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2D-3D PIC CODE BENCHMARKING/ANCHORING COMPARISONS FOR A NOVEL RFQ/RFI LINAC DESIGN*

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Abstract

In this study, comparisons are made between several particle dynamics codes (namely CST Particle Studio [CST PS], General Particle Tracker [GPT] and PARMULT) for a specific accelerator system. The structure used for simulations is a novel 200 MHz, 2.5 MeV, CW RFQ/RFI LINAC designed by Ion Linac Systems (ILS) [1]. The structure models and parameters are provided, simulation techniques are explained, and results from all three code families are presented. These results are then compared with each other, identifying similarities and differences. Various parameters for comparison are used, including the transmission efficiency, Q-factor, E-field on-axis, and beam properties. Preliminary anchoring between modeling and simulation performance predictions and experimental measurements are also shown.

INTRODUCTION

The machine presented in this paper was designed by ILS for use in Boron Neutron Capture Therapy (BNCT). BNCT requires intense neutron fluxes and previously these have been produced using nuclear reactors. To make BNCT more accessible there is now an interest in producing neutron fluxes using accelerator-based sources. To produce a sufficiently high neutron flux, a linear accelerator (linac) must operate in the continuous wave (CW) mode, which can prove challenging due to cooling problems and operational costs. There are a few of these types of accelerators in the world, so the machine described in this paper was designed to fill this gap [1]. The Radio Frequency focused Interdigital (RFI) linac was designed by Don Swenson and is four times more efficient than current Radio Frequency Quadrupoles (RFQ) or Drift Tube Linac (DTL) designs [2]. This RFI design, combined with an efficient RFQ, allows for CW operation at high currents (up to 30-mA) that can produce high neutron fluxes for BNCT.

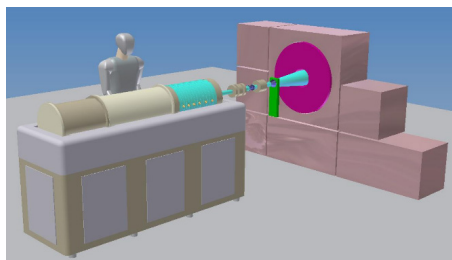


Figure 1: Example of full BNCT setup.

The RFQ structure was originally simulated in PARMTEQ and the RFI in PARMIR. Beam dynamics simulations were also performed using the PARMULT code for the RFQ [3,4]. Now that the structure has been built, there is an interest in modeling the structure in CST MWS, and to perform beam dynamics simulations using CST PS and General Particle Tracer (GPT) to benchmark them and take full 3D effects into account.

This paper is divided into the following sections:

- CST eigenmode (cold tests) vs. experimental results.
- Beam dynamics code comparison for CST PS vs. GPT

CST COLD TESTS VS. EXPERIMENTAL RESULTS

In order to anchor experimental results from the RFQ/RFI structures, the CST MWS Eigenmode solver was used to calculate the eigenmode frequencies and fields.

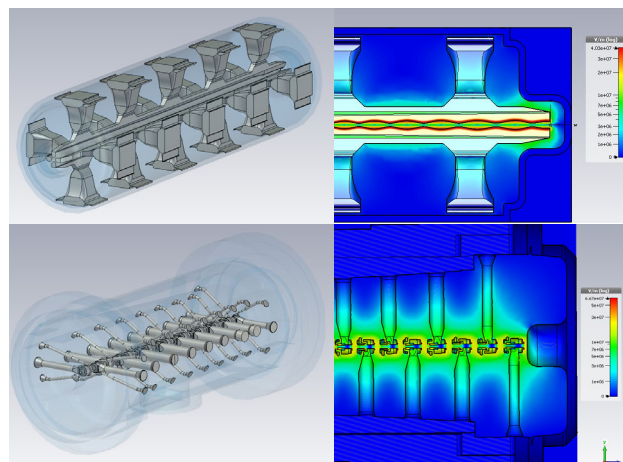


Figure 2: RFQ model and E-field magnitude (top); RFI model and E-field magnitude (bottom).

