AI-coupled HPC Workflows

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Increasingly, scientific discovery requires sophisticated and scalable workflows. Workflows have become the “new applications,” wherein multi-scale computing campaigns comprise multiple and heterogeneous executable tasks. In particular, the introduction of AI/ML models into the traditional HPC workflows has been an enabler of highly accurate modeling, typically reducing computational needs compared to traditional methods. This chapter discusses various modes of integrating AI/ML models to HPC computations, resulting in diverse types of AI-coupled HPC workflows. The increasing need of coupling AI/ML and HPC across scientific domains is motivated, and then exemplified by a number of production-grade use cases for each mode. We additionally discuss the primary challenges of extreme-scale AI-coupled HPC campaigns—task heterogeneity, adaptivity, performance—and several framework and middleware solutions which aim to address them. While both HPC workflow and AI/ML computing paradigms are independently effective, we highlight how their integration, and ultimate convergence, is leading to significant improvements in scientific performance across a range of domains, ultimately resulting in scientific explorations otherwise unattainable.

I. INTRODUCTION

Scientific discovery increasingly requires sophisticated and scalable workflows. Workflows have become the “new applications,” wherein multi-scale computing campaigns comprise hundreds to thousands of heterogeneous executable tasks. Introducing AI/ML models into traditional high performance computing (HPC) workflows has been an enabler of highly accurate modeling, and has been demonstrated to be a promising approach for significant performance improvements.

Advances in statistical algorithms and runtime systems have enabled extreme scale ensemble-based applications [1] to overcome limitations of traditional monolithic simulations. However, in spite of several orders of magnitude improvement in efficiency from these ensemble algorithms, the complexity of phase space and dynamics for modest physical systems require additional orders of
magnitude improvements and performance gains. Integration of traditional HPC workflows with AI/ML methods holds real promise for overcoming such barriers [2].

In many application domains, the integration of AI/ML into a computational workflow is a favorable way to obtain large performance gains, and presents an opportunity to jump a generation of simulation enhancements. For example, one can view the use of learned surrogates as a performance boost that can lead to substantial speedups, as calculation of a prediction from a trained network can be many orders of magnitude faster than full execution of the simulation [3, 4]. In addition to the use of learning for advanced sampling as mentioned above, other simple examples include the use of a surrogate to represent a chemistry potential [5], or a larger grain size to solve the diffusion equation underlying cellular and tissue level simulations [6].

There are various modes (couplings) of integrating traditional HPC methods and simulations, with AI/ML methodologies, resulting in diverse types of AI/ML “enhanced” HPC workflows. This chapter provides an overview the various couplings and how they can result in the adaptive execution of workflow applications comprising heterogeneous tasks. We identify the core characteristics of such workflow applications, as well as discuss state-of-art tools and workflow applications.

II. LEARNING EVERYWHERE PARADIGM

There are two classes of interplay between HPC and ML. In the first, ML directly enhances and impacts applications; in the second class, ML enhances the HPC environment on which those applications operate. This chapter exclusively focuses on the former.

Central to the first class, as well as the re-examination and overcoming the performance barrier, is the need to integrate ML methodologies and HPC. In this approach – learning enhanced simulations and campaigns – we include the use of neural surrogates, with a neural network directly predicting either the full results of simulations, or components thereof. This also includes using learning methods to control and steer simulations, for example, efficient campaigns that steer ensembles smartly through phase space[7–10]. We have identified three high-level modes of integrating ML with HPC [3, 11, 12]: ML-in-HPC, ML-out-HPC, and ML-about-HPC.

ML-in-HPC represents the scenario when an ML model is introduced in lieu of a component of the HPC simulations, or possibly, in lieu of the total simulation itself, i.e., ML model serves as a “total surrogate”. ML-out-HPC captures situations wherein a ML model resides “outside” of the traditional HPC simulation loop, but dynamically controls the progression of the HPC workflow. For example, Active Learning and Reinforcement Learning control of computational campaigns.
FIG. 1. Illustrating the three modes of ML-x-HPC: (1) ML-in-HPC: AI/ML surrogate models are used to replace part or entire simulations. (2) ML-about-HPC: AI/ML complements traditional computational tasks and possibly steers the tasks, improving their scientific results or efficiency (3) ML-out-HPC: A high-level AI/ML based algorithm, such as active learning or reinforcement learning is used to dynamically control the campaign, or steer the workflow as a whole (as opposed to just the tasks). Typically, ML-in and ML-about are directly responsible for producing output for further analysis, while ML-out drives this production.

