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Simulations of particle interactions in a high-current RFQ

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High-intensity beams of composite ions are susceptible to particle interactions that do not affect single ions, such as stripping of electrons and charge exchange. Beam dynamics simulation techniques used in accelerator design do not often include these particle interactions, and so the transmission of the real beam can be significantly different from the design simulations.

We have modified the IMPACT-T code to include particle interactions as part of the beam dynamics simulations, including space-charge effects and beam losses. We have carried out validation simulations of interactions in a molecular hydrogen ion beam through an existing high-intensity deuteron RFQ design, as beam commissioning is often carried out using molecular hydrogen beams, to avoid deuteron–deuteron interactions in the accelerator leading to neutron activation. The new code framework successfully models the interactions within the beam, tracks the different source and product ions through the accelerator, and calculates the collective effects such as space charge from all particles together. We also discuss other simulation codes that could be modified to include similar interaction effects, and possible applications to other types of accelerators.

I. INTRODUCTION

As linear accelerators strive for higher and higher beam intensities, the interactions of particles in the beam with one another becomes more significant. These interactions can lead to changes in the beam dynamics, to beam halo and emittance growth effects, and to collisions with other particles and with surfaces of the accelerator. The end effects are loss of beam current [1], damage to accelerator surfaces and components [2], and increased radiation and activation [3].

Such interactions have been known and studied for many years [4], and mechanisms for beam loss have recently come to the forefront as intensities continue increase and the losses become more and more difficult to control [1].

However, most beam dynamics software does not include such interactions when carrying out accelerator design simulations, meaning that such effects are often added in by hand or overlooked entirely. For lower beam intensities, this is not a significant cause of error, but for new accelerator designs with ever higher beam power and duty factor, the inclusion of these particle interactions in the beam dynamics simulations will be crucial.

We have modified the IMPACT-T simulation code to include a framework for modeling many different interactions together with the beam dynamics, and implemented a number of key interactions for molecular hydrogen ions in a high-current RFQ [5]. We have designed the framework to be easily extensible to different interactions and different applications.

The IMPACT code suite is a three-dimensional multi-particle tracking code, designed for high intensity accelerator applications. It uses the particle-in-cell (PIC) method of modeling space-charge effects, and runs in parallel for scalability. IMPACT-T is the time-dependent implementation. We recently added an RFQ module [6], including benchmarks with TOUTATIS and PARMTEQ. More information on the IMPACT-T code can be found on the project website [7].

In section II, we discuss some of the interactions relevant to high-intensity linacs, and how these could be modeled. In section III, we discuss some existing beam dynamics codes, and how interactions can be handled using those codes. Then, in section IV, we discuss the modifications we have made to IMPACT-T, the application to molecular hydrogen beams, and how the framework can be extended to other applications. The results of our simulations can be found in section V, and we give our final conclusions in section VI.

II. INTERACTIONS

Interactions within the accelerator can be classified into three broad categories: interactions with residual background gas; interactions with other particles in the beam; and interactions with electromagnetic fields. In each of these categories, there are a number of different mechanisms that lead to different interactions. A useful review of many of these mechanisms, especially as relevant to negative hydrogen H^- ion acceleration, can be found in reference [1].

Interactions with the residual background gas include stripping, charge exchange, and ion capture. There are

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also higher order interactions and scattering, which have much smaller cross-sections. Stripping of electrons from beam ions is the most significant mechanism, and can, for example, strip negative hydrogen H^- ions to produce neutral ions [1], or strip the electron from molecular hydrogen H_2^+ ions leaving two protons in the beam [4]. Double stripping is also possible, at measurable levels in existing high-intensity machines, such as H^- to bare protons [8]. Charge exchange, where an ion in the beam picks up an electron from a residual gas molecule, results in changed charge states or neutralization of fast-moving ions, and also ionization of the background gas. Together with ion capture, where ionized background gas particles are accelerated by the RF fields of the accelerator, these lead to neutral or charged fast-moving particles that do not match the design parameters for the accelerator, which can cause significant losses and radiation effects [9].

Interactions with other particles in the beam, sometimes known as intra-beam stripping, were first studied for the LEAR project at CERN [10, 11], and more recently have been discussed in relation to the Spallation Neutron Source (SNS) [12, 13]. For negative hydrogen H^- beams the main interaction is single-electron detachment $H^- + H^- \rightarrow H^- + H^0 + e^-$, and the equivalent interaction for molecular hydrogen H_2^+ ions is $H_2^+ + H_2^+ \rightarrow H_2^+ + 2H^+ + e^-$. Again, the result is neutral or charged fast-moving particles that are not controlled by the beam dynamics design.

