ABSTRACT

Performance tools for emerging heterogeneous exascale platforms must address two principal challenges when analyzing execution measurements. First, measurement of large-scale executions may record mountains of performance data. Second, performance measurements for parallel programs are sparse in two ways: the set of metrics present for any context and the set of contexts present in different threads. For GPU-accelerated applications, an important source of sparsity is that none of the myriad of GPU metrics apply to any of the many CPU contexts. To address these challenges, we developed a novel streaming aggregation approach to postmortem analysis that employs both shared and distributed memory parallelism to aggregate sparse performance measurements from every rank, thread, and GPU stream of an application, and attributes heterogeneous call path profiles and traces to source code. Using the same amount of resources, our approach analyzes large-scale performance measurements of GPU-accelerated applications over an order of magnitude faster than HPCToolkit and its sparse analysis results are as much as three orders of magnitude smaller than HPCToolkit’s dense representation of metrics.

CCS CONCEPTS
• General and reference → Performance; • Computing methodologies → Shared memory algorithms; Distributed algorithms.

KEYWORDS
performance, parallelism

1 INTRODUCTION

Emerging exascale compute platforms pose significant challenges for performance tools. Applications may have performance problems that only become apparent at very large scales, thus performance tools must support measurement and analysis at scale. For applications running on tens of thousands of compute nodes equipped with multicore processors, performance tools may record gigabytes of measurement data per second. Analysis of measurement data becomes more expensive as data volume grows.

Performance measurements for parallel programs are naturally sparse in two ways: the set of metrics present for any context and the set of contexts present in different threads. Metric sparsity can be very significant. For instance, on systems with GPU-accelerated compute nodes, such as the US DOE’s emerging exascale supercomputers, metrics for GPU code are disjoint from those for CPU code. When both CPU and GPU metrics are collected for an application, none of the myriad of GPU metrics apply to any of the many CPU contexts. Context sparsity may also be significant. Threads with different roles typically execute different code in different calling contexts. For tools to efficiently measure and analyze code performance on heterogeneous exascale systems, sparse metrics and contexts must be handled efficiently throughout tool workflows.

In this paper, we present an approach to address the aforementioned challenges: a novel, highly-parallel strategy for postmortem analysis that uses sparse formats and out-of-core methods to analyze performance data. Our approach is particularly effective for analyzing large-scale measurements of GPU-accelerated applications because of their extreme metric sparsity. We implement these methods in HPCToolkit-SA - a tool derived from the open-source HPCToolkit performance tools [22]. HPCToolkit-SA aggregates call path profiles and traces from every CPU thread and GPU stream in the application and associates them with detailed heterogeneous calling contexts that include inlined functions, loops, and calls to device functions within GPU kernels. It does so in a way that is scalable and efficient in both time and space. This paper makes the following contributions:

• it describes HPCToolkit-SA’s novel sparse formats for measurement data and analysis results, designed to accelerate key access patterns for postmortem analysis, presentation, and data analytics;
• it outlines HPCToolkit-SA’s novel, highly-parallel streaming aggregation approach to postmortem analysis, which

\[1\] For example, Riken’s Fugaku supercomputer has 158,976 nodes, each equipped with 48 compute cores [18].
employs both shared and distributed memory parallelism, concurrent data structures, and efficient algorithms to rapidly analyze sparse measurements; and
• it evaluates the effectiveness of HPCToolkit-SA’s approach in terms of storage volume and analysis time.

In our case studies analyzing measurement data for GPU-accelerated executions, HPCToolkit-SA’s use of sparse formats instead of dense ones yielded as much as an order of magnitude reduction in the size of measurement data and three orders of magnitude reduction in the size of analysis results. Our analysis algorithm is capable of processing measurements from tens of thousands of application threads and GPU streams in minutes, using only a small fraction of the resources consumed by the application itself. These results show the promise of our design for analyzing performance data from extreme scale executions.

The remainder of the paper is organized as follows. Section 2 overviews approaches used by other performance tools in this space, with particular focus on scalability. Section 3 describes HPCToolkit-SA’s novel approach to postmortem analysis based on sparse formats and a highly-parallel analysis algorithm. Section 4 provides an empirical analysis of HPCToolkit-SA’s postmortem analysis workflow, comparing against similar open-source postmortem analysis tools. Section 5 summarizes our conclusions.

2 RELATED WORK

Performance tools supporting GPU-accelerated applications differ widely in their approach to large-scale applications and in the level of detail they provide.

Some tools, such as NVIDIA’s Nsight Systems [17] and Extrae [7], rely on traces of an application’s execution. For long-running applications traces become huge and thus extremely slow to analyze, which limits the scalability of these tools. Although HPCToolkit-SA analyzes traces when present, our work focuses on the harder problem of aggregating a set of per-thread or per-GPU-stream call path profiles.

