

## Ray-Tracing Electrons through a Magnetic Lens

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The primary way to understand the trajectory of electrons through a Transmission Electron Microscope (TEM) is through numerical ray-tracing. While free resources are available for optical ray-tracing, to the best of the authors' knowledge, no free and open source package exists which enables ray-tracing for electrons through the electromagnetic lenses of a TEM system.

Here we present a simple TEM system with two dipole deflectors and a round lens to focus the electron beam. Using this simulation, we can understand how minor changes to the beam tilt entering the lenses influence the shape of the beam spot on the detector or image plane. We can also change the field strength of a magnetic field and build an understanding of how the tilt of the beam and lens strength affect the shape and position of the electron beam within the TEM. The model presented here is proof of concept for how to build a full ray-tracing simulation for a TEM, incorporating all the lenses and deflectors within the system.

The ability to trace the electrons through the lens system of the TEM enables users to fully understand the path of the electron beam and how the aberrations occur as the electrons propagate through the system.

The ray-tracing simulation is written in python [1] and will be made freely available. For those with a Nvidia graphics card, there is the option of using Cuda-accelerated ray-tracing functions [2], which allow up to thirty-two thousand rays traced simultaneously in real-time as the user changes the adjustable parameters of the lens system.

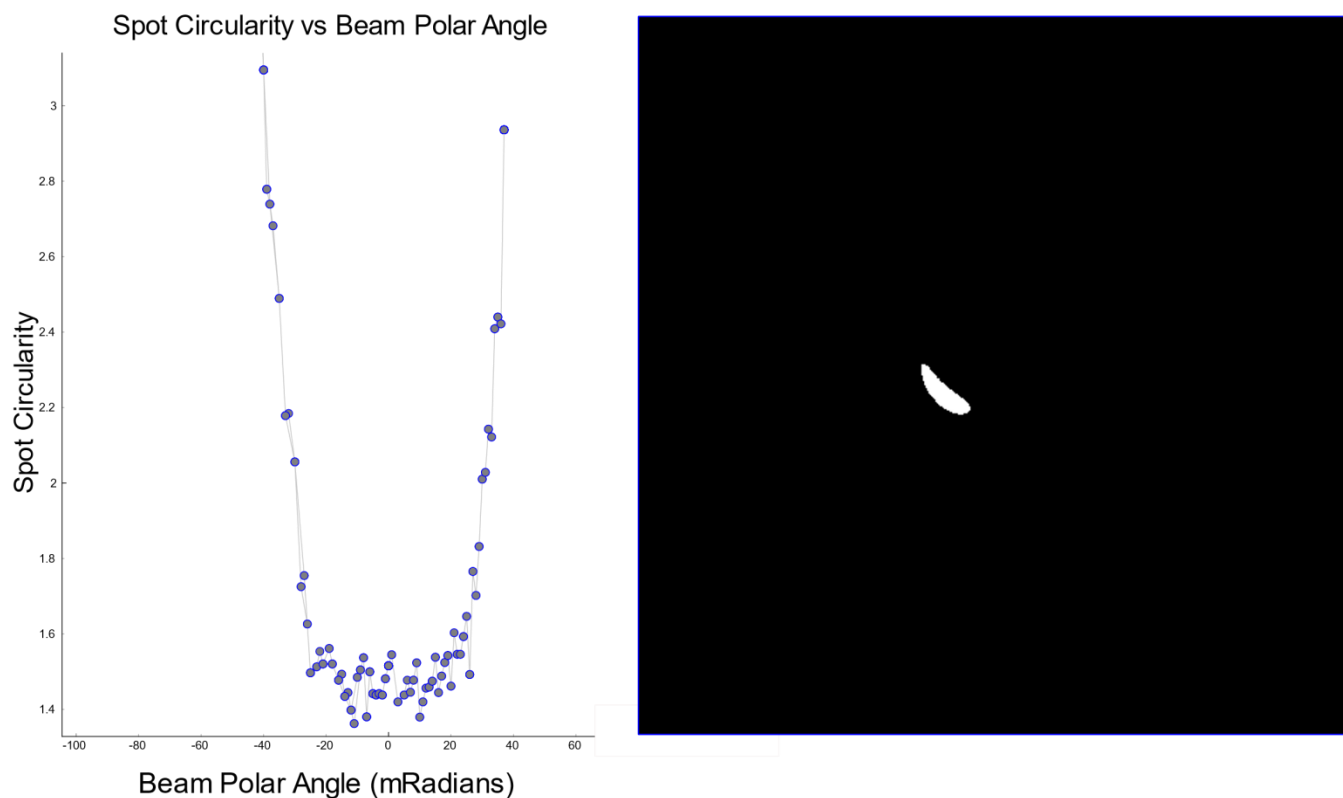
Our software calculates and displays an electron beam spot in real-time, displays a basic 3D model of TEM components, along with electron paths (see Figure 1 and Figure 2), and records spot characteristics associated with the current alignment state via an interactive GUI.

