

Pilot-Abstraction: A Valid Abstraction for Data-Intensive Applications on HPC, Hadoop and Cloud Infrastructures?

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ABSTRACT

HPC environments have traditionally been designed to meet the compute demand of scientific applications and data has only been a second order concern. With science moving toward data-driven discoveries relying more and more on correlations in data to form scientific hypotheses, the limitations of existing HPC approaches become apparent: Architectural paradigms such as the separation of storage and compute are not optimal for I/O intensive workloads (e.g. for data preparation, transformation and SQL workloads). While there are many powerful computational and analytical kernels and libraries available on HPC (e.g. for scalable linear algebra), they generally lack the usability and variety of analytical libraries found in other environments (e.g. the Apache Hadoop ecosystem). Further, there is a lack of abstractions that unify access to increasingly heterogeneous infrastructure (HPC, Hadoop, clouds) and allow reasoning about performance trade-offs in these complex environments. At the same time, the Hadoop ecosystem is evolving rapidly with new frameworks for data processing and has established itself as de-facto standard for data-intensive workloads in industry and is increasingly used to tackle scientific problems. In this paper, we explore paths to interoperability between Hadoop and HPC, examine the differences and challenges, such as the different architectural paradigms and abstractions, and investigate ways to address them. We propose the extension of the Pilot-Abstraction to Hadoop to serve as interoperability layer for allocating and managing resources across different infrastructures providing a degree of unification in the concepts and implementation of resource management across HPC, Hadoop and other infrastructures. For this purpose, we integrate Hadoop compute and data resources (i.e. YARN and HDFS) with the Pilot-Abstraction.

In-memory capabilities have been successfully deployed to enhance the performance of large-scale data analytics approaches (e.g. iterative machine learning algorithms) for which the ability to re-use data across iterations is critical. As memory naturally fits in with the Pilot concept of re-

taining resources for a set of tasks, we propose the extension of the Pilot-Abstraction to in-memory resources. These enhancements to the Pilot-Abstraction have been implemented in BigJob. Further, we validate the abstractions using experiments on cloud and HPC infrastructures investigating the performance of the Pilot-Data and Pilot-Hadoop implementation, HDFS and Lustre for Hadoop MapReduce workloads, and Pilot-Data Memory for KMeans clustering. Using Pilot-Hadoop we evaluate the performance of Stampede, a compute-centric resource, and Gordon, a resource designed for data-intensive workloads providing additional memory and flash storage. Our benchmarks of Pilot-Data Memory show a significant improvement compared to the file-based Pilot-Data for KMeans with a measured speedup of 212.

1. INTRODUCTION

As more scientific disciplines rely on data as an important means for scientific discovery, the demand for infrastructures that support data-intensive tasks in addition to traditional compute-intensive tasks, such as modeling and simulations, is increasing. For example, in biology and astronomy scientific discovery is increasingly based on analysis of data collected from machines, such as genome sequencing machines or observatories [1]. Across disciplines there is a move towards data-driven discovery and with increasing diversity in the source of data (c.f. the Internet of Things and the usage of networked sensors to collect data). The term “fourth paradigm” [2] refers to scientific discovery based on data in addition to theory, experimentation and simulation based discovery.

Data-intensive applications are associated with a wide variety of characteristics and properties, as summarized by Fox et al. [3, 4]. Often, they are more complex and heterogeneous than HPC applications as they typically comprise of multiple stages with different characteristics. Typical stages are: data ingest, pre-processing, feature-extraction and advanced analytics. While some of these stages are I/O bound with potential different I/O characteristics (random vs. sequential access), some stages (e.g. advanced analytics) are compute- and memory bound. Managing and supporting such heterogeneous application workflows on top of heterogeneous resources at scale represents an important challenge.

HPC infrastructures introduced parallel filesystems, such as Lustre or GPFS, to meet the increased I/O demands of data-intensive applications and archival storage to address the need for retaining large volumes of primary simulation output data. The parallel filesystem model of using large, optimized storage clusters exposing a POSIX compliant rich

interface and connecting it to compute nodes via a fast interconnects works well for compute-bound task. It has however, some limitations for data-intensive, I/O-bound workloads that require a high sequential read/write performance. Similarly, high-throughput infrastructures (HTC), such as OSG, rely on separate storage environments, e.g. SRM or iRODS based, to manage data. In clouds, object stores are a common mechanism for persisting data outside of ephemeral VM-based compute resources. To address some of these issues, new – mostly hardware – capabilities have been added to HPC resources to meet the demands of data-intensive applications; machines such as Gordon or Wrangler, provide large memory nodes to facilitate shared memory data analytics tools (e.g. R, Python) and additional storage tiers (e.g. SSD).

Hadoop [5] and the MapReduce abstraction [6] were developed with data as first order consideration and established the de-facto standard for data-intensive computing. The biggest differentiator of Hadoop compared to HPC systems is data-locality: while HPC systems generally rely on fast interconnects between compute and storage, Hadoop co-locates compute and data. The Hadoop ecosystems – in the following referred to as *Apache Big Data Stack (ABDS)* – provides a manifold set of novel tools and higher-level abstractions for data processing. In addition to MapReduce, Spark [7] gained popularity for memory-centric data processing and analytics. ABDS tools and frameworks are increasingly used in sciences (see [8, 9]). While the Hadoop platform has proven its value in scientific applications, challenges remain in deploying ABDS applications on HPC infrastructure and when integrating these with HPC applications, e.g. based on MPI [10, 11].

A main differentiator of ABDS are high-level abstractions that trade-off capabilities and performance; MapReduce and Spark’s RDDs offer the ability to reason about data processing steps (e.g. filtering, transformations and aggregations) without the need to explicitly implement data parallelism. Further important capabilities are offered in the advanced analytics and machine learning domain. MPI provides a good abstraction for implementing parallel applications providing primitives for point-to-point and collective communications; however, it lacks the productivity of higher-level ABDS abstractions.

Over the past decades, the *High Performance Distributed Computing (HPDC)* community has made significant advances in addressing resource and workload management on heterogeneous resources. In contrast, the ABDS ecosystem has been evolving to provide similar levels of sophistication for commercial enterprise. In fact, some conceptual ideas dominant in the HPDC world have already started making an impact in ABDS tools. For example, the concept of multi-level scheduling as manifest in the decoupling workload assignment from resource management via the concept of intermediate container jobs (also referred to as Pilot-Jobs [12]) has made its presence in ABDS after the transition from Hadoop to YARN/Mesos. This concept has been adapted and refined in the ABDS environment allowing frameworks to retain resources (cores, memory, storage) and expand/shrink the resource pool if necessary. It turns out to be the case that multi-level scheduling is even more important for data-intensive applications as often only application-level schedulers can be aware of the localities of the data sources used by a specific application. This mo-

tivated the extension of the Pilot-Abstraction to support data-aware scheduling on application-level [13]. As most HPC schedulers are data agnostic, this is an important/critical extension of capabilities. However, this advance has had the interesting consequence that heterogeneity in ABDS systems is now no longer confined to the filesystems and resource-access mechanisms, but like traditional HPDC systems, the resource management interface and semantics are different.

