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Scanning Horn Simulation Code for Electron Beam Machine Based on Boris Algorithm

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ABSTRACT

A numerical particle simulation code package to estimate the irradiation distribution of an electron beam machine is presented. Particle-to-particle interactions are calculated using particle-in-cell method, while the equation of motion is solved using Boris algorithm. The amplitude of oscillating magnetic field distribution from the scanning horn is obtained using CST magnetic field solver. The code was run using Intel's i7-10700 processor without multithreading. For cases where particle-to-particle interactions are negligible, the simulation requires about 10 000 seconds to finish. The results show that different shapes of signals will result in different irradiation distributions. For a relatively low magnetic oscillation frequency, it is shown that a triangular signal will result in a more evenly distributed irradiation compared to a sinusoidal signal.

INTRODUCTION

The Center for Accelerator Science and Technology, National Nuclear Energy Agency, Indonesia, is currently developing electron beam machines designed to irradiate various types of materials, enhancing their properties. The electron beam machine accelerates electrons using static electric field which boosts the electrons with a maximum energy of 350 keV. The beam of electrons is then intentionally redirected using a time-varying magnetic field which causes the beam to scan the irradiated object. The time-varying magnetic field is produced by two solenoids along with iron cores with a particular shape (see Fig. 1). By varying the electric current in the solenoid with respect to time, a time-varying magnetic field can be obtained [1-3].

The distribution, strength, frequency, and signal shape of the magnetic field, along with the energy and the profile of the electron beam, will generally affect the distribution of the electron irradiation. If an evenly-spread distribution is desired, then an optimization of those parameters is necessary. It is possible to perform a rough calculation to obtaint an approximate irradiation distribution. However, for non-simple magnetic distribution and signal, a numerical simulation is a more sensible approach.

Here, a simulation code package to estimate the irradiation distribution of electron for a set of previously mentioned parameters is presented. The irradiation distribution is calculated at the surface of the titanium foil of the machine. The code was written in C++, which makes the program easier to maintain, more reusable, and readily extended [4]. A numerical simulation program written in C++ is also generally faster compared to the ones written in newer languages such as Java or Python [5], which means that more accurate calculations can be employed without needing too much computational power.

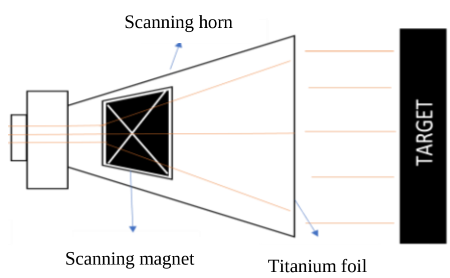

Fig. 1. Scanning Horn Schematic.

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Currently, there are many particle simulation code packages that use particle-in-cell algorithm to calculate particle-to-particle interactions in a particle accelerator [6-8]. The code packages are often intended to simulate particle trajectories in a higher-energy beam, where particle-to-particle interactions a crucial factor in determining beam quality. Unfortunately, those packages are rather inflexible for simulating particles in a time-varying magnetic field for an arbitrary signal shape. For instance, a well-established particle simulation code package called PARMELA was used to simulate the irradiation distribution using static magnetic field [9]. It would not be possible to calculate the irradiation distribution using PARMELA if the magnetic field varies with time. The difference between PARMELA and the package developed in the present work is that the current code package has been made specifically to simulate irradiation distribution easier without further modifications.

In Ref. [10], a beam simulation code package specifically made for the scanning magnet of an electron beam machine is proposed. The method uses integer steps for both position and velocity (or momentum) updates. Several authors have pointed out that non-symplectic methods with same step evaluation between position and velocity such as in Ref. [10] or fourth order Runge-Kutta method will not be as accurate as staggered time algorithms such as Boris method [11,12], especially after a long period of time. There is also another simulation code applied to similar type of machine called electron beam welding [13]. However, the beam in that particular machine is intended to be focused, which means that its deflection coil does not need to be time varying.

The simulation code package presented here was designed to be able to run with various signal shapes applied to magnetic coil. Thus, the specific signal shape which produces the best irradiation distribution for a given initial parameters (and magnetic field distribution) can be searched. The code can also include several scanning magnets on the domain, each of which may have a different frequency.

