Simulation study of ion stability of in-situ generated ions in a 3D ion trap under different gas load conditions

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Introduction

3D ion traps are commonly used for trapping and detection. In-situ ionization combined with a pulsed gas inlet system allows to build very compact and versatile devices.

In real world system ion trapping of in-situ generated ions not only depends on the a- and q-parameters, but also on the place of birth, and kinetic energy of those ions. SIMION simulations were carried out to study the ion stability and instability under different gas loads.

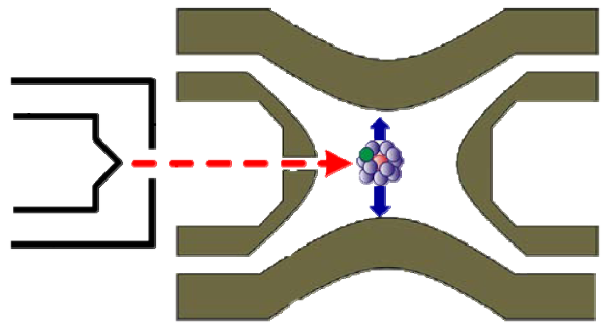
A complete simulation chain was build:
In a first step time-dependent in-situ ion generation by electron impact was simulated using SIMION and a Monte Carlo approach.

In a second step those generated ions were used to investigate ion dynamics and trapping efficiency. Different a- and q-parameter were used to study ion stability and instability under different residual gas and buffer gas loads.

In a third step those results were evaluated by MATLAB programs and compared to theoretical considerations and models under ideal vacuum conditions.

Simulation setup

- Classical Paul-trap: RF signal is applied to the ring electrode while the endcaps are held at ground.
- In-situ ionization with an electron gun (70 eV) attached to the ring electrode

