Spark-MPI: Approaching the Fifth Paradigm of Cognitive Applications

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Abstract—Over the past decade, the fourth paradigm of data-intensive science rapidly became a major driving concept of multiple application domains encompassing and generating large-scale devices such as light sources and cutting edge telescopes. The success of data-intensive projects subsequently triggered the next generation of machine learning approaches. These new artificial intelligent systems clearly represent a paradigm shift from data processing pipelines towards the fifth paradigm of composite cognitive applications requiring the integration of Big Data processing platforms and HPC technologies. The paper addresses the existing impedance mismatch between data-intensive and compute-intensive ecosystems by presenting the Spark-MPI approach based on the MPI Exascale Process Management Interface (PMIx). The approach is demonstrated within the context of hybrid MPI/GPU ptychographic image reconstruction pipelines and distributed deep learning applications.

I. INTRODUCTION

The fourth paradigm of data-intensive science, coined by Jim Gray [1], rapidly became a major conceptual approach for multiple application domains encompassing and generating large-scale scientific drivers such as fusion reactors and light source facilities [2] [3]. Taking its root from data management technologies, the paradigm emphasized and generalized a data-driven knowledge discovery direction that complemented the computational branch of scientific disciplines. The success of data-intensive projects subsequently triggered an explosion of numerous machine learning approaches [4] [5] [6] addressing a wide range of industrial and scientific applications, such as computer vision, self-driving cars, and brain modelling, just to name a few. The next generation of artificial intelligent systems clearly represents a paradigm shift from data processing pipelines towards knowledge-centric applications. As shown in Fig. 1, these systems broke the boundaries of computational and data-intensive paradigms and began to form a new ecosystem by merging and extending existing technologies. Identifying this trend as the fifth paradigm aims to infer common aspects among diverse cognitive computing applications and steer the development of complementary solutions for addressing emerging and future challenges.

The initial landscape of data-intensive technologies was designed after Google’s Big Data stack over 15 years ago. It represented a consolidated scalable platform bringing together database and computational technologies. The open-source version of this platform was further advanced with the Spark framework resolving the immediate requirements of numerous data-intensive projects. The new model of the Spark computing platform significantly extended the scope of data-intensive applications, spreading from SQL queries to machine learning to graph processing. According to the data-information-knowledge-wisdom model [7], these projects eventually elevated data-information pipelines to practical applications of knowledge development. Cognitive systems of the fifth paradigm take the relay baton from data-driven processing pipelines and generalizes their scope with knowledge acquisition processes carried out by rational agents through the exploration of their environments.

In contrast with the MapReduce embarrassingly parallel pipelines, machine learning applications rely on the communication among distributed workers for synchronizing their internal representations. This mismatch led to the development of new distributed processing frameworks, such as GraphLab [8], CNTK [9], TensorFlow [10], and Gorila [11]. As with any standard evolutionary spiral, a variety and growing number of different approaches eventually raised the question of their consolidation. Similar problems are faced by researchers of large-scale scientific experimental facilities and computational projects. Prior to the Big Data era, most scientific algorithms were built within the third computational paradigm based on HPC clusters and Message Passing Interface (MPI) communication model. To address the immediate requirements of emerging applications, the fourth data-intensive paradigm was developed by minimally intersecting with the HPC ecosystem as shown in Fig. 1.
The strategic transition from data-intensive science towards the fifth paradigm of composite cognitive computing applications is a long-term journey with many unknowns. This paper addresses the existing mismatch between Big Data and HPC applications by presenting the Spark-MPI integrated platform aiming to bring together Big Data analytics, HPC scientific algorithms and deep learning approaches for tackling new frontiers of data-driven discovery applications. The remainder of the paper is organized as follows. Section 2 provides a brief overview of the Spark data-intensive and MPI high-performance platforms and outlines the Spark-MPI integrated approach based on the MPI Process Management Interface (PMI). Section 3 and Section 4 further elaborate the approach within the context of the hybrid MPI/GPU psychographic image reconstruction pipelines and distributed deep learning applications. Section 5 provides insights into future directions using the PMI-Exascale library. Finally, Section 6 and Section 7 survey related work and conclude with a summary.

