Predicting **Charged Particle Trajectories**

Simulation helps researchers obtain electromagnetic field solutions for predicting charged particle trajectories in a wide range of industrial, medical and research applications.

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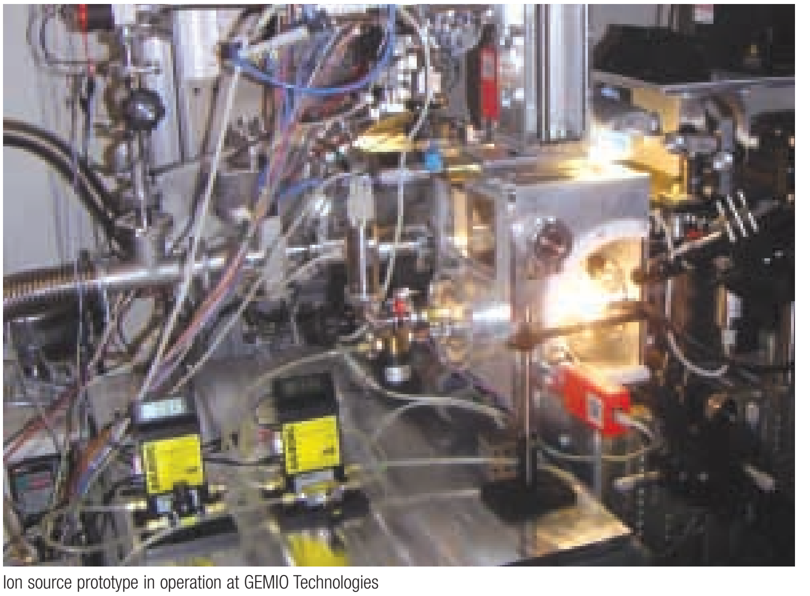
The origins of charged particle optics date back to the mid-1800s, when some of the first studies examined the effects of electric currents in gases, and later when cathode ray tubes were studied. A formal theory of charged particle optics — namely, using electric and magnetic fields to accelerate and guide electrons for imaging applications — was developed in the 1920s, providing the theoretical foundation for the first electron microscopes in the 1930s.

Today, modern applications based on charged particle optics span a wide range of instruments and devices, including electron microscopes, electron-beam lithography machines, vacuum/pressure gauges, x-ray tubes, free electron lasers, electron tubes and related radio-frequency (RF) devices, field emitter–based displays, high-power electron beam guns, ion traps, mass spectrometers, and ion sources. Such instruments are indispensable for building and testing the latest integrated circuit chips, creating advanced medical imaging equipment, and finding molecular biomarkers for the prediction and treatment of human diseases. Specifically, due to the advent of ion sources for biomolecules and the resulting increased importance of mass spectrometry in life science, the field of charged particle optics is experiencing a healthy rejuvenation [1].

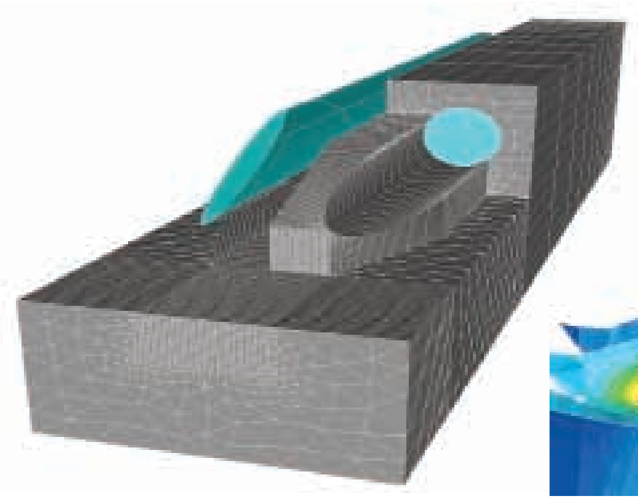
A growing number of these applications are based on ion optics using particles much larger and heavier than electrons. Therefore, researchers must account for far greater mass-to-charge ratios that exceed the ratio relevant for electron optics by factors ranging from approximately 2,000 for hydrogen ions (protons), more than 10^8 for very large macromolecules. Regardless of the types of charged particles used, accurate solutions for the electric and electromagnetic fields in these applications are of critical importance [2].



