MESSI: In-Memory Data Series Indexing

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***Abstract*—Data series similarity search is a core operation for several data series analysis applications across many different domains. However, the state-of-the-art techniques fail to deliver the time performance required for interactive exploration, or analysis of large data series collections. In this work, we propose MESSI, the first data series index designed for in-memory operation on modern hardware. Our index takes advantage of the modern hardware parallelization opportunities (i.e., SIMD instructions, multi-core and multi-socket architectures), in order to accelerate both index construction and similarity search processing times. Moreover, it benefits from a careful design in the setup and coordination of the parallel workers and data structures, so that it maximizes its performance for in-memory operations. Our experiments with synthetic and real datasets demonstrate that overall MESSI is up to 4x faster at index construction, and up to 11x faster at query answering than the state-of-the-art parallel approach. MESSI is the first to answer exact similarity search queries on 100GB datasets in ∼50msec (30-75msec across diverse datasets), which enables real-time, interactive data exploration on very large data series collections.**

***Index Terms*—Data series, Indexing, Modern hardware**

I. Introduction

[Motivation] Several applications across many diverse domains, such as in finance, astrophysics, neuroscience, engineering, multimedia, and others [1]–[3], continuously produce big collections of data series[1] which need to be processed and analyzed. The most common type of query that different analysis applications need to answer on these collections of data series is similarity search [1], [4], [5].

The continued increase in the rate and volume of data series production renders existing data series indexing technologies inadequate. For example, ADS+ [6], the state-of-the-art sequential (i.e., non-parallel) indexing technique, requires more than 2min to answer exactly a single 1-NN (Nearest Neighbor) query on a (moderately sized) 100GB sequence dataset. For this reason, a disk-based data series parallel indexing scheme, called ParIS, was recently designed [7] to take advantage of modern hardware parallelization. ParIS effectively exploits the parallelism capabilities provided by multi-core and multi-socket architectures, and the Single Instruction Multiple Data (SIMD) capabilities of modern CPUs. In terms of query answering, experiments showed that ParIS is more than 1 order of magnitude faster than ADS+, and more than 3 orders of magnitude faster than the optimized serial scan method.

[1]A data series, or data sequence, is an ordered sequence of data points. If the ordering dimension is time then we talk about time series, though, series can be ordered over other measures. (e.g., angle in astronomical radial profiles, frequency in infrared spectroscopy, mass in mass spectroscopy, position in genome sequences, etc.).

Still, ParIS is designed for disk-resident data and therefore its performance is dominated by the I/O costs it encounters. For instance, ParIS answers a 1-NN (Nearest Neighbor) exact query on a 100GB dataset in 15sec, which is above the limit for keeping the user's attention (i.e., 10sec), let alone for supporting interactivity in the analysis process (i.e., 100msec) [8].

[Application Scenario] In this work, we focus on designing an efficient parallel indexing and query answering scheme for *in-memory* data series processing. Our work is motivated and inspired by the following real scenario. Airbus[2], currently stores petabytes of data series, describing the behavior over time of various aircraft components (e.g., the vibrations of the bearings in the engines), as well as that of pilots (e.g., the way they maneuver the plane through the fly-by-wire system) [9]. The experts need to access these data in order to run different analytics algorithms. However, these algorithms usually operate on a subset of the data (e.g., only the data relevant to landings from Air France pilots), which fit in memory. Therefore, in order to perform complex analytics operations (such as searching for similar patterns, or classification) fast, in-memory data series indices must be built for efficient data series query processing. Consequently, the time performance of both index creation and query answering become important factors in this process.

[MESSI Approach] We present MESSI, the *first* in-MEmory data SerieS Index, which incorporates the state-of-the-art techniques in sequence indexing. MESSI effectively uses multi-core and multi-socket architectures in order to concurrently execute the computations needed for both index construction and query answering and it exploits SIMD. More importantly though, MESSI features redesigned algorithms that lead to a further ∼4x speedup in index construction time, in comparison to an in-memory version of ParIS. Furthermore, MESSI answers exact 1-NN queries on 100GB datasets 6-11x faster than ParIS across the datasets we tested, achieving for the first time interactive exact query answering times, at ∼50msec.

When building ParIS, the design decisions were heavily influenced by the fact that the cost was mainly I/O bounded. Since MESSI copes with in-memory data series, no CPU cost can be hidden under I/O. Therefore, MESSI required more careful design choices and coordination of the parallel workers when accessing the required data structures, in order to improve its performance. This led to the development of a more subtle design for the construction of the index and on

[2]http://www.airbus.com/

the development of new algorithms for answering similarity search queries on this index.

For query answering in particular, we showed that adaptations of alternative solutions, which have proven to perform the best in other settings (i.e., disk-resident data [7]), are not optimal in our case, and we designed a novel solution that achieves a good balance between the amount of communication among the parallel worker threads, and the effectiveness of each individual worker. For instance, the new scheme uses concurrent priority queues for storing the data series that cannot be pruned, and for processing these series in order, starting from those whose iSAX representations have the smallest distance to the iSAX representation of the query data series. In this way, the parallel query answering threads achieve better pruning on the data series they process. Moreover, the new scheme uses the index tree to decide which data series to insert into the priority queues for further processing. In this way, the number of distance calculations performed between the iSAX summaries of the query and data series is significantly reduced (ParIS performs this calculation for all data series in the collection). We also experimented with several designs for reducing the synchronization cost among different workers that access the priority queues and for achieving load balancing. We ended up with a scheme where workers use radomization to choose the priority queues they will work on. Consequently, MESSI answers exact 1-NN queries on 100GB datasets within 30-70msec across diverse synthetic and real datasets.

The index construction phase of MESSI differentiates from ParIS in several ways. For instance, ParIS was using a number of buffers to temporarily store pointers to the iSAX summaries of the raw data series before constructing the tree index [7]. MESSI allocates smaller such buffers per thread and stores in them the iSAX summaries themselves. In this way, it completely eliminates the synchronization cost in accessing the iSAX buffers. To achieve load balancing, MESSI splits the array storing the raw data series into small blocks, and assigns blocks to threads in a round-robin fashion. We applied the same technique when assigning to threads the buffers containing the iSAX summary of the data series. Overall, the new design and algorithms of MESSI led to ∼4x improvement in index construction time when compared to ParIS.

[Contributions] Our contributions are summarized as follows.

- We propose MESSI, the first in-memory data series index designed for modern hardware, which can answer similarity search queries in a highly efficient manner.
- We implement a novel, tree-based exact query answering algorithm, which minimizes the number of required distance calculations (both lower bound distance calculations for pruning true negatives, and real distance calculations for pruning false positives).
- We also design an index construction algorithm that effectively balances the workload among the index creation workers by using a parallel-friendly index framework with low synchronization cost.
- We conduct an experimental evaluation with several synthetic and real datasets, which demonstrates the efficiency of the proposed solution. The results show that MESSI is up to 4.2x faster at index construction and up to 11.2x faster at query answering than the state-of-the-art parallel index-based competitor, up to 109x faster at query answering than the state-of-the-art parallel serial scan algorithm, and thus can significantly reduce the execution time of complex analytics algorithms (e.g., *k-NN* classification).

II. Preliminaries

We now provide some necessary definitions, and introduce the related work on state-of-the-art data series indexing.