A fine tetrahedral mesh (~1.6 M tetrahedrons) was used for both structures although simulations were also performed on fine hexahedral meshes (~25 M cells). The tetrahedral mesh was primarily used as it is well parallelized and the simulations are significantly faster. For both structures, the meshes surrounding the beam axis were refined to provide more accurate results for the fields in this region. After running the eigenmode solver, the appropriate modes were identified, longitudinal E-field components found, and the Q-factor calculated assuming the material was pure copper. The results are summarized in Table 1 and Table 2.

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Table 1: Results for the RFQ

Parameter	CST	Measured
Frequency (MHz)	201.5	200.87
Q-factor	6800	5925
Power loss (kW)	189.5	75

Table 2: Results for the RFI

Parameter	CST	Measured
Frequency (MHz)	200.61	200.915
Q-factor	10,024	9247
Power loss (kW)	105	45

The measured power losses for both structures are the powers that need to be supplied during operation due to wall losses and the differences in Q, which are attributed to the coupling slot between the cavities and impurities/finishing effects. From the results we can see that there is less than 0.5% error between the measured and calculated resonant frequencies for the mode of operation. In the CST MWS model, the longitudinal field components were found for the two structures and are shown in Fig. 3.

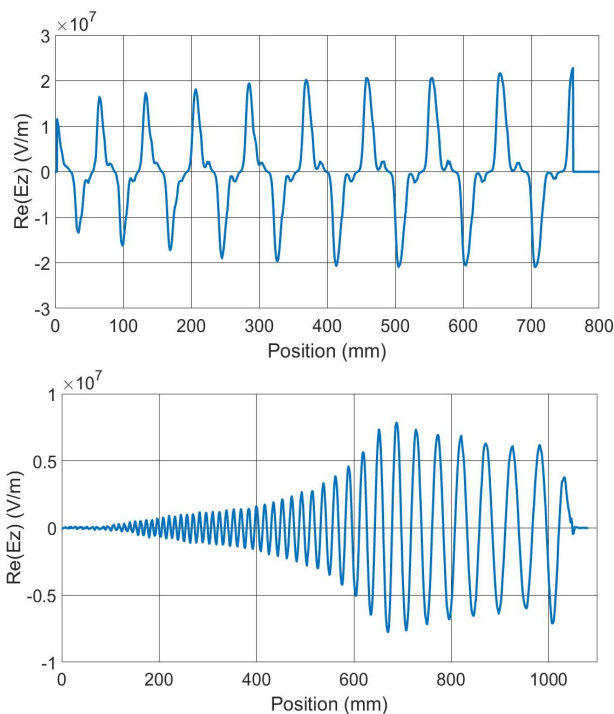


Figure 3: E_z field component on-axis (top RFI; bottom RFQ).

BEAM DYNAMICS CODE COMPARISON

Original beam dynamics studies for the RFQ were performed in PARMULT. Using 10,000 macro-particles, and a beam current of 20-mA, the simulations predict an effective transmission rate of 93.85% with space charge and 94.85% without space charge. To compare results, the CST PS solver and GPT were used.

CST PS Solver Results

For CST PS, the eigenmode fields were exported from the eigenmode solver, imported into the particle solver, and then scaled using the measured and simulated power losses. The original PARMULT particle distribution input files (20-mA, 10 k macro particles) were converted to a .pit file to import into CST. In Fig. 4 we show the results from a 2D particle monitor located at the end of the RFQ vanes which records the position and energy at 0.1 ns intervals. The bunch energy is around the design energy of 750 keV. Introducing an energy cut of ± 50 keV around 750 keV, the effective transmission was calculated to be 85% with space charge, and 92.2% without space charge.

