We run a Markov chain sampling a random many-body spin wavefunction on a $L \times L$ square lattice. Our experiment only studies the sampling process itself against this random wavefunction so that the Hamiltonian is omitted. The total number of samples generated by the MC is proportional to the number of spins:

$$N_{\text{tot}} \propto N_{\text{spin}} = L \times L,$$

because MC needs more steps to decorrelate as system size grows. This experimental setup yields:

$$r_{\text{acc}} N_{\text{proj}} \left( \frac{N_{\text{qty}}}{N_{\text{smp}}} + 1 \right) N_{\text{spin}} \left( 2N_{\text{spin}}^2 + \frac{1}{4N_{\text{spin}}} N_{\text{spin}}^3 \right) = \omega N_{\text{spin}}^3 \text{ MACs}$$

for each system size. Here $r_{\text{acc}}$ is the acceptance ratio since rank-1 (rank-$k$) update is requested every time (every $k$ times) a configuration update is accepted. $N_{\text{qty}}$, $N_{\text{smp}}$ and $N_{\text{proj}}$ correspond to $N_{\text{DataQtySmp}}$, $N_{\text{VMCSample}}$ and $N_{\text{Q}}$ parameters in the mVMC application. The extra $\frac{3}{4}N_{\text{spin}}^2 N_{\text{spin}}$ term inside the bracket accounts for the recalculation of full $X \to X^{-1}$ every $N_{\text{spin}}$ acceptances to remove the accumulated round-up error by fast updates. We set $N_{\text{qty}} = 10$, $N_{\text{smp}} = 10$ and $N_{\text{proj}} = 16$ in our experiment. Acceptance ratios turned out to be $r_{\text{acc}}^{\text{real}} \approx 31\%$ for real Slater determinants and $r_{\text{acc}}^{\text{comp}} \approx 47\%$ for complex ones regardless of $N_{\text{spin}}$. Hence the coefficients $\omega$ become $\omega_{\text{real}} \approx 2050$ and $\omega_{\text{complex}} \approx 3000$ for real and complex Slater determinants, respectively. Since different hardware vendors sometimes count performance data differently, here we use the expression:

$$\text{FLOPs/sec} = \omega_{\text{data}} \times \text{OpCost}_{\text{data}} \times \frac{L^6}{T_{\text{elapsed}}}$$

(38)

to convert time measurements to floating-point performance data, where $\text{OpCost}_{\text{data}}$ is the number of floating-point operations (FLOPs) yielded by each MAC on corresponding data types, hence 2 for real Slater determinants and 8 for complex Slater determinants.

Three CPU variants are selected to be included in this test, each having its own significance in the HPC context:

- Intel® Xeon® Platinum 8260 under Skylake-X microarchitecture with AVX512 vector instructions support;
- AMD EPYC™ 7702 under Zen 2 microarchitecture with AVX2 vector instructions support;
- Fujitsu A64FX based on Armv8 ISA with 512-bit Scalable Vector Extension[38] support.
Figure 3: Benchmark conducted on 3 different CPUs against mVMC’s Markov chain sampling process comparing original version and our block-update optimized version. FLOPs numbers here, given by eq. (38), show how much our method has speed up the mVMC program. Performance draw-back of Intel Skylake-X at $L \geq 20$ is believed to be caused by the block-update’s panel size exceeding processor’s L2 cache[36]. Future work on deploying a hierarchy storage (e.g. one implemented in Low and van de Geijn [37]) to X might address this problem and allow further speed-up.
Results of our blocked-update mVMC compared to the original implementation is shown in Fig. 3. Note that all tests here are conducted single-threaded because mVMC has parallel capability at a higher level. These results show that performance of our blocked algorithm can ramp up quickly with the growth of system size, yielding up to more than 6× performance compared to the original code on all our processors tested, while the latter two tested architectures seem to bear potential for higher speed-up rates on even larger system sizes. Among all test cases here, AMD EPYC™ 7702 yields the most significant speed-up (up to ~ 17.5×) thanks to a new skinny-matrix handling strategy introduced to BLIS[39].

7. Conclusion

We have shown in this article a framework for computing and updating Pfaffians that is fast, flexible and runs across different microarchitectures. mVMC optimized with this framework has achieved significant speed up compared to its original release. Theory as well as library implementation in this work can also be applied to other kinds of variational methods that deals with skew-symmetric wavefunctions, i.e. Fermions, like TurboRVB[24]. On the implementation side, this blocking would also allow potential portings of the related methods onto heterogeneous platforms like a general-purpose GPU machine, although the sequential nature of Markov chains might require additional parallelizations to unleash GPUs' full power. Further, our work shows a new possible pattern of open-source communities collaborating with hardware people to deliver an assembly-level optimized code for HPC applications.

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3The original code is compiled with corresponding vendor compilers under default max-optimization options.
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