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High-Fidelity RF Gun Simulations with the Parallel 3D Finite Element Particle-In-Cell Code Pic3P

A. Candel, A. Kabel, L. Lee, Z. Li, C. Limborg, C. Ng, G. Schussman and K. Ko

SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

Abstract. SLAC's Advanced Computations Department (ACD) has developed the first parallel Finite Element 3D Particle-In-Cell (PIC) code, Pic3P, for simulations of RF guns and other space-charge dominated beam-cavity interactions. Pic3P solves the complete set of Maxwell-Lorentz equations and thus includes space charge, retardation and wakefield effects from first principles. Pic3P uses higher-order Finite Element methods on unstructured conformal meshes. A novel scheme for causal adaptive refinement and dynamic load balancing enable unprecedented simulation accuracy, aiding the design and operation of the next generation of accelerator facilities. Application to the Linac Coherent Light Source (LCLS) RF gun is presented.

Keywords: higher-order finite element time domain (FETD), electromagnetic particle-in-cell (PIC), space charge, electron dynamics, moving window, parallel computing
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INTRODUCTION

A detailed understanding of emission, acceleration and transport phenomena is necessary for advancing the development of high-quality electron guns for next-generation light sources and colliders to be operated at ever more demanding parameter regimes. Joining in this effort, SLAC has developed the first high-performance higher-order Finite Element (FE) 3D Particle-In-Cell (PIC) code Pic3P, for realistic modeling of low energy, space-charge dominated electron dynamics in injectors. Running on large-scale supercomputing facilities, Pic3P provides advanced capabilities that enable RF gun simulations with unprecedented accuracy and speed.

THE PARALLEL CODE PIC3P

In Pic3P, the full set of Maxwell's equations is solved numerically in time domain using parallel higher-order FE methods. Electron macro-particles are pushed self-consistently in space charge, wake- and external drive fields.

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Finite Element Time-Domain Field Solver

Ampère's and Faraday's laws are combined and integrated over time to yield the inhomogeneous vector wave equation for the time integral of the electric field **E**:

$$\left(\varepsilon\frac{\partial^2}{\partial t^2}+\sigma_{\mathrm{eff}}\frac{\partial}{\partial t}+\nabla\times\mu^{-1}\nabla\times\right)\int^t \mathbf{E}(\mathbf{x},\tau)\,\mathrm{d}\tau=-\mathbf{J}(\mathbf{x},t), \tag{1}$$

with permittivity ε and permeability μ. The effective conductivity σ_{eff} provides a simple model for damping in lossy materials.

The computational domain is discretized into curved tetrahedral elements and $\int^t \mathbf{E}\,\mathrm{d}\tau$ in Equation (1) is expanded into a set of hierarchical Whitney vector basis functions $\mathbf{N}_i(\mathbf{x})$ up to order p within each element:

$$\int^t \mathbf{E}(\mathbf{x},\tau)\,\mathrm{d}\tau=\sum_{i=1}^{N_p} e_i(t)\cdot\mathbf{N}_i(\mathbf{x}). \tag{2}$$

Substituting Equation (2) into Equation (1), multiplying by a test function and integrating over the computational domain results in a system of linear equations for the coefficients e_i, second-order in time. Numerical integration is performed with the unconditionally stable implicit Newmark-Beta scheme [1]. More detailed information about the employed methods has been published earlier [2].

Higher-Order Particle-Field Coupling

Electron macro particles are specified by position **x**, momentum **p**, rest mass m and charge q. The total current density **J** in Equation (1) is then approximated as

$$\mathbf{J}(\mathbf{x},t)=\sum_i q_i\cdot\delta(\mathbf{x}-\mathbf{x}_i(t))\cdot\mathbf{v}_i(t), \tag{3}$$

with $\mathbf{v}=\frac{\mathbf{p}}{\gamma m}$, $\gamma^2=1+|\frac{\mathbf{p}}{mc}|^2$. The classical relativistic collision-less Newton-Lorentz equations of motion are integrated using the standard Boris pusher, an explicit method splitting the momentum update into one magnetic and two electric contributions [3].

Maintaining numerical charge conservation during the self-consistent simulation of charged particles and electromagnetic fields is achieved by starting with proper initial conditions and then fulfilling the discrete versions of Equation (1) and the continuity equation

$$\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{J}=\mathbf{0} \tag{4}$$

simultaneously during time integration.

