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INTEGRATION OF CAVITY DESIGN AND BEAM DYNAMICS SIMULATION USING THE PARALLEL IMPACT AND THE ACE3P CODES*

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Abstract

The 3D parallel code IMPACT code suite has been extensively used in the beam dynamics study of photoinjectors while the 3D parallel code ACE3P has been extensively used in RF cavity design. In this paper, we propose integrating the ACE3P cavity design and the IMPACT beam dynamics simulation into a single work flow. Such a workflow enables fast simulation of 3D effects (e.g. from a RF coupler) on high performance computers.

INTRODUCTION

Next generation x-ray free electron laser (FEL) light source and ultra-fast electron diffraction/microscopy (UED/UEM) put stringent requirements for high electron beam quality. In order to design and to optimize accelerators to generate such high brightness beams, high-fidelity simulations that include both self-consistent charged particle interactions among electrons inside the beam and external fields including realistic RF details of beamline components are needed.

While advanced simulation codes for electromagnetics or beam dynamics are available, the former cannot perform efficient beam transport calculations and the latter cannot calculate the electromagnetic fields with sufficient fidelity. The development of an integrated modeling tool that can simulate all these physical characteristics in accelerators will benefit the design, optimization and commissioning of existing and future light sources and UED/UEM applications. The tool would be able to perform large-scale simulations to address system-level 3D effects. In this paper, we propose to integrate the parallel electromagnetics code suite ACE3P [1] for accurate 3D calculation of beamline components EM fields and the parallel beam dynamics particle tracking code IMPACT [2] for beam transport simulation with space charge effects. The code integration provides a unique HPC capability on supercomputers to address critical design and operation issues including beam breakup, beam quality and machine protection for light sources such as LCLS-II.

ACE3P-IMPACT INTEGRATION

We begin with a brief description of the electromagnetics code suite ACE3P, developed at SLAC, and the beam dynamics code framework IMPACT, developed at LBNL.

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ACE3P is a parallel finite element electromagnetics modeling suite developed for accelerator cavity and structure design including integrated multiphysics effects in electromagnetic, thermal, and mechanical characteristics. 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 [3-5]. The modeling capabilities of each ACE3P module [6] are summarized as follows:

(1) Omega3P, an electromagnetic eigensolver in the frequency domain for calculating the resonant modes and their damping in accelerator cavities;

(2) S3P, an electromagnetic solver in the frequency domain for determining the transmission of electromagnetic fields in open accelerator structures;

(3) Track3P, a particle tracking code in the time domain for tracking electrons in accelerator structures under the influence of external static or dynamic electromagnetic fields for studying multipacting and dark current;

(4) T3P, a time domain solver for the computation of wakefield excited by a charged particle beam and for studying transient effects from external electromagnetic excitations;

(5) Pic3P, a full-wave particle-in-cell solver in the time domain for simulations of space-charge dominated devices;

(6) TEM3P, a multi-physics module consisting of thermal and mechanical solvers for the analysis of integrated electromagnetic, thermal and mechanical effects in accelerator cavities and structures. In addition to these application modules, preprocessing tools for handling mesh formats and evaluating mesh entity statistics, postprocessing tools for visualization and analysis of simulation results, as well as a cavity shape optimization tool [7, 8] have also been implemented.

IMPACT is a parallel particle-in-cell code suite for modeling high intensity, high brightness beams in RF proton linacs, electron linacs, and photoinjectors [9-21]. It consists of two parallel particle-in-cell tracking codes IMPACT-Z and IMPACT-T (the former uses longitudinal position as the independent variable and allows for efficient particle advance over large distances such as in an RF linac, the latter uses time as the independent variable and is needed to accurately model systems with

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strong space charge as in photoinjectors), an RF linac lattice design code, an envelope matching and analysis code, and a number of pre- and post-processing codes. Both parallel particle tracking codes assume a quasi-electrostatic model of the beam (i.e. electrostatic self-fields in the beam frame, possibly with energy binning for a beam with large energy spread) and compute space-charge effects self-consistently at each time step together with the external acceleration and focusing fields. 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.

There are six Poisson solvers in the IMPACT suite, corresponding to transverse open or closed boundary conditions with round or rectangular shape, and longitudinal open or periodic boundary conditions. These solvers use either a spectral method for closed transverse boundary conditions, or a convolution-based Green function method for open transverse boundary conditions. The convolution for the most widely used open boundary condition Poisson solver is calculated using an FFT with a doubled computational domain. The computing time of this solver scales like N·log(N), where N is the number of grid points.