II. SPARK-MPI PLATFORM

The integration of data-intensive and compute-intensive ecosystems was addressed by several projects. For example, Geoffrey Fox and colleagues provided a comprehensive overview of the Big Data and HPC domains. Their application analysis [12] was based on several surveys, such as the NIST Big Data Public Working Group and NRC reports, including multiple application areas: energy, astronomy and physics, climate, and others. Overall, from a conceptual perspective, the Spark-MPI platform can be considered as the Spark-based version of the Exascale Fast Forward (EFF) I/O Stack three-tier architecture [13]. The Spark-MPI platform furthermore focuses on the development of a common integrated approach addressing a wide spectrum of applications including large-scale computational studies, data-information-knowledge discovery pipelines for experimental facilities, and reinforcement learning systems.

Fig. 2 shows a general overview of the Spark-MPI integrated environment. It is based on the Spark Resilient Distributed Dataset (RDD) middleware [14] that decouples various data sources from high-level processing algorithms. RDDs are distributed fault-tolerant collections of in-memory objects that can be processed in parallel using a rich set of operations, transformations and actions. The top layer is represented by an open collection of high-level components addressing different types of data models and processing algorithms, including machine learning and graph processing. The interfaces between RDDs and distributed data sources are provided by Connectors that are already implemented for major databases and file systems.

In addition, Spark is designed to cover a wide range of workloads that previously required separate distributed systems encompassing batch applications, iterative algorithms, interactive queries, and streaming. This combination forms a powerful processing ecosystem for building data analysis pipelines and supporting multiple higher-level components specialized for various workloads. The Spark Streaming module [15] further extends the RDD pluggable mechanism with the Receiver framework enabling to ingest real-time data into RDDs from streaming sources, such as Kafka and ZeroMQ. Adherence to the RDD model automatically provided the Spark streaming applications with the same functional interface and strong fault-tolerance guarantees including exactly-once semantics.

The combination of a data-intensive processing framework with a consolidated collection of diverse data analysis algorithms offered by Spark represents a strong asset for its application in large-scale scientific projects across different phases of the data-information-knowledge discovery path. In contrast with existing data management and analytics systems, the Spark in-situ approach does not require the transformation of data into different formats and provides a generic interface between heterogeneous algorithms with heterogeneous data sources. The current version of the Spark programming model, however, is limited by the embarrassingly parallel paradigm and the Spark-MPI approach serves to extend the Spark ecosystem with the MPI-based high-performance computational applications.

MPI is an abbreviation for the Message Passing Interface standard that is developed and maintained by the MPI Forum [16]. The process of creating the MPI standard began in April 1992 and as of now, it is used in most HPC applications. The popularity of the MPI standard was determined by the optimal combination of concepts and methods challenged by two conflicting requirements: scope of parallel applications and portability across different underlying communication protocols.

The MPI standard interface extends the Spark embarrassingly parallel model with a rich collection of communication methods encompassing Remote Memory Access (RMA), pairwise point-to-point operations (e.g., send and receive), master-worker (e.g., scatter and gather) and peer-to-peer (e.g., allreduce) collective methods. In addition, the Barrier method within the collective category provides a synchronization mechanism for supporting the Bulk Synchronous Parallel paradigm. To address the scalability and performance aspects, MPI introduced the concept of Communicators that defined the scope for communication operations. As a result, this approach significantly facilitated the development and integration of parallel libraries using inter- and intra-communicators.

To support the MPI parallel model across different operating and hardware systems, the MPI frameworks are based on a portable access layer. One of its initial specifications, Abstract Device Interface (ADI [17]), was developed within the MPICH project. Later, the MVAPICH project further extended the ADI implementations to support InfiniBand interconnects and GPUDirect RDMA [18]. The OpenMPI team introduced a different solution, Modular Component Architecture (MCA) [19], that was derived as a generalization of four projects [20] bringing together over 40 frameworks. MCA utilizes components (a.k.a. plugins) to provide alternative implementations of key functional blocks such as message transport, mapping
algorithms, and collective operations. As a result, OpenMPI Byte Transfer Layer (BTL) represents an open collection of network-specific components for supporting shared memory, TCP/IP, OpenFabric verbs, and CUDA IPC, just to name a few.