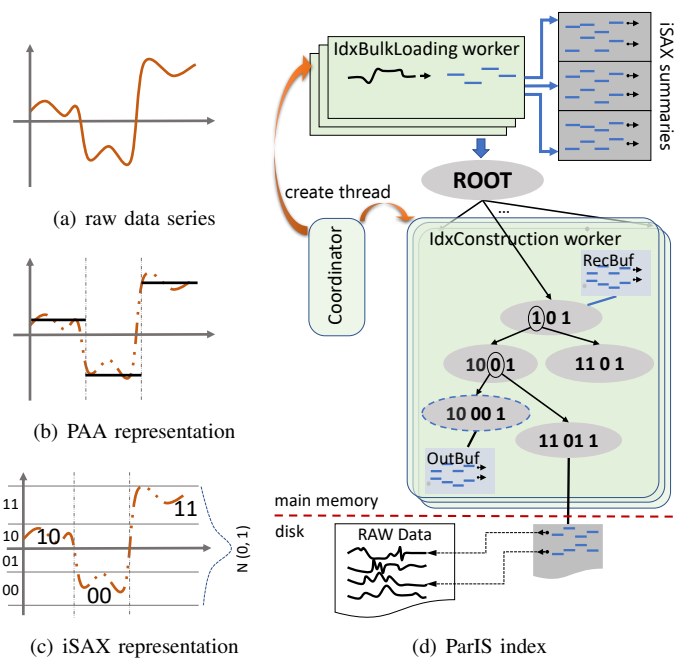
A. Data Series and Similarity Search

[Data Series] A data series, $S = \{p_1, ..., p_n\}$, is defined as a sequence of points, where each point $p_i = (v_i, t_i)$, $1 \leq i \leq n$, is associated to a real value v_i and a position t_i. The position corresponds to the order of this value in the sequence. We call n the *size*, or *length* of the data series. We note that all the discussions in this paper are applicable to high-dimensional vectors, in general.

[Similarity Search] Analysts perform a wide range of data mining tasks on data series including clustering [10], classification and deviation detection [11], [12], and frequent pattern mining [13]. Existing algorithms for executing these tasks rely on performing fast similarity search across the different series. Thus, efficiently processing nearest neighbor (NN) queries is crucial for speeding up the above tasks. NN queries are formally defined as follows: given a query series S_q of length n, and a data series collection $\mathcal{S}$ of sequences of the same length, n, we want to identify the series $S_c \in \mathcal{S}$ that has the smallest distance to S_q among all the series in the collection $\mathcal{S}$. (In the case of streaming series, we first create subsequences of length n using a sliding window, and then index those.)

Common distance measures for comparing data series are Euclidean Distance (ED) [14] and dynamic time warping (DTW) [15]. While DTW is better for most data mining tasks, the error rate using ED converges to that of DTW as the dataset size grows [16]. Therefore, data series indexes for massive datasets use ED as a distance metric [6], [15]–[18], though simple modifications can be applied to make them compatible with DTW [16]. Euclidean distance is computed as the sum of distances between the pairs of corresponding points in the two sequences. Note that minimizing ED on z-normalized data (i.e., a series whose values have mean 0 and standard deviation 1) is equivalent to maximizing their Pearson's correlation coefficient [19].

[Distance calculation in SIMD] Single-Instruction Multiple-Data (SIMD) refers to a parallel architecture that allows the execution of the same operation on multiple data simultaneously [20]. Using SIMD, we can reduce the latency of an operation, because the corresponding instructions are fetched once, and then applied in parallel to multiple data. All modern CPUs support 256-bit wide SIMD vectors, which means that certain floating point (or other 32-bit data) computations can be up to 8 times faster when executed using SIMD.



(a) raw data series (b) PAA representation (c) iSAX representation (d) ParIS index

Fig. 1. The iSAX representation, and the ParIS index

In the data series context, SIMD has been employed for the computation of the Euclidean distance functions [21], as well as in the ParIS index, for the conditional branch calculations during the computation of the lower bound distances [7].

B. iSAX Representation and the ParIS Index

[iSAX Representation] The iSAX representation (or summary) is based on the Piecewise Aggregate Approximation (PAA) representation [22], which divides the data series in segments of equal length, and uses the mean value of the points in each segment in order to summarize a data series. Figure 1(b) depicts an example of PAA representation with three segments (depicted with the black horizontal lines), for the data series depicted in Figure 1(a). Based on PAA, the indexable Symbolic Aggregate approXimation (iSAX) representation was proposed [16] (and later used in several different data series indices [6], [7], [11], [23], [24]). This method first divides the (y-axis) space in different regions, and assigns a bit-wise symbol to each region. In practice, the number of symbols is small: iSAX achieves very good approximations with as few as 256 symbols, the maximum alphabet cardinality, $|alphabet|$, which can be represented by eight bits [18]. It then represents each segment w of the series with the symbol of the region the PAA falls into, forming the word $10_2 00_2 11_2$ shown in Figure 1(c) (subscripts denote the number of bits used to represent the symbol of each segment).

[ParIS Index] Based on the iSAX representation, the state-of-the-art ParIS index was developed [7], which proposed techniques and algorithms specifically designed for modern hardware and disk-based data. ParIS makes use of variable cardinalities for the iSAX summaries (i.e., variable degrees of precision for the symbol of each segment) in order to build a hierarchical tree index (see Figure 1(d)), consisting of three types of nodes: (i) the root node points to several children nodes, 2^w in the worst case (when the series in the collection cover all possible iSAX summaries); (ii) each inner node contains the iSAX summary of all the series below it, and has two children; and (iii) each leaf node contains the iSAX summaries of all the series inside it, and pointers to the raw data (in order to be able to prune false positives and produce exact, correct answers), which reside on disk. When the number of series in a leaf node becomes greater than the maximum leaf capacity, the leaf splits: it becomes an inner node and creates two new leaves, by increasing the cardinality of the iSAX summary of one of the segments (the one that will result in the most balanced split of the contents of the node to its two new children [6], [18]). The two refined iSAX summaries (new bit set to *0* and *1*) are assigned to the two new leaves. In our example, the series of Figure 1(c) will be placed in the outlined node of the index (Figure 1(d)). Note that we define the distance of a query series to a node as the distance between the query (raw values, or iSAX summary) and the iSAX summary of the node.

In the index construction phase (see Figure 1(d)), ParIS uses a coordinator worker that reads raw data series from disk and transfers them into a raw data buffer in memory. A number of index bulk loading workers compute the iSAX summaries of these series, and insert <iSAX summary, file position> pairs in an array. They also insert a pointer to the appropriate element of this array in the receiving buffer of the corresponding subtree of the index root. When main memory is exhausted, the coordinator worker creates a number of index construction worker threads, each one assigned to one subtree of the root and responsible for further building that subtree (by processing the iSAX summaries stored in the coresponding receiving buffer). This process results in each iSAX summary being moved to the output buffer of the leaf it belongs to. When all iSAX summaries in the receiving buffer of an index construction worker have been processed, the output buffers of all leaves in that subtree are flushed to disk.

For query answering, ParIS offers a parallel implementation of the SIMS exact search algorithm [6]. It first computes an approximate answer by calculating the real distance between the query and the best candidate series, which is in the leaf with the smallest lower bound distance to the query. ParIS uses the index tree only for computing this approximate answer. Then, a number of lower bound calculation workers compute the lower bound distances between the query and the iSAX summary of each data series in the dataset, which are stored in the *SAX array*, and prune the series whose lower bound distance is larger than the approximate real distance computed earlier. The data series that are not pruned, are stored in a candidate list for further processing. Subsequently, a number of real distance calculation workers operate on different parts of this array to compute the real distances between the query and the series stored in it (for which the raw values need to be read from disk). For details see [7].

