Adjoint Optimization for Electrostatic Charged Particle Lens in 3D

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We present a method for efficient calculation of the design sensitivities of electrostatic charged particle lensing systems, based on adjoint design sensitivity analysis[1]. Electrostatic lenses obey a nonlinear, coupled system comprising the Laplace equation for the electric potential and an equation of motion based on Lorentz force law and Newton's second law. These governing equations can rarely be solved together analytically, so computation has been essential for engineering devices such as electron microscopes and mass spectrometers. Moreover, systems with many designable parameters (e.g. dimensions and applied voltages) are computationally burdensome to optimize. However, to improve the device design one would desire to know how its performance changes under perturbations to its shape, dimensions, and operating conditions. This design sensitivity can be obtained by simulating each possible perturbed device in turn, a computationally costly approach requiring at least one extra calculation per design parameter. Adjoint design sensitivity analysis is a method to obtain all of the design sensitivities at once for a nearly-fixed computational cost[1] and thus enables rapid optimization of complex systems.

We demonstrate the applicability of this method to electron optics by deriving the framework and employing the method for the tuning of a three element Einzel lens to focus electrons at oblique angles (Fig. 1). For this, we use a commercial finite-element simulator (COMSOL Multiphysics) to obtain the fields, and simulate the particle trajectories employing an in-house custom particle dynamics simulator. To validate the derived method, we demonstrate system gradients and optimization results. For parameters to which the system is sensitive, the gradients obtained using finite differentiation and the dual system are in excellent agreement with up to 5% error (Fig. 2). Due to the computational advantage of the adjoint method, we can optimize the system for 16 parameters simultaneously and the desired focal spot of the Einzel lens decreased significantly (by three orders of magnitude, Fig.3). This proves the usability of the adjoint method for such a design problem. This is, to our best knowledge, the first published demonstration of the adjoint method for such a system.

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[1] Giles, M. B., & Pierce, N. A. (2000). An introduction to the adjoint approach to design. *Flow, turbulence and combustion*, 65(3-4), 393-415.

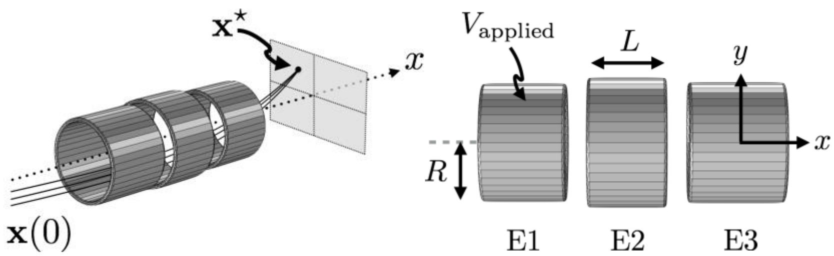

Figure 1: Geometry and Problem description: Schematic of focusing by three-element Einzel lens and overview of changeable parameters. The desired focal point is at x*. The optical axis of the system is x. Three electron paths are shown entering the lens from the left and focusing to x*. The length L, Voltage $V_{applied}$, radius R and the position in y, x and z of each electrode E_{1-3} are the design parameters of the optimization problem.

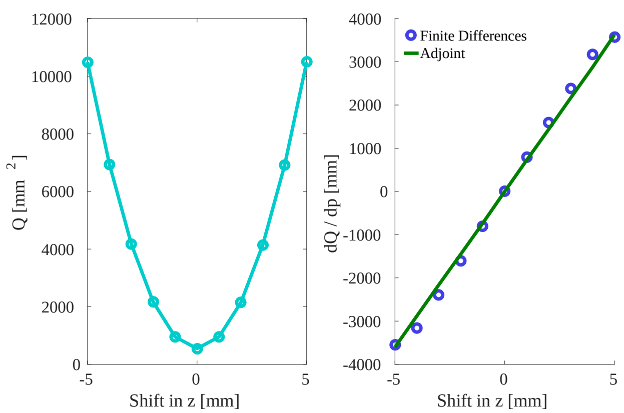

Figure 2: Sensitivity analysis: Sensitivity of objective function (spot size) Q to shift of the center electrode position. The system is strongly sensitive to this parameter and the finite difference and adjoint results agree.

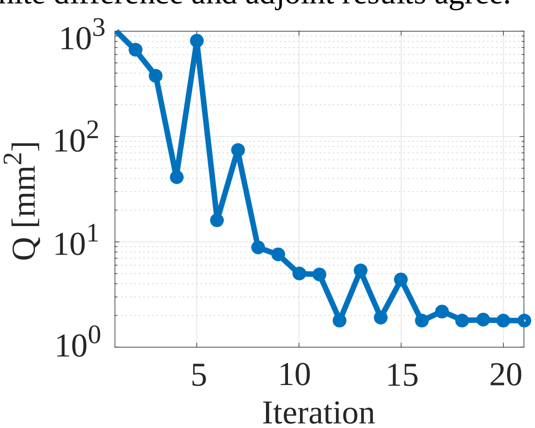

Figure 3: Optimization process: The first demonstrated optimization: Improvement of Q with the change of the design parameters for 21 iterations. The value of Q changes around 3 orders of magnitude.