DEVELOPMENT OF ADVANCED MODELS FOR 3D PHOTOCATHODE PIC SIMULATIONS*

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Abstract

Codes for simulating photocathode electron guns invariably assume the emission of an idealized electron distribution from the cathode, regardless of the particular particle emission model that is implemented. The output of such simulations, a relatively clean and smooth distribution with very little variation as a function of the azimuthal angle, is inconsistent with the highly irregular and asymmetric electron bunches seen in experimental diagnostics. To address this problem, we have implemented a recently proposed theoretical model [1] that takes into account detailed solid-state physics of photocathode materials in the VORPAL particle-in-cell code [2]. Initial results from 3D simulations with this model and future research directions are presented and discussed.

INTRODUCTION

Future advances in fundamental research in high-energy physics require more powerful particle accelerator facilities, such as the Next Linear Collider (NLC), than those currently in use. A key component of the NLC is its photoinjector electron gun. Free electron lasers (FEL) [3] also require significant advances in beam brightness from photocathode electron guns. Modeling photoinjectors permits design improvement and optimization without the cost of construction.

Codes for simulating photocathode electron guns use specific particle distribution functions (e.g. a cigar or an ellipsoid shapes) for the loading of electrons "emitted" from the cathode, regardless of the particular physics of the emission process [4]. As a result, the output data of such simulations shows a relatively clean and smooth distribution with very little variation as a function of the azimuthal angle, are inconsistent with the highly irregular electron bunches observed in experiments. This is a fundamental problem that must be resolved to facilitate new ideas and designs within the electron gun community leading to the order-of-magnitude performance increase needed by the NLC and other next-generation accelerators.

The opportunity presented by this challenge is to take advantage of recent advances in the theoretical understanding of the photo emission process from various cathode materials [1, 5]. The idea is to implement these theoretical models in a high-performance 3-D particle-in-cell (PIC) code that is general and flexible enough to accurately simulate the laser pulse, the emission process, and the subsequent electron beam dynamics. The VORPAL PIC code [2] meets these requirements and was selected for this purpose.

In the next section we briefly introduce the VORPAL simulation framework. Then, we describe the currently implemented capabilities to model radio frequency (RF) photoinjectors with VORPAL and present results from Copper photocathode simulations. We conclude with a summary of the current progress in implementing photocathode models in VORPAL and discuss our future development plans.

THE VORPAL SIMULATION FRAMEWORK

The VORPAL code is under active development at Tech-X Corp. for the purpose of simulating intense laser-plasma physics.

The VORPAL framework currently can model the interaction of electromagnetic fields with conducting boundaries, charged particles (of both constant and variable weight), and charged fluids. Included in the fluid implementations are both a cold (pressureless) fluid and a scalar-pressure fluid. VORPAL also has field ionization production of particles and a Direct Simulation Monte Carlo treatment of neutral and charged fluids, i.e., self collisions for the particle representations.

The VORPAL framework uses C++ templating over both dimension and floating point types, so that one can build 1D, 2D and 3D codes, in both single and double precision, using a single source code base. Output is in the form of Hierarchical Data Format V.5 files, a binary, cross-platform, self-describing data format. VORPAL can run on a parallel Beowulf cluster or on the parallel IBM SP RS/6000 through use of the Message Passing Interface (MPI). On OS X, VORPAL works with the LAM MPI implementation.

VORPAL was designed from the outset to be flexible through use of object-oriented methods. These methods have permitted easy addition of different electromagnetic field solvers, particle dynamics, and charged fluids. For example, VORPAL makes available both an electrostatic solver and an implicit electromagnetic solver.

VORPAL simulations are currently applied to study a number of problems: generation of laser wake fields and optical injection of particles into wake fields [6], electron cooling of ion beams, photonic band gap systems, RF heating of fusion plasmas, magnetic reconnection.

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DEVELOPMENT OF PHOTOINJECTOR MODELING IN VORPAL

There were two main problems to be solved to enable photoinjector modeling in VORPAL. Firstly, code infrastructure was needed for support of photocathode objects initialization and, more importantly, development of an algorithm for loading electron macro particles in the simulation in response to (photo and thermal) emission. Secondly, implementation of photocathode models was needed to enable the calculation of emitted current density during the interaction of a laser pulse with a photocathode.

We designed and implemented code to instantiate photocathode emitter and dispenser cathode objects only if data in a VORPAL input file request a simulation with a photocathode. Once the objects of these two types are initialized, the actual loading of electrons emitted from a photocathode happens at each time step.