Collectively, the above features and trends point to the possibility and need for consilience between the HPDC and ABDS approaches for resource management. The aim of this paper is to examine the need for consilience in resource management approaches between ABDS and traditional HPDC approaches, understand some of the challenges on the path to doing so and explore the Pilot-Abstraction as one possible way to address some of the challenges.

Another concern of this paper is to understand how to address the issues of interoperability: There is a great need to integrate both HPDC and Hadoop, e.g. due to the necessity to co-locate data/compute or to combine compute-centric HPC applications (e.g. linear algebra solvers) with ABDS applications (e.g. MapReduce and Spark). In this paper, we explore the usage of the Pilot-Abstraction inside an ABDS environment, as well as a path for the interoperable use of ABDS applications on HPDC infrastructure.

This paper makes the following contributions: (i) We propose several extensions to the Pilot-Abstraction [12] to better facilitate data processing and advanced analytics on HPDC and to support interoperability with Hadoop; specifically, we design and implement Pilot-Abstractions that provides a common approach for data-aware resource management on and across HPC, cloud and Hadoop infrastructures. By supporting Hadoop’s resource manager YARN, the Pilot-Abstraction can be used as standard application framework simplifying the usage of HPC application on Hadoop. (ii) We extend an implementation of the Pilot-Abstraction to facilitate the deployment and execution of ABDS applications on HPC. Pilot-Hadoop enables the dynamic, ad-hoc creation of Hadoop or Spark clusters on HPC infrastructures. (iii) We extend Pilot-Data for distributed in-memory computing that is essential for scalable analytics, such as iterative machine learning. Pilot-Data Memory provides a unified way to access distributed memory within data-intensive applications that is integrated with the data-affinity model of Pilot-Data. Pilot-Data offers a unified approach for data management across complex storage hierarchies comprising of local disks, cloud storage, parallel filesystems, SSD and memory. (iv) Finally, we validate the proposed abstractions and tools on XSEDE using Stampede and Gordon (machine designed for data-intensive applications). We investigate the performance of HDFS and Lustre using a MapReduce workload and of KMeans running on different ABDS and HPC-backends using the Pilot-Abstraction.

This paper is structured as follows: In section 2 we survey the ABDS ecosystem and compare the provided tools and abstractions with the HPC environment. We continue with a discussion of the new Pilot-Data capabilities that support Hadoop/HPC interoperability as well as advanced analytics and machine learning applications in section 3. The results of our experimental validation are presented in section 4. We conclude with a discussion of the contributions and lessons learned as well as relevant future issues in section 5.

2. BACKGROUND AND RELATED WORK

Hadoop emerged separate from high-performance computing in enterprise environments inspired by Google’s cloud infrastructure based on the Google Filesystem and MapReduce [6]. Apache Hadoop evolved to a general purpose cluster computing framework suited for many kinds of data-intensive applications [14]. While Hadoop MapReduce lacks behind some capabilities, e.g., high-performance inter-process communication, a set of novel, high-level abstractions and runtime environments emerged on top of the core Hadoop services, the Hadoop Filesystem (HDFS) and the YARN resource manager. YARN allows the deployment of any application on a Hadoop cluster without the need to retrofit applications into the MapReduce model as required for Hadoop 1.

In this section, we summarize our previous work in analyzing the characteristics and properties HPC and Hadoop Infrastructures as well as related work to provide abstractions and runtime environment for such applications.

2.1 HPC and ABDS Abstractions

This section describes abstractions and runtime systems for data-intensive computing in the HPC and ABDS domains. As alluded to earlier, data-intensive applications are typically more heterogeneous than compute-intensive simulations. Data-intensive applications are often modeled as a pipeline of tasks (from data ingest, storage, processing to analytics) or a direct acyclic graph with tasks corresponding to nodes in the graph. We use the term *workflow* to refer to multi-stage data-processing; *data pipeline* is often used as a synonym for this.

A common concern is the provision of a scalable environment support different stages of data processing and analytics workflows: from coarse-grained data parallelism for data-filtering with MapReduce to fine-grained parallelism for machine learning that often relies on scalable linear algebra libraries. In this section, we give a brief overview of HPC libraries and abstractions and investigate their usage within data-intensive workflows. We further compare and contrast these approaches to abstractions developed in the ABDS world.

Communication-Abstractions (MPI)

Analytics and machine learning algorithms can often be expressed and transformed into matrix operations and thus, require efficient linear algebra implementation. MPI and OpenMP are the standard abstraction for implementing parallel applications on HPC infrastructures. While they provide an important building block for scalable analytics, they lack the usability of higher-level abstractions (such as the R dataframe). Several parallel, numerical libraries (MPI/OpenMP-based) that support analytics have been developed, e.g. ScaLAPACK [15] or ARPACK [16]. These parallel libraries are based on the lower-level libraries LAPACK and BLAS. While they provide an important building block for scalable analytics, they lack the usability of higher-level abstractions. Which the introduction of YARN, the execution of MPI applications on Hadoop clusters is well supported, e.g. MPICH2-YARN and Hamster, an YARN application master for OpenMPI.

File-based Abstractions

Scientific applications are commonly based on files. Many abstractions for improving file management in the HPC context emerged: Filecules [17] e.g. simplify the the processing of file groups. Similarly, other data management systems, such as iRods often work on collection/groups of files. However, file-based data management is often associated with inefficiency in particular for temporary data, e.g. intermediate data of iterative machine learning applications. iRods [18] utilizes so-called collections to group and manage files. While these tools allow a logical grouping of data, they provide limited support for data-parallel processing of these files as data partitioning and processing is done outside of these tools.

Pilot-Jobs and Workflows

Pilot-Jobs [12] have been developed to support ensembles of fine-grained tasks in HPC environments; examples of Pilot-Jobs are Condor-G/GlideIn [19] or BigJob [20]. By using a set of placeholder jobs distributed across multiple resources, the system can accommodate dynamic task workloads through a dynamically adjusting resource pool improving the overall utilization at the same time. Pilot-Jobs have been successfully used to enhance the performance of scientific workflows.

Scientific workflows popularized the direct acyclic graphs (DAGs) abstraction as fundamental way to express workflows; examples of such systems are Pegasus [21] and Taverna [22]. Many of these system focus on the higher-level workflow abstraction lacking a high-performance, vertically integrated runtime system (as provided by the ABDS stack). Another constraint is the fact that the dataflow is often based on files. In ABDS similar DAG abstractions emerged, which are implemented on top of ABDS primitives, such as MapReduce, and are discussed in the following section.

Pilot-Jobs have been extended to facilitate data management (mainly on file-basis) and for dataflow-oriented workflows. Falcon [23] provides a data-aware scheduler on top of a pool of dynamically acquired compute and data resources [24]. The so called data diffusion mechanism can cache data on Pilot-level enabling the efficient re-use of data. Another area of research is the utilization of distributed memory for data-intensive, task-based workflows. Swift/T [25] is a rewrite of the Swift to utilize the MPI-based Turbine engine for processing of data-intensive workflows benefiting from MPI features, such as effective collective communications.

