ElasticBroker: Combining HPC with Cloud to Provide Realtime Insights into Simulations

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Abstract. For large-scale scientific simulations, it is expensive to store raw simulation results to perform post-analysis. To minimize expensive I/O, “in-situ” analysis is often used, where analysis applications are tightly coupled with scientific simulations and can access and process the simulation results in memory. Increasingly, scientific domains employ Big Data approaches to analyze simulations for scientific discoveries. However, it remains a challenge to organize, transform, and transport data at scale between the two semantically different ecosystems (HPC and Cloud systems). In an effort to address these challenges, we design and implement the ElasticBroker software framework, which bridges HPC and Cloud applications to form an “in-situ” scientific workflow. Instead of writing simulation results to parallel file systems, ElasticBroker performs data filtering, aggregation, and format conversions to close the gap between an HPC ecosystem and a distinct Cloud ecosystem. To achieve this goal, ElasticBroker reorganizes simulation snapshots into continuous data streams and send them to the Cloud. In the Cloud, we deploy a distributed stream processing service to perform online data analysis. In our experiments, we use ElasticBroker to setup and execute a cross-ecosystem scientific workflow, which consists of a parallel computational fluid dynamics (CFD) simulation running on a supercomputer, and a parallel dynamic mode decomposition (DMD) analysis application running in a Cloud computing platform. Our results show that running scientific workflows consisting of decoupled HPC and Big Data jobs in their native environments with ElasticBroker, can achieve high quality of service, good scalability, and provide high-quality analytics for ongoing simulations.

Keywords: HPC, cloud computing, in-situ data analysis, scientific workflows.

1 Introduction

HPC and Big Data ecosystems are significantly different from each other, and are designed and manufactured for their own purposes, respectively. In the HPC
world, systems are designed for faster execution of large-scale parallel programs. Hundreds of thousands of processes run across a large number of compute nodes. Those compute nodes are high-end servers equipped with many CPU cores and large-size memories, and are tightly connected by fast interconnects such as InfiniBand. Simple and minimal operating system kernels and software stacks are used in those computer nodes for efficient operation. Often, the low-level, highly portable and efficient message-passing parallel programming model (MPI) is used, such that processes in different address spaces can work collaboratively and talk with each other through point-to-point or collective communications.

Big Data is a totally different world, where applications are designed to collect, process, and analyze large amounts of data to gain knowledge. Software in a Big Data ecosystem such as Apache Spark or Hadoop can use the high-level MapReduce programming model to execute data analysis jobs on clusters of commodity machines. More recently, cloud computing technologies such as container and service-oriented architecture have further hidden the complexity of parallel software packages, and have made Big Data platforms more accessible to developers. Overall, the general architecture and design commonly found in Big Data ecosystems, help users process and analyze data at large scale affordably and reliably. More details of the comparison between the HPC and Big Data ecosystems have been discussed and presented by Reed and Dongarra.

In practice, many scientific computing applications not only have long execution time, but also generate “big” amounts of data. For instance, peta-bytes of data may be generated from a single run of a scientific simulation. The generated data is traditionally stored in a parallel file system, then copied to another site, and read again by different analysis applications for further investigation or exploration. Such a data storage/movement/post-analysis pattern can be extremely expensive, and hence there is an inevitable trend to pursue in-situ data analysis, where analysis applications can continuously process and analyze the in-memory data structures while the simulation applications are running.

However, existing in-situ analysis frameworks often run in the scope of HPC ecosystem. The main problem is that almost all data analytics and machine learning (ML) applications have been written using Big Data programming languages and libraries (e.g., Python, Scala, MapReduce, Spark, etc.), and are often deployed to Cloud computing platforms. In addition, these data analytics or ML software and tools have already been widely accepted by the Big Data community, and fully tested on Cloud platforms/services such as Apache Spark or Google Dataflow. Hence, the question is: can a system be designed that can run scientific workflows which consist of both native HPC and Big Data applications? Since it is almost impossible to port all data analytics/ML libraries from the Big Data ecosystem to the HPC ecosystem (or vice versa), we strive to bridge the gap and integrate HPC with Cloud environments, so that we may utilize the elastic services and native software in the Cloud to analyze HPC simulations efficiently.