Finally, **ML-about-HPC** represents the situation where ML models are concurrent and coupled to the main HPC tasks. Figure 1 illustrates these primary modes coupling AI/ML to HPC workflows. These three modes are not mutually exclusive, and will increasingly be used collectively.

The *learning everywhere* paradigm [3, 11, 12] contends that increasingly, scientific applications will achieve performance gains and methodological advances by using all three modes of combining learning approaches with HPC simulation-based techniques. In the next section, we will discuss multilevel drug selection as a canonical example of learning-everywhere paradigm, but additional prominent examples include materials design and earth-systems modeling [4].

There are many open challenges that implementing and translating the paradigm to practice poses. For example, how and where can ML effectively enhance or accelerate HPC simulations? How to make ML methods that work in tandem with HPC simulations scalable, robust, and reliable? For a given computational campaign what is the optimal mix and execution plan of ML-in, out and about HPC? Furthermore, there are system and software challenges and opportunities
in combining ML and HPC systems software, hardware, and overall infrastructure. What are the correct programming models and abstractions to manage the diverse “computational tasks” viz., ML training & inference along with traditional HPC workloads? What runtime systems are needed to manage the heterogeneous workload effectively? What are the general motifs of interaction between ML and HPC, and their influence on design of runtime systems?

A leitmotif of the learning everywhere paradigm is effective performance, i.e., the performance improvement obtained by substituting a traditional HPC method with an integrated HPC and learning method. Effective performance measures the improvement in application performance metric (e.g., computational cost, improved time-to-solution, or the achievement of scientific objective) when using ML methods in conjunction with HPC, as compared to using HPC methods stand-alone. For example, effective performance can be measured as the time-to-solution ratio of the traditional approach vs. the learning-enhanced approach. If a traditional parameter study ran 1000 simulations to determine an optimal engineering design, while a model-based optimizer produced the same optimum in 100 simulations, the effective performance of the learning enhanced application is 10. If, additionally, the ML-based approximations in the simulation accelerated computation by a factor of 10, the effective performance would be 100. These orders-of-magnitude increase in effective performance as learning-enhanced high-performance computing takes root [13] are at the heart of the motivation for this new paradigm of computation.

III. LEARNING EVERYWHERE EXAMPLES

This section provides an overview of various use cases and exemplar applications, across scientific domains which couple HPC and ML/AI. Table I groups use cases and exemplar applications using the three modes described in Sec. II. Use cases and applications were selected to provide a representative overview of the ML techniques currently employed to couple ML with HPC, and to cover diverse scientific domains in which this coupling is bringing innovation and unprecedented performance improvement.

A. ML-in-HPC

Workflows in high energy physics are multi-scale, comprising quantum field theoretic calculations, detector simulations, and classical reconstruction of physical objects. Each scale has considerable computational requirements and, using only traditional methods, it is impossible to produce
| Mode            | Domain                        | Application     | Coupling Mechanism               |
|-----------------|-------------------------------|-----------------|----------------------------------|
| ML-in-HPC       | High Energy physics           | Atlfast3        | Surrogate methods                |
|                 | Molecular Dynamics            | DeePMD-kit      | Surrogate methods                |
| ML-about-HPC    | Atomistic simulations         | Proxima         | Runtime surrogate tuning         |
|                 | Material engineering          | Colmena         | Runtime model (re)training/configuration |
|                 | RAS protein/Cancer            | MuMMI           | Runtime ML-based selection       |
| ML-out-HPC      | Cancer research               | DeepHyper       | Automated machine learning       |
|                 | Cyberinfrastructure           | SIOX            | Offline ML                       |
|                 | Materials Science             | EXARL           | ML-guided simulations            |

TABLE I. Examples of ML-x-HPC modes across scientific domains.

sufficient numbers of Monte Carlo events to maintain statistical adequacy with recorded data. As such, ML techniques, including generative adversarial networks, are becoming an increasingly attractive alternative to standard frameworks implementing step-by-step model predictions.