Some tools reduce the performance data volume by eliding details at scale, this includes Intel’s VTune Profiler [9], ARM MAP [6], and ScalaTrace [15]. VTune only provides summary statistics for MPI, I/O, GPU and CPU performance. MAP retains a limited (1000 by default) number of samples for each application thread or GPU stream. ScalaTrace compresses MPI traces by recognizing repetitive structure within and across traces. Details of problems that arise at large scales may be elided by these approaches. Also, without detailed performance attribution, the causes behind issues become unnecessarily difficult to recover. The work in this paper feasibly includes complete performance data for each application thread.

Tools based on the Score-P [11] measurement infrastructure exploit a single dimension of sparsity using the CUBE data format [21], this includes Scalasca [23], TAU [20], and Vampir [10]. In our experiments in Section 4.1.1 we find that for GPU-accelerated programs two dimensions of performance data are highly sparse, exploiting only one is insufficient at scale. Our sparse profile formats exploit both dimensions of sparsity for significant space reductions.

HPCToolkit [22] attributes performance to complete heterogeneous calling contexts spanning both GPU and CPU code. Figure 1 shows the calling contexts surrounding a GPU kernel launch, lines above the highlighted line indicate the host-side launch site while lines below show a loop and in-lined function calls within a device-side kernel. Some tools only attribute GPU performance at the kernel-launch level, this includes Score-P [11], Scalasca [23], and TAU [20]. Other tools, such as Intel’s VTune [9] and NVIDIA’s Nsight Compute [16] only support “flat” line-level attribution on the device side. According to David Richards (LLNL), Mercury [12]–a next-generation, general-purpose radiation transport code–has O(100K) lines of code in a single kernel; the causes of performance losses in such a code can’t be fully understood without detailed attribution within an kernel. HPCToolkit-SA supports detailed attribution of metrics within GPU kernels by using HPCToolkit’s measurement infrastructure to collect performance data.

Finally, many tools do not use parallelism past a single compute node in their postmortem performance analysis phases, this includes NVIDIA’s NSight Systems [17], Intel’s VTune Profiler [9], TAU [20] and Vampir [10]. Extrae [7] provides an MPI-based merger that integrates a collection of traces into a single Paraver trace file. Scalasca’s Scout [23] uses MPI-OpenMP parallelism to assemble profile results as

Figure 1: A segment of a heterogeneous call path containing functions, loops, and inline code on both CPU and GPU.
dense blocks of metrics in the CUBE format. HPCToolkit’s hpcprof-mpi [3] uses pure-MPI parallelism to integrate multiple performance profiles into a dense tensor indexed by application thread, calling context, and metric. Our highly-parallel analysis approach uses both thread-level and process-level parallelism to perform postmortem performance analysis, producing a compact sparse representation.

3 APPROACH
To address the challenge of analyzing very large profiles (and optionally traces) for large-scale executions on either homogeneous (CPU) or heterogeneous (CPU+GPU) scalable parallel systems, we created HPCToolkit-SA. HPCToolkit-SA differs from the open-source implementation of HPCToolkit for GPU-accelerated systems [22] in two key ways: it uses novel sparse representations for performance data and it uses a novel streaming aggregation approach for highly-parallel postmortem analysis of large, sparse performance measurement data. Section 3.1 describes the design of HPCToolkit-SA’s sparse representations. Section 3.2 presents HPCToolkit-SA’s streaming aggregation approach.

3.1 Sparse Formats for Performance Data
Applications running on tens of thousands of compute nodes can generate gigabytes of measurement data per second. Unsurprisingly, postmortem analysis of large measurement data also produces large analysis results. For GPU-accelerated programs, metrics are numerous and very sparse. The sparsity appears in two ways: metrics and contexts. Below, we list a few factors that contribute to metric and context sparsity for GPU-accelerated programs.

- Metrics accumulate within expensive leaf functions; often distant calling context ancestors representing high-level functions will have no exclusive metrics.
- Many metrics apply only to instructions or code regions executed on a particular compute device, such as stall metrics for GPU instructions (12 kinds on NVIDIA GPUs) or CPU metrics for work, resource utilization, or waste.
- Some metrics apply only to very specific contexts such as GPU kernels (e.g., GPU utilization, block count) or GPU data movement operations (e.g., copy costs in bytes and time).
- Threads with different roles (e.g., main thread, OpenMP worker thread, GPU progress thread, MPI I/O helper thread) typically execute different code in different calling contexts. After postmortem analysis, threads will have zero-valued metrics for contexts only present in other threads.

![Figure 2: HPCToolkit-SA’s sparse format for measurement data.](image)

The number of metrics affected by these kinds of sparsity is large in practice, for instance our measurements of GPU-accelerated programs described later in Section 4 use a single CPU metric but 62 GPU metrics. As part of the postmortem analysis, most of these exclusive metrics are augmented with inclusive metric costs and may be inputs to derived metrics. None of the many GPU metrics apply to any CPU context, which are typically more numerous than GPU contexts.