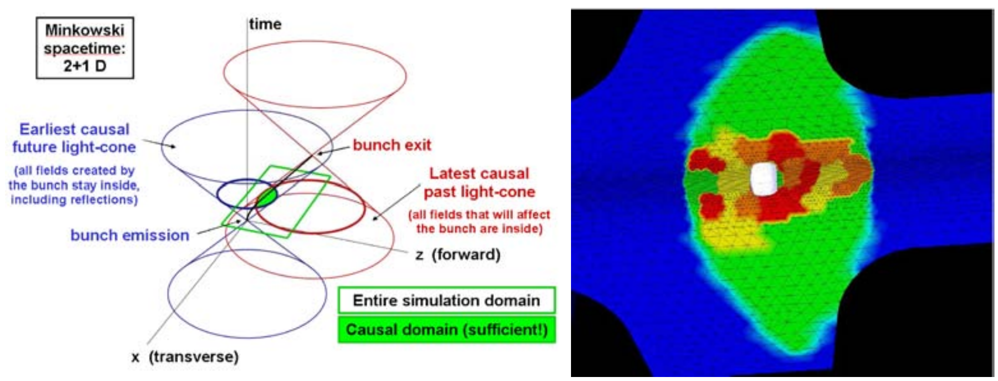
The use of higher-order finite elements not only significantly improves field accuracy and dispersive properties [4], but also leads to intrinsic higher-order accurate particle-field coupling equivalent to, but much less laborious than, complicated higher-order interpolation schemes commonly found in finite-difference methods.

Causal Moving Window

The methods used in Pic3P are based on unstructured meshes of up to second-order curved tetrahedral elements – this allows modeling of small geometric features and scattering effects with high accuracy. In combination with higher-order field representation, highly efficient use of computational resources and unprecedented simulation accuracy are obtained.

Furthermore, orders of magnitude in computational resources can be saved, without sacrificing modeling accuracy, by restricting field computations to the causal field region around the particle bunch. This 'moving window' technique can be efficiently implemented using adaptive p-refinement – every element in the overall domain uses an individual basis order $p \geq 0$.

Figure 1a) shows a Minkowski spacetime diagram indicating the causal domain for a bunch transiting through a compact structure. Figure 1b) shows the corresponding parallel dynamic load balancing of the causal field domain during a typical RF gun PIC simulation with Pic3P, where both the field calculation and communication efforts are balanced.



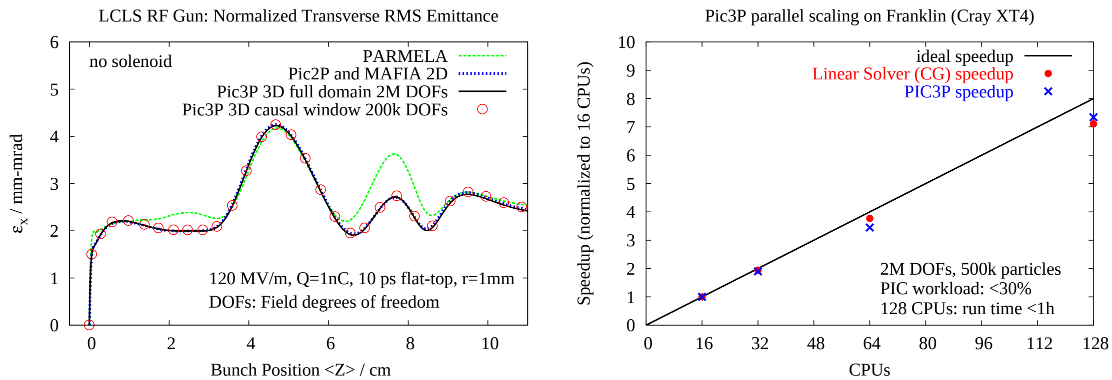
(a) (b)

FIGURE 1. Snapshot in time during bunch transit through compact structure with causal moving window technique. (a) Minkowski spacetime diagram indicating the causal domain.
(b) Pic3P simulation of a quarter model of an RF gun with particle bunch in transit. Elements in non-causal domain are omitted in the field computations ($p = 0$). Elements and fields in the causal domain ($p > 0$) around the particle bunch are partitioned onto all CPUs with dynamic parallel load balancing.

RESULTS

PIC simulations of the 1.6-cell S-band LCLS RF gun are presented [5]. In the simulations, the gun is driven by the π-mode with a peak accelerating field gradient of 120 MV/m at the cathode (the cavity wall). A cold, uniform, 10 ps flat-top, cylindrically symmetric electron bunch of 1 mm radius is emitted, centered around a phase of -58° with respect to the crest. Solenoidal focusing fields are neglected for simplicity. These parameters allow comparisons between the 3D results from simulations with Pic3P and PARMELA and the 2D results from simulations with Pic2P and MAFIA.

For Pic3P simulations, a conformal, unstructured 3D (1/4) mesh model with 305k tetrahedral elements is used, with mesh refinement along the center of the beam pipe. High fidelity cavity mode fields are obtained with the parallel FE frequency domain code Omega3P and directly loaded into Pic3P as drive fields. Figure 2a) shows a comparison of transverse emittance results by the different codes and Figure 2b) shows the parallel scalability of Pic3P.



