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A Unifying Framework to Enable Artificial Intelligence in High Performance Computing Workflows

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Abstract

Current trends point to a future where large-scale scientific applications are tightly-coupled HPC/AI hybrids. Hence, we urgently need to invest in creating a seamless, scalable framework where HPC and AI/ML can efficiently work together and adapt to novel hardware and vendor libraries without starting from scratch every few years. The current ecosystem and sparsely-connected community are not sufficient to tackle these challenges, and we require a breakthrough catalyst for science similar to what PyTorch enabled for AI.

A Unifying Framework to Enable Artificial Intelligence in High Performance Computing Workflows

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The potential for scientific discovery is on the cusp of a seismic change because of a confluence of factors, such as rapid advances in Artificial Intelligence and Machine Learning (AI/ML) and their demand for low-precision, diverse and customizable hardware, and rapid advances in traditional High Performance Computing (HPC). It is imperative for the scientific community to start building sustainable software infrastructure that can harness this potential effectively. Challenges abound because of multiple axes of growth and their need to keep up and interoperate with one another. To prepare for the arrival of exascale platforms, the United States Department of Energy launched the Exascale Computing Project (ECP)[1] seven years ahead of the delivery of the first machine, Frontier, at Oak Ridge National Laboratory. This endeavor was a concerted effort to consolidate the gains of two decades of research and growth in HPC software and hardware and computational science into a robust computing ecosystem.

It would be impossible to repeat the ECP for every generation of new development in hardware, especially because it is becoming harder to predict what that hardware might look like. Additionally, the explosive growth in AI/ML utility, scaling, and national interest[2] occurred during the lifetime of the ECP, but only a handful of mission-critical codes were in a position to benefit from it. In part, this is linked to the fact that commercial competition in the AI space led to rapid developments of siloed software ecosystems which lack uniform, stable, and scalable APIs to interface with conventional HPC software.

[1]`https://www.exascaleproject.org`
[2]`https://www.youtube.com/watch?v=NFwZi94S8qc`

Together, these developments have created a perfect storm where the software ecosystem to exploit the advances in HPC and AI/ML together for science is nearly nonexistent. Computational science needs immediate investment and commitment to develop a framework where HPC and AI/ML interoperate efficiently, scale well, and can evolve with the challenges of growing complexity in workflows without having to go back the drawing board for each new generation of platforms, models, and algorithms.

Similar to siloed AI software ecosystems [1], a siloed funding and development structure fostered the state of HPC software that we are in today, which on the surface appears coherent. However, if one would create a compatibility matrix—not just theoretically but on a practical level—of all packages in Spack[3], the result would be much sparser than expected. Incentive structures paired with these incompatibilities in solvers, libraries, languages, tools, etc., then leads to further inefficiencies, fragmentation and redundant research and developments. While challenging the status quo is occasionally beneficial [2], a consolidation of efforts, e.g., as seen recently in the compiler [3] or the performance analysis communities [4], benefits everyone but especially the ones who matter most: the users!

Another dismal example is the various programming frameworks, especially when targeting accelerators. Although successful in their intended goal, state-of-the-practice approaches to programming frameworks lack a holistic program view that is crucial for attaining performance, approachability, and interoperability. Frameworks often focus on executing task graphs and providing portable computations at the kernel level, which are only a part of modern-day performance engineering. Scientific codes, however, are workflows consisting of multiple components, i.e., languages, numerical and communication libraries, frameworks, surrogate AI models, and runtime memory management—all of which need to be carefully orchestrated to minimize memory footprint and data movement. As a result of this decoherence, many optimization opportunities are missed.

We are a group of computer and computational scientists who believe that the HPC community should be deeply concerned about the imminent barrier to innovation that will come from not being able to use future resources in a timely fashion. Additionally, the next iteration of code refactoring must take a fundamentally different approach than the ECP, because the pace of change in hardware and its specialization is likely to be faster than the pace in which a typical team can adapt their code(s) to the target hardware. Therefore, we have put together ideas—based on our own prior experiences—for a viable application-facing framework, that, we hope and expect would be able to support a large class of tightly-coupled HPC/AI hybrids through several generations of hardware evolution. Here, we describe our ideas that we believe can not only meet the needs of several mission-critical science domains, but also provide a blueprint for software where our design may not be directly applicable.

