SELF-CONSISTENT WARPX MODELING OF SPACE-CHARGE NEUTRALIZATION IN WHAM-RELEVANT NEUTRAL BEAMS

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Abstract

This work presents Particle-in-Cell (PIC) simulations using WarpX [1] to study neutral beam injection (NBI) [2] physics in Wisconsin HTS Axisymmetric Mirror (WHAM) [3]-class beamlines as part of a DOE INFUSE collaboration between Realta Fusion and Lawrence Berkeley National Laboratory. The goal is to develop a self-consistent model that couples beam extraction, gas neutralization, re-ionization, and space-charge compensation. The neutralization model is verified against an analytic matrix formulation for charge-state evolution, and the accelerator model is benchmarked against a published WHAM-relevant positive-ion NBI configuration. WarpX reproduces the single-aperture extracted current and captures the reference downstream beam divergence. The coupled simulation further shows that primary electrons generated by impact ionization reduce the beam potential by about 80%, identifying the dominant space-charge neutralization mechanism. These results establish a benchmarked positive-ion NBI modeling workflow for future multi-aperture WHAM simulations and advanced negative-ion or photo-neutralized beam concepts.

INTRODUCTION

Neutral beam injection (NBI) is a mature and widely used technique for plasma heating in magnetic confinement fusion devices [4]. However, predictive modeling of NBI systems remains challenging because beam extraction, neutralization, and space-charge compensation are strongly coupled. In particular, downstream transport is not determined only by accelerator optics or gas neutralization efficiency, but also by the charged-particle population created by beam–gas interactions.

This work was performed as part of a U.S. DOE INFUSE collaboration between Realta Fusion and Lawrence Berkeley National Laboratory to develop a self-consistent WarpX modeling capability for Wisconsin HTS Axisymmetric Mirror (WHAM)-class neutral beam systems. The immediate objective is to benchmark WarpX against a positive-ion neutral beam configuration relevant to the WHAM NBI system. The broader motivation is to establish a validated simulation framework for future negative-ion and photo-neutralized NBI concepts [5,6], where space-charge effects are expected to play a central role.

The central physics question addressed here is how space-charge neutralization develops in the beamline. Conventional ion-optics calculations often represent compensation using an assumed neutralization factor. In contrast, WarpX evolves charged particles and electrostatic fields self-consistently, allowing compensation to arise from physical beam–gas processes such as charge exchange, impact ionization and re-ionization. This enables direct study of which charged species dominate the compensation and how that compensation affects beam divergence and transmitted neutral current.

PHYSICAL AND NUMERICAL MODEL

The WarpX model evolves the coupled hydrogen beam phase space, charge-state composition, and space-charge compensation in a neutral beamline. The calculation is organized into two connected stages. First, a single aperture accelerator model generates the extracted positive-ion beam from an upstream plasma source and embedded-boundary grid geometry. Second, the extracted beam is transported through a prescribed neutral gas region, where charge exchange, stripping, impact ionization, and re-ionization modify the beam composition.

The simulation is performed in electrostatic particle-in-cell (PIC) mode. Rather than imposing an idealized injected beam or a prescribed space-charge compensation factor, the extracted distribution is produced self consistently from the plasma source, applied grid biases, aperture geometry, and beam space-charge. This provides the initial transverse phase space, current, and energy spread entering the neutralizer. For this benchmark, the model represents a single aperture of a WHAM-relevant positive-ion accelerator and produces an approximately 40 keV hydrogen beamlet.

For reference, the idealized neutralization model is described by the evolution of a beam species fraction vector, $\mathbf{F} = \begin{bmatrix} f_+ & f_0 & f_- \end{bmatrix}^T$, where f_+, f_0, and f_- represent the positive-ion, neutral, and negative-ion fractions. For a beam passing through a prescribed neutral gas target, the charge-state evolution can be written as

$$\mathbf{F}(s) = \exp\left[\mathbf{M} \int_0^s n_{\text{gas}}(s')\, ds'\right] \mathbf{F}(0), \tag{1}$$

where n_{gas} is the background gas density and $\mathbf{M}$ is a reaction matrix containing the relevant charge-changing and ionization cross sections [7]. This matrix model provides