There are several challenges to achieve the goal. Firstly, the data formats between HPC systems and Cloud services are usually different. It is a non-
trivial task to offload data from HPC simulations to Cloud applications, and apply necessary data transformations correctly and efficiently. Also, the bandwidth between HPC and Cloud systems is limited, and bridging services between the two ecosystems must be carefully designed to minimize the data transmission overhead. Furthermore, the mapping between simulation processes and data analysis processes should be optimized to minimize data flow stalls. To tackle those challenges, we present ElasticBroker, which bridges the ecosystems of HPC and Cloud. When MPI-based HPC applications are linked with the ElasticBroker library, the simulation data will be transformed to Cloud-native data objects and continuously streamed to the data analysis services deployed in Cloud systems, where the data objects together with scheme information are organized and analyzed.

To showcase our system, we develop a real-world cross-ecosystem scientific workflow, which has:

– a parallel MPI-based computational fluid dynamics (CFD) simulation running in HPC, and
– a distributed online Dynamic Mode Decomposition (DMD) application using stream processing service deployed in Cloud.

We build and execute this workflow on the IU Karst HPC [7] and XSEDE Jetstream Cloud systems[8,9]. From the experimental results, we observe that by linking CFD applications with ElasticBroker, we can effectively migrate the simulation data from HPC system, and by using the remote Cloud analysis services, we can provide in-time insights into the ongoing fluid dynamics.

2 Background

In this section, we first introduce Cloud-based stream processing. Then, we present the background knowledge of Dynamic Mode Decomposition, which is an analysis method we have deployed in our Cloud-based stream processing service.

2.1 Cloud-based stream processing data analytics

Nowadays it has become common that data is generated continuously over time. For example, sensor data generated from IoT devices or web logs are produced from multiple sources and can accumulate everyday. Instead of storing the data and doing post-processing in future, stream processing can be used to give real-time insights of the data. The advantage of being “real-time” is essential in various scenarios such as online fraud detection and emergency handling, where it can help early decision-making.

In stream processing, “unbounded” datasets (or “data streams”) are used as input. New data records are continuously added to those data streams, where they can be analyzed on the fly. Popular stream processing frameworks (e.g., Apache Kafka [10], Flink [11], Storm [12], and Spark Streaming [13]) have been extensively used in different areas to provide in-time analytics for various data...
sources. Popular Cloud providers now offer data analytics as a service (e.g., Google DataProc [14], Amazon Kinesis Streams [15]), so that users can interact with the service using their favorite programming languages regardless of platform infrastructure.

In the case of computational fluid dynamics (CFD) in the HPC domain, the simulations can run over days or even months. Analysis of data generated while the simulation is in progress can help scientists discover patterns and understand behaviors, which they would otherwise have to wait till the simulation finishes. In this work, we explicitly utilize the convenience and advantages of Cloud-based stream processing to provide timely insights to the running simulations.

2.2 Dynamic Mode Decomposition

In fluid dynamics, the flow fields are organized in a complex, high-dimensional dynamical system. It is well known that important flow features can be recognized through visual inspections of the flow, even when there are perturbations and variations [16]. This means that some coherent structures exist in the fluid fields, which contain useful dynamical information of the fluids and can help researchers understand the patterns/behaviors of the fluid flows. To mathematically extract those coherent structures from such dynamical systems, modal analysis techniques, such as Dynamic Mode Decomposition analysis (DMD [17]), are often used. Specifically, DMD analysis relies solely on snapshots (or measurements) of a given system, and provides the spatial-temporal decomposition of those data into a set of dynamical modes [18]. Since DMD is data-driven and doesn’t need to model the governing equations of the fluids, it is considered as an “equation-free” and “data-driven” method. Traditionally, DMD analysis has been used to study fluid structures from dynamic flow geometries [19]. In this work, we use DMD as an analysis example, and show how it can be deployed in the Cloud as a part of the distributed stream processing service, to analyze CFD simulations at real time.