Interactions with electromagnetic fields come about because in the rest frame of the beam, there is an electrostatic force that can pull loosely-bound electrons away from the beam ions. This is known as Lorentz stripping, and can arise from the focusing magnets or even from black-body radiation. For strong cyclotron magnets, Lorentz stripping can cause problems [14]. However, in most linac applications, this effect is not significant, as the magnetic fields are not strong enough and the energy is not high enough for Doppler-shifted black-body photons to cause a problem [1].

III. EXISTING CODES

To include such interactions in beam dynamics design simulations for high-intensity linacs requires the following four elements to work together:

1. Representations of beamline elements;
2. Calculation of particle trajectories;
3. Calculation of space-charge effects;
4. Modeling of interactions acting on beam ions.

All beam dynamics design codes must include the first two elements, and most modern codes also calculate space-charge fields and their effects on the beam dynamics, usually by the particle-in-cell (PIC) method. However, modeling of interactions is not often included.

Conversely, simulation codes focusing on particle interactions (usually using Monte Carlo methods) are often not well suited to beam dynamics design applications, and may be missing one or two of the other vital elements.

Table I shows the features of several key simulation codes.

PARMTEQ is the standard design code for RFQs, produced by Los Alamos National Laboratory [15]. It is specialized to RFQ design, and does not handle other beamline elements natively. It includes space charge using the PIC method [16], but does not include any other interactions. As the code is closed, it is not possible to add interactions to run at the same time as the main beam dynamics simulation, although it is possible to combine PARMTEQ simulations with other codes.

TRACEWIN is a beam dynamics code capable of simulating many different kinds of accelerators, produced by CEA Saclay [17]. It was initially developed to fulfill specific requirements for high-intensity linear accelerators [18]. It includes many different beamline elements, with the ability for the user to define their own elements, and implements multiple PIC space-charge models. It already includes some interaction code, simulating scattering on background gas and stripping of electrons on residual gas and in magnetic fields. It is under constant development, and users can request new features to be added, but the code is not open and so users cannot add arbitrary features. It implements RFQ simulations by incorporating the TOUTATIS code as a submodule.

TOUTATIS was also developed at CEA Saclay, focused on high-intensity RFQ beam dynamics [19]. Rather than using analytical approximations of the RFQ vane shapes, it uses the finite difference method with a multigrid solver to take into account real vane shapes [20]. It can be used as a stand-alone program or integrated with the TRACEWIN interface, but unfortunately the stripping and scattering effects modeled in TRACEWIN cannot be used within the TOUTATIS RFQ simulation.

OPAL is a massively parallel 3D code, mainly developed at PSI for charged-particle optics in accelerator structures and beam lines [21]. The code is open-source and in active development, and already includes

TABLE I. Features of relevant simulation codes.

Code	Beamline elements	Particle tracking	Space charge	Interactions
PARMTEQ	RFQ	Yes	Yes	No
TRACEWIN	Many	Yes	Yes	Some
TOUTATIS	RFQ	Yes	Yes	No
OPAL	Many	Yes	Yes	Yes
EPOCH	No	Yes	No	Yes
GEANT4	No	Yes	No	Yes
G4BEAMLINE	Some	Yes	Yes	Yes
BDSIM	Many	Yes	No	Yes
IMPACT-T	Many	Yes	Yes	No

a number of particle–matter interactions using Monte Carlo methods [22]. It includes a number of beam elements, but unfortunately not an RFQ element [23]. RFQs can be included using field maps.

EPOCH is a code initially developed for laser-plasma interactions, from Warwick University [24]. As a plasma-focused code, it does not include RFQs and other beamline elements in its built-in input blocks. However, it does include a variety of different interaction types, and is open-source and extensible [25].

GEANT4 is the leading software code for the simulation of particles through matter, developed at CERN [26]. It is under constant development, is open-source and extensible, and allows the user to write their own application software using the powerful underlying toolkit [27]. It is not a beam dynamics design code itself, but the following two design codes are built on top of the GEANT4 toolkit, making use of its interaction code.