For example, Fig. 2 shows an illustration of the ATLAS Collaboration’s “fast” simulation framework, Atlfast3 [14], where ML-based techniques are used in place of intensive Geant4 [15] simulations. In this configuration, surrogates are employed in lieu of full Geant4 simulations for specific particle types, energies and subdetectors to reduce overall simulation times up to several orders of magnitude. At the same time, those surrogates allow to maintain accurate detector modeling for new physics searches, statistically-limited analyses, background processes, and detector upgrades.

Another significant example of ML-in-HPC can be found in the traditional *ab initio* MD (AIMD) methods for modeling atomistic phenomena. Due to demanding computational requirements (cubic scaling in the number of electronic degrees of freedom), most AIMD applications are limited to \(O(1000)\) atoms. However, AIMD plays a major role in addressing many issues related to, e.g., drug discovery, complex chemical processes and nanotechnology. As such, tremendous efforts have been afforded to more efficient methods, including ML.

Jia et al. [5] offer a powerful example of ML-in-HPC applied to AIMD. Jia’s approach employs an ML-based simulation protocol which uses surrogates (Deep Potential MD) in conjunction with a highly-optimized code (a GPU-accelerated DeePMD-kit [16]) to simulate \(O(10^8)\) nanosecond-long trajectories in 24 hours. This record-setting accomplishment efficiently scaled to the whole 4,560 nodes of the Summit supercomputer, reaching double/mixed-single/mixed-half precision performance of 91/162/275 PFLOPS. Compared to other state-of-the-art, Jia et al. showed more than
FIG. 2. Illustration of ML-in-HPC, showing a configuration of different surrogate modules replacing Geant4 in the ATLAS detector. Different ML-based components can be employed, depending on the type of process being modeled, specific subdetectors, particle types and energies. Image from [14].

$O(10^{-3})$ reduction in time-to-solution (TTS) [s/step/atom].

Ref. [5] is a prime example of how ML-in-HPC, which is on the cusp of a paradigmatic change as learning approaches influence the way both ODE and PDEs are being solved. For example, Karniadakis et al [17] are investigating how to solve and discover new PDEs via deep learning. For partial differential equations (PDEs), neural operators directly learn the mapping from any functional parametric dependence to the solution. Thus, they learn an entire family of PDEs, in contrast to classical methods which solve one instance of the equation [18].

B. ML-about-HPC

Replacing computationally intensive computations with surrogate approximators aims to reduce TTS often by sacrificing accuracy with respect to more complete models. Optimally balancing TTS and accuracy is a non-trivial task, and the former is often neglected in order to reach the desired accuracy. Proxima [19], provides real-time feedback from executing simulations and it has been utilized to develop systematic and automated methods for dynamically tuning surrogate configurations. An iterative simulation workflow, representative of the ML-about-HPC mode, evaluates uncertainties associated with the use of surrogates, concurrently updating configurations based on a distance metric to learn features and an accuracy metric to evaluate prediction. Between iterations, surrogates evolve and replace less optimized ones, providing the coupling between concurrent surrogate tuning and the main HPC campaign.
The Proxima framework has been demonstrated in a Monte Carlo sampling application, where the first-principles Hartree-Fock [20] prediction target is replaced with a Proxima-managed surrogate. Mean absolute error (MAE) and TTS comparisons are made between Proxima and a surrogate strategy with a fixed distance threshold (based on scientific trial-and-error). In certain scenarios, the fixed strategy outperforms Proxima in terms of TTS. However, the utility of user-defined error bounds ensures more robust results with Proxima. By determining values for surrogate configurations automatically during workflow execution, Proxima is able to satisfy error bounds while achieving as much as 5.5x speedup in TTS.