The scanning horn simulation code package here uses particle-in-cell algorithm to calculate interactions between particles in the beam. It is assumed that the relative velocities between particles are low enough that inter-particle magnetic fields can be ignored. The inter-particle electric field is combined with external electromagnetic field using Lorentz equation, which directs the movement of the particles in the beam. The Lorentz equation is numerically solved using Boris algorithm, which currently is the standard for integrating particle motion under electromagnetic field [14]. Boris algorithm was chosen because the method is accurate enough but only requires a single evaluation each step, thus making it fast. The numerical error of Boris algorithm is also bounded even if electric and magnetic fields are applied simultaneously in the domain.

The magnetic field used in testing this program was obtained from magnetic field simulations using CST magnetic solver program, since a direct magnetic field measurement has not been done. The code was then benchmarked using CST particle tracking solver. The benchmark involved single-particle tracking to see whether the code package would give approximately identical results with the results obtained using CST particle tracking or not.

NUMERICAL METHODS

Theoretical background

The equation of motion of a charged particle can be determined using Lorentz equation, Eq. (1), provided that the initial conditions are known.

$$\vec{F} = q\vec{E} + q\vec{v} \times \vec{B} \tag{1}$$

For relativistic cases, the left-hand side of Eq. (1) is given by Eq. (2).

$$\vec{F} = \frac{d\vec{p}}{dt} \tag{2}$$

In Eq. (2), the momentum $\vec{p}$ is given by $\vec{p} = \gamma m\vec{v}$ with γ representing the Lorentz factor $\gamma = \sqrt{1 - \frac{v^2}{c^2}}$. Relativistic Lorentz equation can be numerically solved by using Boris algorithm [15]. The discretization of equation of motion goes as follows:

$$\frac{\vec{u}^{n+1} - \vec{u}^{n}}{\Delta t} = \frac{q}{m}\left(\vec{E}(\vec{x}^{n+0.5}) + \bar{\vec{v}} \times \vec{B}(\vec{x}^{n+0.5})\right) \tag{3}$$

$$\frac{\vec{x}^{n+1.5} - \vec{x}^{n+0.5}}{\Delta t} = \vec{v}^{n+1} \tag{4}$$

In Eqs. (3) and (4), $\vec{u} = \gamma\vec{v}$ and the average velocity $\bar{\vec{v}}$ depends on $\vec{u}^{n+1}$. For Boris algorithm, the average velocity is defined by Eq. (5), as in [16].

$$\bar{\vec{v}} = \frac{\vec{u}^{n+1} + \vec{u}^{n}}{2\gamma^{n+0.5}}. \tag{5}$$

It is more convenient to separate electric field and magnetic field from Eq. (1) into particle-to-particle interaction part and particle with external field interaction part. For a realistic beam simulation, many particles need to be calculated simultaneously; thus, particle-to-particle interactions will generally take effect. Each of the particle will interact electromagnetically with each other; however, assuming that the relative velocities between particles are much lower than the speed of light, it can be expected that magnetic interactions between particles will be much smaller than electric interactions, and thus can be ignored [17].

The sheer number of particles for a typical value of beam current means that simulating every single one of them is practically impossible. Thus, the simulation will be done using macroparticles instead, where each of them represents a fixed number of particles. Macroparticles move just like the particle they represent, but with different values of charge and mass. Both the charge and the mass of macroparticles are w_m times as large as the charge and the mass they represent. The ratio of charge to mass stays the same, thus from Lorentz equation, Eq. (1), the trajectory of the macroparticles would be similar to the smaller particles they represent. However, since the charges are different, the electric fields obtained from Coulomb equation would also be different. The result will mimic particle-to-particle interactions between a larger number of particles.

