Computing Double Precision Euclidean Distances using GPU Tensor Cores

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Abstract—Tensor cores (TCs) are a type of Application-Specific Integrated Circuit (ASIC) and are a recent addition to Graphics Processing Unit (GPU) architectures. As such, TCs are purposefully designed to greatly improve the performance of Matrix Multiply-Accumulate (MMA) operations. While TCs are heavily studied for machine learning and closely related fields, where their high efficiency is undeniable, MMA operations are not unique to these fields. More generally, any computation that can be expressed as MMA operations can leverage TCs, and potentially benefit from their higher computational throughput compared to other general-purpose cores, such as CUDA cores on Nvidia GPUs. In this paper, we propose the first double precision (FP64) Euclidean distance calculation algorithm, which is expressed as MMA operations to leverage TCs on Nvidia GPUs, rather than the more commonly used CUDA cores. To show that the Euclidean distance can be accelerated in a real-world application, we evaluate our proposed TC algorithm on the distance similarity self-join problem, as the most computationally intensive part of the algorithm consists of computing distances in a multi-dimensional space. We find that the performance gain from using the tensor core algorithm over the CUDA core algorithm depends weakly on the dataset size and distribution, but is strongly dependent on data dimensionality. Overall, TCs are a compelling alternative to CUDA cores, particularly when the data dimensionality is low (≤4), as we achieve an average speedup of 1.28× and up to 2.23× against a state-of-the-art GPU distance similarity self-join algorithm. Furthermore, because this paper is among the first to explore the use of TCs for FP64 general-purpose computation, future research is promising.

Index Terms—Tensor Cores, Euclidean Distance, GPU, Similarity Searches

I. INTRODUCTION

Tensor cores (TCs) are a type of Application-Specific Integrated Circuit (ASIC), and are specifically designed for Matrix Multiply-Accumulate (MMA) operations. The high specificity of TCs makes them typically more efficient at computing MMA operations, than other more general-purpose cores such as CPU cores or GPU CUDA cores. Given four matrices $A, B, C$, and $D$, TCs are designed to compute $D = A \times B + C$ (where $C$ and $D$ may be the same matrix). Over the past few years, TCs have been heavily used for machine learning and other fields requiring linear algebra, and few papers have examined broadening the use of TCs for other algorithms. Despite their high specificity, TCs may also be very versatile: any computation expressed with MMA operations, as defined above, should be able to leverage TCs and consequently, benefit from their high computational throughput.

Several companies have proposed a version of TCs, each with its own different characteristics. In this paper, we focus on the Nvidia GPU TCs. These TCs were first introduced with the Volta generation in 2017. Since this first iteration, they have been implemented in several GPU models and have greatly improved over time. In particular, while the first generation of TCs was only capable of computing in half precision using 16-bit floats (FP16), TCs are now capable of double precision computing using 64-bit floats (FP64) with the Ampere generation. This enables TCs to be used for applications where high precision is critical. Furthermore, their number, as well as their theoretical computational throughput, have continued to increase, making them an attractive alternative to the general-purpose CUDA cores.

As mentioned above, in this paper we focus on TCs proposed by Nvidia on their GPUs. In addition to the CUDA API to access GPU functionalities, we also leverage the Warp Matrix Multiply-Accumulate (WMMA) API, which provides programmatic access to TCs. While other libraries also give access to TCs, they are all higher level than the WMMA API and less versatile, thus less suited to our use case. However, there are some limitations when using the WMMA API. In particular, matrix sizes are limited to a few options, and not all compute precisions are available or can be combined (e.g., FP32 for both multiplication and accumulation is not available, and FP16 multiplication can not be combined with FP64 accumulation).

The Euclidean distance is a metric commonly used in many scientific applications, particularly for data analysis algorithms such as the distance similarity self-join, the $k$NN, or the Density-Based Spatial Clustering of Applications with Noise (DBSCAN) algorithms. Within these algorithms, distance calculations are usually the most time-consuming fraction of the total computation. In this paper, we propose to improve the throughput of Euclidean distance calculations by leveraging TCs on the GPU, and consequently also improve the overall performance of the algorithms mentioned above. To
illustrate greater applicability to these other algorithms, we use the distance similarity self-join algorithm as a representative example case for the other data analysis algorithms mentioned above. Given a dataset $D$ in $d$ dimensions, the distance similarity self-join algorithm finds all pairs of points $(a, b)$ that are within a distance threshold $\epsilon$ of each other; $\text{dist}(a, b) \leq \epsilon$, where $a, b \in D$, and $\text{dist}$ is the Euclidean distance function.

This paper makes the following contributions:

• We propose a new algorithm for computing Euclidean distances using TCs, leveraging the Nvidia Ampere architecture TCs [2] supporting double precision (FP64) computations.

• We integrate the aforementioned method into the distance similarity self-join algorithm, that we name Tensor Euclidean Distance Join (TED-JOIN). We show that TED-JOIN is competitive with the best parallel distance similarity self-joins in the literature for multi-core CPUs and GPU CUDA cores.

• The solution we propose here extends beyond the distance similarity self-join algorithm and can be integrated into other algorithms that use the distance similarity self-join, or more generally Euclidean distance calculations, as a building block.

• We evaluate TED-JOIN across a broad range of datasets, that span several distributions, sizes and dimensionalities, and compare it to a state-of-the-art GPU CUDA cores (GDS-JOIN [6]) and two multi-core CPU distance similarity join algorithms, SUPER-EGO [7] and FGF-HILBERT [8]. We conclude that TED-JOIN should always be preferred over SUPER-EGO and FGF-HILBERT, and should be preferred over GDS-JOIN when the dimensionality $d \leq 4$, where it achieves an average speedup of $1.28 \times$ (and $1.07 \times$ when considering all the experiments we conducted), and up to $2.25 \times$.

• To our knowledge, this paper proposes the first Euclidean distance calculation for TCs using FP64 computation, and the first use of TCs for the distance similarity self-join.