Estimating properties of large collections of molecules is often necessary to find candidates for medical therapeutics, next-generation batteries, etc. However, the number of possible candidates for a single application, and therefore the number of different experimental configurations required to test them all, is often intractable. Large-scale workflows have thus come to adopt methodologies to provide an ML model training and retraining runtime to decide which computations to perform based on previous outputs.

The Colmena framework [21] facilitates a user-defined steering for workflow execution. Using an example application involving an ML-guided search of $10^5$ molecules with high resistance to oxidation electrolyte design, the Colmena workflow provides components to actively train and learn as simulations are executed. Colmena performs a concurrent execution mode, having ML and traditional simulations running side-by-side throughout the workflow. Candidacy of molecules is evaluated using ML models which are scored based on selection criteria and then are ordered based on their score. Molecules appearing at the top of the ordered list reflect most suitable candidates, and subsequently additional simulations are executed. Colmena is reported to find candidate molecules at rates 100 times that of traditional computational solutions, and scaling up to 1024 nodes (65,636 cores) on Theta supercomputer.

A naturally more complicated scenario is the development of therapeutics. This type of R&D can take years or decades to come to fruition due to the complicated computational modeling involved in searches for candidate drugs and strict FDA approval procedure. In the context of cancer treatments, for example, it is suggested that Ras proteins are involved in nearly a third of all human cancers in the US [22]; however, many physiochemical properties of Ras-Raf-membrane dynamics are not fully understood. The inherent multi-scale nature of such processes makes computational modeling challenging, and each scale is traditionally simulated separately.

The massively parallel Multiscale Machine-Learned Modeling Infrastructure (MuMMI) [23, 24] couples three resolution scales with ML-based selection, effectively promoting important configu-
rations from coarse-grained to all atomistic (highest resolution). The autonomy and full power of MuMMI is realized through dynamic co-scheduling of tasks which is achieved by tying together application and coordination layers of the workflow. MuMMI achieves a 98% GPU occupancy for more than 83% of 600,000 node hours, coordinating 24,000 jobs and managing several terabytes of data daily. Furthermore, the split architecture, separating the workflow application from coordination, permits generalizability, making the infrastructure attractive beyond drug design.

C. ML-out-HPC

Increasing computational power helps to produce more rapidly predictive models, larger volumes of collected data enables higher fidelity predictions. However, improving models typically implies introducing additional complexity such as substantially increasing trainable parameters. As such, building ML models for complex diseases—such as cancer—requires a significant amount of trial-and-error, and intervention from both epidemiologists and ML experts, making diagnosis, detection, prognosis and prediction extremely time-consuming tasks.

Work from Balaprakash et al. [25] introduces a reinforcement, learning-based neural architecture search for autonomous deep learning development. By targeting specific class of cancer data, the automated approach finds neural architectures requiring fewer trainable parameters—thus reducing training time—which produce equivalent or better accuracy to manually finely-tuned architectures. Scalability is demonstrated using 1024 nodes of the Theta supercomputer, with the best neural architecture outperforming the manually designed network in terms of scientific results, and having $11.5 \times$ fewer trainable parameters and $2.5 \times$ faster training time. These results suggest ML-driven neural architecture search has the potential to accelerate cancer research, allowing researchers in the field to automate neural architecture discovery using HPC.

To accommodate needs of scientists and non-ML experts, a recent effort providing flexible user tools for distributed and scalable reinforcement learning (RL) is the EXARL [26] from the Co-Design Center for Exascale Machine Learning Technologies (ExaLearn). EXARL enables interfacing with existing exascale applications—e.g., LAMMPS [27] and NWChem [28]—which domain scientists can guide using RL algorithms and associated neural network architectures. In addition to the miniGAN proxy application [29], the ExaLearn team has demonstrated its usefulness and exercise its scalable RL to a block copolymer application [30]. This is generally a complicated problem as materials may evolve toward generic states or become trapped in a metastable state, and thus requiring hundreds of experimental trials to reach a target state. By mapping this problem
to RL, wherein a NN is trained to update annealing temperatures for subsequent block copolymer simulations, EXARL was able to show learning convergence for guiding the annealing process to both equilibrium and non-equilibrium states. Ongoing and future work includes expanding to new scientific domain use-cases, and enablement of further scaling and execution of multi-process applications.

