VELOC: VEry Low Overhead Checkpointing in the Age of Exascale

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ABSTRACT
Checkpointing large amounts of related data concurrently to stable storage is a common I/O pattern of many HPC applications. However, such a pattern frequently leads to I/O bottlenecks that lead to poor scalability and performance. As modern HPC infrastructures continue to evolve, there is a growing gap between compute capacity vs. I/O capabilities. Furthermore, the storage hierarchy is becoming increasingly heterogeneous: in addition to parallel file systems, it comprises burst buffers, key-value stores, deep memory hierarchies at node level, etc. In this context, state of art is insufficient to deal with the diversity of vendor APIs, performance and persistency characteristics. This extended abstract presents an overview of VeloC (Very Low Overhead Checkpointing System), a checkpointing runtime specifically design to address these challenges for the next generation Exascale HPC applications and systems. VeloC offers a simple API at user level, while employing an advanced multi-level resilience strategy that transparently optimizes the performance and scalability of checkpointing by leveraging heterogeneous storage.

KEYWORDS
HPC, checkpoint-restart, state preservation, resilience

1 INTRODUCTION
High performance computing (HPC) applications produce massive amounts of checkpointing data during their runtime, which is often used for defensive purposes, i.e. to employ a checkpoint-restart resilience strategy in case of failures. In addition, the increasing convergence between HPC, big data analytics and artificial intelligence prompted many new scenarios for checkpointing, both productive (e.g., algorithms that revisit previous intermediate results, coupling of workflow components, introspection to understand the evolution of a computation or data), and administrative (e.g., out-of-core computations, co-scheduling of batch jobs and on-demand jobs using suspend-resume).

Checkpointing in the context of HPC is a challenging I/O pattern, because the data coming from a large number of distributed processes typically is coordinated to form a globally consistent state. This generates high write concurrency that overwhelms the I/O bandwidth of the system, leading to large performance overheads and poor scalability. In the quest to reach Exascale, many architectural trade-offs are necessary, including a high degree of parallelism and a growing gap between the compute capacity and I/O capabilities, which means less I/O bandwidth will be available per compute unit, thereby making checkpointing even more challenging.

To avoid this issue, many applications have switched from writing checkpoints directly to an external storage repository (e.g. a parallel file system) to more advanced approaches, such as multi-level checkpointing. The idea is to use the faster and less reliable local storage of the compute nodes (or that of neighboring nodes) to implement "lighter" resilience levels that hold the checkpoints. This enables applications to survive a majority of failures without interacting with an external storage repository, thereby conserving the scarce I/O bandwidth.

Despite promising potential, multi-level checkpointing as implemented by state of art are not sufficient at Exascale and many challenges remain. First, the storage stack is increasingly heterogeneous both regarding compute nodes (deep memory hierarchies combined with local storage) and external repositories (burst buffers, key-value stores, parallel file systems). Therefore, it is increasingly difficult to design optimal I/O and resilience strategies that can take advantage of all storage options simultaneously. Second, in a quest to differentiate from competition, vendors propose storage solutions with different performance/resilience characteristics and custom APIs. Therefore, it is important to solve the problem of portability for both I/O and resilience. Third, performance and scalability requirements have prompted a transition from blocking to asynchronous strategies (i.e., block the application only while writing to the fastest level, while performing the rest of the operations in the background). However, background operations may compete with the application for resources, generating runtime interference that is not well understood and needs to be minimized through mitigation strategies.

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This extended abstract proposes VELOC, a low overhead checkpointing system that is part of the Exascale Computing Project (ECP) and aims to build a production-ready solution that is specifically designed to address the challenges mentioned above. For the rest of this paper, we briefly introduce the main features of VELOC and discuss several recent results.

2 VELOC: AN OVERVIEW

Hidden Complexity of Heterogeneous Storage. To address the challenge of complexity due to heterogeneous storage, we propose a simple API that enables each application process to declare "critical" memory regions that need to be part of a global checkpoint. When a global checkpoint needs to be taken, all processes call a collective checkpointing primitive that handles all details transparently. Using this approach, users never have to worry what types of storage are available and how to use them. Furthermore, the separation between fine-grained declarations of critical memory regions and the actual checkpoint request opens several optimization opportunities compared with writing the critical data directly to a local storage device or external repository, such as: optimized serialization, fine-grain allocation and movement of checkpoint chunks between different types of storage based on memory layout and access patterns, synergies between resilience strategies, etc. For example, recent work enables VELOC to take advantage of heterogeneous node-local storage to minimize the duration of blocking for asynchronous flushing to an external repository. In this case, there are non-obvious producer-consumer patterns that form under I/O concurrency, for which using the fastest storage may be suboptimal [4].

Optimized Asynchronous Multi-Level Strategies. We propose an advanced multi-level approach that is based on the idea of leveraging idle resources in order to advance the asynchronous checkpointing strategies in the background without causing significant interference. To this end, we envision two possible complementary approaches. First, if the behavior of the application is predictable (which is the case of many iterative HPC applications that naturally exhibit a repetitive behavior), then the background operations can be scheduled in such a way that they use different resources than those needed by the application at a given moment. To this end, machine learning techniques based on sequence-to-sequence models are a promising tool in predicting the application behavior [6]. Second, the background operations can be scheduled such that they run with lower priority. In this case, the operating system will reduce contention by giving the application a large time slice at the expense of making the background operations less predictable. To this end, performance modeling using micro-benchmarks focused on interference patterns can be used to control the priority.