We combat the increase in data volume by exploiting these two kinds of sparsity with a series of new sparse formats. In addition to lower space requirements, data accesses need to be efficient to ensure the performance of postmortem analysis and responsiveness of a graphical browser for analysis results. Therefore, a guarantee of efficient data accesses is a requirement of these new formats.

Our solution was inspired by the Compressed Sparse Row (CSR) format for sparse matrices [8]. Section 3.1.1 describes our sparse format for measurement data. Section 3.1.2 describes our two sparse formats for analysis results.

3.1.1 Sparse Measurement Format. HPCToolkit profiles each CPU thread and GPU stream of an application, storing the per-thread profiles in separate measurement files. Each measurement file includes a representation of the calling context tree observed in that thread or stream. HPCToolkit stores metric values collected exclusively for each calling context in a dense vector stored as part of the calling context tree node. In contrast, HPCToolkit-SA’s measurement subsystem stores metric values in a separate region of a measurement file using the format shown in Fig. 2 and described below.

The left side of Fig. 2 shows a dense matrix storing metric values for all metrics and all calling contexts. Each element of this matrix is the metric value $v$ measured for a metric $m$ in a calling context $c$. Our sparse format is shown on the right, consisting of an $(m, v)$ vector listing non-zero metric values and a $(c, i)$ vector mapping contexts to contiguous ranges of the $(m, v)$ vector. The $(c, i)$ vector is sorted by $c$ and the $(m, v)$ vector by $m$ within each contiguous context range. These two sorts enable the use of binary search to access the data for an individual context or metric.

\[ (m, v) : \begin{bmatrix} (1, 5) & (0, 2) & (2, 6) & (1, 3) \\ (c, i) : \begin{bmatrix} (0, 0) & (1, 1) & (3, 3) & (7, 4) \end{bmatrix} \end{bmatrix} \]

$^2$For example, GPU utilization = $\frac{\text{measured GPU PC samples}}{\text{expected GPU PC samples across all threads}}$

$^i$ is the index of the first $(m, v)$ associated with a calling context $c$. The end of $c$’s range directly precedes the following $i$ or ending $\text{T, T}$ sentinel.
This format takes advantage of both kinds of sparsity present in this measurement matrix. First, “empty” calling contexts with all zero metric values are elided from the \((c, i)\) vector. Second, zeros in the metric values for any context are elided from the \((m, v)\) vector. In short, we exploit both row-wise and column-wise sparsity within this matrix.

Let \(\mathcal{V}, \mathcal{M}\) and \(C\) be the number of non-zero metric values, metrics and non-empty calling contexts respectively. The space cost of our sparse format is \(O(\mathcal{V} + C)\). In \((m, v)\), referencing the start of the range for a calling context \(c\) can be done in \(O(\log C)\) time with a binary search, while accessing a specific value takes another \(O(\log M)\) time binary search within the mapped range.

### 3.1.2 Sparse Analysis Result Formats

A browser interactively exploring performance analysis results requires efficient access to metrics both within a single profile and for selected contexts across multiple profiles. For instance, a developer may investigate the performance of an individual CPU thread across all calling contexts, or check for load imbalance across threads within a particular calling context. Today, HPCToolkit outputs one dense result file for each CPU thread and each GPU stream. This is acceptable for the first scenario but not the second, as a browser would need to read a single value from each of thousands of files, each of which may be quite large.

To support efficient access for both use cases while reducing space requirements, for HPCToolkit-SA we developed two formats for these two use cases, respectively: Profile Major Sparse (PMS) format and Context Major Sparse (CMS) format. Each format contains the entirety of the analysis results in a single file to avoid large numbers of files. Their main difference is in the order in which the performance data is stored, allowing readers to read the file best suited for their use case. Figure 3 shows a high-level visualization of these formats. For brevity we only detail the PMS format, CMS is similar with dimensions transposed as shown in Fig. 3.

Our PMS format consists of \(\mathcal{P}\) “planes” of data each representing the analysis results for a single profile \(p\). Each plane contains results for every calling context \(c\) and metric \(m\) for that profile in the CSR-like format shown in Fig. 2, which exploits both metric and context sparsity. Planes are referenced by byte offset in a \(\mathcal{P}\)-sized “table of contents” header, allowing planes to appear in the file in any order. Since every profile generally has at least one non-zero analysis result, we do not need to use a sparse representation for this mapping.