G4BEAMLINE is a particle tracking simulation program based on GEANT4, produced by Muons Inc. [28]. It can be used to simulate a variety of different beamline elements and includes all of the physics processes that can be modeled with GEANT4, but unfortunately does not include code for modeling RFQ accelerators [29]. It is, however, open-source and extensible.

BDSIM (Beam Delivery Simulation) is a high-level program developed at Royal Holloway, University of London, which uses a suite of toolbox utilities including GEANT4, CLHEP and ROOT to build a 3D model of a beamline and simulate the acceleration of particles, including interactions with matter [30]. It includes a variety of beamline elements, supporting RFQ simulations via import of a field map [31]. Space charge calculations are not yet included.

As can be seen from Table I and the discussion above, there is no code that currently fulfills all the requirements for this investigation. This leaves three ways to tackle the program: to write an entirely new code; to add interactions to an existing beam dynamics design code; or to add RFQ tracking and design features to an existing Monte Carlo code. We investigated each of these options, and here we present the second choice, starting from the IMPACT-T beam dynamics code and adding extra modules for interactions.

IV. MODIFICATIONS TO IMPACT-T

IMPACT-T was first developed for high-brightness light sources, focusing on efficient and accurate parallelized multi-physics simulation using the PIC method to calculate self-consistent space-charge forces [32]. It has now been expanded for many other applications, including high-intensity linacs and plasma wakefields, and has a fully symplectic 3D space-charge algorithm [33]. There are two different ways to include RFQ accelerators, either with an imported field map to which sinusoidal time variation is applied, or using the eight-term analytical field approximation produced directly from the RFQ cell parameters [6]. This latter method enables direct import of the cell parameters from the output of the PARMTEQ design code, making the design and simulation stages much more closely integrated.

The main element for simulation in IMPACT-T is the *beam bunch*. Each beam bunch has a reference particle, which defines the time progression of the bunch, and a certain number of macro-particles, which define the collective effects such as space charge. In order to facilitate interactions between different charge states and species of particles in the beam, we differentiated the model at the beam bunch level. For example, for a beam that starts with molecular hydrogen H_2^+ ions and models interactions that produce protons, the simulation would start with two types of bunches: one type dedicated to molecular hydrogen ions and one type dedicated to protons, as shown in Figure 1. At the beginning of the simulation, all particles would be molecular hydrogen ions and the proton bunches would be empty. As interactions take place in the simulation, particles are removed from the molecular hydrogen bunches and added to the proton bunches. The advantage of this method is that IMPACT-T is already set up to handle multiple bunches with different properties, to accelerate the different ions correctly, and to combine the collective effects such as space charge. This means that the interactions code mainly needs to be concerned with modeling the interactions themselves and the movement of particles between bunches, without needing major changes to other parts of the code, and so can rely on existing code validation and verification results.

Our changes to the IMPACT-T code include the following key elements:

- New `Interactions` class;
- Modifications to the `BeamBunch` class to add and remove particles to and from bunches, and to interface with the `Interactions` class;
- A new input file for interactions, which defines the

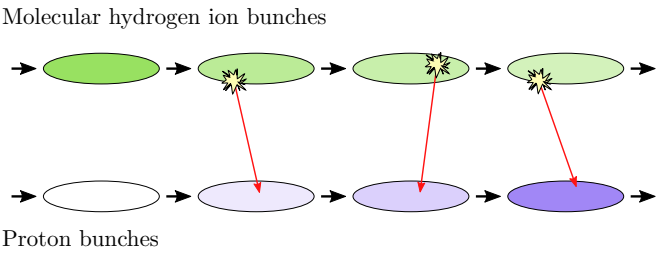

FIG. 1. Schematic representation of interactions and transfer between bunches. In this example, Molecular hydrogen H_2^+ ions are the beam ions, and protons are the interaction products. Proton bunches start empty and increase in particle count as protons are produced by interactions. H_2^+ bunches start full and decrease in particle count as ions are lost through interactions.

interactions to include and the types of particles affected.

We also made the following smaller changes to fit the interaction processes into the existing code:

- Modifications to the `AccSimulator` class to include calls to the `Interactions` class, and to handle empty bunches correctly;
- An additional (optional) flag in the main input file that switches the interactions module on or off;
- Modifications to the `Input` and `Output` classes to handle the new input files and interaction bunches;
- New utility classes `Calculation` and `QuickSort`.

Source code for these changes is available from the authors on request.

