kEDM: A Performance-portable Implementation of Empirical Dynamic Modeling using Kokkos

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ABSTRACT
Empirical Dynamic Modeling (EDM) is a state-of-the-art non-linear time-series analysis framework. Despite its wide applicability, EDM was not scalable to large datasets due to its expensive computational cost. To overcome this obstacle, researchers have attempted and succeeded in accelerating EDM from both algorithmic and implementational aspects. In previous work, we developed a massively parallel implementation of EDM targeting HPC systems (mpEDM). However, mpEDM maintains different backends for different architectures. This design becomes a burden in the increasingly diversifying HPC systems, when porting to new hardware. In this paper, we design and develop a performance-portable implementation of EDM based on the Kokkos performance portability framework (kEDM), which runs on both CPUs and GPUs while based on a single codebase. Furthermore, we optimize individual kernels specifically for EDM computation, and use real-world datasets to demonstrate up to 5.5x speedup compared to mpEDM in convergent cross mapping computation.

CCS CONCEPTS
• Computing methodologies → Parallel computing methodologies; • General and reference → Performance; • Applied computing → Mathematics and statistics.

KEYWORDS
Empirical Dynamic Modeling, Performance Portability, Kokkos, GPU, High Performance Computing

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1 INTRODUCTION
Empirical Dynamic Modeling (EDM) [2] is a state-of-the-art non-linear time-series analysis framework used for various tasks such as assessing the non-linearity of a system, making short-term forecasts, and identifying the existence and strength of causal relationships between variables. Despite its wide applicability, EDM was not scalable to large datasets due to its expensive computational cost. To overcome this challenge, several studies have been conducted to accelerate EDM by improving the algorithm [10] and taking advantage of parallel and distributed computing [14].

We tackle this challenge by taking advantage of modern HPC systems equipped with multi-core CPUs and GPUs. We have been developing a massively parallel distributed implementation of EDM optimized for GPU-centric HPC systems, which we refer to as mpEDM. In our previous work [22], we have deployed mpEDM on the AI Bridging Cloud Infrastructure (ABCI) to obtain an all-to-all causal relationship map of all 10^5 neurons in an entire larval zebrafish brain. To date, this is the first causal analysis of a whole vertebrate brain at single neuron resolution.

Although mpEDM has successfully enabled EDM computation at an unprecedented scale, challenges remain. The primary challenge is performance portability across diverse hardware platforms. Recent HPC landscape has seen significant increase in the diversity of processors and accelerators. This is reflected in the design of upcoming exascale HPC systems, for example, the Frontier system at the Oak Ridge National Laboratory will use AMD EPYC CPUs and Radeon GPUs while the Aurora system at the Argonne National...
Laboratory will employ Intel Xeon CPUs and Xe GPUs; additionally, the Fugaku system at RIKEN uses Fujitsu A64FX ARM CPUs.

The current design of HPC applications has failed to keep up with this trend of rapidly diversifying HPC systems. Computational application kernels are developed with the native programming model for the respective hardware (e.g., CUDA on NVIDIA GPUs). mpEDM is no exception and maintains two completely independent backends for x86_64 CPUs and NVIDIA GPUs. However, this design becomes a burden when supporting a diverse set of hardware platforms because a new backend needs to be developed and maintained for every platform. Based on this trend, various performance portability frameworks [3, 4] have emerged to develop performance-portable applications from single codebase.

In this paper, we use the Kokkos [1] framework and develop a performance-portable implementation of EDM that runs on both CPUs and GPUs, herein referred to as kEDM. This new implementation is based on a single-source design and facilitates the future development and porting to new hardware. Furthermore, we identify and take advantage of optimization opportunities in mpEDM and achieve up to 5.5× higher performance on NVIDIA V100 GPUs.

The rest of this paper is organized as follows: Section 2 first introduces EDM briefly and discusses the challenges in mpEDM; Section 3 presents kEDM, a novel implementation of EDM based on the Kokkos performance portability framework; Section 4 compares kEDM and mpEDM using both synthetic and real-world datasets and assesses the efficiency of kEDM; and finally Section 5 concludes the paper and discusses future work.

