Simulation of Ion Kinetic Energies from an NO REMPI Laser Plasma with Spherically Symmetric and Gaussian Beam Geometry

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GDCh AnalytChem

IDSimF

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Introduction & Methods

Pulsed PI (photoionization) sources of appropriate intensity and wavelength are capable of producing charged particle clouds with high-energy photoelectrons. These highly transient phenomena cannot reliably be simulated using CFD or similar methods, which are reliant on equilibrium assumptions. *Kinetic codes*, which directly calculate the trajectories of individual particles, extend simulations into this non-equilibrium regime.

The expansion of an $NO^+ + e^-$ cloud generated by a pulsed REMPI laser source (Figure 1) was simulated using
a) a simplified 1D program and
b) the in-house open Ion Dynamics Simulation Framework **IDSimF**[1].
IDSimF uses a Barnes-Hut method, which was extended with a multipole expansion to allow for bipolar charge distributions. The most relevant output is the *Ion Energy Distribution Function* (IEDF), which was compared between simulations.
A spherically symmetric and a physically more accurate *Gaussian beam shape* starting distribution were modeled. Particles were initiated at uniform density in the spherical case, and according to both quadratic intensity scaling and a (1+1) REMPI kinetic model[2] for the beam simulations.

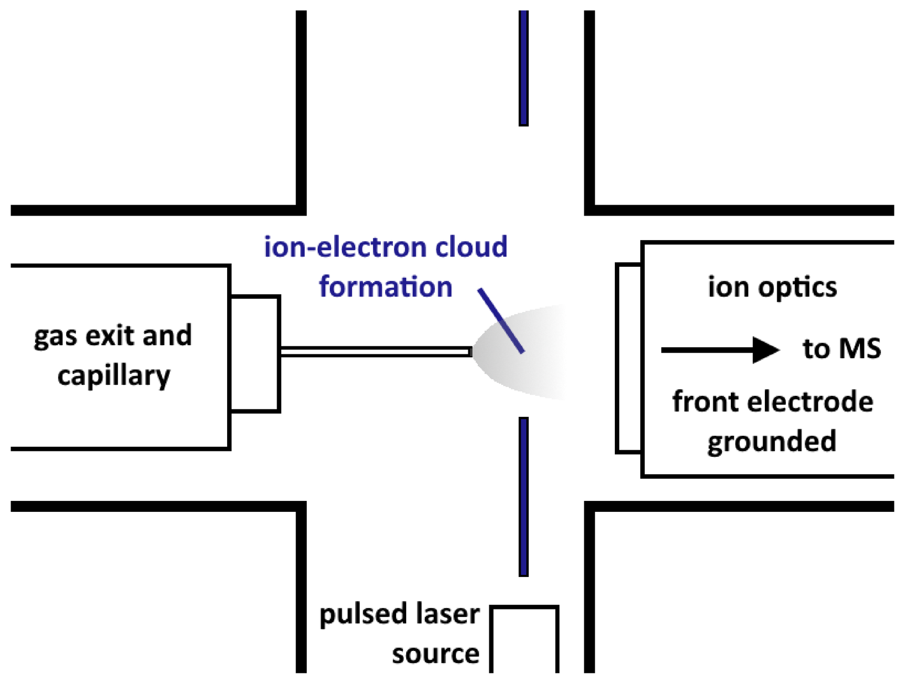

Figure 1: NO REMPI laser experiment

Results

Despite the huge differences in simplification between the simple 1D model and IDSimF, results for EEDFs and IEDFs were in good agreement for a spherical starting distribution (see Table 1).
Higher initial charge densities generally yielded higher deviation between the two models, which could be explained by the increased relevance of particle-particle interactions ("Coulomb collisions") missing in 1D and at least partially handled explicitly in IDSimF. Average and maximum kinetic energies are used to represent IEDFs.

