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INTEGRATED ACCELERATOR SIMULATION WITH ELECTROMAGNETICS AND BEAM PHYSICS CODES*

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Abstract

This paper presents a high-performance computing (HPC) integrated simulation capability for accelerators including electromagnetic field and beam dynamics effects. The integrated codes include the parallel finite-element code suite ACE3P for electromagnetic field calculation of beamline components, the parallel particle-in-cell (PIC) code IMPACT for beamline particle tracking with space-charge effects, and the parallel self-consistent PIC code Warp for beam and plasma simulation. The integration between the application codes requires efficient data transfer, where the common data format, openPMD, has been adopted for field and particle I/O and transfer. One integration is to employ ACE3P for 3D realistic electromagnetic field calculations in accelerator cavities, which are then used for particle tracking in IMPACT for studying beam qualities such as emittance growth in accelerator beamlines. Another integration is to combine ACE3P electromagnetic field calculation and Warp plasma simulation for investigating plasma processing for operational performance of RF cavities. Realistic simulation requires the development of a mapping of CAD geometry used in ACE3P to Warp Cartesian grid representation. Furthermore, an efficient integrated simulation workflow has been implemented to enable the execution of integrated simulation using these codes on HPC systems. Examples for integrated simulation of the LCLS-II injector using ACEP-IMPACT and plasma ignition in SRF cavities using ACE3P-Warp will be presented.

KEYWORDS

High-performance computing, Electromagnetic field, Beam dynamics, Particle-In-Cell, Particle accelerators, openPMD

INTRODUCTION

Accelerator activities rely on advanced computer modelling which requires an integrated set of accelerator simulation software to speed up design and innovation in accelerator science and technologies. Through the support of DOE, advanced simulation codes which are used at many institutions have been developed and used worldwide for the modelling of particle beams and the design of particle accelerators. A progressive transition from the current state of the codes to an integrated solution that builds upon DOE's cumulative investment while maintaining continuity, thus minimizing disruptions to the users and the developers is ongoing. The main goal is to transform the existing collection of codes into a modular ecosystem of interoperable components that facilitate cooperation and reuse, while fostering creativity and constructive competition.

This paper presents two ecosystem code integrations works. The related codes are ACE3P, IMPACT and Warp.

CODE INTEGRATION

ACE3P (Advanced Computational Electromagnetic 3D Parallel) is a comprehensive set of conformal, higher-order, parallel finite element electromagnetics modelling suite developed for accelerator cavity and structure design including integrated multiphysics effects in electromagnetic, thermal, and mechanical characteristics with two unique features: 1). Based on higher order curved finite elements for high-fidelity modelling and improved solution accuracy; 2). Implemented on massively parallel computers for increased memory (problem size) and speed. The electromagnetic modules of the program are discretized in the frequency domain and time domain for the computational volume inside an accelerator cavity, while the thermal and mechanical solvers are formulated in the frequency domain for the computational volume of the cavity walls and their surroundings. Six simulation modules have been developed in ACE3P to address different physics aspects of accelerator applications [1-3].

IMPACT is a parallel particle-in-cell code suite for modelling high intensity, high brightness beams in RF proton linacs, electron linacs, and photoinjectors [4-6]. It consists of two parallel particle-in-cell tracking codes IMPACT-Z and IMPACT-T, an RF linac lattice design code, an envelope matching and analysis code, and a number of pre- and post-processing codes. The 3D Poisson equation is solved in the beam frame at each step of the calculation. The resulting electrostatic fields are Lorentz transformed back to the laboratory frame to obtain the electric and magnetic self-forces acting on the beam.

Warp[7-9] is a particle-in-cell (PIC) Python package designed to simulate high current particle beams and plasmas in a range of applications, incorporating a broad variety of integrated physics models and extensive diagnostics, most of which work in multiple dimensions to allow examination of modeling idealizations within a common framework. The Python interpreter user interface allows flexible problem descriptions in Python scripts, giving the advantage of the full versatility of Python and allowing inter-

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active steering of runs. Warp has a hierarchy of multi-species physics models which has been used in a wide range of applications.

OPENPMD I/O

The ACE3P discretization scheme is based on a finite element method, while both IMPACT and Warp use a finite difference method. Therefore, a general and efficient conversion tool will be needed to convert the unstructured ACE3P data to a standard structured data format for input to the IMPACT and Warp.