While HPC drives much of scientific research and discovery, the platforms themselves require continuous performance analysis and optimizations to reach their full potential. This is particularly difficult for I/O systems which are commonly bottlenecks in computing systems, trailing in performance with respect to computational capabilities by several orders of magnitude. This is due to complexity of I/O systems, requiring intimate knowledge of the underlying components and potentially thousands of parameters need to mutual optimization.

The SIOX Project [31] monitors, diagnoses and optimizes I/O system parameters of HPC platforms. The modular design of SIOX provides plug-and-play capability, allowing to use diverse monitoring tools for data production. Plugins use offline ML to predict the performance gains or losses for different optimization actions and online ML to perform anomaly detection. SIOX implements actuator tasks to apply the selected optimizations and evaluator tasks to measure achieved performance.

D. Learning EveryWhere: A Canonical Example

The three modes of coupling ML with HPC are not mutually exclusive. In fact, the most ambitious multi-scale or multi-stage campaigns involve all three modes. For example, considering the universe of about $10^{68}$ possible drug compounds, efficient and high throughput frameworks for early stage drug discovery [32] are needed. *In silico* methodologies need to be improved to better select lead compounds that can proceed to later stages of the drug discovery protocol accelerating the entire process [33–35]. Innovations that integrate AI and simulation at multiple levels are demonstrating promise in overcoming fundamental limitations.

We discuss IMPECCABLE as a representative campaign that is comprised of ML-in-, ML-out-, and ML-about-HPC workflows, supplanting traditional HPC with learning everywhere. Although, IMPECCABLE was developed for COVID19 therapeutics, the multi-stage and AI-HPC integrated campaign is representative of a range of campaigns in material and molecule design, climate science, inter alia.

The campaign consists of an iterative loop initiated with ML predictions (ML1), followed by
FIG. 3. IMPECCABLE is a virtual drug discovery pipeline, from hit to lead through to lead optimization. The constituent components are deep-learning based surrogate model for docking (ML1), Autodock-GPU (S1), coarse and fine-grained binding free energies (S3-CG and S3-FG) and ML-enhanced MD simulations.

data processing stages S1, S2, S3. ML/AI techniques (ML1 and S2) interfaced with physics-based methods estimate docking poses of compounds that are promising leads for a given protein target (S1) and binding free-energy computations (S3). Put together, the campaign glues together learning methods with innovative physics-based methods, with iterative algorithms allowing both upstream and downstream feedback to overcome fundamental limitations of classical in silico drug design [8]. It includes high-throughput structure-based protein-ligand docking simulations, followed by iterative refinements to these virtual screening results to filter out compounds that “show promise” in biochemical or whole-cell assays, safety and toxicology tests.

ML techniques overcome the limitations of S1 and S3 by predicting the likelihood of binding between small molecules and a protein target (ML1), and accelerating the sampling of conformational landscapes to bound the binding free-energy values for a given protein-ligand complex (S2). Interfacing ML approaches with physics-based models (docking and MD simulations), we achieve at least three orders of magnitude improvement in the size of compound libraries that can be screened with traditional approaches, while simultaneously providing access to binding free-energy calculations that can impose better confidence intervals in the ligands selected for further (experimental or computational) optimization.
S1 is an example of ML-in-HPC mode (i.e., training and using a surrogate in lieu of computations), while S2 [36] represents a common instance of the ML-about-HPC mode. Although ML-out-HPC was not implemented on HPC platforms at the time of publication, prototypes were used to determine optimal allocation of computational resources across S1-S3 [37].

The impact of the algorithmic, methodological and infrastructural innovations resulted by measuring both raw throughput—defined as ligands per unit time, scientific performance—defined as effective ligands sampled per unit time, as well as the quality of ligands selected [8, 9, 38, 39]. Thus, the IMPECCABLE [9, 38] drug discovery pipeline is the quintessential example of the learning everywhere paradigm.

