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Benchmarking of CST and Trak in the simulation of an electron gun for a future C^{6+} ion source

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Abstract: This study benchmarks the CST Studio Suite and Trak codes in simulating an electron gun for a future C^{6+} hadrontherapy installation. CST Studio Suite offers 3D simulation capabilities, allowing detailed modelling of complex geometries and electromagnetic fields. Trak, on the other hand, offers efficient 2D simulations, which can significantly reduce computational time while still providing valuable results.

These studies are being conducted in the framework of a project dedicated to the design of the initial stage of a C^{6+} hadrontherapy linac. The electron gun studied is based on the MEDeGUN developed at CERN. This study provides an overview of the results obtained so far and outlines plans for future improvements and development.

Keywords: Accelerator modelling and simulations (multi-particle dynamics, single-particle dynamics); Ion sources (positive ions, negative ions, electron cyclotron resonance (ECR), electron beam (EBIS))

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Contents

1 Introduction

In recent years, there has been a growing interest for ion therapy, particularly involving carbon ions C^{6+}, due to their significant medical benefits. Carbon ions deposit most of their energy at a narrow depth range known as the Bragg peak. This characteristic allows them to spare surrounding healthy tissue, thereby minimizing side effects while enhancing therapeutic efficacy. Compared to traditional C^{4+} ions, the use of C^{6+} ions provides several advantages in hadrontherapy installations, including improved acceleration efficiency and reducing the need for strippers.

One of the challenges of future hadron installations is the development of an ion source that can directly produce C^{6+} ions while meeting specific requirements for current, low impurity levels, and temporal pulse structures (short, intense pulses with high repetition rates). Currently, high-intensity pulsed sources, such as the EBIS, represent the most suitable solution for generating ions with these characteristics and have been chosen as a first approach. The electron gun (figure 1) studied in this context is based on the Brilloun electron gun called MEDeGUN [1, 2] developed at CERN.

This study benchmarks the CST Studio Suite [3] and Trak Charged Particle Toolkit [4] codes in simulating said electron gun. CST Studio Suite offers 3D simulation capabilities, allowing detailed modelling of complex geometries and electromagnetic fields. Trak, on the other hand, offers efficient 2D simulations, which can significantly reduce computational time while still providing valuable results.

2 Model

The electron gun studied is a Brillouin type electron gun, composed of a cathode, an anode, a focusing electrode known as the Wehnelt and the Wehnelt insulator. The electrostatic model can be seen in figure 1. The cathode has a radius of 6.0 mm.

The guiding magnetic field is generated by a superconducting 2 T solenoid, located at around 128 mm with a length of 1.22 m, and a magnetic shielding structure significantly reduces the magnetic field on the cathode (figure 2).

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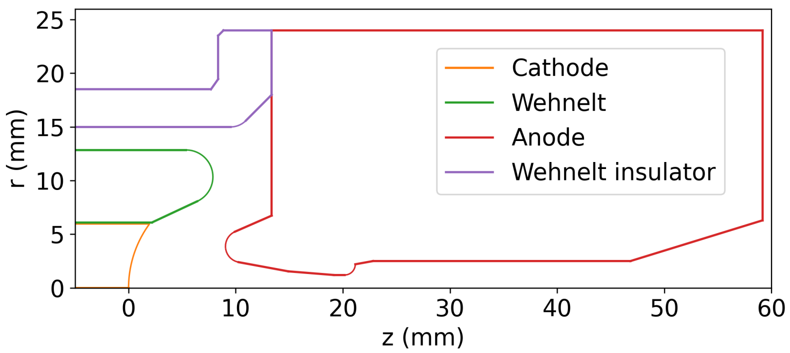

Figure 1. Electrostatic model of the electron gun. The anode can be seen in red, the Wehnelt or focusing electrode in green, the cathode in orange and the Wehnelt insulator in purple.