The parallel implementation includes both a 2D domain decomposition approach for the 3D computational domain and a particle-field decomposition approach to provide the optimal parallel performance for different applications on modern supercomputers. Besides the fully 3D space-charge capability, the IMPACT suite also includes detailed modeling of beam dynamics in RF cavities (via field maps or z-dependent transfer maps including RF focusing/defocusing), various magnetic focusing elements (solenoid, dipole, quadrupole, etc), allowance of arbitrary overlap of external fields (3D and 2D), structure and CSR wakefields, tracking of multiple charge states and bin/bunches, an analytical model for laser-electron interactions inside an undulator, and capabilities for machine error studies and correction.

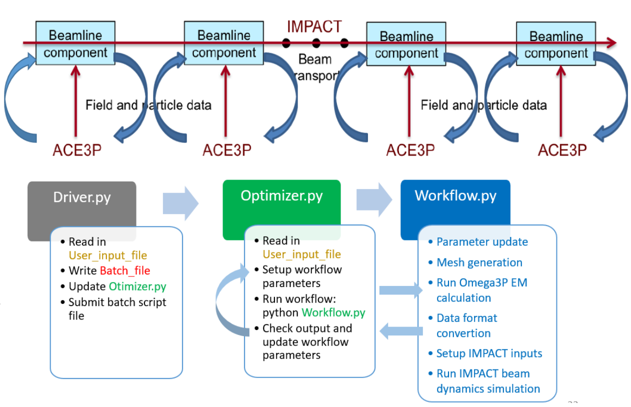

Figure 1: A schematic flow diagram of integrated ACE3P-IMPACT simulation workflow.

A schematic flow diagram of the integrated ACE3P-IMPACT simulation is shown in Fig. 1. A typical accelerator system consists of a number of beamline components such as accelerator cavities, focusing magnets, etc., connected by drift tubes. The integrated simulation starts with the calculation of electromagnetic fields of the beamline components using ACE3P, and then the field data is transferred to IMPACT for beam particle tracking along the accelerator system. In this study, we adopted the Python program environment for the integration development. A workflow python script file, Workflow.py, is developed to run both the ACE3P and the IMPACT simulations. This workflow includes updating parameters in the input files, generating meshes for cavity EM calculations, running Omega3P for EM calculations to attain realistic 3D fields, converting data format to the standard OpenPMD format [22], setting up the IMPACT inputs, and running the IMPACT beam dynamics simulation. This workflow will be included as an objective function into another Python program, Optimizer.py, for integrated EM and beam dynamics optimization. Another Python program Driver.py is used to set up global input parameters, to prepare a batch file script, and to launch the integrated simulation.

The ACE3P discretization scheme is based on a finite element method, while IMPACT uses a particle-in-cell 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. The OpenPMD standard [22], short for open standard for particle-mesh data files, 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.

BENCHMARK WITH THE LCLS-II INJECTOR DESIGN

As a test of the above ACE3P-IMPACT workflow, we simulated a 100pC photo-electron beam generation and transporting through the LCLS-II injector design using either the 3D field generated by ACE3P directly or the 2D azimuthal symmetry field constructed from the on-axis longitudinal electric field. 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 buncher cavity, eight 9-cell 1.3 GHz Tesla like superconducting cavities, and two transverse focusing solenoids.

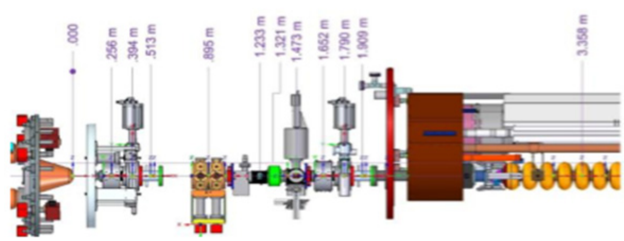

Figure 2: Layout of the LCLS-II injector.

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Firstly, we performed a benchmark through the RF gun. Figure 3 shows the electric field distribution and the on-axis electric field distribution inside the gun from the ACE3P calculation. Using these fields, we ran the beam dynamics simulation through the gun using the IMPACT code. Figure 4 shows the transverse rms size and the projected emittance evolution through the gun from the simulation using the 3D field and the 2D azimuthally symmetric field. It is seen that both rms size and emittance evolution from the two types of the fields are very similar. This is because the RF gun has been carefully designed so that the quadrupole component induced by the two RF couplers have a negligible effect on the beam.

