 Lifetime-based Method for Quantum Simulation on a New Sunway Supercomputer

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**Abstract**—Faster classical simulation becomes essential for the validation of quantum computer, and tensor network contraction is a widely-applied simulation approach. Due to the memory limitation, slicing is adopted to help cutting down the memory size by reducing the tensor dimension, which also leads to additional computation overhead. This paper proposes novel lifetime-based methods to reduce the slicing overhead and improve the computing efficiency, including: interpretation for slicing overhead, an in place slicing strategy to find the smallest slicing set, a corresponding iterative method, and an adaptive path refiner customized for Sunway architecture. Experiments show that our in place slicing strategy reduces the slicing overhead to less than 1.2 and obtains 100-200 times speedups over related efforts. The resulting simulation time is reduced from 304s (2021 Gordon Bell Prize) to 149.2s on Sycamore RQC, with a sustainable mixed-precision performance of 416.5 Pflops using over 41M cores to simulate 1M correlated samples.

**Index Terms**—quantum simulation, tensor network contraction, slicing, Sunway architecture

I. INTRODUCTION

Quantum computers provide exponentially speedups over classical counterparts in some special cases. The declaration “Quantum Supremacy” refers to these tasks in which the time costs are only reasonable by using quantum computers, and otherwise would be unacceptable \(^1\)[2][3]. However, despite such advantages in the computing capability, low fidelity is still the major challenge for quantum computers \(^4\). Results from classical simulation are therefore important to provide basic validations \(^5\). Furthermore, scientists and researchers in areas that heavily rely on reliable computing resource, such as quantum algorithm, quantum programming language, and quantum compiler, can work on classical simulators and obtain close performance\(^6\). Considering both the exponential complexity and the urgent demand, reducing the computation costs of quantum simulation becomes essentially necessary.

Random quantum circuit (RQC) is an typical task to demonstrate the “Quantum Supremacy”\(^1\). Similar to the classical circuit model, RQC is consists by qubits and quantum gates. Users prepare an \(n\) qubits of initial state as input, and get one of \(2^n\) possible output states in a sampling process. With \(k\) samples \(s_1, s_2, \ldots, s_k\) \((k \approx 10^6\) in Google\(^1\)) obtained by experiments, linear cross-entropy benchmarking (Linear XEB) is calculated for validation\(^7\):

\[
\mathcal{F}_{\text{XEB}} = \frac{2^n}{k} \sum_{i=1}^{k} p_C(s_i) - 1 \tag{1}
\]

where \(p_C(s_i)\) comes from classical simulation. To simulate the process of quantum sampling, there are two major strategies, i.e., state vector\(^8\) and tensor network contraction\(^9\). The difficulty of the former comes from the exponential memory complexity\(^10\). To get rid of memory barrier, though many strategies\(^11\)[12] are developed, a general-purpose and sufficiently effective method that reduces the memory demand is still less to be seen. Tensor network contraction can resolve the memory problem by slicing, but suffers from the exponentially increasing computation cost when the RQC becomes deeper\(^13\), while the increasing becomes polynomial in terms of state vector method.

In tensor-based strategy, qubits and quantum gates are represented as tensors. The complete RQC can be considered as a tensor network\(^14\). The amplitude of a state is generally represented as tensors. The complete RQC can be considered as a tensor network\(^14\). The state vector comes from classical simulation. To simulate the process of quantum sampling, there are two major strategies, i.e., state vector\(^8\) and tensor network contraction\(^9\). The difficulty of the former comes from the exponential memory complexity\(^10\), To get rid of memory barrier, though many strategies\(^11\)[12] are developed, a general-purpose and sufficiently effective method that reduces the memory demand is still less to be seen. Tensor network contraction can resolve the memory problem by slicing, but suffers from the exponentially increasing computation cost when the RQC becomes deeper\(^13\), while the increasing becomes polynomial in terms of state vector method.

Unlike previous efforts that largely use heuristic algorithms, this work introduces a new conception, *lifetime*, in order to provide better interpretability for the slicing optimization in tensor network contraction. Based on the analysis of *lifetime*, a novel strategy for tuning the contraction path and selecting the slicing set is obtained, well resolves problems such as computation overheads, and achieves better time-to-solution.

Major contributions of this work include:
A conception, *lifetime* of indices, is proposed to explain what makes up the slicing overhead and the optimization space, and to select the best strategy in different conditions.

- Guided by *lifetime*, a dynamic slicing method with a new target function is proposed, successfully finds the smallest slicing set, and acquires 100-200 times speedups compared with related efforts. The iterative version using tree tuning is able to reduce the overhead caused by the structure of contraction tree.