In the in-memory version of ParIS, the raw data series are

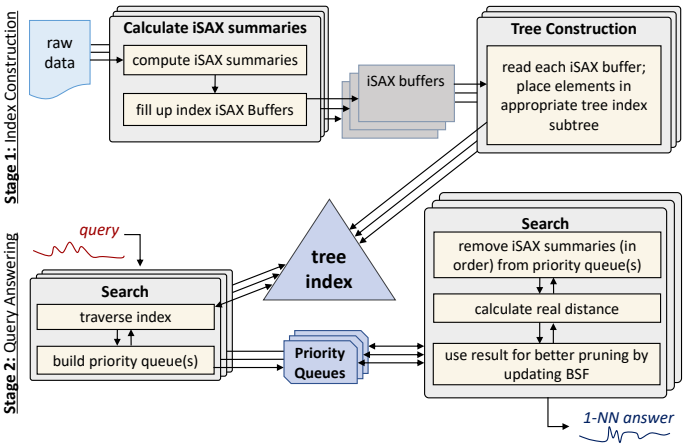


Fig. 2. MESSI index construction and query answering

stored in an in-memory array. Thus, there is no need for a coordinator worker. The bulk loading workers now operate directly on this array (split to as many chunks as the workers). In the rest of the paper, we use ParIS to refer to this in-memory version of the algorithm.

III. The MESSI Solution

Figure 2 depicts the MESSI index construction and query answering pipeline. The raw data are stored in memory into an array, called $RawData$. This array is split into a predetermined number of chunks. A number, N_w, of *index worker* threads process the chunks to calculate the iSAX summaries of the raw data series they store. The number of chunks is not necessarily the same as N_w. Chunks are assigned to index workers the one after the other (using Fetch&Inc). Based on the iSAX representation, we can figure out in which subtree of the index tree an iSAX summary will be stored. A number of *iSAX buffers*, one for each root subtree of the index tree, contain the iSAX summaries to be stored in that subtree.

Each index worker stores the iSAX summaries it computes in the appropriate iSAX buffers. To reduce synchronization cost, each iSAX buffer is split into parts and each worker works on its own part[3]. The number of iSAX buffers is usually a few tens of thousands and at most 2^w, where w is the number of segments in the iSAX summaries of each data series (w is fixed to 16 in this paper, as in previous studies [6], [7]).

When the iSAX summaries for all raw data series have been computed, the index workers proceed in the constuction of the tree index. Each worker is assigned an iSAX buffer to work on (this is done again using Fetch&Inc). Each worker reads the data stored in (all parts of) its assigned buffer and builds the corresponding index subtree. Therefore, all index workers process distinct subtrees of the index, and can work in parallel and independently from one another, with no need for synchronization[4]. When an index worker finishes with the current iSAX buffer it works on, it continues with the next iSAX buffer that has not yet been processed.

When the series in all iSAX buffers have been processed, the tree index has been built and can be used to answer similarity search queries, as depicted in the query answering phase of Fig. 2. To answer a query, we first perform a search for the query iSAX summary in the tree index. This returns a leaf whose iSAX summary has the closest distance to the iSAX summary of the query. We calculate the real distance of the (raw) data series pointed to by the elements of this leaf to the query series, and store the minimum of these distances into a shared variable, called BSF (Best-So-Far). Then, the index workers start traversing the index subtrees (the one after the other) using BSF to decide which subtrees will be pruned. The leaves of the subtrees that cannot be pruned are placed into (a fixed number of) minimum priority queues, using the lower bound distance between the raw values of the query series and the iSAX summary of the leaf node, in order to be further examined. Each thread inserts elements in the priority queues in a round-robin fashion so that load balancing is achieved (i.e., all queues contain about the same number of elements).

As soon as the necessary elements have been placed in the priority queues, each index worker chooses a priority queue to work on, and repeatedly calls DeleteMin() on it to get a leaf node, on which it performs the following operations. It first checks whether the lower bound distance stored in the priority queue is larger than the current BSF: if it is then we are certain that the leaf node does not contain any series that can be part of the answer, and we can prune it; otherwise, the worker needs to examine the series contained in the leaf node, by first computing lower bound distances using the iSAX summaries, and if necessary also the real distances using the raw values. During this process, we may discover a series with a smaller distance to the query, in which case we also update the BSF. When a worker reaches a node whose distance is bigger than the BSF, it gives up this priority queue and starts working on another, because it is certain that all the other elements in the abandoned queue have an even higher distance to the query series. This process is repeated until all priority queues have been processed. During this process, the value of BSF is updated to always reflect the minimum distance seen so far. At the end of the calculation, the value of BSF is returned as the query answer.

Note that, similarly to ParIS, MESSI uses SIMD (Single-Instruction Multiple-Data) for calculating the distances of both, the index iSAX summaries from the query iSAX summary (*lower bound distance calculations*), and the raw data series from the query data series (*real distance calculations*) [7].

A. Index Construction

Algorithm 1 presents the pseudocode for the *initiator* thread. The initiator creates N_w index worker threads to execute the

[3] We have also tried an alternative technique where each buffer was protected by a lock and many threads were accessing each buffer. However, this resulted in worse performance due to the encountered contention in accessing the iSAX buffers.

[4] Parallelizing the processing inside each one of the index root subtrees would require a lot of synchronization due to node splitting.

Algorithm 1: $CreateIndex$

Input: **Index** $index$, **Integer** N_w, **Integer** $chunk\_size$

1 **for** $i \leftarrow 0$ **to** $N_w - 1$ **do**
2 create a thread to execute an instance of IndexWorker($index$, $chunk\_size$,i, N_w);
3 wait for all these threads to finish their execution;

Algorithm 2: $IndexWorker$

Input: **Index** $index$, **Integer** $chunk\_size$, **Integer** pid, **Integer** N_w

1 CalculateiSAXSummaries($index$, $chunk\_size$,pid);
2 barrier to synchronize the IndexWorkers with one another;
3 TreeConstruction($index$, N_w);
4 exit();

index construction phase (line 2). As soon as these workers finish their execution, the initiator returns (line 3). We fix N_w to be 24 threads (Figure 9 in Section IV justifies this choice). We assume that the $index$ variable is a structure (struct) containing the $RawData$ array, all iSAX buffers, and a pointer to the root of the tree index. Recall that MESSI splits $RawData$ into chunks of size $chunk\_size$. We assume that the size of $RawData$ is a multiple of $chunk\_size$ (if not, standard padding techniques can be applied).

The pseudocode for the index workers is in Algorithm 2. The workers first call the $CalculateiSAXSummaries$ function (line 1) to calculate the iSAX summaries of the raw data series and store them in the appropriate iSAX buffers. As soon as the iSAX summaries of all the raw data series have been computed (line 2), the workers call $TreeConstruction$ to construct the index tree.

The pseudocode of $CalculateiSAXSummaries$ is shown in Algorithm 3 and is schematically illustrated in Figure 3(a). Each index worker repeatedly does the following. It first performs a Fetch&Inc to get assigned a chunk of raw data series to work on (line 3). Then, it calculates the offset in the $RawData$ array that this chunk resides (line 4) and starts processing the relevant data series (line 6). For each of them, it computes its iSAX summary by calling the ConvertToiSAX function (line 7), and stores the result in the appropriate iSAX buffer of $index$ (lines 8-9). Recall that each iSAX buffer is split into N_w parts, one for each thread; thus, $index.iSAXbuffer$ is a two dimensional array.

Each part of an iSAX buffer is allocated dynamically when the first element to be stored in it is produced. The size of each part has an initial small value (5 series in this work, as we discuss in the experimental evaluation) and it is adjusted dynamically based on how many elements are inserted in it (by doubling its size each time).