The openPMD [10] is a standard for metadata and naming schemes. openPMD provides naming and attribute conventions that allow sharing and exchanging particle and mesh-based data among various scientific simulations and experiments. openPMD is suitable for any kind of hierarchical, self-describing data format, such as ACE3P data in NetCDF format.

A standalone tool with parallel processing I/O capability for converting unstructured finite element data format based on NetCDF in ACE3P to structured finite difference data format based on openPMD has been developed. The tool facilitates the integrated simulation workflow of combined ACE3P electromagnetics and IMPACT beam dynamics simulation. The development for openPMD format field data communication between ACE3P and Warp is on progress.

ACE3P-IMPACT CODE INTEGRATION

A schematic flow diagram [11][12] of the integrated ACE3P-IMPACT simulation is shown in Fig. 1. The user interface of ACE3P-IMPACT code integration is the Python interpreter with dynamically loaded compiled modules.

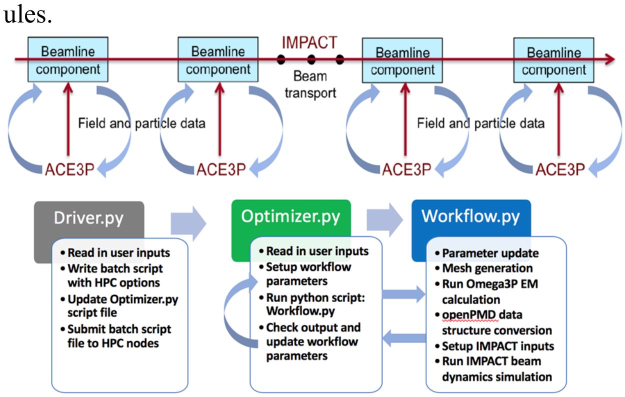

Figure 1: A schematic flow diagram of integratedACE3P-IMPACT simulation workflow.

A 100pC photo-electron beam generation and transporting through the LCLS-II injector design has been used to test the ACE3P-IMPACT workflow. A layout of the LCLS-II injector is shown in Fig. 2. It consists of a 186MHz normal conducting RF gun, a two-cell 1.3GHz normal conducting bunched cavity, eight 9-cell 1.3 GHz Tesla like superconducting cavities, and two transverse focusing solenoids.

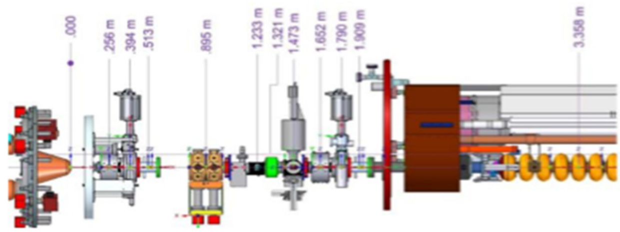

Figure 2: Layout of the LCLS-II injector.

For comparison, both 3D field generated by ACE3P directly and 2D azimuthal symmetry field constructed from the on-axis longitudinal electric field are used as inputs for IMPACT. Benchmark through the RF gun, bunch cavity and eight cryomodule superconducting boosting cavities, which will be presented below, are all performed. Figure 3 shows 3D electric field distribution and transverse field distribution along the axis from the ACE3P calculation. The use of the RF coupler on both ends of the cavity breaks the azimuthal symmetry of the field inside cavity and induces non-zero on-axis transverse electric fields. The amplitude of those transverse fields is three-orders of magnitude smaller than the longitudinal accelerating field on axis. Figure 4 shows the transverse rms size and projected emittance evolution through the boosting cavities using the 3D field from the ACE3P and the 2D azimuthally symmetric field. It is seen that there is noticeable difference of emittance evolution between the 3D field and the 2D field. The extra emittance growth from 3D field is due to on-axis transverse electric field that provides a skew quadrupole like kick to the beam and causes the increase of the emittance.

