Simulation of isotherm HiKE-IMS – MS Transfer Stage

Robin Hillen[1]; Walter Wissdorf[1]; Maria Allers[2]; Hendrik Kersten[1]; Stefan Zimmermann[2];
Thorsten Benter[1]

[1]: Physical & Theoretical Chemistry
Wuppertal, Germany
Institute for Pure and Applied Mass Spectrometry

[2]: Leibniz University Hannover,
Institute of Electrical Engineering and Measurement Technology

Introduction

To elucidate the chemical dynamics prevailing in a High-Kinetic-Energy-IMS (HiKE-IMS), a Time-Of-Flight (TOF) mass analyzer is planned to be coupled to the HiKE-IMS. The transfer stage between IMS and MS has to transfer ions from a pressure range of 10-40 mbar into the high vacuum of the mass analyzer. Ideally, this ion transfer should maintain the same effective ion temperature as in the drift space of the HiKE-IMS and should not mass discriminate towards low masses. The current transfer stage is realized by a printed circuit board (PCB) quadrupole and a PCB ion funnel. Numerical simulations of the quadrupole are performed to describe ion trajectories and ion energy distributions.

Methods

Simulations:

- SIMION® 8.1 with hard sphere collision model (HS1) and custom Lua scripts [1]
- Sparta open source DSMC Code (feb19) [2]

CAD-Software:

- OpenSCAD 2019.5 [3]
- Autodesk Inventor 2019 [4]

Data Analysis:

- Python 3 with numpy, pandas and scipy libraries
- ParaView 5.6 [5]

Machine:

- Dell Precision T7500 with eight physical cores (two Xeon E5530 CPUs) and 24 GB RAM

Experimental setup

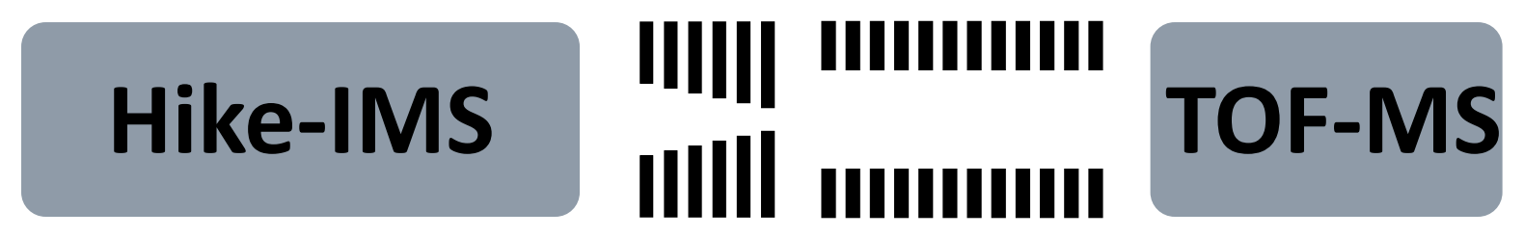

Fig 1: Schematic drawing of the experimental setup

Analyte ions are generated and separated in the HiKE-IMS. Instead of a faraday plate detector, a TOF mass analyzer is coupled to the IMS. Therefore, the ions must be transferred into a low-pressure region. This is realized by a PCB ion funnel and a PCB quadrupole.

Goals

- investigation of differences between 3D- and 2D-SPARTA simulations in view of the accuracy of the results
- perform high resolution 2D axisymmetric SPARTA simulations to calculate pressure and velocity profiles
- ion trajectory simulations in SIMION considering the background gas flow profile to estimate ion motion and collision energy distributions

SPARTA simulations

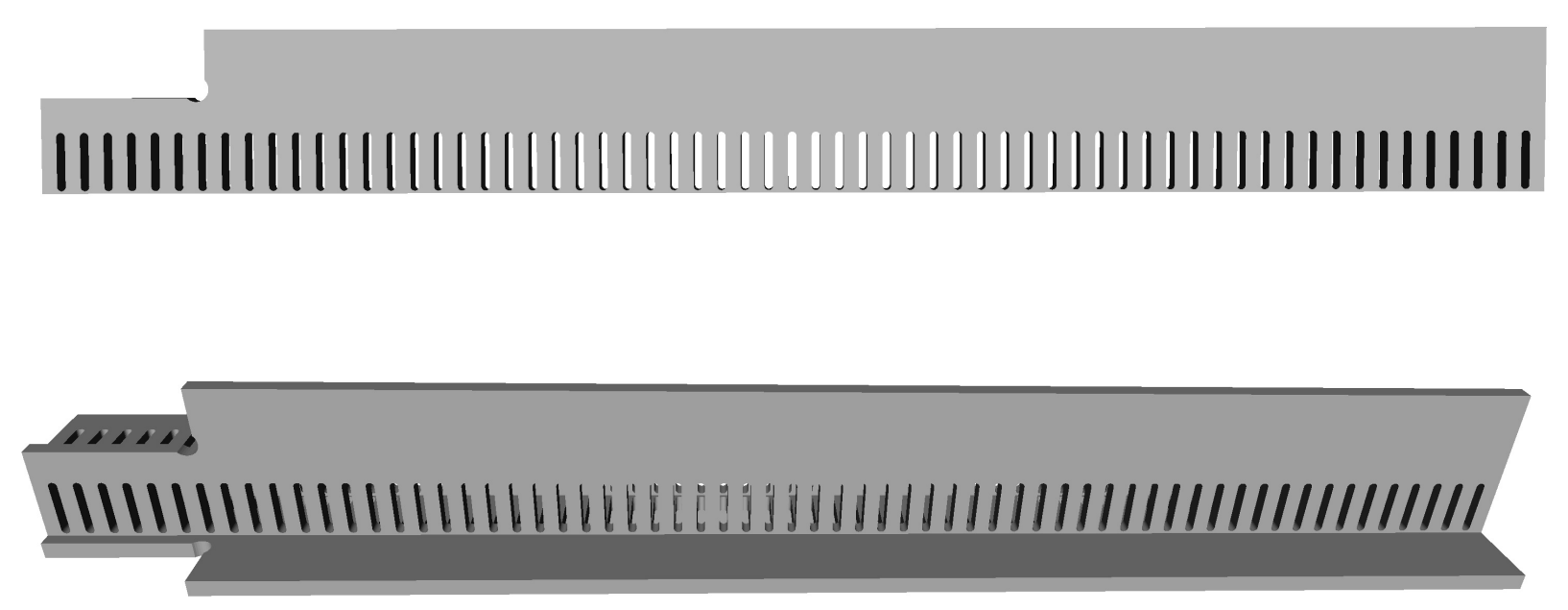

Fig 2: CAD model of the PCB quadrupole

Initially, the three-dimensional model of the quadrupole is transformed to a two-dimensional axisymmetric model. To ensure that the 2D axisymmetric model is valid, also full 3D SPARTA simulations are performed. Fig. 4 shows the pressure profile on the x-axis for a 2D and a 3D SPARTA simulation. The two profiles differ at most by a factor of 1.75 and the end pressure is nearly the same. Due to this small difference, the 2D model is chosen for better computing performance.

