

NEW PARTICLE-IN-CELL CODE FOR NUMERICAL SIMULATION OF COHERENT SYNCHROTRON RADIATION*

Balša Terzić, Rui Li, Jefferson Lab, 12000 Jefferson Avenue, Newport News, VA 23606, USA

Abstract

We present a first look at the new code for self-consistent, 2D simulations of beam dynamics affected by the coherent synchrotron radiation. The code is of the particle-in-cell variety: the beam bunch is sampled by point-charge particles, which are deposited on the grid; the corresponding forces on the grid are then computed using retarded potentials according to causality, and interpolated so as to advance the particles in time. The retarded potentials are evaluated by integrating over the 2D path history of the bunch, with the charge and current density at the retarded time obtained from interpolation of the particle distributions recorded at discrete timesteps. The code is benchmarked against analytical results obtained for a rigid-line bunch. We also outline the features and applications which are currently being developed.

INTRODUCTION

Coherent synchrotron radiation (CSR) is an effect of curvature-induced self-interaction of a microbunch with a high charge as it traverses a curved trajectory. It can cause a significant emittance degradation, as well as fragmentation and microbunching of the electron bunch. Numerical simulations of the CSR effects have proven to be extremely challenging because of: (i) the memory requirement associated with storing the history of the beam bunch; (ii) difficulty to accurately account for retardation; (iii) large cancellation between \mathbf{E} and \mathbf{B} fields in Lorentz force; (iv) sensitivity to numerical noise, exacerbated by presence of gradients in relevant equations; (v) scaling of the self-interactions in computations. Here we focus on the self-consistent 2D CSR code developed by Li [1, 2]. The code is based on integration of the retarded potential for a 2D charge distribution (no vertical size). The present work transforms Li's original code from a particle-particle to a particle-in-cell (mean-field) form, thereby enabling superior performance in terms of efficiency and spatial resolution.

EQUATIONS OF MOTION

The dynamics of an electron in the bunch is governed by the following equation:

$$\frac{d}{dt}(\gamma m_e \mathbf{v}) = e(\mathbf{E} + \boldsymbol{\beta} \times \mathbf{B}), \quad (1)$$

where $\boldsymbol{\beta} \equiv \mathbf{v}/c$, $\mathbf{E} \equiv \mathbf{E}^{\text{ext}} + \mathbf{E}^{\text{self}}$, $\mathbf{B} \equiv \mathbf{B}^{\text{ext}} + \mathbf{B}^{\text{self}}$. Here \mathbf{E}^{ext} and \mathbf{B}^{ext} are external electromagnetic (EM)

fields, and \mathbf{E}^{self} and \mathbf{B}^{self} are the EM fields from bunch self-interaction, which depend on the history of the bunch charge distribution ρ and current density \mathbf{J} via the scalar and vector potentials ϕ and \mathbf{A} :

$$\mathbf{E}^{\text{self}} = -\nabla\phi - \frac{1}{c}\partial_t\mathbf{A}, \quad (2a)$$

$$\mathbf{B}^{\text{self}} = \nabla \times \mathbf{A}, \quad (2b)$$

where

$$\phi(\mathbf{r}, t) = \int \frac{d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \rho\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c}\right), \quad (3a)$$

$$\mathbf{A}(\mathbf{r}, t) = \int \frac{d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \mathbf{J}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c}\right). \quad (3b)$$

For an ultrarelativistic bunch on a circular orbit, the EM self-fields are dominated by CSR effects.

