Advanced optimization with SIMION for charged particle optics design and development

H. Q. Hoang, R. Pureti, K. Huber
Advanced Instrumentation for Nano-Analytics (AINA), SIPT Unit, Luxembourg Institute of Science and Technology, 41 rue du Brill, L-4422 Belvaux, Luxembourg
hung.hoang@list.lu

Optimization of Charged Particle Optics (CPO) design and simulation is critical for advancing scientific instrument development such as electron/ion microscopes, energy/mass spectrometers, or other complex CPO systems. Optimizing the design and simulation of these complex systems typically requires a high-dimensional parameter space (electrode geometries and arrangements, electrical/magnetic excitation, etc.) and multi-objective (transmission, beam spot size, energy/mass resolution, etc.) optimization.

SIMION, a valuable ion/electron optics simulation software, offers a robust platform for modeling and optimizing electrostatic, low-frequency RF, and magnetic fields for CPO designs [1]. Optimization in SIMION is mainly performed with its Simplex optimizer [2]. However, the typical workflow using the Simplex optimization algorithm in SIMION is limited by the number of parameters and a single objective that can be optimized, often converging to local minima rather than the global minimum due to its heuristic nature. Therefore, using SIMION's Simplex optimizer to optimize complex multi-parameter and multi-objective CPO systems is typically insufficient.

In this context, we have developed two advanced optimization platforms to work with, but not limited to, SIMION. The first platform upgrades the Simplex optimization algorithm to optimize multiple parameters with multi-objective capability. The second platform uses a multi-objective genetic algorithm (MOGA) based on the open DEAP framework [3]. Both optimization platforms allow the simultaneous and independent optimization of many parameters of different types (up to 10 with the Simplex algorithm running on a typical personal computer, and, in principle, non-limited with MOGA) for two objectives. We also incorporate parallel processing to enhance computational efficiency, addressing the time-intensive nature of potential/field calculation and ray tracing by SIMION. Figure 1 shows the architecture and workflow of the optimization platform using MOGA. Automated communication between MOGA and SIMION is done via a ZeroMQ-based interface. A comprehensive post-data analysis can evaluate the robustness of the optimized solutions against parameter deviations.

Here, we will review the two optimization platforms and present benchmarking and showcases in different CPO simulation scenarios on various secondary ion mass spectrometer (SIMS) designs for FIB-SIMS platforms.

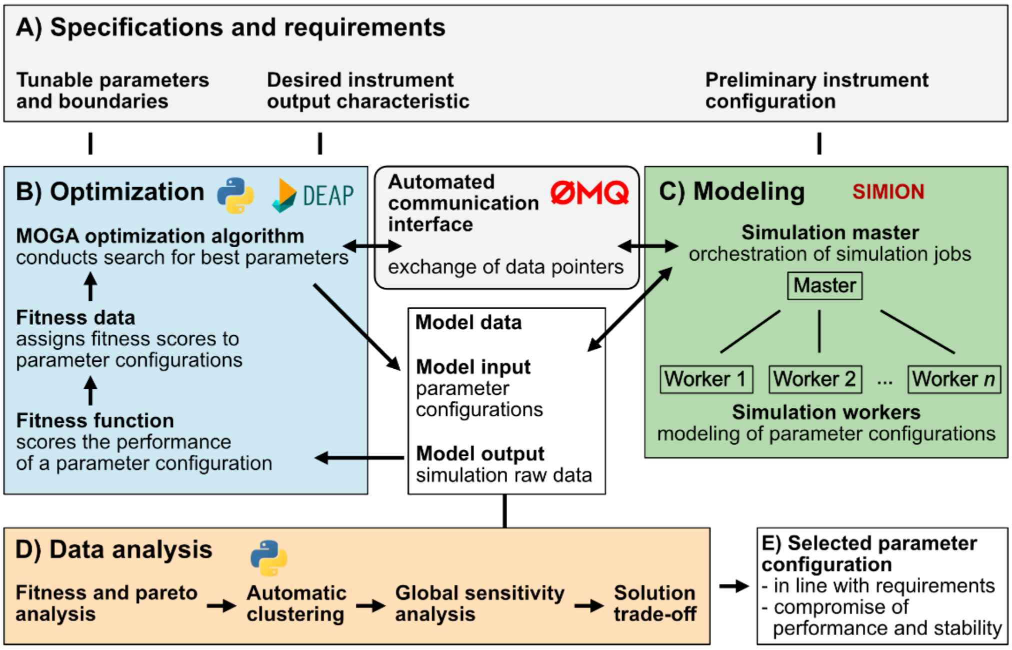

Figure 1. Optimization platform using MOGA for CPO modeling with SIMION. The modular architecture, ZeroMQ-based communication interface, and parallel processing allow a flexible and efficient multi-dimensional, multi-objective optimization with SIMION.

Reference

1. David A. Dahl, SIMION for the Personal Computer in Reflection, Int. J. Mass. Spectrom., **200**, 3 (2000).
2. Saša Singer and John Nelder, Nelder-Mead algorithm, Scholarpedia, **4**, 2928 (2009).
3. K. Huber, T. Wirtz, H. Q. Hoang, CPOpt: A modular framework for genetic algorithm optimization and post-optimization analysis in complex charged particle optical design", Nucl. Instrum. Methods. Phys. Res. A, **1067**, 169702 (2024).