Instrument Modeling: Simulation, Field Analysis, Synthesis, and Space-Charge

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At the HEMS 2019 workshop, we introduced some ideas about using SIMION™ for field analysis and synthesis. In this presentation, we will make a quick review of those concepts, and then return to some of the newer possibilities with SIMION™ as well as other readily available software tools. The problem of harsh environment mass spectrometer design very often involves considerable compromises to the design that is typically further from the ideal designs made for the laboratory to accommodate space, power constraints, cost, etcetera.

Most of us engaged in the design of mass spectrometer technology have made use of some form of ion optics modeling software including SIMION, somewhere along the way. However, recently personal computers with many computational cores and GPU technology with hundreds to thousands of cores with double precision processing are available and within reach of the typical instrument designer. To be sure the exploration of all of these capabilities defies most researchers' time constraints. So this presentation will show examples using these capabilities to motivate a deeper understanding of what can be done with these tools and how the user can expand the software to address many of the problems of mass spectrometer design and optimization.

We start with a review of the field analysis method. Followed then by a look at SIMION to see how we can control or even replace almost any aspect of the SIMION. Finally, we will discuss using the SIMION Poisson solver applied to space charge simulation.

We hope that these examples capture enough of the new capabilities to provoke the imagination of the audience with the further hope of generating interest in a general mass spectrometer simulation interest group.