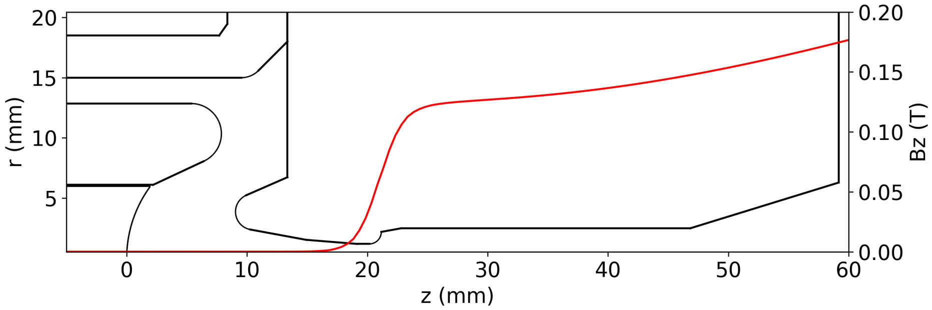

Figure 2. Electrostatic model of the electron gun and longitudinal magnetic field distribution in red.

The simulated perveance of the studied electron gun is 9.5×10^{-7} A/V$^{3/2}$. In our simulations, for the anode voltage, the potential of the cathode and Wehnelt electrode, the potential difference was fixed at -10 kV, for which it can deliver a simulated current of 1.0 A.

3 Simulation methods

Particle tracking simulations of the electron gun, including the superconducting solenoid and its shielding, were carried out using two commercial simulation tools: CST Studio Suite and Trak Charged Particle Toolkit. This section provides a comparison of the methods used in each code, focusing on the key differences and similarities in the approaches.

3D simulations were carried out using the CST Studio Suite package. This software offers multiple specific simulation modules to study different problems through a graphical user interface. In our case, the CST Particle Studio and the CST EM Studio modules were used [5].

2D Simulations were carried out using Trak: 2D Charged Particle Tool Kit. Trak is a versatile program for charged-particle optics. The following components were used for the simulations: Mesh, (meshing), EStat (electric-field solutions), PerMag (magnetic-field solutions) and Trak (trajectories and fields).

3.1 Meshing and geometry

In CST, 3D geometries are defined on a computational grid or mesh. The meshing subdivides the geometry into discrete cells, determining both the precision of the geometry and the accuracy of the results. CST has the options to use hexahedral or tetrahedral meshing. In this simulation, a refined hexahedral mesh was imposed in the electron gun region, where precision is critical.

In contrast, Trak uses a 2D subdivision of the geometry, generating triangular meshes through its Mesh module. The geometries are defined in terms of coordinate points that create lines on a 2D plane, and the mesh can be adjusted for different areas. Like CST, a refined mesh was applied in the electron gun region for beam tracking simulations.

Both codes handle independent meshes for electric and magnetic fields that overlap in common regions. While CST uses a more detailed 3D meshing approach, Trak simplifies the process by relying on 2D triangular meshes, which results in faster computations but may affect spatial accuracy.

3.2 Magnetic field simulations

In CST, the magnetic field simulations were carried out using the magnetostatic solver (MS) (figure 3), which solves magnetic problems where sources are defined by currents, coils, or permanent magnets The current of the solenoid was set to 2×10^6 A as stranded model and the material for the shield was set as iron (permeability of 1000 H/m). The solenoid was modeled with a stranded conductor model for compatibility with the meshing. A hexaedral mesh was used with a total of 10 million mesh cells and a finer mesh in the region of the beam. The accuracy was set to 1×10^{-9}. Magnetic boundary conditions were set to "add space if,", which virtually extends the boundary to infinity, and symmetry planes were employed to improve computation efficiency. The resulting field map was exported for use in the electron tracking simulations.

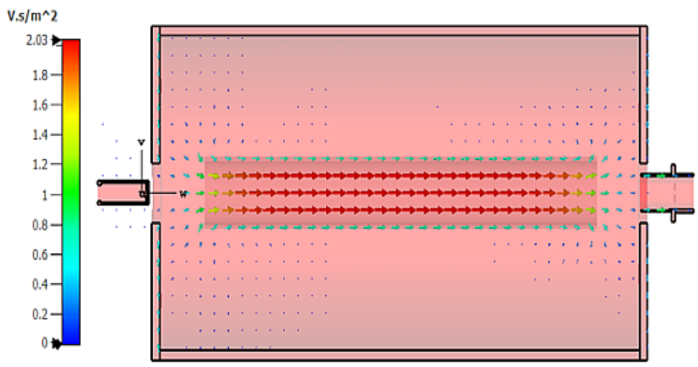

Figure 3. Magnetic field distribution in the MS solver in CST. The red arrows show the 2 T magnetic field inside the solenoid. The magnetic shielding can be seen on the edges of the model.