MapReduce & Higher-Level Abstractions

MapReduce [6] proofed an effective abstraction for processing data in a parallel way decoupling storage backend, data formats and processing engine. Hadoop MapReduce established itself as de-facto standard for scalable data processing – in contrast to file-based approaches found in the scientific workflow community – MapReduce hides complex details, such as data organization, formats, data partitioning and aggregation. While MapReduce simplified the creation of data-intensive application (particularly applications that need to process vast volumes of data), the MapReduce abstraction is limited in its expressiveness as pointed out by various authors [26, 27] and lead to manifold higher-level abstractions for implementing sophisticated data pipelines.

In addition, the native APIs provided by Hadoop are com-

plex: the creation of a simple application requires an implementation of a map and reduce function, as well as various configurations and auxiliary functions. Also, the creation of more complex data pipelines or iterative machine learning applications consisting of multiple MapReduce jobs is very complex. Thus, a set of high-level APIs, such as Apache Crunch [28], Cascading [29], Apache Flink [30] and Spring XD [31], emerged. While the expressiveness of the API was better than MapReduce, they still were constrained by the MapReduce runtime system.

With the emergence of YARN, several new processing engines emerged in the Hadoop ecosystems that improved the support for workflows. Framework, such as Spark [7] and Tez [32], provide richer abstractions that are built on modern processing engines that can retain resources across task generations and effectively utilize distributed memory. Spark's reliable distributed dataset (RDD) abstraction provides a powerful way to manipulate distributed collection stored in the memory of the cluster nodes. Spark is increasingly used for building complex data workflows and advanced analytic tools, such as MLLib [33] and SparkR [34].

As alluded, the ability to utilize efficient collectives is important for advanced analytics implementations that often require fast linear algebra implementations. Some hybrid frameworks have been proposed to provide MPI-style collective operations in conjunction with data-intensive abstractions, such as MapReduce. For example, Harp [35] proposes the usage of collective operations in the map-phase of a MapReduce application – the model is referred to MapCollective. This model is similar to the bulk-synchronous communication model or the MPI communication model; Harp however aims to provide a higher-level abstraction than MPI. In contrast to other abstraction, such as MapReduce, the user is required to manually manage data partitions and processes. Different implementations and algorithms for the HARP collective layer have been investigated, e.g. based on based e.g. on the Netty and Azure inter-role communication mechanism. A constraint is that the collective framework of Harp currently only supports a static group of resources.

Dataset and Dataframe Abstractions

The *dataset* or *dataframe* abstractions originally introduced in R (respectively his predecessor S) exposes data in a tabulated format to the user and supports the efficient expression of data transformations and analytics [36]. A dataframe typically stores data matrix of different types of data (e.g. numeric, text data and categorical data). The dataframe abstraction supports various functions for manipulating data stored inside the data structures, e.g. to subset, merge, filter and aggregate data, using well-defined primitives or SQL. Similar abstractions emerged for other languages and runtime environments, e.g. Pandas [37], Scikit-Learn [38] and Dato SFrame [39] for Python. For Mahout a dataframe abstraction has been proposed.

While the dataframe abstractions are very expressiveness and well-suited for suited for implementing advanced analytics, they traditionally lacked the ability to scale-out. The MLI-inspired Spark Pipeline API [40] for Spark, H2O [41], and Blaze [42] for Python attempt to introduce similar abstractions also supporting scalable backends - however, they currently lack in the variety of analytics frameworks and algorithms available for these tools. Another constraint is that

many of these framework, e.g. Spark, are Java-based making it difficult to integrate these with native libraries, e.g. parallel linear algebra libraries from the scientific computing domain. HPC abstractions in contrast to the dataframe or MapReduce abstraction focus on low-level functions (e.g. MPI for communications). Thus, they often do not provide an easy way to explore data-parallelism. Further, higher-level dataset/dataframe abstractions designed for domain scientists are typically not available.

The ability to combine different frameworks and abstractions is the key for implementing end-to-end data-intensive workflows with multiple stages with different workload characteristics. To address these complex requirements, it can be expected, that the design space for abstractions will be further explored and more hybrid approaches will emerge allowing for efficiently supporting end-to-end data pipelines (including analytics). Another constraint is the fact, that the majority of the available runtime systems is based on Java. Python – a popular language for scientific computing – is typically only supported as secondary option.

2.2 HPC and Hadoop

The heterogeneity of distributed infrastructures is still increasing: HPC and Hadoop e.g. following dramatically different design paradigms. In HPC environments traditionally storage and compute are separated connected by an high-end network (e.g. Infiniband). To address the increasing need to process large volumes of data on HPC, the capacity of these storage systems and the networks. System, such as Wrangler [43], maintain this separation. Wrangler in particular deploys a mix of a Lustre storage system, a SSD-based high-end storage system and local storage. In addition archival storage systems often based on HPSS are used to store cold data.

Resource Management: The fine-grained data-parallelism of data-intensive applications is ideally suited for multi-level scheduling. Multi-level scheduling [44] originated in HPC environments and proved as efficient mechanism to managed ensembles of tasks. By decoupling system-level and application-level scheduling and by taking into account system-level, such as resources utilization and allocation policies, as well as application-level objectives, e.g. dynamic resource requirements for every application stage, in most cases a superior performance can be achieved. Pilot-Jobs [12] provided a powerful abstraction for implementing multi-level scheduling on HPC systems. While Hadoop originally only provided a rudimentary scheduling system, the new YARN scheduler provides efficient support for application-level scheduling.

YARN address the need that with the uptake of Hadoop, the requirements with respect to resource management increased: more complex data localities (memory, SSDs, disk, rack, datacenter), long-lived services, periodic jobs, interactive and batch jobs need to be supported on the same environment. Multi-level scheduling serves as the basic architectural principle to support this requirement. YARN [45], Hadoop's resource, aims to address these limitations. In contrast, to traditional batch schedulers, YARN is optimized for data-intensive environments supporting data-locality and the management of a large number of fine-granular tasks (found in data-parallel applications). YARN enables applications to deploy their own application-level scheduling routines on top of Hadoop-managed storage and com-

pute resources. While YARN manages the lower resources, the higher-level runtimes typically use an application-level scheduler to optimize resource usage for the application. Applications need to initialize their so-called Application-Master via YARN; the Application Master is then responsible for allocating resources – containers – for the applications and to execute tasks in these containers. Data locality, e.g. between HDFS blocks and container location need to be manually managed by the application master (by requesting containers on specific nodes/racks etc.). Other resource management systems addressing similar needs emerged, e.g. Mesos [46] Omega [47] Google’s distributed scheduler.