(a) (b)

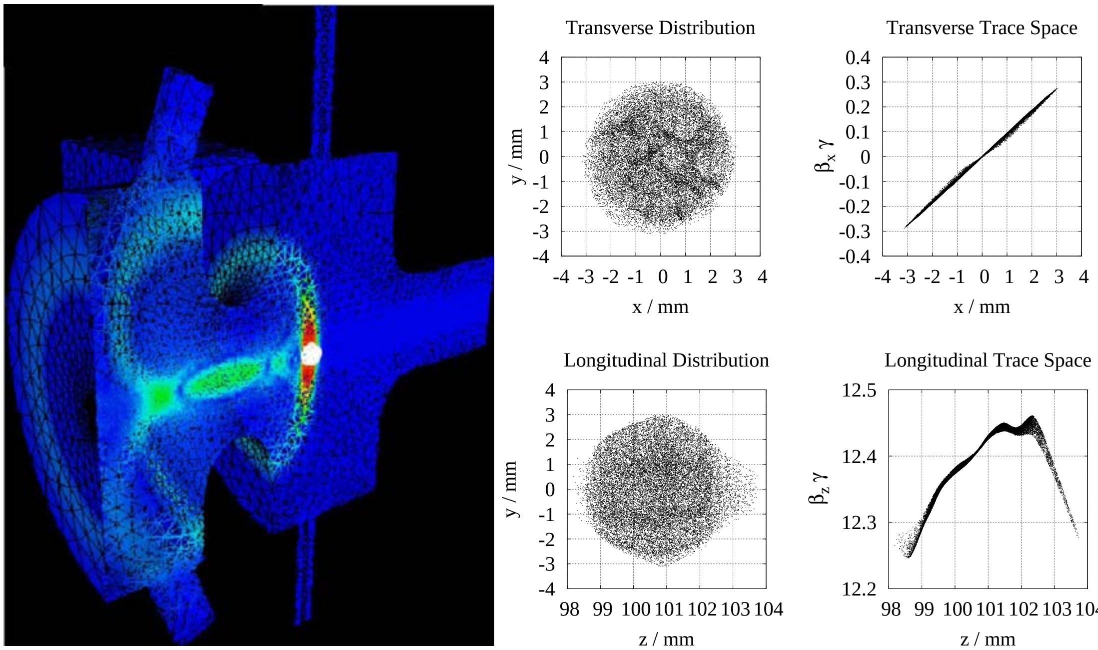
FIGURE 2. (a) Comparison of normalized transverse RMS emittance as a function of beam position in the LCLS RF gun as calculated with PARMELA, Pic2P and MAFIA 2D (both agree), and Pic3P, where the causal moving window technique reduces the problem size by one order of magnitude.
(b) Parallel scalability of Pic3P for the full domain simulation with 2M DOFs.

Excellent agreement between 3D results from Pic3P and the 2D results from Pic2P and MAFIA is found, as expected from the high cylindrical symmetry in the fields and the convergence behavior of the codes. PARMELA results differ as space-charge effects are significant, presumably because wakefield and retardation effects are ignored, as detailed in a previous study [2].

Pic3P allows large-scale 3D PIC simulations of RF guns with realistic particle distributions, including intra-bunch effects. Starting with an initial particle distribution obtained from measurements, another LCLS RF gun simulation was performed. Figure 3a) shows a snapshot of the scattered fields during bunch transit. Figure 3b) shows the transverse and longitudinal phase phase of the particle bunch near the exit of the gun.

CONCLUSIONS

The first successful implementation of a parallel Finite Element 3D electromagnetic PIC code is presented. The new code Pic3P was used to model space-charge effects in the LCLS RF gun from first principles, including wakefield and retardation effects. It employs state-of-the-art parallel Finite Element methods on conformal, unstructured meshes with unconditionally stable time integration and self-consistent higher-order particle-field coupling. In combination with novel causal moving window techniques and dynamic load balancing, Pic3P allows unprecedented accurate and efficient simulations of low-emittance electron injectors, aiding the design and operation of the next generation of light sources and colliders.



(a) (b)

FIGURE 3. Snapshot during LCLS RF gun simulation with Pic3P, starting with a non-uniform electron bunch distribution obtained from measurements. (a) Scattered electric fields (b) Phase space

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REFERENCES

1. N. M. Newmark, “A method of computation for structural dynamics”, Journal of Eng. Mech. Div., ASCE, vol. 85, pp. 67-94, July 1959.
2. A. Candel et al., “Parallel Higher-order Finite Element Method for Accurate Field Computations in Wakefield and PIC Simulations”, Proc. ICAP 2006, Chamonix Mont-Blanc, France, Oct. 2-6, 2006.
3. J. P. Boris, “Relativistic plasma simulation-optimization of a hybrid code”, Proc. Fourth Conf. Num. Sim. Plasmas, Naval Res. Lab, Wash. D.C.,pp. 3-67, Nov. 2-3, 1970.
4. M. Ainsworth, “Dispersive properties of high-order Nedelec/edge element approximation of the time-harmonic Maxwell equations”, Philos. trans.-Royal Soc., Math. phys. eng. sci., vol. 362, no. 1816, pp. 471-492, 2004.
5. L. Xiao et al., “Dual Feed RF Gun Design for the LCLS”, Proc. PAC 2005, Knoxville, Tennessee, May 15-20, 2005.