3 Methodology

In this section, we present the design of our software framework and the decisions we have made to solve the challenges of offloading analytical tasks to Cloud systems from the running simulations. The ElasticBroker framework contains two major components:

1. A C/C++ brokering library in HPC, which transforms data from a simulation-domain format to a Cloud-compatible format.
2. A distributed stream processing analysis service deployed in Cloud.

Between HPC and Cloud, data is converted from the simulation by ElasticBroker, and then transferred to the distributed stream processing analysis service using available inter-site bandwidth.
3.1 HPC components

On the HPC side, commonly used I/O libraries, such as MPI-IO [20] and ADIOS [21], provide interfaces to output simulation data to the file system. We provide a similar interface for HPC applications so that it is easy for existing simulation code to adapt to the ElasticBroker services, as shown in Listing 1.1.

In Listing 1.1, a Cloud service consists of several endpoints. Each of them is specified using service_ip and service_port. The broker_init function initializes the connections between HPC and Cloud by registering data fields from the simulation with remote Cloud service endpoints. Those data fields are differentiated by the field_name variable in the API, such as “pressure” or “velocity_x”. We divide the MPI processes in a simulation into groups (using group_id), so that processes in one group will register themselves with one corresponding Cloud endpoint for future writes, as shown in Figure 1. During the main iterations of the simulation, the broker_write function is called iteratively, to transform field data from the simulation process into stream records, which are sent to the Cloud endpoint that process has connected to. Each stream record contains the time-step information and the serialized field data of the simulation process. In the Cloud, stream records received from all endpoints will be indexed, aggregated and partitioned by the stream processing service, which will be discussed in Section 3.2.

Listing 1.1: The ElasticBroker C/C++ API used by HPC applications.

```c
struct CloudEndpoint{
    char* service_ip;
    int service_port;
};

// A Cloud service can provide several endpoints
struct CloudEndpoint endpoints[NUMGROUPS];

// Initialize the broker service, by connecting each MPI
// process with one of the Cloud endpoints.
broker_ctx* broker_init(char* field_name, int group_id);

// Write a chunk of in-memory data (void* data) to the broker.
broker_write(broker_ctx* context, int step, void* data, size_t data_len);

// Finalize the broker services
broker_finalize(broker_ctx* context);
```

Dividing HPC processes into groups enables us to assign each group to a designated Cloud endpoint for achieving a higher data transfer rate, as shown in Figure 1. Process groups also provide a higher degree of flexibility. Users can decide how many endpoints are necessary based on the outbound bandwidth of each HPC node and inbound bandwidth of each Cloud endpoint.
3.2 Cloud-based data analysis components

In this subsection, we will first introduce how we setup the Cloud stream processing service, and then describe how different components in the Cloud service work together to provide insights to the incoming streamed simulation data.

**Preparation** We choose Spark Streaming [13] as our stream processing engine, which supports scalable, high-throughput, fault-tolerant stream processing of live data streams. By utilizing the core Spark functionality, we can apply basic operations such as map, reduce, filter, join, and advanced algorithms using Spark Machine Learning and Graph Processing libraries to data streams. Currently, we deploy our Spark cluster and Cloud endpoints within a Kubernetes cluster in the Jetstream Cloud. As a popular container orchestration system, Kubernetes provides an abstraction layer above different Cloud providers [22]. This way our stream processing setup can be easily reproduced with different Cloud providers like Google Cloud Platform or Amazon AWS.