ML-Optimized Checkpoint Intervals. The combination of asynchronous techniques that leverage heterogeneous storage makes it very difficult if not impossible to determine an optimal checkpoint interval analytically (due to sheer complexity) or by simulation of the failure scenarios (due to a large number of parameters that result in a massive number of failure scenarios). Under such circumstances, a promising direction is the use of machine learning to reduce the search space of the simulation-based approaches. Specifically, by sampling a subset of representative failure scenarios, the aim is to train a ML model that is capable of filling the missing gaps in the search space in order to predict the optimal checkpoint interval with high accuracy. In this regard, preliminary work [1] shows that models based on neural networks can be particularly effective for this task, outperforming other approaches such as random forest.

Flexibility through Modular Design. We propose a modular design that encapsulates each I/O and resilience strategy as an independent module that is part of a pipeline. Whenever a checkpoint request is issued, the pipeline will trigger each module one after another based on a pre-defined priority. Each module is individually responsible to react to a checkpoint request and can do so (or simply pass) based on its own internal state (e.g. optimal checkpoint interval) and/or the outcome of the other modules invoked earlier in the pipeline. Using this approach, a module can be activated or deactivated at runtime as needed using a simple switch. Furthermore, custom modules can be easily added in the pipeline (e.g., conversion between output formats, compression, integrity checks based on checksumming) and control when they are triggered by customizing their priority with respect to the other modules. The pipeline is managed by an engine that can run it either synchronously (in which case the engine is linked into the application directly as a library) or asynchronously (in which case the engine lives is a separate process called the active backend). This is illustrated in Figure 1.

3 PRODUCTIVE CHECKPOINTING: THE CASE FOR DEEP LEARNING

As mentioned in Section 1, productive use case of checkpointing make it a valuable tool in the design of new algorithms and approaches that revisit previous states. At the intersection of HPC and deep learning, systematic approaches such as guided model
discovery and sensitivity analysis illustrate the need to capture intermediate snapshots of the DNN model in order to study its evolution in time and potentially reuse it later.

For example, outlier detection is critical for evaluating, curating, and using biomedical data sets used to train DNN models. In this case, approaches such as [7] build deep learning ensembles and workflows to construct a system for automatically identifying data subsets that have a large impact on the trained models. Specifically, the goal is to evaluate many training variations with and without considering subsets of the training samples. However, these training variations need not be trained independently from scratch, they can share a common training path up until a point when they begin to diverge. Therefore, the model can be checkpointed and replicated in order to be able to branch off in different directions, which greatly speeds up the exploration.

Our work on DeepFreeze [3] illustrates DNN checkpointing techniques based on the idea of augmenting the execution graph with fine-grain tensor copy operations, which can run in parallel with gradient computations and weight updates involving different layers during the back-propagation. Using this approach, a full checkpoint of the DNN model can be produced in-memory or on local storage with minimal impact on the learning performance, which can then be again transferred asynchronously to the memory of a different GPU and/or remotely to a different compute node. This can be further improved with techniques such as DeepClone [5]: the augmentation techniques for the execution graph during the back-propagation can be extended with additional techniques such as zero-copy transfers of tensors and optimized reconstruction that efficiently replicates a DNN model in the memory of remote nodes without involving stable storage. Furthermore such techniques can take advantage of already existing replicas that are naturally produced by large-scale data-parallel training techniques.

Such considerations have inspired new data models such as data states [2], which are intermediate snapshots of datasets (e.g., DNN models) that can be either captured or cloned asynchronously at scale, while making them discoverable and accessible a lineage, making it easy to navigate through their evolution and/or search for interesting snapshots that can be reused.

4 EXASCALE ECOSYSTEM

VELOC is developed as part of the Exascale Computing Project (ECP) and is designed as a production-ready multi-level asynchronous checkpointing solution based on the features mentioned above. Currently, it serves several ECP applications, including HACC, LatticeQCD and EXAALT.

It is in use and regularly tested on several pre-Exascale testbeds, including Theta (4392 Intel Xeon Phi KNL nodes, peak: 11.69 PFLOPS), Summit (9126 POWER9 CPUs, 27648 NVIDIA Tesla V100 GPUs, peak: 200 PFLOPS peak), Sierra (architecture similar to Summit, peak: 135 PFLOPS). Other platforms where VELOC is currently being evaluated include Frontera (8008 Intel Xeon nodes, peak: 38.7 PFLOPS) and Fugaku (158976 ARM64 nodes, peak: 442 PFLOPS).

A recent run on Summit at full scale for the HACC application achieved an I/O throughput of up to 224 TB/s for writing local in-memory checkpoints in a blocking fashion, while generating a negligible runtime overhead for flushing the local checkpoints to a Lustre parallel file system in the background.

We aim to integrate VELOC with alternative external storage repositories that complement parallel file systems. Notably, a recent effort has targeted DAOS, a scalable object storage system developed by Intel. To this end, we developed an experimental module that leverages an optimized low-level put/get API for key-value pairs.

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