Efficient computation of electromagnetic fields for round lenses in charged particle optics

Timothy R. Groves, University at Albany, SUNY

Numerical simulation of charged particle optics systems can be regarded as a two-step process consisting of (1) computation of the electromagnetic fields, and (2) computation of the resulting particle trajectories. These computations are based on analytical theory which is well-described in textbooks [1-3]. This theory forms the basis of computer simulation for optical properties.

Computing the electromagnetic fields for arbitrary geometry in four-dimensional space-time is challenging. Generally, an efficient computation is one for which the required accuracy is achieved with relatively few computation steps. A large class of useful systems have static fields and high spatial symmetry. For example, round lenses have axial symmetry of the electrodes or pole pieces. Consequently, the field components can be specified in cylindrical coordinates by two spatial dimensions, radial and axial. Low dimensionality generally enables efficient computation.

The purpose of this study is to describe a novel method for the round lens field computation whose input condition is the scalar potential (electric or magnetic) along a single curve which traces out the boundary surface in a meridional plane. Effectively the problem is reduced to one dimension, thereby optimizing computational efficiency. The method is a variant of the surface charge density approach [4]. The known potential on the boundary is given by the line integral involving the surface charge density along the boundary curve as follows:

$$\Phi(\rho_i, z_i) = \frac{1}{\pi\epsilon_0} \oint ds_j \, \rho_j \, \sigma(\rho_j, z_j) \, [\, (z_i - z_j)^2 + (\rho_i + \rho_j)^2 \,]^{-1/2} \, K(m_{ij}),$$

where

$$m_{ij} = \frac{4\rho_i \rho_j}{(z_i - z_j)^2 + (\rho_i + \rho_j)^2},$$

where σ is the surface charge density, and K is the complete elliptic function of the first kind. The boundary surface is discretized into n annular segments and the equation solved for σ by Gauss-Jordan elimination for the matrix inversion. The resulting potential on the symmetry axis is

$$\Phi(z) = \frac{1}{4\pi\epsilon_0} \sum_{k=1}^{n} \frac{\Delta q_k}{[\, (z - z_k)^2 + \rho_k^2 \,]^{1/2}}$$

where

$$\Delta q_j \;=\; \sigma_j \cdot (2\pi\rho_j) \, \Delta s_j$$

is the charge on the j^{th} annular segment. This form for Φ is easily differentiated to high order with respect to the axial coordinate z, enabling high accuracy for points close to the optic axis. We show that the axial potential and its even axial derivatives through 8^{th} order agree to within a few parts in 10^8 with the analytic solution for the test case consisting of two coaxial cylinders at different potentials. This represents an exceptionally efficient computational approach.

[1] Hawkes P.W. and Kasper E. 1996, *Principles of Electron Optics*, Vols. 1-3, Elsevier (present), Academic Press (original).

[2] Rose H. 2013, *Geometrical Charged Particle Optics*, Second edition, Springer Series in Optical Sciences, ISBN-13: 978-3642321184.

[3] Groves T.R. 2014, *Charged Particle Optics Theory, an Introduction*, CRC Press, ISBN-13: 978-1482229943.

[4] Lencova B, Lenc M. 1984, The computation of open electron lenses by coupled finite element and boundary integral methods, *Optik* Vol. 68, pages 37-60.