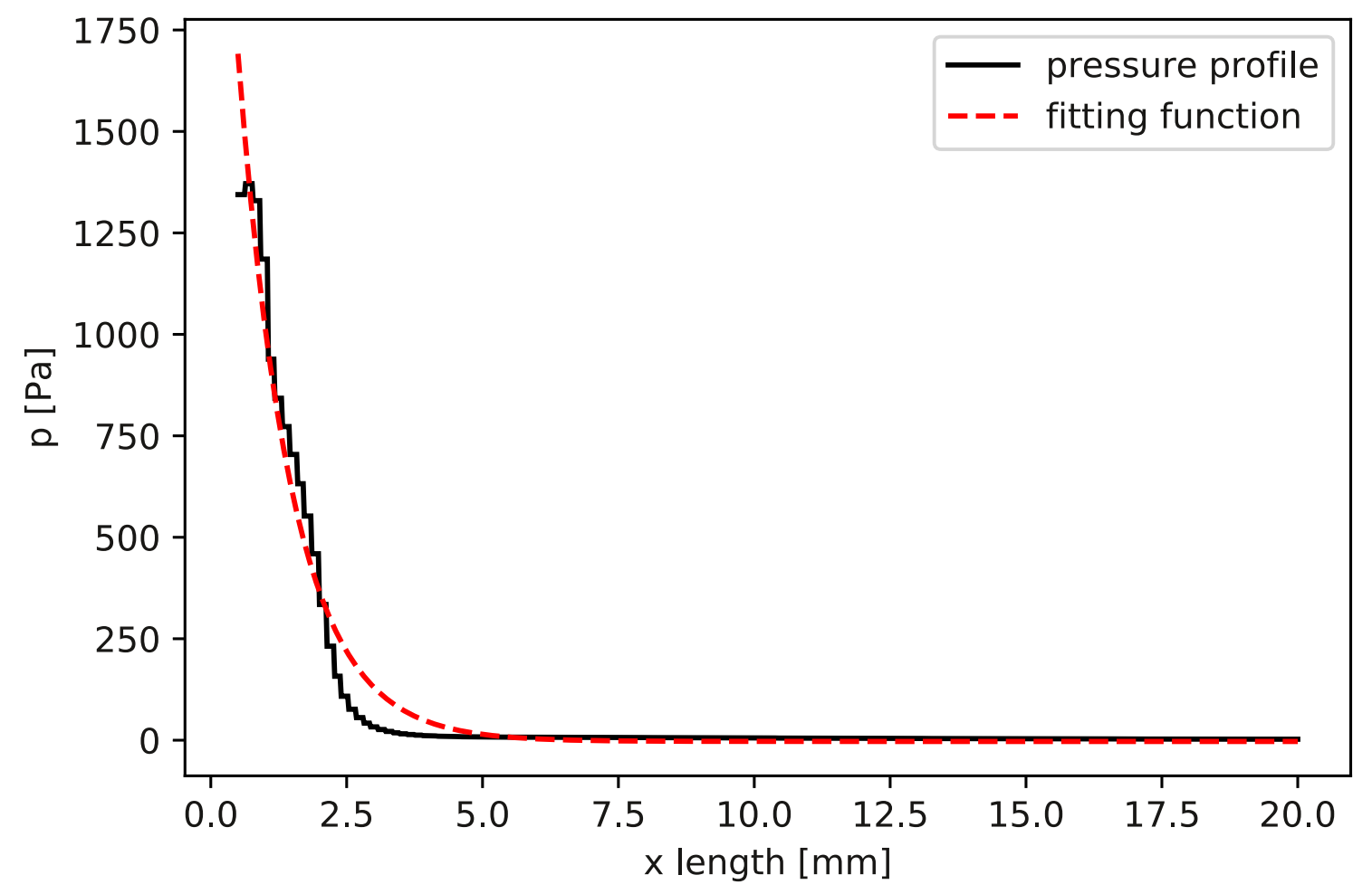

Fig 5: Pressure profile along the center axis

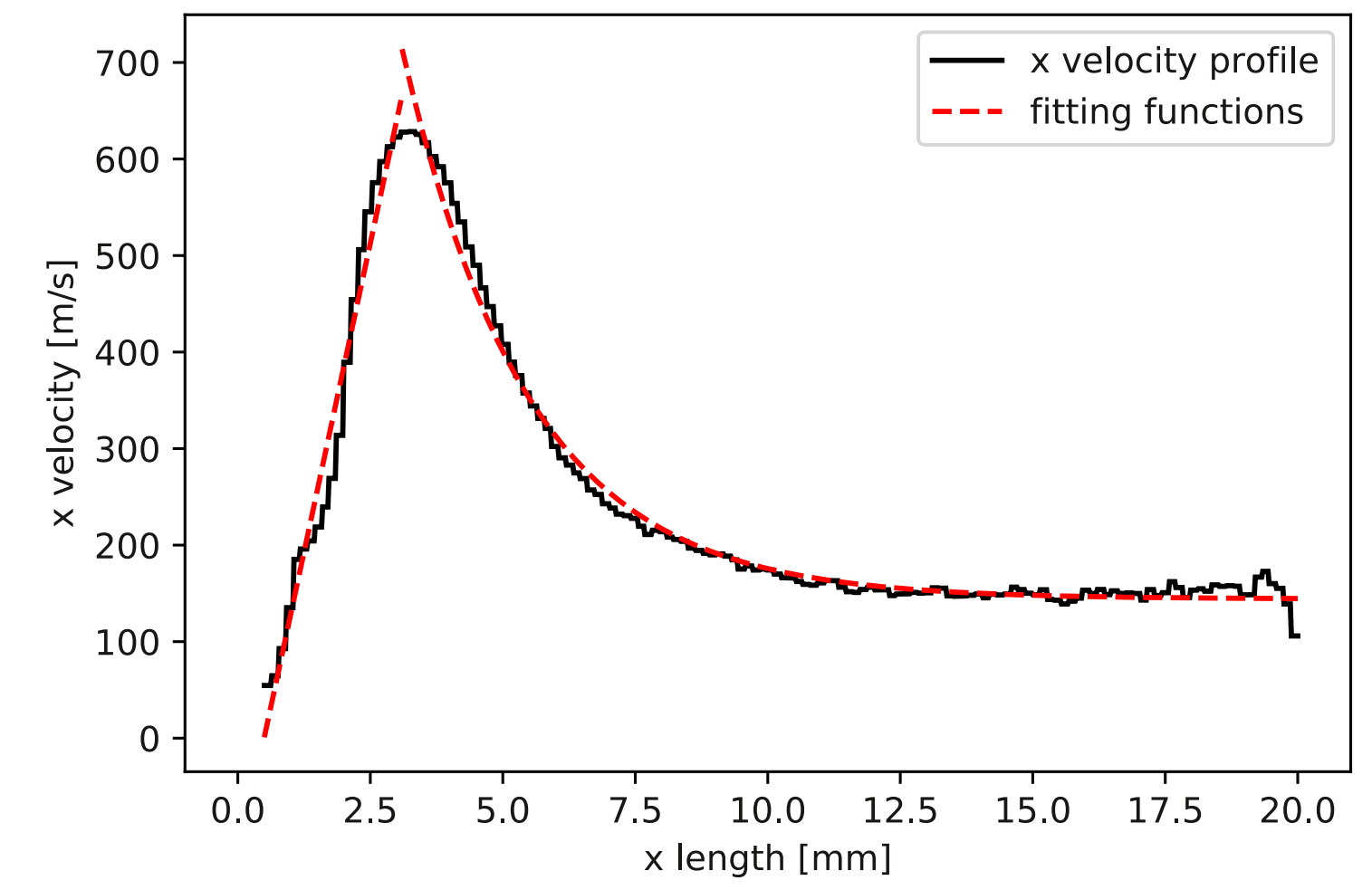

Fig 6: Velocity in x direction along the center axis

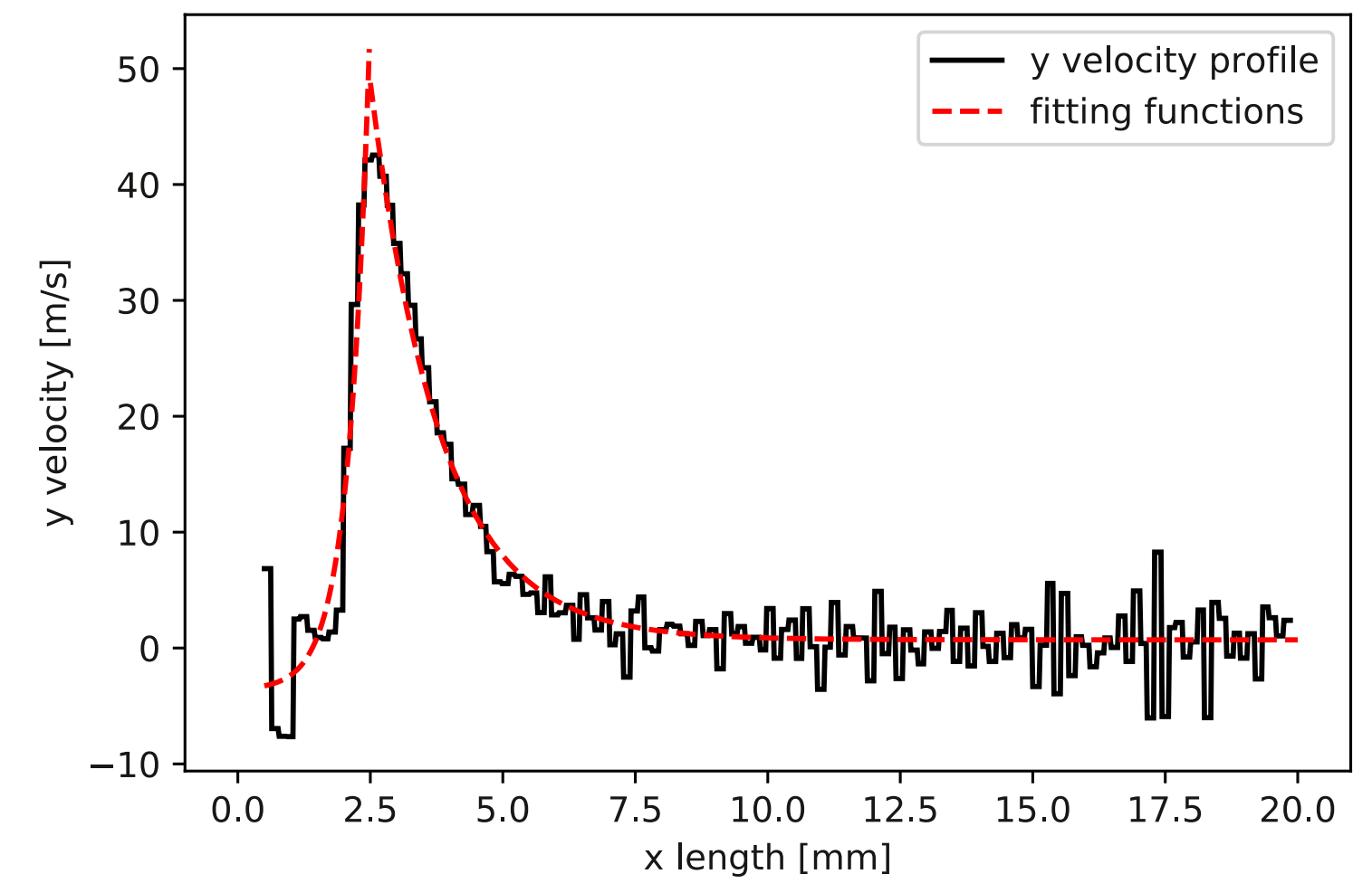

Fig 7: Velocity in y direction along the center axis