Trak, on the other hand, uses the PerMag module for magnetic field simulations (figure 4). The solenoid was defined with a superconducting current of 2×10^6 A, as in CST, and the shield material was defined by importing a B-H curve for iron. 2 million mesh elements were used. The accuracy or residual target was set to 1×10^{-8} and Omega, a parameter to control the iterative matrix solution was set to 1.95.

Although the same physical system was modeled, the 2D nature of Trak simplifies the geometry definition and simulation process. The magnetic field maps generated by PerMag were later used for tracking the electron beam.

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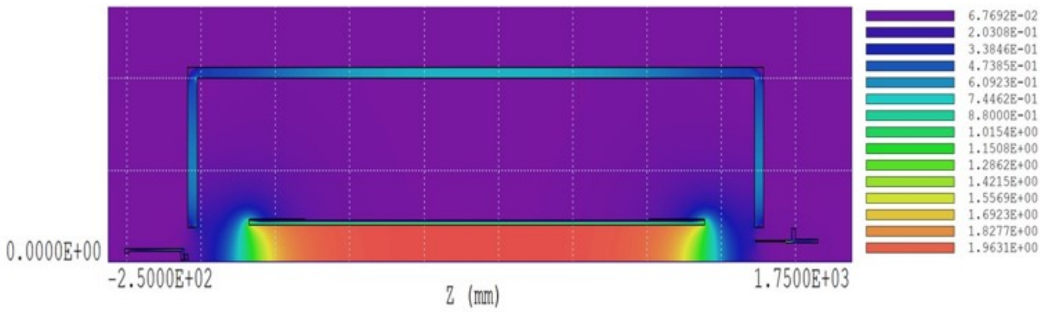

Figure 4. Magnetic field distribution in the PerMag module of Trak. The red color shows the 2 T magnetic field inside the solenoid. The shieldings can be seen in blue.

3.3 Electric field and electron tracking simulations

In CST, the electron beam tracking was performed using the particle tracking solver (Trk) (figure 5), which calculates electrostatic potentials and tracks charged particles through pre-calculated fields. The electric field was resolved with an accuracy of 1×10^{-9}. The solver was configured with 10 k time steps, 5 particle pushes per cell, and a dynamic time step of 1.2, adjusted according to particle energy. The electron source was defined on the cathode surface, and the gun iteration module was enabled to model the space charge potential with a charge residual goal of -80 dB and a relaxation setting of 0.3 to balance simulation time and stability. The emission distance was set to relative 1 (equivalent to 0.25 mm), because orbit calculations would not be possible if particles were created in the surface, due to the Child condition of zero electric field which implies that zero energy particles would not move.

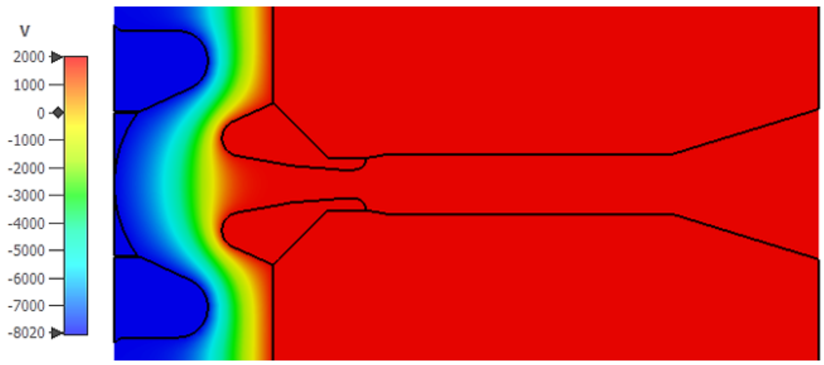

Figure 5. Electrostatic potential applied to the electron gun components in color scale, in CST.

In Trak, the electrostatic simulations were carried out in the EStat module (figure 6), were the potentials were defined. The accuracy or residual target was set to 2×10^{-8} and Omega was set to 1.95, as in the magnetic field calculations.

Then the Trak module imports both magnetic and electric field solutions to carry out the tracking simulations. The electron beam was also initiated on the cathode surface, with the SCHARGE mode. The solver was configured to a time step of 5×10^{-13} and maximum integration steps of 900000. The distance from the emission surface to the generation surface was set to 0.04 mm.