We note that we also tried a design of MESSI with no iSAX buffers, but this led to slower performance (due to the worse cache locality). Thus, we do not discuss this alternative further.

As soon as the computation of the iSAX summaries is over, each index worker starts executing the $TreeConstruction$ function. Algorithm 4 shows the pseudocode for this function and Figure 3(b) schematically describes how it works. In

Algorithm 3: $CalculateiSAXSummaries$

Input: **Index** $index$, **Integer** $chunk\_size$, **Integer** pid

1 **Shared integer** $F_c = 0$;
2 **while** *(TRUE)* **do**
3 $b \leftarrow$*Atomically* fetch and increment F_c;
4 $b = b * chunk\_size$;
5 **if** ($b \geq$ size of the $index.RawData$ array) **then** break ;
6 **for** $j \leftarrow b$ **to** $b + chunk\_size$ **do**
7 $isax = ConvertToiSAX(index.RawData[j])$;
8 ℓ = find appropriate root subtree where $isax$ must be stored;
9 $index.iSAXbuf[\ell][pid] = \langle isax, j \rangle$;

Algorithm 4: $TreeConstruction$

Input: **Index** $index$, **Integer** N_w

1 **Shared integer** $F_b = 0$;
2 **while** *(TRUE)* **do**
3 $b \leftarrow$*Atomically* fetch and increment F_b;
4 **if** ($b \geq 2^w$) **then** break ; // the root has at most 2^w children
5 **for** $j \leftarrow 0$ **to** N_w **do**
6 **for every** $\langle isax, pos \rangle$ pair $\in index.iSAXbuf[b][j]$ **do**
7 $targetLeaf \leftarrow$ Leaf of $index$ tree to insert $\langle isax, pos \rangle$;
8 **while** $targetLeaf$ is full **do**
9 SplitNode($targetLeaf$);
10 $targetLeaf \leftarrow$ New leaf to insert $\langle isax, pos \rangle$;
11 Insert $\langle isax, pos \rangle$ in $targetLeaf$;

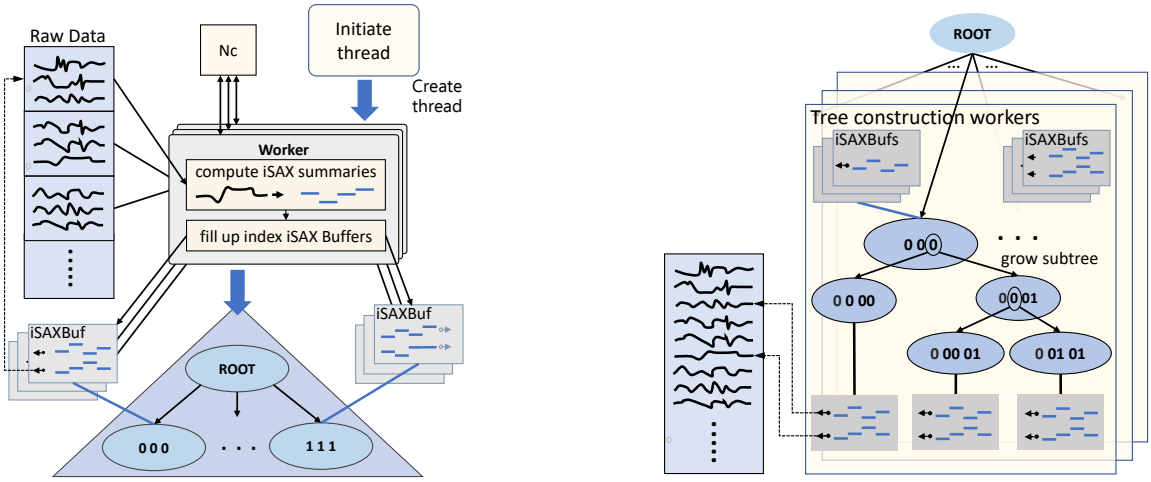
$TreeConstruction$, a worker repeatedly executes the following actions. It accesses F_b (using Fetch&Inc) to get assigned an iSAX buffer to work on (line 3). Then, it traverses all parts of the assigned buffer (lines 5-6) and inserts every pair $\langle$iSAX summary, pointer to relevant data series$\rangle$ stored there in the index tree (line 7-11). Recall that the iSAX summaries contained in the same iSAX buffer will be stored in the same subtree of the index tree. So, no synchronization is needed among the index workers during this process. If a tree worker finishes its work on a subtree, a new iSAX buffer is (repeatedly) assigned to it, until all iSAX buffers have been processed.

B. Query Answering

The pseudocode for executing an exact search query is shown in Algorithm 5. We first calculate the iSAX summary of the query (line 2), and execute an approximate search (line 3) to find the initial value of BSF, i.e., a first upper bound on the

Algorithm 5: $ExactSearch$

1 **Shared float** BSF;
Input: **QuerySeries** QDS, **Index** $index$, **Integer** N_q
2 QDS_iSAX = calculate iSAX summary for QDS;
3 BSF = approxSearch(QDS_iSAX, $index$);
4 **for** $i \leftarrow 0$ **to** $N_q - 1$ **do**
5 $queue[i]$ = Initialize the ith priority queue;
6 **for** $i \leftarrow 0$ **to** $N_s - 1$ **do**
7 create a thread to execute an instance of SearchWorker(QDS, $index$, $queue[]$, i, N_q);
8 Wait for all threads to finish;
9 **return** (BSF);



(a) CalculateiSAXSummaries (b) TreeConstruction

Fig. 3. Workflow and algorithms for MESSI index creation

actual distance between the query and the series indexed by the tree. This process is illustrated in Figure 4(a).

During a search query, the index tree is traversed and the distance of the iSAX summary of each of the visited nodes to the iSAX summary of the query is calculated. If the distance of the iSAX summary of a node, nd, to the query iSAX summary is higher than BSF, then we are certain that the distances of all data series indexed by the subtree rooted at nd are higher than BSF. So, the entire subtree can be pruned. Otherwise, we go down the subtree, and the leaves with a distance to the query smaller than the BSF, are inserted in the priority queue.

The technique of using priority queues maximizes the pruning degree, thus resulting in a relatively small number of raw data series whose real distance to the query series must be calculated. As a side effect, BSF converges fast to the correct value. Thus, the number of iSAX summaries that are tested against the iSAX summary of the query series is also reduced.

Algorithm 5 creates $N_s = 48$ threads, called the *search workers* (lines 6-7), which perform the computation described above by calling $SearchWorker$. It also creates $N_q \geq 1$ priority queues (lines 4-5), where the search workers place those data series that are potential candidates for real distance calculation. After all search workers have finished (line 8), $ExactSearch$ returns the current value of BSF (line 9).

We have experimented with two different settings regarding the number of priority queues, N_q, that the search workers use. The first, called *Single Queue* (SQ), refers to $N_q = 1$, whereas the second focuses in the Multiple-Queue (MQ) case where $N_q > 1$. Using a single shared queue imposes a high synchronization overhead, whereas using a local queue per thread results in severe load imbalance, since, depending on the workload, the size of the different queues may vary significantly. Thus, we choose to use N_q shared queues, where $N_q > 1$ is a fixed number (in our analysis N_q is set to 24, as experiments our show that this is the best choice).