The result of these changes is a new framework for interactions, which is modular and extensible. The framework handles the reading of the interaction definitions, the creation of source and product beam bunches, and the application of the interactions to the beam bunches during the simulation. The main IMPACT-T simulation code handles the time evolution of these beam bunches, and collective effects such as space charge. Within the `Interactions` class, each individual type of interaction is implemented by defining both an initialization and an interaction routine.

We have implemented three different interaction types in the module, and applied these to the acceleration of molecular hydrogen H_2^+ ions in an RFQ accelerator. The first interaction type is molecular dissociation, where the single electron of the H_2^+ ion is stripped by the residual background gas, breaking the molecular bond and leaving two protons in the beam as interaction products: $H_2^+ \rightarrow 2H^+ + e^-$. The second interaction type is a charge exchange reaction, where an H_2^+ ion captures an electron from the residual gas, which neutralizes the ion and adds a neutral hydrogen molecule to the beam: $H_2^+ + e^- \rightarrow H_2$. The third interaction type is an example of a compound reaction, where an initial electron capture is then followed by dissociation into two neutron hydrogen atoms: $H_2^+ + e^- \rightarrow 2H$. There are plenty of other types of reaction that could be considered, but these three offer a way of evaluating the effectiveness of the interaction code in creating and tracking different types of interaction product.

For interactions with the background gas, the probability P of an interaction in a certain space ds and time dt is calculated by the code as:

$$P = \sigma \frac{p}{k_B T} I_p \, ds \, dt, \tag{1}$$

where σ is the interaction cross-section, p and T are the pressure and temperature of the residual background gas with k_B being the Boltzmann constant, and I_p is the particle current I/qe for particles of charge q.

The framework allows different ways of determining the cross-section based on the particle energy. In the simulations below, we used a simple relationship:

$$\sigma = \begin{cases} \sigma_{max} \dfrac{E}{E_{max}}, & \text{if } E \leq E_{max} \\ \sigma_{max} \dfrac{E_{max}}{E}, & \text{otherwise,} \end{cases} \tag{2}$$

which represents a linear increase in cross-section up to the peak energy, and a fall-off with $1/E$ above this peak energy. The maximum cross-section and peak energy are inputs to the simulation.

V. SIMULATION RESULTS

The cross-sections for these interactions are specified in the new interactions input file. In order to produce results that clearly show the functionality of the new interactions module, we first ran some simulations where the cross-sections are artificially high, so the beam will undergo many interactions during the acceleration process. For the application, we modeled the acceleration of a 50 mA continuous-wave (CW) molecular hydrogen H_2^+ ion beam through a 1.8 m RFQ, based on an existing design for accelerating deuterons from 50 keV to 1 MeV [34]. This type of high-intensity molecular hydrogen ion beam is often used during the commissioning of deuteron accelerators, to avoid problems of neutron activation when using deuteron beams [35]. Table II lists the details and parameters of the simulation.

TABLE II. Beam parameters and interaction cross-sections for the test simulation. Interaction parameters are set artificially high to validate the interaction modeling process.

Target ion	molecular hydrogen H_2^+	
RFQ length	1.8	m
Frequency	162.5	MHz
Input energy	0.5	MeV
Output energy	1.0	MeV
Beam current	50.0	mA
Input x-emittance (norm. rms)	0.20	πmm $\cdot$ mrad
Input y-emittance (norm. rms)	0.20	πmm $\cdot$ mrad
Number of macroparticles	100 000	
Dissociation cross-section	5.0×10^{-19}	m^2
Dissociation peak energy	100	keV
Charge exchange cross-section	1.0×10^{-19}	m^2
Charge exchange peak energy	100	keV
Compound reaction cross-section	3.0×10^{-20}	m^2
Compound reaction peak energy	100	keV