- Indicated by *lifetime*, a contraction tree tuning algorithm that fits well with the Sunway architecture is presented. It can be easily projected that the resulting simulation time is reduced from 304s (the work that won the 2021 Gordon Bell Prize) to 149.2s, with a sustainable mixed-precision performance of 416.5 Pflops using 107,520 nodes (more than 41 million cores) to simulate 1M correlated samples of quantum supremacy circuits.

## II. BACKGROUND

### A. Tensor Network Contraction and Slicing

1) **Notation:** A tensor network can be treated as an undirected graph, when tensor and dimension are denoted by vertex and edge, respectively. We define the notation similar with the work of Cotengra[17].

We denote a graph by \( G = (V, E) \). \( V \) is the vertex set, and \( E \subseteq \{(u, v) : u, v \in V\} \) is the edge set. A map \( w : E \rightarrow \mathbb{R} \) denotes the edge weight, as well as the size on each dimension. The incidence set \( s_v \) is defined as \( s_v = \{e : e \in E, v \in e\} \), for vertices set \( s_V = \{e : e \in E, e \cap V \neq \emptyset\} \). Vertex contraction, which merges two vertex to one by removing shared edge and keeping the rest, can be represented as a map: \( \text{Cont} : P \rightarrow V_P \), where \( V_P \) is the image set that contains all the elements of \( V \). The new vertex after contraction, \( P = \{(u, v) : u \in V_P, v \in V_P\} \) is the set of pair of vertices. \( \text{Cont}(u, v) \) is a new vertex under the rules of \( s_{\text{Cont}(u,v)} = \{e : e \in \{s_u \cup s_v - s_u \cap s_v\}\} \). Based on these definitions, tensor network contractions can be represented as vertex contractions.

If we perform the pairwise contraction sequentially till there’s only one vertex left, the contraction order would form a contraction path. Obviously some subsets of the contraction whose preimage set have empty intersection are independent from each other. So the contraction path are not a decisive expression. All equivalent paths can be uniquely described by a tree structure. A contraction tree \( B \) is defined as \( B = (N_B, E_B) \), with each edge denoted by a vertex of original graph or an intermediate vertex generated by contraction. Specially, the edges connecting to leaf nodes are denoted by vertices in \( V \). Nodes expressed as triplet \( node = (e_1, e_2, e_3) \) refer to contractions. In particular, leaf nodes such as \((1, e_1, e_1)\) can be treated as a multiplication with a scalar 1. Then leaf nodes can represent the reading process. A certain contraction path determines the direction of each contraction. By adding the final contraction as the root, as shown in Fig 1, a rooted binary tree is acquired.

![Fig. 1: Tensor Network and One of its Contraction Tree](image)

2) **Related Work:** To find the best path, exhaustive search with dynamic programming approach ensures an optimal result[18]. However, as an \#P problem[19] or worse, low efficiency caused by combinatorial explosion makes it impractical even for a 40-tensors graph. As a compromise, people are committed to an near-optimal but much faster algorithm,
to find a high-quality path in an acceptable period, where a number of challenges have been levied\[20\][21].

Cotengra\[17\] integrates several anytime methods and claims over $10000 \times$ speedup compared to the estimation made by Google\[1\]. This work mainly contributes two strategies, reducing the search space and introducing heuristic. After the pre-process implemented in \[22\], rank-1 and rank-2 tensors are absorbed, and the tensor network is largely simplified.

Methods based on graph partition often offer better results. GN method by Girvan and Newman\[23\] divides a graph by community detection. Another partitioner Kahypar\[24\][25\] can divide a hypergraph into $k$ parts with an assigned imbalance factor, minimizing the cut-edges or another target function called ‘connectivity’. With a graph partition, people can get a series of subgraphs unconnected to each other, and just perform the inner contractions before contracting the intermediate edges. The search space can be significantly reduced, as the primary search space comes from the interaction of tensors. To find a contraction path in the small subgraph, even exhaustive search can help. Contengra offers a greedy strategy \[26\] to find indices to slice: repeatedly choose one index which causes least time complexity increase. Such strategy will frequently fall into local minimum, and the complexity after slicing is over hundreds of times than before. Specific to the contraction of 20-cycle Sycamore circuit, Cotengra can offer a path with $10^{18.8}$ times complexity, slicing overhead of 4, and a 14.7% FLOPS efficiency.

### III. KEY IDEA

#### A. Lifetime

We first explain where does the slice overhead come from. Fig \[3\] shows a contraction process on a $4 \times 2$ tensor network. If we apply a contraction path and slice tensors as shown in the figure, the path and sliced index are obviously far from optimal. The two sliced tensors drops one dimension each time. The slicing strategy is a dynamic process. While basic logic same as Contengra, they perform local tuning of contraction tree between two steps of slicing picking. This work can provide $10^{18.8}$ times complexity, slicing overhead of 4, and a 14.7% FLOPS efficiency.