Electric interactions between particles can be calculated directly. For instance, assuming there are N simulated macroparticles, for i^{th} particle, the resultant force is given by Eq. (6).

$$\vec{F}_i = \sum_{j\neq i}^{N} \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{\left|\vec{x}_i - \vec{x}_j\right|^3} \left(\vec{x}_i - \vec{x}_j\right). \tag{6}$$

Note that the force in Eq. (6) is just for a single i^{th} particle. Thus, for a single simulation step, typically $N^2 - 2N$ 3-vector calculations are needed. For a large number of particles, this is computationally very demanding. Therefore, in this simulation, the particle-in-cell method is used to calculate particle-to-particle interactions instead.

Particle-in-cell calculation is done by transforming continuous space into discrete space with a specific mesh [18]. The values of all quantities of interest are defined on the nodes of the meshes. The calculation of electrical interaction itself is done using Poisson equation, Eq. (7).

$$\nabla^2\phi = -\frac{\rho}{\varepsilon_0}\,. \tag{7}$$

The charge density ρ which is defined on each node is calculated using $\sum_i q_i n_i$ where q_i is the charge of each species of the charged particles, and n_i is the macroparticle number density. After charge density is known, the electric potential ϕ defined on each node can be calculated. The electric field can be calculated numerically on each node using $\vec{E} = -\vec{\nabla}\phi$ which is true if relative velocities between particles are small compared to the speed of light. The resulting electric field is then combined with electric and magnetic field from external sources to calculate Lorentz equation, resulting in a new position and velocity for each of macroparticle.

Standard numerical procedure

The equations mentioned in the previous section are calculated numerically with the following procedure: (i) Initial value problems are solved using Boris algorithm, because of its high accuracy in integrating Lorentz equation; (ii) The domain is meshed into structured hexahedral mesh; (iii) Particle number density is calculated on each node using first order scatter algorithm; (iv) Poisson equation is solved using Gauss-Seidel algorithm; (v) Electric field from particle-to-particle interactions is calculated using second-order forward (or backward) difference method for nodes on the boundaries, and first order central difference method for the rest of the nodes; (vi) Electric and magnetic field at the position of each particle are calculated using first order interpolation algorithm; (vii) If a macroparticle steps outside of the domain, the last position of macroparticle within the domain is saved and the particle is deleted; (viii) Irradiation distribution can be calculated by plotting last positions of macroparticles just before they stepped outside the domain.

Note that the external electric and magnetic fields need to be loaded from external files first. The files are generated by other solvers, such as static magnetic solver from CST Studio Suite that will be shown in the next section.

Simulation setup

The simulation was separated into three parts. First, the single particle trajectory simulation was benchmarked using CST particle tracking solver. Second, the emittance of beams with and without particle-to-particle interactions were compared. Particle-to-particle interactions take an incredibly long time to simulate for a finer mesh. Thus, if it turned out that particle-to-particle interactions for the case at hand did not really affect the beam dynamics, as shown by the beam emittance, then simulation without particle-to-particle interactions could be used instead. The last step was to calculate irradiation distribution for two different signal shapes.

Single particle benchmark

The code package developed was benchmarked using the particle tracking solver in CST Studio Suite, which is a professional tool for particle tracking simulation. For this benchmark, only the single particle case was simulated. Both of the code package and the particle tracking solver had an almost identical setup, such as same initial conditions (position and velocity), same simulation domain, and same magnetic field distribution. It must be noted that there are several parameters that cannot be modified in CST, such as the step width of the simulation, the domain meshing, and the interpolation scheme. Even so, as long as the choice of parameters are fine enough, the difference in the scheme will not severely affect the result. An approximately identical result would indicate that both of the tracking part and field interpolation part are accurate enough to be used for a more complex simulation, such as irradiation distribution calculation.

The benchmark parameters used for single particle simulation can be seen in Table 1.

Table 1. Benchmark parameters.

No.	Parameter	Values
1.	Initial velocity	v_y = -2.3×10^8 m/s (directed to y- axis)
2.	Initial position	$\vec{x}$ = (0, 0.14, 0) m
3.	Domain (Box)	$\vec{x}_{min}$ = -(0.23883, 0.13883, 0.14433) m $\vec{x}_{max}$ = (0.23883, 0.19883, 0.14433) m
4.	Domain meshing	n_x = 61 n_y = 31 n_z = 21
5.	Magnet domain	$\vec{x}_{min}$ = -(0.19, 0.118, 0.0955) m $\vec{x}_{max}$ = (0.19, 0.118, 0.0955) m
6.	Magnet domain meshing	n_x = 300 n_y = 186 n_z = 151
7.	Coil current	1 A
8.	Coil number of turns	154

The magnetic field distribution was calculated using CST magnetic solver program and the model is presented in Fig. 2. The magnetic field result was then imported to the scanning horn code.

