A faster hafnian formula for complex matrices and its benchmarking on the Titan supercomputer

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Abstract

We introduce new and simple algorithms for the calculation of the number of perfect matchings of complex weighted, undirected graphs with and without loops. Our compact formulas for the hafnian and loop hafnian of $n \times n$ complex matrices run in $O(n^2 2^{n/2})$ time, are embarrassingly parallelizable and, to the best of our knowledge, are the fastest exact algorithms to compute these quantities. Despite our highly optimized algorithm, numerical benchmarks on the Titan supercomputer with matrices up to size $56 \times 56$ indicate that one would require the 288000 CPUs of this machine for about a month and a half to compute the hafnian of a $100 \times 100$ matrix.

1 Introduction

Counting perfect matchings in a graph is an important problem in graph theory [1] and has diverse applications [2]. For a bipartite graph the number of perfect matchings is given by the permanent of the associated adjacency matrix, which has been shown to be #P-complete to compute exactly [3]. Various algorithms have been developed for fast computation of permanents [4, 5, 6] (see Ref. [7] for a recent and detailed benchmarking of different algorithms for the computation of permanents using supercomputers). For a more general graph (one that is not bipartite), the number of perfect matchings is given by the hafnian of the associated adjacency matrix of the graph [8]. The hafnian can be thought as a generalization of the permanent. Whereas the permanent counts the number of perfect matchings in a bipartite graph, the hafnian counts the number of perfect matchings in an undirected graph. For the related problem of approximating the hafnian several methods have been developed for restricted sets of matrices [9, 10, 11, 12].

In this manuscript we develop a new algorithm to compute hafnians of general complex matrices that runs in $O(n^2 2^{n/2})$ time where $n$ is the size of the matrix. Our algorithm builds on the hafnian algorithm of Cygan and Pilipczuk [13], here adapted to the field of complex numbers using elementary tools from linear algebra. Compared to the general ring hafnian algorithm of Cygan and Pilipczuk, our algorithm is a factor $n$ faster. The new algorithm is, to the best of our knowledge, the fastest exact algorithm to compute the hafnian of a complex matrix.

A second motivation behind studying fast computation of hafnians stems from quantum computing. Recent developments in quantum complexity theory have provided renewed impetus for the study of combinatorial sampling problems. The most prominent of these developments is perhaps Aaronson and Arkhipov’s Boson Sampling problem [14]. In Boson Sampling $n$ photons are sent through a (linear) lossless optical device that has $n^2$ inputs and outputs. The probability that a certain arrangement of detectors click is proportional to $|\text{per}(U_S)|^2$, where $U_S$ is a submatrix of a unitary matrix $U$ representing the optical device and ‘per’ stands for permanent [4]. Aaronson and Arkhipov argue that for large enough $n$ it will be impossible for a classical computer to generate samples in polynomial time from the event distribution (of click detections) of the optical circuit just described. This observation has prompted a significant effort to understand how fast a classical computer can calculate permanents [7] or sample from Boson Sampling distributions that depend on permanents [15, 16].

Recently Hamilton et al. [17, 18] introduced a related problem called Gaussian Boson Sampling. Their problem is almost identical to Boson Sampling except that now the light sent into the optical device is not single photons but squeezed light [19]. Hamilton et al. show that this “small” change can significantly simplify the experimental challenges in constructing a Boson Sampler. In Gaussian Boson Sampling the probability of the detectors clicking is now proportional to the modulus squared of the hafnian [1] of a submatrix constructed from the unitary matrix representing the circuit and the values of intensities of the squeezed light going into the device.

With the development of new quantum sampling problems that are less complex to implement experimentally it becomes important to understand where the limits of classical computers with the best possible algorithms lie [20]. Thus the results presented here should be of relevance for any claim of quantum supremacy using Gaussian Boson Sampling.

1.1 Earlier Work The exact calculation of the number of perfect matchings for general graphs has been investigated by several authors in recent years. An algorithm running in $O(n^2 2^n)$ time was given by Björklund...
and Husfeldt [21]. In the same paper an algorithm running in $O(1.733^n)$ time was presented using fast matrix multiplication. Koivisto [22] gave an $O^*(\phi^n)$ time and space algorithm, where $\phi = (1 + \sqrt{5})/2 \approx 1.618$ is the Golden ratio and the notation $O^*$ is used to indicate that polylogarithmic corrections have been suppressed in the scaling. Nederlof [23] provided a polynomial space algorithm running in $O(1.942^n)$ time.

