

# A 2D STEADY-STATE SPACE CHARGE SOLVER FOR AZIMUTHALLY SYMMETRIC PROBLEMS OF ARBITRARY DEGREE

A. Gold\*, S. Tantawi

SLAC National Accelerator Laboratory, Menlo Park, United States

## Abstract

Correctly and rapidly simulating the steady-state interaction between particle beams and electromagnetic fields is crucial to the design and optimization of accelerator and radio-frequency (RF) source components. Iteratively solving for the self-consistent interaction between particles and fields can prove challenging and highly susceptible to numerical noise and mesh induced instabilities. We present herein two new approaches to solving the self-consistent trajectories of particles in the presence of external and self fields. The first method reformulates the integrated self field contribution as a path integral. The second method uses a hybrid Eulerian framework and produces an interpolated continuous current density, resulting in 1-2 orders of magnitude fewer particles required to obtain an accurate solution. We conclude with benchmarking results which show this method is as accurate as state of the art PIC solvers, while running 80-120X faster.

## INTRODUCTION

With complex geometries and features covering a wide spatio-temporal range, next-generation electron guns and RF sources have proven challenging to model accurately. Existing simulation codes which model the relativistic beam-wave interaction in these devices are exceedingly time consuming (on the order of hours to days) with accuracy subject to the mesh and macro-particle distribution. These factors significantly impede the rapid iteration process required for the design and optimization of new guns and RF sources.

Motivated by these considerations, we have been developing a new approach to simulate the beam-wave interaction. While similar to existing methods in that we iteratively solve for the fields, determine the particle trajectories, and repeat until the solution converges, our approach differs in several key respects [1, 2]. The calculation of the source terms (current and space charge density) from the particle trajectories is one such respect. In our frequency domain, Lagrangian based finite element (FE) formulation these source terms drive the fields through interaction terms in the Lagrangian, given by eq. 1. Upon perturbing the system, these terms result in load vectors in the final FE matrix equation.

$$\mathcal{L}_{\omega, \text{int}} = \int -\rho_{\omega} \phi_{\omega}^* - \rho_{\omega}^* \phi_{\omega} + \vec{A}_{\omega} \vec{J}_{\omega}^* + \vec{A}_{\omega}^* \vec{J}_{\omega} dv \quad (1)$$

Here,  $\rho_{\omega}$  and  $\vec{J}_{\omega}$  are the Fourier coefficients of  $\rho$  and  $\vec{J}$ :

$$\rho_{\omega} = \frac{1}{T} \sum_a \int_0^T \rho_a(t) e^{i\omega t} e^{im\phi} dt \quad (2)$$

$$\vec{J}_{\omega} = \frac{1}{T} \sum_a \int_0^T \vec{J}_a(t) e^{i\omega t} e^{im\phi} dt \quad (3)$$

We present two computationally efficient and robust methods for computing these interaction terms from the macroparticle trajectories. We have implemented both methods for structures with azimuthal symmetry of degree  $m \geq 0$ , and have benchmarked it using several electrostatic test problems.

## PATH INTEGRATED LINE CURRENTS

Instead of calculating  $\rho_{\omega}$  and  $\vec{J}_{\omega}$  directly, one approach is to substitute Eqs. (2) and (3) into the expression for Eq. (1). Given a set of macro-particle trajectories,  $a$ , we can treat each trajectory as a discrete line current along the trajectory path,  $\vec{r}_a$ :

$$\rho_a(t) = q_a \delta(\vec{r} - \vec{r}_a(t)), \quad \vec{J}_a(t) = q_a c \beta_a(t) \delta(\vec{r} - \vec{r}_a(t)) \quad (4)$$

Substituting this into the Lagrangian volume integral, the delta function can be integrated over the volume, resulting in only the integral over time. Through a change of variable  $\frac{ds_a}{dt} = |\beta_a|$ , this integral can be rewritten as a path integral along the macroparticle trajectories,  $s_a$ :

$$\mathcal{L}_{\omega, \text{int}} = \frac{2}{T} \text{Re} \sum_a q_a \int \left( \phi(s_a) + \vec{A} \cdot \vec{\beta}(s_a) \right) \frac{e^{i\omega t(s_a)}}{|\vec{\beta}_a(s_a)|} ds_a \quad (5)$$

In the context of the finite element field solver, this integral is computed without reference to the mesh but only with respect to the particle trajectories (the four-potential is recovered via polynomial interpolation over the domain). In contrast, particle-in-cell (PIC) methods usually assign charge density to the mesh nodes based on the position of point charges within the mesh element before numerically integrating the contribution over the volume. In applications where the source terms are localized relative to the mesh, the path based approach thus offers higher resolution.