In order to avoid singularity at $|\mathbf{r} - \mathbf{r}'| = 0$, the integration is performed in polar coordinates of the lab frame:

$$\begin{bmatrix} \phi(\mathbf{r}, t) \\ \mathbf{A}(\mathbf{r}, t) \end{bmatrix} = \sum_{i=1}^{M_{\text{int}}} \int_0^{R_{\text{max}}} \int_{\theta_{\text{min}}^i}^{\theta_{\text{max}}^i} \begin{bmatrix} \rho\left(\mathbf{r}', t - \frac{R'}{c}\right) \\ \mathbf{J}\left(\mathbf{r}', t - \frac{R'}{c}\right) \end{bmatrix} dR' d\theta', \quad (4)$$

where, in numerical implementation, M_{int} is the number of ‘‘cuts’’ of the grid by the circle of causality (up to 4), similar to what has been done in [3]. R_{max} is computed from the circle of causality.

Frames of Reference

The algorithm for efficient computation of retarded potentials requires that we work in two different coordinate systems (frames): *Frenet frame* (FF) and the *lab frame* (LF). These two have been used in the original implementation of Li's code. In addition to these two frames, and for the purposes of the gridded mean-field modification of Li's code, we also use the *grid frame* (GF).

Frenet frame (x, s) is defined so that $x \equiv r - r_0$ is the horizontal offset from the designed orbit, and $s \equiv r_0\theta$ is the longitudinal coordinate:

$$\begin{aligned} x &= r - r_0 \\ s - s_p &= r_0\theta, \end{aligned} \quad (5)$$

where s_p is the position along the beam line at the end of the previous lattice element, r and θ are polar coordinates of the curved orbits, and r_0 is the radial coordinate of the designed orbit.

Lab frame (X, Y) is defined as the Cartesian coordinates in the plane of the beam lattice. The transformation between the FF and LF depends on the type of the section of the lattice (drift or bend).

* Authored by Jefferson Science Associates, LLC under U.S. DOE Contract No. DE-AC05-06OR23177.

Grid frame (\tilde{X}, \tilde{Y}) is defined as the Cartesian coordinates tilted by angle α in LF (see Figure 2), and normalized so that it is always given by $[-0.5, 0.5] \times [-0.5, 0.5]$.

PARTICLE-IN-CELL REPRESENTATION

In order to improve the phase-space resolution of Li's code [1, 2], a better sampling of the DF is needed. Accomplishing this by increasing the number of gaussian macroparticles is computationally prohibitive, as the computation of retarded fields scales as $\mathcal{O}(N^2)$. We now consider an alternative approach to obtain a representation of the DF (or, more precisely, its moments $\rho(\mathbf{r}, t) = \int f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}$ and $\mathbf{J}(\mathbf{r}, t) = \int \mathbf{v} f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}$): sampling the DF by a large number of point-charge particles and binning them on a discrete grid, in order to obtain a mean-field approximation. We thereby convert a point-to-point method of [1, 2] to a mean-field one.

As an illustration, Figure 1 shows an analytically known particle distributions on a 32×32 grid (left column) sampled by 32^2 gaussian macroparticles (middle column) and sampled by 50×32^2 point-charge particles (right column). It is visually evident that the distribution's small-scale structure is much better represented by the point-charge particle model, as can also be quantified by the signal-to-noise ratio.

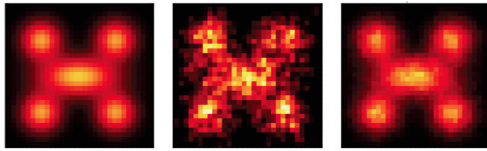


Figure 1: Fictitious charge distribution on a grid: exact (left), using gaussian macroparticles, as in [1, 2] (middle), and using point charge particles deposited on the grid (right).

