Interdisciplinary simulations: Integrating accelerator RF and particle-matter interaction codes

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1 Needs for radiation simulation in accelerator structures

Radiation induced by dark current in accelerating cavities is one of the main concerns for accelerator designers and operators. The radiation may cause damage to cavities operating at high gradients, which leads to shortened lifetimes of the devices and a radiation safety hazard for the surrounding environment. These consequences have been observed at many facilities, such as the CEBAF, LCLS-II, ANL, etc. Sufficient shielding is required to properly contain the radiation, which in turn requires a good understanding and prediction of radiation levels through simulations.

One of the major challenges for high gradient accelerating structures is the dark current generated from field emission at material surfaces. These emitted electrons may create radiation safety hazards when they are accelerated in the RF field and then bombard the surface again. In superconducting RF (SRF) structures, the radiation not only raises safety concerns, but also makes accelerator operations less reliable. Performing a dark current simulation involves different kinds of electromagnetic calculations, including RF field calculation in an accelerator structure and then subsequent tracking of electrons in the structure. In order to modeling radiation effects caused by dark current for accelerator systems, users need a simulation environment to model the physics processes of field emitted electrons in RF cavities and continuation of cascade events through the cavity enclosures. This capability can be provided by particle-matter interaction calculations such as the Fluka and Geant4 simulation toolkits [1], which are widely applied in the high energy physics community to model particle physics processes, such as detector response. It has also been used in simulations for joint HEP-accelerator projects, such as in the data processing and simulation framework for the international Muon Ionization Cooling Experiment (MICE).

2 Integrated tools for accelerator and radiation codes

In the following, we will demonstrate the computational requirements for performing such interdisciplinary calculations that include accelerator modeling and radiation simulation codes. As an example, we use the parallel RF simulation codes ACE3P for cavity field calculation and the particle-matter interaction code Geant4 for radiation calculations to describe what major components need to be added in order to provide a tool that can address the above multi-physics simulation for accelerators.

ACE3P [2] is a comprehensive set of parallel multi-physics codes. It is based on high-order curved finite elements for high-fidelity modeling, and has been implemented on massively parallel computers for increased problem size and speed. Its eigensolver module Omega3P is used widely in RF structure simulations, and its particle tracking module Track3P module models multipacting and dark current effects in the structure. Both modules are highly parallelized; running on high performance computing (HPC) platforms with thousands or more cores. The use of high-order finite elements on tetrahedral conformal meshes with quadratic surfaces enables accurate and fast solutions. ACE3P has been well accepted by the accelerator community as a benchmark and guidance for structure optimizations with large-scale simulations.

Geant4 is fully open source and allows users to customize physics processes of interest in a customized geometry, such as low to medium energy electron interactions with beam stops, or proton interactions with human tissues in proton therapy. However, one of the challenges of using Geant4 is that a user needs to be very familiar with C++ programming to use the libraries correctly and get the correct program response to the physics model. Furthermore, converting a 3D engineering model used in ACE3P to a Geant4-compatible format is also a time-consuming programming task.

The integrated simulation environment starts with the simulation of the physics processes at the surface and within a RF structure, and then interfaces the electromagnetic field and particle tracking codes of ACE3P/Track3P with Geant4 radiation calculations (referred to as the G4ACE3P environment hereafter). This is an environment that seamlessly integrates RF and radiation modeling for accelerator design and optimization. It should be able to work with geometries defined in a CAD file and control the particle tracking workflow such that Geant4 and ACE3P can communicate with each other with particle information that contains more than just the 6D phase space coordinates; such as the parentID, PDGcode, etc. Furthermore, it should eventually avoid all the I/O for intermediate particle distribution files and eliminate the need for one program to wait for the other to finish and transfer particle files. Since ACE3P already takes advantages of large scale computation on DOE high performance computing facilities, such as NERSC at LBNL, and Geant4 can use multiple processors by employing threading, it will require the development of a hybrid model to address the different program paradigms for parallelism used in the respective codes.

The model has to ultimately be compared and benchmarked with experimental data using real accelerating cavities, which is a joint effort between the RF cavity designers and experimental users. A collaboration between the code authors and the industry can greatly accelerate the process. Furthermore, we propose to develop a user-friendly graphical user interface that can help users

visualize the radiation effects under various operational configurations.

3 Outlook

The development of G4ACE3P serves as another attractive addition to the development of a modular ecosystem of accelerator and beam modeling tools that would enable the modeling capabilities of the community to reach another level of breadth and depth [3]. This new simulation environment can further integrate more physics models and algorithms such as new space charge calculations, new photocathode emission processes, faster tracking routines, etc.

References

- [1] the Geant4 collaboration. "GEANT4: A Simulation Toolkit". In: *Nucl. Instrum. Meth. A* 506 (2003).
- Cho-Kuen Ng et al. "Advances in Parallel Finite Element Code Suite ACE3P". In: IPAC 2015 proceedings MOPMN002 (2015).
- [3] Jean-Luc Vay et al. "A modular community ecosystem for multiphysics particle accelerator modeling and design". In: *Snowmass21 LOI* (2020).