Let \(\mathcal{V}, \mathcal{M}\) and \(C\) be the number of non-zero values, metrics and non-empty calling contexts respectively, averaged across all \(\mathcal{P}\) profiles. The space cost of our PMS format is \(O(\mathcal{P}(\mathcal{V} + C))\). The plane for any particular profile can be obtained from the “table of contents” in \(O(1)\) time. Then as noted before, the range for a particular context can be referenced in \(O(\log C)\) time and any specific value in an additional \(O(\log M)\) time using binary search. Similar algorithms with transposed dimensions can be used in the CMS format to access the data for an individual context and metric in logarithmic time. In total, our PMS and CMS formats provide efficient access to all analysis results while exploiting sparsity to compress the contained performance data.

### 3.2 Streaming Aggregation

We require an efficient approach to correlate and aggregate data measured from thousands of application threads or GPU streams. We divide the postmortem analysis performed by HPCToolkit-SA into three classes based on common dataflow properties: class 1 analyses are produced for each performance profile of a single CPU thread or GPU stream, while class 2 analyses correlate and class 3 analyses aggregate data from multiple profiles. Specifically, HPCToolkit-SA produces the following analyses:

- (Class 1) Inclusive and exclusive cost metrics for every calling context within a single thread or stream,
- (Class 1) Execution traces of each thread or stream, composed of a sequence of samples containing a timestamp and calling context,
- (Class 2) Unified source-level calling context tree, in which each node represents a unique call path observed at runtime,
- (Class 2) Unified source files and application binaries, in which each node represents a unique source file or binary used by the application, and
- (Class 3) Inclusive and exclusive cost statistics for every calling context and metric, summarizing the full application execution.

To produce these analyses, HPCToolkit-SA employs a novel thread-parallel approach we call streaming aggregation to process performance data, described in Section 3.2.1. This approach provides excellent performance and makes use of
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Per-Profile (Class 1) Output

Input Profiles

Concurrent Data Structures

Correlated/Aggregated (Class 2/3) Output

Figure 4: Conceptual diagram of the streaming aggregation thread-parallel approach, discussed in Section 3.2.1. Numbered blocks indicate operations of the numbered class, as defined in Section 3.2.

shared-memory algorithms to provide better efficiency than a purely MPI-based approach. For scalability, HPCToolkit-SA also uses conventional distributed-memory parallelism across multiple compute nodes in a hybrid approach, described in Section 3.2.2. Finally, in Sections 3.2.3 and 3.2.4 we detail the parallelizations we chose for a selection of the algorithms required for producing our analysis.

3.2.1 Thread-level Parallelism. To analyze performance data from large-scale executions, our thread-parallel streaming aggregation approach exploits formal properties of the three classes of analyses HPCToolkit-SA produces. First, since class 1 analyses are produced for every input performance profile, much of their processing is independent of other profiles and can be performed in parallel. Second, class 2 and 3 analyses do not enforce any particular order, they are associative, commutative, and class 2 analyses are also idempotent.

Figure 4 shows the conceptual layout of our streaming aggregation approach. Class 1 analyses are performed using conventional embarrassing parallelism, each thread reads and processes data from an input profile and writes the class 1 analysis results directly to the output before moving on to the next profile. This design means class 1 data does not reside in memory for the lifetime of the analysis, in our approach class 1 data effectively "streams" from the input profiles to the output analysis results.

This design also means that producing class 2 and 3 analyses requires communication across the threads. Since class 2/3 analyses can be freely reordered, we implemented this communication as a series of shared concurrent data structures where the result of every operation integrates a class 2/3 datum. This design means only the class 2/3 analysis results reside in memory, "aggregated" from the data parsed from each input profile. Conventionally this aggregation would be done using reduction phases, our decision to use concurrent data structures was informed by the preliminary experiment described later in Section 4.2.1, which finds that this use of shared concurrent data structures significantly outperforms conventional reduction-based approaches.

Class 2 analyses differ from class 3 analyses in that class 2 analyses are required to output class 1 analyses, while class 1 analyses are aggregated to form class 3 analyses. An important class 2 example is calling context identifiers, which must be unique to each calling context but consistent across profiles. To support these cases we perform class 2 analyses as early as possible, for instance we assign identifiers exactly when a new, unique calling context has been added to the shared data structures. These class 2 analyses are not allowed to change afterward, thus providing the consistency across profiles while retaining the high degree of parallelism afforded by our thread-parallel approach.

3.2.2 Process-level Parallelism. To exploit multiple compute nodes for portmortem analysis, we use more conventional distributed-memory parallelism implemented with MPI. Each

Correlated/Aggregated (Class 2/3 Output)

Figure 5: Conceptual diagram of our process-parallel approach, discussed in Section 3.2.2. Each of the n ranks use t threads. Numbered blocks indicate instances of streaming aggregation limited to the numbered classes of operations.
MPI rank in this approach uses our thread-parallel streaming aggregation approach to efficiently use the threads available on each compute node.