2 BACKGROUND

2.1 Empirical Dynamic Modeling (EDM)

Empirical Dynamic Modeling (EDM) [2, 25] is a non-linear time series analysis framework based on the Takens’ embedding theorem [6, 19]. Takens’ theorem states that given a time-series observation of a deterministic dynamical system, one can reconstruct the latent attractor manifold of the dynamical system using time-delayed embeddings of the observation. While the reconstructed manifold might not preserve the global structure of the original manifold, it preserves the local topological features (i.e., a diffeomorphism).

Convergent Cross Mapping (CCM) [13, 18, 21] is one of the widely used EDM methods that identifies and quantifies the causal relationship between two time series variables. Figure 1 illustrates the overview of CCM. To assess if a time series $\hat{Y}(t)$ (hereinafter called target) causes another time series $X(t)$ (hereinafter called library), CCM performs the following four steps:

1. **Embedding**: Both time series $X$ and $Y$ are embedded into $E$-dimensional state space using their time lags. For example, embedding of $X$ is denoted by $x$, where $x(t) = (X(t), X(t-\tau), \ldots, X(t-(E-1)\tau))$. Here, $\tau$ is the time lag and $E$ is the embedding dimension, which is empirically determined and usually $E < 20$ in real-world datasets.

2. **k-Nearest Neighbor Search**: For every library point $x(t)$, its $E+1$ nearest neighbors in the state space are searched. These neighbors form an $E$-dimensional simplex that encloses $x(t)$ in the state space. We refer to these nearest neighbors as $x(t_1), x(t_2), \ldots, x(t_{E+1})$ and the Euclidean distance between $x(t)$ and $x(t_i)$ as $d(t, t_i) = \|x(t) - x(t_i)\|$.

3. **Lookup**: The prediction $\hat{y}(t)$ for a target point $y(t)$ is a linear combination of its neighbors $y(t_1), y(t_2), \ldots, y(t_{E+1})$.
we were unable to modify or tune the k-NN search to suit our use; however, when applying to EDM, the time-delayed embedding distances for every query point. This interface is simple and easy-to-use; however, when applying to EDM, the time-delayed embedding needs to be performed on the CPU in advance and then passed on to ArrayFire. This hinders performance because it increases the memory consumption and memory copies was also challenging because ArrayFire implicitly allocates, deallocates and copies arrays. Another potential optimization opportunity is the partial sort function topk() invoked in the k-NN search. ArrayFire uses NVIDIA’s CUB\(^3\) library to implement partial sort. CUB is a collection of highly optimized parallel primitives and is being used by other popular libraries such as Thrust\(^4\). ArrayFire’s topk() function divides the input array into equal sized sub-array and then calls CUB’s parallel radix sort function to sort each sub-array. It then extracts the top-k elements from each sub-array and concatenates them into a new array. This is recursively repeated until the global top-k elements are found. Even though this implementation is well-optimized, it may not be optimal for EDM because the target k is relatively small (\(\leq 20\)).

Finally, we were unable to implement efficient lookups on GPU using ArrayFire. ArrayFire provides a construct for embarrassingly parallel computation called GFOR that allows one to perform independent for-loops in parallel. Although we were able to implement lookups using GFOR, the attained performance was poor. Managing memory consumption and memory copies was also challenging because ArrayFire implicitly allocates, deallocates and copies arrays.

2.2 Challenges in mpEDM

This subsection discusses the two major challenges in mpEDM\(^2\), our previous parallel implementation of EDM.

2.2.1 Performance portability across diverse hardware. The GPU backend of mpEDM was based on ArrayFire [11], a general purpose library for GPU computing. We chose ArrayFire primarily for its productivity and portability. ArrayFire provides CUDA and OpenCL backends to run on OpenCL devices. Although it also provides a CPU backend, most of the functions provided by the CPU backend are neither multi-threaded nor vectorized. We therefore developed our own implementation for CPUs using OpenMP.

As a result, mpEDM had an ArrayFire-based GPU implementation and an OpenMP-based CPU implementation of EDM, which double the maintenance cost. Considering the diversifying target hardware, a unified implementation that achieves consistent and reasonable performance across a diverse set of hardware is required.