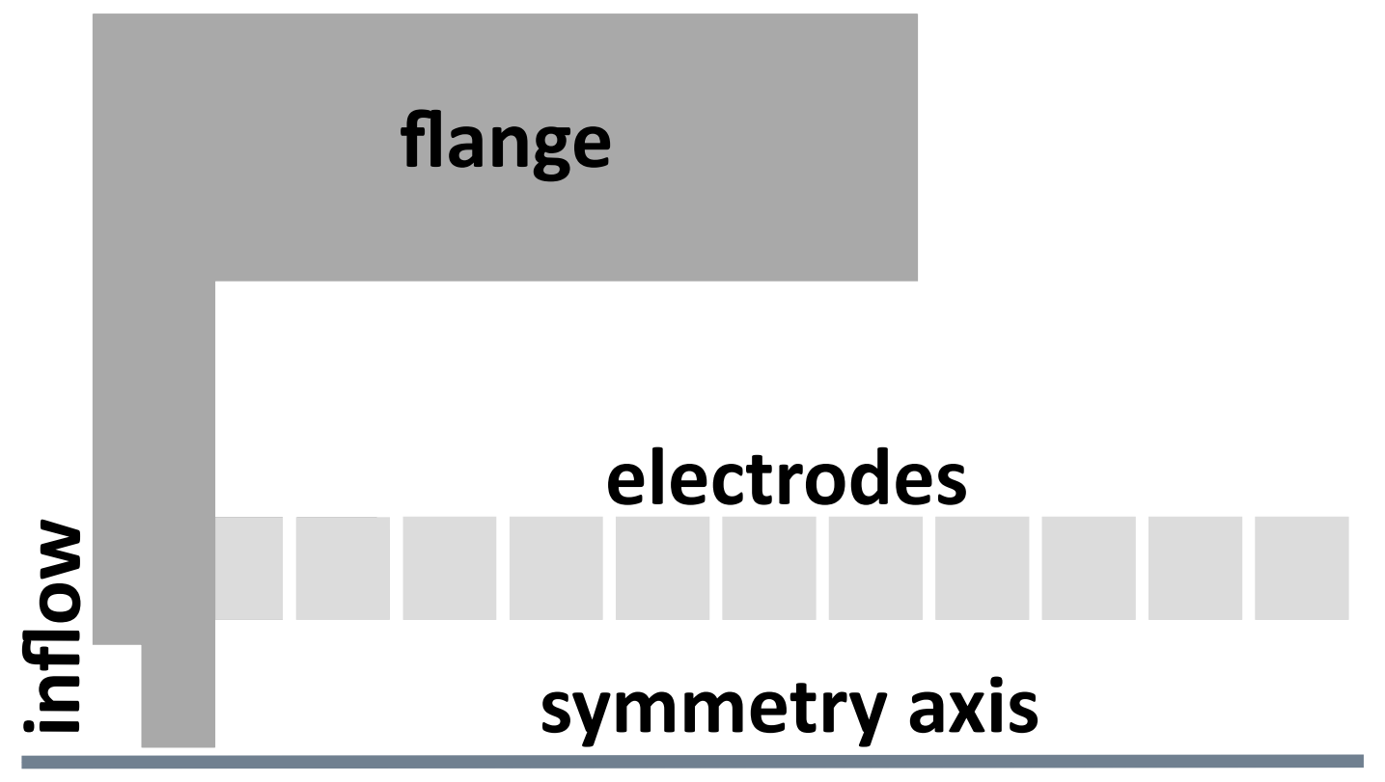

Fig 3: Two-dimensional axisymmetric model of the inelt system and the quadrupole

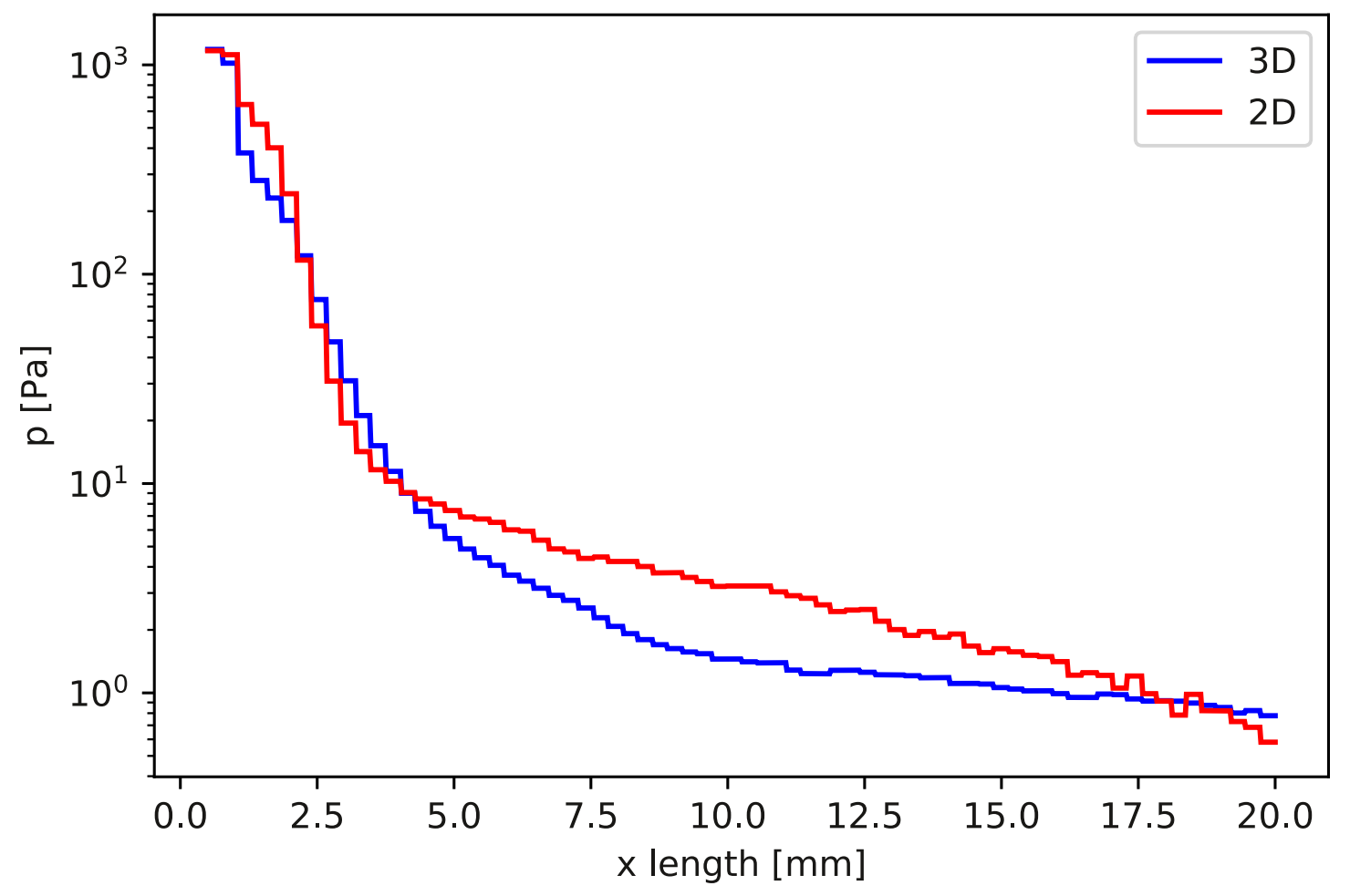

Fig 4: Comparison of pressure profile on the x axis for a 3D and 2D SPARTA simulation