Running parallel programs on HPC clusters requires interactions with external process and resource managers, such as SLURM and Torque, to enable the MPI processes to discover each other’s communication endpoints. Within the MPI ecosystem, this topic is typically addressed by the Process Manager Interface (PMI [21]). While the implementation of the PMI specification was never standardized, libraries nearly always consist of two parts: client and server. The client code is linked with the MPI program and provides messaging support to the server - it has no a priori knowledge of the overall application, and must rely on the server to provide any required information.

The PMI server is instantiated on each node that supports an MPI process and has both the ability to communicate with its peers (usually over an out-of-band Ethernet connection) and full knowledge of how to contact those peers (e.g., the socket upon which each peer is listening). The server is typically either embedded in the local daemon of the system’s resource manager, or executed as a standalone daemon started by a corresponding launcher such as \textit{mpirun}.

The Spark-MPI approach extends the scope of the PMI mechanism for integrating the Spark and MPI frameworks. Specifically, it complemented the Spark conventional driver-worker model with the PMI server-worker interface for establishing MPI inter-worker communications as outlined in Fig. 3 and Fig. 4.

The first version of the Spark-MPI approach was validated with the primary internal process manager, Hydra, used by two MPI projects (MPICH and MVAPICH). The Hydra Process Manager (PM) is started by the MPI launcher \textit{mpirun} on the launch node which subsequently spawns a tree-based collection of interconnected proxies on the allocated nodes. Each proxy locally spawns one or more application processes and then acts as the PMI server for those processes. During initialization, each process “publishes” its connection information to the proxy, which then performs a global collective operation to share the information across all proxies for
eventual distribution to the application. Within the Spark-MPI integrated platform, MPI application processes are started by the Spark scheduler (see Fig. 4). Hydra local proxies therefore were modified to suppress their launching functionality.

Recently, the Spark-MPI approach was integrated with the Open MPI framework. The OpenMPI Modular Component Architecture further streamlined its implementation as the sparkmpi plugin of the OpenRTE Daemon’s Local Launch Subsystem (ODLS). The following sections will demonstrate this approach within the context of the hybrid MPI/GPU ptychographic image reconstruction pipelines and deep learning applications.

### III. Ptychographic Image Reconstruction Pipelines

Ptychography is one of the essential image reconstruction techniques used in light source facilities. It was originally proposed for electron microscopy [22] and lately applied to X-ray imaging [23] [24]. The method consists of measuring multiple diffraction patterns by scanning a finite illumination region, also called the probe, on an extended specimen (the object). The redundant information encoded in overlapping illuminated regions is then used for reconstructing the sample transmission function. Specifically, under the Born and paraxial approximations, the measured diffraction pattern for the jth scan position can be expressed as:

$$I_j(q) = |Fq_j|^2$$  \hspace{1cm} (1)

where \(F\) denotes Fourier transformation, \(q\) is a reciprocal space coordinate, and \(q_j\) represents the wave at the exit of the object \(O\) illuminated by the probe \(P\):

$$q_j = p(r - r_j)O(r)$$  \hspace{1cm} (2)

Then, the object and probe functions can be computed from the minimization of the distance \(||\Psi - \Psi^0||^2\) as [25]:

$$\epsilon = ||\Psi - \Psi^0||^2 = \sum_j \sum_r |q_j(r) - P^0(r - r_j)O^0(r)|^2$$  \hspace{1cm} (3)

\[ \frac{\partial \epsilon}{\partial P^0} = 0 : P^0(r) = \frac{\sum_j q_j^*(r + r_j)O^*(r + r_j)}{\sum_j |O(r + r_j)|^2} \]  \hspace{1cm} (4)

\[ \frac{\partial \epsilon}{\partial O^0} = 0 : O^0(r) = \frac{\sum_j q_j^*(r)P^*(r + r_j)}{\sum_j |P(r - r_j)|^2} \]  \hspace{1cm} (5)

