NEEDS AND CONSIDERATIONS FOR A CONSORTIUM OF ACCELERATOR MODELING*

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Abstract

Thanks to sustained advances in hardware and software technologies, computer modeling is playing an increasingly important role in the design of particle accelerators. This rise in importance is further fuelled by the economic pressure for reducing uncertainties and costs of development, construction and commissioning, thus pushing the field toward an increase use of "virtual prototyping". Until now, the development of accelerator codes has been left to projects without mandate and programmatic funding for coordination, distribution and user support. While this is adequate for the development of relatively small-scale codes on targeted applications, a more coordinated approach is needed to enable general codes with user bases that extend beyond individual projects, as well as cross-cutting activities. In light of this, it is desirable to strengthen and coordinate programmatic activities of particle accelerator modeling within the accelerator community. This increased focus on computational activities is all the more timely as computer architectures are transitioning to new technologies that require the adaptation of existing - and emergence of new - algorithms and codes.

INTRODUCTION

Particle accelerators are essential tools of science and technology, with over 30,000 accelerators in operation around the world, in support of discovery science, medicine, industry, energy, the environment and national security [1]. The size and cost of the accelerators are a limiting factor for many applications, and there is active research worldwide targeted at the development of smaller and cheaper accelerators. Computer modeling is playing a key role in the progress toward bringing the size and cost down. It is essential for the optimization of existing accelerators, cost effective design and the development of game changing technologies. Thanks to sustained advances in hardware and software technologies, computer modeling is playing an increasingly important role. This rise in importance is further fuelled by the economic pressure for reducing uncertainties and costs of development, construction and commissioning, thus pushing the field toward an increase use of "virtual prototyping".

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Many computer simulation codes have been developed (over 70 worldwide) for the modeling of particle accelerators and beam transport. There has been little coordination of the development of the accelerator physics codes whose aggregate involves a mix of complementarity and duplication, and they are not all actively developed and maintained. Many of the codes have been developed by a single developer (often a physicist) for a specialized purpose or accelerator. Several multi-physics frameworks were developed by small teams, some in large part with the support of SciDAC, and are capable of incorporating many physics models. A substantial fraction of the codes is serial, but a number of the codes have been ported to parallel computers and some are capable of handling massive parallelism. A small fraction of the codes were ported to GPUs. Many of the codes are written in FORTRAN, C or C++, with a growing number combining the compiled language modules (for number crunching) with a Python scripting interface.

THE VIEW OF THE COMMUNITY

The key roles of computing, and the needs for a more cohesive approach to development, maintenance, support and training have been recognized by the community, in the 2013 DOE-HEP Snowmass report [2], the 2014 Report from the Topical Panel Meeting on Computing and Simulations in High Energy Physics [3], and the 2014 P5 report [4].

Reports [2] and [3] recommended an increased coordination of modeling effort, dedicated support of code modernization, maintenance & dissemination, increase emphasis on use & development of common tools, better user support, and more training in HEP computational physics. In addition, [3] calls for the establishment of an HEP distributed center for computational excellence (single point-of-contact, cross-cutting activities). As a result, a Forum for Computational Excellence was created [5] aiming at promoting excellence in computing,

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simulation, and data management across all of HEP science and technology.

The P5 report [4] underlines the key role of both accelerator research and computing, stating that:

- "the future of particle physics depends critically on transformational accelerator R&D to enable new capabilities and to advance existing technologies at lower cost."
- "The use of high-performance computing, combined with new algorithms, is advancing full 3-D simulations at realistic beam intensities of nearly all types of accelerators."
- "This will enable "virtual prototyping" of accelerator components on a larger scale than is currently possible."

These led to the recommendation 29 about computing that proposes to "strengthen the global cooperation among laboratories and universities to address computing and scientific software needs, and provide efficient training in next-generation hardware and data-science software relevant to particle physics. Investigate models for the development and maintenance of major software within and across research areas, including long-term data and software preservation."

