



Ion Dynamics Simulation Framework (IDSimF): An Open Source Trajectory Simulation Framework

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Introduction

The numerical simulation of ion trajectories at complex physical conditions is an integral part of the research and design efforts for the development of mass spectrometric devices. There is yet no established open source simulation code for this task available to the community. We present an extensible, open, simulation framework "IDSimF". It allows to perform complex ion trajectory simulations, including performant space charge calculations, and it can freely be adapted to any simulation requirement by the user community.

Open Source Project

IDSimF is available to the public as open source project.

The open repository is available at <https://github.com/IPaMS/IDSimF>

IDSimF is licensed under the *GNU General Public License v3.0*. Thus, the source code has to be available for every public compiled binary version of the program.

Code Application Examples

Example 1: Ion Trajectories with Space Charge: FT-Ring Trap

Ions can be stored and detected in an ion trap geometry, consisting of stacked rings and two cap electrodes. The basic operation is similar to a classical FT-quadrupole ion trap (Paul-trap). The storage conditions in the trap can be modified by manipulating the potentials on the ring electrodes.

IDSimF was used to calculate ion trajectories in a stacked ring ion trap geometry to investigate the sensitivity of different trap configurations to space charge effects.

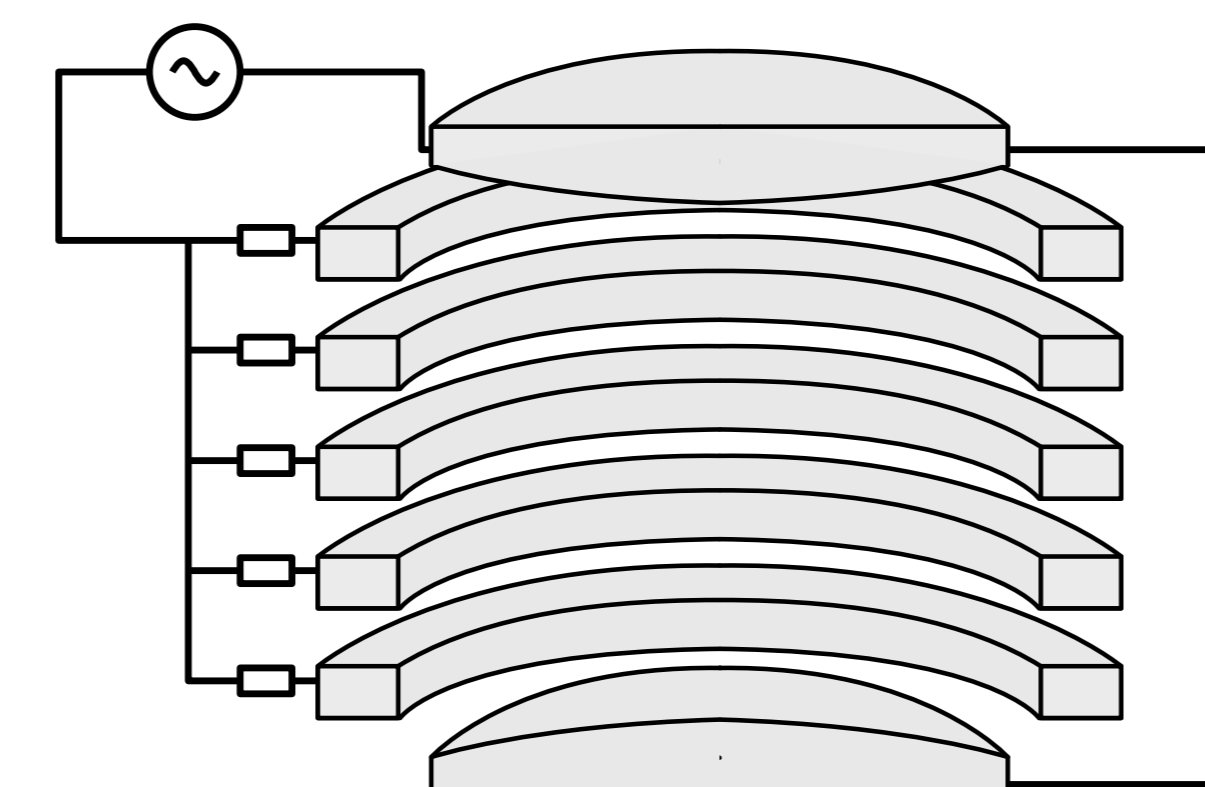


Fig 1: Schematic view of the stacked ring trap

The mirror current transients simulated with IDSimF and the resulting FT-spectra in Fig X clearly show complete peak fusion when space charge is considered with 4000 ions of 100 and 102 Da.

