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LATEST PROGRESS OF ACE3P MULTIPHYSICS MODELING CAPABILITIES*

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Abstract

ACE3P is a parallel multiphysics electromagnetics (EM) simulation toolkit running on supercomputers for virtual prototyping of accelerators and RF components to facilitate their design, optimization, and analysis. ACE3P has been continuing to serve the computational needs of the accelerator community through developing new physics modeling capabilities and integrating its EM modules with beam dynamics and radiative transport codes to expand its multiphyscis capabilities. In this paper, we will present the latest progress on these efforts. First, for the time domain solver T3P, modeling of nonlinear materials with high-order electric susceptibilities has been developed. It can be used to design devices for THz accelerators and quantum information science (QIS). Second, for the particle tracking module Track3P, external DC fields calculated by ACE3P electrostatic solver can be loaded to model the use of DC bias in mitigating multipacting (MP) in accelerator structures. Third, the code integration of ACE3P and the beam dynamics code IMPACT has been used for accelerator injector start-to-end EM and beam dynamics simulation. The code integration of ACE3P and the radiative transport code Geant4 has been developed for dark current radiation analysis in high gradient accelerator structures. The applications using these new modeling capabilities will be presented.

INTRODUCTION

ACE3P codes are based on high-order finite element (FE) methods for discretizing the partial difference equations that model the physical systems with curved surface tetrahedral elements for high-fidelity modeling. Implemented on massively parallel computer architectures such as the supercomputers at National Energy Research Scientific Commutating Center (NERSC), ACE3P can model large-scale accelerator structures at system level. ACE3P codes, written in C++ and using MPI for parallel communication among processes, have been developed over two decades containing multiphysics modeling capabilities for integrated electromagnetic (EM), thermal, and mechanical characteristics. ACE3P code suite consists of seven application modules tailored to accelerator design and optimization [1,2]. In the following sections, we will present the latest progress of ACE3P multiphysics modeling capabilities and their applications.

NONLINEAR MATERIAL MODELING

THz accelerators and optical devices in quantum information science (QIS) use nonlinear materials. At the atomic level, the polarization $\boldsymbol{P}$ is expressed as a power series in the electric field $\boldsymbol{E}$ in Eq. (1):

$$\boldsymbol{P} = \varepsilon_0\left(\chi^{(1)}\boldsymbol{E} + \chi^{(2)}\boldsymbol{E}^2 + \chi^{(3)}\boldsymbol{E}^3 + \cdots\right). \tag{1}$$

T3P, the time domain solver in ACE3P code suite, calculates transient field responses to imposed fields or beam excitations in an RF structure by solving the vector wave equation for the time integral of electric field $\boldsymbol{E}$ as shown in Eq. (2):

$$\left(\mu\varepsilon\frac{\partial^2}{\partial t^2} + \mu\sigma\frac{\partial}{\partial t} + \nabla\times\nabla\times\right)\int_0^t \boldsymbol{E}.dt = -\mu\boldsymbol{J}, \tag{2}$$

where $\sigma = \omega\varepsilon_0\varepsilon_r$ is the electric conductivity.

Under SLAC LDRD support, electrical nonlinearities including second and third high-order electric susceptibilities $\chi^{(2)}$ and $\chi^{(3)}$ have been implemented in T3P using nonlinear methods including "linearized" models by interfacing to PETSc SNES nonlinear solvers. T3P strong parallel scaling of the new developed nonlinear solver up to 10k processors on NERSC Perlmutter supercomputer is shown in Fig. 1. The number of degrees of freedom (DOF) is 1.1 million for the example used in Fig. 1.

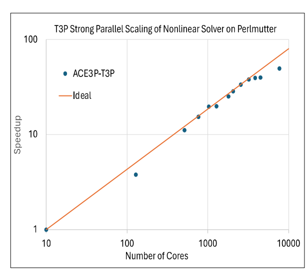

Figure 1: Strong parallel scaling of T3P nonlinear solver.

The nonlinear solver in T3P has been used to simulate the wakefield excited by short electron bunches transiting an X-Band cavity with an electro-optic material LN as shown in Fig. 2. The bunch length is 1 mm with a charge of 100 pC, and the bunch spacing is 0.1 m. The simulated wakefields with and without the laser pumping at the waveguide port are shown in Fig. 3. High frequency wakefield can be controlled through harmonic interactions. This technique can be used in advanced wakefield accelerator beam diagnostics and other applications [3].

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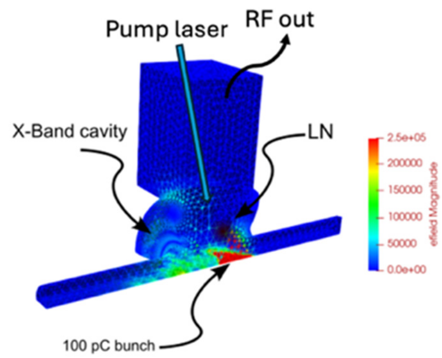

Figure 2: Wakefield excitation with nonlinear material.

