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A massively parallel particle-in-cell code for the simulation of field-emitter based electron sources

Arno E. Candel[a,*], Micha M. Dehler[b], Matthias Troyer[c]

[a]Theoretische Physik, Eidgenössische Technische Hochschule, CH-8093 Zürich, Switzerland
[b]Paul Scherrer Institut, Villigen PSI, Switzerland
[c]Theoretische Physik, Eidgenössische Technische Hochschule, CH-8093 Zürich, Switzerland

Abstract

For the realistic simulation of electron sources using field emitter arrays, the sub-micron resolution required for the emitters leads to simulation models not suitable for current serial codes. Thus, a parallel high-performance 3D Particle-In-Cell code, called *Capone*, has been implemented in C++ using the POOMA II framework on the Linux platform. Sophisticated C++ expression templates techniques deliver Fortran performance combined with high-level programming and development comfort. For the computation of external fields, matching parallel field solvers are in development with the electrostatic one being completed.

The Maxwell field solver is based on the Finite Integration Algorithm on a non-uniform rectilinear grid. Anisotropic ε and μ constants and perfect electric/magnetic materials stored in triangulated grid cells are supported as well as open, electric and magnetic boundary conditions. Self-consistent macro-particle pushing is accomplished by integrating the classical relativistic equations of motion in combination with charge-conserving current scattering onto the computational grid.

Parallelization is performed by partitioning the calculation domain into patches associated to individual processors. Fields are statically distributed while Particles are concurrently distributed to processors according to their position to allow fast local interpolation.

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1. Introduction

1.1. Physical background

After the successful completion of the synchrotron light source project SLS at the Paul Scherrer Institut (PSI), PSI is looking forward at options for a Free Electron Laser (FEL) used as a complementary research tool to the SLS.

Our focus is on compact Angstrom wavelength FEL sources with a modest beam energy and a short saturation length of the undulator. The challenge is the required quality of the generating e^- beam, mainly determined by the electron source. The upper limit for the required transverse emittance scales with the beam energy. A compact FEL working at reduced beam energies needs emittances orders of magnitudes below current designs. Our design goal is in the order of a few times 10^{-2} mm mrad.

The current approach towards a suitable electron source consists of using field emitter arrays (FEA) as a cold, high intensity electron cathode [1]. This cathode is used in a DC gun, driven by a 1 MV, 200 ns FWHM pulse [2], which is currently under development.

An example for a field emitter structure suited to our application is shown in Fig. 1. Here, the required field is

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[*] Corresponding author. Stanford Linear Accelerator Center, 2575 Sand Hill Road, M/S 27, Menlo Park CA 94025, USA.

E-mail addresses: arno@candel.org, candel@slac.stanford.edu (A.E. Candel).

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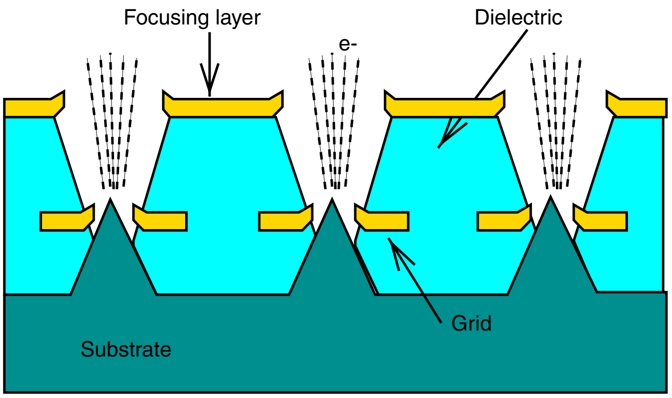

Fig. 1. Field emitter with additional grid and focusing layers.

applied via a conducting gate layer at a distance in the μm range from the substrate. The small distance yields relatively small turn on voltages in the order of 100 V, which in turn allows the use of fast pulse electronics to create short pulses. Having only a gate would lead to a divergent beamlet. In order to combine an array of these beamlets minimizing the emittance of the total beam, an additional focusing layer is mandatory, acting as a set of electrostatic lenses, thus creating an array of parallel beamlets.