The paper is outlined as follows: we present essential material in Section II including an overview of TCs. We then present in Section III our solution that uses TCs to compute Euclidean distances and its integration into the distance similarity self-join algorithm. We show in Section IV the performance of our solution compared to the state-of-the-art distance similarity self-join algorithms, and we conclude and propose future research directions in Section V.

II. BACKGROUND

A. Problem Statement

For two points $a$ and $b$ in $d$ dimensions, and where $a_i$ represents the $i^{th}$ coordinate of the point $a$, and where $i = 1, \ldots, d$, the Euclidean distance between $a$ and $b$ is defined as follows:

$$\text{dist}(a, b) = \sqrt{\sum_{i=1}^{d} (a_i - b_i)^2}. \quad (1)$$

The distance similarity self-join algorithm, as described above, takes a dataset $D$ in $d$ dimensions as well as a search distance $\epsilon$ as inputs, and finds all the pairs of points $(a, b)$ such that $\text{dist}(a, b) \leq \epsilon$ where $a, b \in D$, and where the distance function is, in this case, the Euclidean distance defined in Equation [1]. For a query point $a$, finding all the other points in $D$ that are within $\epsilon$ from $a$ is called a range query, and there are thus $|D|$ range queries in total.

B. Tensor Cores (TCs)

TCs on GPUs are an Application-Specific Integrated Circuit (ASIC) designed for Matrix Multiply-Accumulate (MMA) operations. Given four matrices $A$, $B$, $C$ and $D$, this MMA operation is expressed as $D = A \times B + C$. Matrices $C$ and $D$ are the accumulators and may be equivalent. In hardware, TCs are designed to process $4 \times 4$ MMA operations. However, the WMMA API only gives access to larger matrices (e.g., $16 \times 16$). Therefore, several TCs are used concurrently to perform MMA operations larger than $4 \times 4$. Due to their highly specific design, TCs are significantly more efficient at MMA operations than CUDA cores: double precision computation is presented as twice as efficient when using TCs compared to CUDA cores on the Nvidia A100 GPU [2]. This significantly higher processing throughput is our motivation to transform Euclidean distance calculation into MMA operations, and yield higher computational throughput.

The WMMA API [4], [5] provides some low-level access to TCs, giving us the highest versatility possible. However, several limitations come along with this WMMA API. In particular, it is limited to certain matrix sizes and compute precisions. Among the options available, only a few are relevant to our work. In this paper, we focus on FP64 computation, which limits us to only one size for each of our matrices. Let $M_{m,n}$ be a matrix with $m$ rows and $n$ columns. The matrices that we can use with double precision are thus $A_{8,4}$, $B_{4,8}$, $C_{8,8}$, and $D_{8,8}$. We refer the reader to the documentation [4] for the other TCs options.

Programmatically, the matrices proposed by the WMMA API are called fragments, and are stored into the GPU threads registers. The WMMA API defines several functions to use these fragments:

• load_matrix_sync(): Load a matrix fragment from memory.

• store_matrix_sync(): Store a matrix fragment into memory.

• mma_sync(): Perform an MMA operation using TCs.

• fill_fragment(): Fill a matrix fragment with a specified value.

As their name suggests, these function calls are synchronized. Hence, all 32 threads of the warp are blocked until the operation is complete. The load and store functions take, among other arguments, a stride between the elements comprising the matrix rows. Hence, all the elements consisting of a row in the target matrix need to be coalesced in memory. Furthermore, the individual elements of the matrix fragments are stored in an unspecified order in the registers. Thus, contrary to regular arrays, the first element of a matrix may not be stored in the first element of the fragment. Consequently, operations on an individual element of a matrix fragment need to be applied to all the other elements, similar to a map function, and using a loop iterating over all of the elements of the fragment.
C. Tensor Cores in the Literature

As mentioned above, the literature concerning TCs heavily revolves around machine learning and other closely related fields, and not many other types of applications employing TCs [13]–[17]. We present in this section a selection of papers that discuss the use of TCs for applications that are more focused on computational/data-enabled science, similarly to this paper. Moreover, since most of the literature seems to focus on low precision computations, we believe that this paper is the first to propose an implementation combining the TCs and FP64 computations.

Dakkak et al. [13] propose a method to perform reduction and scan operations, using the WMMA API to leverage TCs. Their reduction algorithm consists of multiplying a matrix whose first row are ones and the rest are zeros with a matrix containing the values to reduce, and accumulated with a matrix containing the result from previous reductions. Their scan solution is similar but uses an upper triangular matrix filled with ones and where the rest are zeros, instead of a single row filled with ones. Their proposed solutions achieve a speedup of 100× for the reduction and 3× for the scan, compared to other state-of-the-art methods not using TCs.

Ji and Wang [14] propose using TCs to improve the performance of the DBSCAN algorithm. They mainly use TCs to compute distance matrices between the points that might form a cluster, using the cosine similarity formula (in contrast to the Euclidean distance used in this paper). In addition, they use TCs to perform reduction operations, which are used to determine whether points belong to a cluster or not. Their solution using TCs achieves a speedup of up to 2.61× to compute distance matrices compared to using the CUDA cores. While this work is very relevant to us, it differs in that they use a different distance metric (cosine similarity vs. Euclidean distance), they do not use an index structure, and part of their work is exclusive to the DBSCAN algorithm, whereas our solution essentially concerns the Euclidean distance calculations and, therefore, more applications than the distance similarity self-join that we just take as an example for this paper.

Ahle and Silvestri [15] theorize using TCs to compute similarity searches. They use TCs to compute either the Hamming, squared $L_2$ distances, or cosine similarity through an inner product operation, expressed as matrix multiplications. Additionally, they opt for the Local Sensitivity Hashing (LSH) method, reducing the overall complexity of the computation similarly to an indexing structure used by other similarity join solutions [6]–[8]. However, and contrary to these solutions, the LSH method typically yields an approximate result.