Managing resources on top of YARNs is associated with several challenges: while the default design particularly facilitates the fine-grained data parallelism of MapReduce, for certain application characteristics it is desirable to retain resources during longer periods, e.g. to longer cache data that is often re-used in-memory, to have readily available resources for interactive applications or to facilitate iterative processing. Several higher-level frameworks for YARN addressing specific application characteristics emerged: Llama [48] offers a long-running application master for YARN designed for the Impala SQL engine. Apache Slider [49] supports long-running distributed applications on YARN with dynamic resource needs allowing applications to scale to additional containers on demand. TEZ [32] is a DAG processing engine primarily designed to support the Hive SQL engine allowing the application to hold containers across multiple phases of the DAG execution without the need to de-/re-allocate resources. REEF [50] is a similar runtime environment that provides applications a higher-level abstraction to YARN resources allowing it to retain memory and cores supporting heterogeneous workloads. REEF Retainers can re-use JVM and store data in the JVM’s memory.

Interoperability: To achieve interoperability, several frameworks explore the usage of Hadoop on HPC resources. Resource managers, such as Condor and SLURM, provide Hadoop support. Further, various third-party systems, such as SAGA-Hadoop [51], JUMMP [52] or MyHadoop [53], exist. A main disadvantage with this approach is the loss of data-locality, which the system-level scheduler is typically not aware of. In addition there are several other limitations associated with that approach: e.g. the necessity to load data into HDFS and the ability to achieve higher cluster utilization by more fine-grained resource sharing.

For Hadoop deployments typically local storage is preferred; nevertheless some deployments use a HPC-style separation of compute and storage systems. Hadoop workloads on these HPC systems is supported via a special client library, which improves the interoperability with Hadoop; it limits however data locality and the ability for the application to optimize for data placements since applications are commonly not aware of the complex storage hierarchy. Another interesting opportunity is the usage of Hadoop as active archival storage – in particular, the newly added HDFS heterogeneous storage support is suitable for supporting this use case.

Summary: Understanding performance in a heterogeneous, distributed environment is complex. In the remainder of the paper, we investigate the Pilot-Abstraction as unifying concept to efficiently support the interoperability

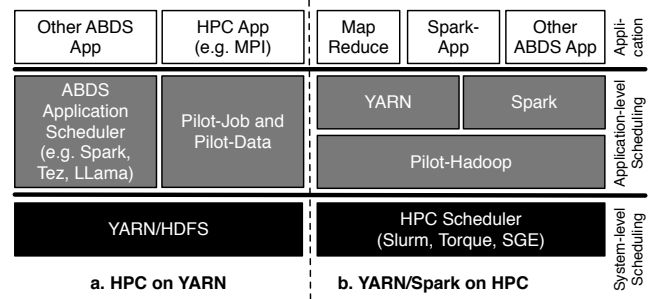


Figure 1: Hadoop and HPC Interoperability: There are two options: **a. Running HPC applications inside a YARN cluster**, **b. spawning a YARN or Spark cluster on a HPC environment**.

between HPC and Hadoop. By utilizing the multi-level scheduling capabilities of YARN, Pilot-Data can efficiently manage Hadoop cluster resources providing the application with the necessary means to reason about data and compute resources and allocation. On the other side, we show, how the Pilot-Abstraction can be used to manage ABDS application on HPC environments.

3. PILOT-ABSTRACTION FOR HADOOP: DESIGN AND IMPLEMENTATION

The Pilot-Abstraction [12] has been successfully used in HPDC for supporting a diverse set of task-based workloads on distributed resources. A Pilot-Job provides the ability to utilize a placeholder job as a container for a dynamically determined set of compute tasks. The Pilot-Data abstraction [13] extends the Pilot-Abstraction for supporting the management of data in conjunction with compute tasks. The Pilot-Abstraction defines the following entities: A Pilot-Compute allocates a set of computational resources (e.g. cores); a Pilot-Data represents space on a physical storage resource. Further, the abstraction defines a Compute-Unit (CU) as a self-contained piece of work represented as executable that is submitted to the Pilot-Job. A Data-Unit (DU) represents a self-contained, related set of data.

The Pilot-Job and Pilot-Data abstractions have been implemented within BigJob [12, 20], an interoperable Pilot-Abstraction framework for supporting heterogeneous task-based workloads on heterogeneous infrastructures. In this section, we present the extensions made to the Pilot-Abstraction to facilitate a broader set of data-intensive applications and infrastructures, such as Hadoop. We explore several options for integrating HPC and Hadoop environments as depicted in Figure 1 using the Pilot-Abstraction. By providing support for Hadoop inside BigJob (Figure 1a) HPC applications can run on Hadoop YARN clusters without modification. Pilot-Hadoop enables the execution of ABDS applications inside environments managed by traditional HPC schedulers (Figure 1b).

In section 3.1, we describe how the Pilot-Abstraction and the BigJob implementation was extended to support Hadoop resource manager, i.e. YARN and Mesos, and HDFS storage. We continue with a discussion of Pilot-Hadoop for running YARN as application-level scheduler on HPC resources

in section 3.2. Finally, we present Pilot-Data Memory- an infrastructure-agnostic in-memory runtime for analytics applications in section 3.3.

3.1 Pilot-Abstraction: Interoperable Access and Management of Hadoop Resources

With the introduction of YARN, arbitrary applications can be executed within Hadoop clusters. Nevertheless, utilizing an Hadoop environment outside of higher-level frameworks, such as MapReduce and Spark, is a difficult task. Established abstractions that enable the user to reason about compute and data resources across infrastructures (i. e. Hadoop, HPC and clouds) are missing. Also, the new generation of schedulers that emerged in the YARN space impose a more stringent requirements on the application. While schedulers such as YARN or Mesos effectively facilitate application-level scheduling, the development efforts for YARN and Mesos applications are very high. YARN provides e. g. only a very low-level abstraction for resource management – the application must be able to work with a subset of the requested resources. Also, allocated resources (the so called YARN containers) can be preempted by the scheduler. Data/compute locality needs to be manually managed by the application scheduler by requesting resources at the location of a file chunk. To address this, various frameworks that aid the development of such applications have been proposed, e. g. Apache Slider [49] and Spring YARN [54]. While these frameworks simplify development, they do not address concerns such as interoperability and support for geographically distributed resources.

To provide a unified, infrastructure-agnostic abstraction, the Hadoop resource model as exposed by YARN and HDFS must be mapped to the Pilot-Abstraction. The Hadoop resource model primarily relies on cores and memory for modeling compute and storage space modeling data resources. While HPC resources typically only allocate compute cores and nodes, the memory requirement can be easily translated to a Pilot-Compute description of a YARN-based Pilot. Similarly HDFS space can be mapped to the space parameter of the Pilot-Data description.

To facilitate physical access to Hadoop resources, several adaptors had to be developed inside the Pilot-Framework BigJob. As shown in Figure 2, the Pilot-Framework is able to spawn and manage Compute-Units and Data-Units on different kinds of compute and storage resources using a set of adaptors. The new YARN, Mesos and HDFS adaptors enables applications to take advantage of new infrastructures and manage their CUs and DUs on dynamic resource pools located in an Hadoop environment. A particular challenge for the implementation of the YARN adaptor is the multi-step resource allocation process imposed by YARN, which as alluded differs significantly from HPC schedulers. The YARN adaptor for BigJob implements a so-called YARN Application Master, which is the central instance for managing the resource demands of the application. Once the Application Master is started, subsequent resource requests are handled by it. The BigJob Application Master will then request the specified number of YARN container. Once these are allocated by YARN, the Pilot-Agent will be started inside these containers. The dispatching of the CUs is done via the normal Pilot-Framework internal mechanisms without involvement of YARN.