This hybrid MPI+SA approach is depicted conceptually in Fig. 5. Since class 2 analysis is required for correct class 1 output from each rank, we reduce and distribute class 2 analysis results prior to performing class 1 analysis on any rank. A similar reduction is done at the end of execution to aggregate class 3 data. Class 1 data is never communicated across ranks, instead every rank writes out class 1 data to disk in parallel as discussed in Section 3.2.1. This allows our hybrid MPI+SA approach to retain the same "streaming" qualities of standard streaming aggregation, using MPI communication only during the "aggregation" across multiple ranks.

Both reductions in our hybrid approach are implemented using conventional reduction trees, however unlike a pure-MPI reduction tree we process the reduction inputs in parallel at every rank, using the thread-level parallelism afforded by streaming aggregation. In this case a $t$-ary reduction tree has minimal depth and an optimally short critical path, where $t$ is the number of threads available in each rank. Thus for our hybrid approach we use $t$-ary reduction trees for the two reductions, which reduces to a single-round reduction when $t$ is larger than the number of ranks. By using only two reductions in our MPI+SA hybrid approach, we retain much of the parallelism provided by our base streaming aggregation approach.

3.2.3 Generating Source-level Calling Context. HPCToolkit’s measurement infrastructure records observed calling contexts as the addresses of individual instructions encountered during a call stack unwind, specifically as byte offsets within application binaries. To provide useful performance analysis, HPCToolkit-SA expands these instruction-level contexts into source-level (lexical) calling context, including functions, inlined function calls, nested loops and source lines, as shown in Fig. 6. For simplicity, we perform this expansion for every context read for a profile, creating only the expanded sequence of contexts shown on the right of the figure in the shared context tree.

In this design, each context present in a profile requires a lookup in the source-level mappings available for an application binary, which can be obtained from DWARF debugging information or pre-calculated with HPCToolkit’s hpcstruct tool. We parse both of these formats serially, which for large binaries may cause unwanted serialization. To combat this, we aggregate application binaries from profiles first, and eagerly load source mappings for every new binary found. After the first thread observes a binary, other threads do not wait for these mappings to be loaded until they require it for a calling context expansion later, and wait using a fine-grained atomic flag. Since application binaries will often be identical across threads and MPI ranks within an execution, this is generally an effective way to parse the source mappings of multiple binaries in parallel.

3.2.4 Parallel Output to a Shared File. As described in Section 3.1, all class 1 analysis results reside in two files in our PMS and CMS formats. To prevent this from causing undue serialization, our PMS format does not require a particular order for the profiles. This allows us to use a shared atomic counter to "allocate" space in the PMS output immediately before writing a profile's class 1 analysis results to disk, when extended for MPI this counter is shared across ranks$^4$.

We generate our CMS format in a separate phase after our PMS output is complete, pre-calculating the location of every calling context’s data before copying and transposing blocks of data in parallel. Each thread in this phase uses a heap to efficiently sort the PMS data in context-major order without checking every profile, since each profile is in context-major order in our PMS format this heap is only as large as the number of profiles. This design allows this additional phase to take up very little total time in HPCToolkit-SA and avoid becoming a significant performance bottleneck.

$^4$We found that MPI one-sided communication introduced significant latency for this case, we avoided this by using a dedicated "server" thread.
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System Properties:
Theta[4]: Intel Knight’s Landing Architecture
4 threads/core, 64 cores/node
Lustre file system, peak 6 GiB/s
Perlmutter[14]: AMD EPYC 7763 + NVIDIA Ampere A100
2 threads/core, 64 cores/node, 4 GPUs/node
All-flash Lustre file system, aggregate 5 TiB/s

Analysis Tool Launch Parameters:
Theta[4]:
Scalasca Same threads/ranks as application
HPCToolkit 1 thread/rank, 128 ranks/node
HPCToolkit-SA 128 threads/rank, 1 rank/node
Perlmutter[14]:
HPCToolkit 1 thread/rank, 63 ranks/node
HPCToolkit-SA 63 threads/rank, 1 rank/node

AMG2013[1] Execution Parameters (Theta[4]):
Metrics 1 CPU metric
AMG 8K 8192 threads, 64 nodes, 0:22 runtime
AMG 16K 16384 threads, 128 nodes, 0:23 runtime
AMG 65K 65536 threads, 512 nodes, 0:32 runtime
AMG 262K 262144 threads, 1024 nodes, 0:57 runtime

LAMMPS[19] Execution Parameters (Perlmutter[14]):
Metrics 1 CPU metric + 62 GPU metrics
LAMMPS 1K 512 threads + 512 GPUs, 128 nodes, 4:40 runtime
LAMMPS 4K 2048 threads + 2048 GPUs, 512 nodes, 6:30 runtime

PeleC[2] Execution Parameters (Perlmutter[14]):
Metrics 1 CPU metric + 62 GPU metrics
PeleC 1K 512 threads + 512 GPUs, 128 nodes, 1:24 runtime
PeleC 4K 2048 threads + 2048 GPUs, 512 nodes, 0:48 runtime

Table 1: Properties and parameters used to generate the named series of input performance data sets. All data sets include both per-thread/GPU profiles and execution traces.