However, the majority of applications of interest to the accelerator community do not require such fidelity but rather lose accuracy due to the discrete nature of the macroparticles, which are in fact approximating a continuous distribution. In conventional particle in cell (PIC) methods, this necessitates some minimum number of particles simulated per mesh cell (a general rule of thumb is approximately 10 particles per cell). Using our line integral method results in a similar

\* vrieliink@stanford.edu

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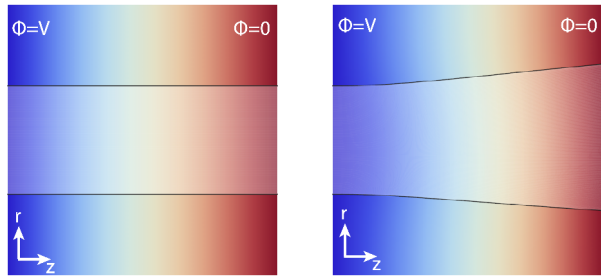


Figure 1: A 2D cross-section of a parallel disc geometry with an applied voltage and macroparticle trajectories in white. The image on the left shows the results with no space charge while the converged trajectories are on the right.

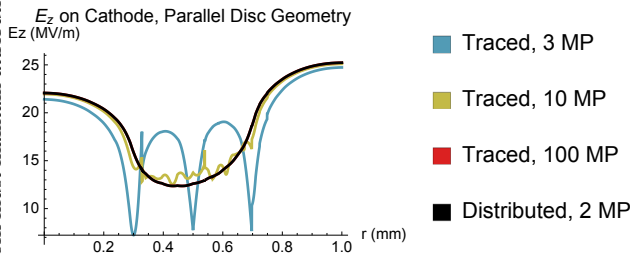


Figure 2: The discrete nature of path integral approach: several macroparticle (MP) trajectories must be calculated to reasonably approximate a uniform beam. Using the HE approach, we can obtain the same accuracy with only 2.

requirement on the number of macroparticles and even with a large number of particles, the discrete nature of the self-field contribution tends to adversely affect the convergence of the beam trajectory. The effect is particularly noticeable at the cathode where the beam is low-energy and most susceptible to noise in the transverse fields.

To illustrate the issue, we consider a relatively simple electrostatic problem: a uniform annular beam in a parallel disc geometry as shown in Fig. 1. The solution for the  $E_z$  field on the cathode is plotted for increasing macroparticle quantities in Fig. 2. Unsurprisingly, modeling this continuous beam with only 3 particles produces inaccurate results and 50 - 100 macroparticles are required before the solution converges. The large number of particles required to model a current distribution that is, in fact, quite simple prompted the development of a new algorithm where macroparticle trajectories are not considered as discrete line currents but as the bounds of a continuous current distribution. The source terms are then determined on the mesh points within these bounds via the charge conservation law. This produces a smooth and physically accurate distribution for use in calculating the space charge contribution in Eq. (1) without using any arbitrary mesh-based or heuristic smoothing factor. The benefit of this approach is clear from the trace labeled “distributed” in Fig. 2, which was obtained using only 2 particles instead of the 100 required using the path integral method.