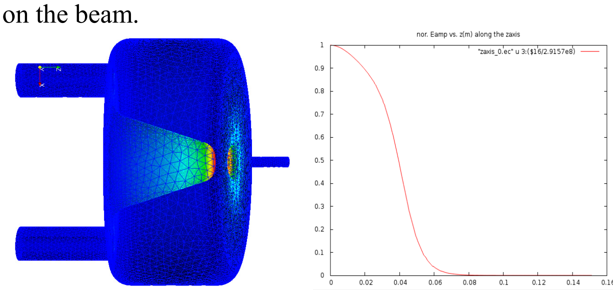

Figure 3: 3D electric field distribution inside the RF gun (left) and the on-axis electric field distribution.

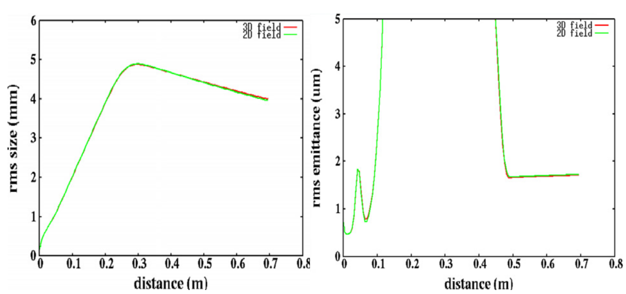

Figure 4: Transverse rms size (left) and emittance evolution (right) through the RF gun using the 3D field and the on-axis 2D field.

Next, we performed a benchmark simulation through the buncher cavity. The buncher cavity provides velocity bunching of the electron beam and compresses the beam longitudinally from 10ps to about 5ps. Figure 5 shows the transverse rms size and the transverse projected emittance evolution through the buncher cavity using the 3D field from the ACE3P and the 2D azimuthally symmetric field. The two solutions nearly overlap with each other through the cavity. The cavity has been designed with two additional perpendicular dummy ports on each cell. The 3D fields induced from the couplers and dummy ports are almost azimuthally symmetric on the beam axis, and thus have negligible effects on the beam dynamics through the cavity.

Then we performed benchmark through the eight cryomodule superconducting boosting cavities. After passing through those cavities, the electron beam energy will be accelerated to around 100MeV. Figure 6 shows the 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 7 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 the 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.

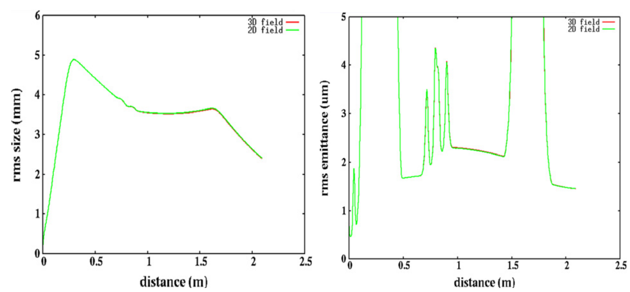

Figure 5: Transverse rms size (left) and emittance evolution (right) through the buncher cavity using the 3D field and the on-axis 2D field.

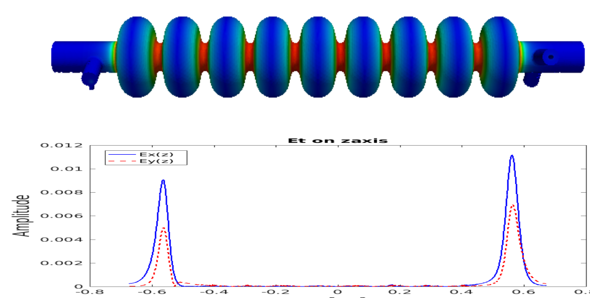

Figure 6: 3D electric field distribution (top) and transverse electric along the axis (bottom) in the boosting cavity.

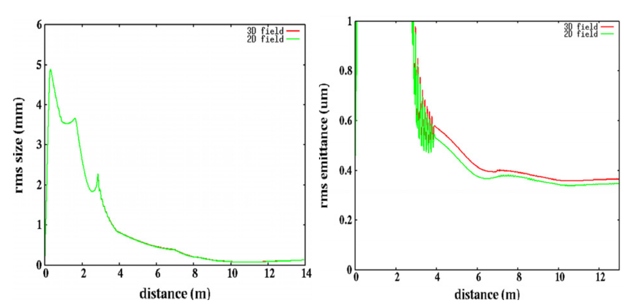

Figure 7: Transverse rms size (left) and emittance evolution (right) through the boosting cavities using the 3D field and the on-axis 2D field.

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