D. Distance Similarity Joins

We discuss in this section several state-of-the-art parallel distance similarity self-join algorithms [6]–[9], which we use as reference implementations for our experimental evaluation. These selected algorithms have in common that they use an indexing structure to prune the number of distance calculations, which is a commonly used optimization [18], [19]. When using an index, it is first searched to yield a set of candidate points for each query point. The set of candidate points is then refined using distance calculations to keep pairs of query and candidate points that are within $\epsilon$ of each other.

Kalashnikov [7] proposes SUPER-EGO, a parallel CPU algorithm to compute a distance similarity join, which is an improvement over the Epsilon Grid Order (EGO) algorithm proposed by Böhm et al. [19]. SUPER-EGO performance relies on a grid index and which is dependent on the search distance $\epsilon$, where a grid with cells of size $\epsilon \times \epsilon$ is laid on the search space to efficiently prune the candidate points to refine. Furthermore, the author proposes to reorder the dimensions of the points based on their variance, so dimensions with the highest variance are considered first when computing the distance between two points. Hence, their cumulative distance is more likely to reach $\epsilon$ sooner, allowing the short-circuiting of the distance computation, and thus to not consider the remaining dimensions. SUPER-EGO has been since improved by Gallet and Gowanlock [9], as part of a CPU-GPU distance similarity self-join algorithm. Among the changes, their version of SUPER-EGO is capable of FP64 computation while performing better than SUPER-EGO proposed by Kalashnikov [7]. As such, further references to SUPER-EGO in this paper will refer to the work conducted by Gallet and Gowanlock [9], rather than Kalashnikov [7].

Perdacher et al. [8] propose FGF-HILBERT, a parallel CPU distance similarity join algorithm also based on an epsilon grid order, but using space-filling curves as their indexing method. Using an EGO-sorted dataset, space-filling curves are used to determine, for each query point, a range of consecutive candidate points in the dataset. The authors further improve the performance by using the OpenMP API and low-level vectorized instructions, making their solution highly optimized. Because FGF-HILBERT typically performs better than SUPER-EGO, particularly in higher dimensions, it is considered a state-of-the-art CPU distance similarity join algorithm. Because of some of its optimizations, FGF-HILBERT is only capable of FP64 computation.

Gowanlock and Karsin [6] propose GDS-JOIN, a GPU algorithm for high-dimensional distance similarity self-joins. Their optimizations related to the high-dimensional case include reordering the dimensions of the points based on their variance, so these with the highest variance would be considered first when computing distances. Similarly to SUPER-EGO presented above, this particularly pairs well with distance calculation short-circuiting. Overall, dimensions with a higher variance are susceptible to increase the cumulative distance more than dimensions with lower variance and are thus more likely to trigger short-circuiting the distance calculation. They also propose to index the data in fewer dimensions than the input dataset dimensionality, making their grid index efficient even in higher dimensions, as the cost of searching their grid index is bound by the number of dimensions that are indexed. Furthermore, as their source code is publicly available, it appears that new optimizations have been added to the GDS-JOIN algorithm since the first publication, including the use of
Instruction-Level Parallelism (ILP) in the distance calculation, which significantly improves the performance of the algorithm. Our experiments show that this newer version of GDS-JOIN is more efficient than the published version [6]. Thus, we choose to use the newer more efficient version, as it is fairer than comparing TED-JOIN with the original algorithm.

III. DISTANCE CALCULATIONS USING TENSOR CORES

We present our algorithm, TED-JOIN, that leverages TCs for Euclidean distance calculations, and show how it is integrated into a distance similarity self-join algorithm.

A. Adapting the Euclidean Distance Formula

Using the Euclidean distance formula defined above (Equation 1) between two points $a$ and $b$ in $d$ dimensions, we can expand this formula as follows:

$$\text{dist}(a, b) = \sqrt{(a_d - b_d)^2 + \ldots + (a_1 - b_1)^2 + 0}. \quad (2)$$

We observe that from right to left, the computation consists of a series of multiply-and-accumulate operations, where the distance in dimension $i$, computed as $(a_i - b_i)^2$ (hence a multiplication of two terms) gets accumulated with the distance previously computed in dimension $i - 1$, where $1 < i < d$.

Let $x, y, z$ and $t$ be four points in $d$ dimensions and where we want to compute their Euclidean distance to each other. For illustration purposes, let $A$, $B$, and $C$ be $4 \times 4$ matrices. Using the Euclidean distance formula described in Equation 1 (and its equivalent in Equation 2), we can compute the distance between $x$ and all the other points (including itself) as follows:

**Algorithm 1** Pseudo-code for Euclidean distance calculations using tensor cores

```plaintext
1: procedure EUCLIDEANDISTMMA(x, points, D)
2: result [4×4], tmp [4×4]
3: fill_matrix(D, 0)
4: for $i \in d$, $i = i + 4$ do
5:     load_matrix_sync(A, x + i, 0)
6:     load_matrix_sync(B, points + i, d)
7:     B = B × (-1.0)
8:     mma_sync(C, A, I, B)
9:     store_matrix_sync(tmp, C)
10:    load_matrix_sync(A, tmp, 0)
11:    load_matrix_sync(B', tmp, 0)
12:    mma_sync(D, A, B', D)
13:    store_matrix_sync(result, D)
14: return result
```

$$A = \begin{pmatrix}
    a_{11} & a_{12} & a_{13} & a_{14} \\
    a_{21} & a_{22} & a_{23} & a_{24} \\
    a_{31} & a_{32} & a_{33} & a_{34} \\
    a_{41} & a_{42} & a_{43} & a_{44}
\end{pmatrix} \quad B = \begin{pmatrix}
    x_1 & x_{i+1} & x_{i+2} & x_{i+3} \\
    y_1 & y_{i+1} & y_{i+2} & y_{i+3} \\
    z_1 & z_{i+1} & z_{i+2} & z_{i+3} \\
    t_1 & t_{i+1} & t_{i+2} & t_{i+3}
\end{pmatrix}$$

Figure 1. Illustration of matrices $A$ and $B$ when using Algorithm 1

The Euclidean distance calculation using TCs MMA operations, as outlined in the pseudo-code in Algorithm 1 works as follows: we first set the result matrix $D$ to 0 (line 3). Then, and because we consider that matrices are $4 \times 4$, we loop over the $d$ dimensions four at a time (line 4). Then, we fill the row-major matrix $A$ with the coordinates of the point $x$ (line 5), replicated across all the matrix’s rows, and we fill the also row-major matrix $B$ with the coordinates of the points $y, z$ and $t$ (line 6) with one point per row. We illustrate how matrices $A$ and $B$ are filled in Figure 1.