Algorithm 6: $SearchWorker$

Input: **QuerySeries** QDS, **Index** $index$, **Queue** $queue[]$, **Integer** pid, **Integer** N_q

1 **Shared integer** $N_b = 0$;
2 $q = pid \mod N_q$;
3 **while** *(TRUE)* **do**
4 $i \leftarrow$*Atomically* fetch and increment N_b;
5 **if** $(i \geq 2^w)$ **then** break;
6 $TraverseRootSubtree(QDS, index.rootnode[i], queue[], \&q, N_q)$;
7 Barrier to synchronize the search workers with one another;
8 $q = pid \mod N_q$;
9 **while** *(true)* **do**
10 $ProcessQueue(QDS, index, queue[q])$;
11 **if** *all queue[].finished=true* **then**
12 break;
13 $q \leftarrow$ index such that $queue[q]$ has not been processed yet;

The pseudocode of search workers is shown in Algorithm 6, and the work they perform is illustrated in Figures 4(b) and 4(c). At each point in time, each thread works on a single queue. Initially, each queue is shared by two threads. Each search worker first identifies the queue where it will perform its first insertion (line 2). Then, it repeatedly chooses (using Fetch&Inc) a root subtree of the index tree to work on by calling $TraverseRootSubtree$ (line 6). After all root subtrees have been processed (line 7), it repeatedly chooses a priority queue (lines 9, 13) and works on it by calling $ProcessQueue$ (line 10). Each element of the $queue$ array has a field, called $finished$, which indicates whether the processing of the corresponding priority queue has been finished. As soon as a search worker determines that all priority queues have been processed (line 12), it terminates.

We continue to describe the pseudocode for $TraverseRootSubtree$ which is presented in Algorithm 7 and illustrated in Figure 4(b). $TraverseRootSubtree$ is

Algorithm 7: $TraverseRootSubtree$

```
   Input: QuerySeries QDS, Node node, queue queue[], Integer *pq,
          Integer N_q
1  nodedist = FindDist(QDS, node);
2  if nodedist > BSF then
3  |   break;
4  else if node is a leaf then
5  |   acquire queue[*pq] lock;
6  |   Put node in queue[*pq] with priority nodedist;
7  |   release queue[*pq] lock;
8  |   // next time, insert in the subsequent queue
9  |   *pq ← (*pq + 1) mod N_q;
10 else
11 |   TraverseRootSubtree(node.leftChild, queue[], pq, N_q);
12 |   TraverseRootSubtree(node.rightChild, queue[], pq, N_q)
```

Algorithm 8: $ProcessQueue$

```
   Input: QuerySeries QDS, Index index, Queue Q
1  while node = DeleteMin(Q) do
2  |   if node.dist < BSF then
3  |   |   realDist = CalculateRealDistance(QDS, index, node);
4  |   |   if realDist < BSF then
5  |   |   |   acquire BSFLock;
6  |   |   |   BSF = realDist;
7  |   |   |   release BSFLock;
8  |   else
9  |   |   q.finished = true;
10 |   |   break;
```

Algorithm 9: $CalculateRealDistance$

```
   Input: QuerySeries QDS, Index index, node node, float BSF
1  for every (isax, pos) pair ∈ node do
2  |   if LowerBound_SIMD(QDS, isax) < BSF then
3  |   |   dist = RealDist_SIMD(index.RawData[pos], QDS);
4  |   |   if dist < BSF then
5  |   |   |   BSF = dist;
6  return (BSF)
```

recursive. On each internal node, nd, it checks whether the (lower bound) distance of the iSAX summary of nd to the raw values of the query (line 1) is smaller than the current BSF, and if it is, it examines the two subtrees of the node using recursion (lines 11-12). If the traversed node is a leaf node and its distance to the iSAX summary of the query series is smaller than the current BSF (lines 4-9), it places it in the appropriate priority queue (line 6). Recall that the priority queues are accessed in a round-robin fashion (line 9). This strategy maintains the size of the queues balanced, and reduces the synchronization cost of node insertions to the queues. We implement this strategy by (1) passing a pointer to the local variable q of $SearchWorker$ as an argument to $TraverseRootSubtree$, (2) using the current value of q for choosing the next queue to perform an insertion (line 6), and (3) updating the value of q (line 9). Each queue may be accessed by more than one threads, so a lock per queue is used to protect its concurrent access by multiple threads.

We next describe how $ProcessQueue$ works (see Algorithm 8 and Figure 4(c)). The search worker repeatedly removes the (leaf) node, nd, with the highest priority from the priority queue, and checks whether the corresponding distance stored in the queue is still less than the BSF. We do so, because the BSF may have changed since the time that the leaf node was inserted in the priority queue. If the distance is less than the BSF, then $CalculateRealDistance$ (line 3) is called, in order to identify if any series in the leaf node (pointed to by nd) has a real distance to the query that is smaller than the current BSF. If we discover such a series (line 4), BSF is updated to the new value (line 6). We use a lock to protect BSF from concurrent update efforts (lines 5, 7). Previous experiments showed that the initial value of BSF is very close to its final value [25]. Indeed, in our experiments, the BSF is updated only 10-12 times (on average) per query. So, the synchronization cost for updating the BSF is negligible.

In Algorithm 9, we depict the pseudocode for $CalculateRealDistance$. Note that we perform the real distance calculation using SIMD. However, the use of SIMD does not have the same significant impact in performance as in ParIS [7]. This is because pruning is much more effective in MESSI, since for each candidate series in the examined leaf node, $CalculateRealDistance$ first performs a lower bound distance calculation, and proceeds to the real distance calculation only if necessary (line 3). Therefore, the number of (raw) data series to be examined is limited in comparison to those examined in ParIS (we quantify the effect of this new design in our experimental evaluation).

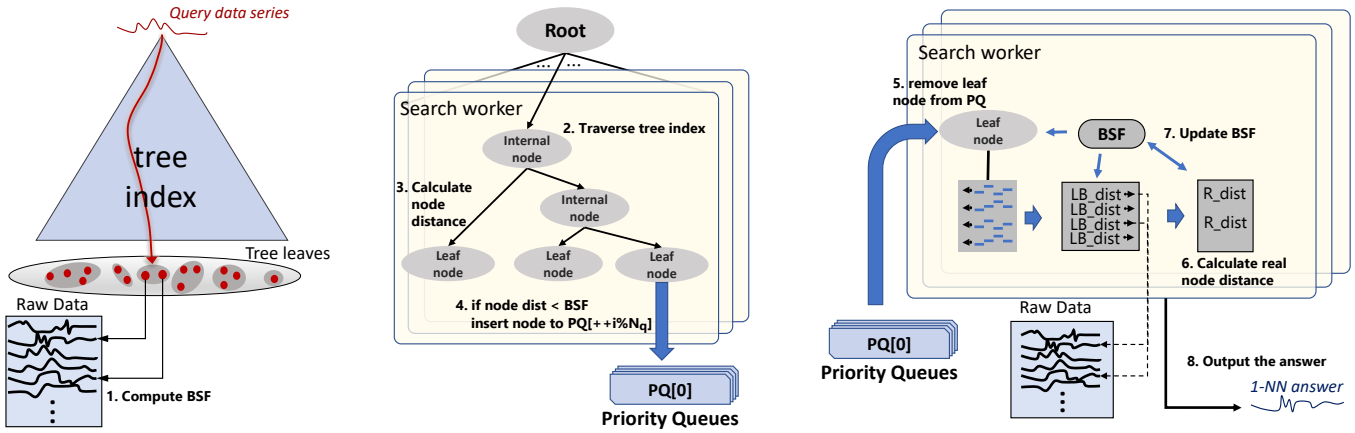
IV. Experimental Evaluation

In this section, we present our experimental evaluation. We use synthetic and real datasets in order to compare the performance of MESSI with that of competitors that have been proposed in the literature and baselines that we developed. We demonstrate that, under the same settings, MESSI is able to construct the index up to 4.2x faster, and answer similarity search queries up to 11.2x faster than the competitors. Overall, MESSI exhibits a robust performance across different datasets and settings, and enables for the first time the exploration of very large data series collections at interactive speeds.