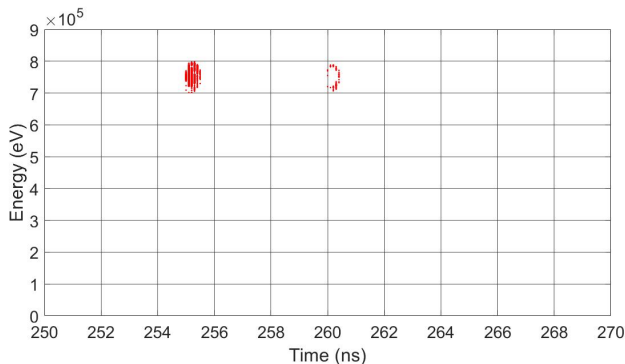


Figure 4: Energy vs. time at the RFQ end (0.1 ns interval).

For simulations aligned closer to experimental measurements, a larger number of particles were used to mimic a 20-mA, H^+ -ion CW beam injected over 10 RF periods (10x10 k). A phase space shot taken at 1 ns intervals for 5 ns (~ 1 RF period) is shown in Fig. 5, showing that the bunches are accelerated to the design of 750 keV. Again, a 2D particle monitor was used to record the number of particles and their energy crossing a plane at a set distance (end of the RFQ) at 0.1 ns intervals.

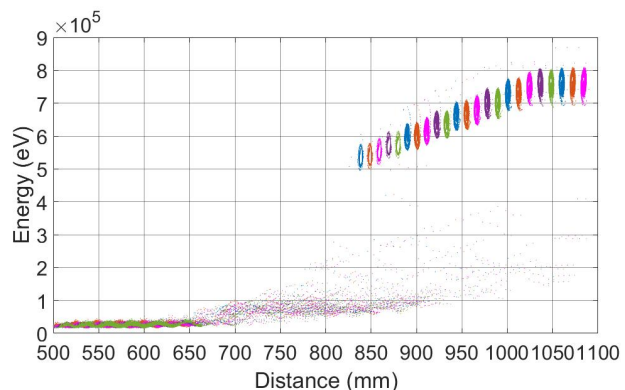


Figure 5: Five overlaid snapshots over 5 ns at 1-ns intervals for the RFQ.

The particles form 11 instead of 10 bunches, and have an average energy of 753.1 keV, although some have much lower energies than the design value, as seen in Fig. 6. To calculate the effective transmission, 9 central bunches were used. By applying a ± 50 keV-energy cut around the design particle energy, the transmission was found to be 83.4%

without space charge effects and 78.8% with space charge. CST PS simulations for the RFI structure, and full end-end simulations are currently ongoing, and will be used to anchor and understand experimental results in the near future.

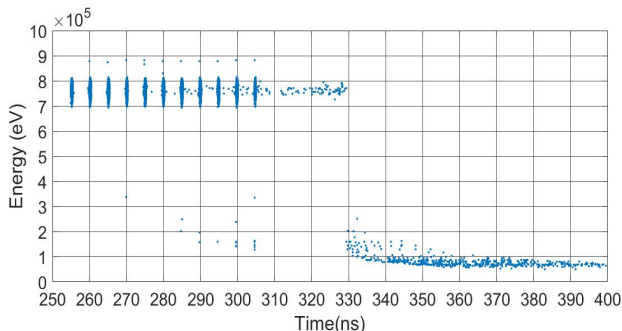


Figure 6: Particle energy vs. time at the end of the RFQ.

GPT Results

The fields calculated by the eigenmode solver of CST were also imported into GPT and scaled. We assumed 75 kW for the RFQ and 45 kW for the RFI wall losses. In GPT, both the RFI and RFQ structures were simulated, providing some end to end results. The RFI field was imported at $z = 1100.41$ mm with a phase shift of π , because the structures (RFQ and RFI) were operated in the $\pi/2$ mode with a resonant coupler in between (cavity) [5]. Simulations over 1 RF period (10 k particles) and 10 RF periods (100 k particles) were performed both with and without space charge effects.