Figure 2 shows the overall layout of such Cloud settings. Currently we use Redis server instances as our Cloud endpoints. Redis, which is an in-memory data structure store, is used to accept data streams from the HPC components. We use spark-redis connector [23] to let the Redis instances forward structured data to Spark stream processing services deployed in Cloud. All Redis instances export TCP port 6379 to the outside of the Cloud system. All of our Cloud services (Spark stream processing engine and Redis server instances) are containerized and are scheduled using Kubernetes’s native scheduling, which makes it easy to adapt to different Cloud providers. Specifically, a Spark-executor container is comprised of the Python-based DMD analysis library PyDMD [24], and related Scala software packages such as spark-redis. More details about the software we use in the Cloud services are provided in Section 4. We create and manage the Kubernetes cluster from a “gateway” VM (virtual machine) in Jetstream Cloud, using the Magnum Openstack Plugin [25]. After the cluster is set up, we use the
spark-submit command from the gateway VM, to launch the Spark-executor containers to the Kubernetes cluster.

Fig. 2: The deployment of our Cloud components. Each Redis-server container acts as an endpoint, and exposes the same TCP port to outside. The Spark-executor containers will read available data streams from Redis-server containers. All containers are scheduled in the Kubernetes cluster deployed in Jetstream, and use the in-cluster network to communicate with each other.

Data Processing in Cloud When data is aggregated from different endpoints, Spark-executors will read records from data streams sent by all MPI processes. Fluid data (snapshots) from different simulation processes are added to the separate data streams over time. Figure 3 shows how data records in one data stream are aggregated as Spark “Dataframes”, which are then processed by analysis code.

Fig. 3: Data processing in the Cloud. Each MPI process sends data through a data stream, then unbounded data in each data stream is re-arranged into micro-batches (aka Spark Dataframes). Micro-batches from multiple data streams are treated as partitions of one Resilient Distributed Dataset (RDD). The rdd.pipe function then sends each partition to the external Python script exactly once.

We let Spark manage the scheduling and parallelism, so that multiple executors can be mapped to different data streams and process the incoming data concurrently. We use the rdd.pipe function in Spark to send Dataframe data from the main Spark context to external programs (in our case the Python interpreter). This operation happens concurrently with all data streams, thanks to the design of Spark which enables a high degree of parallelism. The results of
all Spark-executors are then collected using the `rdd.collect` function so that they can be visualized/presented.

## 4 Experiments

We perform two sets of experiments to evaluate the performance of scientific workflows using ElasticBroker. The first set of experiments use a real-world CFD simulation running in HPC, with DMD analysis deployed in Cloud, to show workflows with ElasticBroker can achieve good end-to-end time. The second set of experiments use synthetic data generator processes in HPC and the same DMD analysis deployed in the Cloud to evaluate ElasticBroker’s throughput and quality of service at different scales.

We use IU Karst as our HPC platform, which has specifications shown in Table 1a. We deploy our Cloud analysis applications in XSEDE Jetstream Cloud [8,9], whose information is shown in Table 1b.

| Information         | Information          |
|---------------------|----------------------|
| CPU                 | VM image             |
| 2 Intel Xeon        | Fedora-Atomic-29    |
| E5-2650 v2.60 GHz CPUs |                      |
| # cores             | VM type              |
| 16 cores per node   | ml.large             |
| Main memory         | VM vCPUs             |
| 32 GB per node      | 10                   |
| Secondary storage   | VM memory            |
| 250 GB per node     | 30GB                 |
| Network             | Kubernetes version   |
| 10-gigabit Ethernet | 1.15.7               |
| MPI                 | Spark version        |
| OpenMPI 2.1         | 2.4.5                |
| Compiler version    | Redis version        |
| GCC 5.4             | 5.0                  |
| OpenFOAM            |                      |
| v1906               |                      |

(a) Karst System

| Information         | Information          |
|---------------------|----------------------|
| VM image             | Spark version        |
| Fedora-Atomic-29    | 2.4.5                |
| VM type              | Redis version        |
| ml.large             | 5.0                  |
| VM vCPUs             |                      |
| 10                   |                      |
| VM memory            |                      |
| 30GB                 |                      |
| Kubernetes version   |                      |
| 1.15.7               |                      |
| Spark version        |                      |
| 2.4.5                |                      |
| Redis version        |                      |
| 5.0                  |                      |

(b) Jetstream System

Table 1: Hardware and software information of the IU Karst HPC system and the XSEDE Jetstream Cloud system.