#### B. New Sunway Supercomputer

As the key approach to look for the near optimal contraction path, and a time- and memory-consuming part, performing the actual contraction generally requires support from sophisticated supercomputers. A new Sunway supercomputer is selected in this work.

The new-generation Sunway supercomputer has a similar architecture as Sunway TaihuLight\[28\], with the major computing capability provided by core-groups (CGs). A heterogeneous many-core processor, SW26010pro, is designed for this supercomputer. Fig \[3\] shows the structure of the chip. Each processor chip has 6 CGs. The computing processing elements (CPEs) of each CG are arranged in an 8 by 8 grid. A loop network-on-chip (NoC) connects the CGs and undertakes the task of communication.

Each CG contains 16GB main memory, and each CPE contains 256KB local data memory (LDM). A direct memory access (DMA) with a bandwidth of 51.2 GB/s is provided between LDM and main memory. Remote memory access (RMA) is designed for data exchange between CPEs within one CG. RMA provides similar function-like communication without waiting, and results in a quite different computation-communication overlapping options compared with the TaihuLight \[28\] system.
contracted tensors, the calculation without the sliced index will be doubled.

![Diagram](image)

Fig. 4: Origin of Slicing Overhead

Based on the analysis above, this work proposed a new concept, **lifetime**, to describe the scope of influence of a sliced index during the slicing. The definition, and application of **lifetime** will be provided hereafter, and the notation comes from section [II-A1](#).

**Definition 1**: Given a contraction tree \( B = (N_B, E_B) \), the concept **life-time** of index \( k \) refers to a set of edges(tensors) \( \{T_{i_1}, T_{i_2}, \ldots, T_{i_m}\} \subseteq E_B \), if \( k \in s_{N_i} \), for all \( 1 \leq j \leq n \).

**Definition 2**: Given a contraction tree \( B = (N_B, E_B) \), the concept correlated contractions of index \( k \) refers to a set of nodes(contractions) \( \{N_{i_1}, N_{i_2}, \ldots, N_{i_m}\} \subseteq N_B \), if \( k \in s_{N_i} \), for all \( 1 \leq j \leq m \).

Based on above definitions, **lifetime** has some good properties, and the most important one is linearity.

**Lemma 1**: Given a contraction tree \( B = (N_B, E_B) \), for any index in \( s_{E_B} \), if it involves the corresponding contraction, it will only be in the two incidence edges of a node. Otherwise, it will not exist at all in \( s_{node} \).

Conservation describes a common condition that an index involves a contraction. If contracted, it will only exist in the two contracted tensors; otherwise, it will be kept from one of the contracted tensors to the generated tensor. An interesting corollary from this theorem is that, contractions do not create or diminish index. Instead, they connect two tensors that share common index. Another inference is that, a correlated contraction of an index contains two tensors which exist in the indices’ **lifetime**. Furthermore, for every index, all contractions of the tree involved by tensors in its **lifetime** form a correlated contraction set. Therefore, **lifetime** and correlated contractions demonstrate a linear structure:

**Theorem 1**: Given a contraction tree \( B = (N_B, E_B) \) and an index \( k \), there exists a path on the tree from one leaf node to another. The set of edges the path goes through is equivalent to the **lifetime** of \( k \), and the set of nodes on the path is equivalent to the correlated contraction set of \( k \).

With the definition of **lifetime** and correlated contractions, the overhead caused by one sliced index \( k \) can be clearly described. Memory complexity of tensors in the **lifetime** of \( k \) will reduce by half, and will remain the same for the other tensors. The time complexity of correlated contractions will remain the same, and will be doubled for the other contractions. More in-depth discussion will be given in the following part.

### B. The Origin of Slicing Overhead

The property Linearity makes **lifetime** a powerful tool for the complexity analysis. Take the problem of multi-indices slicing for example. Considering that **lifetimes** of different indices are independent, slicing index \( a \) has nothing to do with the **lifetime** of index \( b \). So each sliced index can be analysed one by one. For each tensor, if it contains \( s \) sliced indexes, it will be divided into \( 2^s \) smaller tensors. For \( 2^m \) subtasks, there will be \( 2^{n-s} \) times of redundant data. Similarly, for correlated contractions with \( s \) sliced indices involving calculation, the time complexity will be multiplied by \( 2^{n-s} \) times. These result can be represented by the overlapping of **lifetimes**, as is shown in Fig 5. The density of **lifetimes** overlapping plays a decisive role on memory and computation complexity on a region.

![Diagram](image)

Fig. 5: Overlap of **Lifetime**

So far, we have discussed the overhead due to the computation complexity. However, it could become even worse when the memory demand is not appropriately satisfied. For a certain contraction tree, if the dimensions of all tensors drop and becomes no more than the target dimension after slicing \( s \) indices, a \( s + 1 \) indices slicing set will introduce redundancy.