4 EXPERIMENTAL RESULTS

To evaluate the benefits of our novel approach to performance analysis, we compared HPCToolkit-SA’s space requirements and analysis time against Scalasca’s Scout [23] and HPCToolkit’s hpcprof-mpi [3], two postmortem performance analysis tools exploiting multi-node parallelism.

The system and launch parameters used for our experiments are listed in Table 1. To provide inputs for the tools, we collected performance measurements from short runs of AMG2013[1], LAMMPS[19] and PeleC[2] on the Theta[4] supercomputer at Argonne National Laboratory and Perlmutter[14] at the National Energy Research Scientific Computing Center. These measurement data sets include both execution profiles and traces, and are run up to moderate scales for the systems. In particular, the two 4K data sets are from executions taking up approximately a third of NERSC’s Perlmutter [14] supercomputer, an allocation of similar size to the entirety of Argonne’s Polaris[5] supercomputer.

The launch parameters used for the analysis tools in our experiments are designed to provide consistent compute power across tools within their individual limitations. Scalasca’s Scout can only be run with the same parameters as the application. HPCToolkit’s hpcprof-mpi uses a single thread per MPI rank, we maximize its number of ranks per node. HPCToolkit-SA uses both thread-based and MPI-based parallelism, for consistency we use the same number of threads per node as base HPCToolkit.

In the rest of the section, Section 4.1 evaluates the sparsity of current profiles and shows the benefits of our sparse storage formats. Section 4.2 shows the performance and scalability of our streaming aggregation approach.

4.1 Evaluation of Sparse Formats

Very sparse data recorded in a dense format wastes storage. Section 4.1.1 shows the benefits of our sparse formats and that the density of non-zero values in analysis results is often lower than 1%. Section 4.1.2 compares the storage requirements for HPCToolkit-SA against those for HPCToolkit and Scalasca.

4.1.1 Sparsity Case Studies. Table 2 presents density statistics and size comparisons for a selection of the experiments discussed in Section 4. The upper half presents statistics for the measurement data, and the lower half presents statistics for the analysis results.

For each application, the first density column lists the percentage of calling contexts with at least one non-zero metric value. The second density column lists the percentage of non-zero metric values per calling context on average. These values are then averaged across all profiles in the dataset. These two density columns demonstrate the high sparsity of performance data in both the context and metric dimensions.

5AMG2013 is a CPU-based parallel algebraic multi-grid solver for linear systems implemented using hybrid MPI/OpenMP.
6LAMMPS is a CPU and GPU-based parallel molecular dynamics simulation implemented using hybrid MPI/OpenMP/CUDA.
7PeleC is a GPU-based code for parallel adaptive-mesh compressible hydrodynamics implemented using hybrid MPI/CUDA.
we observed at most a
we do not need to collect many metrics before the sparsity be-
to the unification of calling contexts across threads, along
format, which includes additional derived metric values for
metric sparsity, thus this table only compares performance
data sets, less than 2.3% of the contexts are not empty, and for
each context on average, less than 1.4% of the metric values
are not zero. Pruning insignificant calling contexts will not
suffice to mitigate this degree of sparsity. Our PMS format
provides a reduction ratio of up to 6003
in dense format to
with the addition of lexical contexts such as source lines,
inlined functions and nested loops. In all of the considered
data sets, less than 2.3% of the contexts are not empty, and for
each context on average, less than 1.4% of the metric values
are not zero. Pruning insignificant calling contexts will not
suffice to mitigate this degree of sparsity. Our PMS format
provides a reduction ratio of up to 6003× (AMG2013 [1] with
7 CPU metrics) by exploiting both kinds of sparsity in the
performance analysis results.

4.1.2 Storage Comparisons. Table 3 compares the storage re-
quirements for measurement data including traces and analy-
sis results among Scalasca, HPCToolkit, and our HPCToolkit-
SA. This comparison illustrates the benefits of our sparse
formats in practice.

To show the actual storage requirements in practice, Ta-
ble 3 lists the size of all data. For each application and config-
uration pair, the first column lists the size of measurement
data (In), which this time, includes traces. The second col-
umn lists the size of analysis results (Out). In this column,
our sparse formats include both PMS and CMS output files,
and execution traces as well.

Scalasca [23] outputs much larger measurement data than
current HPCToolkit [3] and uses much more resources, de-
tailed in Section 4.2.2. Therefore, Table 3 focuses on compar-
ing HPCToolkit and HPCToolkit-SA’s sparse formats.