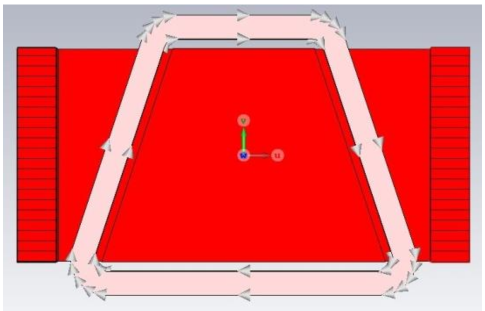

Fig. 2. Cross-sectional image of the scanning horn magnet.

Beam emittance comparison

To see how much particle-to-particle interactions affect beam shape, beam emittance for cases with and without particle-to-particle interactions need to be investigated. One can refer to [19] for the procedure of rms emittance calculation. For this case, it is preferable to exclude external magnetic fields, to make simulation easier. The beam emittance comparison parameters can be seen in Table 2.

Table 2. Beam emittance comparison parameter.

No.	Parameter	Values
1.	Initial velocity (homogenous)	v_y = -2.3×10^8 m/s (directed to y- axis)
2.	Initial position (center of beam)	$\vec{x}_c$ = (0, 0.14, 0) m
3.	Domain (Box)	$\vec{x}_{min}$ = -(0.19, 0.13883, 0.0955) m $\vec{x}_{max}$ = (0.19, 0.14883, 0.0955) m
4.	Domain meshing	n_x = 101 n_y = 41 n_z = 51
5.	Beam length	2.3 cm
6.	Beam initial radius	2 cm
7.	Beam current	50 mA 1 A 50 A

Three different values of beam current were used in this comparison, to see how high the current needs to be to cause beam emittance to significantly diverge from the case without particle-to-particle interactions.

Irradiation distribution simulation

After it is decided whether particle-to-particle interactions have a significant effect on beam emittance or not, the irradiation simulation can be carried out. A beam of reasonable current and initial conditions affected by external scanning magnet was simulated. When some of the particles on the beam stepped outside the domain, their final positions were recorded, with the domain being the scanning horn. After a reasonable duration has passed (at least a half of period of magnetic oscillation), all of the recorded final positions are compiled and then plotted. Several simulation parameters can be varied, such as magnetic field strength, signal shape, or particle initial condition, to obtain the best outcome. To make this paper concise, however, only signal variation is considered. Simulation parameters for irradiation distribution simulations are presented in Table 3.

Table 3. Irradiation distribution parameter.

No.	Parameter	Values
1.	Initial velocity (homogenous)	v_y = -2.3×10^8 m/s
2.	Initial position (center of beam)	$\vec{x}_c$ = (0, .0.14, 0) m
3.	Domain (Box)	$\vec{x}_{min}$ = (-0.19, -0.13883, -0.0955) m $\vec{x}_{max}$ = (0.19, 0.14883, 0.0955) m
4.	Domain meshing	n_x = 101 n_y = 41 n_z = 51
5.	Magnet frequency	50 kHz
6.	Magnet domain (box)	$\vec{x}_{min}$ = (-0.19, -0.118, -0.0955) m $\vec{x}_{max}$ = (0.19, 0.118, 0.0955) m
7.	Initial beam radius	2 cm
8.	Beam current	50 mA
9.	Coil current	1 A
10.	Coil number of turns	154

Note that the domain only covers the scanning horn. This means that the plot was based on the last position of particles just before they stepped outside of the scanning horn. The plot was not made on the irradiated sample itself, which would require scattering calculations when electrons hit the titanium foil when they stepped out of the scanning horn.