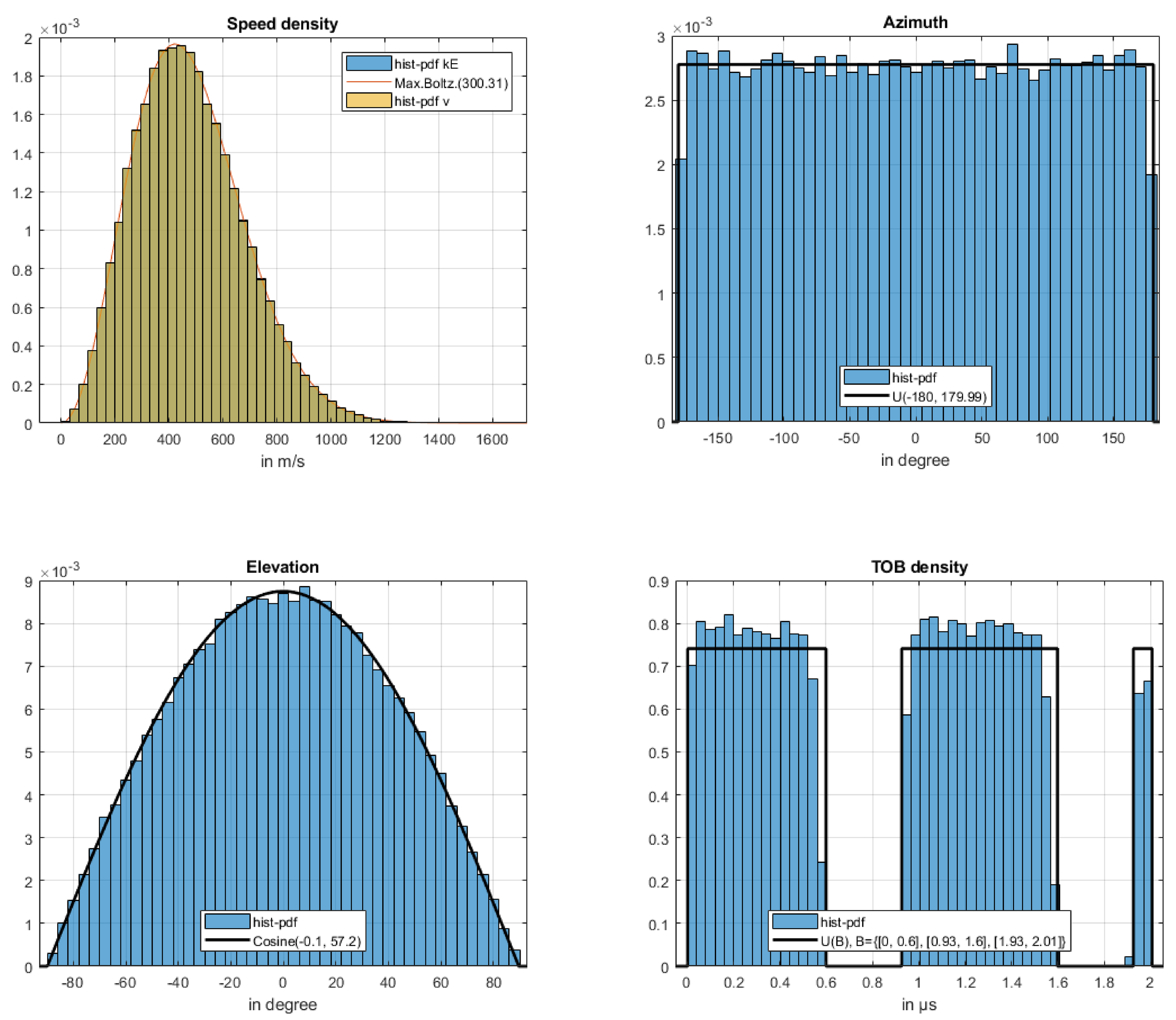


- The simulations in SIMION do not take space charge effects and coulomb's law into account

Ion generation

Electron impact simulations were done to investigate the place of birth (PoB), time of birth (ToB) and kinetic energy (KE) of generated ions. Ion generation simulations are very time consuming due to the large number of simulated particles (electrons). Thus, a statistical model for the ion generation process was developed and used for all following simulations.

Following distributions and parameters were found for 40 amu Argon ions:



The simulation results show good agreement with theoretical considerations.

PoB distribution

A 3D kernel density estimator was developed showing good agreement with the simulated place of birth distribution.

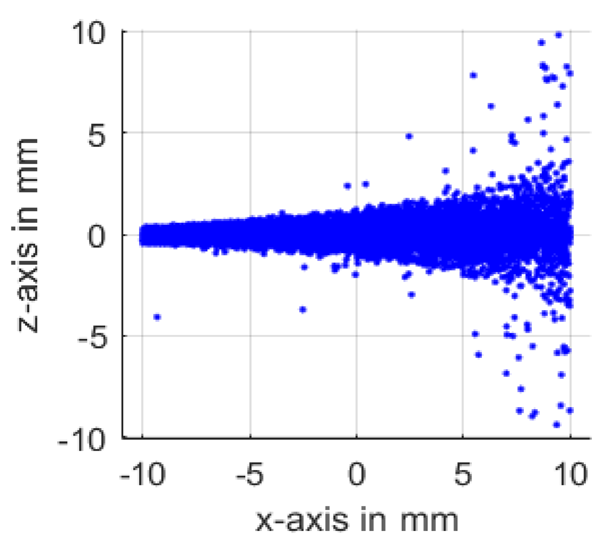


Fig. 1:
Position of simulated ions
Total number of ions: 22500

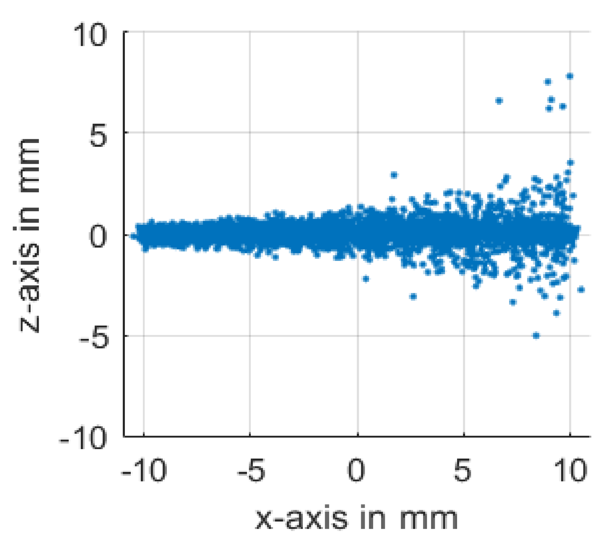


Fig. 2:
Position of generated ions with kernel density
Total number of ions: 6000

