# IMPACTX SPACE CHARGE MODELING OF HIGH INTENSITY LINACS WITH MESH REFINEMENT[*]

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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, modernized language features, and automated testing. While the code contains features that support the modeling of both linear and circular accelerators, we describe recent code development relevant to the modeling of high-intensity linacs (such as beam transport for the Fermilab PIP-II upgrade), with a focus on space charge benchmarking and the impact of novel code capabilities such as mesh refinement.

## BACKGROUND

High-intensity proton and ion linacs are critical to meet the needs of future colliders, spallation neutron sources, and neutrino sources. Accurate beam modeling requires high spatial resolution and particle statistics, with the ability to resolve low-density beam halo and particle loss. To enable integrated start-to-end modeling with reasonable computing times, to enable large ensembles of simulation runs for optimization and for training of machine learning (ML) models, and to prepare for future Exascale computing systems, existing software must be modernized to take advantage of state-of-the-art computer hardware, including GPUs. The Beam pLasma & Accelerator Simulation Toolkit (BLAST) is an open ecosystem of codes, that can be combined with each other and with machine learning frameworks to enable integrated start-to-end simulation of accelerator beamlines for accelerator design [1]. Examples of BLAST tools include the PIC codes WarpX and ImpactX.

## IMPACTX FEATURES

ImpactX [2,3] is a GPU-capable C++ successor to the Fortran code IMPACT-Z [4,5], built on the AMReX software framework [6], 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 [4]. All tracking methods are symplectic by design, and maps are used where possible for efficient particle pushing. By default, the 3D space-charge fields are computed with an iterative Multi-Level Multi-Grid (MLMG) Poisson solver [6], providing support for adaptive mesh refinement. The code provides support for commonly-used elements (drifts, quads, solenoids, dipoles, multipoles, and cavities), as well as some specialized elements (plasma lens models, IOTA nonlinear elliptic magnet). Exact nonlinear maps are implemented for several elements (sector bends, drifts, uniform electrostatic gaps, and thin multipoles). The code is fully open to the community, and it is integrated into the BLAST software stack for interoperability with other BLAST codes.

### *Capabilities Added in SciDAC*

ImpactX originated in an LBNL-supported LDRD as a code supporting magnetic lattice elements and high resolution space charge. As part of an ongoing HEP SciDAC-5 project [7,8], the code has undergone active development to facilitate the modeling of high intensity linacs, as part of a collaborative effort with FNAL to develop a “virtual test stand” of the PIP-II accelerator complex (Fig. 1) [9]. Capabilities added include:

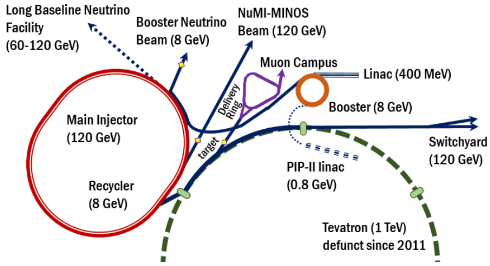

Figure 1: The Fermilab accelerator complex in preparation for the PIP-II upgrade. $H^-$ ions are accelerated to 800 MeV in the superconducting PIP-II linac and injected into the Booster synchrotron. From there they are delivered to further accelerators and experiments.

- user control of mesh refinement (for MLMG solver)
- a 3D IGF Poisson solver with open boundaries [10]
- RF cavity models - using on-axis electric field data
- openPMD standardized format for particle output [11]
- elliptical and rectangular transverse apertures
- lost particle phase space diagnostics
- support for rotation and misalignment errors
- soft-edge magnet fringe field models (quads, solenoids)

Additional relevant tools include Python scripts for postprocessing (e.g., Twiss optics, beam visualization) and optimization (e.g., matching).

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## SPACE CHARGE VALIDATION

ImpactX is benchmarked after each code change, using automated testing, against a suite of (now 89) test problems for validation. Currently $\sim$10 of these tests target the validation of 3D space charge in bunched beams. A collection of benchmark problems used for space charge validation is described in [12].

As one example, Fig. 2 illustrates the field component $E_x$ in a 1 nC Gaussian bunch at rest in free space, for several values of beam aspect ratio. The solid lines denote the exact result, while points are obtained from the ImpactX MLMG solver [12]. The domain used is 3 times larger than the bunch, to emulate open boundaries. A larger domain (7×) is needed for large aspect ratio $r = 0.2$ (with a correspondingly larger number of grid points), to ensure convergence to the exact free-space result. This motivated the addition of a second Poisson solver, using an integrated Green function method for open boundary conditions [10].