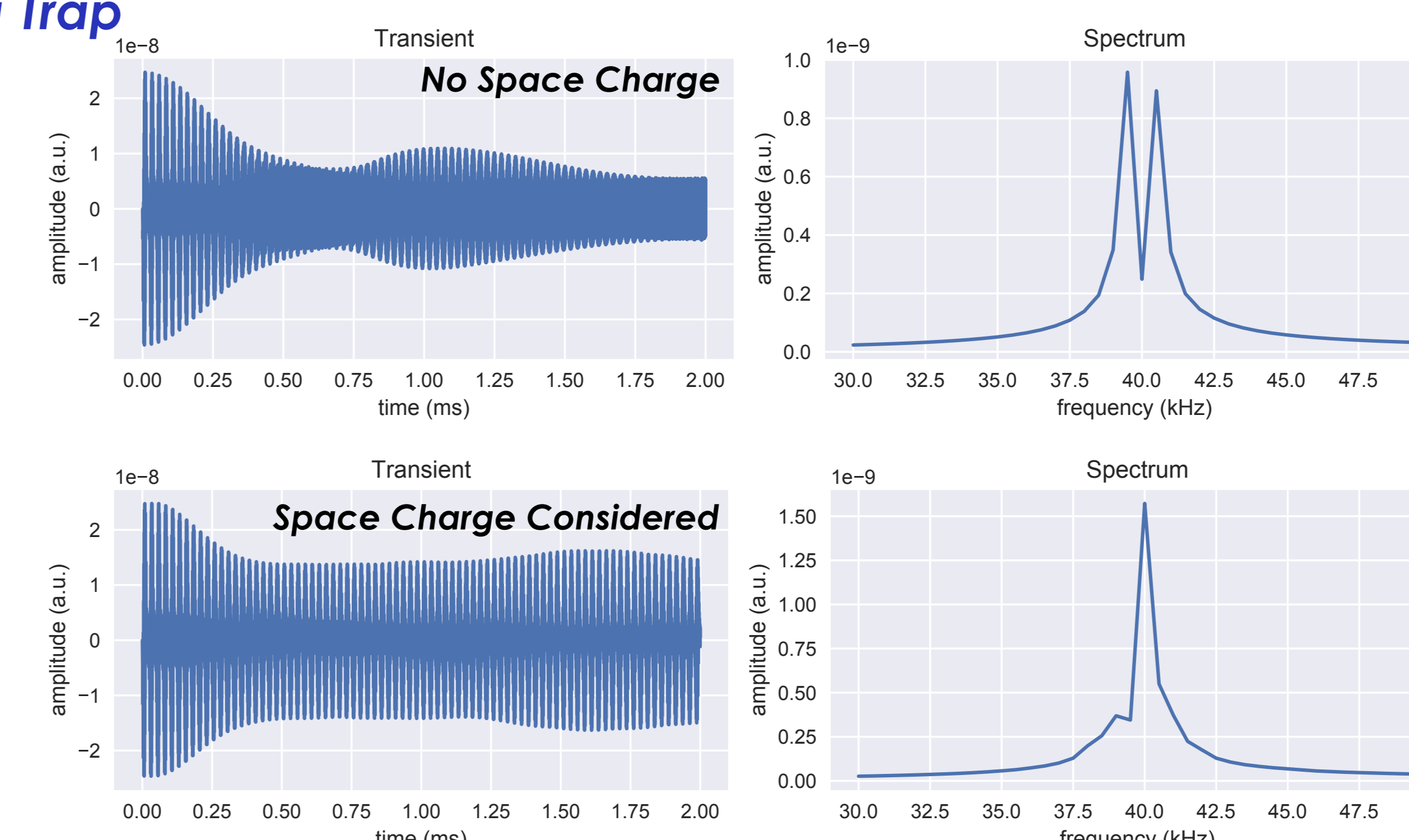


Fig 2: Simulated transients and FT-spectra in a ringed ion trap. The total peak fusion due to space charge is clearly visible.