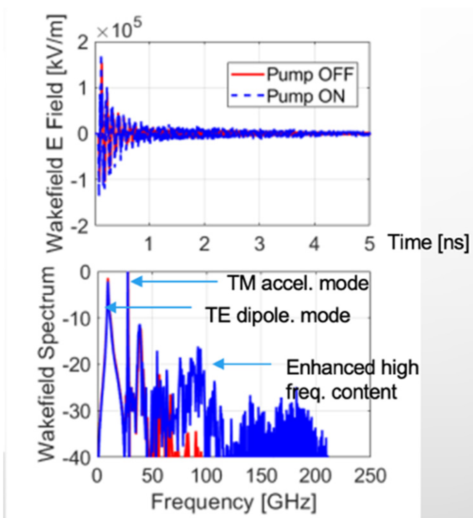

Figure 3: Wakefield (above) and frequency spectrum (below) from T3P nonlinear solver.

PARTICLE TRACKING WITH ELECTROSTATIC FIELDS

SLAC led a multi-lab collaboration to develop a low emittance, high-gradient CW quarter wave (QW) SRF gun operating at 185.7 MHz for LCLS-II-HE LEI [4]. ACE3P codes have been used to design and optimize SRF gun cavity shape to aim for high shunt impedance and low surface peak EM fields as well as multipacting (MP) suppression.

Track3P traces charged particles under the electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ fields from ACE3P frequency solvers Omega3P or S3P using the Lorentz force equation in Eq. (3)

$$\frac{d(m\boldsymbol{v})}{dt} = q(\boldsymbol{E} + \boldsymbol{v}X\boldsymbol{B}), \qquad \frac{d\boldsymbol{r}}{dt} = \boldsymbol{v} \tag{3}$$

MP has been found in initial SRF gun cavity shape with a long oval anode wall shape from Track3P as shown in Fig. 4. A dome anode wall shape has been adopted to suppress MP in the SRF cavity. MSU designed the SRF gun 3D features including the fundamental power coupler and cathode stalk. SLAC/MSU SRF gun cavity 3D design is shown in Fig. 5.

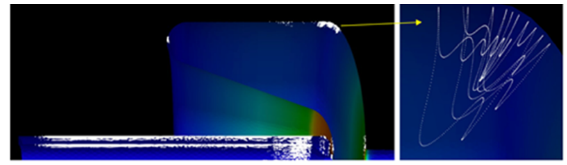

Figure 4: Resonant particles in initial SRF cavity shape.

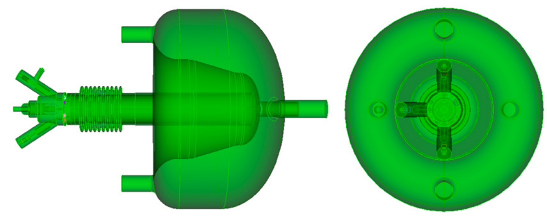

Figure 5: SLAC/MSU SRF gun cavity.

The SRF gun cathode stalk includes coax, bellows, DC break, and end stool. Some typical resonant particles in DC break found from Track3P are shown in Fig. 6.

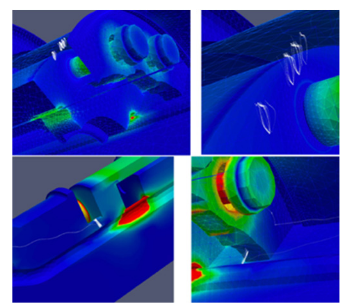

Figure 6: Resonant particles in SRF gun cathode stalk DC break region.

The MP in the cathode stalk is mitigated through DC bias. The calculated 3D electrostatic fields in DC break from ACE3P electrostatic solver are shown in Fig.7. Track3P traces the charged particles under the sum of RF and DC fields. The simulations show that no resonant particles found in the cathode stalk when the DC voltage is larger than 175 V.

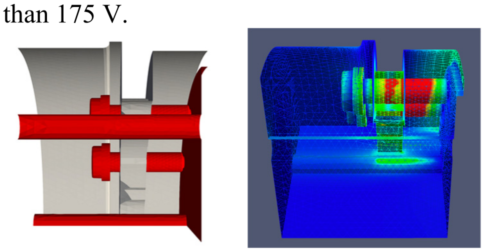

Figure 7: Cathode stalk geometry (left) with ground surface in grey, high voltage surface in red, and electrostatic fields (right).

