Concurrent Cloud Distributed Simulation with Space Charge using SIMION

Mr. Mark Osgood - United States - Ashwood labs
Ms. Ayla Osgood - United States - Ashwood labs

Abstract

To design, characterize and optimize recirculating devices such as ion traps it is often necessary to simulate with a sufficiently large number of particles and with space charge effects accounted for. This is a computationally intensive task and can quickly exceed the computing resources of a single workstation. In this work we present an architecture developed that allows particle trajectory and space charge accounting to be distributed across arbitrarily scalable cloud-based computing resources. This same arbitrarily scalable architecture also enables massively paralleled exploration of operational parameter space for the purposes of device optimization. Post processing of large simulation result data sets is implemented in Jupyter notebooks taking full advantage of big data tools such as pandas data frames and various visualization frameworks such as matplotlib, seaborn and others.

Biography - Mark Osgood

Mark Osgood has over 25 years of experience in the design, construction and commercialization of mass spectrometers and analytical instrumentation. He served as a R&D physicist and project manager for TOF-MS product development at Bruker Daltonics, and was the Vice President and Director of Engineering of Excellims Corporation. In 2021 Mark Co-founded the Ashwood Labs where he serves as a principal R&D Engineer and Physicist. He holds numerous patents in the analytical field and received his BS in Physics from the University of New Hampshire.

Keywords

SIMION, Distributed computing, Simulation, Cloud, Space charge