All shown 2D SPARTA simulations were performed with a background pressure of 2 Pa and an inflow pressure of 1,300 Pa. The simulated gas is pure nitrogen. The grid resolution was 9,600 grid cells per meter. The original length of the quadrupole of 142 mm is clipped to 20 mm for all simulations to reduce computing demand. The simulated time is 300 µs with a timestep lenght of 2 ns.

Flow profile fitting

Fig. 5 shows the pressure profile along the x coordinate. The end pressure of 2 Pa is reached after 3 mm and remains stable. The pressure profile is represented by an exponential function. The velocity in x direction is shown in dependence on the x position (Fig. 6). The maximum is at approximately 3 mm. The pressure profile is described by a linear increase followed by an exponential decrease. An upper limit is set to avoid an overestimation in the maximum region. Fig. 7 shows the velocity in y direction analogously to Fig. 6. The first part of the profile is described with an exponential function. The parameterized fitting functions were used in the hard sphere collision model of SIMION. The axisymmetric flow profile from the 2D SPARTA simulation is rotated around the symmetry axis numerically to gain an approximate 3D flow profile as SIMION input.

Sensitivity analysis

A sensitivity analysis was carried out on the 2D SPARTA simulation. The influence of the simulated time and the factor between simulated and physical particles (fnum) is comparatively small. The differences in the simulation results are between 5 and 10 %. However, the grid resolution has a significant influence on the results. Therefore all 2D SPARTA simulations were performed with high grid resolutions.