The HDFS adaptor access the Hadoop Filesystem using

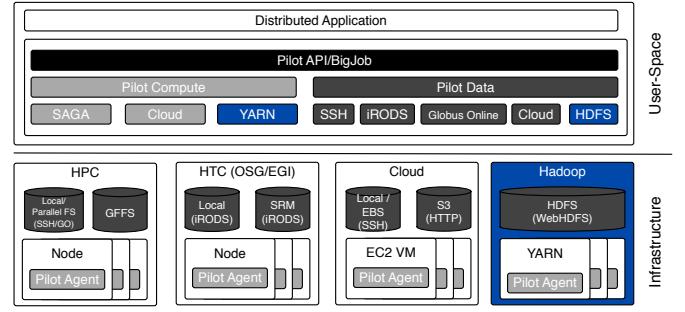


Figure 2: Pilot-Framework Big Job on Heterogeneous Infrastructure: BigJob provide a unified abstraction for compute and data resources. The extension for Hadoop are encapsulated in a YARN adaptor for Pilot-Compute and HDFS adaptor for Pilot-Data.

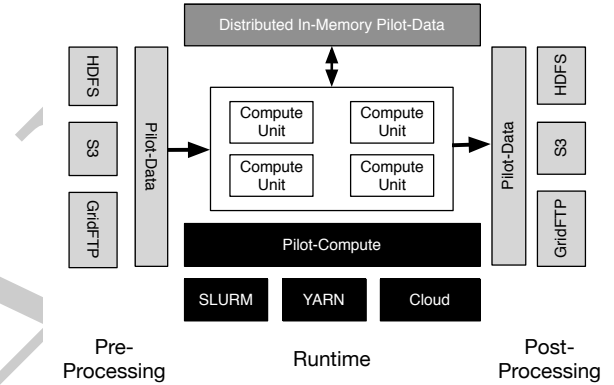


Figure 3: Pilot-Abstraction for Data-Parallel Processing: Pilot-Compute allows the flexible allocation of resources across heterogeneous infrastructures, Pilot-Data enables Compute Units to seamless access datasets on different storage infrastructures. The In-Memory Data-Unit facilitates data-parallel processing using a group of Compute-Units.

the WebHDFS API. Pilot-Data supports access to data from different sources: data may reside on a local or mounted shared storage system (e. g. Lustre storage), HDFS, iRods or another cloud object store. Pilot-Data will ensure that the data will be available before the Compute-Unit is started. As shown in Figure 3 the Pilot-Abstraction enables the implementation of complex data workflows, i. e. the stage-in/out and processing of data residing in different sources. In section 3.3, we discuss the usage of Pilot-Data for caching data during complex processing steps. Pilot-Data is data format agnostic, i. e. the implementation of access to the data structure is done on application-level (in the CU). It supports standard formats, such as text files, CSV but also advanced columnar formats (bcolz) or HDF5.

The Pilot-API provides a unified API across heterogeneous resources and gives application-level control to storage and compute resources. The new adaptors enable applications to seamlessly utilize Hadoop resources inside their data-intensive workflows. Depending on the application

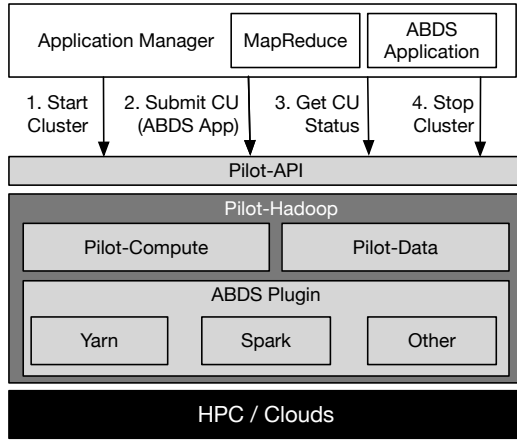


Figure 4: Pilot-Hadoop for HPC and Cloud Infrastructures: Pilot-Hadoop provides uniform framework to managing Hadoop and Spark clusters on resources managed by HPC schedulers, such as PBS, SGE and SLURM. The Pilot-API provides a unifying interface for allocating a YARN/Spark cluster on HPC and for managing Compute-Units that marshal a YARN, Spark or other ABDS application.

requirements the API is suited for implementing complex data-intensive workflows as well as running scalable analytics kernels (optimized for complex storage and memory hierarchies) on the data. The API relies on affinity labels to manage the co-location of data and compute (see [13]). Using the API developers can model complex storage hierarchies consisting of archival storages, cold data storage for raw data, warm and hot storage for pre-processed data used in the model fitting phase and memory for intermediate results of iterative machine learning algorithms. The runtime system will ensure that data/compute will be co-located if possible to improve performance.

3.2 Pilot-Hadoop: Supporting Application-Level Interoperability for ABDS and HPC

Having discussed the extensions to the Pilot-Abstraction to support Hadoop resources, we explore the usage of Hadoop and other ABDS frameworks on HPC resources in this section (see Figure 1 (b)). Pilot-Hadoop [55] provides a framework for executing ABDS applications written for YARN (e.g. MapReduce) or Spark on HPC and cloud resources. Pilot-Hadoop has been developed as successor to SAGA-Hadoop [51] utilizing the handling of multi-node cluster environments of the Pilot-Agent.

Figure 4 illustrates the architecture of Pilot-Hadoop. Pilot-Hadoop uses the Pilot-Abstraction and the BigJob implementation to manage Hadoop clusters inside an environment managed by an HPC scheduler, such as PBS, SLURM or SGE, or clouds. The Pilot-Framework is used for dispatching a bootstrap process that generates the necessary configuration files and for starting the Hadoop processes. The specifics of the Hadoop framework (i.e. YARN and Spark) are encapsulated in an adaptor. The bootstrap process is then responsible for launching YARN’s resource and node manager processes respectively the Spark

master and worker agents on the nodes allocated by the Pilot-Framework. While nearly all ABDS frameworks (e.g. MapReduce, Tez and also Spark) support YARN for resource management, Spark provides a standalone cluster mode, which is more efficient for dedicated resources. Thus, a special adaptor for Spark is provided.

Once the cluster is setup, users can to submit applications by using the Pilot-API’s Compute-Unit API to start and manage application processes. Compute-Units with type Hadoop and Spark are then forwarded to the YARN respectively Spark resource manager, which then handles the management of these tasks. With this capability, the Pilot-Abstraction can be used to manage highly heterogeneous workloads, e.g. bag-of-tasks, coupled tasks, MPI, Hadoop and Spark applications, via a single interface.