RESULTS AND DISCUSSION

There are several sets of results that are going to be presented here. They are the benchmark results, the emittance comparison results, and the irradiation results.

Benchmark results

Figure 3 shows the benchmark results on the position of a single particle during simulation.

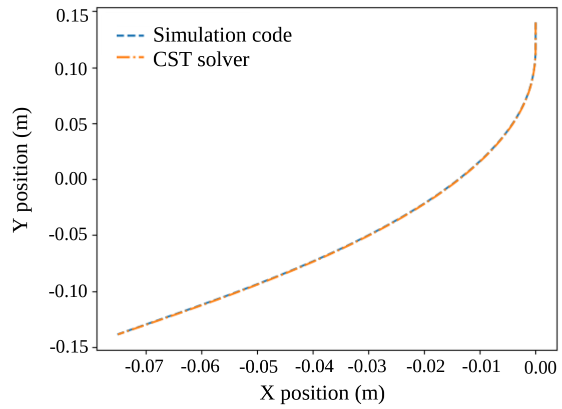

Fig. 3. Comparison of particle position using CST and the scanning horn simulation code.

From Fig. 3, it can be seen that the particle trajectory obtained from the scanning horn simulation code package is approximately identical to the particle trajectory obtained from CST. However, it is not completely identical; by zooming in to one end of the trajectory, difference of particle positions in the two simulations were observed. It is presented in Fig. 4.

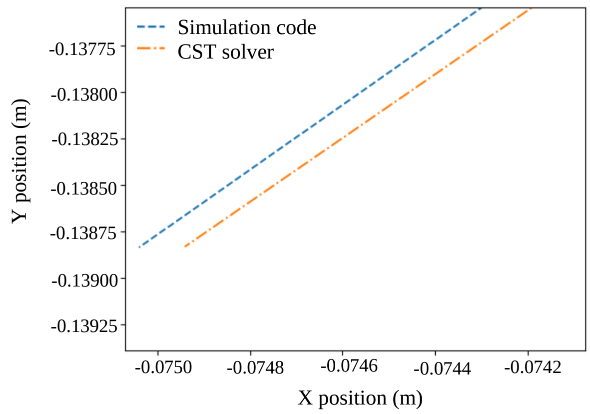

Fig. 4. Comparison of particle position using CST and the scanning horn simulation code (zoomed in).

It is clear that the trajectories do not completely coincide with each other. The difference on the final position is approximately 0.13 %, which can be attributed to the fact that several parameters in CST particle tracking solver are not easily tunable. This applies, for instance, to the step width of the particle trajectory integrator. Nevertheless, the difference is minute and it can be said that the trajectories are identical. Additionally, the step width of integrator CST cannot be set explicitly, thus making the benchmark not have exactly the same parameters.

The identical results mean that, for the same simulation setup, if CST Studio Suite has a solver that is able to calculate irradiation distribution of a scanning horn with a time-varying magnetic field that has a specific signal shape, then the same result would be reproduced. Since the current version of CST Studio Suite does not have this capability (especially the part on the time varying external field with an arbitrary signal shape), then the single particle tracking is good enough to be used as benchmark.

Beam emittance results

In this subsection, the beam normalized emittances for several cases are presented. The results are shown in Figs. 5(a)-(d).

One of the emittances is calculated without particle-to-particle interactions, to see whether other cases diverge significantly from this case or not. It is clear that in the case without particle-to-particle interactions, all of the particle on the beam still retains their initial velocity, no transversal velocities emerge. For plausible values of beam current, such as 50 mA, it can be seen that transversal velocities start to emerge. The emittance shows that the beam is not focused at all, as expected (no focusing device involved). A particle with positive deviation from the center acquires positive velocity and vice versa.

Nevertheless, the velocities are not high enough that the beam really diverges from its original shape during the simulation period (from when the particles are spawned until when the beam stepped outside the domain). This is also true for a larger values of beam current such as for 1-A case. A current that high is really hard to produce in a laboratory, especially for an electron beam machine, and thus is only considered for theoretical curiosity. A more extreme case was also considered, where a 50-A beam current is injected to the simulation domain. For this case, it can be seen that beam divergence is still relatively small but significant. This example was only used to verify that a higher beam current would make the electric repulsion stronger, which turned out to be the case.