Finally, Björklund [24] and later Cygan and Pilipczuk [13] provided $O(\text{poly}(n)2^{n/2})$ time and polynomial space algorithms for the calculation of the general ring hafnian. These algorithms are believed to be close to optimal unless there are surprisingly efficient algorithms for the Permanent. This is because these two algorithms can also be used to count (up to polynomial corrections) the number of perfect matchings for bipartite graphs with the same exponential growth as Ryser’s algorithm for the permanent [4]. Equivalently, if one could construct an algorithm that calculates hafnians in time $O(\alpha^{n/2})$ with $\alpha < 2$ one could calculate permanents faster than Ryser’s algorithm (which is the fastest known algorithm to calculate the permanent [25]). This is because of the identity

$$\text{haf} \left( \begin{bmatrix} 0 & W \\ W^T & 0 \end{bmatrix} \right) = \text{per}(W),$$

which states that a bipartite graph with two parts having $n/2$ elements can always be thought as a simple graph with $n$ vertices. It should be noted that improving over Ryser’s algorithm is a well-known open problem: e.g. Knuth [26] asks for an arithmetic circuit for the permanent with less than $2^n$ operations. Also note that since the exact calculation of the permanent of $(0,1)$ matrices is in the #P complete class [3] the above identity shows that deciding if the hafnian of a complex matrix is larger than a given value is also in the #P complete class.

1.2 Our Contribution
In this paper we improve upon recently developed algorithms for counting the number of perfect matchings of undirected graphs [24, 13] and the calculation of hafnians. Furthermore these algorithms are generalized to allow for the inclusion of graphs that contain loops. Finally, we provide benchmarks of the algorithms developed using the Titan supercomputer of the Oak Ridge National Laboratory. The results presented here should provide a stepping stone for our understanding of how fast Hafnians can be calculated in classical computers and delimit the realm of quantum supremacy for (Gaussian) Boson Samplers.

2 Hafnians and Perfect Matchings
The hafnian of an $n \times n$ symmetric matrix $A = A^T$ is defined as

$$\text{haf}(A) = \sum_{M \in \text{PMP}(n)} \prod_{(i,j) \in M} A_{i,j},$$

where $\text{PMP}(n)$ stands for the set of perfect matching permutations of $n$ (even) objects. For $n = 4$ the set of perfect matchings is

$$\text{PMP}(4) = \{(0,1)(2,3), (0,2)(1,3), (0,3), (1,2)\},$$

and the hafnian of a $4 \times 4$ matrix $B$ is

$$\text{haf}(B) = B_{0,1}B_{2,3} + B_{0,2}B_{1,3} + B_{0,3}B_{1,2}.$$ More generally, the set $\text{PMP}(n)$ contains

$$|\text{PMP}(n)| = (n-1)!! = 1 \times 3 \times 5 \times \ldots \times (n-1),$$

elements and thus as defined it takes $(n-1)!!$ additions of products of $n/2$ numbers to calculate the hafnian of $A$. Note that the diagonal elements of the matrix $A$ do not appear in the calculation of the hafnian and are (conventionally) taken to be zero.

The hafnian function has an interesting connection with graph theory: if $A$ is the adjacency matrix of a loopless, unweighted, undirected graph (i.e., $A$ is a $(0,1)$ matrix with zeros along the diagonal) then $\text{haf}(A)$ is precisely the number of perfect matchings of the graph represented by $A$. Indeed, each element of the set of perfect matchings asserts whether the partition of the graph leaves no edge unmatched. For the set $\text{PMP}(4)$ in Eq. (2.3) one can easily visualize the corresponding matchings of a graph with four vertices as the first three partitions in the top row of Fig. 1.

The notion of perfect matching is easily generalized from $(0,1)$ adjacency matrices to matrices over any field. The hafnian of a (symmetric) matrix $A$ will be then the sum of weighted perfect matchings of an undirected graph with adjacency matrix $A$.