In both CST and Trak, the electron gun simulations were carried out using Child-Langmuir emission models, which simulate non-relativistic, high-current electrons with self-consistent space charge effects.

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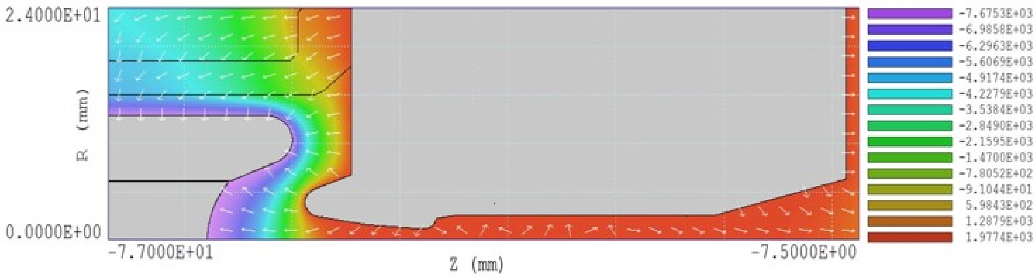


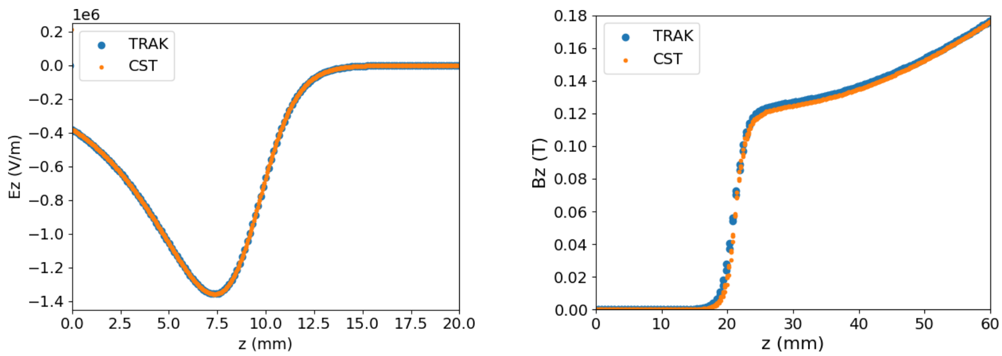
Figure 6. Electrostatic potential distribution in color scale and arrows showing the electric field, in the EStat module in Trak.

4 Results

This section presents a comparative analysis of the simulation results obtained using CST and Trak. The main goal of this analysis is to assess the accuracy and consistency of the magnetic and electric fields generated by each code, as well as to evaluate the differences in the trajectories of the electron beams.

In both simulation codes, the magnetic and electric fields are resolved separately. The meshing process plays a crucial role in determining the accuracy of the fields and, consequently, the simulation results, including the particle trajectories. Therefore, careful adjustment of the mesh is essential. While finer meshing can significantly enhance resolution, it also increases simulation time and memory usage very rapidly. To mitigate these issues, fine meshing was applied mainly in the cathode and beam region, where precision is most critical.

The magnetic and electric fields generated by CST and Trak show a very good agreement, with only minor discrepancies observed. These discrepancies are largely attributed to differences in the meshing techniques and numerical algorithms employed by each code. Figure 7 shows the comparison of the longitudinal electric and magnetic fields generated by the two codes.



(a) (b)

Figure 7. (a) Longitudinal electric and (b) longitudinal magnetic fields at r = 0 mm along the z axis.

The emission model used in both codes is described by the Child-Langmuir law and compute the transport and acceleration in a similar iterative way taking the space charge into account. Parameters such as the maximum number of cycles, residual error, and the number of timesteps are consistently defined for each code to ensure comparable results.