Besides, redundant slicing will introduce more calculations, and increase the algorithmic complexity. Here we use a path with two slice indices, whose **lifetime** are respectively between \( T_{i_1}, T_{j_1} \), and \( T_{i_2}, T_{j_2} \) to explain. Without loss of generality, we assume \( i_1 < m < i_2, j_1 < n < j_2 \). Based on the analysis of **lifetime**, if the two sliced indices have no overlapping part in their **lifetimes**, the whole computation will at least be doubled, and is certainly higher than a single slicing across \( m \) and \( n \). Obviously, even if there is an overlapping part, its length is less than \( n-m \), and is the shortest length of region whose time complexity is kept by single slicing, let alone the quadruple parts. So it is necessary to avoid redundant slicing.
In conclusion, the slicing overhead mainly comes from the lifetime of sparsely overlapping of sliced indices, and the redundant slicing. Based on the discussion above, it maybe helpful to have slicing indices with long lifetimes which include more large tensors.

C. Limitation and Improvement

Obviously, if we have more tensors whose dimension exceeds the memory demand during a lifetime of sliced indices, less overhead will be resulted in. A straightforward method is to repeatedly choose an index who has the longest lifetime until the memory bound is achieved. However, such operation will mislead the optimization to some degree. As an intuitive conception to describe the influence of time cost by an index, lifetime treats all tensors that share an index in the tree with the same weight. But considering the huge difference in dimensions, the assumption is not realistic.

To solve this problem, we can consider the region with intensive computation only. Recent work led by Alibaba [27] presented an observed structure that is stem from Sycamore RQC[1], and is defined as a path formed by high-weights tensors. However, the definition lacks generality, as it is an observation on a particular tensor network. In this work, we present a quantitative definition of stem, and make it a general conception. There are \( n^2 \) continuous paths from a leaf node to another leaf node on the \( n - \text{leaves} \) contraction tree. Time complexity of these path can be defined as the summation of complexity of all contractions. Stem refers to a certain path with the highest time complexity. Based on the definition, we can find a stem on an arbitrary contraction tree for every tensor network. The rest parts outside the stem on the contraction tree are referred to as branches. If regarding the branches as pre-contraction tensors, we can see tensors on the stem sequentially absorb branches.

The advantage of introducing stem is that we can ignore the behavior between most of low dimension tensors. We can redefine lifetime of a index as its scope of influence on the stem. Dominance of the stem is the central problem we concern. Fortunately, heavy branches occasionally appear. A simple example can provide interpretation for the generality of dominant stem: two huge tensors contract \( m \) indices and form a \( n \)-dimensional tensor, the complexity will be \( 2^{m+n} \). However, a huge one sequentially absorb small tensors, i.e. contraction by steps, have a heaviest step no more than \( 2^{m+n} \), since contracted indices are distributed. An additional benefit is that stem is a linear structure, then we can discuss the overlap problem clearly on a broken line. Using a contraction tree of Sycamore[1] as an example, Fig 6 shows the distribution of time complexity on the stem as the blue graph, and also present the multiplier of each parts as the orange one. It’s easy to find that the upper two pictures can be somehow mapped, and best mapping minimizes the time complexity.

D. Route of Slicing Optimization

We have proved that slicing overhead mainly comes from redundant calculation, so there are two potential optimization strategies, choosing better indices for slicing, and improving data reuse. This part explains under what conditions data reuse strategy can be applied. Hereafter dimension exceeded tensor denotes those tensors whose dimension exceeds the memory demand. In the discussion below, we can see that the strategy is determined by the distribution of the dimension exceeded tensor.

On a stem-dominant tree, if dimension exceeded tensors are clustered on one part of the stem, data reuse is not very practical. We can find at most one part on the stem, where the lifetime of all indices are overlapped, and only in this part the time complexity is kept. The other parts can be treated as two categories, branch and both ends (head and tail) of the stem. Branches are far more complex than the whole tree, but carry few or zero sliced indices. Contractions will be repeated and consume most of the execution times. We can simply perform a pre-contraction to avoid such redundancy, though in most conditions the overhead is not significant (the observed benefits is less than one ten thousandth for Sycamore RQC[1]).

As for the head/tail ends of the stem, sliced indices enter the tree one by one along the stem. After all sliced indices entered, the lifetime of all indices overlaps until the first index leaves. When a sliced index enters, the number of homologous tensors at corresponding position is doubled. With the number of tensors required to be stored increases, together with the increase of dimension, the data easily exceeds the main memory capacity in a very short time. In conclusion, the redundant calculation can hardly be reused. Under such circumstance, looking for a better set of index for slicing shall be a more practical way for optimization.