3.3 Pilot-Data Memory: A Processing Engine for Machine Learning

The Pilot-Abstraction provides a low-level mechanisms to manage the data across different, possible distributed, data stores in conjunction with their task-based computing focusing on the stage-in and out of data related to a set of CUs. Also, it required the developer to either manually implement data parallelism or use a higher-level framework, such as Pilot-MapReduce [56]. Another constraint is the fact that only persistent storage can be used. The usage of (distributed) memory for caching of input or intermediate data (e.g. for iterative machine learning) is not supported. While this disk-based model is effective for doing many forms of large volume data processing, iterative processing, e.g. for machine learning, requires more sophisticated ways to manage intermediate data.

Pilot-Data Memory adds in-memory capabilities to Pilot-Data and makes it available via the Pilot-API. A particular challenge is the integration of the in-memory layer with the compute layer, which typically requires support for a manifold set of tools and programming languages. We focus on providing a Python-based API and runtime; many scientific applications are implemented in Python, which makes it easy to integrate native code to achieve a good performance. Further, there is a lack of in-memory frameworks and tools for Python – Pilot-Data Memory is an attempt to address these limitations. A particular gap is the ability to manage large amounts of distributed memory - while it is fairly simple to manage memory on a single node (using e.g. memory mapped files), support for distributed memory typically requires specialized runtime and processing environments that are not compatible with traditional Posix file APIs.

To process data in an in-memory DU, we extend the DU interface to provide a higher-level MapReduce-based API for expressing transformations on the data. Using a map and reduce functions, applications can express abstract operations on data without manually creating CUs for partitioning and processing the data. The API utilizes a key/value pair tuples as input for the map and reduce function. The runtime system generates the necessary application tasks (Compute-Units) and run these in parallel considering data locality and other aspects. Users have the possibility to control this placement using a simple, label-based affinity model, which allows reasoning about compute and data and provides the runtime system with hints for optimizing execution. The system is data format agnostic and supports heterogeneous data schemes (schema on read).

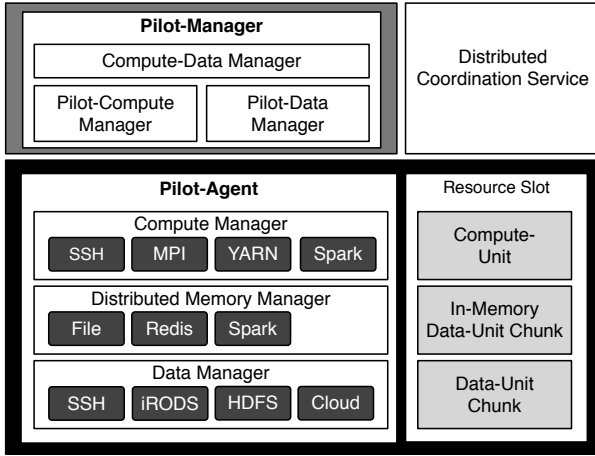


Figure 5: Pilot-Data Memory Architecture: The Pilot-Manager handles manages a set of queues from which the agents are pulling CUs. Data management is carried out at the Pilot-Agent-level. The Pilot-Agent will stage-in and out data via the Data Manager. The Distributed Memory Manager handles the caching of data. CUs are executed via the Compute Manager.

Figure 5 illustrates the architecture of the Pilot-Data Memory framework. There are multiple levels of coordination and decision making: The Compute-Data-Manager manages a set of memory and disk-backed Pilot-Data and Pilot-Compute. Applications can submit Compute-Units (CUs) and Data-Units (DUs) to the Pilot-Manager, which exposes control over Pilots, CUs and DUs via the Pilot-API. The Compute-Data-Manager will assign submitted Compute-Units and Data-Units to a Pilot taking into account the current available Pilots, their utilization and data locality. The Pilot-Agent will stage-in and out data via the data manager. The Distributed Memory Manager handles the caching of data required for the computation. CUs are executed via the Compute Manager. The architecture enables late decision making at runtime: depending on the current utilization CUs can be processed by different Pilots. Currently, the Pilot-Manager considers both the utilization of the Pilot and data locality. In the future, we plan to support further resource characteristics, such as the amount of available memory (critical for memory centric computing), as well as the characteristics of the CU workload (providing support for co-placing CUs or streaming data between two subsequent CUs).

An important design objective for Pilot-Data Memory is extensibility and flexibility. Thus, Pilot-Data provides an adaptor mechanism to support different in-memory backends. Currently three different backends are supported: (i) file-based, (ii) in-memory Redis and (iii) in-memory Spark. Pilot-Hadoop can be used to setup the necessary Spark infrastructure on a HPC resource. We further evaluate support for Tachyon [57] and the HDFS In-Memory storage tier [58]. The adaptor service interface specifies the capabilities that need to be implemented by the in-memory backend; it consists of functions for allocating/deallocation memory, for loading data and for executing a map and reduce func-

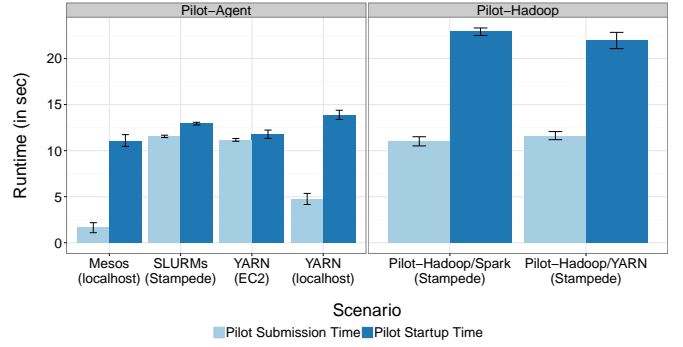


Figure 6: Pilot-Data: Interoperable Use of Pilot-Data on HPC, Cloud and Hadoop Resources: Pilot-Data supports different compute infrastructure using an adaptor mechanism and SAGA (left facet). Further, it supports running ABDS frameworks, such as Hadoop’s YARN and Spark, on HPC and Cloud environments (right facet).

tions on the data. Depending on the backend the processing function need to be implemented either manually, e.g. for the file-based and Redis backend adaptor, or can be directly delegated to the processing engine as for Spark. The Redis and file backends use the Pilot-Job framework for executing the CUs generated by Pilot-Data Memory.

In summary, the Pilot-Abstraction and Pilot-Data Memory allows applications to seamlessly move data between different forms of storage and memory providing the basis for the implementation of complex data workflows, e.g. for fusing different data sources, data filtering, feature extraction and for execution complex analytics on top of the data. As described in the following section (section 4), Pilot-Data Memory enables the efficient implementation of advanced analytics algorithms allowing e.g. the efficient storage of intermediate data in memory for iterative processing.

4. EXPERIMENTS

We proposed several extensions to the Pilot-Abstraction to accommodate Hadoop infrastructures. In this section, we investigate the characteristics of the Hadoop adaptor for the Pilot-Framework BigJob and Pilot-Hadoop. Further, we evaluate the performance of Hadoop MapReduce on HPC resources and compare HDFS and Lustre. Finally, we use KMeans to validate the suitability of Pilot-Data Memory for data analytics applications.