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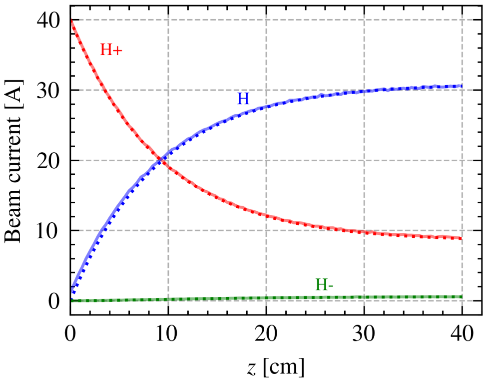

Figure 1: Comparison between the analytic matrix neutralization model (dashed line) and the WarpX Monte Carlo collision model (solid line) for hydrogen charge-state evolution in a prescribed gas target without self-consistent space-charge effects. The agreement verifies the collision implementation in the benchmark limit.

the analytic reference limit for charge-state evolution in a prescribed gas target.

In WarpX, the same reaction physics is implemented as a particle-based Monte Carlo collision operator. At each particle step, the local gas density, particle energy, path length, and tabulated cross sections determine the probability of a reaction. If a collision occurs, the reaction channel is selected according to the relative cross sections of the available processes, and the resulting particle products are placed in the corresponding species. Fast neutrals then propagate ballistically, while charged products remain coupled to the self-consistent beam fields.

To verify the collision model independently of beam self-fields, Fig. 1 compares the charge-state evolution obtained from Eq. (1) with the corresponding WarpX Monte Carlo result in a prescribed gas target. In this benchmark, space-charge forces are disabled so that the comparison isolates the species-conversion physics. The agreement demonstrates that the particle-based implementation reproduces the expected neutralization and re-ionization dynamics in the analytic limit.

After this isolated verification, the same collision physics is coupled back to the self-consistent WarpX beam model. In the full simulation, charge exchange determines the useful neutral beam fraction, while impact ionization and re-ionization produce charged particles that modify the beam potential. The simulation therefore does not require a prescribed compensation factor; instead, the compensating charge density emerges from the local beam–gas interaction history.

BENCHMARK AGAINST WHAM-RELEVANT BEAM DATA

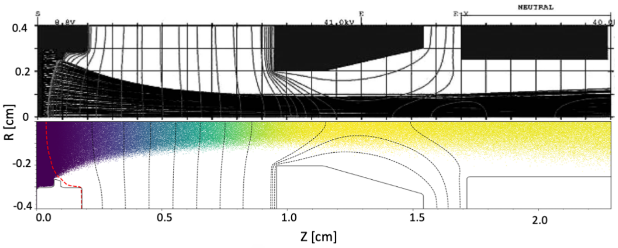

Figure 2: Single-aperture WHAM-relevant beamlet benchmark. The upper panel shows the published reference ion-optics solution, while the lower panel shows the corresponding WarpX simulation.

Table 1: Single-Aperture WHAM-Relevant Beamlet Benchmark

Quantity	**Reference**	**WarpX**
Extracted current [A]	0.0658	0.0640
Beam radius [cm]	0.13	0.16
Neutral divergence [mrad]	20	19
Transmitted neutral current [A]	24	14

The beamline validation step was a single-aperture benchmark against a published WHAM-relevant ion-optics configuration. Figure 2 compares the published reference solution [8] with the corresponding WarpX simulation. The WarpX model uses an electrostatic PIC formulation with boundary accelerator grids and self-consistent beam extraction. The model reproduces the extracted beam trajectory and downstream beam envelope while evolving the plasma meniscus [9] and beam space-charge self-consistently.

The benchmarked beam properties are summarized in Table 1. WarpX reproduces the extracted current with good agreement and captures the reference downstream beam divergence. The modest difference in beam radius and the lower transmitted neutral current indicate that the downstream result is sensitive not only to the extracted current, but also to the beamlet phase space, space-charge compensation, and transport model.

To isolate the role of the initial angular phase space, the post-grid beam distribution was projected to the WHAM diagnostic distance of 2.5 m. The realistic WarpX case matches the reference divergence closely, even though the divergence is not prescribed but emerges from the extraction and transport physics.

The control case is useful for interpreting the current discrepancy. When the initial neutral divergence is artificially set to zero, the projected neutral current recovers the reference value, but the resulting divergence is reduced to approximately 8 mrad, well below the reference value. Since the neutralization model has been verified independently, this suggests that the remaining current discrepancy is not caused by the charge-state conversion model alone, but by missing or simplified information in the downstream projection, source phase space, beamlet packing, or space-charge compensation used in the reference comparison. Thus, the available reference comparison does not uniquely constrain both transmitted current and divergence, motivating direct comparison with WHAM operation.