In this manuscript we will also study a generalization of the hafnian function where we will consider graphs that have loops, henceforth referred to as ‘haf’ (loop hafnian). The weight associated with said loops will be allocated in the diagonal elements of the adjacency
matrix $A$ (which were previously ignored in the definition of the hafnian in Eqs. (2.2) and (2.4). To account for the possibility of loops we generalize the set of perfect matching permutations PMP to the single-pair matchings (SPM). This is simply the set of perfect matchings of a complete graph with loops. Thus we define

$$
\text{lhaf}(A) = \sum_{M \in \text{SPM}(n)} \prod_{(i,j) \in M} A_{i,j}.
$$

Considering again a graph with 4 vertices we get a total of 10 SPMs:

$$
\text{SPM}(4) = \{(0,1)(2,3), (0,2)(1,3), (0,3)(1,2),
(0,0)(1,2)(3,3), (0,2)(1,1)(3,3),
(0,0)(2,2)(1,3), (0,0)(3,3)(1,2), (0,3)(1,1)(2,2),
(0,0)(1,1)(2,3)(3,3)\}.
$$

and the lhaf of a $4 \times 4$ matrix $B$ is

$$
\text{lhaf}(B) = B_{0,1}B_{2,3} + B_{0,2}B_{1,3} + B_{0,3}B_{1,2} + B_{0,0}B_{1,1}B_{3,3} + B_{0,2}B_{1,3} + B_{0,0}B_{3,3}B_{1,2} + B_{0,3}B_{1,2}B_{3,3}.
$$

More generally for a graph with $n$ vertices ($n$ even) the number of SPMs is

$$
|\text{SPM}(n)| = T \left(n, \frac{1}{2}, \frac{1}{\sqrt{2}}\right)
$$

where $T(a, b, r)$ is the Toronto function (cf. page 509 of Ref. [27]). A derivation of this formula and some comments on the asymptotic super polynomial scaling of the ratio

$$
\frac{|\text{SPM}(n)|}{|\text{PMP}(n)|} = T \left(n, \frac{1}{2}, \frac{1}{\sqrt{2}}\right) / (n-1)!!
$$

are presented in Appendix A.

Finally, let us comment on the scaling properties of the haf and lhaf. Unlike the hafnian the loop hafnian function is not homogeneous in its matrix entries, i.e.

$$
\text{haf}(\mu A) = \mu^{n/2} \text{haf}(A) \text{ but,} \\
\text{lhaf}(\mu A) \neq \mu^{n/2} \text{lhaf}(A).
$$

where $n$ is the size of the matrix $A$ and $\mu \geq 0$. However if we split the matrix $A$ in terms of its diagonal $A_{\text{diag}}$ part and its offdiagonal part $A_{\text{off-diag}}$

$$
A = A_{\text{diag}} + A_{\text{off-diag}},
$$

then it holds that

$$
\text{lhaf}(\sqrt{n} A_{\text{diag}} + \mu A_{\text{off-diag}}) = \mu^{n/2} \text{lhaf}(A_{\text{diag}} + A_{\text{off-diag}}) = \mu^{n/2} \text{lhaf}(A).
$$

Later we will show that the new formulas we derive here for the hafnian and loop hafnian explicitly respect these scaling relations.

3 The Algorithm

As mentioned in the previous section, the hafnian and loop hafnian functions count the number of perfect matchings in a graph. The topology of the graph is encoded in the adjacency matrix that is input into either function. In the following sections we present an algorithm that allows to count the number of perfect matchings of a graph with $n$ vertices in time $O(n^3 2^n)$ for (unweighted) graphs with and without loops and then generalize it to weighted graphs. Our algorithm and its analysis largely follows that of Cygan and Pilipczuk [13] with one crucial exception. Whereas the terms in their formula are computed by an $O(n^4)$ dynamic programming tabulation, we reduce the terms to efficiently computable functions of the traces of the first $n/2$ powers of a matrix. This enables us to gain a factor of $n$ in the running time by first computing the eigenvalue spectrum with a known $O(n^3)$ time algorithm. We can than use standard trace identities to compute all traces of the matrix powers more efficiently than by explicitly constructing the matrix powers.

3.1 Notation and Terminology

Let $G = (V, E)$ be an undirected graph with loops, and let $n = |V|$ be even. A perfect matching in $G$ is a subset $E' \subset E$ of edges such that every vertex in $V$ is part of exactly one edge $e \in E'$. Note again that $e$ may be a loop from a vertex $v$ to itself. We consider here the problem of enumerating all possible perfect matchings of $G$, a quantity we will denote by $M(G)$.