Because the Euclidean distance consists of the product of a difference (Equation 1), we first need to compute the difference between the points’ coordinates. Thus, we normalize matrix $A$ by a factor of $-1$ (line 7), and compute a first MMA on line 8 where we multiply matrix $A$ with identity matrix $I$ and accumulate matrix $B$. Hence, matrix $C$ contains the difference between matrices $A$ and $B$. We store $C$ in memory, and load it into matrices $A$ and $B'$ (lines 9 to 11), where $B'$ is a column-major matrix. We then compute a second MMA operation where matrices $A$ and $B$ are multiplied and accumulated with matrix $D$, which contains the Euclidean distance between $x$ and $y, z$ and $t$.

A severe limitation of using the Euclidean distance shown in Equation 1 and represented with the pseudo-code in Algorithm 1 is that this solution is only capable of computing the distance between one point and several other points. Consider $D_{1,1}$ as the element in the first column of the first row of matrix $C$. The result of Algorithm 1 is that this solution is only capable of computing the distance between one point and several other points. Consider $D_{1,1}$ as the element in the first column of the first row of matrix $C$. The result of Algorithm 1 is that $D_{1,1} = \text{dist}(x, x)$, $D_{2,2} = \text{dist}(x, y)$, $D_{3,3} = \text{dist}(x, z)$ and $D_{4,4} = \text{dist}(x, t)$.

In other words, out of the $4 \times 4 = 16$ results that matrix $D$ can store, only four correspond to the actual Euclidean distance between $x$ and the other points. Consequently, while TCs have a higher peak throughput than CUDA cores, only a fraction of the computation is actively used to compute Euclidean distances, which yields inefficient resource utilization. Consequently, we propose to use the expanded and equivalent form of the Euclidean distance outlined in Equation 1 which we detail as follows:

$$\text{dist}(a, b) = \sqrt{\sum_{i=1}^{d} a_i^2 - 2a_ib_i + b_i^2}. \quad (3)$$

Similarly to Equation 2, we can expand Equation 3 yielding the following equation:

$$\text{dist}(a, b) = \sqrt{a_1^2 + (-2a_2b_2 + b_2^2) + \ldots + a_d^2 + (-2a_1b_1 + b_1^2)}. \quad (4)$$

Using Equation 4, we highlight which part of the computation will be carried out by TCs and which part by the CUDA cores. While the entire computation could be computed by TCs, it would be less efficient than using a combination of TCs and CUDA cores. Let $T_i = -2a_ib_i + b_i^2$ be the MMA operation done by TCs. To compute $\text{dist}(a_1, b_1)$, we need to calculate $a_1^2 + T_1$. To use TCs, we need to transform this into an MMA operation, computing either $a_1^2 \times I + T_1$, or $T_1 \times I + a_1^2$, where $I$ is the identity matrix. In either case, an element of the multiplication needs to correspond to the identity matrix to
keep the other element of the multiplication as is, and therefore only perform an accumulation. From Equation 3, we thus identify the part of the computation that benefits the most from TCs, and the part that benefits the most from CUDA cores. Furthermore, using Equation 3, we can compute the Euclidean distance between the four points $x, y, z$ and $t$ at once, using the method outlined in the pseudo-code in Algorithm 2 and which was not possible using Equation 1 and Algorithm 1. Finally, we observe that when computing the Euclidean distance between multiple points, and as will be the case when computing a distance similarity self-join, a part of the computation can be reused. The squared coordinates of the points ($a_i^2$ and $b_i^2$), are often reused throughout the computation. Indeed, the squared coordinates of a point are used for all the distance calculations with other points and do not change throughout the computation. Thus, the squared coordinates of the points can be precomputed to further improve the performance of the algorithm. As we still consider the use of $4 \times 4$ matrices for illustrative purposes, we store in an array the squared and accumulated coordinates of each point, four coordinates at a time. Considering that $x$ is our first point, the element 0 of this precomputed array is $x_0^2$ + $x_1^2 + x_2^2 + x_3^2$. For a dataset $D$ in $d$ dimensions, this array represents a memory overhead of only $|D| \times [d/4]$.

Algorithm 2 Pseudo-code for Euclidean distance calculations using tensor and CUDA cores

```plaintext
1: procedure EUCLIDEANDISTMMA_v2(points, squaredPoints)
2:     result [4 \times 4], resultTmp [4 \times 4]
3:     for $i \in d$, $i = i + 4$ do
4:         load_matrix_sync(A, points + i, d)
5:         load_matrix_sync(B, points + i, d)
6:         load_matrix_sync(C, squaredPoints + (i/4), (d/4))
7:         fill_matrix(D, 0)
8:         A = A \times (-2.0)
9:         mma_sync(D, A, B, C)
10:        store_matrix_sync(resultTmp, D)
11:    result ← result + resultTmp + squaredPoints
12: return result
```

Figure 2. Illustration of matrices $A$ and $B$ when using Algorithm 2

We present in Algorithm 2 the pseudo-code for the version of our Euclidean distance calculation method using TCs and which is based on Equation 3. Similarly to Algorithm 1, we iterate over the $d$ dimensions, four by four (line 3). Then, for each loop iteration, we fill matrices $A$ and $B$ with the points and their corresponding coordinates (lines 4 and 5), represented in Figure 2. We then fill matrix $C$ with the squared coordinates of the candidate points that are in $B$, and where it occupies a full row per candidate point. We then fill the result matrix $D$ with zeros (line 7), normalize matrix $A$ by a factor of $-2.0$ (line 8), and compute the MMA using matrices $A$, $B$, $C$ and $D$ (line 9) using TCs. We then accumulate these intermediate distances with the distances from previous loop iterations (stored in the array result) and the squared coordinates (line 11) of the query points that are in $A$, this time using the CUDA cores. We finally return the result array (line 12), which contains the Euclidean distances between the points $x, y, z$ and $t$ (i.e., the $16$ Euclidean distances).