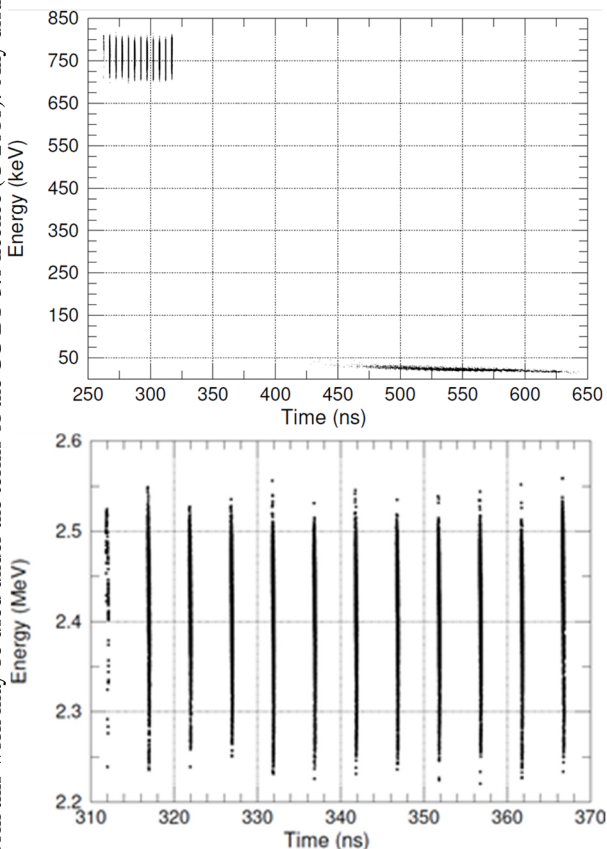


Figure 7: Particle energy vs. time at the end of the RFQ (top) and RFI (bottom).

The input transverse emittances and energy spreads were derived from the original PARMULT input file; with 10 k macro-particles the transmission was calculated to be 84.7% with space charge and 92.9% without space charge. For 100 k macro-particles and energies below a 150-keV cut, the RFQ transmission ($z = 1048$ mm) was 89% with space charge effects and 91.1% with space-charge effects turned off. Fig. 7 shows bunches at the end of the RFQ and RFI. The particle distribution along the longitudinal z direction are also shown in Fig. 8 with the final transmission ratio being 66.4% with space charge and 71.4% without space charge. (RFI transmission was 74.5% from the end of the RFQ.) In PARMULT, the effect of including space charge was a minimal $\sim 1\%$ difference, so the larger differences in GPT and CST need to be investigated further.

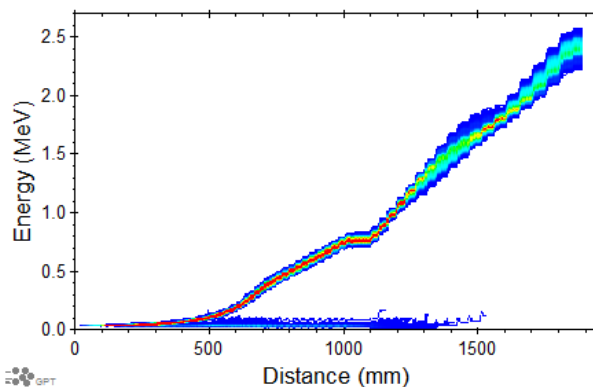


Figure 8: Particle energy distribution along the z axis through the RFQ and RFI. The color represents the density of the particles in the bin (red is densest).

CONCLUSION

Cold test results from the CST eigenmode solver are presented along with experimental data from a novel RFQ/RFI design, showing similar resonant frequencies and the correct longitudinal field components. The RFQ transmission efficiencies for a 20-mA, H^+ , CW (100 k) ion beam with space charge are also calculated using CST and GPT simulations (78.8%, 89.0%). All three code families agree (to within 3%) with the predicted RFQ transmission for a 10 k particle bunch with no space charge. Full end-end simulations are performed in GPT giving a total transmission of 66.4%. The RFI structure will be simulated in CST PS along with end-end simulations to compare with the GPT results, understand differences between the two, and anchor with experimental measurements. These will be presented in the future.

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