We write $[m]$ for a positive integer $m$ as the set

$$
[m] = \{0, 1, \ldots, m-1\}.
$$

The vertices $V$ of the graph will be associated with the set $[n]$. A walk is a sequence of vertices $\hat{w} = (w_0, w_1, \ldots, w_\ell)$ where $\forall i < \ell : (w_i, w_{i+1}) \in E$. The length of the walk is $\ell$.

For a subset $A \subseteq E$, we say a walk $\hat{w} = (w_0, w_1, \ldots, w_\ell)$ is $A$-alternating, if and only if

- $\forall i < \ell$, $i$ is odd : $(w_i, w_{i+1}) \in A$,
- $\forall i < \ell$, $i$ is even : $(w_i, w_{i+1}) \notin A$, and
- either $\ell$ is even and $\hat{w}$ is closed ($w_0 = w_\ell$), or $\ell$ is odd and the endpoints are loops ($w_0 = w_1$ and $w_{2\ell-1} = w_\ell$).

An $A$-tangle is a set of $A$-alternating walks passing through edges in $A$ exactly $n/2$ times in total, possibly by traversing some edges several times.

3.2 Perfect matchings in exponential time

For a subset $Z \subseteq [n/2]$, define the edge set $A(Z) = \{(w_2i, w_{2i+1}) : i \in Z\}$. Let $G_Z$ be the input graph $G$ with the edges $A(Z)$ added to it. The algorithm uses the following inclusion–exclusion formula for the perfect
We have
\[\sum_{Z \in P([n/2])} (-1)^{n/2-|Z|} f_G(Z),\]
(3.16a)
\[f_G(Z) = \#\{a : a \text{ is an } A(Z) \text{ - tangle in } G_Z\}.\]
(3.16b)

In Eq. (3.16a), \(P(Z)\) denotes the set of all the subsets of \(Z\) and \(\#\{x : Q(x)\}\) indicates the number of \(x\)s that satisfy the clause \(Q(x)\). Note that for a set of cardinality \(n/2\) there are \(2^{n/2}\) subsets. We will show in the next section that the function \(f_G(Z)\) is polynomial time computable.

First consider a perfect matching \(M\) in \(G\). Note that \(M \cup A([n/2])\) is exactly the edge set of an \(A([n/2])\)-tangle in \(G_{[n/2]}\); cf. Fig. 2. That is, the matchings together with the added alternating edges form even length cycles and paths with loops at both ends. This \(A([n/2])\)-tangle will only be counted once in Eq. (3.16b), namely for \(Z = [n/2]\). It will not be counted for any other \(Z\) as it traverses every edge in \(A([n/2])\) and at least one of them is missing in \(G_Z\) for \(Z \subset [n/2]\).

Second, any \(A([n/2])\)-tangle that traverses all of \(A([n/2])\) in \(G_{[n/2]}\) represents a unique perfect matching. This is because if one removes the edges in \(A([n/2])\) one is again left with a perfect matching in \(G\). So the equation at least counts perfect matchings, but we also must convince ourselves that it does not overcount.

To this end, consider a \(A([n/2])\)-tangle \(\tau\) that does not traverse all edges in \(A([n/2])\), say it only traverses \(A(Y)\) for some \(Y \subset [n/2]\). Then \(\tau\) will be counted once in \(G_Z\) for all \(Z, Y \subset Z \subset [n/2]\) but with sign \((-1)^{n/2-|Z|}\).

We have
\[\sum_{Y \subseteq Z \subseteq [n/2]} (-1)^{n/2-|Z|} = \sum_{W \subseteq [n/2] \setminus Y} (-1)^{|W|} = 0,\]
(3.17)
since there are as many odd as even sized subsets of a finite non-empty set. Hence, such a \(\tau\) will not be counted in Eq. (3.16).