B. Tensor Cores for Distance Similarity Joins

As we outlined in Section 1-D, most of the distance similarity self-join algorithms in the literature reduce the overall computational complexity by using an index data structure and, compared to a brute-force approach, typically reduces the number of candidate points that need to be refined per query point. In particular, the distance similarity self-join algorithms that we leverage here, GDS-JOIN, uses a grid index with cells of size $c_d$. For each query point in the dataset $D$, we thus search the grid indexing for neighboring cells, yielding a set of candidate points for each of the query points, which are then refined by computing the Euclidean distance between them and the query point. Because TED-JOIN and GDS-JOIN use the same index, both algorithms yield the same candidate points to be refined using distance calculations. This allows us to compare the performance of CUDA and TCs in a self-consistent manner, where the performance differences are directly attributable to distance calculations.

A characteristic of the grid index we are using is that all the query points from the same cell share the same candidate points. This characteristic is particularly important, as it is necessary to efficiently make use of Equation 3 and Algorithm 2. Indeed, the query points we use in matrix $A$ must compute their Euclidean distances, in matrix $B$, to the same set of candidate points. Hence, the query points used in matrix $A$ should come from the same grid cell, as they share the same set of candidate points.

Another optimization used by Gowanlock and Karsin is the batching of the execution. Because the final result of the similarity self-join might exceed the memory size of the GPU, the entire execution is split across multiple batches. As a positive side-effect, multiple batches allow for hiding data transfers between the host and the GPU with computation. Indeed, batches are computed by several parallel CUDA streams, where the data transfers of a stream can overlap the computation of another stream. However, as a batch corresponds to a set of query points to compute, we must ensure in our case that the query points we send in a batch can be computed by our TCs algorithm. More specifically, when assigning query points from a batch to a warp on the GPU, we must ensure that these query points belong in the same grid cell and are not from different cells. Otherwise, we would be unable to use Algorithm 2.

Because we choose to compute Euclidean distances using FP64, only one combination of matrix sizes is available. Namely, matrix $A$ will contain up to four coordinates of up to eight query points, matrix $B$ up to four coordinates of up
to eight candidate points, matrix $C$ the squared coordinates of up to eight candidate points, and matrix $D$ up to sixty-four Euclidean distances between the query points in $A$ and the candidate points in $B$. As such, and because TCs operate at a warp level using the WMMA API, we assign up to eight query points to a warp, which will then compute the Euclidean distance to all the candidate points, as determined by the use of the grid index. Note that in the case where the number of query points, candidate points, or coordinates is insufficient to fill the remaining rows or columns of the matrices, we must fill them with zeros. Consequently, and because we process four coordinates at a time, up to $[d/4]$ steps are necessary to compute the Euclidean distance. Similarly to GDS-JOIN [6], we allow the distance calculation to be short-circuited, which may happen after every MMA operation, i.e., for every 4 dimensions. However, all currently computed Euclidean distances between all the query points and candidate points of the warp must short-circuit to trigger this optimization.

IV. EXPERIMENTAL EVALUATION

In this section, we detail the experimental evaluation we conducted. We start by comparing our TCs algorithm and another optimized TCs algorithm to compute Euclidean distances. We then compare our proposed algorithm TED-JOIN to other state-of-the-art distance self-join algorithms.

A. Datasets

We evaluate the algorithms using a wide range of real-world and synthetic datasets, spanning several sizes, dimensionalities, and distributions. Synthetic datasets are generated following either a uniform or exponential distribution, and their name is prefixed by either $Unif$ or $Exp$, respectively, followed by the dimensionality and the number of points (e.g., $Exp3D2M$ is an exponentially distributed 3-D dataset containing 2M points). We summarize the different synthetic datasets that we use in Table I and the real-world datasets in Table II. $Gaia50M$ and $OSM50M$ are the first 50M points of the original datasets, as described by Gowanlock [20]. We choose to use different distributions to better evaluate the performance of TCs under different workloads: when a dataset is uniformly distributed, TCs should all have a similar workload, while when a dataset is exponentially distributed, some TCs will have a higher workload than other TCs.

We denote the selectivity as $S$, which represents the average number of neighboring points found within $\epsilon$ of each query point when performing a similarity self-join, excluding each query point finding itself. The selectivity is calculated as follows: $S = \frac{|R| - |D|}{|D|}$, where $R$ is the result set of the similarity self-join, and $D$ the dataset. This metric is used in the literature to quantify the complexity of the search for a given value of $\epsilon$: increasing $\epsilon$ typically results in more work to compute, as well as a higher selectivity. It can also be used to ensure that the result size of the distance similarity self-join is practical, and to ease comparisons between test cases by using a similar selectivity.

B. Methodology

We conducted our experiments on the following platforms:
• Platform 1: 2 $\times$ AMD Epyc 7542 CPU (2 $\times$ 32 cores, 2.90GHz) with 512 GiB of RAM and an Nvidia A100 GPU.
• Platform 2: Intel Xeon W-2295 CPU (18 cores, 3.00GHz) with 256 GiB of RAM.