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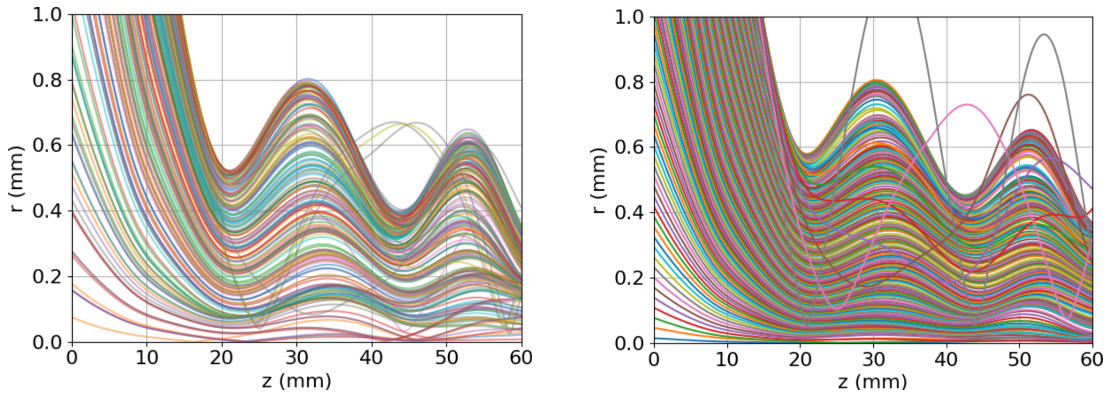
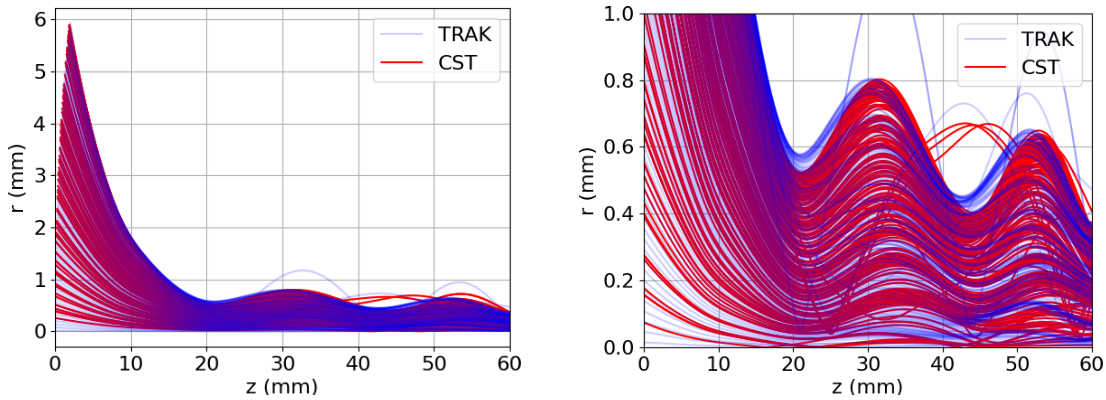
Particle trajectories were also computed in both codes, and their results are shown separately in figure 8 and a more detailed comparison can be seen in figure 9. While the overall patterns of the trajectories are similar, there are slight differences between the two simulation tools. These differences are primarily due to the varying resolutions of the electromagnetic fields and the differences in tracking algorithms, as well as the fact that CST employs a 3D simulation approach, while Trak operates in 2D. The trajectories in Trak show a better laminarity while in CST for small radii some of the trajectories cross, pressumably due to the convergence of the simulations. For larger radii, in both codes, the particles that cross are coming from the edges of the cathode and are a bit more focused by the Wehnelt electrode.



(a) (b)

Figure 8. Electron beam trajectories in (a) CST and (b) Trak.



(a) (b)

Figure 9. Electron beam trajectories comparison in CST and Trak, (b) zoom into the cathode area.

Despite these differences, both codes produced consistent results. Overall, the results indicate that both CST and Trak are capable of producing accurate simulations of electron dynamics, with discrepancies attributable to meshing choices and convergence in the simulations.

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5 Conclusions

This study benchmarks the performance of CST Studio Suite and Trak in simulating an electron gun for C^{6+} ion source, with the goal of comparing their performance in modeling the electromagnetic fields and the particle trajectories. This study helps us better understand both tools for the future studies and optimization of the electron gun. The results show a good agreement, the magnetic and electric fields generated agree within a small range, but the difference between the trajectories' results is more noticeable.

During the benchmarking process, we encountered significant convergence issues, particularly with CST. These issues are largely attributed to the meshing, which directly impacts the resolution of the simulations and the accuracy of the trajectory results.

The study is ongoing, and future work will focus on refining the meshing techniques and improving the convergence criteria to achieve more consistent and reliable results across both simulation codes.

Acknowledgments

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