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ImpactX MODELING OF BENCHMARK TESTS FOR SPACE CHARGE VALIDATION*

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Abstract

The code ImpactX represents the next generation of the particle-in-cell code IMPACT-Z, featuring s-based symplectic tracking with 3D space charge, parallelism with GPU acceleration, adaptive mesh-refinement, and modernized language features. With such a code comes a renewed need for space charge validation using well-defined benchmarks. For this purpose, the code is continuously checked against a test suite of exactly-solvable problems. The suite includes field calculation tests, dynamical tests involving coasting or stationary beams, and beams matched to periodic focusing channels. We evaluate the code performance on documented space charge benchmarks appropriate for high-intensity bunched beams.

CODE DESIGN

ImpactX [1, 2] is a GPU-capable C++ successor to the code IMPACT-Z [3], built on the AMReX software framework [4], for modeling relativistic charged particle beams in linacs or rings. Similar to IMPACT-Z, tracking is performed with respect to the path length variable s, and space charge is included using a second order operator splitting [5]. All tracking methods are symplectic by design, and maps are used where possible for efficient particle pushing. The 3D space-charge fields are computed with an iterative Multi-Level Multi-Grid (MLMG) Poisson solver [4], providing support for adaptive mesh refinement. The code is continuously benchmarked (after every code change) against a suite of >20 test problems, designed to validate each feature of the code. The space charge benchmarks, to be described, are valid for bunched beams in the presence of open boundary conditions.

BENCHMARK PROBLEMS

The code was used to reproduce the space charge benchmark problems described in Refs. [6] and [7]. However, the first problem in [7], involving a matched K-V beam in a periodic focusing channel (appropriate for beams with 2D space charge), has been replaced by a Kurth beam in a periodic focusing channel [8] (appropriate for bunches with 3D space charge). In each case, the boundary used by the Poisson solver is placed sufficiently far from the beam to reproduce the free-space space charge fields.

Space Charge Fields in a Gaussian Bunch

This benchmark is described in detail in Ref. [6]. In Fig. 1, the space charge fields within a 1 nC Gaussian electron bunch (at rest) produced by ImpactX are compared against the exact results for several values of the beam aspect ratio. Some visible discrepancy appears in the values of E_x for large aspect ratio ($r \leq 0.2$). In the future, the case of large aspect ratio will be addressed more efficiently using integrated Green function techniques [9].

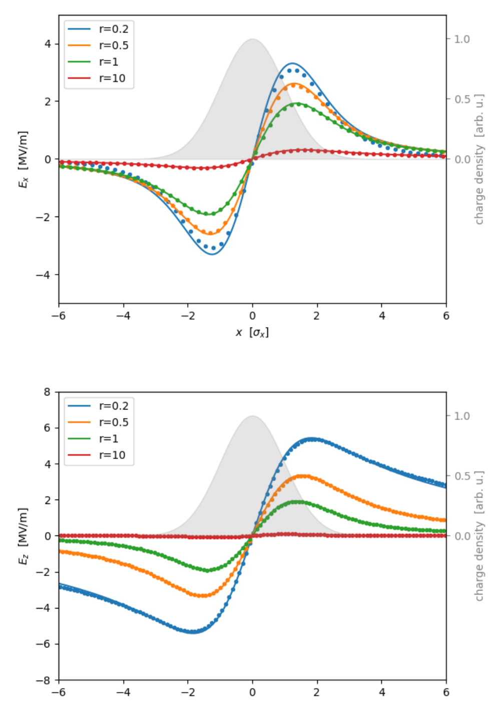

Figure 1: Electric field in a Gaussian bunch using ImpactX, 1 M particles and [128, 128, 256] grid (dots) and from Eq. (1) of Ref. [6] (lines) for various aspect ratios $r = \sigma_z/\sigma_\perp$. The bunch charge is 1 nC, with $\sigma_x = \sigma_y = \sigma_\perp = 1$ mm. (Upper) Along the line $y = 0$, $z = 0$. (Lower) Along the line $x = 0$, $y = 0$. Compare Fig. 1 of Ref. [6].