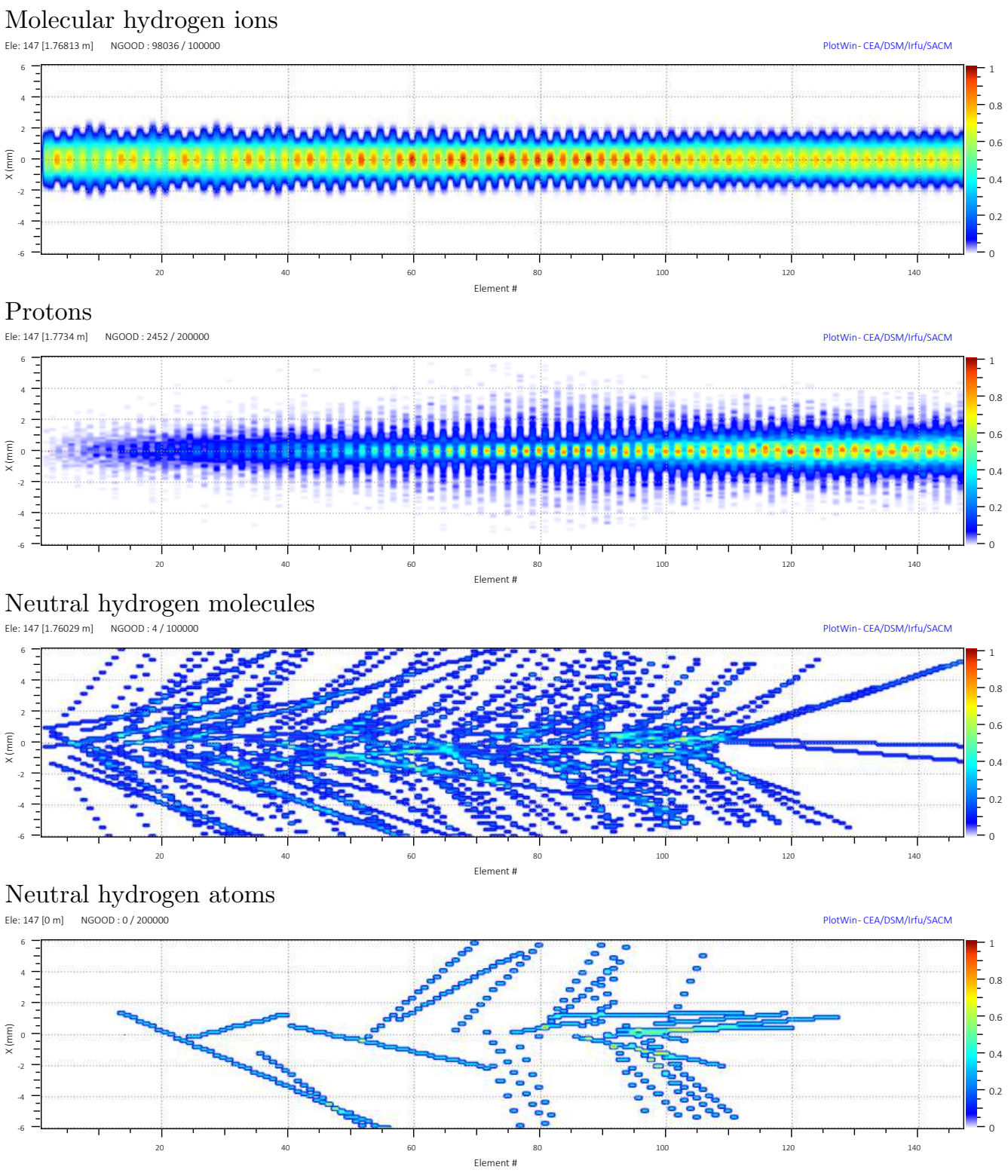

FIG. 2. Tracks of different particle species along the length of the simulated RFQ. Produced using PLOTWIN [37].

In order to promote reproducibility of simulation results, we used the software code REPRODUCIBLE produced at Lawrence Berkeley National Laboratory [36]. This enables us to store the simulation parameters and input files in a GIT repository, where the source code and simulation data can be referenced by unique identifiers, which can be used to exactly reproduce the simulation at a later date. The simulation reported here is run `333fb20`, using source code version `5cb8c4f`.

Figure 2 shows the tracks of different types of particles along the length of the RFQ. Although the simulation handles all collective calculations with all particle species together, the separate beam bunch method allows us to plot the tracks for each particle species separately.

The results for molecular hydrogen H_2^+ ions show that the target ion species is accelerated well, with no direct losses, but approximately 2 % of ions undergo some kind of interaction and are effectively lost from the main beam.

As protons have the same charge-to-mass ratio as the target H_2^+ ions, many of the protons produced by stripping reactions are captured by the RF buckets and accelerated along with the molecular hydrogen ions. By the end of the simulation, the particle count for protons is 2.5 % of the initial particle count, as each stripping reaction produces two protons.

The neutral particles (H_2 molecules and atomic hydrogen) are not controlled by the electromagnetic fields in the RFQ, and so follow straight paths from the interaction locations. Most of these particles will collide with the RFQ vanes close to the place where they were produced.