Example 2: Trajectories of Reactive Ions in Diluted Gas: HiKE-IMS

Classical ion mobility spectrometry (IMS) separates ions by their different collision cross sections in a gas filled drift tube with a static electric field. The high kinetic energy IMS (HiKE-IMS) [2] is a drift tube instrument, which combines low background pressure with strong electric drift fields. This leads to low absolute reaction rates, high effective ion temperatures and very short residence times of ions in the drift region. Thus, even very fast chemical reactions of analyte ions can be resolved in HiKE-IMS.

IDSimF was used to simulate the trajectories of reactive proton bound water cluster ions ($H+(H_2O)_n$) in a HiKE-IMS drift tube. The interaction with the background gas was modeled with a Hard-Sphere collision model. The modeling of the cluster formation and fragmentation reactions considered the effective ion temperature caused by the strong drift field (reduced field strength in the range of 100 Td).

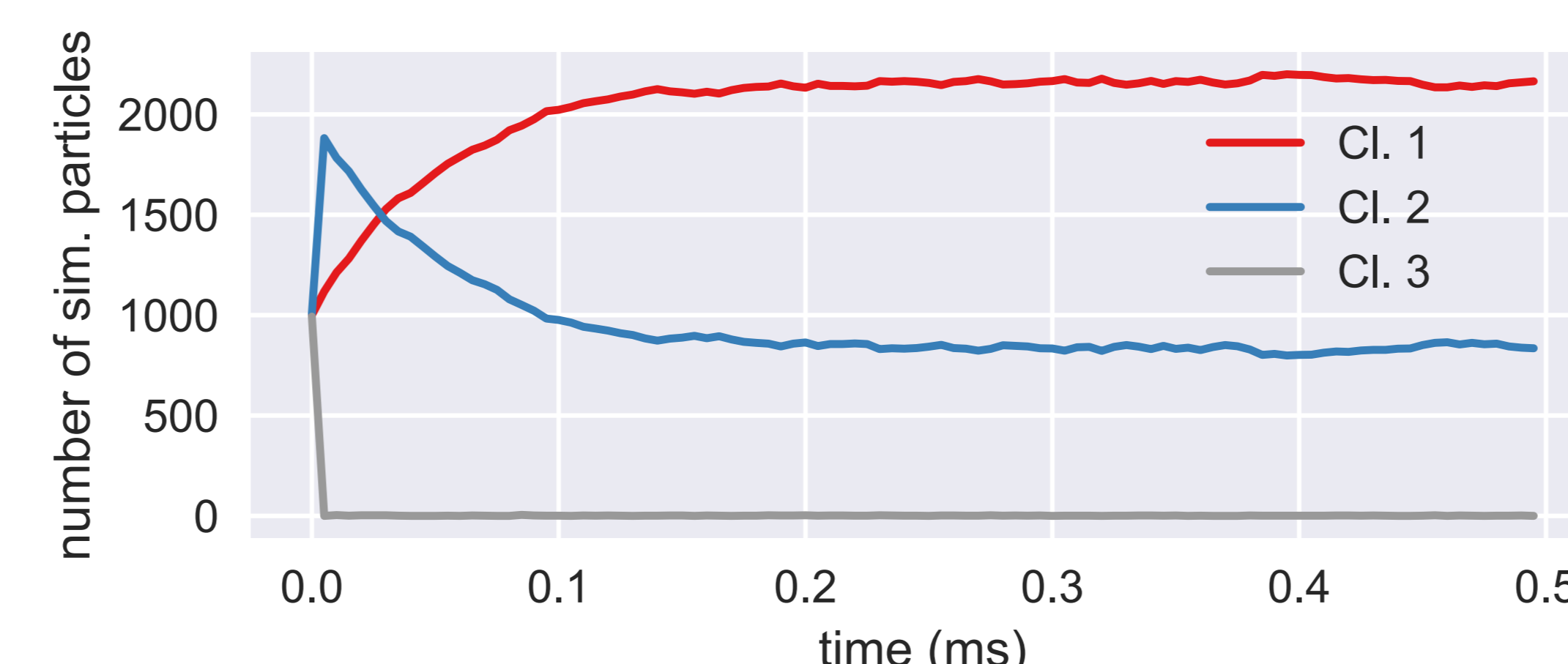


Fig 4: Concentration profile of the water cluster particle ensemble in the HiKE-IMS simulation.