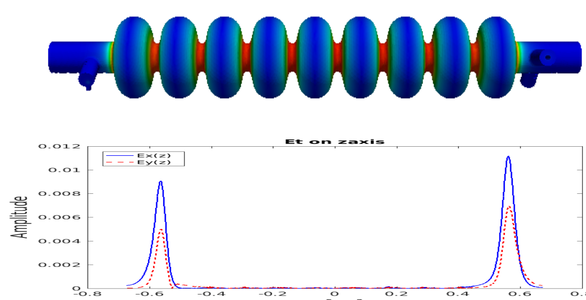

Figure 3: 3D electric field distribution (top) and transverse electric along the axis (bottom) in the boosting cavity.

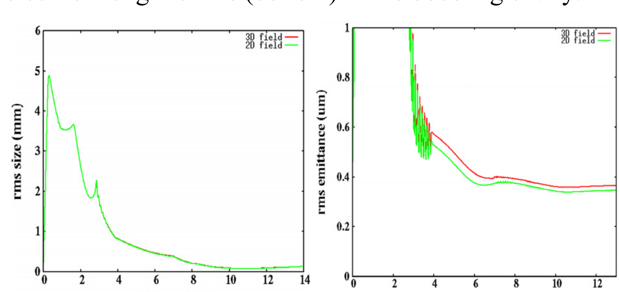

Figure 4: Transverse rms size (left) and emittance evolution (right) through the boosting cavities using the 3D field and the on-axis 2D field.

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ACE3P-WARP CODE INTEGRATION

An integrated simulation capability using ACE3P electromagnetic field calculation for Warp plasma simulation to study plasma processing in accelerator cavities has been launched. The integration requires field data transfer and geometry shape mapping from ACE3P unstructured grids to Warp Cartesian grids. The field data transfer is currently done through ASCII files and will be enabled by openPMD in the future. For geometry shape transfer, a conversion tool has been implemented to convert the CAD surface represented by a triangular grid in ACE3P to individual triangles inputted by Warp to calculate the minimum distances of the triangle vertices to coordinates in a Cartesian grid is shown in Fig. 5.

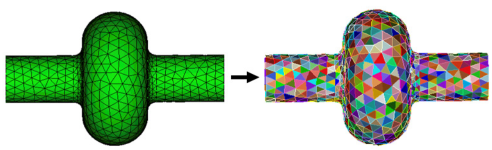

Figure 5: Conversion of surface grid used in ACE3P to individual surface triangles inputted into Warp.

Figure 6 shows an integrated ACE3P-Warp simulation for a simple single-cell superconducting cavity. The surface mesh and cavity field are transferred to Warp to simulate plasma ignition in a neon gas with background electrons. The ionized electron distribution agrees well with that obtained by direct build of the metal boundary in Warp using analytical definitions of curves.

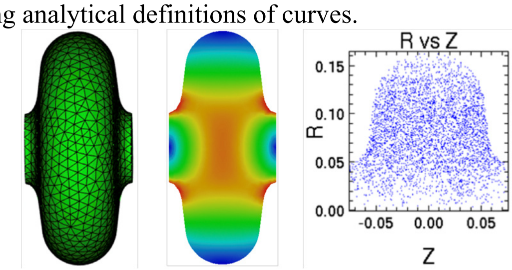

Figure 6: Integrated ACE3P-IMPACT simulation of cavity: (Left) Surface mesh; (Middle) Electric field of operating mode; (Right) Ionized electrons from neon gas.

The present approach bypasses this cumbersome procedure in previous calculation and will facilitate modeling for 3D complex geometries, such as plasma cleaning which increase SRF cavity gradient. It will be used for field gradient enhancement of LCLS-II SRF cavities as shown in Fig. 7.

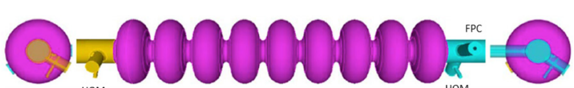

Figure 7: LCLS-II SRF cavity.

The integrated simulation using ACE3P cavity field as input for Warp plasma simulation has been demonstrated for studying gas ignition in superconducting cavities Fig. 7. The process requires significant effort in manual manipulation between the two codes. A Python script will be developed to streamline the simulation process with a tightly coupled code infrastructure to handle the interactions between the two codes. The python-based workflow driver could be further extended to couple ACE3P to WarpX, where the embedded boundary capabilities from the adaptive mesh refinement package AMReX could provide better approximation to cavity geometry that is commensurate with ACE3P finite element representation.

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