The algorithms we use in our experiments, TED-JOIN, GDS-JOIN, SUPER-EGO and FGF-HILBERT, are configured as follows:
• TED-JOIN: Our proposed TCs algorithm is executed on Platform 1, configured with 256 threads per block (8 warps), up to 8 query points per warp, and using distance calculations short-circuiting, as explained in Section III-B.
• GDS-JOIN: Parallel GPU algorithm proposed by Gowanlock and Karsin [6] and further optimized since the original publication, executed in Platform 1. This algorithm is configured with 256 threads per block, $ILP = min(8, d)$ and uses distance calculations short-circuiting, as presented in Section II-D.
• SUPER-EGO: Parallel CPU algorithm proposed by Kalashnikov [7], optimized by Gallet and Gowanlock [9] and executed on Platform 1 using 64 threads/cores (the number of physical cores on the platform).
• FGF-HILBERT: Parallel CPU algorithm proposed by Perdacher et al. [8], executed on Platform 2 (the only platform with AVX-512 instructions, which is required for this algorithm) and using 18 threads/cores (the number of physical cores on the platform).

While we would have preferred to use a single platform to conduct all our experiments, and thus have the same number of threads/cores for all CPU algorithms, prior experiments we conducted showed us that both SUPER-EGO and FGF-HILBERT had a relatively poor scalability. Hence, if we were able to run FGF-HILBERT using 64 threads/cores, as we did for SUPER-EGO, the results we show in the following sections would not have been significantly different. Furthermore, note that despite using fewer threads/cores, FGF-HILBERT typically outperforms SUPER-EGO.

All the algorithms are using double precision (FP64) to compute, and are compiled using the NVCC compiler v11.2 (for TED-JOIN and GDS-JOIN) or the GCC compiler (v8.5 for SUPER-EGO, and v9.4 FGF-HILBERT) using the O3 compiler option.

### Table I

**SYNTHETIC DATASETS USED IN THE EXPERIMENTAL EVALUATION.**

| Distribution   | $d$   | $n$   |
|----------------|-------|-------|
| Uniform        | 2, 3, 4, 6, 8 | 10M   |
| Exponential    | 2, 3, 4, 6, 8 | 2M, 10M |

### Table II

**REAL-WORLD DATASETS USED IN THE EXPERIMENTAL EVALUATION.**

| Dataset         | $d$   | $n$   |
|-----------------|-------|-------|
| SW2DA           | 2     | 1.86M |
| OSM50M          | 2     | 50M   |
| SW3DA           | 3     | 1.86M |
| BigCross        | 57    | 11M   |
| SW2DB           | 2     | 5.16M |
| Gaia50M         | 2     | 50M   |
| SuSy            | 18    | 5M    |
| Songs           | 90    | 515K  |
optimization. Note that during our experiments, many scenarios using FGF-HILBERT did not produce the correct self-join results, which are consequently not included. We believe that the issues encountered with FGF-HILBERT are due to the width of the vectorized instructions: 512-bits, or 8 FP64 values, which may not be working when \( d < 8 \). Furthermore, SUPER-EGO happened to fail in several low-dimensional cases without a clear understanding of the reason, and we thus also do not report the execution time of these experiments. However, we consider that the successful experiments should be sufficient to accurately evaluate the performance of TED-JION compared to the other algorithms. Finally, note that the four algorithms, TED-JION, GDS-JION \(^3\), SUPER-EGO \(^7\), and FGF-HILBERT \(^8\), are publicly available.

C. Results: Comparison of Brute-force TC Approaches

We compare the performance of TCs and CUDA cores for performing Euclidean distance calculations when using brute-force computation, which is \( O(|D|^2) \). Here, we use the algorithm TED-JION (TCs), to which we removed all optimizations, including indexing, and compare to a highly optimized MMA reference implementation by Nvidia \(^27\), that leverages the WMMA API similarly to TED-JION, denoted as WMMA-REF. We selected this implementation instead of a library such as cuBLAS \(^9\) or CUTLASS \(^10\) (with the latter built upon the WMMA API), as it is the best direct comparison between approaches.

We outline two major differences between WMMA-REF and TED-JION, as a consequence of matrix size, as follows:

1) The matrix sizes are dependent on data dimensionality and impact performance \(^28\), \(^29\). WMMA-REF is designed and optimized for large MMA operations, whereas TED-JION targets smaller matrices. For instance, in Algorithm \(^2\) on line \(3\) the values of \( d \) for real-world datasets are \( \leq 100 \), and as shown in Table \(\text{II}\), we evaluate \( d \leq 90 \).

2) TED-JION uses small matrices, and thus computes many small \( 8 \times 8 \) distance matrices and leverages shared memory. In contrast, WMMA-REF computes the entire \( |D|^2 \) distance matrix, thus requiring a much larger memory footprint. Consequently, when using WMMA-REF, and to be able to use it on large datasets that would exceed global memory capacity, we store the result matrix using unified memory, which automatically pages data between main and global memory. Furthermore, as cuBLAS and CUTLASS work similarly to WMMA-REF, they have the same drawback related to the use of unified memory.

Figure \(3\) plots the performance of TED-JION and WMMA-REF using brute-force searches (i.e., without using an index) to compute Euclidean distance calculations on a 16-D exponentially distributed synthetic datasets, spanning \( 2^{17} \) points (we omit datasets with other dimensionalities as we observed similar results). Note that \( 2^{18} \) points overflows main memory when using WMMA-REF. We observe that the performance of WMMA-REF degrades quicker than TED-JION as the dataset size increases. We attribute these results to the use of unified memory by WMMA-REF, which is required to store the large result matrix \( (|D| \times |D|) \), and which is paged between GPU global and main memory when its size exceeds global memory capacity. In addition to the poor performance attributed to unified memory, using WMMA-REF, which computes on large matrices and thus on the \( d \) dimensions of a dataset at a time, limits the use of several optimizations, which are explored in the following sections. Namely, this inhibits short-circuiting the distance calculations when the cumulative distance between points exceeds \( \epsilon \).