Then we consider the condition where high dimensional tensors are clustered in several unconnected parts. Similar with the work in [5], a tensor network is firstly divided into two subgraphs with \( k \) edge connected with each other. If the value of \( k \) is quite small compared with the connectivity of each subgraph, a considerable contraction order is to contract all subgraphs into single tensors, and perform contraction between subgraphs. Here we assume there are \( m, n, \) and \( s \) sliced indices in part A, part B, and the connecting edges between A and B, respectively. According to the definition of lifetime, indices in part A only have a lifetime in the subtree
A, and have nothing to do with B, so are the indices in B. Meanwhile, lifetime of indices between A and B can lie across the demarcation point between A and B. Therefore, data reuse can be applied by executing $2^{m+s}$ and $2^{n+s}$ subtasks to perform contraction of subgraph A and subgraph B, respectively. While the contraction of A is completed, we merge each $2^m$ subtasks into 1 task, representing contractions of the m sliced indices.

Here $C_A, C_B$ denote the time complexity of A and B, respectively. $C = C_A + C_B + 2^k$ and $P_A = C_A/C, P_B = C_B/C$. $2^k$ is much smaller than C, and can be neglected. The accelerating ratio after reuse is:

$$\text{ratio} = \frac{2^{m+n} \times (C_A + C_B)}{2^m \times C_A + 2^n \times C_B} = \frac{2^n}{1 + (2^{n-m} - 1) \times P_B}$$

(5)

Obviously, the ratio relies on m, n and $P_B$. Since the dimension of tensors plays significant roles to the time complexity, we can expect $n - m$ often has a positive correlation with $P_B$. Therefore, if n is much larger than m, $P_B$ is considered large. So "1" can be ignored, and the ratio is approximately equivalent to $2^n/P_B$. Otherwise, $P_B$ is considered small. So $2^{n-m}$ can be neglected compared to 1, and the ratio is approximately equivalent to $2^n/P_B$. If $m = n$, the ratio is $2^n$.

Since the number of sliced index is divided in to $m + n + s$, we should select less slicing index between subgraphs, in order to achieve better performance. However, such circumstance relies on a small k, a nearly-balanced complexity distribution between A and B, as well as the property of community[30]. So the good result can hardly be obtained within a tree with an agglomerate stem.

IV. SLICING STRATEGY GUIDED BY LIFETIME

A. Problem Statement

To minimize overhead while fitting memory bound describes an optimization problem with constraints. Given a contraction tree $B = (N_B, E_B)$, the target function can be described by the total time complexity after slicing.

$$C(B, S) = \sum_{V \in N_B} 2^{|S| + |S| - |S \cap S|}$$

(6)

where $S$ is the set of sliced indices. For the stem, the target function combines the multiply curve and the time complexity curve. Large value of $|S|_{s}$ represents a computation intensive region. To minimize $C(B, S)$, the two curves shall be aligned in a sense.

The target size which does not exceed the memory capacity is denoted as $t$. For every $e \in E_B$, $|S \cap s_e| \geq |s_e| - t$. The target function and the formula together can determine the optimization problem.

B. Slicing Strategy

Now it has been proved that redundant slicing leads to higher overhead. So selecting the smallest slicing set is able to help achieve the best result. Since small tensors have nothing to do with the memory constraints, they can be removed from the stem. The new stem holds a linear structure and does not break any of the lifetime, only making some of them shorter. If the original stem is dominant in terms of the computing time, the new stem $M = \{T_1, T_2, \ldots, T_N\}$ will only contains all dimension exceeded tensors. Assuming the optimal size of the slicing set is $s_1$, the stem is then separated into two continuous parts: $M = M_1 + M_2$, and the optimal size of $M_1$ is $s_1$. For $M_1$, there is a number of candidate sets that share the same size $s_1$. In the new $M_2$ where $s_1$ is removed, we have to choose the best set to shrink and find the smallest value of $s_2$.

For slicing, an important lemma is that: the length of lifetime does not determine the slicing overhead, unless the lifetime of an index is the subset of the another’s, as shown in Fig 7. It is the same for the effect of reducing memory. Therefore, if there is such a set $S_1$, for any other candidates, we can find a one-to-one correspondence between each index in the two sets. And in every pair, the lifetime of the index from other set is a subset of the one in $S_1$. $S_1$ is the optimal set to minimize $s_2$. For an arbitrary separation, it may be difficult to find the optimal set. But it is easy to separate edge tensors one by one. The discussion above is concluded in our proposed Algorithm[1] which ensures that the smallest slicing set can be found.

Besides being capable of finding a minimum size of the slicing set, the proposed algorithm is able to improve the performance as well. For previous state-of-the-art efforts (Cotengra[17]) that applies greedy method, it has to exhaustly traverse in the worst case to find a local optimal. However, in our algorithm, all indices only needs to be traversed once to calculate lifetime. What’s more, in terms of finding the slice index, we only need to traverse all indices in the smallest tensor, which could be hundred of times faster than the performance of Cotengra[17].

