# SIMION Beyond Ion Simulation: Field Analysis, Synthesis, and Harmonic Analysis for MS Design

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The problem of harsh environment mass spectrometer design very often involves considerable compromises to the nearer ideal designs made for the laboratory, in order to accommodate space, power constraints, cost, etc. Most of us engaged in the design of mass spectrometer technology have made use of some version of the SIMION™ ion optics simulation software somewhere along the way. However, over the past decade we have seen an explosion of computing power and added capabilities in SIMION, all controlled by the LUA scripting language and leading the release SIMION 8.2. To be sure the exploration of all of these capabilities defies most researchers time constraints, so this presentation will show examples using these capabilities with the goal of motivating a deeper look at what can be done with SIMION and how the user can expand the software to address many of the problems of Mass spectrometer design and optimization. We show that it is now possible within SIMION to analyze and mathematically characterize the fields created by the structures we design in order to understand the observed simulated ion motion and thereby the instrument performance. In order provide a very quick tutorial we utilize non-ideal ion traps and show how to grasp quickly and directly in SIMION the non-linear behavior and the effects on your instrument using spatial Fourier characterization of the mathematical form of the fields. We then show how new designs can be synthesized by modifying these fields and how to generate new electrode structures. It is hoped that the methods in these examples capture enough of the new capabilities to provoke the imagination of the audience with the further hope of generating interest in a SIMION user group or possibly a more general mass spectrometer simulation interest group.