2.2.2 Kernels tailored for EDM. Since mpEDM was relying on ArrayFire’s k-nearest neighbor search function nearestNeighbor(), we were unable to modify or tune the k-NN search to suit our use case and missed opportunities for further optimization. ArrayFire’s nearest neighbor function accepts arrays of reference and query points, and returns arrays of closest reference points and their distances for every query point. This interface is simple and easy-to-use; however, when applying to EDM, the time-delayed embedding needs to be performed on the CPU in advance and then passed on to ArrayFire. This hinders performance because it increases the amount of memories copies between the CPU and the GPU and memory reads from GPU memory.

Another potential optimization opportunity is the partial sort function topk() invoked in the k-NN search. ArrayFire uses NVIDIA’s CUB\(^3\) library to implement partial sort. CUB is a collection of highly optimized parallel primitives and is being used by other popular libraries such as Thrust\(^4\). ArrayFire’s topk() function divides the input array into equal sized sub-array and then calls CUB’s parallel radix sort function to sort each sub-array. It then extracts the top-k elements from each sub-array and concatenates them into a new array. This is recursively repeated until the global top-k elements are found. Even though this implementation is well-optimized, it may not be optimal for EDM because the target k is relatively small (\(\leq 20\)).

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3 kEDM

3.1 Overview

kEDM\(^5\) is our performance-portable implementation of EDM based on the Kokkos framework. We retain the high-level design of mpEDM, but reimplement the whole application using Kokkos and optimize the bottleneck kernels (\(i.e., \)all k-nearest neighbor search and lookup). To ensure the correctness of the implementation, outputs from kEDM are validated against mpEDM as well as the reference implementation of EDM (cppEDM\(^6\)), using automated unit tests.

Prior to implementing kEDM, we have examined a number of popular performance portability frameworks. These include OpenMP, OpenACC, OpenCL and SYCL. We chose Kokkos because recent studies [3, 4, 12] have shown that it delivers portable performance on a large set of devices compared to its alternatives. In addition, it has already been adopted by multiple production applications [5, 8, 17]. SYCL and OpenMP are certainly attractive choices as they have grown rapidly over the last few years in terms of hardware coverage and delivered performance, but we still consider them immature compared to Kokkos at the point of writing this paper. Therefore, we choose Kokkos to implement kEDM.

3.2 Kokkos

Kokkos [1] is a performance portability framework developed at the Sandia National Laboratories. The aim of Kokkos is to abstract away the differences between low-level programming models such as OpenMP, CUDA and HIP, and exposes a high-level C++ programming interface to the developer. Kokkos allows developers to build cross-platform and performance-portable applications on a single codebase.

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\(^1\)https://nvlabs.github.io/cub
\(^2\)https://github.com/NVIDIA/thrust
\(^3\)https://github.com/SugiharaLab/cppEDM
\(^4\)https://github.com/keichi/kEDM
\(^5\)https://github.com/keichi/mpEDM
\(^6\)https://github.com/SugiharaLab/cppEDM
To parallelize a loop in the Kokkos programming model, the developer specifies (1) the parallel pattern, (2) computational body, and (3) execution policy of the loop. Available parallel patterns include parallel-for, parallel-reduce and parallel-scan. The computational body of a loop is given as a lambda function.

The execution policy defines how a loop is executed. For example, RangePolicy defines a simple 1D range of indices. TeamPolicy and TeamThreadRange are used to launch teams of threads to exploit the hierarchical parallelism of the hardware. For example, on a GPU, teams and threads map to hardware threads within thread blocks and cores. On a CPU, teams map to physical cores and threads map to hardware threads within cores. TeamPolicy gives access to team-private and thread-private scratch memory, an abstraction of shared memory in GPUs. Each execution policy is bound to an execution space, an abstraction of where the code runs.

The latest release of Kokkos supports Serial, OpenMP, OpenMP Target, CUDA, HIP, Pthread, HPX and SYCL as execution spaces. Views are fundamental data types in Kokkos that represent homogeneous multidimensional arrays. Views are explicitly allocated by the user and deallocated automatically by Kokkos using reference counting. Each view is associated to a memory space, an abstraction of where the data resides.

Listing 1 shows a vector addition kernel implemented in Kokkos. In this example, a parallel-for loop is launched that iterates over the iD range [1, N]. Listing 2 shows a matrix vector multiplication kernel leveraging hierarchical parallelism. The outer parallel-for loop launches M teams that each computes one row of the output vector y. The inner parallel-reduce computes the dot product between one row in A and x.