Ion stability in vacuum

In order to create a stability diagram under real world conditions (to detect field errors and geometric limits), ions with different starting parameters were used and trapping efficiencies were investigated:

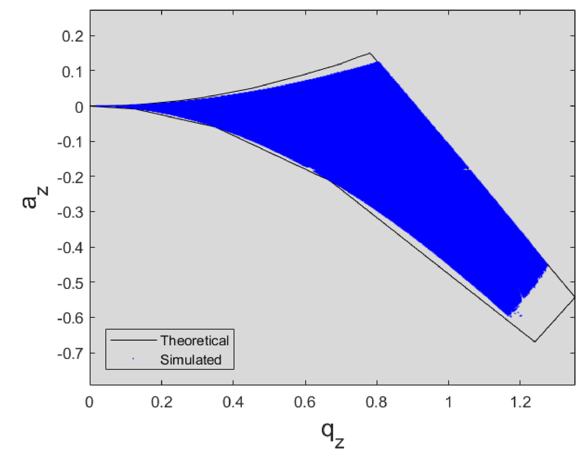


Fig. 3

Starting Parameters
- Ion position: 2 mm off-center
- Kinetic energy: 0.0367 eV
- Mass: 40 amu (Argon)
- Without background gas

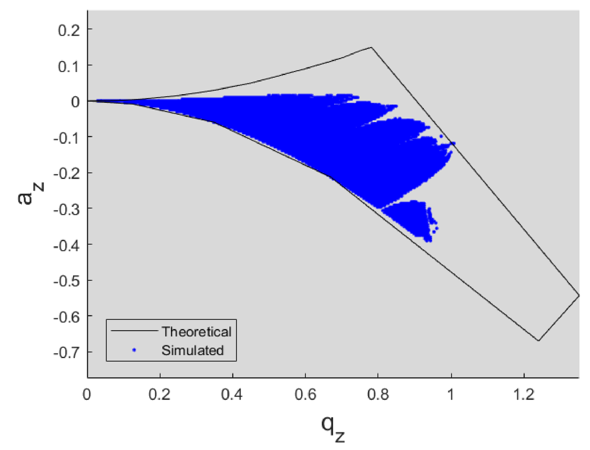


Fig. 4

Starting Parameters
- Ion position: 4 mm off-center
- Kinetic energy: 0.0367 eV
- Mass: 40 amu (Argon)
- Without background gas

Trapping efficiency is better for ions generated closer to the center of the trap. Those ions also show a better approximation of the theoretical ion stability.

Ion stability under gas load

The following results are generated with the same starting parameters as in Fig. 4, but this time with different gas loads.