We profile TED-JION and WMMA-REF on the \( 2^{17} \) points 16-D dataset we show in Figure \(3\). With this dataset size, unified memory needs to be paged between global and main memory throughout the execution. We measure that WMMA-REF transfers 687.84 GB between the L1 and L2 caches, and 503.61 GB between the L2 cache and global memory. In comparison TED-JION transfers 558.57 GB and only 0.046 GB, respectively, as we rely on shared memory to store small \( 16 \times 16 \) results matrices, rather than a large \( |D| \times |D| \) matrix in global memory like WMMA-REF. This results in lower L1 and L2 hit rates: 19.35\% using WMMA-REF vs. 50.32\% using TED-JION for the L1 hit rate, and 72.45\% vs. 99.99\% for the L2 hit rate. In summary, the unified memory required by WMMA-REF negatively affects performance in the case of distance calculations, and thus TED-JION should be preferred.

D. Results: Optimized TC and CUDA Core Approaches

We investigate in this section the performance of TED-JION, as compared to other state-of-the-art algorithms from the literature: GDS-JION, SUPER-EGO, and FGF-HILBERT.

1) Uniformly Distributed Datasets: We start this result section with uniformly distributed synthetic datasets, detailed in Table \(\text{II}\). We select this distribution as all the query points will have a similar number of candidate points to refine, allowing us to evaluate the performance of TCs when their workload is relatively uniform.

We show in Figure \(4\) the execution time of TED-JION compared to GDS-JION, SUPER-EGO, and FGF-HILBERT on a selection of uniformly distributed synthetic datasets.
these cases, we can see that SUPER-EGO is consistently performing worse than all of the other algorithms, except on the Unif8D10M dataset when $\epsilon = 0.08$ (Figure 5(d)). Furthermore, we observe that TED-Jjoin performs similarly or better than GDS-Jjoin in most cases, except on Unif8D10M when $\epsilon < 0.32$. From these results, it seems that TED-Jjoin performs similar to GDS-Jjoin when $\epsilon$ is low, and therefore when the workload is low as well, potentially indicating an overhead from using TCs. But when $\epsilon$ increases, and thus the workload, the higher computational throughput of TCs outperforms the CUDA cores used by GDS-Jjoin.

We also observe that the speedup is the highest on the 2-D and 4-D datasets since all 2 or 4 dimensions can be computed at once using TCs, as we compute 4 dimensions at a time. The speedup is the lowest on the 6-D datasets since we need to compute the distances in two iterations (as many as for the 8-D datasets), but where 2 dimensions are zeros and thus that the CUDA cores in GDS-Jjoin do not have to compute.

2) Exponentially Distributed Datasets: In this section we present the results on the same algorithms as in Section IV-D1 on the exponentially distributed synthetic datasets, detailed in Table IV. We select this distribution as it creates a large workload variance between the query points, where some query points may have many candidate points to refine, and other query points very few, which allows us to evaluate the performance of the TCs when their workload varies.

Figure 4 reports the execution time of TED-Jjoin compared to GDS-Jjoin, SUPER-EGO, and FGF-Hilbert on a selection of exponentially distributed synthetic datasets. Note that FGF-Hilbert did not run correctly on the 2-D and 6-D datasets (Figures 5(a) and (c)). We observe that in these experiments, TED-Jjoin typically performs similarly or better than GDS-Jjoin, particularly as $\epsilon$ increases. SUPER-EGO is consistently outperformed by the other algorithms, while FGF-Hilbert performs the best on the Expo4D10M dataset (Figure 5(b)), but is outperformed by both TED-Jjoin and GDS-Jjoin on the Expo8D10M dataset (Figure 5(d)). Because these datasets are exponentially distributed, the workload throughout the computation of the similarity self-join can vary a lot. The query points in the denser regions of the dataset will have many candidate points to refine, and the query points in the sparse regions of the dataset may have only a few candidate points. Hence, and despite a highly varying workload, TED-Jjoin remains more efficient in most cases compared to GDS-Jjoin, and all compared algorithms in general, particularly in lower dimensions ($2 \leq d \leq 4$).

3) Real-World Datasets: We present in this section the results of TED-Jjoin, GDS-Jjoin, SUPER-EGO, and FGF-Hilbert on a selection of the real-world datasets (Table IV), as shown in Figure 6. We observe that TED-Jjoin and GDS-Jjoin perform very similarly, particularly on the higher dimensional datasets (Figures 6(b)–(d)), while TED-Jjoin outperforms GDS-Jjoin on the SW3DA dataset as $\epsilon$ increases (Figure 6(a)). FGF-Hilbert also performs quite similarly to TED-Jjoin and GDS-Jjoin, while SUPER-EGO is often outperformed by the other algorithms. Overall, these experiments show that TED-Jjoin and GDS-Jjoin may perform similarly as dimensionality increases, while TED-Jjoin yields an advantage in lower dimensions (Figure 6(a)), as we observed in previous Figures 4 and 5. These experiments show us that in higher dimensions (Figures 6(b)–(d)), TED-Jjoin may not yield an advantage compared to GDS-Jjoin.

E. Discussion: When Tensor Cores Should Be Employed

We summarize the results of TED-Jjoin as compared to the SUPER-EGO [9], FGF-HILBERT [8], and GDS-JJOIN [6] algorithms that we obtained across experiments, including those that were omitted due to space constraints. The experiments covered a wide range of data dimensionalities, sizes, and distributions, resulting in an insightful picture of the overall performance of using TCs in TED-Jjoin compared to the use of CUDA cores in GDS-Jjoin. We report the speedup of TED-
Figure 6. Response times of TED-JOIN, GDS-JOIN, SUPER-EGO, and FGF-HILBERT on a selection of real-world datasets (Table II). $S$ is in the range (a) 163–5373, (b) 5–1090, (c) 1–1104 and (d) 127–998. The legend in (a) corresponds to all subfigures.