These minimization conditions need to be augmented with the modulus constraint (1) and included in the iteration loop. For example, the comprehensive overview of different iterative algorithms is provided by Klaus Giewekemeyer [26]. At this time, the difference map [27] is considered as one of the most generic and efficient approaches to address these types of imaging problems. It finds a solution in the intersection of two constraint sets using the difference of corresponding projection operators, \(\pi_1\) and \(\pi_2\), composed with associated maps, \(f_1\) and \(f_2\):

$$\psi^{n+1} = \psi^n + \beta \Delta(\psi^n)$$

$$\Delta = \pi_1 \circ f_2 - \pi_2 \circ f_1$$

$$f_i(\psi) = (1 + \gamma_i)\pi_i(\psi) - \gamma_i \psi$$  \hspace{1cm} (6)

where \(\gamma_{1,2}\) are relaxation parameters. In the context of ptychographic applications, these projection operators are associated with the modulus (1) and overlap (2) constraints. By selecting different values of relaxation parameters, the difference map (6) can be specialized to different variants of phase retrieval methods and hybrid projection-reflection (HPR) algorithms. Further developing HPR, Russel Luke [28] introduced the relaxed averaged alternating reflections (RAAR) approach:

$$\psi^{n+1} = [2\beta \pi_0 \pi_a + (1 - 2\beta)\pi_a + \beta(1 - \pi_0)]\psi^n$$  \hspace{1cm} (7)

The RAAR algorithm was implemented in the SHARP program [31] at the Berkeley Center for Advanced Mathematics for Research Applications (CAMERA).

SHARP is a high-performance distributed ptychographic solver using GPU kernels and the MPI protocol. Since most equations with the exception of (4) and (5) are framewise intrinsically independent, the ptychographic application is naturally parallelized by dividing a set of data frames among multiple GPUs. Then, for updating a probe and an object, the partial summations of (4) and (5) are combined across distributed nodes with the MPI Allreduce method as shown in Fig. 5.

Fig. 5. MPI communication model of the SHARP solver

The SHARP multi-GPU approach significantly boosted the performance of ptychographic applications at the NSLS-II light source facility and immediately highlighted the path for developing near-real-time processing pipelines. Table I compares the performance results for processing 512 frames on different numbers of GPUs.

| Application   | Time (s) vs Number of GPUs (Tesla K80) |
|---------------|--------------------------------------|
| SHARP-NSLS2   | 22.7 13.6 8.6  |

In the experimental settings, the time interval between frames takes approximately 50 ms, in other words 25 seconds for 512 frames. And according to Table I, the Spark-MPI application demonstrated the feasibility of the near-real-time scenario. This direction is especially important from the perspective of a new category of emerging four-dimensional tomographic applications that combine series of ptychographic projections generated at different angles of object rotation.
In these experiments, each ptychographic projection is reconstructed from tens of thousands of detector frames and the MPI multi-GPU version becomes critical for addressing the GPU memory challenges.

The Spark-MPI integrated platform immediately provided a connection between MPI applications and different types of distributed data sources including major databases and file systems. Furthermore, the Spark Streaming module reused and extended the RDD-based batch processing framework with a new programming abstraction called discretized stream, a sequence of RDDs, processed by micro-batch jobs. These new batches are created at regular time intervals. Similar to batch applications, streams can be ingested from multiple data sources like Kafka, Flume, Kinesis and TCP sockets.

For evaluating the Spark-MPI approach, the SHARP ptychographic pipeline was tested with the Kafka streaming platform, an Apache open source project that was originally developed at LinkedIn [30]. The corresponding simulation-based scenario is described with a conceptual diagram (see Fig. 6).

According to this scenario, the input stream represents a sequence of micro-batches. The Spark driver waits for a topic-init record and processes each micro-batch with the run_batch method. At the beginning of this method, the Kafka data are ingested into the Spark platform as the Kafka RDDs. To achieve a higher level of parallelism, records of micro-batches are divided into topics that are consumed by Kafka Receivers on distributed Spark workers. Each Kafka Receiver creates a topic-specific RDD and the Spark driver logically combines them together with a union operation. As a result, it prepares a distributed RDD to be processed with the MPI application.

The acceleration of image processing algorithms with the next generation of GPU devices further strengthened the direction by creating the necessary conditions for augmenting photographic pipelines with optimization procedures. The modern ptychographic approaches depend on many parameters and their choice is important for achieving the most accurate reconstruction results. For example, Fig. 7 and Fig. 8 demonstrate reconstructed object phases for different choices of constraints.

