Shape Optimization of Electrostatic Ion Beam Systems with a 3D Adjoint Boundary Element Method

L.T. Neustock, L. Hesselink
Department of Electrical Engineering, Stanford University, Stanford, CA 94305
larstn@stanford.edu

For decades, researchers have used simulations and their underlying numerical models as foundational tools for designing and studying ion beam systems. While these models can predict the behavior of a design at hand, finding a more optimal design can only be achieved by varying design parameters manually and rerunning the updated simulation. Such an approach makes a problem with many design parameters intractable as the required computational effort grows exponentially with the number of design parameters.

The adjoint variable approach can overcome this issue.[1] By only solving one additional linear system, the adjoint system, this approach calculates the gradient of a function specifying the success criterion of a design for any large number of design parameters at once. As a result, the adjoint system's computational complexity is independent of the number of design parameters.

In our earlier work, we have shown the ability of an adjoint-based tool based on the Finite-Element Method (FEM) to design ion-optical lens systems restricted to 2D or cylindrical symmetry.[1] Yet, FEM-based systems are often not accurate enough compared to Boundary-Element Method (BEM) systems used as the gold standard for highly sensitive ion optics simulation (e.g., in SimIon).[2]
Here, we show – to the best of our knowledge – the first implementation of a 3D-mesh adjoint design tool based on the BEM method for electrostatics and the Störmer-Verlet-Method for particle trajectories simulations. We compare BEM- and FEM-based design tools and show optimized designs. *Fig.2* shows an illustrative optimization. In this example, we minimize the potential at the center of an icosphere with a voltage distribution $V(x) = \frac{1}{4\pi\sqrt{(x-0.9)^2+y^2+z^2}}$. The device's shape is defined by 492 design parameters. The potential was reduced more than 3.5-fold in 96 iterations. Compared to manual optimization, the presented tool achieves a more than 28,000-fold reduction in computational cost. Therefore, the tool paves the way for comprehensive computer-aided design for ion optical devices as well as quantum computing hardware in 3D. Such a design technology has galvanized design and innovation in fields like aeronautics or photonics.

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1 Neustock, Lars Thorben, Paul C. Hansen, Zachary E. Russell, and Lambertus Hesselink. "inverse Design tool for ion optical Devices using the Adjoint Variable Method." Scientific Reports 9, no. 1 (2019): 1-12.

2 Singer, Kilian, Ulrich Poschinger, Michael Murphy, Peter Ivanov, Frank Ziesel, Tommaso Calarco, and Ferdinand Schmidt-Kaler. "Colloquium: Trapped ions as quantum bits: Essential numerical tools." Reviews of modern physics 82, no. 3 (2010): 2609.

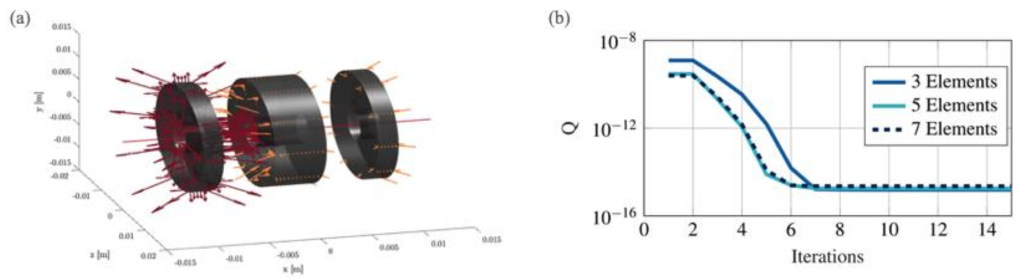

Figure 1: Sensitivity Analysis and Optimization of an Ion Lens System: (a) Illustration of a sensitivity analysis of an ion lens system using our FEM design tool. A sensitivity analysis shows how much the objective function Q would change for a variation of each studied surface point. (b) Spot size of the ion optical lens system throughout an optimization of its shape. *(Both graphs are reproduced from our previous work[3])*

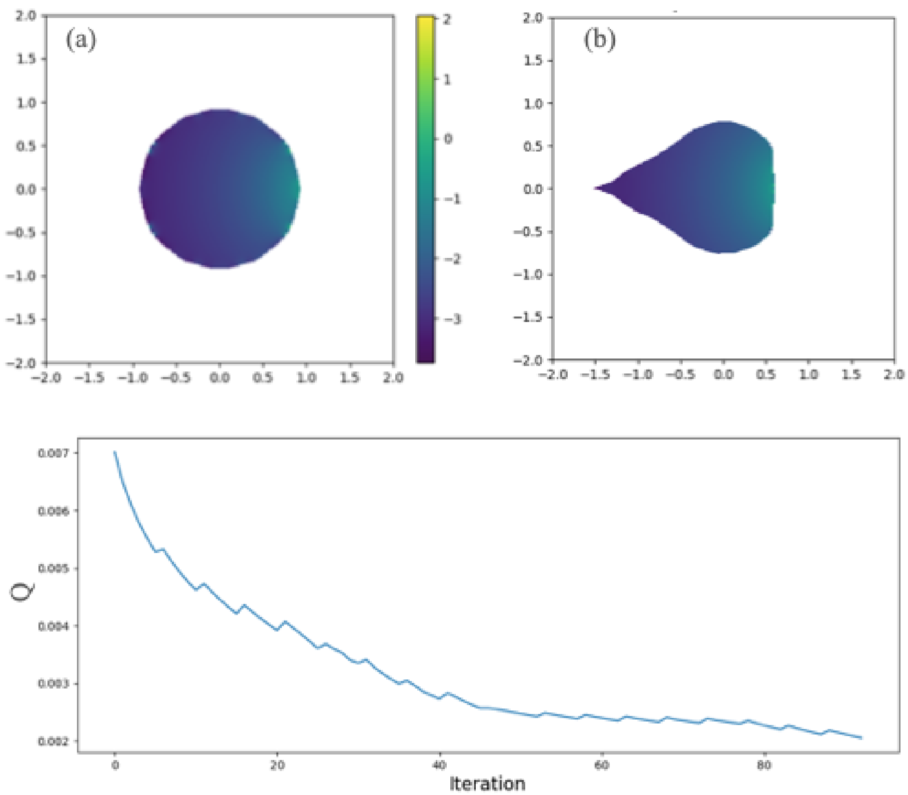

Figure 2: *Optimization of an Interior Laplace Problem*: (a), (b) Initial and Optimized shape. The plots show the *x,y*-plane at *z=0*. Both graphs display the logarithm of the voltage inside the device as well as its shape. (c) Downward trend of the objective function Q, measuring the magnitude of the voltage in the center of the device.

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[3] Neustock, Lars Thorben, Paul C. Hansen, Zachary E. Russell, and Lambertus Hesselink. "inverse Design tool for ion optical Devices using the Adjoint Variable Method." Scientific Reports 9, no. 1 (2019): 1-12.