A. Setup

We used a server with 2x Intel Xeon E5-2650 v4 2.2Ghz CPUs (12 cores/24 hyper-threads each) and 256GB RAM. All algorithms were implemented in C, and compiled using GCC v6.2.0 on Ubuntu Linux v16.04.

[Algorithms] We compared MESSI to the following algorithms: (i) ParIS [7], the state-of-the-art modern hardware data series index. (ii) ParIS-TS, our extension of ParIS, where we implemented in a parallel fashion the traditional tree-based exact search algorithm [16]. In brief, this algorithm traverses the tree, and concurrently (1) inserts in the priority queue the nodes (inner nodes or leaves) that cannot be pruned based on the lower bound distance, and (2) pops from the queues nodes for which it calculates the real distances to the candidate series [16]. In contrast, MESSI (a) first makes a *complete pass* over the index using lower bound distance computations and then proceeds with the real distance computations; (b)



(a) Approximate search for calculating the first BSF

(b) Tree traversal and node insertion in priority queues

(c) Node distance calculation from priority queues

Fig. 4. Workflow and algorithms for MESSI query answering

it only considers the *leaves* of the index for insertion in the priority queue(s); and (c) performs a *second* filtering step using the lower bound distances when popping elements from the priority queue (and before computing the real distances). The performance results we present later justify the choices we have made in MESSI, and demonstrate that a straight-forward implementation of tree-based exact search leads to sub-optimal performance. (iii) UCR Suite-P, our parallel implementation of the state-of-the-art optimized serial scan technique, UCR Suite [15]. In UCR Suite-P, every thread is assigned a part of the in-memory data series array, and all threads concurrently and independently process their own parts, performing the real distance calculations in SIMD, and only synchronize at the end to produce the final result. (We do not consider the non-parallel UCR Suite version in our experiments, since it is almost 300x slower.) All algorithms operated exclusively in main memory (the datasets were already loaded in memory, as well). The code for all algorithms used in this paper is available online [26].

[Datasets] In order to evaluate the performance of the proposed approach, we use several synthetic datasets for a fine grained analysis, and two real datasets from diverse domains. Unless otherwise noted, the series have a size of 256 points, which is a standard length used in the literature, and allows us to compare our results to previous work. We used synthetic datasets of sizes 50GB-200GB (with a default size of 100GB), and a random walk data series generator that works as follows: a random number is first drawn from a Gaussian distribution N(0,1), and then at each time point a new number is drawn from this distribution and added to the value of the last number. This kind of data generation has been extensively used in the past (and has been shown to model real-world financial data) [6], [16]–[18], [27]. We used the same process to generate 100 query series.

For our first real dataset, *Seismic*, we used the IRIS Seismic Data Access repository [28] to gather 100M series representing seismic waves from various locations, for a total size of 100GB. The second real dataset, *SALD*, includes neuroscience MRI data series [29], for a total of 200M series of size 128, of size 100 GB. In both cases, we used as queries 100 series out of the datasets (chosen using our synthetic series generator).

In all cases, we repeated the experiments 10 times and we report the average values. We omit reporting the error bars, since all runs gave results that were very similar (less than 3% difference). Queries were always run in a sequential fashion, one after the other, in order to simulate an exploratory analysis scenario, where users formulate new queries after having seen the results of the previous one.

B. Parameter Tuning Evaluation

In all our experiments, we use 24 index workers and 48 search workers. We have chosen the chunk size to be 20MB (corresponding to 20K series of length 256 points). Each part of any iSAX buffer, initially holds a small constant number of data series, but its size changes dynamically depending on how many data series it needs to store. The capacity of each leaf of the index tree is 2000 data series (2MB). For query answering, MESSI-mq utilizes 24 priority queues (whereas MESSI-sq utilizes just one priority queue). In either case, each priority queue is implemented using an array whose size changes dynamically based on how many elements must be stored in it. Below we present the experiments that justify the choices for these parameters.

Figure 5 illustrates the time it takes MESSI to build the tree index for different chunk sizes on a random dataset of 100GB. The required time to build the index decreases when the chunk size is small and does not have any big influence in performance after the value of 1K (data series). Smaller chunk sizes than 1K result in high contention when accessing the fetch&increment object used to assign chunks to index workers. In our experiments, we have chosen a size of 20K, as this gives slightly better performance than setting it to 1K.

Figures 6 and 7 show the impact that varying the leaf size of the tree index has in the time needed for the index creation

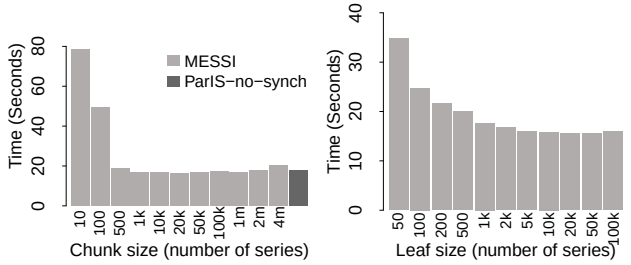


Fig. 5. Index creation, vs. chunk size

Fig. 6. Index creation, vs. leaf size

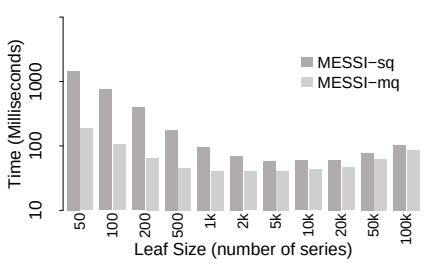


Fig. 7. Query answering, vs. leaf size

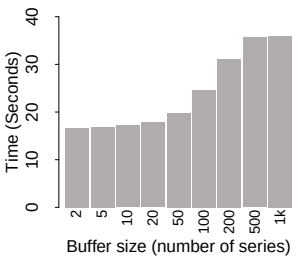


Fig. 8. Index creation, vs. initial iSAX buffer size

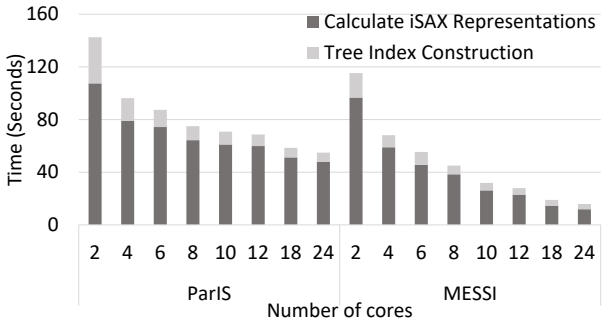


Fig. 9. Index creation, varying number of cores

and for query answering, respectively. As we see in Figure 6, the larger the leaf size is, the faster index creation becomes. However, once the leaf size becomes 5K or more, this time improvement is insignificant. On the other hand, Figure 7 shows that the query answering time takes its minimum value when the leaf size is set to 2K (data series). So, we have chosen this value for our experiments.