1.2. Simulation strategy

Given the complexity of the problem, the dynamics of the emitted electrons in a given setup can only be simulated with a self-consistent, parallel 3D Maxwell Particle-In-Cell (PIC) code consisting of a Maxwell field dynamics solver, a static field solver and a relativistic particle pusher. Currently, a reasonable spatial resolution in 3D cannot be accomplished without parallelization due to high memory needs. Existing available codes like MAFIA [3] are either not fully 3D, not self-consistent, restricted to special cases or are only serial, and therefore not suited to our problem.

Over the last two years, a massively parallel high-performance 3D Maxwell PIC code has been implemented in C+ + using the POOMA II framework for parallel computing on the Linux platform. Sophisticated C+ + expression templates techniques deliver Fortran performance combined with high-level programming and development comfort. The simulation code is compatible to MAFIA's PIC modules TS2/TS3 which are used as reference. The code is called *Capone*, which stands for Charged Accelerated Particles Outta Next-generation Emitters.

2. Methods

2.1. Dynamic field solver

The numerical simulation of the electromagnetic field dynamics uses the Finite Integration Technique (FIT) [4].

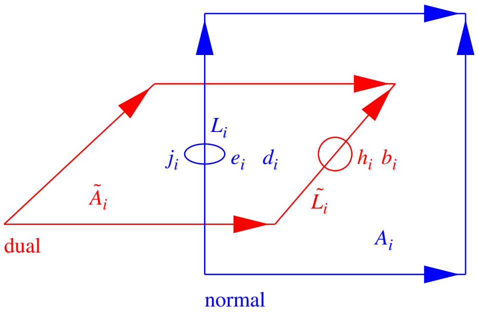

Fig. 2. Topological structure of the Finite Integration Algorithm.

A complete discretization of the calculation volume on two dual rectilinear grids G, $\tilde{G}$ is done, described by cells with volumes V_i, $\tilde{V}_i$, cell faces A_i, $\tilde{A}_i$ and grid lines L_i, $\tilde{L}_i$. Integrated field components $e_j = \int_{L_j} \vec{E}\, d\vec{s}$ etc. are stored at positions indicated in Fig. 2.

Maxwell's equations are mapped to this topological space, using discrete curl and divergence operators C, $\tilde{C}$, S, $\tilde{S}$ as well as discrete material operators D_ε, D_μ, resulting in the following set of discrete Maxwell's equations:

$$Ce = -\frac{\partial b}{\partial t} \tag{1}$$

$$\tilde{C}h = \frac{\partial d}{\partial t} + j \tag{2}$$

$$\tilde{S}d = q \tag{3}$$

$$Sb = 0 \tag{4}$$

$$d = D_\varepsilon e \tag{5}$$

$$b = D_\mu h. \tag{6}$$

Non-homogeneous distributions of ε and μ are permitted, with material boundaries given by cell boundaries and cell diagonals. In addition to Dirichlet and Neumann boundary conditions, open boundaries have been implemented.

The system is solved in the time domain by integrating the two curl equations using the leap frog algorithm [13]. Due to the orthogonality of the discrete curl and div operators, the continuity equations remain fulfilled throughout the iteration process. There is no systematic accumulation of spurious space charges [5].

The discrete electric current density j in (2) is obtained with a Nearest-Grid-Point (NGP) scatter interpolation in combination with a scheme fulfilling the continuity equation in discrete space [6]. A spatial filter is used to smoothen the electric current density at every time step.

2.2. Static field solver

For the generation of a consistent initial electrostatic field solution, exactly the same grid and the same material distribution as for the FIT solver are used. In our parallel approach, we are using an iterative conjugate gradient solver together with an incomplete Cholesky