Figure 2 shows the phase space of an initially cold Gaussian 1 nC electron bunch after drifting a distance of 1 m, comparing the final particle populations of ImpactX and

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IMPACT-Z for the same numerical resolution, showing reasonable agreement. (Compare Fig. 4 of Ref. [6].)

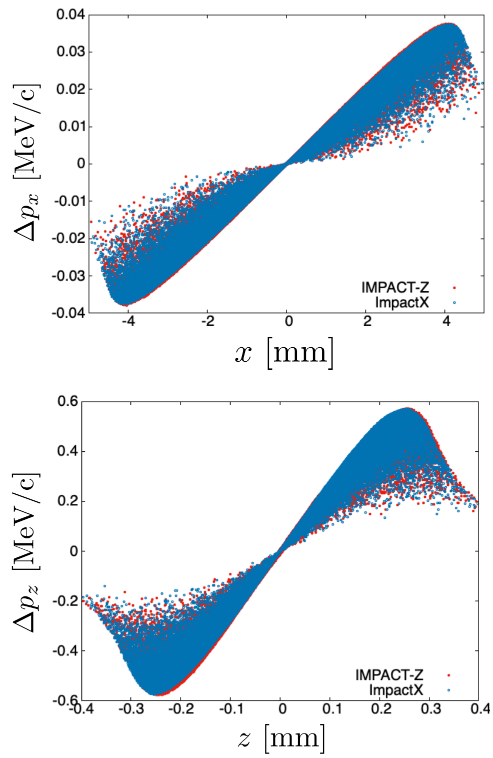

Figure 2: Phase space at the end of a 1 m drift, for an initial Gaussian electron bunch with $(\sigma_x, \sigma_y, \sigma_z) = (1, 1, 0.1)$ mm, 1 nC of charge, and 10 MeV total energy moving the z-direction. The initial momentum spreads are zero. Both codes used 1 M particles and [128,128,256] grid. Compare Fig. 4 of Ref. [6].

Waterbag Beam in a Constant Focusing Channel

This is a simple dynamical test involving the interplay between exernal focusing and space charge defocusing. The test case consists of a 10 nC proton bunch with a kinetic energy of 2 GeV and an unnormalized rms emittance of 1 µm in each plane. The beam is matched to a constant focusing section of strength $k = 1\ \mathrm{m}^{-1}$ and length 2 m, using the rms envelope equations. (The longitudinal focusing is chosen so that the bunch is radially symmetric in the beam rest frame.) We verify that the three rms beam sizes and emittances remain stationary. The beam distribution is not fully stationary, since nonlinear space charge will result in emittance growth on long time scales.

Kur8h Beam in a Periodic Focusing Channel

ImpactX provides intrinsic support for generation of both 4D and 6D distributions of Kurth type [8, 10]. Such distributions provide exact, self-consistent solutions of the Vlasov-Poisson equations for a 2D or 3D beam in an s-dependent isotropic focusing system. The test case consists of a 10 nC proton bunch with a kinetic energy of 2 GeV propagating in a periodic channel comprised of alternating drift spaces and constant linear focusing sections ($k = 0.7$/m). The bunch and the external focusing are radially symmetric in the bunch rest frame. The bunch has an rms unnormalized emittance of 1 µm in each plane, yielding a (depressed) phase advance per period of 74°. Figure 3 illustrates the matched beam size over a single period, comparing the values from ImpactX against the rms envelope equations, showing good agreement. The space charge forces within the bunch are linear, so any emittance growth is purely numerical. Figure 4 shows the numerical emittance evolution over 100 periods. The emittance fluctuations decrease as the resolution is improved.

