Title:
SimELIT: A GUI Based Ion Trajectory Simulation Software

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Abstract:
Electron and ion optics simulations are performed using a few available simulation programs, however existing programs do not have the capability to model the full scope of ion transport in multiphysics fields (pressure scales, gas dynamics and electrodynamics) under one platform. Thus, combining results from multiple simulation platforms and import results to perform ion trajectory simulations has been the norm. While this slows down ion optics design, we describe herein a new comprehensive solver SimELIT which enables ion trajectory simulations in multiphysics environments of mass spectrometry systems.
SimELIT is based on an OpenFOAM (an open-source tool for defining and solving computational mechanics problems, differential equations etc.) solver as its computational core. The solver allows users to select from among multiple physics that need solution (e.g., Electrostatics, electrodynamics, vacuum, static gas, incompressible gas flows and compressible gas flows). Ion trajectories are evolved using either Lagrangian or Eulerian treatment of ion dynamics. Collisional models enable treatment of collisions with the background dependent on the pressure regime of the domain where ion trajectories are being computed. In addition to the comprehensive solver, a graphical user interface to allow user friendly simulation case setup was built. This enables bypassing the otherwise text based and somewhat non-intuitive input definition inherent with the use of OpenFOAM for computations.
We will report on the GUI utility in simulation setup and running ion trajectory simulations using SimELIT. Several test cases of ion trajectories in typical mass spectrometry ion optics situations and validation of the computations will be reported.