### Listing 1: Basic data parallel loop

```cpp
Kokkos::parallel_for(RangePolicy<ExecSpace>(N),

KOKKOS_LAMBDA(int i) {
  y(i) = a * x(i) + y(i);
});
```

### Listing 2: Hierarchical data parallel loop

```cpp
parallel_for(TeamPolicy<ExecSpace>(M, AUTO),

KOKKOS_LAMBDA(const member_type &member) {
  int i = member.team_rank();
  float sum = 0.0f;
  parallel_reduce(TeamThreadRange(member, N),

  [=] (int j, float &tmp) {
    tmp += A(i, j) * x(j)
  }, sum);
  single(PerTeam(member),

  [=] () {
    y(i) = sum;
  });
});
```

3.3 **All k-Nearest Neighbor Search**

We implement the all k-NN search using an exhaustive approach similar to [7]. That is, we first calculate the pairwise distances between all embedded library points in the state space and obtain a pairwise distance matrix. Subsequently, each row of the obtained distance matrix is partially sorted to find the distances and indices of the top-k closest points.

#### 3.3.1 Pairwise distances

As discussed in Section 2.2, storing the time-delayed embeddings in memory and then calculating the pairwise distances is inefficient since it increases memory access. Instead, we simultaneously perform the time delayed embedding and distance calculation.

Algorithm 1 shows the pairwise distance calculation algorithm in kEDM. Using Kokkos’ TeamPolicy and TeamThreadRange, we map the outer-most i-loop to thread teams and the j-loop to threads within a team. A consideration on CPU is which loop to vectorize. Since the inner-most k-loop is short ($E \leq 20$) in our use case, vectorizing it is not profitable. We therefore use Kokkos’ SIMD types\(^1\) to vectorize the j-loop. SIMD types are short vector with overloaded operators that map to intrinsic functions. SIMD types are mapped to scalars on GPUs and do not impose any overhead.

To increase the degree of parallelism and reuse of precomputed distance and index matrices, we implement batched lookups. That

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\(^1\)https://github.com/Kokkos/simd-math
is, we perform the lookups for multiple target time series in parallel. CCM requires the library time series to be embedded in the optimal embedding dimension of the target time series. Therefore, we first group the target time series by their optimal embedding dimensions and then perform multiple lookups for target time series that have the same optimal embedding dimension in parallel.

Algorithm 3 shows our lookup algorithm. The outer most i-loop iterates over all time series of which optimal embedding dimension is E. The loop is parallelized using TeamPolicy, where each team performs prediction of one target time series. The j-loop is parallelized using TeamThreadRange, where each thread makes a prediction for each time point within a time series. The inner most serial k-loop is unrolled to increase instruction-level parallelism. Since Kokkos currently lacks a feature to indicate loop unrolling, we use the #pragma unroll directive here. The loop body requires indirect access to the target time series using the indices table. To speed up random memory access, we cache the target time series in team-private scratch memory.

Algorithm 3: Lookup

| Input: Array of target time series y, top-k distance matrix Dk and index matrix Ik computed from the library time series |
| Output: Array of predicted time series y |
| // TeamPolicy |

```plaintext
parallel for i ← 1 to N do |
    // TeamThreadRange |
    parallel for j ← 1 to L do |
        y(i, j) ← 0 |
        for k ← 1 to E + 1 do |
            y(i, j) ← y(i, j) + Dk(j, k) * y(Ik(j, k)) |
        end |
    end |
end |
```

In case the raw prediction is unneeded but only the assessment of the predictive skill is needed, kEDM does not write out the predicted time series to global memory. Instead, Pearson’s correlation is computed on-the-fly. Kokkos’ custom reduction feature is used to implement parallel calculation of the correlation coefficient. The algorithm is based on a numerically stable algorithm for computing covariance proposed in [15].

4 EVALUATION

In this section, we compare kEDM with mpEDM using micro benchmarks and real-world datasets. Furthermore, we conduct a roofline analysis of kEDM to assess the efficiency of our implementation.