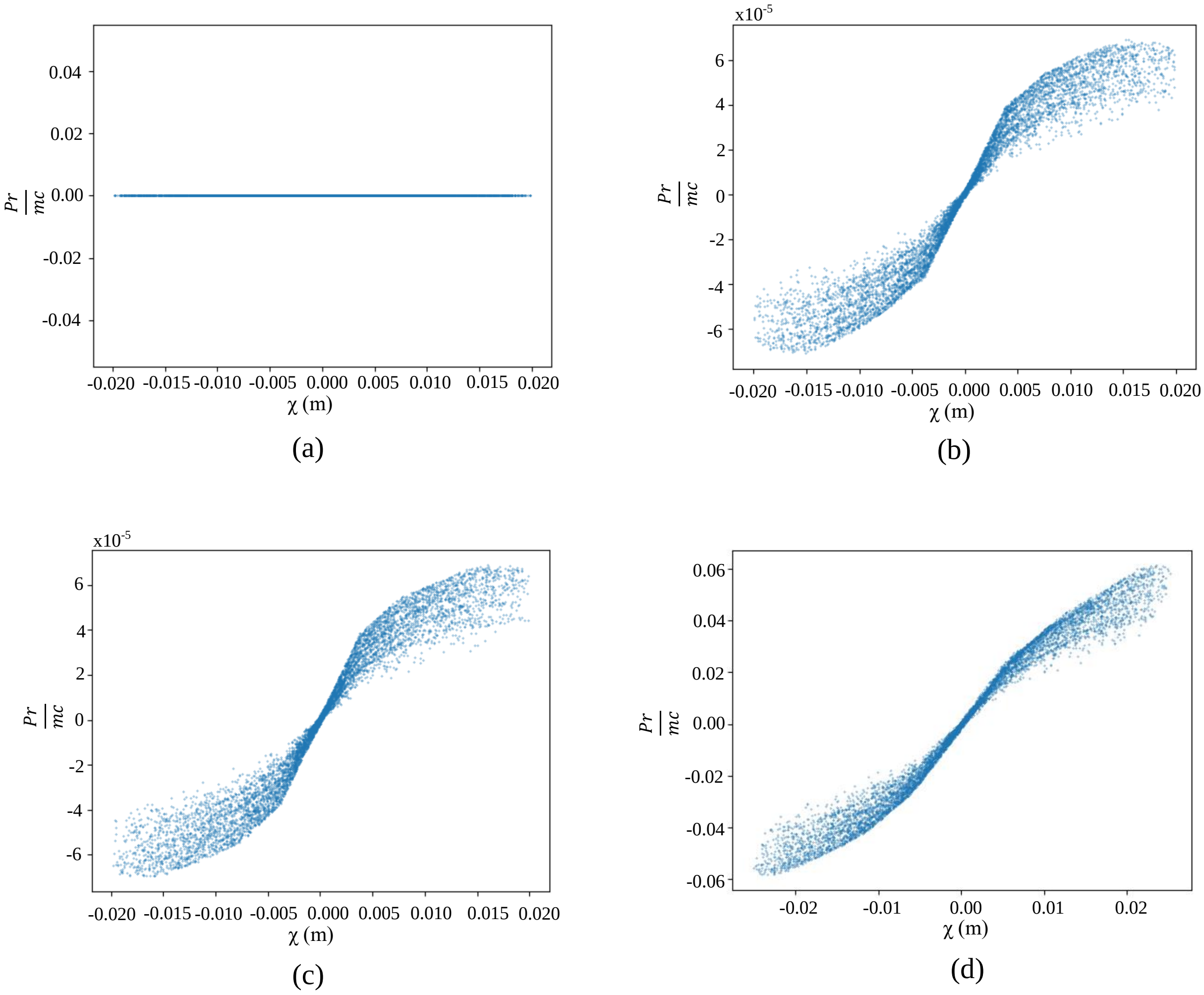

Fig. 5. Normalized emittance for (a) beam without particle-to-particle interactions; (b) 50 mA beam current; (c) 1 A beam current; (d) 50 A beam current.