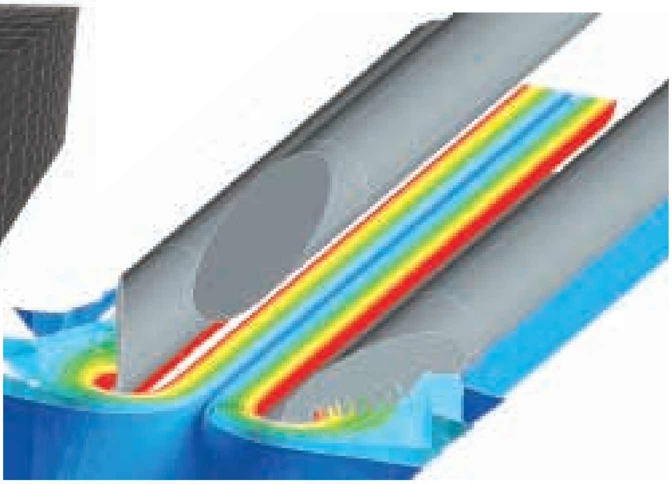
Ion source prototype in operation at GEMIO Technologies

For most conventional configurations in charged particle optics, analytical mathematical expressions have been developed for determining the fields and particle trajectories. For example, in an electric mirror time-of-flight configuration (also referred to as reflectron TOF), the trajectory of an ion has an analytical mathematical solution. These mathematical expressions are extremely valuable in understanding how variations in key parameters affect the operation of such devices.

Simulations based on finite element analysis (FEA) may be used in cases in which no exact, or even approximate, mathematical expression exists, or when additional physical effects acting on the particles or the device itself must be taken into account. Numerical simulation is also useful in accounting for imperfections due to variations in manufacturing, thermal expansion, mechanical stress, or aging of field-generating components, such as



Finite element model of quadrupole tip region



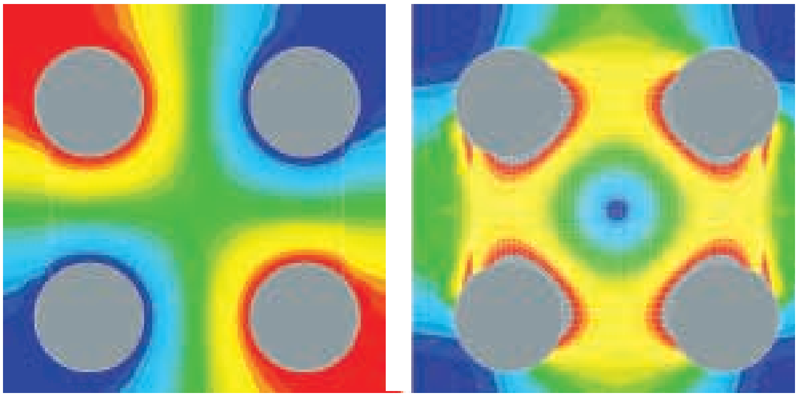
Isosurface plots of electric field

electrodes, isolators and current-carrying conductors. Such variations usually break certain symmetries in the device or particular spatial ratios that are frequently assumed in the mathematical expression. In these cases, simulation is usually the only option that can provide more depth of understanding for the situation. For many practical problems, the electromagnetic simulation capabilities provide field solutions for extremely complicated geometries with sufficiently high accuracy.

Charged particle trajectory simulations based on these field solutions need to satisfy different and frequently conflicting requirements. The experienced computational physicist, therefore, must carefully balance these demands and choose the appropriate numerical methods and techniques for the simulation.

Among such constraints are:

- Degree of spatial accuracy of the final position of a trajectory
- Long-term stability of a solution (trajectory)
- Execution speed of the computation (the ability to simulate a very large number of trajectories using techniques such as Monte Carlo simulation)
- Degree of smoothness of a trajectory [3]
- Relevance of coupled effects (particle-field coupling such as space charge, induced currents, etc.) and other more advanced effects, usually relevant only in high-energy physics applications



Electric potential (left) and electric field magnitude (right) for a cross section through the quadrupole

In one recent study of a complex trajectory problem, physicists at GEMIO Technologies, a company that utilizes advanced numerical methods to design ion optical devices for life science applications, used ANSYS Emag capabilities for the simulation of an RF quadrupole, a system of four parallel rods that can act as a guide or filter for charged particles. Very good mathematical approximations for the electric field inside an infinitely long quadrupole can be developed, and stability conditions for trajectories can be derived [4]. However, no accurate mathematical relationships are available characterizing the electric field and particle behavior at the tip of a quadrupole. As a result, researchers are heavily dependent on simulation at that critical location.

In this study, first the researchers created a finite element model representing the 3-D geometry of the quadrupole tip region. They used the simulation results to generate 3-D isosurface plots of the electric field resulting from applying various potentials to the rods. The simulation also provided information about the electric potential and magnitude of the electric field in a cross section of the quadrupole. The numerical values obtained from the simulation solution are remarkably accurate and require little numerical effort while using fairly coarse discretization. At the axis of the quadrupole, the predicted potential has a relative error of less than 10^{-8}, while that of the predicted electric field is only 10^{-6} relative to the maximum value inside the quadrupole.