Finding the most optimal parameters can be automated with conventional optimization approaches. In addition, the pipelines can be further advanced with modern machine learning techniques for image analysis and steering reconstruction algorithms.

**IV. Deep Learning Applications**

The Spark-MPI platform was designed for building a new generation of composite data-information-knowledge discovery pipelines for experimental facilities. Deep learning applications advanced the scope and requirements of large-scale scientific projects to the next level. From the perspective of the fifth paradigm, Spark-MPI can be considered as a generic front-end of composite agent models for interacting with heterogeneous environments.

Historically, distributed deep learning frameworks were developed within the fourth paradigm of data-intensive processing platforms. On the other hand, compute-intensive tasks have been already successfully addressed with a HPC stack of hardware and MPI applications from the third computational paradigm. The parallel acceleration of deep learning algorithms was then pursued by several MPI-based projects, such as CNTK [9], TensorFlow-MaTex [31], FireCaffe [32], and S-Caffe [33].

CNTK and TensorFlow are deep learning toolkits developed by Microsoft and Google, respectively. For distributed training, CNTK relies on the MPI communication platform and can be directly deployed on HPC clusters. In contrast, the original implementation of the TensorFlow distributed version is based on Google’s gRPC interface developed for cloud computing systems using Ethernet. To leverage the HPC low latency interconnects, the TensorFlow-MaTEx project added two new
TensorFlow operators, Global_Broadcast and MPI_Allreduce, and correspondingly modified the TensorFlow runtime. The FireCaffe and S-Caffe distributed approaches were developed around single-node Caffe deep learning solvers according to the data-parallel architecture. In addition, they further accelerated the data-parallel communication schema by replacing a parameter server with the allreduce communication pattern based on a reduction tree. Recently, the TensorFlow project was extended with a hybrid communication interface based on the combination of gRPC and MPI protocols. In contrast with other deep learning applications, the TensorFlow framework provides a pluggable mechanism for registering different communication interfaces that can be interchanged with other more advanced or application-specific versions.

Within the beamline composite pipeline platform, the Spark-MPI approach was evaluated with Horovod [34], a MPI training framework for TensorFlow. The Horovod team adopted Baidu’s approach [35] based on the ring-allreduce algorithm [36] and further developed its implementation with the NVIDIA’s NCCL library for collective communication. As a result, the ring-allreduce approach replaced parameter servers of the TensorFlow distributed version with an efficient mechanism for averaging gradients among the TensorFlow workers. Their integration with the Horovod distributed framework consists of two primary steps as illustrated by the horovod_train method in Fig. 9. First, Horovod and MPI is initialized with hvd.init. And then, the TensorFlow worker’s optimizer is wrapped by hvd.DistributedOptimizer, a Horovod’s ring-allreduce distributed adapter.

```python
def horovod_train():
    # initialize Horovod
    hvd.init()
    # Extract the MNIST dataset ...
    # Build the TensorFlow model ...
    loss = ...
    opt = tf.train.RMSPropOptimizer(0.001 * hvd.size())
    # Add the Horovod distributed optimizer.
    opt = hvd.DistributedOptimizer(opt)
    # Make training operation ...
```

Fig. 9. Horovod-TensorFlow example

The Spark-MPI pipelines enable to process the same method on Spark Workers within Map operations as shown in Fig. 10. To establish MPI communication among the Spark Workers, the Map operation needs only to define PMI-related environmental variables (such as PMIX_RANK and a port number) for connecting the Horovod MPI application with the PMI server.

Implementing deep learning applications on the MPI parallel framework immediately extended the scope of the Spark-MPI ecosystem with composite pipelines as shown in Fig. 11.

For light source facilities, the development of composite pipelines involves two major topics: application of deep learning approaches for analyzing reconstructed images and development of machine learning feedback systems for steering reconstruction algorithms. According to the survey by Geert Litjens and colleagues [37], deep learning techniques pervade every aspect of medical image analysis: detection, segmentation, quantification, registration, and image enhancement. The feedback system can be viewed from the perspective of a rational agent that interacts with a reconstruction pipeline representing its environment. Depending on the applications, an agent can be built with different learning techniques. One of the most important breakthroughs is associated with the introduction of a deep Q-network (DQN) model for reinforcement learning [5]. The DQN-based approach demonstrated state-of-the-art results in various applications [38] ranging from playing video games to robotics. As shown in Fig. 11, Spark-MPI provides a generic front-end for distributed deep reinforcement learning platforms on the HPC cluster.

