End-to-End Virtual Accelerators (EVA)

(Contribution to Snowmass21)

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Abstract

The growing importance of particle accelerators to society, together with their increasing complexity and high cost, demands that we bring the most advanced computing tools to bear on their design. Modeling of beams at extreme intensities and densities (toward the quantum degeneracy limit), and with ultra-fine control (down to the level of individual particles), calls for integrated predictive tools that can take advantage of the largest supercomputers, with an ultimate goal of creating End-to-end Virtual Accelerators (EVA) that model particle accelerators from start to end. Ultimately, with the help of surrogate models, such virtual accelerators could have many of the characteristics of a Virtual Reality (VR) simulator, allowing the operator to quickly and efficiently model operation of the accelerator for its intended application in real time.

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1 Existing accelerator codes capabilities

No major accelerator project can proceed without being thoroughly modeled by comprehensive, detailed simulations. There is a need - in addition to fast, reduced models - for full physics 6-D computer simulations (often based on the Particle-In-Cell method). Although there are many beam and accelerator codes in existence (developed independently, with accessibility ranging from open-source communities to fully closed source), predictive end-to-end simulations of particle accelerators that accurately take into account subtle effects such as halo are for the most part out of reach.

Detailed simulations are used to model and design magnets, RF cavities, beam generation and evolution in accelerator sections, beam collisions or final interaction with a target, etc., but are usually not integrated in end-to-end, all encompassing, computer models. In fact, multiple codes exist to model each of these and have typically been developed by single (or very few) developer(s) with little or no coordination to enable interoperability, as was noted in the 2015 HEPAP report:

> Computer simulations play an indispensable role in all accelerator areas. Currently, there are many simulation programs used for accelerator physics. There is, however, very little coordination and cooperation among the developers of these codes. Moreover there is very little effort currently being made to make these codes generally available to the accelerator community and to support the users of these codes. The CAMPA framework is an exception, and such activities should be encouraged.
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> — HEPAP report, 2015

As a result, accelerator physicists usually simulate the accelerator by parts (injector, magnet, beam dynamics, etc), eventually missing important couplings of physical effects as well as opportunities for more efficient working points that can be achieved only from system optimization of the entire accelerator. Workflows for end-to-end modeling of particle accelerators have emerged recently, in application to free electron lasers [1, 2, 3], but also in application to high-energy physics experiments. For example, the integration of RF, beam dynamics and plasma codes provides a unique HPC accelerator modeling toolset to virtual prototyping from start to end of a possible RF injector for the future HEP facility FACET-III. The groundwork for this kind of code integration using HPC has been laid during the past several years through the HEP CAMPA [4] support for streamlining the use of different HPC accelerator modeling codes including developing a unified format for data transfer (based on the openPMD standard [5, 6]). Further development of the simulation workflow using HPC will enable realistic modeling including all the essential physics components for the accelerator system. End-to-end tools also enable global optimizations in the design and operation of accelerator systems.

2 Challenges

Many challenges exist that can slow the emergence of end-to-end, multi-physics, solutions. Many codes are naturally developed by domain scientists in support of specific projects, often without adopting standards or coordination between projects. This is a result of a relative lack of dedicated funding for accelerator and beam code development and maintenance. The situation is not new and has not changed fundamentally since the 2012 Office of HEP Accelerator R&D Task Force report:

> Software should help researchers optimize operating regimes and reduce the overall risk that underlies all modern accelerator design. Much of the current software has not taken advantage of the many computer improvements that have been developed in the last few decades. Such progress includes vastly increased processor speed, exploding memory capabilities, disk storage growth and cloud computing. There is not enough overall commercial demand for such high performance accelerator design software to have confidence this problem will be solved without US government intervention.
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> ...
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> Accelerators across the board also need advanced simulation studies, and long-term support for code development and maintenance is therefore needed.
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> — Office of HEP Accelerator R&D Task Force report, 2012

While some codes have since been modernized and can now run efficient on parallel CPU-based computers, only a fraction can efficiently run on parallel GPU-based computers. In fact, most codes in the community do not run on GPUs at all. It was already noted, nonetheless, in the 2015 HEPAP report that the progress in computer hardware opens new possibilities:

> Advances in simulations, as well as in computational capabilities, raise the exciting possibility of making a coherent set of comprehensive numerical tools available to enable virtual prototyping of accelerator components as well as virtual end-to-end accelerator modeling of beam dynamics. It should be possible to construct real-time simulations to support accelerator operations and experiments, allowing more rapid and detailed progress to be made in understanding accelerator performance.
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> — HEPAP report, 2015

3 End-to-End Virtual Accelerators (EVA)

Future needs, as outline in, e.g., the Grand Challenges (GC) presented in [7]:

- **GC #1 (beam intensity)**: How do we increase beam intensities by orders of magnitude?
- **GC #2 (beam quality)**: How do we increase beam phase-space density by orders of magnitude, towards the quantum degeneracy limit?
- **GC #3 (beam control)**: How do we measure and control the beam distribution down to the level of individual particles?
- **GC #4 (beam prediction)**: How do we develop predictive "virtual particle accelerators"?

drive the need toward the type of end-to-end virtual accelerators that was envisioned in the 2015 HEPAP report. Pushing the limits in beam intensity, quality and control demands more accurate, more complete and faster predictive tools, with an ultimate goal of virtual accelerators. The development of such tools requires continuous advances in fundamental beam theory and applied mathematics, improvements in mathematical formulations and algorithms, and their optimized implementation on the latest computer architectures. Full integration of machine learning tools [8] will be essential to enable efficient use of these end-to-end virtual accelerators for practical applications.

The realization of such ambitious goal call for a more effective coordination of the code development and maintenance across the community - which should be encouraged among laboratories, academia and industrial partners - together with the development of ecosystems of modeling tools for multiphysics particle accelerator modeling and design [9], standards and end-to-end workflows [6]. To maximize efficiency and benefits to the community, these should be developed using modern software best practices [10] and adopt open science principles (except when contraindicated by well-justified reasons such as export control) [11]. The resulting interchangeability and comparability of the simulation tools ensure an increased level of confidence in the simulation predictions and continuity of the simulation capabilities. The effort can also benefit widely by leveraging the tools and practices developed by programs such as the DOE SciDAC and Exascale Computing Projects. Dedicated support for consortiums (e.g., CAMPA) and dedicated Center(s) for accelerator and beam physics modeling [12] would critically benefit this endeavour.

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