ACCELERATOR INJECTOR EM AND BEAM DYNAMICS SIMULATIONS

LCLS-II-HE LEI SRF gun is symmetric to eliminate RF dipole component on the beam axis. However, transverse fields on the beam axis can be induced from cavity imperfections due to fabrication errors, and thus adversely affect beam performance. To resolve the small transverse fields along the beam axis induced from the fabrication errors,

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fourth-order basis functions plus denser mesh in the beam region were used in Omega3P simulations to distinguish the transverse fields which is three orders of magnitude lower than the longitudinal field. The total number of DOFs is 11 millions running on 16 cores in about 10 mins. The 3D EM fields from ACE3P were then imported into beam dynamics code IMPACT for beam performance evaluation.

IMPACT simulated LCLS-II injector with the SRF cavity front plate shifted by 500 µm. The electrical fields from Omega3P in the imperfect SRF cavity and beam emittance growth along LCLS-II injector from IMPACT are shown in Fig. 8. This kind of SRF cavity imperfection can increase the beam emittance by 35% relative to an ideal cavity.

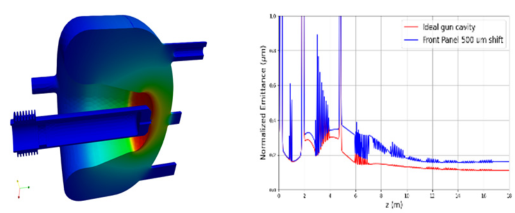

Figure 8: Electrical fields from Omega3P in an SRF gun with the front plate offset by 500 µm along the vertical direction (left) and the beam emittance comparison results from IMPACT in LCLS-II injector with the deformed SRF gun cavity (right).

DARK CURRENT RADIATION ANALYSIS IN HIGH GRADIENT ACCELERATOR

A code integration tool of ACE3P and the radiative transport code Geant4 has been developed and applied for the dark current radiation analysis in KEK S-Band 56-cell constant gradient structure as shown in Fig. 9. The work is supported by HEP US-Japan Science and Technology Cooperation Program [5].

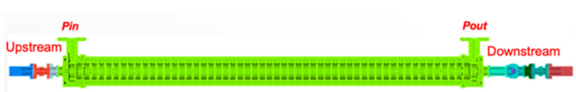

Figure 9: KEK S-Band accelerator structure CAD model.

S3P, S-Parameters solver in ACE3P code suite, was used to simulate the EM fields at the operating frequency of 2856 MHz as shown in Fig. 10. There are 20 millions of DOFs which cannot be solved using commercial EM software due to lack of computational power and memory. Running on Perlmutter supercomputers at NERSC, it can be solved using ACE3P within a few minutes using 256 processors on 4 nodes.

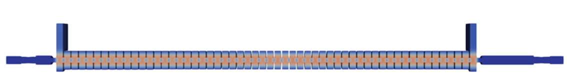

Figure 10: Electric field distribution in KEK accelerator structure.

Track3P traced the emitted particles calculated using Fowler–Nordheim (FN) emission model up to 30 RF cycles. The simulated dark current at downstream Faraday cup is shown in Fig. 11, which shows similar behavior as KEK measurements.

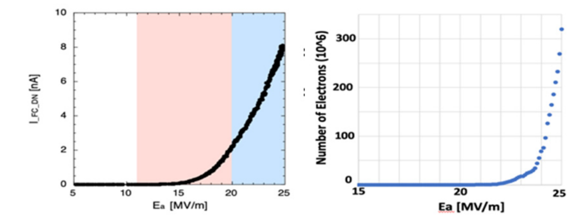

Figure 11: Dark current measurements (left) and simulations (right) in KEK accelerator structure.

The particles impact data on the cavity wall from Track3P are transferred into Geant4 for radiation analysis. The radiation dose distributions along the KEK accelerator structure from KEK measurements and SLAC simulations are shown in Fig. 12.

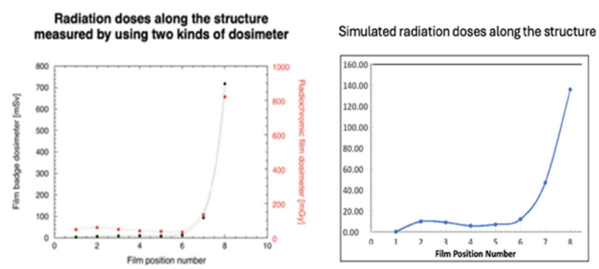

Figure 12: Radiation dose measurements (left) and simulations (right) in KEK accelerator structure.

SUMMARY

ACE3P, a mature set of RF modeling tools, has been developed over more than two decades under the support of DOE's HPC initiatives (SciDAC), GARD and SLAC programs. Its HPC capabilities enable accelerator designers to model and simulate accelerator and RF components and systems with enhanced scale, complexity and speed. New modeling capabilities have been added in support of accelerator community and beyond. To expand ACE3P multiphysics modeling capabilities, ACE3P has been integrated with beam dynamics code IMPACT and radiative transport code Geant4 to further broaden the user base.

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