SIMION simulations

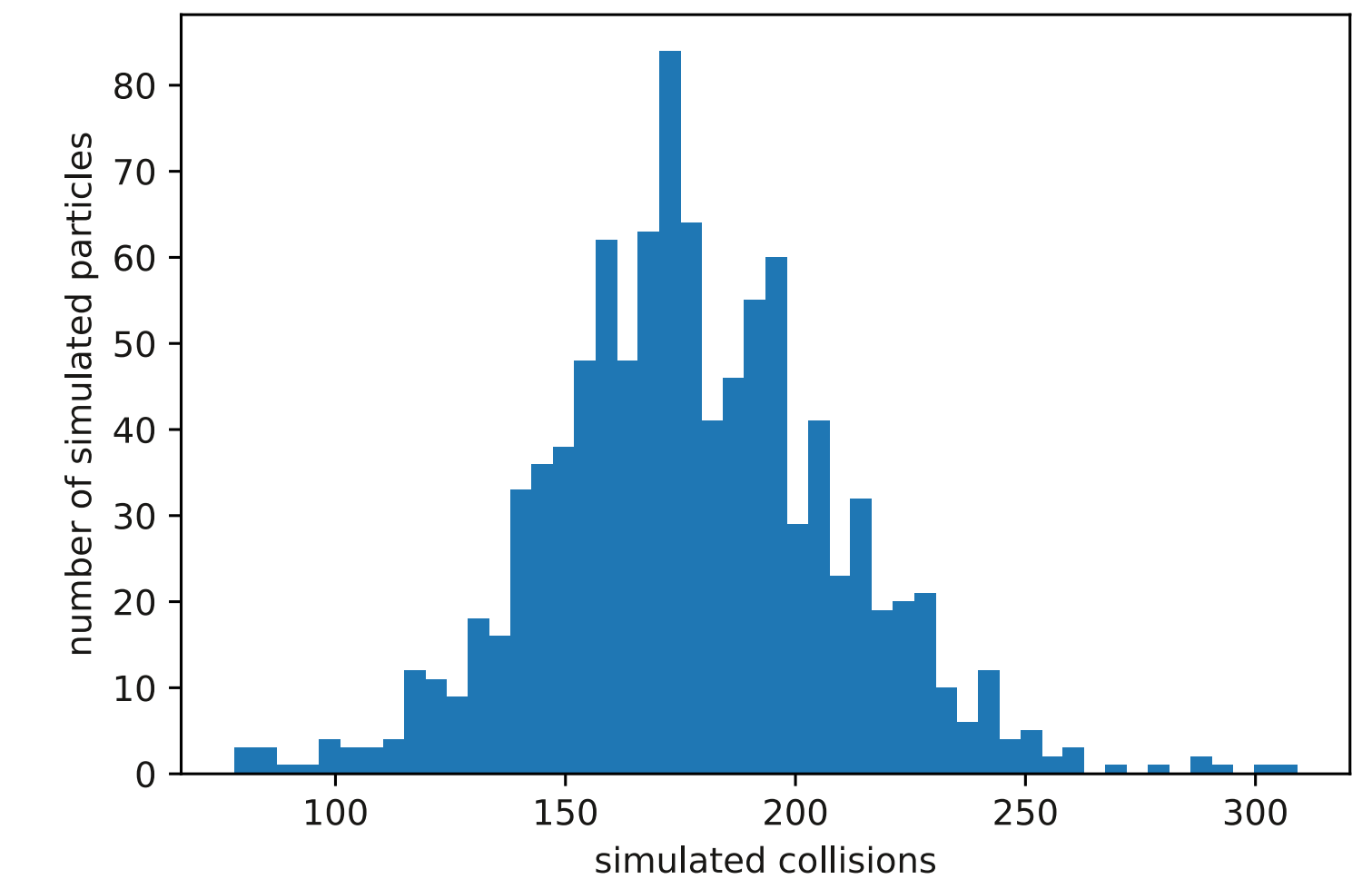

Fig 8: Histogram of the number of simulated collisions

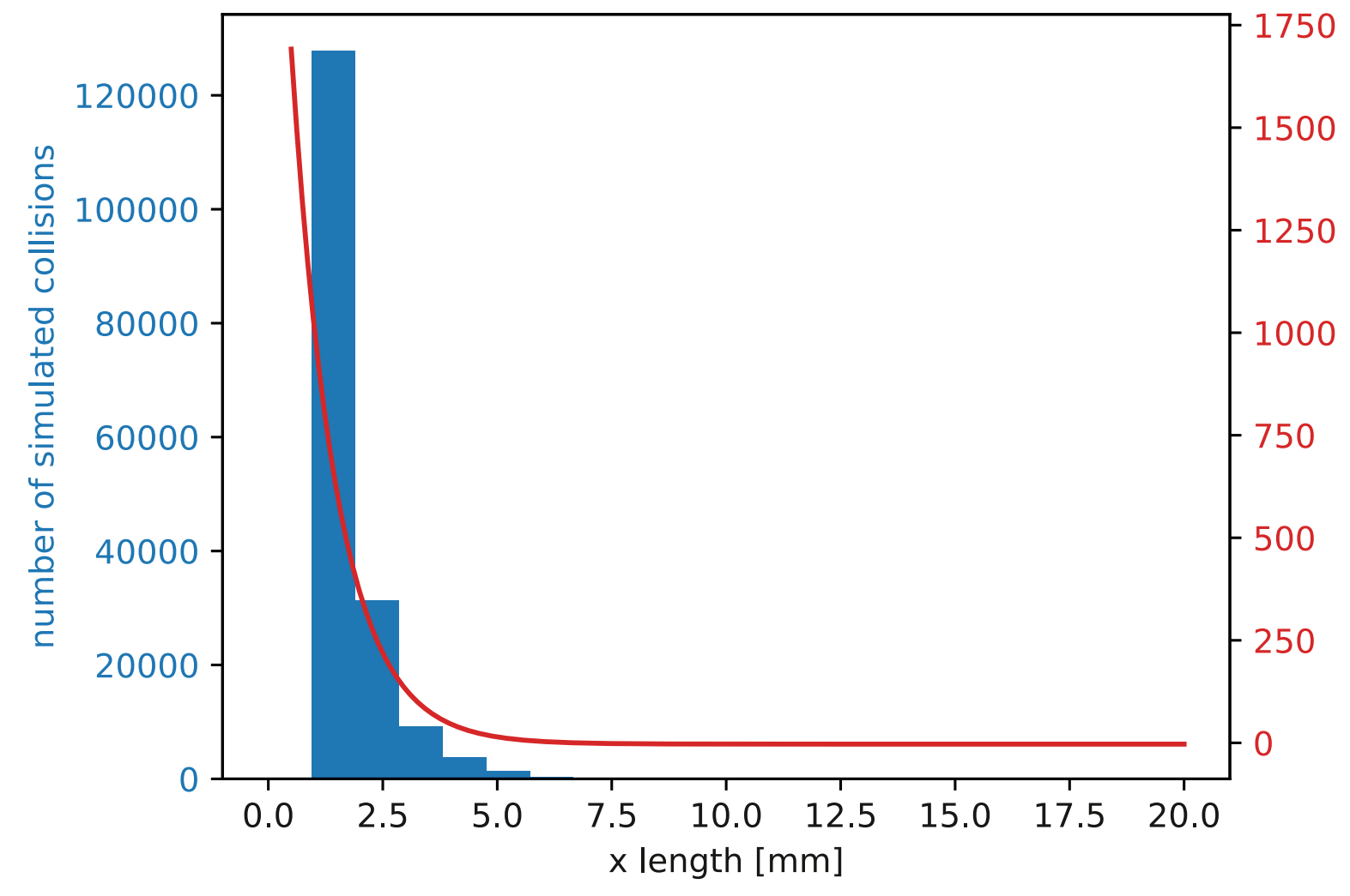

Fig 9: Histogram of the x positions of the collisions in association with the local pressure

Collisions and local pressure

The 3D model of the quadrupole was used for all shown SIMION simulations. For one run 1,000 ions with mass 50 Da, with a single positive charge and a kinetic energy of 0.3 eV are initialized. As in the SPARTA simulations, only the first 20 mm of the quadrupole are simulated. The kinetic energy is calculated from the velocity of the ions. As shown in Fig. 8 the ions undergo 100 to 250 collisions during the transmission through the quadrupole. The maximum is at approximately 170 collisions. Most of the collisions occur within the first 4 mm due to the high local pressure. Furthermore, the ion density is highest near the x-axis, so that approximate pressure and velocity profiles can be used (see Fig.10). Fig. 11 shows that some ions gain additional kinetic energy during the flight.