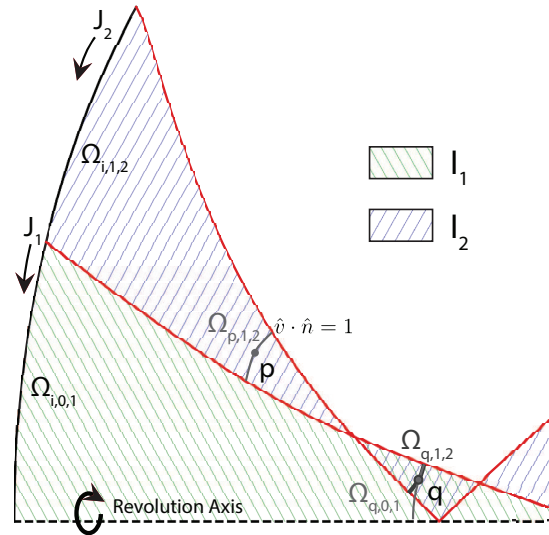


Figure 3: Calculating the source term from the macroparticle trajectories.

## HYBRID EULERIAN APPROACH

We titled this distributed current density technique a hybrid Eulerian approach as it combines the simplicity and computational efficiency of using macroparticles in the particle tracking phase (a Lagrangian representation of the beam) with the improved accuracy in the space charge calculation obtained by modeling the beam as an Eulerian flow field. A similar technique has been applied in other fields, but to our knowledge, this is the first time it has been applied in this context [3].

Starting with the charge conservation law, given by Eq. (6), one can integrate over the volume and apply the divergence theorem to produce Eq. (7) at steady state.

$$\frac{\partial J^\mu}{\partial x^\mu} = \frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \quad (6)$$

$$\int_V \nabla \cdot \vec{j} dx = \int_{\partial V} \vec{j} \cdot \hat{n} dS = \text{const} = I \quad (7)$$

Assuming laminar particle flow between macroparticles, the current contained between macroparticle trajectories is constant. The current density at any mesh point  $p$  located between two trajectories,  $k, k+1$  can thus be calculated from Eq. (7). A surface,  $\Omega_{p,k,k+1}$ , is first determined which contains  $p$ , is bounded by  $k$  and  $k+1$ , and for which  $\hat{j} \cdot \hat{n} = 1$  everywhere. Having done so, we use Eq. (7) as follows to obtain the approximate current density at  $p$ :

$$I_{k,k+1} = \int_{\Omega_{p,k,k+1}} \vec{j} \cdot \hat{n} dS = |\vec{j}_{k,k+1}| A_{\Omega_{p,k,k+1}} \quad (8)$$

$$\Rightarrow \vec{j}_{k,k+1} = \frac{I_{k,k+1}}{A_{\Omega_{p,k,k+1}}} \hat{n} \quad (9)$$

An illustration of this concept is provided for a two dimensional example in Fig. 3. In the case where macroparticle trajectories are crossing, we must consider the contribution from multiple current regions. This concept is illustrated for point  $q$  in Fig. 3, for which the current density would be

calculated as:

$$\vec{j}_q = \frac{I_1}{A_{\Omega_{q,0,1}}} \hat{n}_{q,0,1} + \frac{I_2}{A_{\Omega_{q,1,2}}} \hat{n}_{q,1,2} \quad (10)$$

The case of crossed trajectories returns us to, and seemingly contradicts, the assumption of laminar flow made previously. While most physical designs of interest do involve laminar flow, particularly when space charge is accounted for, the algorithm handles non-laminar beams as well. The assumption on laminar flow need only be valid locally, between trajectories, even if globally the solution is non-laminar. In the limit of a sufficient number of macroparticle trajectories, this local condition is adequately approximated. The number of macroparticle trajectories required will depend on how non-laminar the flow is but in the worst case should be equivalent to the number of particles required in a PIC code, and generally tends to be 1 - 2 orders of magnitude less. Figure 4 illustrates this concept as applied to an electrostatic gun design with an overfocused beam. The solution converges using 5-10 particles while a 2D PIC code would require at least 100-1000 particles before converging. By

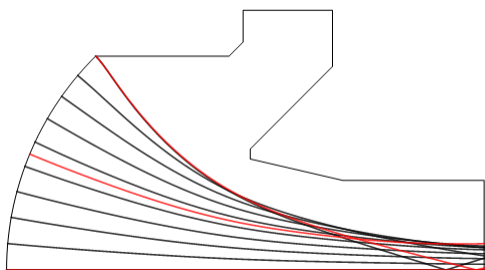


Figure 4: Particle trajectories through an overfocused electron gun demonstrating highly non-laminar flow. While 3 macroparticles are insufficient to capture the beam dynamics, after 10 macroparticles the solution has converged.