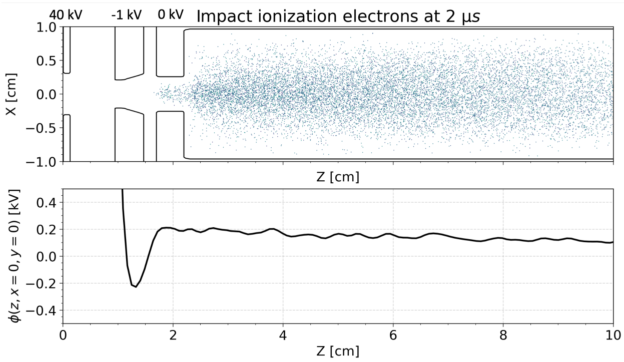

Figure 3: Space-charge neutralization in the start-to-end single-beamlet WarpX simulation. The upper panel shows electrons generated through impact ionization penetrating beyond the extraction grids into the downstream beam region. Note that the horizontal and vertical scales differ. The lower panel shows the corresponding reduction of the beam electrostatic potential.

SPACE-CHARGE NEUTRALIZATION MECHANISM

The key physics result of this study is the identification of the dominant source of space-charge compensation. In the positive-ion beamline, uncompensated space-charge would drive rapid transverse expansion of the ion beam and reduce the useful neutral current transported downstream. The WarpX simulations show that compensation is not an externally imposed parameter, but instead develops self-consistently through beam–gas interactions.

By tracking the charged products generated in the neutralizer, the simulation shows that primary electrons produced by impact ionization provide the dominant contribution to the compensating charge density. Figure 3 shows that these electrons penetrate through the accelerator region and accumulate within the beam transport volume, reducing the beam potential from approximately 1 kV to 0.2 kV. This corresponds to about 80% space-charge neutralization and provides a physical explanation for why gas neutralization and beam transport cannot be treated independently: the same beam–gas collisions that convert ions into neutrals also create the charged particles that regulate the beam potential.

The result also shows why a prescribed neutralization factor is not sufficient for predictive beamline modeling. The compensating charge density depends on where electrons are created, how they are confined or lost, and how they overlap with the positive beam charge. These quantities depend on the gas profile, beam energy, cross sections, grid geometry, and downstream boundary conditions. As a result, the same nominal compensation level may produce different beam envelopes if the spatial distribution of the compensating particles is different. A self-consistent PIC treatment is therefore needed to connect the local beam–gas reaction physics to the global beam transport.

CONCLUSION AND NEXT STEPS

This work establishes a WarpX workflow for modeling neutral beam transport with self-consistent space-charge effects. The goal was to test whether the key physics needed for predictive NBI modeling—beam optics, neutralization, and space-charge compensation—can be treated in a single particle-based framework rather than as separate prescribed inputs.

The model was validated progressively. In the prescribed gas-target limit, with space-charge forces disabled, the WarpX Monte Carlo collision model agrees with the analytic matrix model for charge-state evolution. The accelerator calculation then reproduces the main features of a published WHAM-relevant single-aperture benchmark, including extracted current and downstream divergence. These comparisons provide confidence that the coupled calculation captures the beam phase space and charge-state evolution that control transport.

With the full model enabled, the simulations show that space-charge neutralization develops through charged products generated by beam–gas interactions. Primary electrons from impact ionization provide the dominant compensation, reducing the beam potential by about 80%. This explains why neutralization and transport cannot be fully separated: the gas interactions that set the useful neutral fraction also generate the charged particles that regulate the beam potential and beam envelope.

The next step is to extend the model to a realistic multi-aperture accelerator grid and compare directly with WHAM operation, including beamlet packing, overlap, aperture-to-aperture variation, and full beamline transport. After that validation, the same framework will be applied to negative-ion beams and photon-driven neutralization. This extension is motivated by Realta's next-step tandem-mirror devices, where beam energies above 200 keV are expected to require negative-ion NBI for efficient neutralization [10]. In this regime, detached electrons, residual ions, and re-ionized particles can strongly modify the beam potential, making space-charge effects even more critical. The positive-ion benchmark developed here therefore provides the foundation for evaluating advanced photo-neutralized NBI concepts under fusion-relevant conditions.

ACKNOWLEDGMENTS

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