4.1 Application Framework and Backend Interoperability

In the following, we investigate the performance of the new Pilot-Data adaptors for YARN and Mesos as well as Pilot-Hadoop. For this experiments, we utilize Mesos 0.14, Hadoop 2.6 and Spark 1.1 as well as Amazon EC2 and the XSEDE machine Stampede.

Figure 6 summarizes the results. The left part illustrates the usage of the native Pilot-Data to manage CUs on HPC (Stampede) and on YARN and Mesos clusters (in this case hosted on Amazon Web Services). For short-running jobs the scheduler often represents a bottleneck, e.g. the startup of a YARN application typically requires several seconds

mainly to due the overhead induced by the JVM startup as well as the complex startup process; resources have to be requested in two stages: first the application master container is allocated followed by the containers for the actual compute tasks.

For the Pilot-Hadoop scenarios we utilize the Stampede supercomputer. In addition to the normal overhead for starting the Pilot-Agent (see left facet of Figure 6), some extra time is needed for setting up a YARN respectively Spark cluster on Stampede. In both cases, we will spawn the YARN and Spark daemons without HDFS assuming that data will be read from the Lustre storage cluster. Both YARN and Spark show a comparable startup time.

4.2 Exploring Hadoop on HPC

Pilot-Hadoop enables users to start YARN and Spark clusters on HPC resources managed by a scheduler, such as PBS, SLURM or SGE. While the mechanics of launching Hadoop on HPC resources are well understood, a challenge remains the configuration of Hadoop in an optimal way taking into account the specifics of the resource, such as the available memory, storage (flash vs. disks) etc., as these can vary even within a single infrastructure, such as XSEDE.

The objective of this experiment is to explore the usage of Hadoop on two XSEDE resources: Stampede and Gordon. On Stampede the storage space is partitioned into home, work, scratch and archival storage. The home, work and scratch directories are located on a Lustre filesystem; they differ with respect to their quota, backup and purge policy. The archival storage is located on a remote system and not directly mounted on the compute nodes. The amount of local space is constrained to 80 GB in the /tmp directory. Some resources started to cater more data-intensive workloads. Gordon e.g. offers 280 GB flash-based local storage per node. However, since the space is transient, this space is mainly suitable for intermediate data – otherwise data needs to be initially copied to this space. In addition to different storage option, we investigate the usage of the new HDFS In-Memory feature [58].

In the first step we analyze the HDFS and in particular the HDFS in-memory performance. For this purpose, we deploy an HDFS cluster on Stampede using Pilot-Hadoop using up to 512 cores and 32 nodes. HDFS is configured to use the local filesystem (/tmp) as data directory. Half of the data nodes memory is reserved for the in-memory cache. Further, we compare the HDFS performance with the Lustre storage available on Stampede. Figure 7 summarizes the results of our experiments on Stampede.

HDFS 2.6 provides storage policies, which enable clients to directly store data in the memory of the data node without the need to wait for the persistence and replication of the data. This feature requires that the native libraries for Hadoop are in place and that the memory parameter for HDFS data node (`datanode.max.locked.memory`). We see a consistent minor improvement of the write performance when using the in-memory option. However, the overall write performance is determined by the non-parallel write to HDFS. We investigate two kinds of read performances: (i) the read performance using a single client that executes a get command and (ii) the parallel read using a MapReduce job. The larger the cluster size, the better the parallelism for MapReduce parallel reads – as expected Hadoop scales near linear in this case. For the in-memory case, we see no

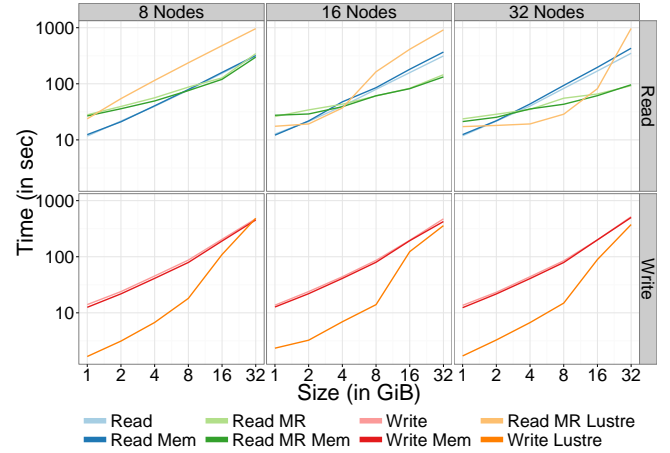


Figure 7: HDFS and Lustre Performance on Stampede: The figure shows the time to read/write different data sizes data to/from HDFS and Lustre. Lustre performs well for small data sizes, while HDFS has a better performance for MapReduce-based parallel reads of larger data sizes on larger clusters.

performance improvements for normal reads (case (i)); for (ii) we see a minor benefits.

Further, we investigate the performance of Lustre. In particular for small file sizes, Lustre performs well. Surprisingly, also the read performance using a non parallel-I/O client was in many cases lower than in the non-parallel HDFS client (case (i)). Obviously, for MapReduce workloads HDFS clearly outperforms Lustre. MapReduce utilizes data locality when assigned map tasks to data file chunk. While there is a Hadoop Lustre plugin as part of the Intel Enterprise Lustre edition available that utilizes a similar mechanism, it is currently not available on Stampede. Thus, by default when running Hadoop MapReduce on top of Lustre data-locality is not considered.

Another concern is the performance of different environments; in the following we compare the performance of Stampede and Gordon. Figure 8 shows the performance of both environments. Gordon clearly shows a better performance for HDFS mainly due to the local flash storage and more memory in the machines. The performance improvement for the in-memory option is in average 9% in comparison to Stampede where the speedup for in-memory is in average 14%.

HDFS heterogeneous storage supports provides a uniform interface for reasoning about storage across a single namespace, which allows a simplification of existing data flows. However, not all YARN/HDFS based tools optimally utilize these capabilities. MapReduce e.g. does not utilize the in-memory HDFS features. In the future, it can be expected that frameworks such as Spark will make use of these capabilities.

4.3 Advanced Analytics: KMeans

KMeans is a classical example of an advanced analytics algorithms used for clustering data that shares characteristics with a broad set of other analytics algorithms. The algorithms requires multiple iterations on the data – in each

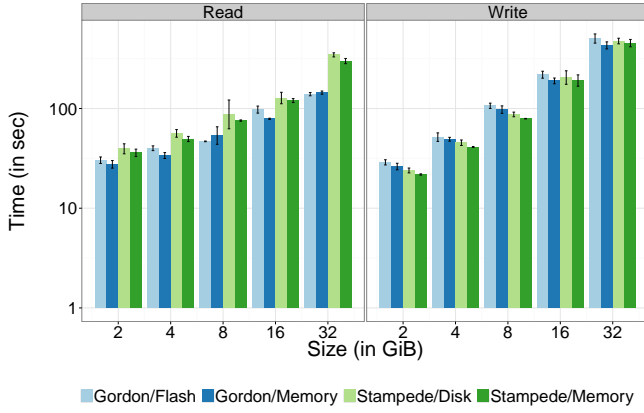


Figure 8: Gordon vs. Stampede on 8 Nodes/128 Cores: The HDFS performance on Gordon is significantly better mainly due to the usage of local flash drives compared to disks. The speedup between flash storage and memory on Gordon is as expected lower than between disk and memory on Stampede.

iterations a new candidate location for the cluster centers.