### 4.1 Implementation of a cross-environment CFD scientific workflow

Our cross-environment in-situ scientific workflow has two applications: CFD simulation and DMD analysis. To implement the CFD simulation application, we use the parallel OpenFOAM software [27,28], deployed in IU Karst. In OpenFOAM, a “solver” is the simulation algorithm and a “case” describes the physical condition of the simulation problem. We choose the `simpleFoam` as our solver, which is a steady-state solver for incompressible, turbulent flow, using the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm. The simulation problem we choose to solve is the WindAroundBuildings, as shown in Figure 4. This case simulates how wind flows behave around a group of buildings in an...
urban area. To enable the in-situ workflow execution by using ElasticBroker, we need to replace the original runTime().write function in the simpleFoam solver with our broker_write function. We divide the simulation problem domain into different processes along the Z (height) axis. The velocity fields of each process region are sent out through the broker, and will be analyzed by the stream processing service deployed in the Jetstream Cloud.

The analysis application reads data streams from HPC processes through the Cloud endpoints described in Section 3.1. Figure 4 shows the visualization results of DMD analysis on 16 data streams received by 1 Cloud endpoints. Each subplot corresponds to the fluid data sent from one simulation MPI process, and shows how the fluid dynamics change over time for this process region. This figure can inform users how stable the fluids in each process region is, while the simulation is running.

4.2 End-to-end workflow time

One concern of using in-situ processing is that it can slow down simulation applications, increasing the overall end-to-end time of the workflow. Traditionally, simulation applications write simulation output to parallel file systems. The stored files can be used for future post-analysis. Such file-based I/O is usually expensive, and can also potentially slow down the primary simulation applications. To investigate how the simulation application and the combined workflow (with Cloud-based DMD analysis) can be affected by different I/O methods, we configure the simpleFoam solver (with 16 processes) in three different modes:

1. File-based: simulation output data is written to parallel Lustre file system using the “collated” write provided in OpenFOAM.
2. ElasticBroker: simulation output data is sent to Cloud endpoints, using the proposed ElasticBroker API.
3. Simulation-only: The simulation runs with data write disabled.
Fig. 5: Analysis results of eigenvalues of DMD low-rank operator from each process region's output. Each subplot shows the average sum of square distances from eigenvalues to the unit circle of that region. Values closer to 0 mean fluids in that region are more stable.

The elapsed time of the simulation application (from simulation starts till simulation finishes) using these different modes are shown in Figure 6. In the figure, there is also an extra column: the workflow end-to-end time, which starts at the beginning of the CFD simulation and stops at the end of the DMD analysis in Cloud. We run the simulation application for 2000 time steps (using the configuration of \( \delta T = 0.2 \) and \( \text{totalTime} = 400 \) in the OpenFOAM control dictionary file). To examine how those I/O modes affect simulation applications, we use different write intervals. For example, with \( \text{interval} = 5 \), the simulation will output simulation results once every 5 timesteps.

From Figure 6 we can see that when the simulation application is configured with long write intervals (e.g. \( \text{write\_interval} = 20 \)), simulation time is similar in different I/O modes. However, when we increase the write frequency (e.g. \( \text{write\_interval} = 5 \)), the file-based method makes the simulation application significantly slower, compared with the simulation-only baseline mode. In comparison, with ElasticBroker, simulation applications can run with only a minimal slowdown. This is due to the fact that ElasticBroker asynchronously writes in-process simulation to data streams, from each simulation process, independently. Compared with the file-based method, no shared file systems are used for output of the bulk simulation, so the simulation can run with much fewer stalls.
In the Cloud side, we configure 16 Spark-executors deployed in a Kubernetes cluster. We configure the DMD analysis to be triggered every 3 seconds for all data streams. Note that the difference between workflow end-to-end time and the ElasticBroker simulation time in Figure 6 is also around 3 seconds, which means, apart from the configured trigger time, there is no significant lag between simulation and analysis applications. In conclusion, plugging CFD simulation with ElasticBroker gives us in-time insights of the running simulation, and it doesn’t harm the performance of the simulation much.