Table 1: Post-expansion ion kinetic energies (KE) for different scenarios

Simulation model	Particle density $\cdot 10^{-13}$ m^3	avg. KE	max. KE
1D	1.19	1.31eV	2.47eV
	2.39	1.51eV	3.29eV
	4.77	1.60eV	4.24eV
IDSimF spherically symmetric	1.19	1.42eV	2.81eV
	2.39	1.58eV	3.53eV
	4.77	1.75eV	4.73eV

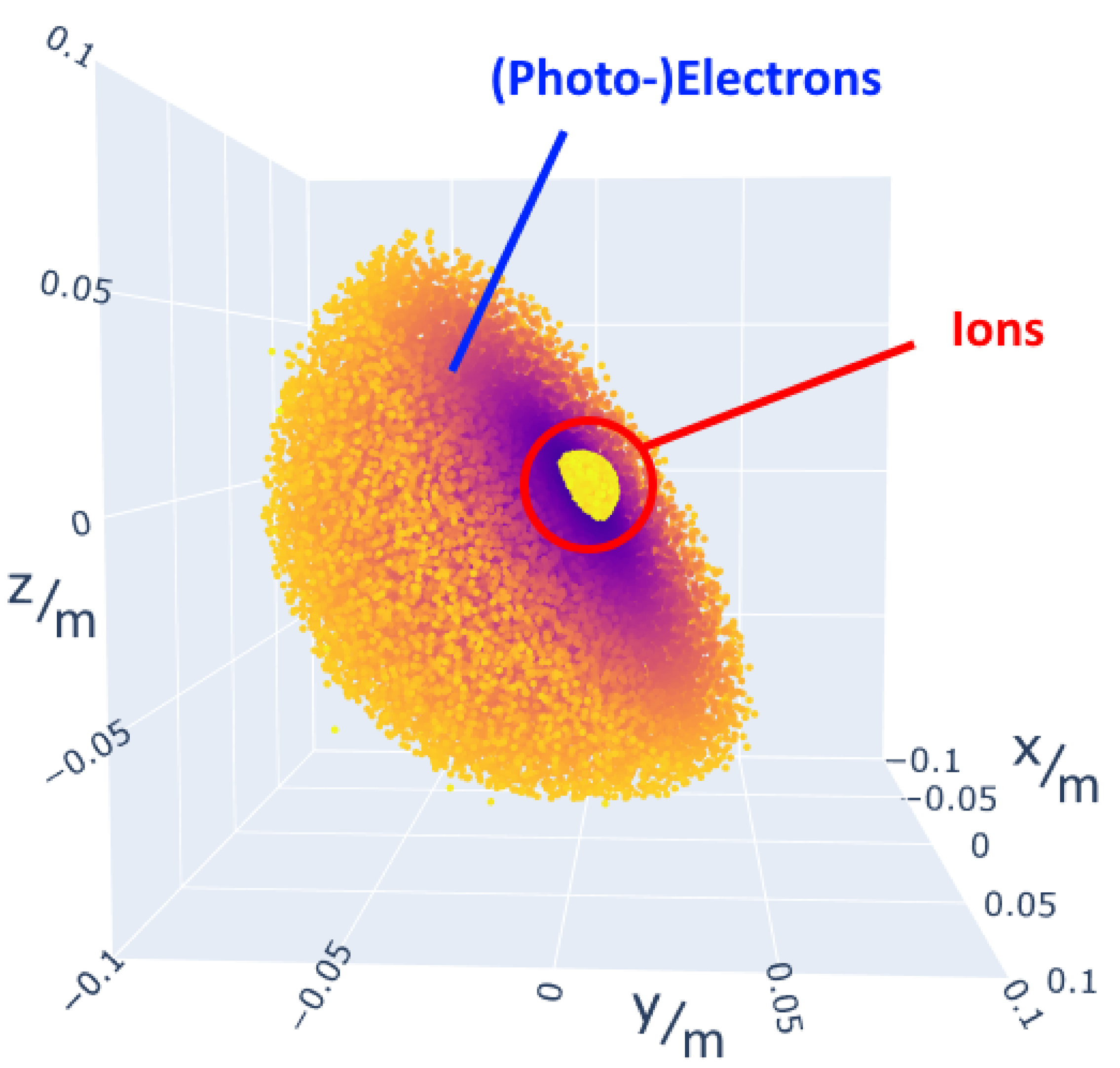

Figure 2: Slice through the particle distribution of a spherical expansion simulated with **IDSimF**

- Multipole treecode is accurate for bipolar charge distributions even with $\theta = 0.9$.
- Ca. 1.5 - 2.0 times higher computational cost compared to monopole tree.
- Performance optimization for higher initial particle densities achieved by downscaling of the simulation timeframe (artificial decrease of ion m/z).
- Downscaling reduces time-to-interact, probably eliminating the greatest source of deviation between 1D and IDSimF.