Table 2: Case study of measurement data excluding traces and analysis results collected by HPCToolkit.

| Application | Density (%) | Size       |
|-------------|-------------|------------|
|              | Measurement data (In) |              |
|             | Contexts | Metrics | Dense (MiB) | Sparse (MiB) |
| AMG 8K      | 69.1      | 100.0    | 103.1       | 139.3       |
| AMG 4K‡     | 22.7      | 20.7     | 458.7       | 217.4       |
| LAMMPS 1K   | 17.7      | 1.8      | 4207.1      | 371.5       |
| PeleC 1K    | 15.8      | 2.0      | 8988.5      | 778.9       |
| Analysis results (Out) |              | (GiB) | (GiB) |
| AMG 8K      | 0.301     | 0.182    | 20.6        | 0.1146      |
| AMG 4K‡     | 0.059     | 0.017    | 1227.5      | 0.2094      |
| LAMMPS 1K   | 2.360     | 1.390    | 262.5       | 0.6495      |
| PeleC 1K    | 0.599     | 0.635    | 2736.1      | 1.8197      |

‡This is a modified version of the data set with 7 CPU metrics.
‡Sparse analysis results in PMS format only.

Table 3: Comparing sizes of measurement data including traces (In) and analysis results (Out).

| Tool          | Size (GiB) |
|---------------|------------|
|               | AMG 8K In  | AMG 8K Out |
| Scalasca [23] | 647        | 1.41       |
| HPC Toolkit   | 0.538      | 9.23       |
| HPC Toolkit-SA| 0.591      | 3.376      |
|               | AMG 16K In  | AMG 16K Out |
| Scalasca [23] | 1310       | 2.87       |
| HPC Toolkit   | 1.19       | 25.1       |
| HPC Toolkit-SA| 1.09       | 25.1       |

|               | LAMMPS 1K In  | LAMMPS 1K Out |
| HPC Toolkit   | 12.3        | 375         |
| HPC Toolkit-SA| 4.42        | 5.19        |
|               |              |              |
| HPC Toolkit   | 76.5        | 2790        |
| HPC Toolkit-SA| 32.1        | 35.6        |

|               | PeleC 1K In  | PeleC 1K Out |
| HPC Toolkit   | 21.2        | 4800        |
| HPC Toolkit-SA| 2.85        | 5.27        |
|               |              |              |
| HPC Toolkit   | 50.7        | 14300       |
| HPC Toolkit-SA| 4.8         | 11.4        |
Table 4: Comparison of different techniques for unifying 32 calling context trees in parallel with 32 threads.

| Technique               | Phase 1 | Phase 2 | Total |
|-------------------------|---------|---------|-------|
| OpenMP Reduction        | 195.1   | 197.6   | 392.7 |
| Tree Reduction          | 183.8   | 66.9    | 250.7 |
| Shared, Intel’s TBB     | 691.9   | –       | 691.9 |
| Shared, Read-Write Locks| 72.1    | –       | 72.1  |

For AMG2013 [1] with only one CPU metric, HPCToolkit’s dense format for measurement data (In) is slightly smaller than HPCToolkit-SA’s full-sparse representation. In this case, there isn’t sufficient sparsity to offset the size of the indices used in the sparse format. When GPU metrics are present, such as for LAMMPS [19] and PeleC [2], HPCToolkit-SA’s full-sparse representation of measurement data is significantly smaller.

For analysis results (Out), HPCToolkit-SA’s full-sparse representation is consistently much smaller than HPCToolkit’s dense format. Including execution traces as well as PMS and CMS output files, with PeleC [2] 4K, we observed as much as a 1254× reduction in the size of HPCToolkit-SA’s sparse results format compared to HPCToolkit’s dense one.

4.2 Evaluation of Streaming Aggregation

Efficiently using the available compute resources for postmortem performance analysis is required for scalable performance tools. Section 4.2.1 shows the benefits of our streaming aggregation approach to thread-based parallelism over more conventional approaches, using a microbenchmark on a smaller related problem. Section 4.2.2 compares the performance of our complete HPCToolkit-SA tool with other parallel postmortem analysis tools.

4.2.1 Performance Benefits of Streaming Aggregation. As discussed in Section 3.2, HPCToolkit-SA correlates and aggregates results from multiple profiles into a single analysis result. The conventional approach for parallel aggregation is to use a separate reduction phase, however we discovered that using shared concurrent data structures instead could provide significantly improved performance. We determined this with a proxy experiment that correlated calling context trees from 32 application threads in parallel using a variety of techniques. The results from our experiment are listed in Table 4. The resulting context tree in each case is made up of context nodes, each containing a hash table to maintain pointers to their child context nodes.