The method above can find a near-optimal slicing set for a given contraction tree. However, different contraction trees show different lower bound of overhead. For instance, if the lifetimes of all indices are so short that no tensor contains all of the sliced indices, the total computation will be increased by at least two times. But in the sense of time complexity of...
there’s $s_0$ slicing index in $T_0$, $s_1$ in $T_1$, $s_2$ in $T_2$, in particular $s_{10}, s_{20}$ sliced index contracted at the first and the second contraction respectively, and $l$ in the whole contraction tree. Let $n = n_0 + n_1 + n_2$, the time complexity before exchange is:

$$C_s = 2^{m+b_1-n_1+l-s_{01}+s_{10}} (1 + 2^{b_2-n_2-s_{02}+s_{10}+s_{20}})$$

Calculating the ratio between time complexity before and after exchanging can show the improvement:

$$ratio = \frac{2^{b_1-n_1-s_{01}+s_{10}}}{2^{b_2-n_2-s_{02}+s_{10}+s_{20}}} \times \frac{1 + 2^{b_2-n_2-s_{02}+s_{10}+s_{20}}}{1 + 2^{b_1-n_1-s_{01}+s_{10}+s_{20}}}$$

If $b_1 - s_{1} \geq b_2 - s_{2}$, with the sugar water inequality, the expression can be simplified as $2^{n_2-n_{10}+s_{10}}$. When $n_2 - s_{20} - (n_1 - s_{10}) \geq 0$ is found, the exchange will reduce the complexity. As a symmetric circumstance, when $b_2 - s_{2} \geq b_1 - s_{1}$, let $n'_1 = b_1 - n_1 - n_0, n'_2 = b_2 - n_2 - n_0, s_{11} = s_1 - s_{10}$, $s_{21} = s_2 - s_{20}$, the expression will be $2^{n'_1-n'_2-s_{11}+s_{21}}$. Therefore, $n'_1 - s_{11} \geq n'_2 - s_{21}$ will lead to exchange as well. If the exchange is performed, the lifetime of some sliced indices will be shorter, while the rest will be longer. We repeatedly perform the exchange till no neighboring branches satisfy the condition. So the branches are organised as a sequence with partial order. After the iterative tuning, the lengthened sliced indices can provide smaller overhead. Another important progress is that, when the condition above is satisfied, $m+b_1-2n_1-s_{01}+2s_{10} > m+b_2-2n_2-s_{02}+2s_{20}$. So the memory complexity is decreased and sometimes the sliced indices is reduced as well.

Now that the slicing algorithm demonstrates better performance, it can be used as an iterating step between one or several steps of exchange to update the slicing set. The corresponding algorithm is described as in algorithm 2. Function `detectStem` is simply implemented by the definition above.

Our sliceFinder is able to find a near-optimal slicing set. After the following branch exchange, the complexity will be largely decreased. For this new contraction tree, sliceFinder is able to find a better slicing set than previous one, and decreases the complexity once more. Therefore, a better result from iterative method can be expected.

V. CUSTOMIZATION FOR SUNWAY ARCHITECTURE

A. FLOPS Efficiency of Tensor Network Contraction on Sunway Supercomputer

In addition to computation complexity, low FLOPS efficiency becomes a problem at the stage of implementation on selected supercomputer. Contraction between tensors is implemented by matrix multiplication. All indices of the tensor can be divided into two groups: $m$ indices are kept and the other $n$ are to be contracted. So a tensor is reshaped as a $M \times N$ matrix, where $M = 2^m$, $N = 2^n$. A high performance library, SWTT[6], based on the General matrix multiplication (GEMM) is used. GEMM applies 2D data distribution for $M$ and $K$ respectively on 68 x 8 CGs, and 6 can be divided as $6 \times 1, 3 \times 2, 2 \times 3$ or $1 \times 6$ for the two directions. Based on this strategy, near optimal FLOPS can be obtained on square-like
Algorithm 2 Procedure tuningSliceFinder

**Input:** Contraction tree $T$, target dim $t$, stride $n$, max repeat num $m$, max fail num $f$

$M = \text{detectStem}(T)$

fail = 0, $i = 0$, $flag = 0$

repeat

$S = \text{sliceFinder}(M, t)$

$k = (flag == 0) ? \text{randomInt}(0, \text{len}(M)) : flag$

for $j \leftarrow 0$ to $n$

if $\text{exchangeCondition}(M, k, k + 1)$ then

exchange$(M, k, k + 1)$

else

fail = fail + 1

break

end if

end for

if fail == $f$ then

for $j \leftarrow 0$ to len$(M)$

if $\text{exchangeCondition}(M, i, i + 1)$ then

$k = flag, stop = False$

break

else

stop = True

end if

end for

end if

fail = 0, $i = i + 1$

until $i == m$ or stop == True

update $T$ by $M$

**Output:** Slicing set $S$, tuned contraction tree $T$

matrix. However, narrow matrix will slow down the FLOPS efficiency.