We use two methods to model the magnetic field of a magnetic lens and magnetic multipoles. For a round lens, we calculate the magnetic potential for a specified axial field distribution. To approximate the field of a multipole (dipole, quadrupole etc.), numerically we solve the Biot Savart law [3] for wires arranged in the desired multipole configuration.

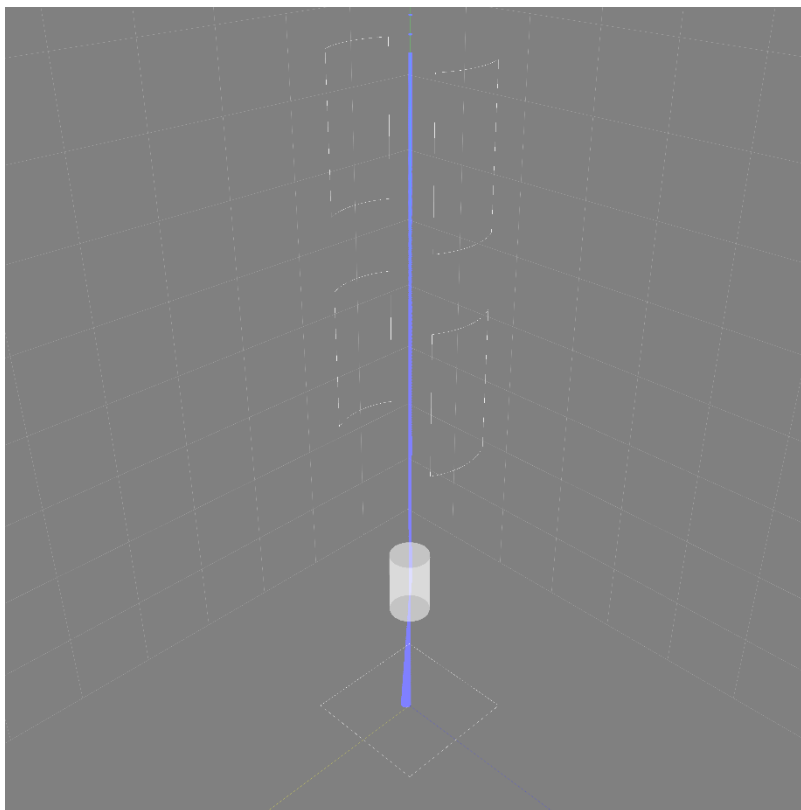
These magnetic fields are then used to solve the Lorentz force numerically [4] and trace electrons in our real time interactive software model created with PyQtgraph [5] This interactive GUI enables a user to

practice alignments such as beam tilt/shift and adjust the magnetic parameters of the model. In addition, spot alignment characteristics such as roundness and position are monitored, which enable an automatic algorithm to complete the pivot point alignment independently.

With this software, our objectives are 2-fold: 1. To create an education platform that enables users to learn the important steps of aligning a TEM without the need to use the instrument, which minimizes the cost of training, and enables more efficient use of resources. 2. Create an environment for the exploration of automated protocols and their applications in the TEM.



**Figure 1.** GUI representation of 4096 electron rays traced through a single lens. Left: Live plot recording spot circularity as a function of the initial polar angle of the beam. Right: Current spot shape on the detector plane after the magnetic lens.



**Figure 2.** 3D model of electron path through two deflectors and a magnetic lens. This 3D model is updated in real time alongside the image of the detector plane.

References:

- [1] G. van Rossum in “Python reference manual”.
- [2] S. Cook in “CUDA programming : a developer’s guide to parallel computing with GPUs”, (Morgan Kaufmann).
- [3] A. J. Mäkinen et al, *J. Appl. Phys.*, vol. 128, p. 063906, (2020), doi: 10.1063/5.0016090.
- [4] M. Szilagyí in “Motion of Charged Particles in Electric and Magnetic Fields”, (Springer US).
- [5] “Welcome to the documentation for pyqtgraph — pyqtgraph 0.12.3 documentation.” <https://pyqtgraph.readthedocs.io/en/latest/index.html> (accessed Feb. 16, 2022).