Achieving highly accurate adjoint sensitivities for charged particle optics: design, optimization and tolerancing

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We introduce the discrete adjoint method for calculation of design sensitivities of charged particle optical devices. Adjoint methods have revolutionized aeronautical, structural and photonic design in recent decades by calculating sensitivities of design performance to perturbations of all points on surfaces and in volumes at low computational cost.[1] We derived and implemented a "discrete" adjoint method using a custom-built electrostatic finite-element method and charged particle dynamics simulator, circumventing the numerical error of "continuous" adjoint methods built with existing simulation software. We calculate the sensitivity of charged particle trajectories to shape perturbations at each point on electrode surfaces. These sensitivities can be directly used for optimization and tolerancing.

Sensitivity analysis is key to design optimization, and the choice of sensitivity method can be crucial. Adjoint methods efficiently calculate the sensitivity of an objective function, e.g. total aberration, to electrode shapes, source properties or applied voltages. Continuous adjoint methods, often implemented using off-the-shelf simulation tools, discretize a physical system's governing equations to calculate the objective function, then separately discretize the physical system's derivatives to calculate the objective function's sensitivity. Because the objective function and its sensitivity are approximated separately, the calculated sensitivity differs from the sensitivity of the calculated objective function. This discrepancy can prevent design optimization algorithms from finding an optimal design. In contrast, discrete adjoint methods differentiate the discretized governing equations to calculate the objective function's sensitivity exactly. To obtain the exact calculated sensitivity we implemented a discrete adjoint system using a custom-built finite-element adjoint Poisson solver and adjoint charged-particle dynamics integrator. Our sensitivities are accurate to less than 1% error (*Fig. 3*). These can be used for optimizations, to determine manufacturing tolerances and to obtain insight into design considerations.

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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.

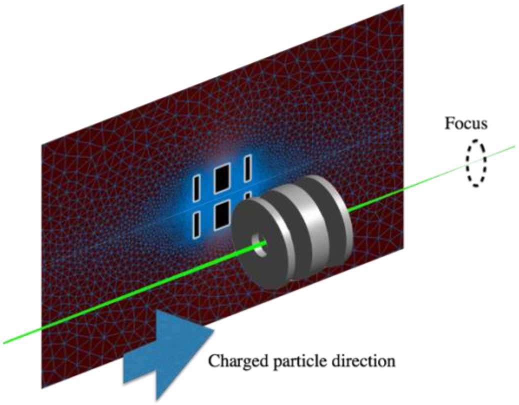

Figure 1: Geometry, Mesh and Particle Trajectories: Schematic of the axial-symmetric Einzel lens with particle trajectories and finite-element mesh. The potential is calculated using a 2D-cylindrical FEM.

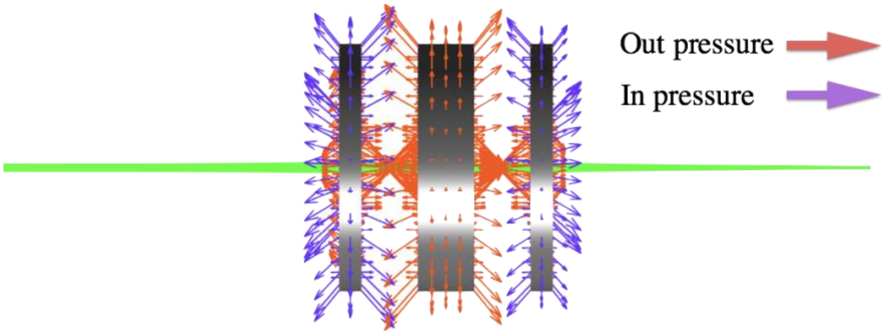

Figure 2: Resulting Design Sensitivities: Einzel lens elements, particle trajectories and arrows showing the sensitivity of the objective function to surface perturbations. Orange arrows indicate outward sensitivity pressure and purple arrows indicate inward pressure.

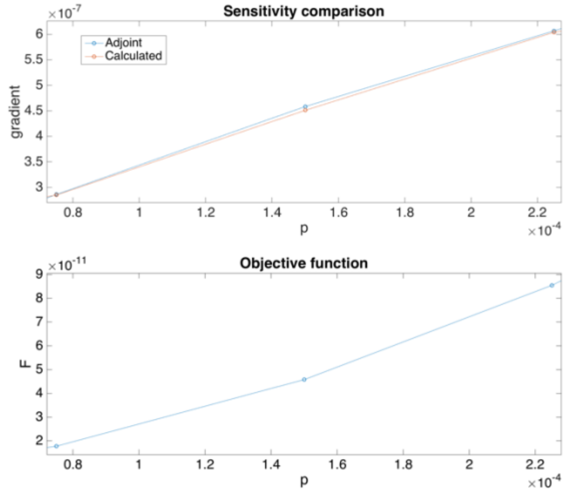

Figure 3: Test of Gradient Accuracy: Comparison of a finite-differenced gradient and the adjoint gradient for the total system optimization. Error is less than 1%.