A particular advantage to having a numerical simulation model is the ability to test the response to certain conditions that are, effectively, impossible to study in most experimental setups. In addition, such ideal conditions provide a method to test the accuracy of the simulation, because frequently the expected result is known. In the case of an RF quadrupole, for example, a particle that is perfectly orthogonally injected into the multipole with certain suitable initial conditions (location, speed and timing) will remain on a stable, periodic trajectory forever. A numerical simulator must be able to replicate such particle capture effects and provide stable long-term solutions. This is somewhat comparable to orbital injection of a satellite around a planet — although gravitational forces are only attractive and obviously static in nature, whereas charged particle capture in multipoles requires RF electric fields, and the resulting trajectories are of more complicated shapes compared with the elliptical orbits of satellites.

Based on certain values for these conditions, the GEMIO team computed the trajectory of an orthogonally injected particle. For this analysis, the quadrupole operates at RF frequencies on the order of 1 MHz with potentials of several hundred volts. Researchers executed the computation in an external module written in FORTRAN™ and based on the field solutions obtained with ANSYS Emag technology. They then imported the resulting data back into software from ANSYS for post-processing.

The particle trajectory simulation indicated that the particle remains on a nontrivial but stable trajectory in a plane orthogonal to the quadrupole axis for a few orbits but, in some rare instances, is suddenly ejected from the plane. From a slightly different angle, the simulation indicated tetrahedrons of nodes in which disturbances of the trajectories occur. Following careful investigation of this unexpected effect, the researchers determined that it was caused by an unusual numerical problem in the external FORTRAN module that executed the trajectory integration. After the team corrected this numerical issue, the effect no longer occurred, and subsequently the team has used this approach to obtain stable trajectories for at least 10^5 RF cycles.

As this study demonstrates, ANSYS Emag simulation features are capable of providing electric and magnetic field solutions with very high accuracy, making these solutions suitable as a basis for different types of charged particle trajectory simulations in a wide range of applications. As always, the numerical behavior of such tools must be carefully evaluated and tested to gain trust in the results. If executed correctly, charged particle simulations provide a valuable solution that substantially reduces physical testing in the development of these systems. Furthermore, simulation continues to represent the only effective method to study configurations for which no analytical mathematical expressions are available. ■

Dr. Andreas Hieke is an internationally recognized expert in computational physics and the founder of GEMIO Technologies. The author welcomes reader feedback and may be contacted at ahi@ieee.org or ah@gemiotech.com.

References

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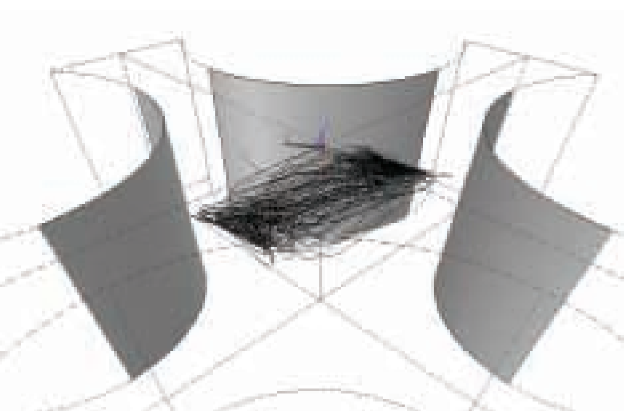
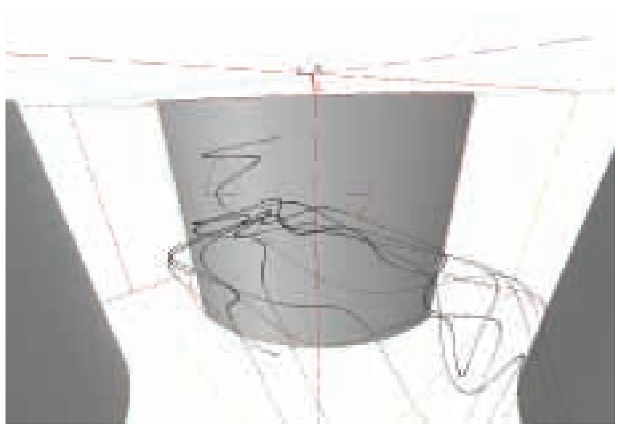


Particle trajectory as predicted based on ANSYS Emag *E* field solutions



Tetrahedrons indicate nodes in which disturbances of trajectories occur.