[3]`https://spack.io`

LATEST IN SCIENTIFIC PROGRAMMING

With the exception of the C++-based tool Kokkos[4], which has seen some adoption, the vast majority of abstractions, programming models, and performance portability tools have not been adopted by more than a handful of scientific applications. Kokkos effectively addresses the challenge of having to maintain multiple code variants for every different hardware target. As a result, cottage industries have grown in many parts of the world where codes are being converted from Fortran to C++, only to be able to use Kokkos. Those efforts still focus on a largely dominant parallel execution model—it has merely switched from distributed memory to a massively parallel model.

For many of the codes in the ECP, the objective was to offload as much work as possible to the GPU, because of its computational and energy efficiency. Orchestration of data and computation movement received very limited attention, and even more limited adoption. Orchestration was meant to be the purview of the task-based runtime systems. Although several have been under development for years, the only success stories they have are when the applications using them were co-designed with the tool itself. Legacy codes, or independently developed codes have had no success with them without deep refactoring, or in a few cases, completely rewriting the code. The latter was up to now unfeasible in our community and whether AI-assisted code translation will be possible without sufficient training data remains an open research question.

Another rapidly growing trend is that Python now dominates as the language of choice for algorithmic innovations in many scientific domains. This trend has been visible for a few years, due to a rich supporting ecosystem and the ease of building prototypes with it. The arrival of AI/ML frameworks with Python interfaces has further accelerated this trend across industry and academia. Transitioning prototypes developed in Python—especially those that are in flux—to performant HPC codes has emerged as a real challenge. We are aware of at least one use case where their toolchain[5] pivoted from being C++-centric to Python-centric because of domain scientists' discomfort with C++, thereby making the use of C++-based abstractions an unsustainable development model.

It may seem impossible to reconcile the growth of Python-based development with the anticipated growth in hardware complexity. However, the path taken by the AI/ML frameworks—enabling plug-and-play code modules with some degree of customization—hints at a way forward for HPC codes as well. For a scientist, a dream come true would be to have an ecosystem where many capabilities they need already exist, and where they can plug in missing capabilities to get results at the cost of having to conform to the coding standards of the framework. Such an approach had some notable successes in the cluster computing era with multiphysics code frameworks that enabled plug-and-play features for physics solvers[6]. We have succeeded in achieving some of these objectives in narrower

[4] `https://kokkos.org`

[5] `https://gridtools.github.io/gt4py/latest/gtscript.html`

[6] E.g. `https://www.cactuscode.org`, `https://flash-x.org`, `https://www.lammps.org`, and `https://www.gromacs.org`.

contexts [5, 6].

We believe that our collective experience positions us well to articulate the design challenges and possible solutions that may meet the needs of domain scientists who require large-scale supercomputers to tackle mission-critical and societal concerns.

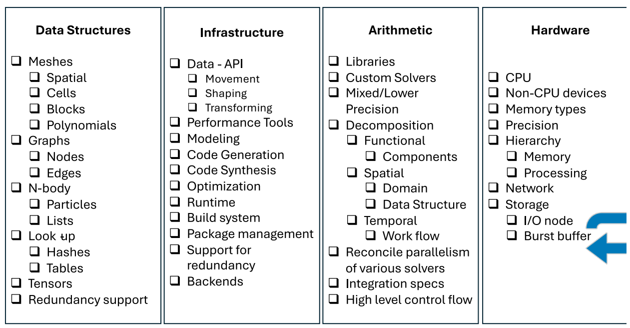


Figure 1: The design space that a multiphysics HPC framework must take into account already in the absence of AI/ML integration or offloading.

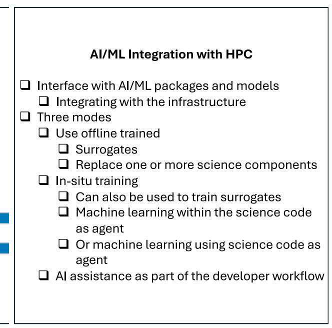


Figure 2: Various ways in which we anticipate use of AI/ML in High-Performance Computing software.

OBJECTIVES AND FEATURES FOR THE FRAMEWORK

We are aware that this is an extremely complicated design space, and that any attempt to implement a general purpose solution would be a very ambitious undertaking. However, we also believe that a concerted effort to crystallize some ideas for how such a framework can be built is already past due. If we had a design and started building the framework now we may have had a possibility of having a partially functional one halfway through the life of the post-exascale platforms. Additionally, past experiences show that attempting to fully specify the design of all aspects of any framework without substantial input from the end-users, the scientists, do not survive the test of deployability. Therefore, the exploration of the design space could, in itself, be a multi-year effort.