IV. MACHINE LEARNING AND SCIENTIFIC WORKFLOW APPLICATIONS

The coupling of AI/ML methods to HPC simulations, poses unprecedented challenges to the development of middleware systems to support the execution of scientific workflow applications on increasingly heterogeneous computing platforms. We outline three main challenges, and discuss how the six use cases introduced in §III address those challenges.

A. Challenges

Traditionally, scientific workflows were defined as either High Throughput Computing (HTC) or High Performance Computing (HPC). The former came to define the distributed workflows of the grid era; the latter epitomized by complex and large DAGs of processing. The increasing importance and popularity of ensembles of HPC simulations, resulted in a convergence of these two primary modes – high-throughput of high-performance computing (HT-HPC). And ultimately workflows involving dependencies between large number of (parallel) tasks, and represented by DAG task-graph. The current workflow middleware reflects these dominant paradigms and trends. Moving forward, they will be supplanted by middleware systems which support ML coupling to HT-HPC workflows at multiple levels of the application.

Integrating ML methods with HPC simulations, results in three primary classes of workflows: (1) Hybrid HPC-HTC workflows; (2) ML-coupled workflows, discussed in §III; and (3) Edge-to-center workflows, which typically involve integrating distributed ML with HPC workflows (e.g., with ML on the edge). This is rapidly becoming an increasingly important type of workflow with distributed data production and ML execution, and their need to couple to large data-centers.
Unsurprisingly, coupling ML to HPC simulations also introduces many challenges — at application, middleware and resource levels. In this chapter we focus on three main middleware development challenges related to resource and task execution management to realize the full potential of ML for scientific workflow applications: (1) task heterogeneity; (2) adaptive execution; and (3) application performance.

ML introduces multiple levels of task heterogeneity. Alongside traditional CPU, GPU and, possibly, multi-node MPI tasks, ML usually requires the execution of high-throughput function calls, often implemented in an interpreted language as Python, and that may depend on datasets distributed across repositories managed by diverse organization and platforms. As a consequence, the middleware that manages the execution of the workflow application, has to be able to concurrently schedule, place and execute MPI executables alongside Python functions with wildly varying execution lifetimes— the former for hours, the latter for as little as fractions of seconds.

One of the main scientific reasons to use ML in workflow applications is to improve the analysis that can be done on the data produced by part of the tasks of the workflow application. While some tasks progress, ML models can be used to learn relevant features and better drive the progress of the workflow at runtime. In order to leverage the potential of ML-based analysis, the workflow application has to become adaptive, i.e., being able to integrate the results of ML inferences and alter the workflow graph accordingly, and define the amount of learning to perform at runtime, especially when that amount cannot be known in advance, before execution [36]: simulations must be paused and restarted with new starting points, and/or a diverse number, type or size of simulations must be started to account for changed requirements, based on ML inferences. Further, ML training can vary at runtime, both in amount per model and across multiple models, when used. That has consequences for the capabilities of the workflow execution middleware. Alongside the capability of traversing an acyclic direct graph (DAG) to produce a concrete execution plan, workflow middleware has to update that DAG, pausing/restarting the execution of some of its nodes, adding/removing some nodes, and/or dynamically changing the amount of resources allocated to those nodes.

Finally, for ML to be useful it must enable improvements in both scientific and execution performance. On one side, the use of ML modeling and inference needs to improve the scientific computation that it drives, e.g., the accuracy and/or physically simulated duration. On the other side, ML has to effectively and efficiently use available resources when integrated within a workflow application. Resource efficiency depends on both the amount of time those resources are used in order to achieve the planned goal of the workflow application, and the percentage of available
resources utilized to achieve that goal. This means that the workflow execution middleware has to manage the concurrent execution of heterogeneous tasks in a way that maximizes resource utilization while minimizing the workflow application total time to completion.

B. Framework and Middleware Solutions

The ML-enabled workflow frameworks described earlier address some or all the challenges of task heterogeneity, adaptive execution and framework’s performance (as opposed to scientific performance), at different levels of the middleware software stack.