The time complexity of GEMM is $\Theta(MNK)$, and the complexity of Reading and Writing is $\Theta(MN + NK + MK)$. Since the peak performance of a Sunway CG is 2.2TFLOPS, and the peak DMA bandwidth is 51.2GB/s, a critical arithmetic intensity is 42.96 Flops/Bytes. When each of $m$, $n$, $k$ is too small, there will be $\Theta(MNK) \approx \Theta(MN + NK + MK)$, and GEMM will change from a computational intensity problem to a bandwidth-constrained problem. Especially for $k, n < 4$ commonly existing on the stem, low bandwidth will make the FLOPS efficiency less than 4%.

Another problem comes from thread distribution. The strategy utilized does not abandon the $n$ direction even if $N$ is less than 8. So some CPEs are idle and the load imbalance becomes a serious issue. The computational kernel makes it even worse. To make full advantage of the 512-bits single instruction multi-data (SIMD), SWTT employed a 8*8 GEMM kernel as basis. When the data alignment can not satisfy the requirement of the kernel, SWTT will do padding, which will introduce 7 times of redundant data in the worst case.

The problem caused by thread distribution and computation kernel can be solved by updating SWTT library. However, bandwidth is a hard constraint. To overcome it, a feasible way is to enlarge $n$ and $k$ with an acceptable increment of time complexity. And, with a larger $k$ and $n$, the negative effect caused by SWTT’s strategy will be reduced simultaneously.

B. Trade-off between Time Complexity and FLOPS Efficiency

On the branch, we simply apply pre-contraction with numpy to avoid such problem. On the stem, branch merging will provide an efficient way. Instead of sequentially contracting with a large tensor, two branches can be pre-contracted with each other first. Following the notation in Section III and IV, we set $n_1 = m - n_1, n_2 = m + b_1 - 2n_1 - n_2 - n_0, n_3 = m - n_1 - n_2, k_1 = b_1 - n_1, k_2 = b_2 - n_2 - n_0, k_3 = b_1 + b_2 - 2n_1 - n_2$. Now analysing lifetime can provide a time complexity for each contraction. With the same computing resources and library, FLOPS efficiency is only related to the data layout. We made a data set concluding the FLOPS efficiency at some combination of $m, n$ and $k$. From the data set we can get $F(M, N, K)$, which denotes the FLOPS efficiency of GEMM with two matrix ($M \times N$ and $N \times K$, respectively). Regarding the executing time proportional to time complexity and inversely proportional to FLOPS efficiency, the time can be expressed similar with the target function in Section IV, with weights representing FLOPS efficiency. Then branch merging will be applied under the following circumstance:

$$\frac{1}{F(m_1, k_1, n_1)} + 2\frac{k_2 - n_1 - s_2 + s_{10} + s_{20}}{F(m_2, k_2, n + n_2)} > 2\frac{k_2 - 2n_1 - n_2 - s_2 + s_{20}}{F(m_3, k_3, n_1 + n_2)}$$

(10)

From the condition we can see, after the merging, if $n$ has a big value, since $b_1 \geq n_1 + n_0, b_2 \geq n_2 + n_0$, the time complexity will be decreased and the FLOPS efficiency will not become worse. If $n_0$ has a small value, $N$ and $K$ will be enlarged to achieve a better FLOPS efficiency, with a increment of time complexity. We can see a trade-off from above analysis. Fortunately, after the merging, the sliced indices on two branches are combined together. So the sliced indices $s_{10}, s_{21}$ on two branches are overlapped, and the time complexity is reduced furthermore. In the implementation, all the merging operations that satisfy the inequality above are performed, till no such neighboring branches are found any longer.

C. The Best Path of All Who Share a Contraction Tree

Different paths corresponding to one contraction tree have same contraction width and very near time complexity. However, the FLOPS efficiency will be various. From the test, there’s an observation that $N$ has a higher width than $K$ when forming the $F(M, K, N)$. On a stem, the path often goes from an end to a intermediate tensor, then stops and restarts from the other end to the one after that tensor, and performs a contraction between them. Considering that a path from end to end on a stem is going with the dimension increasing then decreasing in general, then a path above will reverse a part of downhill to uphill. Uphill means $m + b_1 - 2n_1 > m$, then there will be $N < K$. So we make sure the path is from end to end on the stem.
VI. RESULT

Related efforts (e.g., Cotengra\cite{17}, Alibaba\cite{27} and \cite{6}) have all simulated Sycamore RQC\cite{11}. To make an appropriate comparison, unless otherwise specified, the contraction trees used in this work come from the tensor network of Sycamore as well.