The only viable approach at this late date is for the design specifications to be living documents, which may be subject to change throughout the life of the framework. Meaningful in-depth input from end-users must be central to the evolution of the design. Certain insights from existing frameworks and abstraction tools point to features, listed in Figure 1, which will definitely be needed in the framework. They include a library of data structures for the supported methods and models compatible with known algorithmic constraints; tools to efficiently transform data when migrating between supported data structures and hardware; and embedded tools to monitor and report on runtime behavior. The latter will be necessary for debugging, reasoning about performance, as well as training the AI/ML engines. Figure 2 shows our current view of how AI/ML will be used in this ecosystem. Effectively serving a wide range of science areas, algorithms, and implementation strategies hinges on a set of features, listed hereafter, which are essential to building and maintaining scalable HPC-AI/ML applications.

Desired Features:

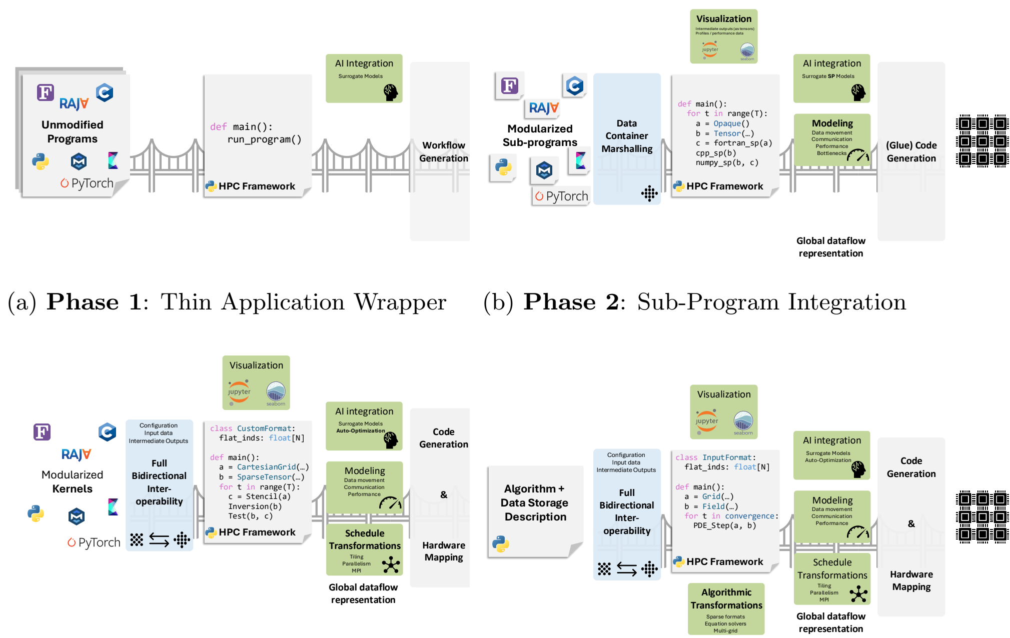
Below we enumerate the high-level features that we believe the framework must have to be successful.

> **Data transformers**. Components that can efficiently convert data structures for different portions of the workflow, i.e., from an HPC friendly data container to AI/ML friendly one.
>
> **Disentangling math from control flow**. The holy grail for domain scientists is to write their equations and have the code generated to solve them. While that is impossible to achieve universally given the multitudes of ways in which equations can be solved, it is possible to enable implementation of numerical algorithms without entanglement with data structures through appropriate abstractions.
>
> **Expressing locality**. Being able to explicitly state the data and computation locality is a critical necessity for efficiency and energy saving.
>
> **Constraining semantics**. Idiomatic richness of the target language is a proportionate burden on the optimizing compiler. Equations do not need this richness; thus, a semantically constrained language subset that is mutually agreed upon by the domain developers and tool developers benefits both sides, and ultimately science. Domain-specific languages follow this idea but relying on new syntax makes them niche solutions.
>
> **Composability**. A very high degree of composability is essential for any framework that aims to support a wide range of scientific workflows while also accommodating non-public code.
>
> **Cost models**. Such models assist in composing the components of an application and guide optimal workflow execution decisions.

The lower levels—especially where competing solutions exist—will require input and careful selections by panels of subject matter experts and users.