Proxima [40] is implemented as a Python library used to wrap a Python function. Based on its inputs, Proxima calculates when to infer via a surrogate model or running the wrapped function. Inferring via a surrogate model is often faster than executing the wrapped function, resulting in an overall speedup. Proxima continually monitors the function execution, dynamically adapting the surrogate configuration parameters and determining when to retrain the surrogate model at runtime. While Proxima executes different types of functions (inference, monitoring, evaluation, configuration and retraining), it is not optimized for HPC and does not concurrently execute those different functions at scale. Proxima implements adaptivity, by retraining at runtime and parametrizing the model. Finally, Proxima performance as Python library is evaluated in terms of Proxima logic, model (re)training, surrogate usage, and inference.

Colmena [21] a general-purpose Python library for steering ensembles of experiments on HPC computing systems. Colmena is designed to execute different types of tasks, including: simulation, inference (via surrogate models) model training, and candidate generation. Different from Proxima, Colmena is designed to scale on HPC platforms, addressing the heterogeneity challenge by coordinating the (possibly concurrent) execution of different types of tasks. Similar to Proxima, Colmena enables adaptivity via surrogate parameterization and (re)training. Colmena uses Parsl as its runtime, avoiding a reimplementation of a ML-specific and general-purpose runtime capabilities. Colmena’s performance is measured in terms of communication overheads (e.g., requests or result object, and data input or output), and scaling performance with different task duration, result size, and number of workers.

EXARL [29] is a Python framework build on OpenAI Gym to enable the implementation of arbitrary reinforcement learning (RL) algorithms and their execution at scale. EXARL implements agents, each based on a learner/actors architecture in which each agent concurrently uses a scalable number of learners. Leaners can be implemented as multi-process or MPI executables; multiple
agents can be executed concurrently. EXARL does not offer specific capabilities for mapping and launching its agents, relying on third party tools like, for example, batch system and an MPI infrastructure. As such, EXARL does not support task heterogeneity and implementing adaptivity requires coding capabilities on top of its agents. Performance is currently under evaluation, in terms of scalability of the size of each learners, and number of concurrent learners and agents.

MUMMI [23, 24] is a Python workflow manager that coordinated the execution of massively parallel multiscale simulations. MUMMI allows to coordinate the concurrent execution of macro- and micro-scale simulation tasks, coupling them via ML methods to decide what space of the macro-scale simulations should be explored by the micro-scale ones. MUMMI uses the Flux job scheduler to coordinate the scheduling and execution of heterogeneous tasks on both CPUs and GPUs, and the Maestro workflow plugin to interface its workflow manager component to Flux. MUMMI enables adaptivity, allowing (re)training of ML models at runtime and using them for steering the simulations. MUMMI’s performance is evaluated in terms of resource utilization and number of concurrent simulations executed.

IMPECCABLE [8, 9] is a drug discovery pipeline that executes heterogeneous tasks (i.e., MD simulations, ML training and inference) on both CPUs and GPUs at scale. Implemented using RADICAL-Cybertools as workflow middleware and runtime systems, it also uses DeepDriveMD. IMPECCABLE enables adaptivity by clustering MD trajectories to steer the ensemble of MD simulations. This may include either starting new simulations (i.e., expanding the pool of initial MD simulations), or killing unproductive MD simulations (i.e., simulations stuck in meta-stable states). IMPECCABLE also supports runtime evaluation of training of docking surrogate(s). IMPECCABLE’s performance is evaluated in terms of resource utilization, framework’s overheads, and total time to completion of the pipeline and each of its stages.

Importantly, the capabilities offered by DeepDriveMD and RADICAL-Cybertools are portable across use cases and computational campaigns. DeepDriveMD and RADICAL-Cybertools capabilities which are utilized for IMPECCABLE, also allowed for coordinating the diverse simulations coupled to ML models, and automate their execution at scale for the #COVIDisAirborne [41] campaign. Work is underway to use RADICAL-Cybertools to support workflow orchestration, heterogeneous task execution and adaptivity at scale.
V. DISCUSSION

The success of ML-enabled HPC workflows brings to the forth several challenges and opportunities: (1) Engineering middleware and frameworks to support for ML-enabled HPC workflows; (2) ML-HPC Benchmarks to measure both execution and effective performance; (3) Online ML model engineering, to name just a few.