V. RELATED WORK

The deployment of the Spark platform on HPC clusters and its comparison with the MPI approaches has been addressed by several projects. The Ohio State University team [39] proposed an RDMA-based design for the data shuffle of Spark over InfiniBand. Alex Gittens and colleagues [40] demonstrated the performance gap between a close-to-metal parallelized C version and the Spark-based implementation of matrix factorization. To resolve this gap, they introduced the Alchemist system for socket-based interfacing between Spark and existing MPI libraries. Michael Anderson and colleagues [41] proposed an alternative approach based on the Linux shared memory file system. The third solution suggested by
Cyprien Noel, Jun Shi and Andy Feng from the Yahoo Big ML team extended the Spark embarrassingly parallel model with the RDMA inter-worker communication interface. Later, this approach was reused by the Sharp-Spark project \cite{42} within the context of ptychographic reconstruction applications. The Sharp-Spark approach followed the Yahoo Big ML peer-to-peer model and augmented it with a RDMA address exchange server that significantly facilitated the initialization phase responsible for establishing Spark inter-worker connections. As a result, the RDMA address exchange server captured the PMI functionality of the MPI implementations and provided a natural transition to the PMI-based Spark-MPI approach.

The similarity between the Spark driver-worker computational model and the data-parallel approach of deep learning solvers triggered the development of a new category of applications such as SparkNet \cite{43}, CaffeOnSpark \cite{44}, TensorFlowOnSpark \cite{45}, and BigDL \cite{46}. SparkNet directly relied on the Spark driver-executor scheme consisting of a single driver and multiple executors running the Caffe or TensorFlow deep learning solvers on its own subset of data. In this approach, a driver communicates with executors for aggregating gradients of model parameters and broadcasting averaged weights back for subsequent iterations. According to the SparkNet-based benchmark, the driver-executor scheme however introduced a substantial communication overhead that was minimized by subdividing the optimization loop into chunks of iterations. Addressing the same problem, the CaffeOnSpark team proposed extending the Spark model with an inter-worker interface providing a MPI Allreduce style method over Ethernet or InfiniBand. Later, the same team began the TensorFlowOnSpark project based on their RDMA extension to the TensorFlow distributed platform. In comparison with these projects, Spark-MPI aims to derive an application-neutral mechanism based on the MPI Process Management Interface for the effortless integration of Big Data and HPC ecosystems.

VI. PATH TOWARDS EXASCALE APPLICATIONS

The validation of the Spark-MPI conceptual solution established a basis for advancing this approach towards the production programming model based on the PMI-Exascale (PMIx) framework. Furthermore, this direction aligns with proposed changes to the MPI standard \cite{47} being supported by the PMIx community.

PMIx \cite{48} was created in response to the ever-increasing scale of supercomputing clusters, and the emergence of new programming models such as Spark that rely on dynamically steered workflows. The PMIx community has therefore focused on extending the earlier PMI work, adding flexibility to existing APIs (e.g., to support asynchronous operations) as well as new APIs that broaden the range of interactions with the resident resource manager.

The initial version of the PMIx standard focused on resolving the scaling challenges faced by bulk-synchronous programming models operating in exascale systems \cite{49} \cite{50}. However, version 2 of the standard directly addressed the needs of dynamic, asynchronous programming models by providing APIs for changing resource allocations (both adding and returning resources, including the ability to “lend” resources back to the resource manager for limited periods of time); controlling application execution (e.g., ordering termination and/or migration of processes, and coordinating requests for application preemption); notification of events such as connection requests and process failures; and connections to servers from “unknown” processes not started by the server.

The Spark-MPI programming model utilizes the last feature as a mechanism by which the processes started by the Spark scheduler can connect to a local PMIx server. The PMIx library includes methods for automatically authenticating connections to the server based on a plugin architecture, thus allowing for ready addition of new methods as required. Servers stores their rendezvous information in files located under system-defined locations for easy discovery, and the client library executes a search algorithm to automatically find and connect to a server during initialization.