In the following, we use our Pilot-Data-based KMeans implementation to evaluate different Pilot-Data Memory backends. The computational kernel, which is called iteratively takes two parameters: (i) a set of multi-dimensional set of vectors to be clustered, remains constant through all the iterations, and (ii) a set of centroid vectors. The centroids vector changes each iteration. For the Pilot-based Redis backend, we utilize one Pilot-Compute managing up to 384 cores on Stampede for running CUs on the Data-Unit stored in a Pilot-Data Memory. The file backend is included for reference purposes. For the Spark scenario, we utilize Pilot-Spark to setup a Spark cluster on Stampede – an XSEDE leadership machine, which is then used to manage both the data and compute inside of Spark (via the Pilot-API). We use Redis 2.8 and Spark 1.1. The experiment demonstrates interoperability in two dimensions: first, it shows how ABDS frameworks can be run on HPC infrastructures, second it demonstrates the versatility of the Pilot-Abstraction for implementing data analytics algorithms on top of different in-memory runtimes in an infrastructure agnostic way.

Figure 9 shows the results of the experiments. We investigated three different K-Means scenarios: (i) 1,000,000 points and 50 clusters, (ii) 100,000 points and 500 clusters and (iii) 10,000 points and 5,000 clusters. Each K-Means iteration comprises of two phases that naturally map to the MapReduce programming model of Pilot-Data Memory: in the map phase the closest centroid for each point is computed; in the reduce phase the new centroids are computed as the average of all points assigned to this centroid. While the computational complexity is defined by the number of points \times number of clusters (and thereby a constant in the aforementioned scenarios), the amount of data that needs to be exchanged during the shuffle phase increases gradually from scenario (i) to (iii), with the number of points.

The performance of Pilot-KMeans improves significantly using the memory-based runtimes for the both the data points and intermediate cluster locations. The Redis back-

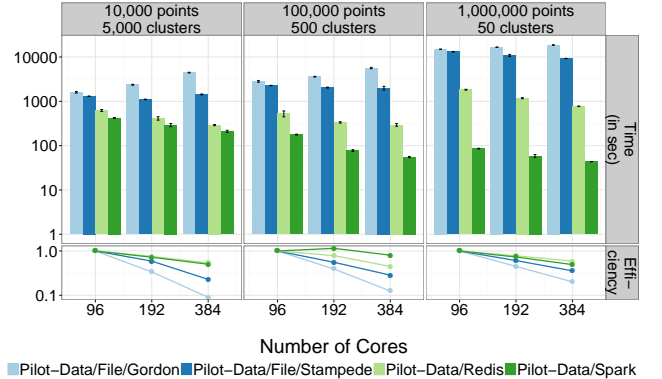


Figure 9: Pilot-Data Memory KMeans: We compare three Pilot-Data backends: (i) file-based and two in-memory-based: (ii) Redis and (iii) Spark. The Redis and Spark scenario are both executed on Stampede. KMeans on Pilot-Data/Spark has the best performance with a speedup of up to 212 compared to the Pilot-Data/File on Stampede. Also the scale-out efficiency of Spark is in most cases better than for Redis.

end achieves only a speedup of up to 11, which is significantly lower than the speedup of up to 212 achieved with Spark. Also, the scale-out efficiency for Spark is better than for Redis in most cases. This is mainly caused by the fact that we utilize a non-distributed Redis server. In the future, we will evaluate a Redis cluster setup. Both in-memory backends scale more efficient than the file-backend.

5. CONCLUSION AND FUTURE WORK

As the needs and sophistication of scientific applications increase, the infrastructures to support these applications are becoming increasingly heterogeneous and trying to accommodate an increasing number and diversity of different workloads. In response, different infrastructures have emerged: HPC for tightly-coupled applications, HTC for task-level parallelism, clouds for elastic workloads and Hadoop for data-intensive workloads. The deluge of tools, abstractions and infrastructures lead to complex landscape of point solutions characterized by a tight coupling of the components and limited interoperability.

In some ways HPC and Hadoop environments are converging: increasingly parallel and in-memory computing concepts have emerged in the ABDS environment, e.g. ML-Lib/Spark utilizes fine-grained parallelism for implementing linear algebra operations for advanced analytics. Although the introduction of ABDS concepts and frameworks have begun, their uptake remains stymied by multiple reasons, one of which is related to finding satisfactory and scalable resource management techniques usable for ABDS frameworks on HPC infrastructure.

Further, there is a need to map different aspects and stages of a data-intensive workflow to the appropriate infrastructure. Choosing the right infrastructure for an application however, is a difficult task: data-intensive workflows typically comprise of multiple stages with different compute and IO requirements. For example, while data filtering and processing is best done with Hadoop (using e.g. the MapReduce

abstraction), the compute-bound parts of that workflow are best supported by HPC environments.

The Pilot-Abstraction and the Pilot-Data implementation enable applications to utilize and explore various paths of running Hadoop on HPC (vice versa) supporting end-to-end data workflows as well as specific steps, such as iterative machine learning. In this paper, we demonstrated the usage of Pilot-Abstraction as a common, interoperable framework for ABDS and HPC, supporting a diverse set of workloads, e. g. both I/O bound data preparations tasks (using MapReduce) as well as memory-bound analytics tasks (such as KMeans). Using the Pilot-Abstraction, applications can combine HPC and ABDS frameworks either by running HPC applications inside YARN or by deploying the YARN resource manager on HPC resources using Pilot-Hadoop. Using these capabilities, applications can compose complex data workflows utilizing a diverse set of ABDS and HPC frameworks to enable scalable data ingest, feature engineering & extractions and analytics stages. Each of these steps has its own I/O, memory and CPU characteristics. Providing both a unifying and powerful abstraction that enables all parts of such a data pipeline to co-exist is critical.

Pilot-Data Memory provides a unified access to distributed memory that is assigned to a Pilot-Compute and shared across a set of tasks. The framework using a plug-gable adaptor mechanism to support different in-memory backends, e. g. based on Redis and Spark. We demonstrated the effectiveness of the abstraction for iterative analytics applications using KMeans as example. Pilot-Data Memory provides a significantly improved performance with speedups of up to 212x compared to the file-based Pilot-Data backend.

In the future, we plan to extend the Pilot-Abstraction on heterogeneous infrastructures using an enhanced set of data-intensive applications. To support further use cases, we will evaluate support for further operations, e. g. to execute collectives on data. Further, we will work on a higher-level API designed for data analytics applications and libraries that supports the expression and execution of data pipelines. Also, infrastructures are evolving – container-based virtualization (based on Docker [59]) is increasingly used in cloud environments and also supported by YARN. Support for these emerging infrastructures is being added to the Pilot-Abstraction.

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