Center(s) for Accelerator and Beam Physics Modeling

(Contribution to Snowmass21)

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Abstract

Computer simulations are key to the success of particle accelerators. All the particle accelerator areas rely on computer modeling at some point, sometimes requiring complex simulation tools and massively parallel supercomputing. Centers of expertise that focus on accelerator and beam physics modeling are necessary to bring the community to the next level, to provide the next generation of simulation tools and the teams that can effectively develop and support them for the community. After all, it is only natural that particle accelerators, which pioneered and embody "big science" projects, need teams to develop and maintain the computational tools that simulate them.

1 Current status and goals

For a large part, efforts in code development and modeling of accelerator and beam physics have been scattered across projects. Without organization of modeling efforts across projects, this has led to the development of many codes (see, e.g., list of beam dynamics codes from the *Beam dynamics codes* section from the Accelerator Handbook edited by A. Chao, 2013).

In fact, the existing set of modeling tools used by the accelerator community encompasses a few large codes that can exploit effectively large supercomputers and new architectures with multiple levels of parallelism (such as Graphical Processing Units, or GPUs); and a fairly large number of smaller codes, which may have unique features, but have typically been developed by single investigators with little emphasis on software sustainability, parallelism, or interconnection with other codes.

The current set of simulation tools is essential to the success of the accelerator community and has been very successful. However, developing the next generation of particle accelerators presents challenges that demand that the community brings the tools - and the teams that are needed to develop and maintain them - to another level [1].

Developing a more coherent set of tools (based on existing and new tools), developed and maintained by coordinated, specialized, dedicated teams, would lead to an ensemble that would be much more capable. In the long run, the new tools would enable projects to benefit from new solutions and run in highly optimized regimes that would be unavailable or unattainable otherwise, resulting in higher science throughput and reduced costs.

2 Challenges

The computational needs in particle accelerator physics are large and varied. Many types of machines are to be modeled: linacs, rings, recirculators, energy recovery systems, fixed-field accelerators, plasma-based accelerators, dielectric-based accelerators, etc. For these machines (which can be combined for a single accelerator complex) the prediction of the final beam(s) before collision (the *end product* of the accelerator) needs tracking from inception and through all acceleration and manipulation processes. This involves modeling from single particle dynamics to tightly coupled many-particles dynamics, including RF fields, magnets, pipes, etc., often for very long times (e.g. in circular machines).

Start-to-end modeling with full physics implies the accounting of many effects: halos, wakefields, impedance, electron cloud, beam-beam, collisions, secondary emission, spin dynamics, (in)coherent synchrotron radiation, painting, etc. Accurate predictions also demand to go beyond idealized accelerator components by coupling these simulations to realistic computer design and analysis of the components. Modeling the interaction of the beam(s) with the target(s) is also often needed. Finally, design implies ensembles of simulations that may need to cover a very large parameter space, aided by multi-objective optimization and increasingly by machine learning.

In addition, the trend is for accelerator physics and projects to increase the demand on capability and accuracy. For example, the four Grand Challenges on Intensity, Quality, Control and Prediction established by the community for the DOE HEP GARD Accelerator and Beam Physics (ABP) thrust roadmap, call for modeling of beams at extreme intensities and densities (toward the quantum degeneracy limit), with ultra-fine control (down to the level of individual particles), and for the development of 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.

While the large modeling needs for accelerator modeling have led to the development of many codes, there is a lot of overlap and duplication in the current set. Examples are particle tracking modules through lattice elements or Poisson/Maxwell solvers for self-fields, which tend to be duplicated in many codes. Development of a small number of libraries and toolkits that can be reused by various codes would alleviate this issue. This would, in turn, free up resources and time to develop new capabilities that cannot be developed otherwise as multiple developers spend time *reinventing the wheel.*

3 Center(s) for Accelerator and Beam Physics Modeling

To move the accelerator modeling capabilities to the next level, we propose to create one or more Center(s) for Accelerator and Beam Physics Modeling. The center(s) can be at a given location or distributed geographically and among institutions across laboratories, academia and industrial partners. The Center(s) would bring together domain scientists (computational accelerator and beam physicists), applied mathematicians, computer scientists and software engineers with collaborations across laboratories, academia and industrial partners. This would follow the successful models from DOE SciDAC and Exascale Computing Projects, which are supporting some of the modeling efforts on which the Centers can build upon.

Depending on the overall size, the center(s) could enable part of all of the following:

- Community development and maintenance of codes using industry-standard quality processes by dedicated, specialized teams [2].
- Libraries for field solvers [3], particle trackers, etc.
- A modular community ecosystem for multiphysics particle accelerator modeling and design [1].
- Standardization of input scripts, output data, lattice description and start-to-end workflows [4].
- Provide compatibility layers to use the same libraries and modules in a number of programming languages.
- End-to-end Virtual Accelerators (EVA) [5].
- User support, high-quality and detailed documentations, online tutorials, and training.
- Easy-to-use user interfaces for preparation and analysis of simulations.
- Automated tools for ensemble simulations for optimization.
- Suite of test problems with well characterized solutions for benchmarking.
- Development, analysis and efficient implementation of novel algorithms and numerical methods (e.g., high-order solvers, adaptive mesh refinement).
- Providing a space to meet (physically or virtually) for the integration of developments from contributors into larger codes, such as PhD projects from external groups, organizing development hackathons, knowledge-transfer, onboarding, etc.
- Developing and organizing workshops for developers and users of codes alike. Inviting national and international speakers/developers (travel/hosting funds).
- Interacting with existing schools, by developing and maintaining state-of-the-art educational resources (e.g. tutorials, lectures) on codes.
- Exploration of novel use of machine learning for accelerator modeling, and, further in the future, of quantum computing [6].

Multiple Centers can be organized through a Consortium (e.g., CAMPA [7]). Except for special restrictions such as export control, it would be desirable for the software developed by the Center to be open source, enabling crosschecking, testing and contribution by the community at large, beyond the participants to the Center(s) [8].

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