DEVELOPMENT APPROACH

Our overarching vision is to allow codes to follow a staggered development and migration. Our collective experience is that any abrupt shift in software architecture will not only be disruptive for science that is relying upon the software



(a) **Phase 1**: Thin Application Wrapper

(b) **Phase 2**: Sub-Program Integration

(c) **Phase 3**: Retargetable Building Blocks

(d) **Phase 4**: Algorithmic Description

Figure 3: Workflow of the proposed HPC framework. Phases enable gradual application integration — the more information provided, the more capabilities can be unlocked to reduce the overhead of utilizing modern hardware.

for discovery, but also a tremendous barrier of entry to adopting new approaches. Application codes are large and complex, and making them compatible with any new programming model or abstraction takes a long time. If no mechanism is provided to keep the code usable while the shift is taking place, scientists cannot continue their work.

We propose beginning with a non-intrusive framework that enables bridging of models through interfaces without any attempts to add new abstractions. This should allow applications to plug into the framework and be able to use features that they may not already have, as shown in Phase 1 of Figure 3. The applications may be able to use limited AI/ML interfaces. As we progress towards later phases, we begin to introduce abstractions where, in exchange for handing some of the control and details over to the framework, the applications gain greater performance and portability while simplifying their own code base. For example, in Phase 2 the framework may become the primary custodian of data containers, with applications indicating what their needs are, allowing them to hand over the communication and data movement to the framework. In the next phase, we can further abstract the knowledge of hardware and control of data from the application so that the framework can internally apply transformations and optimizations as needed. Our final goal is to reach a state where the algorithm writer can express their arithmetic and data storage requirements without binding them to one another. Instead, they can leave the management to the framework.

The use of AI/ML elements is interwoven into the various phases, so as to allow sub-programs to be seamlessly exchanged for surrogate models, as well as use AI to estimate performance models and facilitate automatic optimization without brute-force search.

As the framework grows more sophisticated, one can bring in the state-of-the-art code generation/translation/assembly techniques as integrated capabilities into the framework. Simultaneously, one can integrate necessary tooling to visualize and analyze results, as well as monitor and understand performance.

IMPLEMENTATION PROPOSAL

Given that our HPC community already has a rich ecosystem of existing libraries and tools, we envision a two-pronged approach to the development of the framework. One would begin with a pilot where one can simultaneously study and digest ways in which the existing abstractions and tools are hampered from interoperability by their design choices, and conceptualizing the elements of the framework that would overcome these limitations. In this phase, the backbone elements of the framework would be prototyped and evaluated by the stakeholders and the wider community. This is where the tight coupling with the end user becomes critical for success.

Because we envision existing libraries and tools being integrated into the whole with appropriate refactoring, the approach would be to make a draft design for some selected (usually critical) portion of the library as a component, build the substrate in the framework where the component fits, and then refactor the section of the library to fit into the framework. At this point, it would be feasible to partially evaluate the scalability and efficacy of the design. One could assess the gaps and weaknesses and tweak it as needed. In some circumstances some components of the design may even need a hard reset. The same process can be repeated with other sections of the library, going back to any of the earlier refactored portions and substrates and modifying them if necessary.

Through this incremental and cooperative co-design approach, we should be able to catch design flaws early in the development cycle. We envision several teams working on different aspects of the framework, who are assisted by the latest large-language models to accelerate mundane tasks such as documentations, code transpilations, and interface creation. However, there should always be a degree of overlap among teams and a continuous exchange of information, especially if any team makes non-trivial change in its direction.

CONCLUDING REMARKS

We agree that this is no trivial undertaking. However, the Linux Kernel community, and more recently Deep Learning community with PyTorch et al., have shown what can be achieved by coordinated and targeted efforts. Unfortunately, thus far, HPC lacks this level of coordination, resulting in the field being left behind in the rapidly changing landscape of hardware and software options. We simply cannot afford that every application team struggles with the same challenges in isolation anymore, especially when it comes to code modernization and AI/ML integration.

For efficiency reasons, we urgently need a single scalable framework, into which the majority of relevant scientific algorithms are either integrated or can seamlessly be glued into, to enable HPC-AI/ML hybrids. Data transformers, reuse and composability, code generation, and separation of concerns are the keys to allow computational scientists to focus on algorithms, while computer scientists tackle the efficiency challenges involved in mapping these algorithms onto various processors and distributed architectures.

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