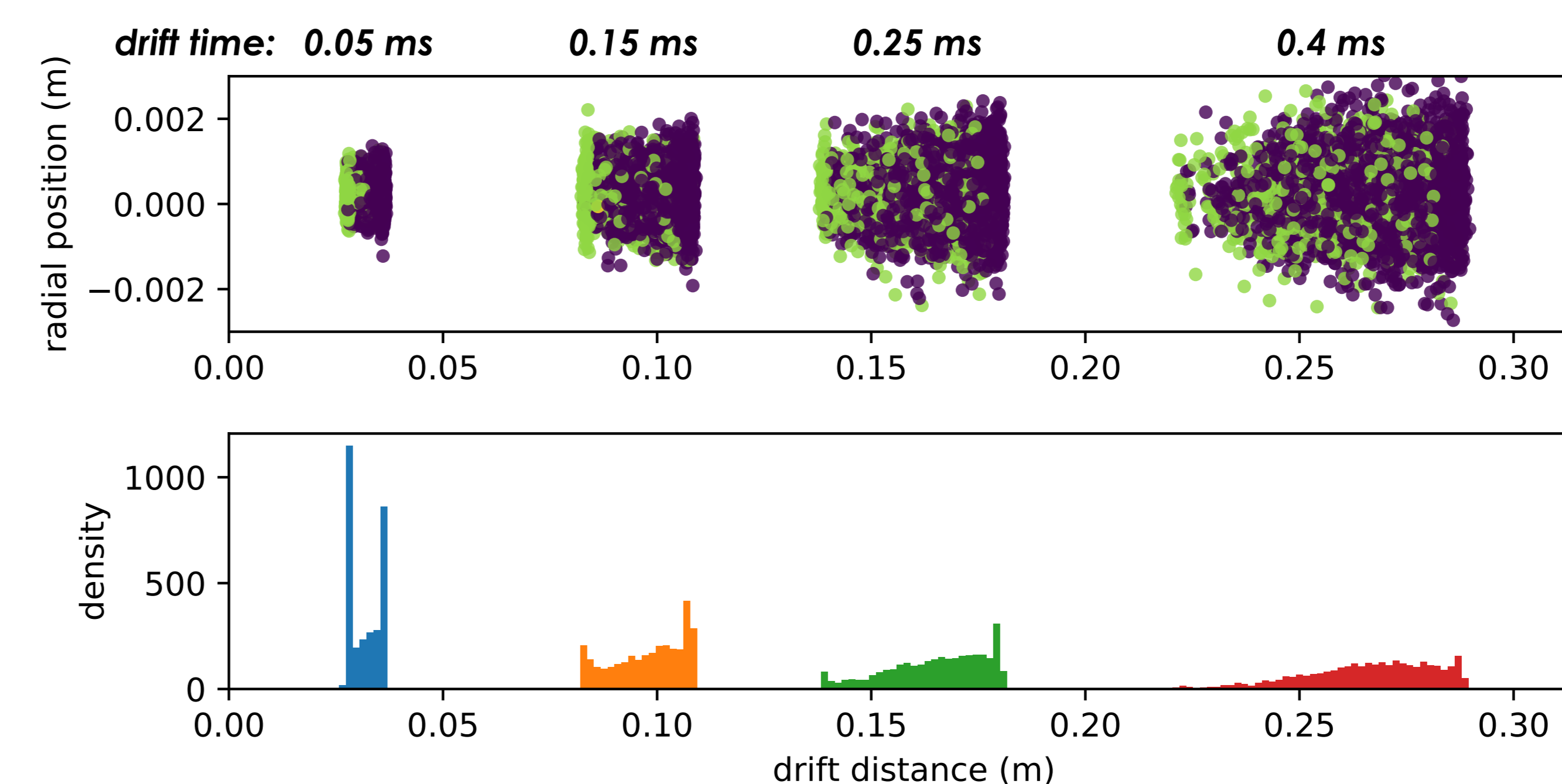


Fig 3: Trajectories and axial density profile of simulated cluster ions in a HiKE-IMS drift tube. Cluster n=2 is green and Cluster n=1 is purple in the scatter plot (top).

The concentration profile (left) clearly shows that at the simulated conditions cluster with n=3 immediately fragments to cluster n=2, which is in a dynamic equilibrium with cluster n=1.

The simulated particle ensemble shows diffusion due to the interaction with the background gas. In addition, particles frequently change their cluster size while drifting due to the dynamic equilibrium between cluster n=1 and n=2. This leads to a fusion of the signals of the individual cluster species: The cluster system merges to one irregularly shaped signal, which is also clearly observed in actual HiKE-IMS experiments.

Conclusions / Outlook

- IDSimF is an open, extensible framework for the simulation of ion trajectories considering space charge, background gas interaction, and chemical reactions.
- IDSimF is in an early development stage. Nevertheless, it was successfully employed for diverse simulation tasks, e.g. simulation of ion traps, transfer quadrupoles, ion mobility analyzers, and differential ion mobility (DMS) cells.
- IDSimF is provided to the public in an open source project to allow the validation, modification, and extension by the interested community.

Outlook:

- We plan to continuously improve and extend the IDSimF codebase.
- Planned improvements for the near future are:
 - Full integration of FMM based space charge simulation with Scafacos
 - Improved background gas interaction models
 - Modelling of internal degrees of freedom / internal energy of ions for reaction simulation

Literature

- [1] Barnes, J., Hut, P.: A hierarchical $O(N \log N)$ force-calculation algorithm. *Nature*. 324, 446–449 (1986).
- [2] Langejuergen, et. al.: High Kinetic Energy Ion Mobility Spectrometry: Quantitative Analysis of Gas Mixtures with Ion Mobility Spectrometry. *Analytical Chemistry*, 86, 7023–7032 (2014).