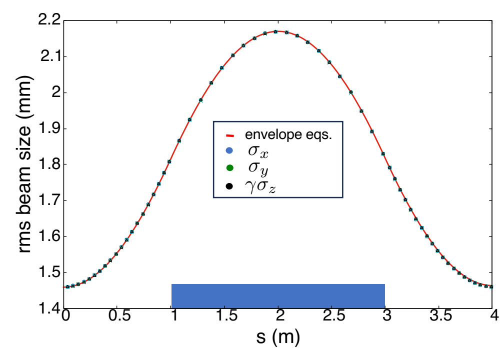

Figure 3: Evolution of the rms beam size $\sigma_x = \sigma_y = \gamma\sigma_z$ over a single period in the focusing channel used for the Kurth beam distribution test. (Line) RMS envelope equations. (Points) Values from ImpactX. The blue rectangle denotes the region of nonzero focusing.

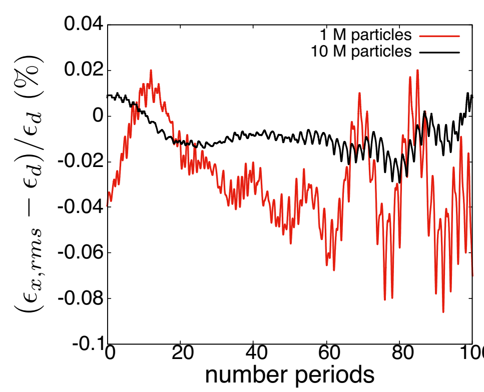

Figure 4: Variation of horizontal emittance from the nominal value $\epsilon_d = 1$ µm for the example in Fig. 3. (Red) 1 M particles, [72,72,72] grid. (Black) 10 M particles, [128,128,128] grid. Emittance growth is purely numerical.

Free Expansion of a Cold Uniform Bunch

This problem describes a cold, uniform ellipsoidal bunch increasing in size (in a drift) due to its own space charge fields [7]. The problem is described exactly by the rms envelope equations. For the special case of a bunch that is spherical in the bunch rest frame ($\sigma_x = \sigma_y = \gamma\sigma_z = R/\sqrt{5}$),

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the drift distance required for the bunch to double in size is given exactly by:

$$\Delta s = \beta\gamma\kappa\sqrt{\frac{R_0^3}{r_c N_b}}, \qquad \kappa = 1 + \frac{\sqrt{2}}{4}\log(3 + 2\sqrt{2}), \quad (1)$$

where R_0 is the initial bunch radius, r_c is the classical particle radius, N_b is the bunch population, and β, γ denote the relativistic factors associated with the design energy. We verify the bunch has the correct second moments at $s = \Delta s$.

Cold Beam in a FODO Channel with RF Cavities

This problem describes a 250 MeV proton bunch of charge $Q = I/f$ (I = 100 mA, f = 700 MHz) matched to a focusing system comprised of a FODO channel with RF cavities added for longitudinal focusing [7]. For a cold uniform bunch, the problem is described exactly by the rms envelope equations. This problem is challenging due to the RF-induced energy evolution and an absence of symmetry among the $x/y/z$ planes. Like its predecessor, ImpactX supports a map-based approach to RF cavities, based on the on-axis electric field [5]. In this problem, the on-axis electric field in each 700 MHz RF cavity is described by the function $E(z) = \exp(-(4z)^4)\cos(\frac{5\pi}{2}\tanh(5z))$ over the cavity length $-0.5 \leq z \leq 0.5$ m. (Note: a typo appears in the corresponding equation of Ref. [7].) Figure 5 illustrates the beam envelopes obtained in ImpactX over a single 3 m period, using the matched initial beam moments obtained from MaryLie/IMPACT.