Those reports and recommendations are consistent with community inputs that were submitted beforehand [6-8].

NEED FOR ADIABATIC TRANSITION

The existing pool of codes is a result of significant investments from the community, and it is essential to minimize disruptions to developers and users, while enabling interoperability and expandability. This can be accomplished by adopting an incremental (near adiabatic) approach for transitioning from the existing collection of codes into a modular ecosystem of interoperable components that facilitate cooperation and reuse. It is also important that innovation in algorithms, which is a strength of the accelerator modeling community, is not hindered by the transition.

Challenges to the coordination of efforts are technical (different programming languages, data formats, parallelism strategies, or code architectures, open vs proprietary sources) and human (resistance to changing habits, different visions, trust, corporatism, rivalry, fear of loss of recognition, distance). A coordination that builds incrementally upon the existing tools and is not binding offers a path toward a smooth transition that mitigates many of the difficulties listed above. Hence, an approach is proposed that is based on bridging the codes at the outer (input and output) and inner (core functions) levels, enabling an incremental and non-disruptive transition, in contrast to the alternatives of down-selecting toward a handful of community codes, or coalescing toward a new unique code or framework. Such a strategy will open the way to creating an ecosystem combining the following: a unified input/output interface, shared functionalities, collaborative development of common units, "natural" down selection of modules, developers and users assembling new functions through creative combinations of individual units that can be viewed as "Lego bricks" or "code genes".

The realization of this strategy is facilitated by the emergence of the scripting language Python as a language of choice in the scientific community for simulations management such as, e.g., steering, chaining, parametric studies, parallel parameter optimization. Thanks to its flexible interface to compiled languages like C, C++ and FORTRAN, it is even used as the frontend of an increasing number of codes: Warp, Synergia, Py-ORBIT, Py-ECLOUD, PyHeadTail, BLonD.

CONSORTIUM FOR ADVANCED MODELING OF PARTICLE ACCELERATORS (CAMPA)

A new collaboration was formed to initiate a Consortium for Advanced Modeling of Particle Accelerators (CAMPA), spanning at present three major U.S. national laboratories (Lawrence Berkeley National Laboratory, SLAC National Accelerator Laboratory and Fermi National Accelerator Laboratory). The consortium is currently funded by the High Energy Physics program of the U.S. Department of Energy Office of Science, and its mission encompasses the following:

- push the frontier of accelerator science through advanced simulation and modeling; push the computing frontier in accelerator science through algorithmic advances;
- provide the scientific community with a comprehensive and integrated toolset of state-of-the-art simulation codes for multi-scale, multi-physics accelerator modeling, in support of the mission of the Office of Science within the Department of Energy (DOE);
- develop and maintain the codes on DOE's supercomputing facilities; distribute and support codes for installation on smaller scale clusters, desktops or laptops;
- support users;
- use the codes as education tools to train students and young researchers on the science and the modeling of accelerators;
- promote collaboration and re-use of accelerator simulation codes and data through common interfaces, data standards, and integrated visualization and analysis capabilities;
- establish a framework aimed at its extension to a national (possibly international) consortium.

BENEFITS

Ultimately, the consortium is expected to benefit science, the funding agencies, the users and the developers. It offers a path toward game changer modeling tools leading to virtual prototyping and experiments, as well as online modeling for real time feedback on experiments. This will speed up design and innovation that will likely result in better accelerator and technology. This, in turn,

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increases the rate of discoveries, providing higher return on investment to the funding agencies. The consortium also provides a singular point of contact for modeling activities to both the funding agencies and the users. To the latter, it also offers an integrated, comprehensive and more capable (multiphysics/multiscale) simulation tool solution. To the developers, the consortium provides a much needed source of funding that is dedicated to user support, algorithmic improvement, code implementation and maintenance, as well as recognition for accelerator software development, and more evident carrier paths.

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