### 3.3 Calculating \(f_G(Z)\) in cubic time

In the last section we showed that the calculation of the hafnian boils down to the calculation of the function \(f_G(Z)\) with \(Z \in P([n/2])\). Before showing how this is done let us introduce some additional notation. For every adjacency matrix \(A\) we introduce its column-swapped version
\[\tilde{A} = X_n A,\]
(3.18)
where
\[X = \bigoplus_{i=1}^{n/2} \sigma_X, \quad \sigma_X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.\]
(3.19)

We label the submatrices of \(\tilde{A}\) by the set \(Z = \{i_0, \ldots, i_{m-1}\} \subseteq [n/2]\) by using the notation \(\tilde{A}^{(Z)}\) to denote the \(2m \times 2m\) square matrix obtained from \(\tilde{A}\) by keeping only rows and columns \(\{2i_0, 2i_0 + 1, \ldots, 2i_{m-1}, 2i_{m-1} + 1\}\) from the original matrix \(\tilde{A}\).

To calculate \(f_G(Z)\) we argue as follows. First count \(A(Z)\)-alternating walks by length, by looking at entries of matrix powers of a matrix obtained from the adjacency matrix \(A\) of \(G\), keeping only the rows and columns representing the vertices spanned by \(A(Z)\), and swapping every pair of columns that are connected in \(A(Z)\); this matrix is precisely \(\tilde{A}^{(Z)}\). To show this note that the \((i,j)\) entry of \(\tilde{A}^{(Z)}\) carries the weight of walking from vertex \(i\) to vertex \(j\) using one original edge, and one “red-dashed” edge (cf. Fig. 2 i.e., an edge added by the edge set \(A(Z)\)).

The trace of \((\tilde{A}^{(Z)})^k\) counts closed alternating walks of length \(2k\) \((k\) original edges and \(k\) red ones), but it counts each walk \(2k\) times. The generating function
\[p(\lambda, B) = \sum_{j=1}^{n/2} \frac{1}{j!} \left( \sum_{k=1}^{n/2} \frac{\text{tr}(B^k) \lambda^k}{(2k)} \right)^j,\]
(3.20)
counts in the monomial \(\lambda^{n/2}\) the number of ways to combine several walks to a total of \(n\) visited edges \((n/2\) original ones and \(n/2\) red ones). Some edges may be counted multiple times here. Finally using an inclusion-exclusion argument [28] it is seen that only combinations of walks that do not use the same edge twice survive in the summation (and there is precisely one such combination of closed alternating walks associated to each perfect matching in the original graph).

One can calculate all the traces appearing in Eq. (3.20) in cubic time by noting that if one uses the Schur decomposition
\[B = QAQ^{-1},\]
(3.21)
with \(A\) upper triangular, then \(\text{tr}(B^k) = \sum_i A^k_{i,i}\). The factorization in Eq. (3.21) can be done in cubic time using standard linear algebra routines [29].

All the quantities appearing in Eq. (3.20) are well defined not only for \((0,1)\) matrices but for matrices over any field which allows us to write a simple and elegant
new formula for the hafnian of an arbitrary matrix $A$

\[
\text{haf}(A) = \sum_{Z \in P([n/2])} (-1)^{n/2-|Z|} \times \frac{1}{(n/2)!} d^{n/2} \left( \lambda, \tilde{A}(Z) \right)_{\lambda=0},
\]

and also for the loop hafnian

\[
\text{lhaf}(A) = \sum_{Z \in P([n/2])} (-1)^{n/2-|Z|} \times \frac{1}{(n/2)!} d^{n/2} \left( \lambda, \tilde{A}(Z), \text{diag}(A(Z)) \right)_{\lambda=0},
\]

where now we have

\[
q(\lambda, B, v) = \sum_{j=1}^{n/2} \frac{1}{j!} \times \left( \sum_{k=1}^{n/2} \frac{\text{tr}(B^k)}{(2k)} + \frac{v(Bx)^{k-1}v^T}{2} \right)^j \lambda^k.
\]

The function \(\text{diag}(B)\) returns the diagonal components of the matrix $B$ as a row vector. If $v = 0$ then $q(\lambda, B, 0) = p(\lambda, B)$ and thus the lhaf reduces to the hafnian when the diagonal entries of the input matrix are zero. Also note that

\[
q(\lambda, \mu B, \sqrt{\mu}v) = q(\mu \lambda, B, v),
\]

for any constant $\mu \geq 0$. This last equation shows explicitly that our loop hafnian formula conforms to the scaling relation in Eq. (2.14).