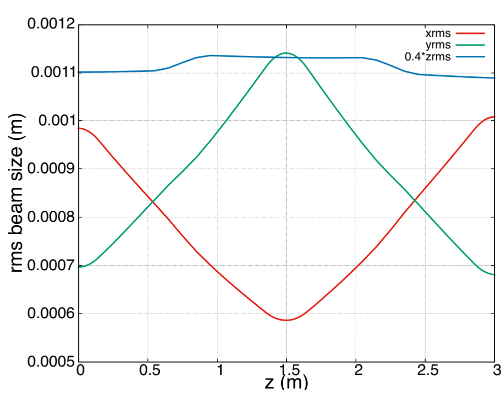

Figure 5: Plot of σ_x (red), σ_y (green), and σ_z (blue, scaled by 0.4 for plotting) versus distance in 1 period of a FODO channel with RF cavities. Compare Fig. 3 of Ref. [7].

Bithermal Beam in a Constant Focusing Channel

This test [7] provides a challenging, self-consistent model of a 3D bunch with a nontrivial core-halo distribution. To treat this case, ImpactX provides intrinsic support for generating a stationary bithermal distribution matched to a radially-symmetric constant focusing channel. The 6D phase space density f has the form:

$$f = c_1 \exp(H/kT_1) + c_2 \exp(H/kT_2), \qquad (2)$$

where H denotes the particle Hamiltonian (including the self-consistent space charge potential), and c_1 and c_2 are normalization factors that control the weights of the core and halo subpopulations. Generation of a bunch of type (2) requires solving a coupled set of ODEs for the space charge potential and the radial distribution function for each population.

The test case consists of a proton beam with kinetic energy of 0.1 MeV with a total charge $Q = I/f$ (I = 100 mA, f = 700 MHz) in a linear focusing channel with $k = 2\pi$/m. The *thermal beam* test case in Ref. [7] consists of a beam with $kT_1 = 36 \times 10^{-6}$ and $c_2 = 0$. In the second, more challenging *bithermal beam* case, the charge is partitioned, with 95% in the core ($kT_1 = 36 \times 10^{-6}$) and 5% in the halo ($kT_2 = 900 \times 10^{-6}$). Figure 6 illustrates the spatial density of the bunch as a function of radius for this case, showing that the beam distribution remains stationary after tracking. A log scale is used to visualize the beam halo. Compare Fig. 4 of Ref. [7].

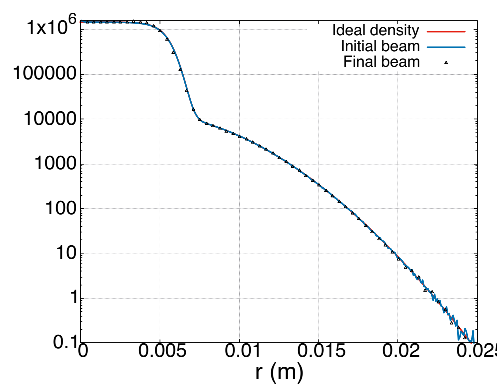

Figure 6: Probability density function (3D) versus radius for a bithermal core-halo distribution generated with 100M particles in ImpactX. The distribution is tracked for 10 focusing periods $\lambda_p = 2\pi/k = 1$ m. A log scale is used, showing the distribution is stationary over range of densities spanning 10^6 down to 10^{-1}. Compare Fig. 4 of Ref. [7].

CONCLUSION

In this work, we have used the code ImpactX to reproduce documented space charge benchmarks appropriate for 3D particle-in-cell codes in the context of high intensity bunched beams [6, 7]. All numerical results shown here are archived in [11], and additional benchmark tests can be found at Ref. [1]. Future plans include detailed code performance and scaling studies, detailed exploration of benchmark tests with mesh refinement, the implementation in ImpactX of 2D and/or 2.5D space charge models appropriate for long or unbunched beams, and the implementation of additional collective effects (including resistive wall wakefields and CSR models). In the future, we hope to participate in benchmarks involving 2.5D space charge appropriate to multi-turn tracking of long beams, such as those described in Ref. [12].

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