Figure 7 indicates that the influence of varying the leaf size is significant for query answering. Note that when the leaf size is small, there are more leaf nodes in the index tree and therefore, it is highly probable that more nodes will be inserted in the queues, and vice versa. On the other hand, as the leaf size increases, the number of real distance calculations that are performed to process each one of the leaves in the queue is larger. This causes load imbalance among the different search workers that process the priority queues. For these reasons, we see that at the beginning the time goes down as the leaf size increases, it reaches its minimum value for leaf size 2K series, and then it goes up again as the leaf size further increases.

Figure 8 shows the influence of the initial iSAX buffer size during index creation. This initialization cost is not negligible given that we allocate 2^w iSAX buffers, each consisting of 24 parts (recall that 24 is the number of index workers in the system). As expected, the figure illustrates that smaller initial sizes for the buffers result in better performance. We have chosen the initial size of each part of the iSAX buffers to be a small constant number of data series. (We also considered an alternative design that collects statistics and allocates the iSAX buffers right from the beginning, but was slower.)

We finally justify the choice of using more than one priority queues for query answering. As Figure 11 shows, MESSI-mq and MESSI-sq have similar performance when the number of threads is smaller than 24. However, as we go from 24 to 48 cores, the synchronization cost for accessing the single priority queue in MESSI-sq has negative impact in performance. Figure 13 presents the breakdown of the query answering time for these two algorithms. The figure shows that in MESSI-mq, the time needed to insert and remove nodes from the list is significantly reduced. As expected, the time needed for the real distance calculations and for the tree traversal are about the same in both algorithms. This has the effect that the time needed for the distance calculations becomes the dominant factor. The figure also illustrates the percentage of time that goes on each of these tasks. Finally, Figure 14 illustrates the impact that the number of priority queues has in query answering performance. As the number of priority queues increases, the time goes down, and it takes its minimum value when this number becomes 24. So, we have chosen this value for our experiments.

C. Comparison to Competitors

[Index Creation] Figure 9 compares the index creation time of MESSI with that of ParIS as the number of cores increases for a dataset of 100GB. The time MESSI needs for index creation is significantly smaller than that of ParIS. Specifically, MESSI is 3.5x faster than ParIS. The main reasons for this are on the one hand that MESSI exhibits lower contention cost when accessing the iSAX buffers in comparison to the corresponding cost paid by ParIS, and on the other hand, that MESSI achieves better load balancing when performing the computation of the iSAX summaries from the raw data series. Note that due to synchronization cost, the performance improvement that both algorithms exhibit decreases as the number of cores increases; this trend is more prominent in ParIS, while MESSI manages to exploit to a larger degree the available hardware.

In Figure 10, we depict the index creation time as the dataset size grows from 50GB to 200GB. We observe that MESSI performs up to 4.2x faster than ParIS (for the 200GB dataset), with the improvement becoming larger with the dataset size.

[Query Answering] Figure 11 compares the performance of the MESSI query answering algorithm to its competitors, as the number of cores increases, for a random dataset of 100GB (y-axis in log scale). The results show that both MESSI-sq and

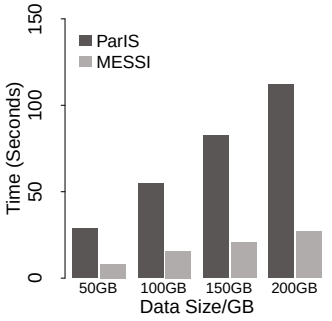


Fig. 10. Index creation, vs. data size

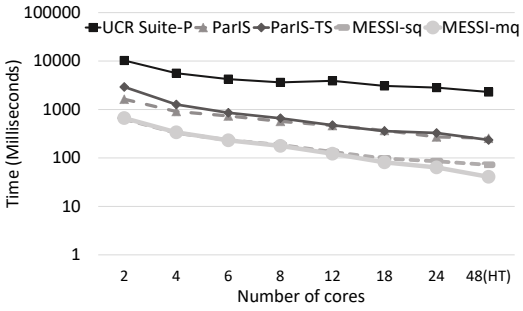


Fig. 11. Query answering, vs. number of cores

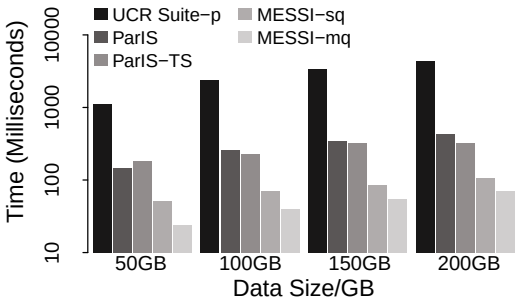


Fig. 12. Query answering, vs. data size

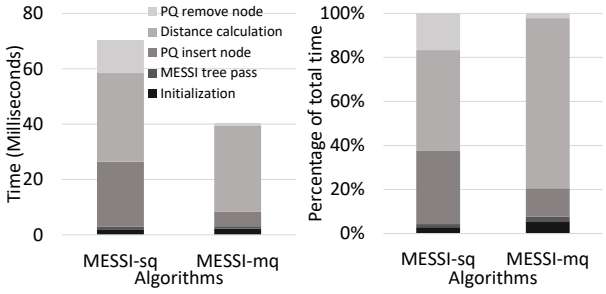
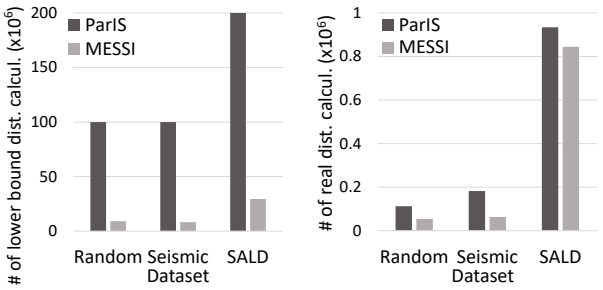


Fig. 13. Query answering with different queue type



(a) Lower bound distance calculations

(b) Real distance calculations

Fig. 17. Number of distance calculations

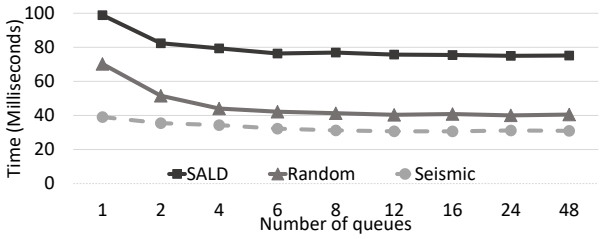


Fig. 14. Query answering, vs. number of queues

MESSI-mq perform much better than all the other algorithms. Note that the performance of MESSI-mq is better than that of MESSI-sq, so when we mention MESSI in our comparison below we refer to MESSI-mq. MESSI is 55x faster than UCR Suite-P and 6.35x faster than ParIS when we use 48 threads (with hyperthreading). In contrast to ParIS, MESSI applies pruning when performing the lower bound distance calculations and therefore it executes this phase much faster. Moreover, the use of the priority queues result in even higher pruning power. As a side effect, MESSI also performs less real distance calculations than ParIS. Note that UCR Suite-P does not perform any pruning, thus resulting in a much lower performance than the other algorithms.

Figure 12 shows that this superior performance of MESSI is exhibited for different data set sizes as well. Specifically, MESSI is up to 61x faster than UCR Suite-p (for 200GB), up to 6.35x faster than ParIS (for 100GB), and up to 7.4x faster than ParIS-TS (for 50GB).