Figure 3 shows the energy spectrum at the end of the RFQ. The main peak comes from the molecular hydrogen H_2^+ ions, but a secondary peak for the protons is very clear. The neutral particles do not show up on the energy spectrum at this scale, as almost all of them are lost before the end of the RFQ.

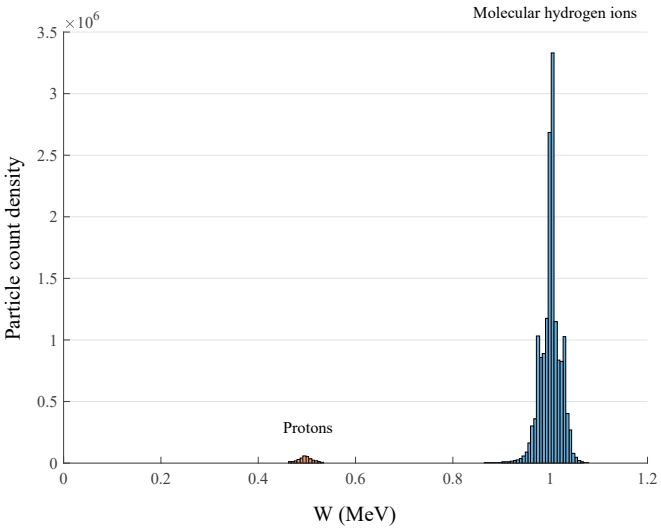

FIG. 3. Energy spectrum at the end of the RFQ, showing a secondary peak for protons generated by the simulated interactions.

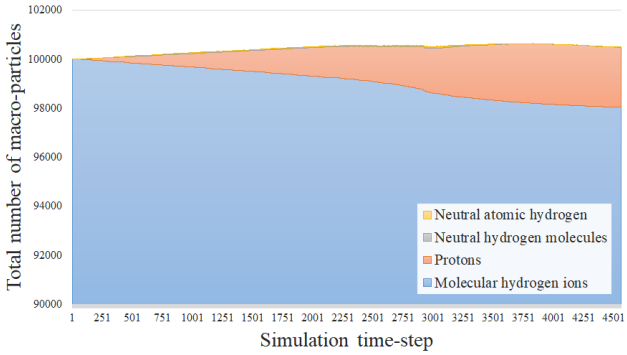

FIG. 4. Number of particles of each species for each time-step in the simulation. Note that the vertical scale starts from 90 000 in order to clarify the comparison.

Figure 4 shows the total number of macro-particles at each simulation time-step, broken down into different particle types. The scale has been modified to focus on the count of secondary particles, as only 2 % of the source H_2^+ ions undergo interactions. The number of protons grows quite steadily, with a requisite decrease in the number of molecular hydrogen ions. Neutral particles are lost soon after being produced, and so do not grow in number.

VI. CONCLUSIONS AND FUTURE WORK

We have developed the IMPACT-T interactions code to the stage where we are quite confident that the mechanisms for producing and tracking secondary particles are robust and ready for use. We have implemented three types of interaction so far, and verified qualitatively that the new particles behave as expected. The next stage for this research is to use known values for interaction cross-sections and quantitatively compare the loss rates with experimental data for high-intensity accelerators. We also intend to add more interaction types to the code in the future, which is the reason for the focus on a modular and extensible approach. In order to make quantitative comparisons with experiment, we need to ensure that all relevant interactions are modeled accurately.

Ideally, the code should use a Monte Carlo method to model the interactions, rather than the probabilistic macro-particle selection process currently implemented. Again, the modular nature of the code should be beneficial, allowing us to try out different particle selection methods and compare the results numerically under the same simulation conditions.

We also are investigating the possibility of integrating with other codes, such as OPAL and BDSIM. These codes already have Monte Carlo routines incorporated, but

need some work to be able to model the RFQ beam dynamics for high intensity beams before they can be directly compared with the IMPACT-T code described here. Both of these software packages are open source and extensible.

In future, this work should be generalizable to many different types of accelerators and beamline elements, and also to many different types of particle interactions, such as the break-up of heavy ions into constituent parts, or interactions with electron clouds in a beam pipe.

As high-resolution multi-particle simulations become more and more important for both the design and operation of high-intensity particle accelerators, the combination of different technologies in a single comprehensive simulation environment becomes ever more vital. This work is just a small part of that ongoing effort.

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