4 Results and Discussion

We now discuss the results of our numerical implementation of the algorithms discussed in the previous section. For increased efficiency, we developed a C-programming-language–CPU-based version of the algorithm for benchmarking together with python wrappers. This library will also be integrated in a future release of the Strawberry Fields platform for ease of use when studying Gaussian Boson Sampling.

Numerical computations are performed using the Titan supercomputer which allowed us to take advantage of hybrid CPU parallelism by combining distributed and shared memory methods using MPI and OpenMP protocols. The Titan supercomputer based at Oak Ridge National Laboratory has a theoretical peak performance of 27 petaFLOPS. It has a Cray architecture and currently ranks among the top 5 supercomputers in the world. Further enhancements to our implementation can be made by using GPUs; this will require new implementations of fast GPU based linear algebra routines for small matrices and will be the subject of a future study.

We considered three different types of graphs to benchmark the accuracy and the speed of the numerical computations:

1. Complete graphs with $n$ vertices: the hafnian of a complete graph, where all vertices are connected to one another with weight 1, without and with loops are known analytically and given by Eqs. (2.5) and (2.9) respectively.

2. Complete bipartite graphs with $n/2$ vertices: If we set the matrix $W$ to have matrix elements $W_{i,j} = 1$...
in Eq. (1.1), the hafnian of the matrix on the left side is simply \( \text{per}(W) = (n/2)! \).

3. In order to test the speed of computations and go beyond the analytically known results, we will consider random symmetric matrices of size \( n \times n \).

For the first two sets of matrices the value of the hafnian is known, hence we used them to not only benchmark the speed of our implementation but also the numerical accuracy of the algorithm.

Fig. 3 shows the performance benchmarks for complete and bipartite graphs by varying the size of matrix (i.e., the number of vertices in the associated graph). The results correspond to a single MPI process and 16 OpenMP threads for loop parallelism. The left panel shows the total computation time in seconds and the right panel shows the scaling of the percentage error defined as

\[
\%\text{Error} = \frac{\text{haf}_{\text{numerical}}(M) - \text{haf}_{\text{exact}}(M)}{\text{haf}_{\text{exact}}(M)} \times 100,
\]

where \( \text{haf}_{\text{numerical}} \) and \( \text{haf}_{\text{exact}} \) refer to numerical and analytical results respectively.

The computation time scales exponentially with matrix size \( n \) (the plots have log-scale on the vertical axis) for all types of graphs including complete and bipartite graphs. As shown in the inset, for a complete graph without loops of size \( n = 54 \) it takes approximately 1000 sec. For a graph with loops and a bipartite graph of the same size, the computation times are 2000 sec and 3000 sec respectively. Note that the exponential behavior is only apparent for \( n > 20 \). For small \( n \) the program spends more time in preprocessing and setting up the computation which is responsible for a knee-like behavior around \( n = 16 \). By fitting the time scaling with the function \( an^{b+c} \) for \( n > 20 \), we obtain \( b \approx 3 \) and \( c \approx 1/2 \) which is the expected scaling behavior. The overall prefactor \( a \approx 3.1 \times 10^{-8} \) sec.

Note that to compute the Hafnian function we need to perform \( \sim n!2^n/2 \) floating point operations and each operation is associated with a small numerical error. We use the standard LAPACK linear algebra package for the computation of the eigenvalues of the submatrices appearing in Eq. (3.22), which is limited to double precision. As \( n \) grows, the number of operations scales exponentially and so does the numerical error in the computation. The right panel of Fig. 3 shows the scaling of the percentage error in the computation (defined as in Eq. (4.26). For \( n = 54 \), the number of operations is \( \sim 4.2 \times 10^{12} \), which comes with an error as large as \( \sim 50\% \) for a complete graph without loops, 10\% for a graph with loops and 5\% for bipartite graphs.

To test the scaling of the computation time, we also consider symmetric random matrices of various sizes in Fig. 4. We find that similarly to the case of complete graphs (with matrix elements all being 1), the computation time scales exponentially with \( n \). Moreover, since the loop hafnian function requires additional computations associated with the diagonal elements, the computation for those is larger as compared to the hafnian function. For a random matrix with \( n = 54 \), the computation time is \( \sim 4500 \) sec and 1600 sec for loop hafnian and hafnian respectively with 16 OpenMP threads. For a fixed size \( n \) the computation times of random matrices are larger than those for matrices corresponding to complete graphs. This is because of the high symmetry of complete graphs which maps to a very simple structure of the eigenvalues of their adjacency matrices.