As a second example, Fig. 3 illustrates the evolution of beam envelopes for an intense, matched proton bunch in a FODO channel with RF cavities added for longitudinal focusing. The beam parameters are chosen so that all three envelopes are matched. A comparison is shown between ImpactX (MLMG solver) and IMPACT-Z using 1 M particles, showing good agreement.

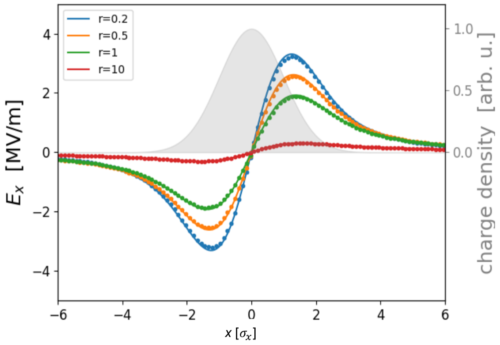

Figure 2: Transverse electric field in a 3D Gaussian bunch using ImpactX, 1 M particles and [128, 128, 256] grid (dots) and the exact result (lines) for various aspect ratios $r = \sigma_z/\sigma_\perp$. The bunch charge is 1 nC, with $\sigma_x = \sigma_y = \sigma_\perp = 1$ mm. The result is shown along the line $y = 0$, $z = 0$.

## MODELING THE PIP-II LINAC

As an application of these capabilities, modeling was performed for a portion of the RF linac designed for the Fermilab complex PIP-II upgrade [9]. Modeling input consisted of a TraceWin [13] lattice file describing transport from the exit of the RFQ (2.1 MeV) to the end of the 800 MeV superconducting linac, together with CST Studio files containing 3D electromagnetic models of 6 distinct RF cavity designs. Conversion of lattice input was performed with the aid of a LUME wrapper for TraceWin [14].

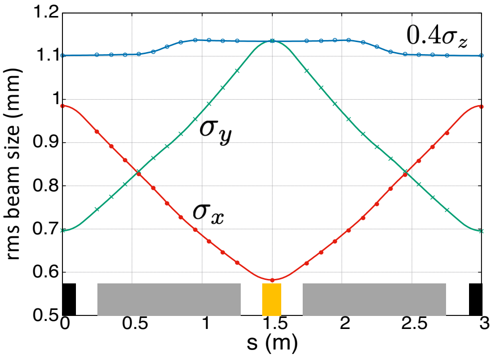

Figure 3: Beam size versus distance for a 100 mA, 250 MeV proton bunch in a FODO channel with 700 MHz RF cavities [12]. Comparison is shown between ImpactX (lines) and IMPACT-Z (points). RF cavities are shown in grey.

Figure 4 illustrates the H$^-$ beam transport from the RFQ through the Medium Energy Beam Transport (MEBT) section, for a beam with 5 mA average current. Comparison between ImpactX and TraceWin output shows good agreement in the rms beam size in each dimension.

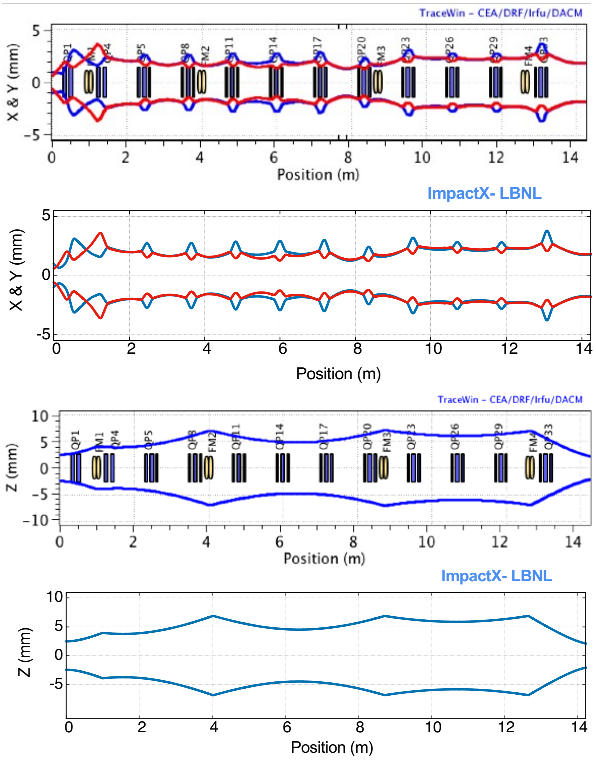

Figure 4: Evolution of the rms beam envelopes of the 5 mA H$^-$ beam in the 2.1 MeV PIP-II MEBT section. (Blue) Horizontal beam size. (Red) Vertical beam size. Results from both TraceWin and ImpactX are shown.