4.3 Throughput

To better understand the performance behavior of running such workflow in the proposed system, we conduct a second set of experiments, in which we illustrate how the system scales when we are using more HPC and Cloud resources.
Differently from the previous end-to-end time experiments, which use real-world CFD software, we use a synthetic data generator in this part, to produce enough data in order to stress the system. The synthetic data generator consists of groups of MPI processes in the HPC side. Data is continuously generated from all processes and streamed to the distributed stream processing service through multiple Cloud endpoints, as we have seen in Figure 1. For larger scale simulations, we increase the number of Spark-executors and Cloud endpoints (i.e., Redis server instances) correspondingly. The ratio among MPI processes, Cloud endpoints, and Spark-executors is set as 16 : 1 : 16.

We evaluate the latency between analysis and simulations, which is from the time when simulation output data is generated, to the time when the data is analyzed by Cloud services. This metric describes the quality of service of our system, which indicates how quickly we can get insights into the running simulations. From Figure 7a, we can see the latency stays between 7 ∼ 9 seconds when using 16 ∼ 128 simulation processes. In Figure 7b which shows the aggregated throughput from all MPI processes, we can observe that when we double the number of MPI processes, the aggregated throughput also increases by around two times. Such scalability benefits from the careful mappings of MPI processes, Cloud endpoints, and Spark-executors. Specifically, MPI processes in one group always write data to a designated Redis endpoint, then the data is analyzed by a fixed subset of the Spark-executors.

5 Related work

Scientific workflows have been widely used to incorporate multiple decoupled applications running on distributed computational resources. To manage data dependencies among different applications, and correctly schedule computational tasks, workflow management systems (e.g., Pegasus [30], Kepler [31]) are used. However, these workflow systems heavily rely on file-based I/O, and only schedule coarse-grain workflow tasks in a sequential manner (i.e., a later task cannot start until all the previous tasks have exited). In the case of ElasticBroker, simulation data is streamed continuously to Cloud services, where data analysis will be conducted while the simulations continue running.

There exist several previous works that deal with different file formats in Big Data and HPC ecosystems. For instance, LABIOS [32] utilizes the label-based I/O system to bridge HPC and Big Data applications. NIOBE [33] uses I/O forwarding nodes and Burst buffer to stage data and offload the data format conversion operations. However, these conversion operations still require a shared file system or shared storage system.

Data transport libraries such as ADIOS [21], Decaf [5], and Zipper [4] do not rely on file-based communications between applications, but they most often require applications to run in an HPC ecosystem. Differently, in ElasticBroker, data can be sent from HPC applications to endpoints exposed by Cloud services, so that decoupled applications can collaborate while residing in their native environments.
6 Conclusion and future work

In this paper, we present our preliminary work that bridges the HPC and Cloud ecosystems and enables cross-system in-situ workflows. We design ElasticBroker, which provides a C/C++ library which MPI applications can be linked to. ElasticBroker can transform simulation data into stream records, and send the stream records to a distributed stream processing service deployed in Cloud. We also show how the Cloud-based stream processing service is setup, and how it partitions, processes and analyzes the stream data continuously. We use the parallel OpenFOAM simulation which runs in IU Karst, and DMD analysis which is deployed in XSEDE Jetstream to demonstrate the effectiveness of our framework. Experimental results show that extending MPI-based simulations with ElasticBroker enables stream processing services deployed in Cloud to provide in-time analysis of ongoing fluid dynamics. The experiments also show good throughput and quality of service of ElasticBroker when we increase both simulation and analysis scales.

In our future work, we plan to extend ElasticBroker to support in-situ workflows with more complex directed acyclic graphs (DAG). More advanced data aggregation functionality can be used in the HPC side so that processes may utilize the bandwidth more efficiently. Additionally, performance models can be designed to automatically decide how to distribute computation tasks of an in-situ workflow to different environments (e.g., HPC and Cloud), based upon application-specific requirements such as computation time, memory consumption, and migration cost.

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