4.1 Evaluation Environment

We evaluated kEDM on two compute servers installed at the Salk Institute: Ika and Aori. Ika is equipped with two sockets of 20-core Intel Xeon Gold 6148 CPUs, one NVIDIA V100 PCIe card and 384 GiB of DDR4 RAM. Aori is equipped with two sockets of 64-core AMD EPYC 7742 CPUs and 1 TiB of DDR4 RAM. kEDM was built with Kokkos 3.2 on both machines. On Aori, we used the AMD Optimizing C/C++ Compiler (AOCC) 2.2.0, a fork of Clang by AMD. On Ika, we used the NVIDIA CUDA Compiler (NVCC) 10.1.

4.2 Micro Benchmarks

We implemented micro benchmarks to measure the performance of the individual kernels we described in Section 3 and compare it with that of mpEDM.

Figure 2 shows the runtime of the all k-NN search kernel of kEDM and mpEDM on NVIDIA V100. Here, we generated a synthetic time series with \(10^4\) time steps and varied the embedding dimension. The results indicate that the pairwise distance calculation in kEDM is significantly faster than mpEDM (up to 6.6×). This is because the time-delayed embedding is performed during the distance calculation on the GPU. The partial sort is also faster than mpEDM if \(E\) is small (6.2× faster if \(E = 1\)). However, kEDM’s partial sort performance degrades as \(E\) increases and slightly under-performs mpEDM when \(E = 20\). Since the local priority queues are stored in shared memory, increasing the capacity of the local queues increases shared memory usage and results in lower multiprocessor occupancy. We confirmed this fact using NVIDIA’s Nsight Compute profiler. Figure 3 shows the runtime on AMD EPYC 7742. kEDM exhibits identical performance as mpEDM on EPYC 7742.

Figures 4 and 5 show the runtime of the lookup kernel (without cross correlation calculation) on V100 and EPYC 7742, respectively. Here, we generated \(10^5\) synthetic target time series each having \(10^4\) time steps and performed lookups from a library time series with the same length. Note that we only executed kEDM on V100 since mpEDM lacks a lookup kernel for GPU as described earlier in Section 2.2.2. These plots indicate that kEDM on V100 consistently outperforms EPYC 7742 by a factor of 3–4×. Interestingly, kEDM slightly outperforms mpEDM on EPYC as well. This might attribute to the fact that we load the target time series to scratch memory before performing lookups. Even though CPUs do not have user-manageable memory as opposed to GPUs, accessing the target time series might have loaded the time series on cache and improved the cache hit ratio.

In Figure 6, we show the runtime of the covariance calculation kernel on both platforms. Here, we generated 1000 synthetic time series with the same length. Note that we only executed kEDM on V100 since mpEDM lacks a covariance calculation kernel for GPU as described earlier in Section 2.2. We can observe that kEDM consistently outperforms mpEDM on V100 by a factor of 2–3×. However, mpEDM outperforms kEDM on EPYC by a factor of 2×. This is because the cycle-accurate simulation of the CPU is not as accurate as the simulation of the GPU. In the future, we plan to improve the accuracy of cycle-accurate simulation of GPUs to improve the accuracy of the benchmarks.

Figures 7 and 8 show the runtime of the cross correlation calculation kernel on both platforms. Here, we generated 1000 synthetic time series with the same length. Note that we only executed kEDM on V100 since mpEDM lacks a cross correlation calculation kernel for GPU as described earlier in Section 2.2. We can observe that kEDM consistently outperforms mpEDM on V100 by a factor of 1.5–2×. However, mpEDM outperforms kEDM on EPYC by a factor of 2×. This is because the cycle-accurate simulation of the CPU is not as accurate as the simulation of the GPU. In the future, we plan to improve the accuracy of cycle-accurate simulation of GPUs to improve the accuracy of the benchmarks.

Figure 9 shows the runtime of the assessment kernel on both platforms. Here, we generated 1000 synthetic time series with the same length. Note that we only executed kEDM on V100 since mpEDM lacks an assessment kernel for GPU as described earlier in Section 2.2. We can observe that kEDM consistently outperforms mpEDM on V100 by a factor of 1.5–2×. However, mpEDM outperforms kEDM on EPYC by a factor of 2×. This is because the cycle-accurate simulation of the CPU is not as accurate as the simulation of the GPU. In the future, we plan to improve the accuracy of cycle-accurate simulation of GPUs to improve the accuracy of the benchmarks.
4.3 Real-world Datasets

We prepared six real-world datasets with diverse number and length of time series that reflect the variety of use cases. We then measured the runtime of kEDN for completing pairwise CCM calculations.