The first two techniques listed in the table use two phases, an embarrassingly parallel phase and a reduction phase. The reduction phase in the first technique is provided by an OpenMP reduction clause, in the second an explicit reduction tree across the threads is used. The latter two techniques use a single parallel phase where all threads insert into a single shared concurrent calling context tree. The third technique uses concurrent hash tables from Intel’s Threaded Building Blocks library in each context node, the fourth and final technique uses simple hash tables in each context node, each table protected by a unique POSIX reader-writer lock.8

Our main takeaway from Table 4 is that using shared concurrent data structures can have significantly better performance than conventional reduction-based approaches. By removing the reduction phase from the critical path we improve our parallel performance significantly. And we also improve the serial performance in each thread by removing the memory allocations for partial results required by a reduction-based approach. To achieve this performance improvement the concurrent data structures must be chosen with care, in our case contention on child hash tables is low enough that the highly dynamic concurrency provided by Intel’s TBB actually degrades the overall performance.

4.2.2 Performance of HPCToolkit-SA. Table 5 compares the performance and scalability of our streaming aggregation approach against the Scout trace analysis tool from Scalasca [23] and the hpcprof-mpi profile and trace analysis tool provided by HPCToolkit [3]. As noted in Section 2 these tools are among the few that make use of parallelism in their postmortem analysis, making them reasonable choices for comparison of parallel postmortem analysis tools.

Of these tools, Scalasca’s Scout is the most expensive, taking as much as 50× as much node-time as the application execution. This is in part because it processes much larger function enter-exit traces, unlike HPCToolkit and HPCToolkit-SA which process smaller performance profiles and sample-based execution traces. Scalasca also cannot run using less compute resources than the application itself, making it impractical for all but small-scale executions.

HPCToolkit and HPCToolkit-SA allow the number of threads to be configured, for consistency we configured both with the same number of active hardware threads. In all configurations and inputs, HPCToolkit-SA completes well before HPCToolkit’s pure-MPI hpcprof-mpi using the same number of hardware threads. HPCToolkit-SA is as much as 41× faster. HPCToolkit also required as many as 16× more compute nodes than HPCToolkit-SA due to its large memory

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8Insertions are performed as follows: first the parent calling context’s lock is acquired in read mode and the requested child is looked up in the children table. If present, the requested child is returned immediately, otherwise the lock is reacquired in write mode and the new child is inserted and returned.
footprint. Because of this, we have observed a node-time reductions of as much as 927× with HPCToolkit-SA for PeleC 1K on 63 threads.

Finally, an important benefit of HPCToolkit-SA is its significantly reduced compute resource requirements compared to the application. We have observed HPCToolkit-SA analyzing performance data from 512 nodes in almost 3 minutes using a single compute node, and as much as 1050× less node-time than the application itself. This ability to perform analysis using a fraction of the compute resources for the application is critical for performance analysis of increasingly large scale executions.

5 CONCLUSIONS AND FUTURE WORK

Our new HPCToolkit-SA postmortem analysis tool shows the promise of our novel approach to analyzing performance data from extreme-scale executions. Use of sparse formats in HPCToolkit-SA reduces its space usage by as much as three orders of magnitude compared to similar dense formats. By efficiently using a fraction of the compute resources for the application, HPCToolkit-SA is able to analyze and attribute performance measurements gathered on approximately a third of NERSC’s Perlmutter [14] supercomputer in mere minutes. These results outperform the current state-of-the-art in both Scalasca [23] and HPC-Toolkit [3]. Compared to base HPCToolkit, HPCToolkit-SA uses as much as 1254× less space for storing analysis results and generates detailed performance analysis results using 927× less node-time.

The main discoveries behind HPCToolkit-SA’s significant improvements are not specific to HPCToolkit. The causes for sparsity listed in Section 3.1 which cause the widespread sparsity quantified in Section 4.1 are general properties of all performance profiles and tools. The extreme sparsity in call path profiles for GPU-accelerated applications with both operation-level metrics for kernels and data copies as well as detailed attribution of instruction-level metrics within GPU kernels highlight the shortcomings of prior approaches that don’t exploit sparsity. The high performance of our streaming aggregation approach as described in Section 3.2 and evaluated in Section 4.2 is a general trait of the problem of aggregating performance profiles. These discoveries are critically important to any performance analysis tool intending to support applications running at full scale on forthcoming exascale machines.

We plan to investigate further performance improvements for HPCToolkit-SA. On conventional distributed file systems, writing a large number of files in one directory from many compute nodes in parallel significantly degrades I/O performance, the metadata server in these infrastructures is commonly a bottleneck. As exascale testbeds become available at larger scale, we plan to assess the impact of emerging file system abstractions such as DAOS [13] to better understand how they might be used to accelerate the I/O associated with HPCToolkit-SA’s performance measurement and analysis workflows.

We also plan to investigate alternative approaches to MPI-based parallelism in combination with our streaming aggregation approach. Currently, the conventional MPI-based reductions used in HPCToolkit-SA cause significant idleness in threads across all MPI ranks. Alternative approaches with better integration with streaming aggregation may provide even better performance and increased scalability.
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