Discrete Grid

The distribution function (DF) of the beam sampled by N point-like particles is given by Klimontovich distribution:

$$f_K(\mathbf{x}, \mathbf{v}, t) = q \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}^{(i)}(t)) \delta(\mathbf{v} - \mathbf{v}^{(i)}(t)), \quad (6)$$

from which the charge density is easily found by integrating over velocities:

$$\rho(\mathbf{x}, t) = q \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}^{(i)}(t)), \quad (7)$$

where q is the charge per particle, and Q is the total charge of the bunch, so that $q \equiv Q/N$. The *coarse-grained DF*, defined on a grid with (N_X, N_Y) gridpoints and resolution $\mathbf{h} \equiv (h_X, h_Y)$ (Figure 2), is given by

$$f(\mathbf{x}, \mathbf{v}, t) = \int_{-\mathbf{h}}^{\mathbf{h}} p(\bar{\mathbf{x}}) f_K(\mathbf{x} + \bar{\mathbf{x}}, \mathbf{v}, t) d\bar{\mathbf{x}}, \quad (8)$$

where $p(\bar{\mathbf{x}})$ is the normalized particle deposition scheme (Figure 3).

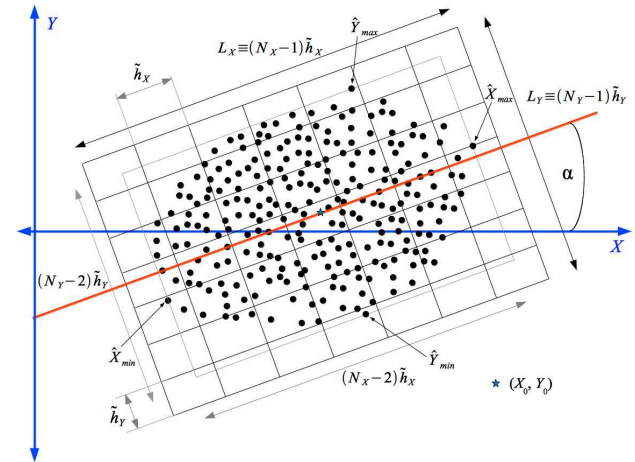


Figure 2: Computational grid. Blue (X, Y) coordinates denote LF, and the computational box defines GF.

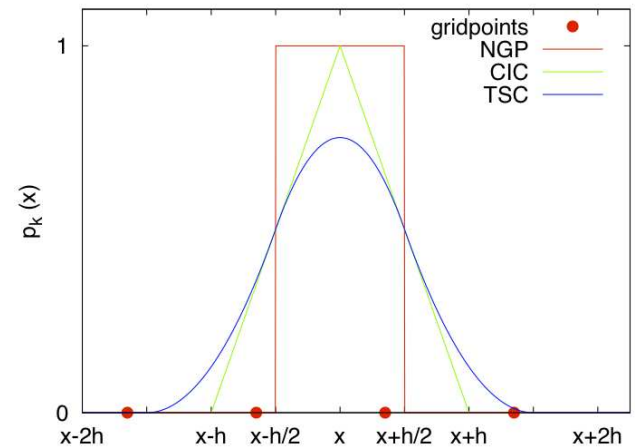


Figure 3: Deposition functions, in increasing order $k = 1, 2, 3$: Nearest Grid Point (NGP), Cloud In Cell (CIC) and Triangular Shaped Cloud (TSC).

Removal of Numerical Noise

The properties of numerical noise in particle-in-cell simulations – due to the finiteness of the computational domain and the graininess of the DF – and its efficient removal using wavelet thresholding, has been studied earlier [4]. This methodology, which yields improvement in both accuracy (“cleaner” physical results) and efficiency (wavelet compression) of the simulations is also implemented in the present algorithm. Simulations can also be ran with this feature turned off. A detailed study of the importance and efficiency of wavelet denoising in the scope of this code is currently underway.

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ALGORITHM OUTLINE

The alternative CSR simulation using discrete grid can be outlined as follows:

Step 1: Sample the DF.

Sample the initial DF with N particles (using, for instance, von Neumann's rejection method) or read it in from a data file.

Step 2: Define grid and deposit particles.

The charged particles are deposited onto a finite grid (Figure 2).

Step 3: Compute spatial and time derivatives of the retarded potentials on the grid.