Once connected to the server, the PMI-aware processes can utilize PMIx to asynchronously request connections to one or more processes. The connect and disconnect APIs in version 2 of the PMIx Standard retain support for bulk-synchronous programming models such as today’s MPI while providing the extensions needed for asynchronous models. Both require that the operation be executed as a collective, with all specified processes participating in the operation prior to it being declared complete - i.e., all processes specified in a call to PMIxConnect must call that API in order to complete the operation. In addition, the standard requires that the host resource manager (RM) treat the specified processes as a new “group” when considering notifications, termination, and other operations, and that no request to “disconnect” from a connected group be allowed to complete until all collectives involving that group have also completed.

Finally, the PMIx community recognized that programming libraries have continued to evolve towards more of an asynchronous model where processes regularly aggregate into groups that subsequently dissolve after completing some set of operations. These new approaches would benefit from an ability to notify other processes of a desire to aggregate, and to allow the aggregation process itself to take place asynchronously.

Accordingly, calls by PMI-aware processes to PMIxConnect are first checked by the PMIx server to see if the other specified participants are available and have also called PMIxConnect - if so, then the connection request will result in each involved process receiving full information about the other participating processes (location, endpoint information, etc.) plus a callback containing the namespace assigned to the connected group. The latter can be considered the equivalent of a communicator and used for constructing that object.

If one or more of the indicated processes has not executed its call to PMIxConnect, then the server will issue an event notification requesting that the process do so. Application processes can register callback functions to be executed upon
receipt of a corresponding event, and events are cached so they can be delivered upon process startup if the event is generated before that occurs. Once receiving a connection request event, the process is given sufficient information in the notification to allow it to join the requesting group, thereby completing the collective operation. Applications can provide an optional timeout attribute to the call to PMIx_Connect so the operation will terminate if all identified participants fail to respond within the given time limit.

Note that any single process can be simultaneously engaged in multiple connect operations. For scalability, PMIx does not use a collective to assign a global identifier to the connect operation, instead utilizing the provided array of process IDs as a default method to identify a specific PMIx_Connect operation. Applications can extend the ability to execute multiple parallel operations by providing their own string identifier for each collective as an attribute to the PMIx_Connect API. Note that all participants in a given collective are required to call PMIx_Connect with the same attribute value.

In cases where the involved hosts are controlled by different RMs, the namespace identifier provided by the host RM for use in PMIx is no longer guaranteed to be unique, thereby leading to potential confusion in the process identifiers. Accordingly, PMIx defines a method for resolving any potential namespace overlap by modifying the namespace value for a given process identifier to include a clusteridentifier - a string name for the cluster that is provided by the host RM, or application itself in the case of non-managed hosts.

The accumulated features of the PMIx distributed framework are identified as a new Exascale cluster service that supplements the conventional resource management and scheduling platform for gluing together HPC and Big Data applications. On HPC clusters, support for PMIx is currently integrated with the Open MPI run-time environment and Simple Linux Utility for Resource Management (SLURM [51]). Therefore, the deployment of the Spark-MPI platform on HPC clusters will be streamlined by adding SLURM into the list of Spark schedulers (see Fig. 2): Standalone, YARN [52], Apache Mesos [53] and Kubernetes [54]. As illustrated by the Spark-MPI psychographic and deep learning examples, this deployment approach is consistent with the Spark computational model. Furthermore, the asynchronous models supported by the PMIx framework highlight the next direction for deploying reinforcement learning architectures [55] on HPC clusters.

VII. CONCLUSIONS

The paper addresses the existing mismatch between Big Data and HPC applications by presenting the Spark-MPI integrated platform for bringing together Big Data analytics, HPC scientific algorithms and deep learning approaches for tackling new frontiers of data-driven discovery applications. The approach was validated with three MPI projects (MPICH, MVAPICH and Open MPI) and established a basis for advancing the Spark-MPI interface towards the Exascale platform using the PMI-Exascale (PMIx) framework. Furthermore, this direction aligns with a paradigm shift from data-intensive processing pipelines towards the fifth paradigm of knowledge-centric cognitive applications. Within the context of new applications, Spark-MPI aims to provide a generic front-end for distributed deep reinforcement learning platforms on HPC clusters. As a result, the Spark-MPI platform represents a triple point solution located at the intersection of three paradigms.

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