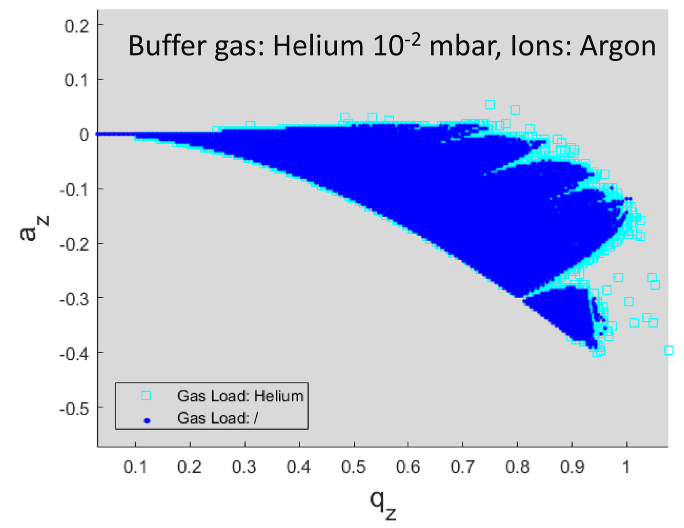


Fig. 5

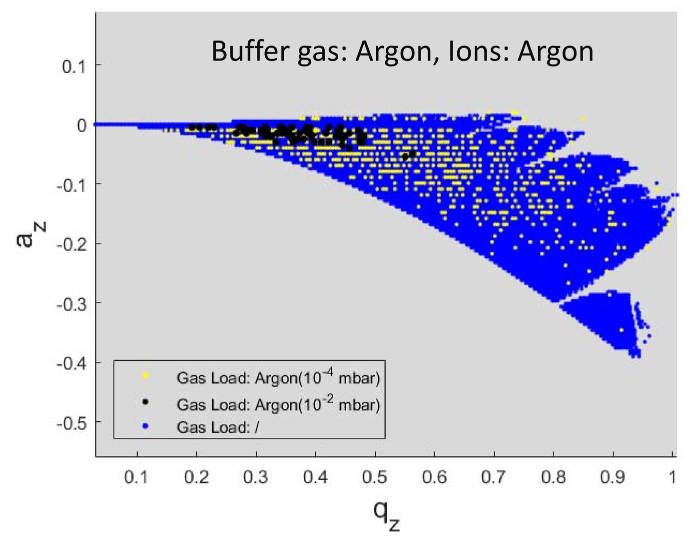


Fig. 6

The desired cooling effect of Helium as background gas does not seem to be relevant in the given pressure regime of 10^{-4} mbar. Even with argon the ion stability is not affected significantly. But this could be due to the fact, that at low pressure only few collisions between the ion and the gas load occur. Fig. 6 shows that collisions with argon at a pressure of 10^{-2} mbar indeed make a huge difference for stability due to ion heating.

Results

The last step was combining all steps. Therefore ions were generated using the statistical model to do some stability studies.

Fig. 7 shows a result of the complete simulation chain. Ions in red are lost, blue ions are safely trapped.

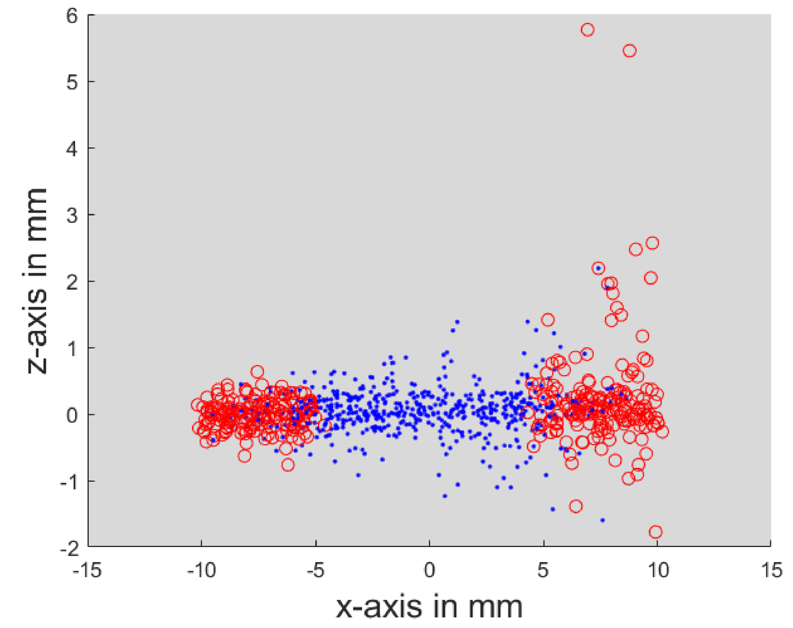


Fig. 7

The further the ion starting positions are away from the center, the more likely they are unstable. 60% of the generated ions are effectively trapped.

Conclusions

- The simulation chain is working, ions can be generated (place of birth, time of birth, speed) with a statistical model without simulating first.
- Helium buffer gas has nearly no effect in the given pressure regime to increase trapping efficiency.
- Place of birth has huge impact if ions are trapped or lost.

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