Table 1 shows the runtime for performing a pairwise CCM on each dataset. Fish1_Normo is a subset of 154 representative neurons of the dominant default zebrafish larva neuronal behaviors collected by lightsheet microscopy of fish transgenic with nuclear localized GCAMP6f, a calcium indicator. Fly80XY is a drosophila melanogaster whole brain lightfield microscopy GCAMP6 recording, where distinct brain areas were identified by independent component analysis with the fly left right and forward walking speed behaviors collected on a styrofoam ball. Genes_MEF contains the gene expression profiles of all genes and small RNAs from mouse embryo fibrobast genes over 96 time steps of two cycles of serum induction and starvation stimulation. Subject6 and Subject11 are whole brain lightsheep microscopy GCAMP6f recordings at whole brain scale and single neuron resolution of larval zebrafish. F1 is a subset of a larval zebrafish biochemically induced seizure recording with three phases: control conditions, pre-seizure and full seizure.

The results clearly demonstrate that kEDM outperforms mpEDM in most cases. In particular, kEDM shows significantly higher (up to $5.5 \times$) performance than mpEDM on NVIDIA Tesla V100 and Intel Xeon Gold 6148. This performance gain is obtained from the optimized $k$-nearest neighbor search and GPU-enabled lookup.

4.4 Efficiency

To assess the efficiency of our implementation, we conducted a roofline analysis [23] of our kernels. The compute and memory ceilings on each platform were measured using the Empirical Roofline Toolkit (ERT)\(^8\) 1.1.0. Since ERT fails to measure the L1 cache bandwidth on GPUs, we used the theoretical peak performance instead. We followed the methodology presented in [24] to measure the arithmetic intensity and the attained FLOP/s. Nvprof 10.1 and likwid [20] 5.0.1 were used to collect the required metrics on GPU and

\(^8\)https://bitbucket.org/berkeleylab/cs-roofline-toolkit
Table 1: Benchmark of CCM runtime using real-world datasets

| Dataset       | # of Time Series | # of Time Steps | V100 & Xeon 6148 | EPYC 7742 |
|---------------|-----------------|----------------|------------------|-----------|
| Fish1_Normo  | 154             | 1,600          | 3s               | 11s       |
|               |                 |                | 3.67x            |           |
| Fly80XY       | 82              | 10,608         | 11s              | 50s       |
|               |                 |                | 4.55x            |           |
| Genes_MEF    | 45,318          | 96             | 344s             | 334s      |
|               |                 |                | 0.97x            |           |
| Subject6     | 92,538          | 3,780          | 22s              | 30s       |
|               |                 |                | 1.36x            |           |
| Subject11    | 101,729         | 8,528          | 96s              | 139s      |
|               |                 |                | 1.45x            |           |
| F1            | 8,520           | 29,484         | 12,145s          | 11,571s   |
|               |                 |                | 0.95x            |           |

Figure 6: Roofline analysis of pairwise distance kernel on V100 ($L = 10^4$)

Figure 7: Roofline analysis of pairwise distance kernel on EPYC 7742 ($L = 10^4$)

Figure 8: Roofline analysis of lookup kernel on V100 ($L = 10^4$, $N = 10^5$)

Overall, these roofline models indicate that kEDM operates close to the ceilings and achieves high efficiency in most cases. Furthermore, the roofline models reveal that EDM is an inherently memory-bound algorithm, primarily bounded by memory or cache.
bandwidth depending on the embedding dimension. It does not enter the compute-bound region of the roofline model in our use cases. This observation suggests that kEDM would benefit from hardware with higher memory, cache, and load/store unit bandwidth.

5 CONCLUSION & FUTURE WORK
We designed and developed kEDM, a performance portable implementation of EDM using the Kokkos performance portability framework. The new implementation is based on a single codebase and runs on both CPUs and GPUs. Furthermore, we removed several several inefficiencies from mpEDM and custom-tailored kernels. Benchmarks using real-world datasets indicate up to 5.5x speedup in convergent cross mapping computation.

In the future, we will implement a Python binding to facilitate adoption by users. We are also planning to evaluate on other hardware platforms such as AMD GPUs and Fujitsu A64FX ARM processors.

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