Loading of electron macro particles is handled by the photochode emitter object provided the emission current is nonzero. The photocathode emitter object obtains the emission current density from the dispenser cathode object. The latter is designed to enable the implementation of different photocathode physics models. Note that the physics of the dispenser cathode generally has different length and time scales than the ones for the PIC simulation. This requires the dispenser cathode object to manage its own physics domain and respond to requests from the photocathode emitter object on the time scales of the PIC simulation.

The photocathode emitter object loads the electron macro particles during each time step according to acceleration in the external fields (e.g., the RF field), the total charge that has to be emitted and the distribution of electron velocities.

The emitted current density is computed in the dispenser cathode object as the sum of the photo $J_\lambda(T_e,\,\Phi)$ and $J_{RLD}(T_e,\,\Phi)$ thermal current densities using Eqn. (14) in Ref. [1]:

$$J_\lambda(T_e,\,\Phi) = q(1-R)\frac{I_\lambda(t)}{\hbar\omega}\times\frac{U(\beta(\hbar\omega-\phi))}{U(\beta\mu)},$$
$$J_{RLD}(T_e,\,\Phi) = A_{RLD}T_e^2\exp(-\beta\phi),$$

where q is the electron charge, T_e is the electron temperature, $\beta = 1/k_BT_e$ with k_B the Boltzmann constant, μ is the chemical potential, Φ is the work function (the difference between the potential barrier maximum and the chemical potential at zero field), and $\phi = \Phi - \sqrt{4QF}$ is the effective potential barrier maximum when the image charge potential and the external electric field are considered [5]. The image charge factor is denoted by Q, F is the magnitude of the electric field, and $\sqrt{4QF}$ is the Schottky barrier lowering. The current density $J_{RLD}(T_e,\,\Phi)$ is calculated in the Richardson approximation [5] ($A_{RLD} \approx 120$ A/cm^{2}T^2 is the Richardson constant). The laser intensity interacting with the photocathode surface at time t is $I_\lambda(t)$, R is the fraction of the reflected laser light, $\hbar\omega$ is the energy of the incident photons with a wavelength λ, and $U(x)$ is the Fowler function [1].

The accurate calculation of the photocathode electron temperature as a function of time represents the most significant problem to solve in order to calculate the emission current. Generally, the electrons and ions in the photocathode have different relaxation times in response to external perturbations (in our case the interaction with the laser pulse). Jensen *et al.* [1] described a general way to model this response and to calculate the electron temperature. They also gave a steady-state approximation model that we implemented first. Results from this model are presented in the next section. The implementation of the general, nonequilibrium, nonlinear, partial differential equations (PDEs) model for the electron and ion temperatures is currently in the development pipeline. All implemented code is for 3D simulations only in Cartesian geometry.

COPPER PHOTOINJECTOR SIMULATION RESULTS

The development of phothocathode models in VORPAL was driven by test simulations of an RF gun with a Cu photocathode so far. The photocathode is specified as a par-

Symbol	Definition	Value
λ	laser wavelength	266.0 nm
l_z	eff. z pulse length	2.544 mm
l_x	eff. x pulse length	3.333 mm
l_y	eff. y pulse length	3.333 mm
Δt	eff. pulse time	6.0 ps
E_0	RF field magn.	50.0 MV/m
ν_{rf}	RF field freq.	1.3 GHz
ϕ_0	RF field phase	248.1 deg.
T_0	Initial cathode temp.	659.0 K
μ	chemical potential	7.0 eV
η	thermal mass factor	1.375
Φ_W	Cu work function	4.6 eV
A_0	e-e relax. time param.	25.1
λ_0	e-ph relax. time param.	0.226
v_s	Cu sound velocity	476000 cm/s
T_D	Cu Debye temp.	347 K
ρ_0	Cu density	8.96 g/cm^3
δ	Cu skin depth	10.416 nm
R	Cu Reflectivity	0.942
n	temp. decrease factor	17.321
L_z	sim. box z length	23 mm
L_x	sim. box x length	30 mm
L_y	sim. box y length	30 mm
dt	sim. time step	0.117 ps
I_0	pulse intensity magn.	10.237 MW/cm^2
$\|Q\|$	beam charge	0.506 nC

Table 1: Selected parameters we used to simulate electron beam generation from a Cu photocathode in an RF gun.

ticle source object at a given simulation boundary. In the simulations here, it was located at the simulation box side with $z = 0$. The laser pulse was modeled as a Gaussian propagating along the direction $-z$ and starting at $3\sigma_z^{rms}$ from the photocathode. The rms widths of the pulse are $\sigma_\alpha^{rms} = l_\alpha/2$ for $\alpha = x,\ y,$ or z. The values of l_α are given in Table 1. The functional form of the RF field is the same as in Ref. [7] and its parameters are given in Table 1. The laser pulse and RF field parameters we used are relevant to photocathode RF gun experiments and are similar reported values in previous simulations [7, 4]. We did the runs without an external solenoidal magnetic field. However, since VORPAL provides an input file space-time function parser, the addition of the solenoidal magnetic field requires only its expression in the input file.