The emittance results indicate that particle-to-particle interactions (in this case only electric repulsion) do not really matter that much for the parameters that are going to be used in irradiation simulation and for the problem that is going to be solved (determining irradiation distribution). Thus, particle-to-particle interactions will not be employed in calculating the irradiation distribution, since the results will predictably be undistinguishable from the without-interaction case, while the computational cost will skyrocket.

Irradiation simulation results

As can be seen from previous results, particle-to-particle interactions can be neglected for a reasonable value of beam current. This will significantly reduce simulation duration without losing much accuracy. Electron simulations would generally need simulation step widths ranging from dt = 10-13 s to dt = 10-11 s to give an accurate trajectory, based on electron plasma frequency [20]. For a magnetic oscillation with a frequency of 50 kHz, one million iterations are needed for the electron beam to cover the whole irradiated object. Thus, for scanning horn simulation, particle-to-particle interactions should only be used if it is found that omitting that procedure will significantly alter the result. Using Intel's i7-10700 CPU without multithreading, the simulation took about $t \approx 10\,000$ seconds. Figure 6 shows the beam trajectory plot for using parameters mentioned in Table 3.

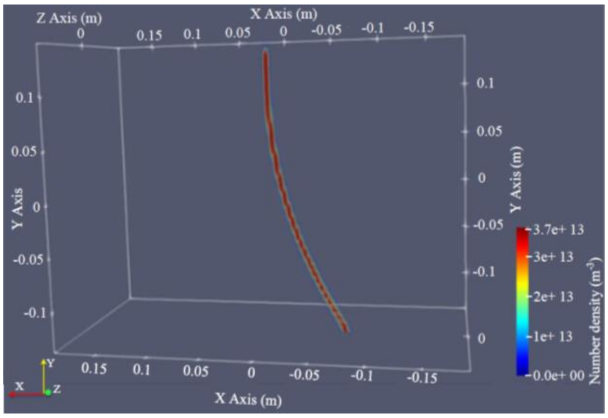

Fig. 6. Beam trajectory for scanning horn. The color indicates the number density of particles, with red means the densest region.

The irradiation distributions for triangular and sinusoidal signals are given in Fig. 7.