The derivatives of the gridded quantities are computed in GF by tri-quadratic interpolation at off-grid points and then transformed from GF to LF.

Step 4: Compute the self-fields on the grid.

Take spatial and temporal derivatives of gridded potentials and combine them to obtain the self-forces in GF. Transform to LF and then to FF by applying transformation matrices.

Step 5: Compute self-forces on each particle.

Self-forces acting on each particle in FF are computed by bi-quadratic interpolation from the previously computed gridded values in FF.

Step 6: Advance particles in time.

The DF sampled by particles is advanced by a small timestep Δt by the leap-frog scheme.

The steps 2-6 are repeated until the end of the simulation.

Computational Efficiency

The computation of charge density and currents from the set of particles is done by simple particle deposition, which is an $\mathcal{O}(N)$ operation. Also an $\mathcal{O}(N)$ operation is solving a set of coupled nonlinear equations needed for computing momenta of each particle. The self-fields are also computed on the grid, so that the computation of the wakefields scales as $\mathcal{O}(N_X^2 N_Y^2)$. Overall, this algorithm scales as $\mathcal{O}(N_X^2 N_Y^2) + \mathcal{O}(N)$. The algorithm in the version of [1, 2] scales as $\mathcal{O}(N^2)$, where N is the number of macro-gaussians. This means that the new algorithm with a resolution of $N_1 \times N_2$ should be computationally as demanding as the earlier implementation of [1, 2] with $N_1 N_2$ macro-gaussians, while possessing much-improved spatial resolution (see Figure 1).

BENCHMARK: RIGID LINE BUNCH

The first test of accuracy of the new code is against a 1D rigid line bunch steady state model for which analytic solutions can be found [5]. Figure 4 shows the effective forces due to the retarded potential at the end of the first bend, computed by the code versus the analytic results. The agreement is excellent.

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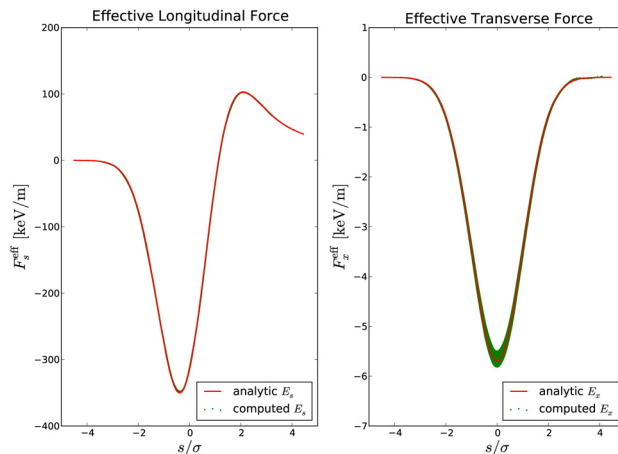


Figure 4: Analytic versus computed effective retarded forces: $N = 512000$ particles on a 64×64 grid. $R = 25.13$ m, $\theta = 11.4^\circ$, $\sigma_z = 50 \mu\text{m}$, $\epsilon = 1$ nm, $Q = 1$ nC, $E = 12$ GeV.

DISCUSSION AND FUTURE WORK

We presented a first look at the new, 2D particle-in-cell code designed to simulate CSR effect in electron beams. The excellent agreement with the rigid bunch benchmark provides the first proof-of-concept.

Our current and future efforts are focused on the following: (i) optimization/parallelization of the code; (ii) more detailed benchmarking of the code; (iii) evaluation and utilization of wavelet methodology in both reducing numerical noise and optimizing algorithms computational efficiency.

Upon successfully benchmarking and optimizing the new code, we expect that the first application will be simulating Jefferson Labs Free Electron Laser and its proposed upgrade JLAMP [6].

Authors would like to acknowledge Philippe Piot for his support of this project. B.T. was partially supported by ONR contract number N00014-36-1-0587 with Northern Illinois University.

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