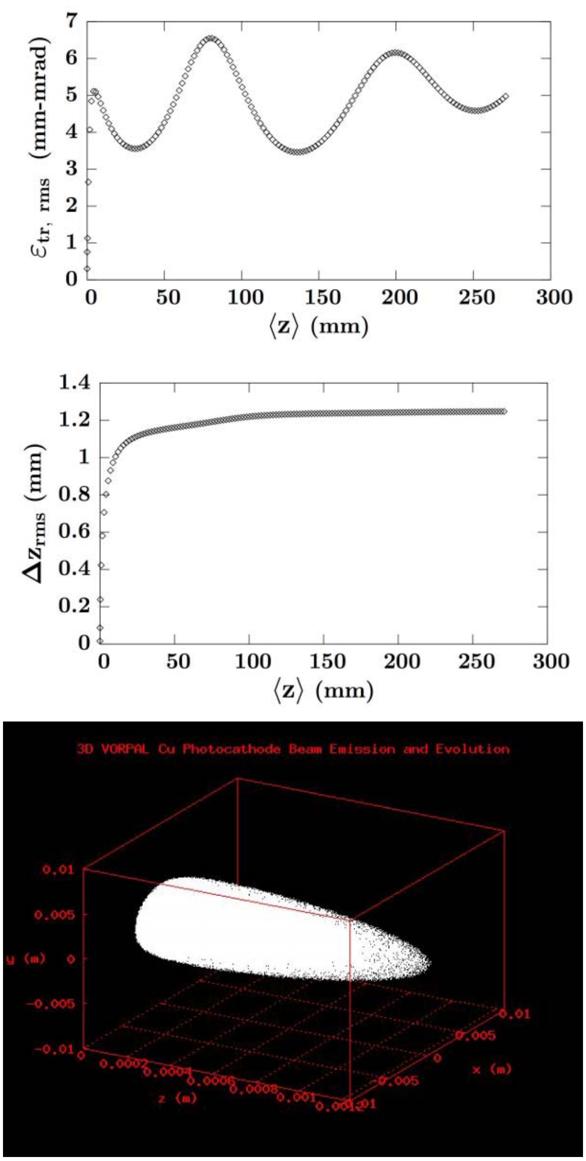

Figure 1: VORPAL and its associated post processing and visualization tools allow the calculation and display of detailed beam properties. A subset of these quantities for the Cu photocathode RF gun simulations are the dependence of the trace space transverse rms emittance (top plot) and the rms bunch length on average beam position $\langle z \rangle$ (middle plot). The beam emission and evolution can be visualized in 3D (bottom plot) The electron macro particles are shown as white dots at $t = 18.9$ ps after the start of the simulations.

Results on the transverse trace-space rms emittance, shown in Fig. 1, reproduce the oscillations with the same frequency as observed in other RF Gun simulation codes [7] with the same RF field. The calculated rms bunch length of $\langle \Delta z_{rms} \rangle \approx 1.25$ mm, middle plot in Fig. 1, after approximately $2\frac{1}{2}$ RF cells propagation is very close to the rms length $\sigma_z^{rms} = l_z/2 \approx 1.27$ mm (Table 1) of the laser pulse indicating that the simulations are done close to the optimum injection phase. The formation of the Gaussian shape of the beam is also seen in a visualization (bottom plot in Fig. 1) of a snapshot of the electron macro particles during the emission process. The beam is followed in the simulations using VORPAL's moving window algorithm. These runs are only practical in parallel and with sufficient CPUs/memory/storage resources available. Larger runs require modern 64 bit computer architectures and operating systems to exceed the 2GB file system partition limitation.

SUMMARY

We implemented the recently proposed steady-state photocathode emission model [1] in the VORPAL PIC code and enabled RF gun simulations with it. The model was applied to simulate beam emission and propagation from a simple metal (Cu) photocathode. These results indicate the potential of this method to provide for the first time detailed photocathode physics modeling in RF gun codes. Future development plans include the implementation of a general, nonequilibrium, nonlinear, PDEs model for the electron and lattice temperatures, modeling of surface roughness, laser pulse modulations, and scattering effects, VORPAL photoinjector code verification and validation.

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