So far, we have only used shared memory parallelism on a single node computer using OpenMP multi-threading. We will now consider a hybrid CPU parallelism: distributing the computation over multiple nodes with OpenMP threads of their own. The time scaling using this hybrid approach for a matrix of size \( n = 50 \) is shown in the left panel of Fig. 5. We consider a range of MPI processes each with varying number of OpenMP threads. The computation turns out to perform extremely well with increasing number of MPI processes. The scaling is almost perfect, i.e. increasing MPI processes by a factor of 2 cuts down the computation time almost by a factor of half. Further enhancement in the computation time can be obtained by harnessing the power of GPU computing, which is beyond the scope of this implementation and is left for future work. The right panel of Fig. 5 shows the associated percentage error in computation. It turns out that choosing different combinations of MPI and OpenMP processes have negligible effect on the accuracy of the results. Using GPUs or other vectorized computing techniques, one may be able to reduce the overall prefactor in the computation time.
scaling, but that leaves the exponential scaling shown in left panel of Fig. 5 unaffected.

From the discussion above, it is clear that evaluating hafnians of large matrices is limited by two factors: (i) speed and (ii) accuracy. For instance a hafnian computation would take \( \sim 14000 \text{ sec} \) = 3.8 hours for \( n = 60 \) and \( \sim 6.8 \times 10^{19} \text{ sec} \) = 2155 years for \( n = 100 \) with 16 processors running in parallel. Utilizing all the 18000 CPU nodes (where each node has 16 CPUs, for a total of 288000 CPUs) of the Titan supercomputer and assuming perfect scaling over distributed nodes, computation of a single \( n = 100 \) hafnian would take at least 1.5 months. This severely constrains the size of the problems where one needs to exactly compute many hafnians of large matrix sizes. For example, generating an (exact) sample for Gaussian Boson Sampling would likely require the evaluation of at least one hafnian of the size of the number of events that are sampled (i.e., the number of detectors that click). The above estimation shows that this problem becomes computationally intractable as the number of inputs on the linear interferometer is increased beyond a few tens. One can hope that for a problem of such extent, an ideal quantum device for Gaussian Boson Sampling may generate a sample in a much smaller time scale hence outperforming classical supercomputers.

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A Number of elements in SPM(n)

For $n$ even one can obtain a closed form expression for the number of elements in SPM(n). Consider first PMP(n) the set of perfect matchings in a graph with $n$ vertices. One can start breaking pairs, i.e., taking a matching such as $(0,1)$ and turn into two loops $(0,0)(1,1)$. If one “breaks” $j$ pairs there are $\binom{n}{j}$ ways of doing this for each perfect matching. However this will overcount the number of partitions. For example if one breaks every matching of the following three perfect matchings $(0,1), (2,3), (0,2), (1,3)$ and $(0,3), (1,2), (3,3)$ one will always get the same set of loops $(0,0), (1,1), (2,2), (3,3)$ thus one needs to account for multiple counting by dividing by the factor $(j-1)!$. We conclude that if one breaks $j$ pairs from the set of perfect matching of $n$ objects one gets $\binom{n-1}{j-1} \binom{n}{j}$ partitions. We now need to sum over all possible $j$ to obtain the total number of partitions

$$|\text{SPM}(n)| = \sum_{j=0}^{n/2} \binom{n}{j} \binom{n-1}{j-1} = T\left(n, -\frac{1}{2}, \frac{1}{\sqrt{2}}\right)$$

(A.1)

where $T(a, b, r)$ is the Toronto function and $M(a, b, z)$ is the Kummer confluent hypergeometric function \cite{hypergeometric}. We also have the following asymptotic limit and bound:

$$\lim_{n \to \infty} M\left(-\frac{n}{2}, \frac{1}{2}, -\frac{1}{4}\right) = 1,$$

(A.2)

$$M\left(-\frac{n}{2}, \frac{1}{2}, -\frac{1}{4}\right) > \exp(\sqrt{n} - \frac{1}{4})/2.$$  

(A.3)