Figure 5 illustrates the energy gain in the first superconducting accelerating section, consisting of 8 half-wave resonator (HWR) cavities operating at 162.5 MHz (Fig. 6) and 8 corresponding soft-edge solenoids. The acceleration is captured accurately using the realistic RF cavity field profile in ImpactX.

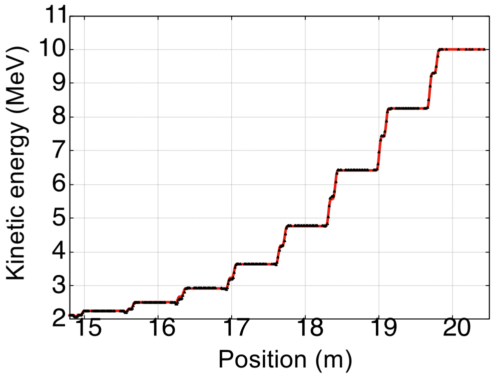

Figure 5: Energy gain in the first (HWR) accelerating section of the PIP-II superconducting linac. (Red line) Using ImpactX. (Black points) Using TraceWin.

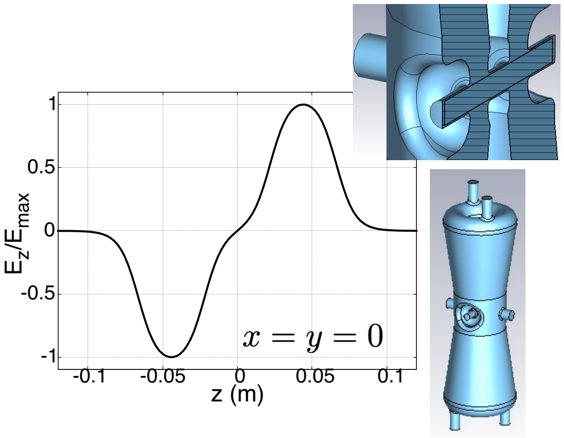

Figure 6: On-axis electric field $E_z$ in the 162.5 MHz HWR cavities. (Insets) Solid model of the HWR cavity and cutaway illustrating the beam pipe.

### *Mesh Refinement*

Figure 7 illustrates the horizontal beam phase space at the exit of the MEBT, modeled using 1 M particles in ImpactX. To demonstrate the use of mesh refinement, two cases are shown. In the leftmost figure, the settings of the MLMG Poisson solver are given by (in the C++ input file):

```
amr.n_cell = 128 128 128
geometry.prob_relative = 3
```

The latter parameter indicates the size of the computational domain relative to the outer beam boundary.

In the rightmost figure, the settings of the MLMG Poisson solver are given by:

```
amr.n_cell = 16 16 16
amr.max_level = 2
amr.ref_ratio = 2
geometry.prob_relative = 3
```

This indicates how the user can specify the number of refinement levels used, as well as the refinement ratio per level. In the latter case with MR, reasonable agreement is obtained with the high-resolution case, despite the coarse grid resolution (16 × 16 × 16) on the outer level.

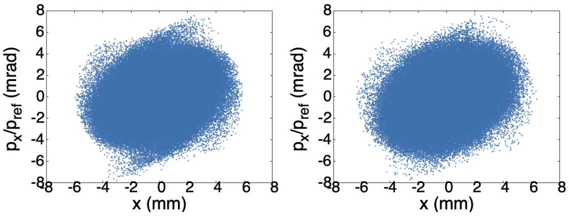

Figure 7: Simulated beam at the exit of the MEBT using 1 M particles in ImpactX. (Left) MLMG solver with $[128, 128, 128]$ grid. (Right) MLMG solver with $[16, 16, 16]$ grid and 2 levels of mesh refinement.

## CONCLUSION

New capabilities have been implemented in the GPU-capable code ImpactX, as part of a SciDAC effort in collaboration with Collaboration for Advanced Modeling of Particle Accelerators (CAMPA), to enable high-intensity beam transport in the PIP-II linac and to facilitate exchange of particle data among codes. High-intensity beam modeling was validated using dedicated space charge benchmarks as well as comparison against existing tools (TraceWin).

The next steps planned include evaluation of CPU to GPU speedup in the presence of mesh refinement, implementation of short-range RF structure wakefields and 1D coherent synchrotron radiation (now ongoing), studies of beam dynamics in the downstream PIP-II linac cryomodules, and implementation of a 2D or 2.5D space charge solver for long or unbunched beams.

## ACKNOWLEDGMENTS

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