requiring only 10 particles instead of 500, the HE code takes only 0.25s compared to 33.8s in COMSOL a commercially available solver which can handle azimuthally symmetric problems. In addition to the qualitative comparison made for the electron gun in Fig. 5, a comparison was made with COMSOL for the annular beam and parallel plate problem depicted in Fig. 1. Comparing the results after each iteration of the field solver and particle tracker, Fig. 6 demonstrates that the HE method converges as effectively as state of the art PIC codes while taking considerably less time to compute. For this problem, the PIC solution took on average 7.8s per iteration, while on the same machine and for a similar mesh, the field solver using the Hybrid-Euler method required only 0.1s. This represents a speed-up in solution time of 78X for the laminar beam and 116X for the non-laminar beam.

## CONCLUSION

We have developed two different approaches to computing the self-field contributions to the self-consistent beam-wave interaction. The path integral approach could be beneficial

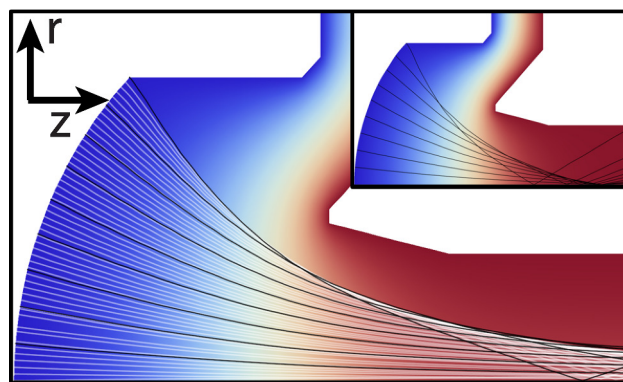


Figure 5: The converged particle trajectories using the HE method compared with a solution from COMSOL. The trajectories solved in COMSOL (in white) agree with those obtained using the HE method, shown in black. The inset shows the solution without space charge, demonstrating the initial highly non-laminar flow.

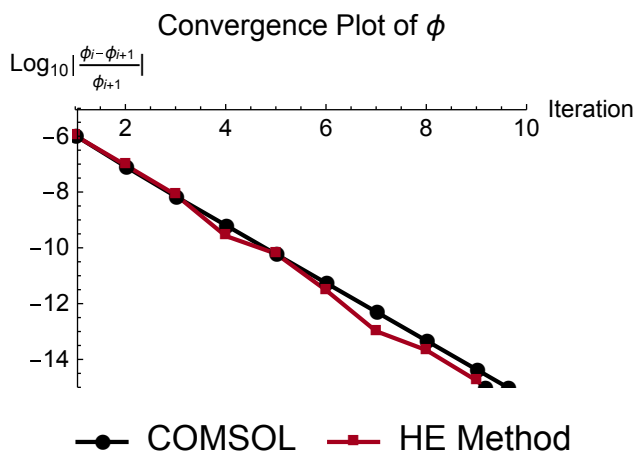


Figure 6: Convergence of the electrostatic potential with iteration number for the problem illustrated in Fig. 1. The mesh resolution was similar for both, consisting of 6282 elements for the COMSOL mode and 6109 elements for the HE based solver. 200 particles were required in the COMSOL model while the HE solver used 2.

in problems where the particle distribution of interest is finer than the mesh resolution but it is susceptible to noise in the solution and requires a large number of macroparticles to approximate continuous distributions. As such, the Hybrid Eulerian method was developed which interpolates the current density by applying the charge conservation law and assuming laminar flow locally between trajectories. Even in the cases where this assumption is only approximated the results are still highly accurate, as demonstrated for the electrostatic gun design. The HE solution converged with only 10 macroparticle trajectories instead of 500, as required in a conventional PIC solver. This resulted in the HE method running 80X - 120X faster than the state of the art PIC code we benchmarked against while maintaining similar solution accuracy.

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