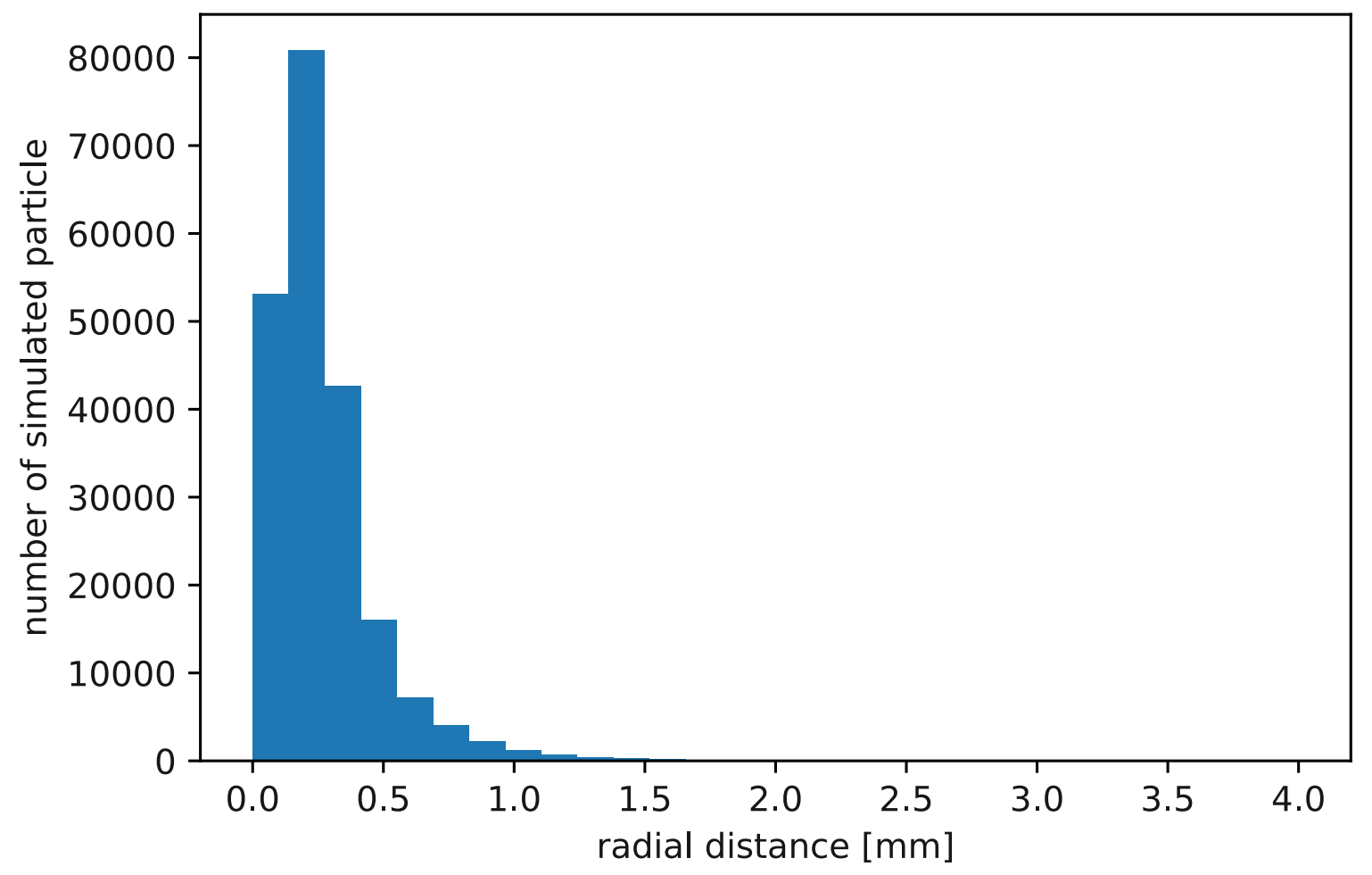

Fig 10: Histogram of the radial distance

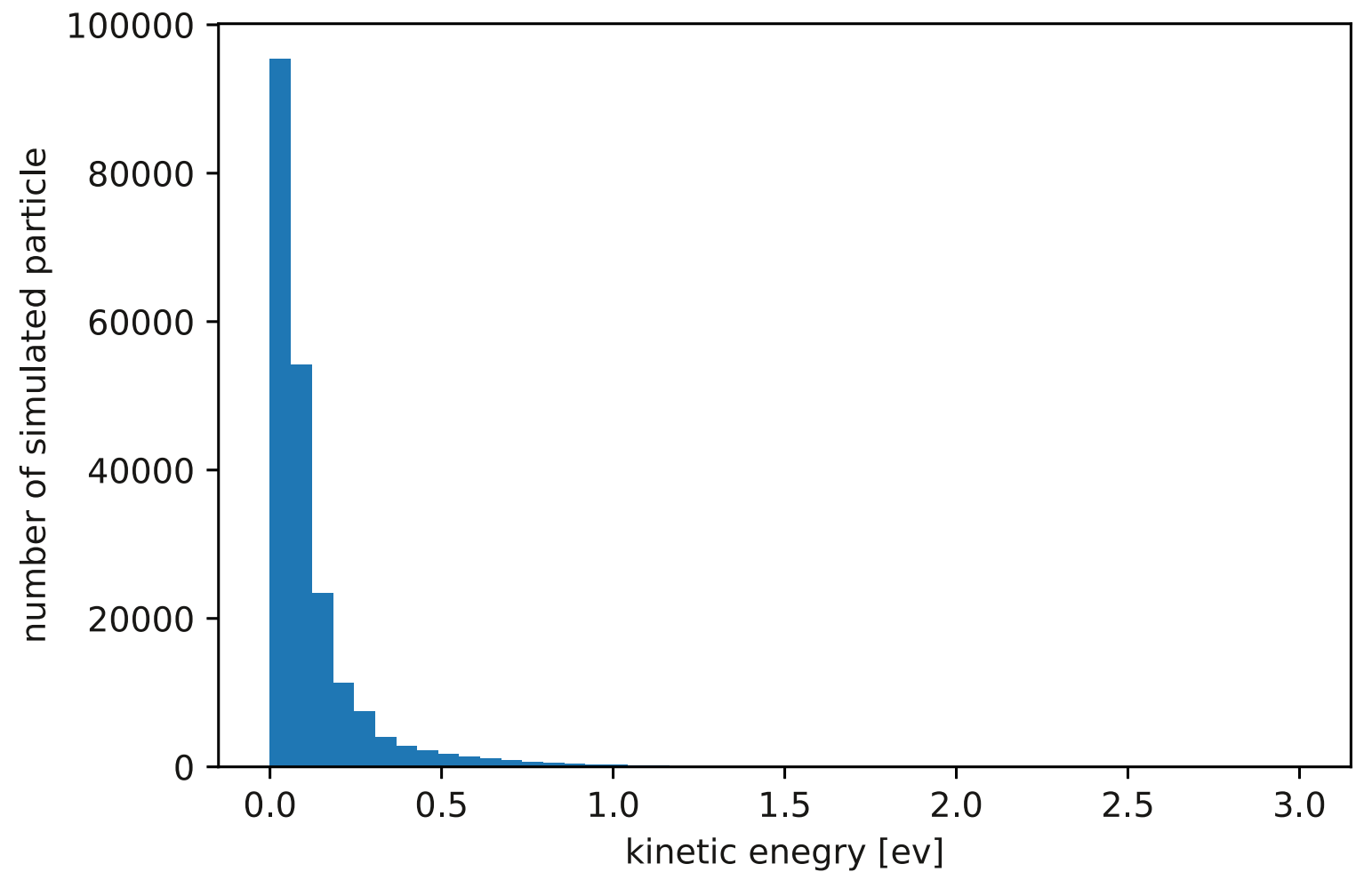

Fig 11: Histogram of the kinetic energy distribution

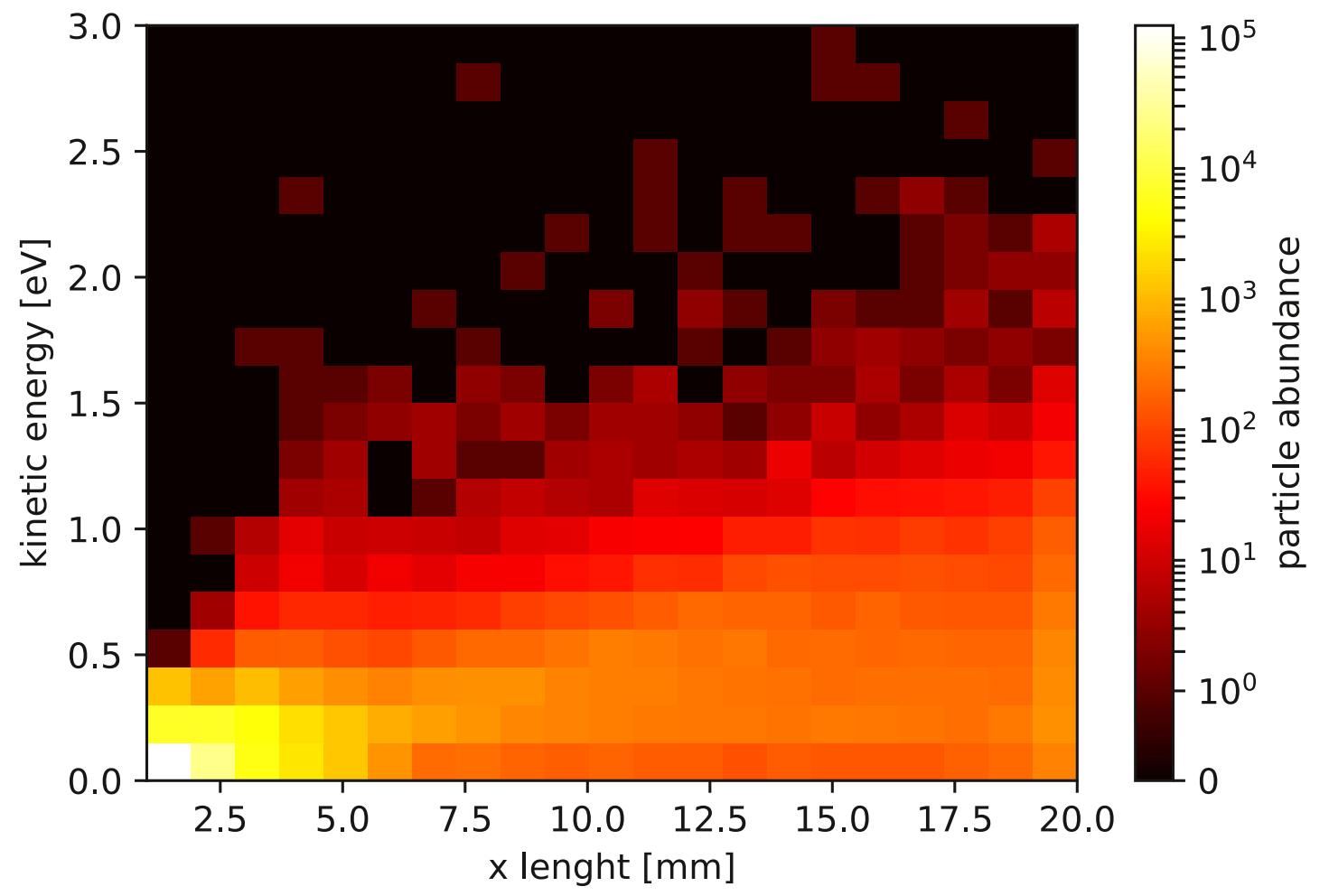

Fig 12: Kinetic energy distribution against the x postions

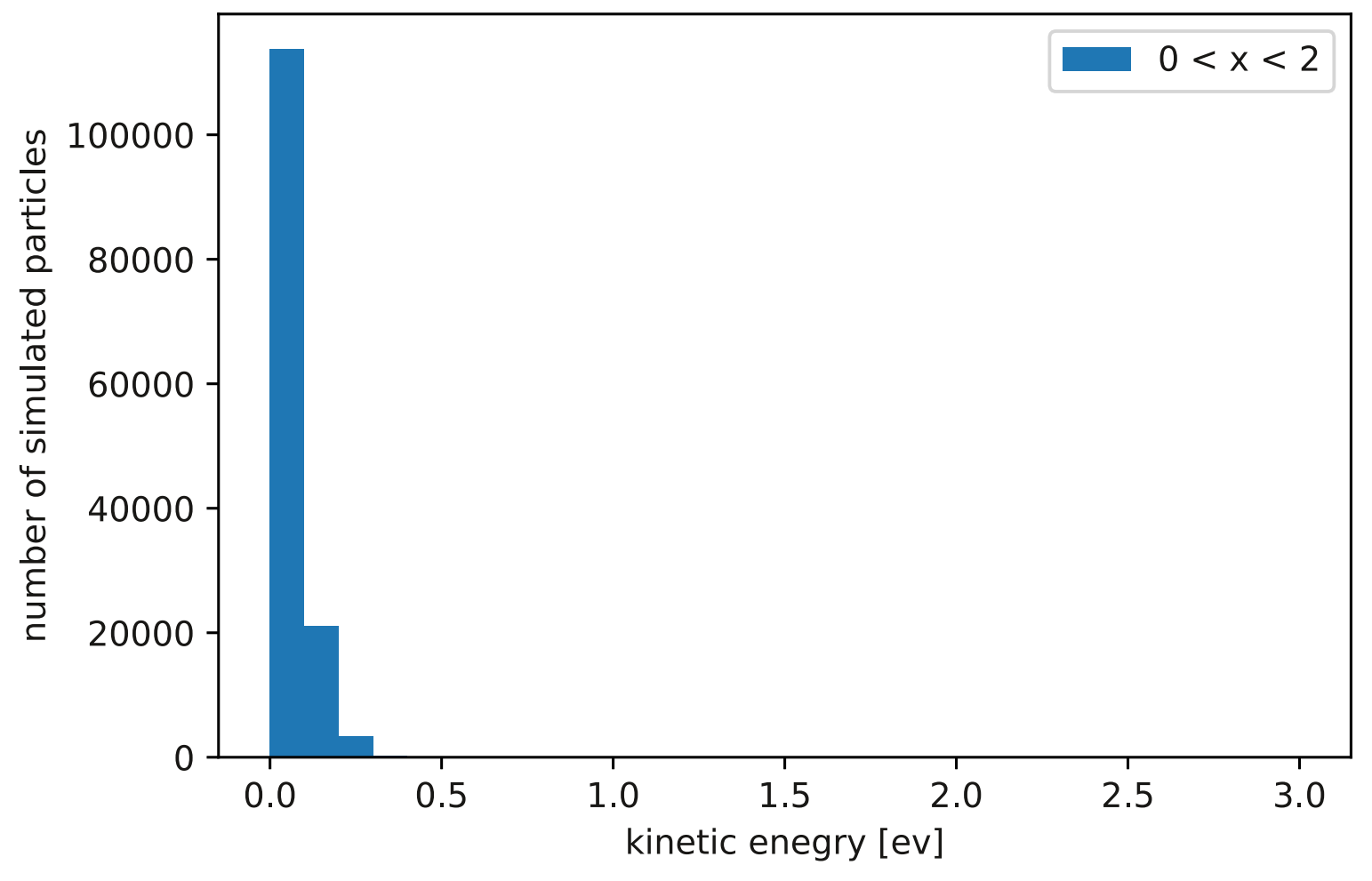

Fig 13: Kinetic energy distribution in the x interval from 0 to 2 mm

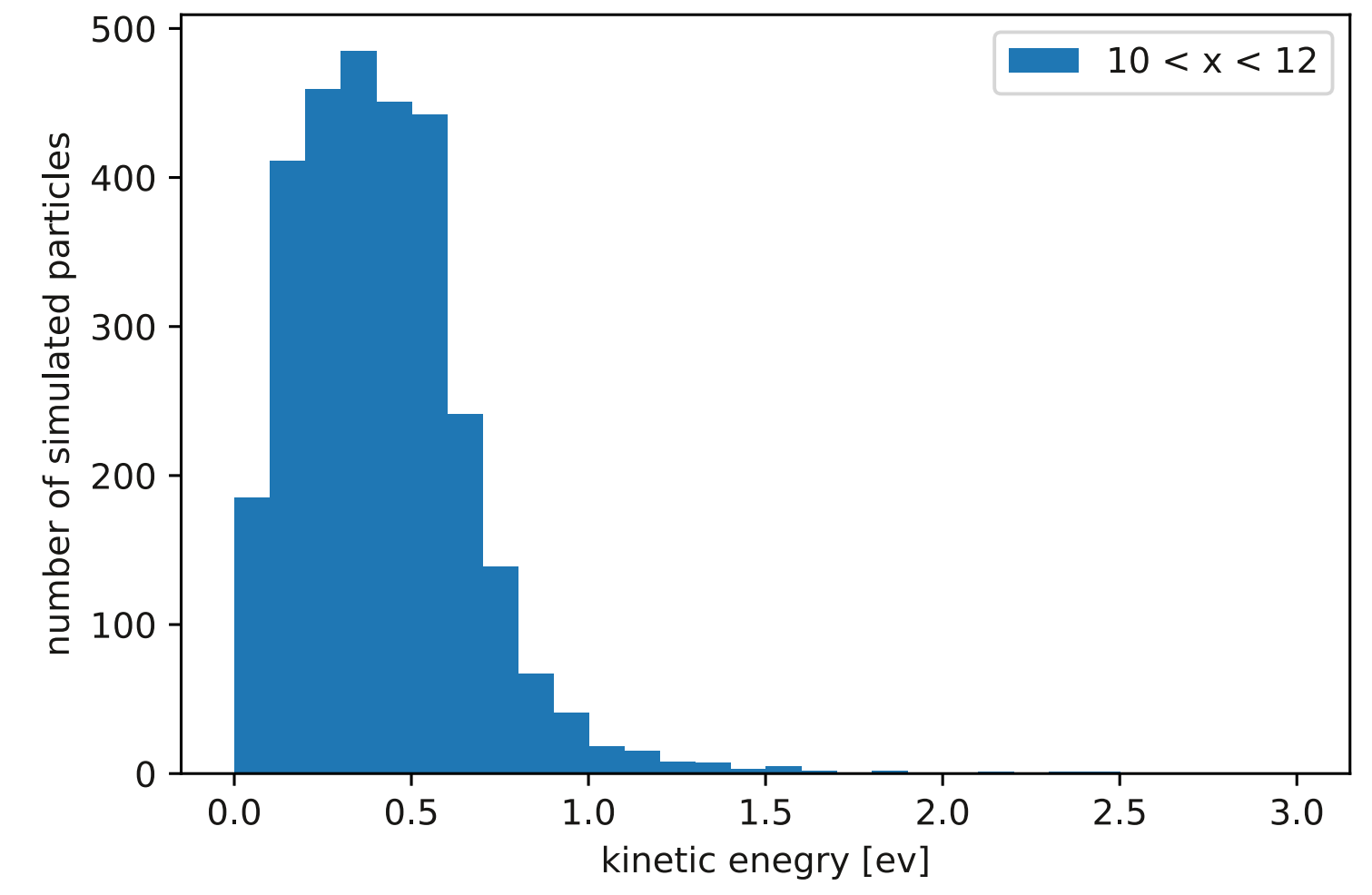

Fig 14: Kinetic energy distribution in the x interval from 10 to 12 mm

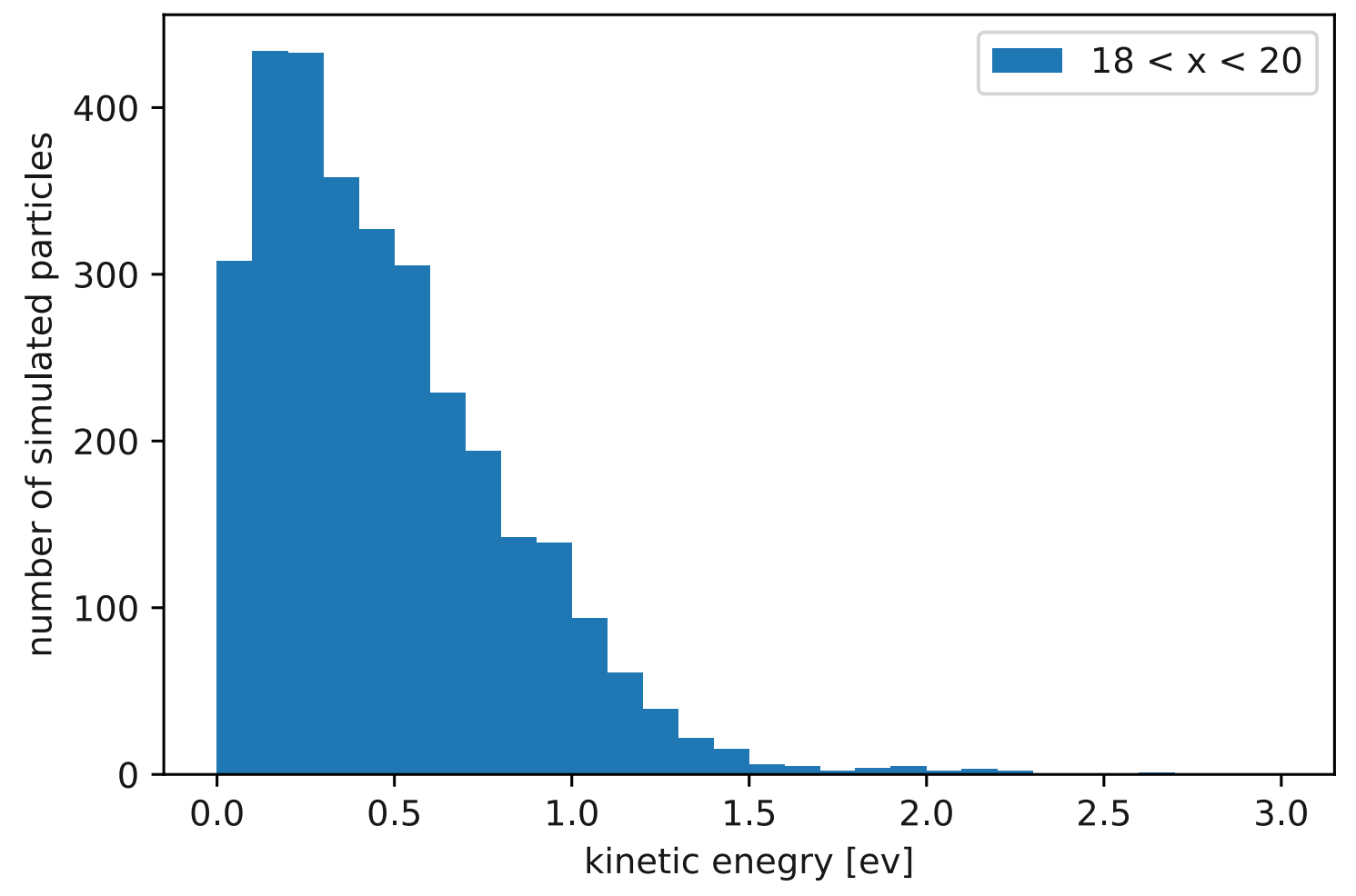

Fig 15: Kinetic energy distribution in the x interval from 18 to 20 mm

Kinetic energy distributions

The kinetic energy and position of all ions is recorded at 1 microsecond intervals. Fig. 12 shows the kinetic energy distribution in dependence of ions' x position. The number of simulated ions is comparatively high at the quadrupole entrance, due to the longer residence time in this region. Fig. 13 to 15 show different intervals of these distributions as histograms. The quantity of simulated ions is high in the entrance region, whereas the kinetic energy is mostly smaller than the start energy (see Fig. 13). By moving forward into x direction, the number of ions per timestep decreases. Furthermore, the amount of collisions, and therefore energy exchange with the background gas, decreases and the energy gain by the electric field gradient increases. That leads to an overall increase of kinetic energy (see Fig. 14). This trend can be observed also at higher x values (see Fig. 15).

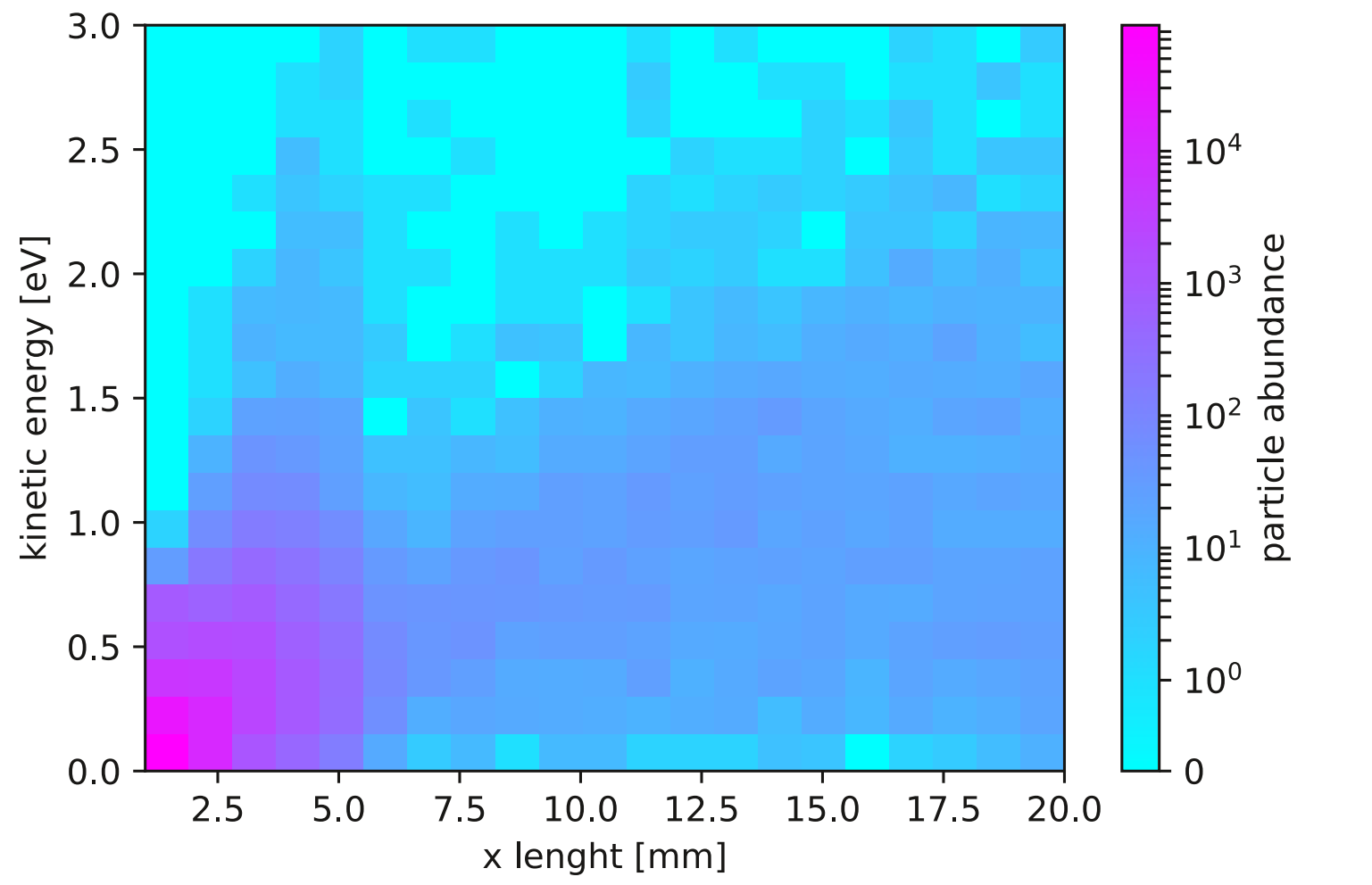