A. Slicing Overhead

According to algorithm \cite{11} we can find a slicing set given a contraction tree. This process is called searching in place. Cotengra has implemented the SliceFinder that provides the same function, and is used in our work for comparison. Due to the greedy strategy, Cotengra often finds a slicing set with local minimum overhead. To overcome this, it needs to repeat the process several times and choose a best one. Such implementation slows down the performance. As is shown in Fig\cite{8} we compare the performance of our work with Cotengra (repeat 16 times in maximum) on the same 100 contraction trees:

Fig. 8: Searching Time Compared by Cotengra

Fig.\cite{8} shows that our proposed sliceFinder can be more than 100 – 200 times faster than Cotengra, in finding a slicing set. The performance improvement enables our algorithm to be fully utilized during the contraction tuning. Cotengra and Alibaba can only distribute steps of slicing searching between local tuning, preventing local searching from the whole slicing information.

We know that slicing overhead is not only determined by the slicing set, but also by the contraction tree itself. To test if our slicing sets achieve the smallest slicing set and a lower overhead, we find contraction trees with different number of sliced indices. For generality, we test more circuits\cite{31} for comparison.

In Fig\cite{9} syc–$m$ denotes $m$–cycle Sycamore circuit, and zn–$m$ denotes $n$–qubits $m$–cycle Zuchongzhi circuit\cite{31}. For all contraction trees, we can see in most cases our work can find a slicing set with equal or smaller size than Cotengra. So our theoretical idea is verified, and the overhead from redundant slicing is effectively eliminated. As for the rest cases, we found that the stems do not contain all of the huge tensors, and do not satisfy our prerequisites. However, these cases can be resolved by simply rearranging several steps on the contraction path. Furthermore, our work indicates a lower bound of the size of slicing set, and this is also strongly correlated with the lower bound of the overhead. As is shown in Fig\cite{10} in most cases, our sliceFinder can work better or equal with Cotengra.

Our algorithm is a memory-oriented method. As a result, when meeting a complicated tensor network which can hardly deal with greedy strategy, we can perform better. The more complex the circuit and the contraction tree are, the better result our algorithm is able to provide. Since for different path, slicing overhead will be various, we tested for hundreds of path for geometric mean and harmonic mean, and found that in most circuits, our algorithm can achieve a lower average overhead.

Due to the high slicing overhead caused by some contraction trees, tree tuning is applied as well. Such strategy is used by Alibaba and the latest version of Cotengra. Alibaba claimed that they can achieve a slicing overhead of 4 times with 25 indices sliced. Cotengra has found a slicing overhead of 419 times. However, with a new function called slicing reconfigure,
the actually overhead was tested through experiments.

On Sycamore circuit, our algorithm achieved a slicing overhead of 1.255 times in the applied path for actual contraction, which is close to the complexity without slicing. The latest version of Cotengra can find a same slicing set with us, and both are better than 4 times claimed by Alibaba’s work.

**B. Computing Efficiency**

We perform the contraction on a new generation Sunway supercomputer. Here we choose 100 different contraction trees and compare the time cost and the computing efficiency (FLOPS) with the recent state-of-the-art work that won the 2021 ACM Gordon Bell Prize [6]. The process-level parallel between subtasks of slicing is barely an embarrassing parallelism, and only one all-reduction operation is required after the computation. So we only need to calculate one subtask, thus the time and FLOPS performance of the who process can be estimated accordingly.

![Fig. 11: FLOPS Efficiency after Branch Merging](image)

Fig. 11 shows that our work is able to significantly improve the computing efficiency from 4% to 20% (single precision) and 1.69% to 7.06% (mixed precision), and reduce the time cost of a subtask from 5.88s to 3.18s. Therefore, we project the simulating time of Sycamore quantum supremacy circuits to is reduced from 304s (2021 Gordon Bell Prize) to 149.2s.

The conception of lifetime proposed in this work demonstrates great potential in facilitating quantum simulation. A series of lemmas and theorems based on lifetime intensify our awareness of a tensor network and the contraction trees. In the field of slicing, it provides a interpretation for slicing overhead, and help us finds the smallest slicing set. Furthermore, based on lifetime, we can distinguish two kinds of tensor network which shall be sliced by different strategy. Based on a specific architecture, i.e., the new-generation Sunway supercomputer, lifetime also helps analyse the time complexity and provides prerequisite inequality.

In addition, lifetime is also very promising in future works in finding contraction path, analysing time complexity, and even helping us explore the structure of tensor network. As a widely applied approach, tensor network can be found in many research fields such as statistical physics, data science, sociology and so on. This work proves that lifetime is essentially helpful for the tensor networks which have an equal edge weight and a dominant stem. However, lifetime can be easily generalized to tensor works with different features and helps analyze both the time- and space-complexities of the contraction.

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