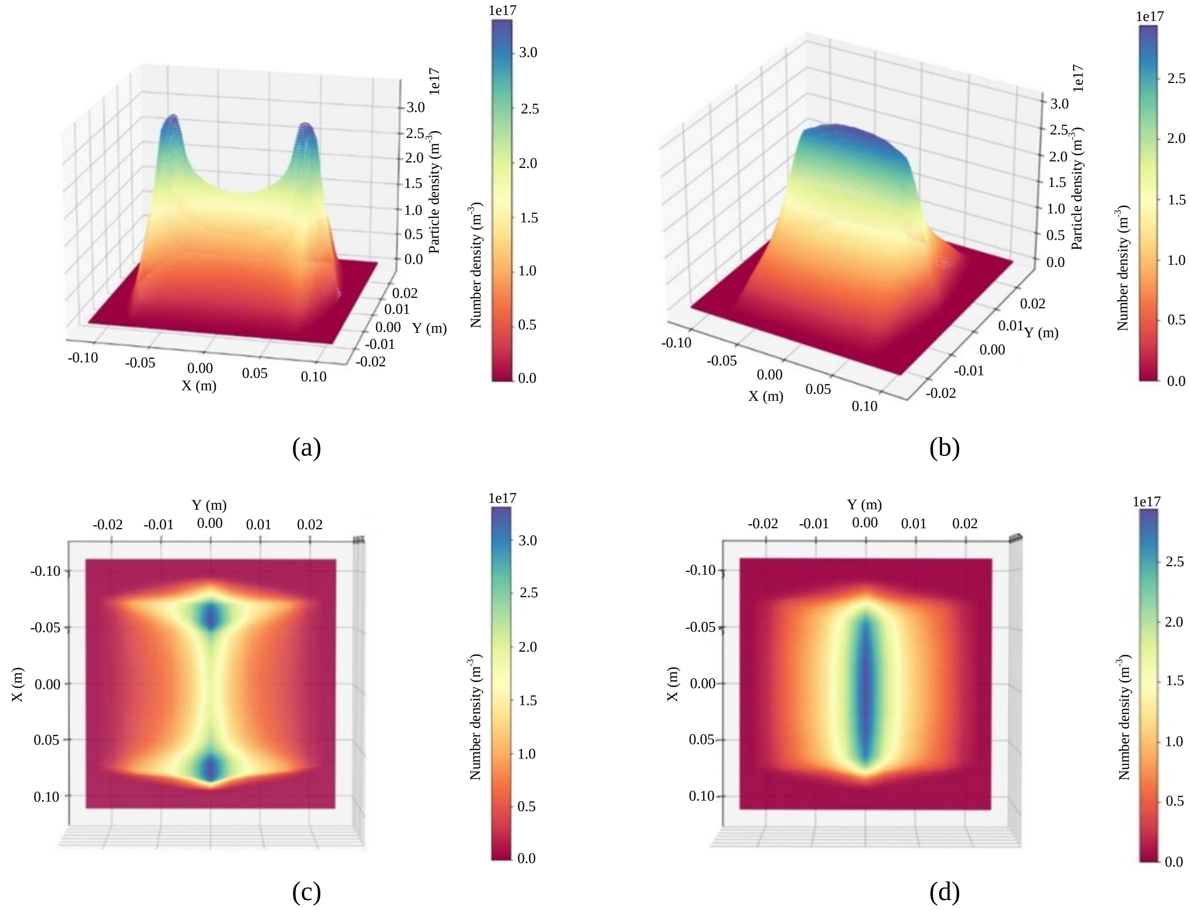

Fig. 7. Irradiation distribution results. The color indicates the number density of particles, with blue means the most irradiated region (a) irradiation distribution for sinusoidal signal; (b) irradiation distribution for triangular signal; (c) and (d) the irradiation distribution as seen from x-y plane perspective for (c) sinusoidal and (d) triangular signal, respectively.

In Fig. 7, different irradiation distributions are shown in different colors. A blueish areas indicates that it is being hit more by electrons, while a reddish area indicates that it is rarely hit by electrons. Thus, the more irradiated the area is, the bluer the area becomes. A good set of irradiation parameters will give a more even irradiation distribution. Here, the choice of parameters mimics the parameters of the currently operational electron beam machine at the Center for Accelerator Science and Technology, except for the beam profile, since the beam profile of the electron beam machine is not measured yet. It is clear that further optimization to get a more evenly spread irradiation distribution is possible.

From Fig. 7, it is clear that different signal shapes will produce different irradiation results. It can be seen that a triangular shape gives a more evenly distributed irradiation compared to a sinusoidal signal. Most the irradiation for sinusoidal signal is concentrated in both ends of irradiated area. This happens because when the beam reaches the ends of the irradiated area, the rate of change of magnetic amplitude is much slower compared to when the beam is at the middle of irradiated area (when the phase is equal to zero or π). Thus, the beam will stay longer near the ends of the irradiated area.

Figure 7 also shows that triangular signal did not give a completely even distribution of irradiation. This means that there is a possibility that there are other shapes of signal out there that will give a better distribution of irradiation. However, this is beyond the scope of this paper and will be further investigated in the future. It also needs to be noted that the irradiation distribution here is calculated on the surface of the titanium foil as shown in diagram. To attain a more accurate result, a Monte Carlo scattering simulation might need to be undertaken. This improvement is also planned for the future refinement of this simulation code. However, it is straightforward that an uneven distribution in the foil will also give uneven distribution on irradiated sample, and vice versa.

CONCLUSION

A code package designed to simulate particle trajectories in a scanning horn of an electron beam has been successfully benchmarked. The code package can be used to estimate the irradiation distribution of a sample, for a set of parameters. It is evident that a triangular-shaped signal gives a much more evenly distributed irradiation compared to the result obtained from a sinusoidal signal.

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AUTHOR CONTRIBUTION

All of the author equally contributed as the main contributor of this paper. All authors read and approved the final version of the paper.

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