Consistent with the current workflow application landscape, many ML methods are being implemented as single-point software solutions, supporting specific user-facing interfaces, use cases and HPC platforms. Nonetheless, as seen in §IVB, some solutions are built over existing middleware, seeking benefits of well-engineered and general-purpose systems. Thus, one of the main requirements in middleware engineering for ML and HPC will be to progressively separate the applications, framework, middleware and platform concerns, enabling ML support across the stack, without having to code a plethora of independent solutions that all implement similar capabilities.

Another of the main items of the ML-enabled HPC workflow applications roadmap, is to promote the integration among existing middleware solutions to support the development of domain-specific ML frameworks. While the middleware layer should be domain-agnostic, offering general-purpose resource and runtime management capabilities, often domain scientists require frameworks tailored to their programming models and abstractions. For example, some scientists may prefer a configuration-based interface to set their applications’ parameters, while others require an API to manage parallelism at loops level. The goal will be to develop frameworks tailored to ML-enabled workflow applications, that leverage runtime capabilities already available, and expose dedicated abstractions to the users while hiding low-level details.

Currently, filesystem performance and implementation of in-memory data sharing are among the main limitations faced by ML-driven workflow applications on HPC platforms. Often, filesystems become bottlenecks for the I/O intensive operations required by ML, especially when performed on data continuously generated at runtime. In-memory approach to data exchange among diverse types of workflow tasks still requires using task-level capabilities[42]. That creates friction between using middleware capabilities to implement coordination protocols and the need to implement those protocols within the tasks themselves because of in-memory communication requirements. That impedes a clean separation of concerns between middleware and tasks, hindering the development of general-purpose, production-grade solutions.

Finally, with the growing number of datasets stored on cloud platforms and the need to leverage diverse programming and computation paradigms, integrating cloud and HPC resources has
become a priority. Developing robust and reliable solutions for such integrations is a sociotechnical challenge. Socially, cloud and HPC resources leverage different economic models, making difficult to reconcile two different resource allocation processes. Technically, the HPC multitenant batch systems with their non-elastic resource allocations, heavily biased towards large and long single MPI jobs, does not match the platform, container and function as a service models implemented by cloud providers. It will be important to develop resource brokering systems, designed to seamlessly execute large-scale, ML-enabled workflow applications on diverse and heterogeneous resources.

Performance will be critical for the future development of ML-enabled workflow applications. Steady-state performance and resource utilization for large-scale workflows is a known challenge. For example, workflows that helped advance research and response to COVID19 and underpinned the Gordon Bell 2020 Special Prize for COVID19 finalists had impressive peak performance, but modest steady-state performance. With increasing heterogeneity and temporal variation in the duration of tasks and services – as can be expected with ML-coupled HPC workflows, improving steady-state performance and resource utilization becomes challenging.

Effective performance, and its measure of scientific improvement over other methods, will have to be complemented by runtime performance to assure effective and efficient utilization of available computing resources. In that context, Benchmarks will play a fundamental role to drive both software and platform development. Benchmarks will have to be accessible and recognized by relevant scientific communities, enabling to compare performance among algorithmic methods and application execution. Without those benchmarks, it will not be possible to converge towards effective algorithmic solutions and, importantly, assess how efficiently future platform architectures will support ML-enabled workflows.

The learning everywhere examples show how ML methods will have to be integrated at multiple levels within workflow applications and the middleware that enable their executions. Whereas the real impact will arise from computational campaigns that integrate ML with HPC, ML methods will also play a fundamental role for the middleware, improving online monitoring, tracing and profiling. ML methods will also enable improved scheduling algorithms, essential for the effective placement of tasks at the upcoming exascale, and preemptive data staging and caching.

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