[Performance Benefit Breakdown] Given the above results, we now evaluate several of the design choices of MESSI in isolation. Note that some of our design decisions stem from the fact that in our index the root node has a large number of children. Thus, the same design ideas are applicable to the iSAX family of indices [4] (e.g., iSAX2+, ADS+, ULISSE). Other indices however [4], use a binary tree (e.g., DSTree), or a tree with a very small fanout (e.g., SFA trie, M-tree), so new design techniques are required for efficient parallelization. However, some of our techniques, e.g., the use of (more than one) priority queue, the use of SIMD, and some of the data structures designed to reduce the syncrhonization cost can be applied to all other indices. Figure 18 shows the results for the query answering performance. The leftmost bar (ParIS-SISD) shows the performance of ParIS when SIMD is *not* used. By employing SIMD, ParIS becomes 60% faster than ParIS-

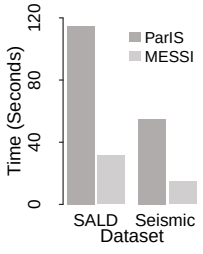


Fig. 15. Index creation for real datasets

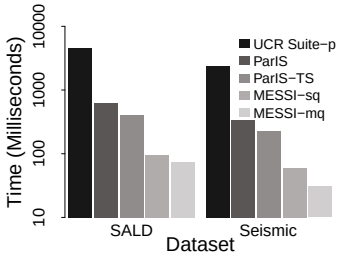


Fig. 16. Query answering for real datasets

SISD. We then measure the performance for ParIS-TS, which is about 10% faster than ParIS. This performance improvement comes form the fact that using the index tree (instead of the SAX array that ParIS uses) to prune the search space and determine the data series for which a real distance calculation must be performed, significantly reduces the number of lower bound distance calculations. ParIS calculates lower bound distances for all the data series in the collection, and pruning is performed only when calculating real distances, whereas in ParIS-TS pruning occurs when calculating lower bound distances as well.

MESSI-mq further improves performance by only inserting in the priority queue leaf nodes (thus, reducing the size of the queue), and by using multiple queues (thus, reducing the synchronization cost). This makes MESSI-mq 83% faster than ParIS-TS.

[Real Datasets] Figures 15 and 16 reaffirm that MESSI exhibits the best performance for both index creation and query answering, even when executing on the real datasets, SALD and Seismic (for a 100GB dataset). The reasons for this are those explained in the previous paragraphs. Regarding index creation, MESSI is 3.6x faster than ParIS on SALD and 3.7x faster than ParIS on Seismic, for a 100GB dataset. Moreover, for SALD, MESSI query answering is 60x faster than UCR Suite-P and 8.4x faster than ParIS, whereas for Seismic, it is 80x faster than UCR Suite-P, and almost 11x faster than ParIS. Note that MESSI exhibits better performance than UCR Suite-P in the case of real datasets. This is so because working on random data results in better pruning than that on real data.

Figures 17(a) and 17(b) illustrate the number of lower bound and real distance calculations, respectively, performed by the different query algorithms on the three datasets. ParIS calculates the distance between the iSAX summaries of every single data series and the query series (because, as we discussed in Section II, it implements the SIMS strategy for query answering). In contrast, MESSI performs pruning even during the lower bound distance calculations, resulting in much less time for executing this computation. Moreover, this results in a significantly reduced number of data series whose real distance to the query series must be calculated.

The use of the priority queues lead to even less real distance calculations, because they help the BSF to converge faster to its final value. MESSI performs no more than 15% of the lower bound distance calculations performed by ParIS.

[MESSI with DTW] In our final experiments, we demonstrate that MESSI not only accelerates similarity search based on Euclidean distance, but can also be used to significantly accelerate similarity search using the Dynamic Time Warping (DTW) distance measure [30]. We note that no changes are required in the index structure; we just have to build the envelope of the LB_Keogh method [31] around the query series, and then search the index using this envelope. Figure 19 shows the query answering time for different dataset sizes (we use a warping window size of 10% of the query series length, which is commonly used in practice [31]). The results show

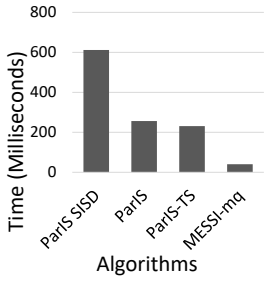


Fig. 18. Query answering performance benefit breakdown

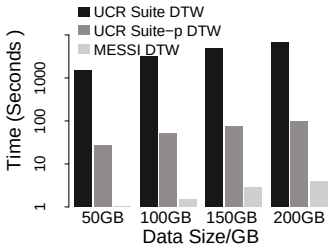


Fig. 19. MESSI query answering time for DTW distance (synthetic data, 10% warping window)

that MESSI-DTW is up to 34x faster than UCR Suite-p DTW (and more than 3 orders of magnitude faster than the non-paralell version of UCR Suite DTW).

V. Related Work

Various dimensionality reduction techniques exist for data series, which can then be scanned and filtered [32], [33] or indexed and pruned [6], [7], [11], [16], [17], [23], [24], [34], [35] during query answering. We follow the same approach of indexing the series based on their summaries, though our work is the first to exploit the parallelization opportunities offered by modern hardware, in order to accelerate in-memory index construction and similarity search for data series. The work closest to ours is ParIS [7], which also exploits modern hardware, but was designed for disk-resident datasets. We discussed this work in more detail in Section II.

FastQuery is an approach used to accelerate search operations in scientific data [36], based on the construction of bitmap indices. In essence, the iSAX summarization used in our approach is an equivalent solution, though, specifically designed for sequences (which have high dimensionalities).

The interest in using SIMD instructions for improving the performance of data management solutions is not new [37]. However, it is only more recently that relatively complex algorithms were extended in order to take advantage of this hardware characteristic. Polychroniou et al. [38] introduced design principles for efficient vectorization of in-memory database operators (such as selection scans, hash tables, and partitioning). For data series in particular, previous work has used SIMD for Euclidean distance computations [21]. Following [7], in our work we use SIMD both for the computation of Euclidean distances, as well as for the computation of lower bounds, which involve branching operations.

Multi-core CPUs offer thread parallelism through multiple cores and simultaneous multi-threading (SMT). Thread-Level Parallelism (TLP) methods, like multiple independent cores and hyper-threads are used to increase efficiency [39].

A recent study proposed a high performance temporal index similar to time-split B-tree (TSB-tree), called TSBw-tree, which focuses on transaction time databases [40]. Binna et al. [41], present the Height Optimized Trie (HOT), a general-purpose index structure for main-memory database systems,

while Leis et al. [42] describe an in-memory adaptive Radix indexing technique that is designed for modern hardware. Xie et al. [43], study and analyze five recently proposed indices, i.e., FAST, Masstree, BwTree, ART and PSL and identify the effectiveness of common optimization techniques, including hardware dependent features such as SIMD, NUMA and HTM. They argue that there is no single optimization strategy that fits all situations, due to the differences in the dataset and workload characteristics. Moreover, they point out the significant performance gains that the exploitation of modern hardware features, such as SIMD processing and multiple cores bring to in-memory indices.

We note that the indices described above are not suitable for data series (that can be thought of as high-dimensional data), which is the focus of our work, and which pose very specific data management challenges with their hundreds, or thousands of dimensions (i.e., the length of the sequence).

Techniques specifically designed for modern hardware and in-memory operation have also been studied in the context of adaptive indexing [44], and data mining [45].

VI. Conclusions

We proposed MESSI, a data series index designed for in-memory operation by exploiting the parallelism opportunities of modern hardware. MESSI is up to 4x faster in index construction and up to 11x faster in query answering than the state-of-the-art solution, and is the first technique to answer exact similarity search queries on 100GB datasets in ∼50msec. This level of performance enables for the first time interactive data exploration on very large data series collections.

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