Fig 16: Kinetic energy distribution before a simulated collision againt the x position

The maximum position is almost constant, but the distribution becomes wider. The difference between the kinetic energy distribution in Fig. 12 and in Fig. 16 is that in the latter only colliding ions are recorded. The kinetic energy distributions of the ions and the collisions are comparable. The results are within expectations. Most of the collisions occur in the first few millimeters of the quadrupole. The energy distribution changes during the transport of the ions through the quadrupole due to the electric field gradient and the collisions with the background gas. Subsequent simulations will consider ions with an initial kinetic energy based on a distribution function, which corresponds with the physical distribution at the end of the transfer funnel. Additionally, the effect of the parameters of the transfer quadrupole will be investigated in detail.

Conclusion

- 2D and 3D SPARTA simulations were performed to assess the applicability of 2D axial symmetric simulations
- Pressure and velocity profiles were calculated, analytical functions were fitted to the simulated profiles
- Resulting profiles were successfully incorporated in ion trajctory simulations in SIMION
- Most collisions occur in the higher pressure regime within the first 5 mm of the quadrupole
- Initial SIMION simulations show an increase of the average kinetic energy of the simulated ions under the given conditions inside the quadrupole

Outlook

- Validation of simulation results with experimental data
- Refinement of the pressure and velocity profiles, usage of fully resolved flow data
- Modification of the initial kinetic energy of the ions with a distribution function, which represents the energy of the ions at the end of the transfer funnel
- Investigation of the kinetic energy distribution of the ions in dependence of the electric parameters of the quadrupole
- Moving from SIMION trajectories simulations to a custom ion dynamics simulation framework (IDSimF) to consider space charge effects and improve numerical performance
- Inclusion of a chemical reaction model for simulated particles in IDSimF based on e.g. RRKM
- Development of an interface to directly use SPARTA results (pressure and velocity profiles) as input parameters for the IDSim framework

Literature

1. Scientific Instrument Services, Inc., Ringeos, NJ, www.simion.com.
2. M. A. Gallis, J. R. Torczynski, S. J. Plimpton, D. J. Rader, T. Koehler: Direct Simulation Monte Carlo: The Quest for Speed. 29th Intl Symposium in Rarefied Gas Dynamics.1628, 27 (2014).
3. M. Kintel: Open source software OpenSCAD, www.openscad.org.
4. Autodesk, San Rafael, CA, USA.
5. Ahrens, James, Geveci, Berk, Law, Charles: Paraview: An End-User Tool for Large Data Visualization, isualization Handbook, Elsevier, 2005 and Ayachit, Utkarsh: The ParaView Guide: A Parallel Visualization Application, Kitware, 2015.

Acknowledgement

Support is gratefully acknowledged:

- Deutscher Akademischer Austauschdienst, Bonn, Germany
- German Research Foundation (DFG), BE2124/8-1
- iGenTraX UG, Haan, Germany