- [3] Wissdorf, W., et. Al.: Monte Carlo Simulation of Ion Trajectories of Reacting Chemical Systems: Mobility of Small Water Clusters in Ion Mobility Spectrometry. *Journal of the American Society for Mass Spectrometry*, 24, 632–641 (2013).

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Code Overview / Code Structure

IDSimF is implemented in C++ and follows a framework approach inspired by OpenFOAM, an open source fluid dynamics code. IDSimF itself provides data structures and algorithms in modularized libraries.

Simulation applications are compact C++ programs, which use the provided framework to solve actual calculation tasks. This flexible structure allows to quickly adapt IDSimF to new simulation tasks.

Core Features and Capabilities:

Trajectory Integration	Space Charge Simulation	Gas Interaction	Chemical Reactions (RS)
analytical fields external field import	Barnes-Hut Tree FMM (Scafacos)	Hard Sphere Model Statistical High Pressure Model External Flow Field Import	Stand Alone Mode Reactive Particle Trajectory Integration Multiple Reaction Types

IDSimF has currently no integrated solver for electric fields, but external fields calculated by other solvers (e.g. SIMION, Comsol) can be imported.

Code Modules:

core	Basic data structures, base classes	BackgroundInteraction	Background gas collision models
ParticleSimulation	Time integration, simulation management	RS	Reaction Simulation: Chemical species and chemical reactions
BTree	Barnes-Hut Tree for space charge simulation	IDSimF Analysis	Python based simulation analysis and visualization library

The Python based analysis and visualization library (*IDSimF Analysis*) is a separate project and will be released in a separate open source repository.

Code Dependencies:

IDSimF has some external dependencies to other open source libraries and projects as shown on the right.

We plan to minimize the required bindings to external projects to simplify the installation / compilation process of IDSimF.