Figure 7. Speedups of TED-JOIN over (a) SUPER-EGO and (b) FGF-HILBERT across datasets presented in Tables I and II for all values of $d$ we used, and as a function of the dimensionality. The dashed horizontal lines correspond to the average speedups of TED-JOIN over a compared algorithm, and the dotted horizontal lines represent no speedup.

Figure 8. The same as for Figure 7 but plotting the speedup of TED-JOIN over GDS-JOIN.

Table III

|                      | SUPER-EGO | FGF-HILBERT | GDS-JOIN ($d \leq 4$) |
|----------------------|-----------|-------------|-----------------------|
| CPU Average          | 5.00×     | 2.09×       | 1.07× (1.28×)         |
| CPU Maximum          | 27.22×    | 9.46×       | 2.23× (2.23×)         |

regardless of the dimensionality, dataset distribution, or size.

Figure 7(b) plots the speedup of TED-JOIN over the CPU algorithm FGF-HILBERT [8]. Because many of our experiments could not be correctly conducted using the FGF-HILBERT algorithm, it makes it harder to draw a clear conclusion regarding the performance TED-JOIN compared to FGF-HILBERT. However, in the successful experiments, our TCs solution achieved an average speedup of 2.09× with a maximum of 9.46×, and the majority of the speedups are above 1. Hence, and similarly to SUPER-EGO, there is no clear disadvantage of using TED-JOIN over FGF-HILBERT.

Observing the speedup of TED-JOIN over the CUDA core algorithm GDS-JOIN (Figure 8), we achieve the best performance when $d \leq 4$, and is best on exponentially distributed synthetic and real-world datasets. However, as the dimensionality $d$ increases, the speedup of TED-JOIN over GDS-JOIN decreases, resulting in an average speedup of only 1.07×, but achieving a maximum of 2.23× on the Expo3D2M dataset. If we only consider datasets where $d \leq 4$, TED-JOIN achieves an average speedup of 1.28× over GDS-JOIN. Furthermore, note that while TCs should be up to two times faster than CUDA cores on the A100 GPU [2], the maximum speedup that we achieve is higher than this theoretical speedup. This is because TED-JOIN does not use exclusively TCs, but also CUDA cores, allowing us to achieve better speedup in certain circumstances. As for the relatively low speedup in higher dimensions, TCs are designed for large matrix multiplications, where data can be reused when computing tiles of the resulting matrix. In the case of TED-JOIN, we are unable to reuse such data, thus limiting the performance.

From these results, we conclude that TCs should be used when the dimensionality is low ($2 \leq d \leq 4$). Furthermore, there are cases where the dimensionality does not evenly divide by 4 (the dimension of the matrices as defined by the WMMA API for FP64). In total, $[d/4]$ MMA operations are needed to compute distance calculations, meaning that an additional MMA operation needs to be performed for cases where $d \mod 4 \neq 0$, which performs excess work. For example, because 6-D datasets are stored as 8-D datasets, where the last two dimensions are filled with zeros, TCs cannot achieve peak performance.

In summary, TCs should be used under the following scenarios instead of the reference implementations on their respective architectures:

- Compared to using CUDA cores, TCs should be used on low-dimensional datasets ($2 \leq d \leq 4$).
- There is no drawback of using TCs over multi-core CPUs.
In this paper, we presented a novel approach to computing Euclidean distances leveraging TCs on Nvidia GPUs. TCs are designed solely for Matrix Multiply-Accumulate operations, and yield a much higher peak throughput than CUDA cores for this operation [2]. While TCs have been extensively used in fields such as machine learning, their usage remains very limited for more general-purpose applications. Hence, to our knowledge, this paper presents the first use of TCs for FP64 Euclidean distance calculations, where FP64 TCs computation has only been possible using the Ampere generation of Nvidia GPUs. This makes our algorithm suitable for scenarios where precise computation using FP64 is required. As such, our algorithm can provide the foundation for improving the performance of other data analysis applications where distance calculations are used (e.g., distance similarity searches, kNN, and DBSCAN [6–11], [14]). In these cases, our TC GPU kernel can be adapted to refine candidate points independently of the index that is used.

Comparison to tensor algorithms: we compared TED-JOIN to a reference MIMA implementation, WMMA-REF, from Nvidia [27], where we did not use any optimizations (including an index). We find that TED-JOIN outperforms WMMA-REF, because the latter algorithm requires unified memory to store the $|D| \times |D|$ distance matrix. Libraries such as cuBLAS and CUTLASS have the same drawbacks as WMMA-REF, and are thus also unsuitable for moderately sized input datasets.

Comparison to similarity search reference implementations: we compared TED-JOIN to the GPU algorithm GDS-JOIN [6]. Despite an average speedup of 1.07× over GDS-JOIN when 2 ≤ d ≤ 90, we achieve a maximum speedup of 2.23× over this algorithm. We find that TED-JOIN yields the best performance when d ≤ 4 with an average speedup of 1.28× over GDS-JOIN. Because TED-JOIN and GDS-JOIN use the same index, this performance improvement is a direct result of employing TCs. While the maximum speedup is expected to be 2× due to the maximum throughput of TCs compared to CUDA cores [2], we achieve a lower speedup on average because we rely on operations using CUDA cores.

Compared to the multi-core CPU algorithms SUPER-EGO [7] and FGF-HILBERT [8], we find that TED-JOIN typically outperforms these algorithms.

Future work: (1) we will profile and model TC performance in determining to which scenarios they should be leveraged instead of CUDA cores. (2) we will investigate using other precisions available for TCs, such as FP16 where the peak throughput of TCs is 16× higher than FP64 TCs on the A100 GPU. (3) we will incorporate our TC GPU kernel into other algorithms, such as other proximity search algorithms including kNN [10], or particle simulations such as those in molecular dynamics [30].

V. CONCLUSION AND FUTURE WORK

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