The more physically accurate Gaussian beam shape, as shown at a late stage in the plasma expansion in Figure 4, had a lot more particle density crammed into its focus region ($r = 125\,\mu$m), resulting in higher peak kinetic energies. At the employed laser intensities, a saturation of the excited A $^2\Sigma^+$ state in NO is expected, resulting in a failure of naive quadratic intensity scaling. The difference between the kinetic model according to Swain et al.[2] and naive J^2 scaling is documented in Figures 3 and 5.

The attenuated energy redistribution from electrostatically bound photoelectrons to the expanding ion cloud in the focus region becomes evident.

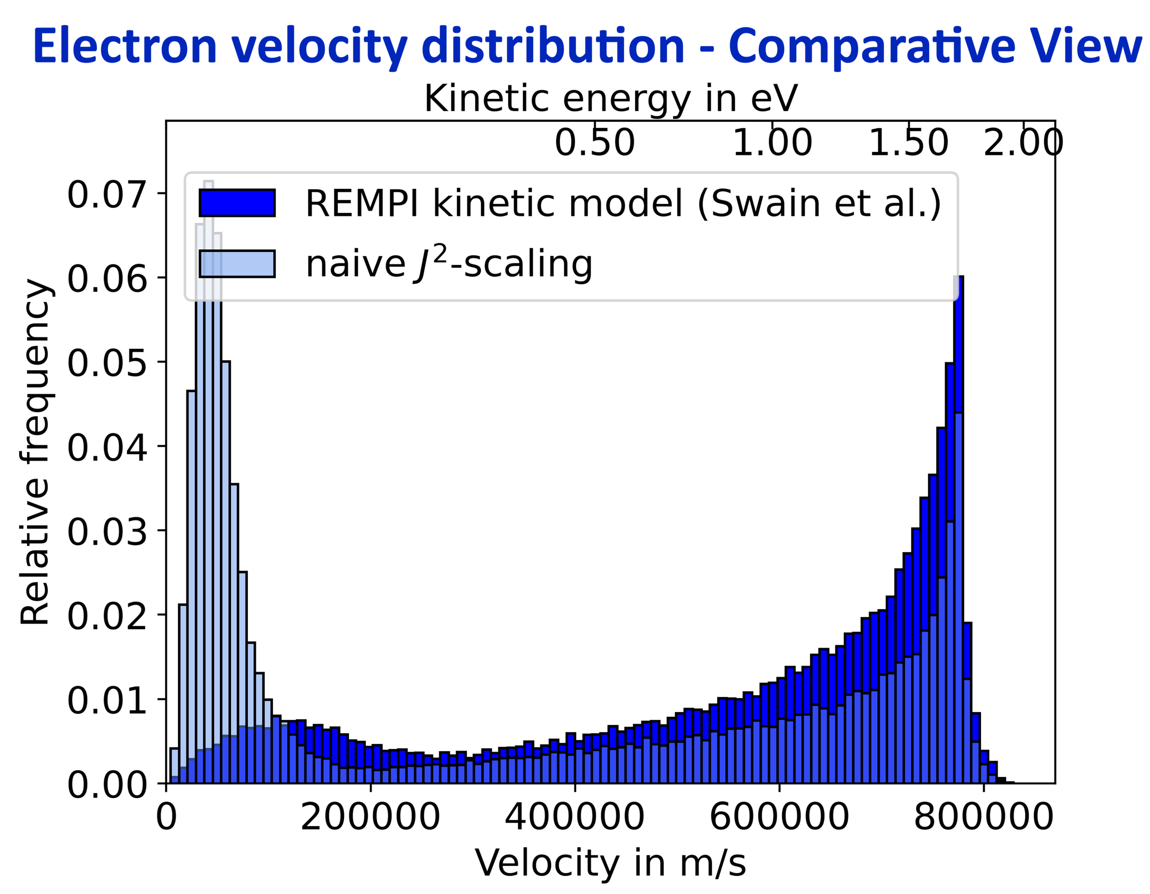

Figure 3: Post-expansion EEDFs in **IDSimF** for 1e7 particles distributed including saturation vs naively

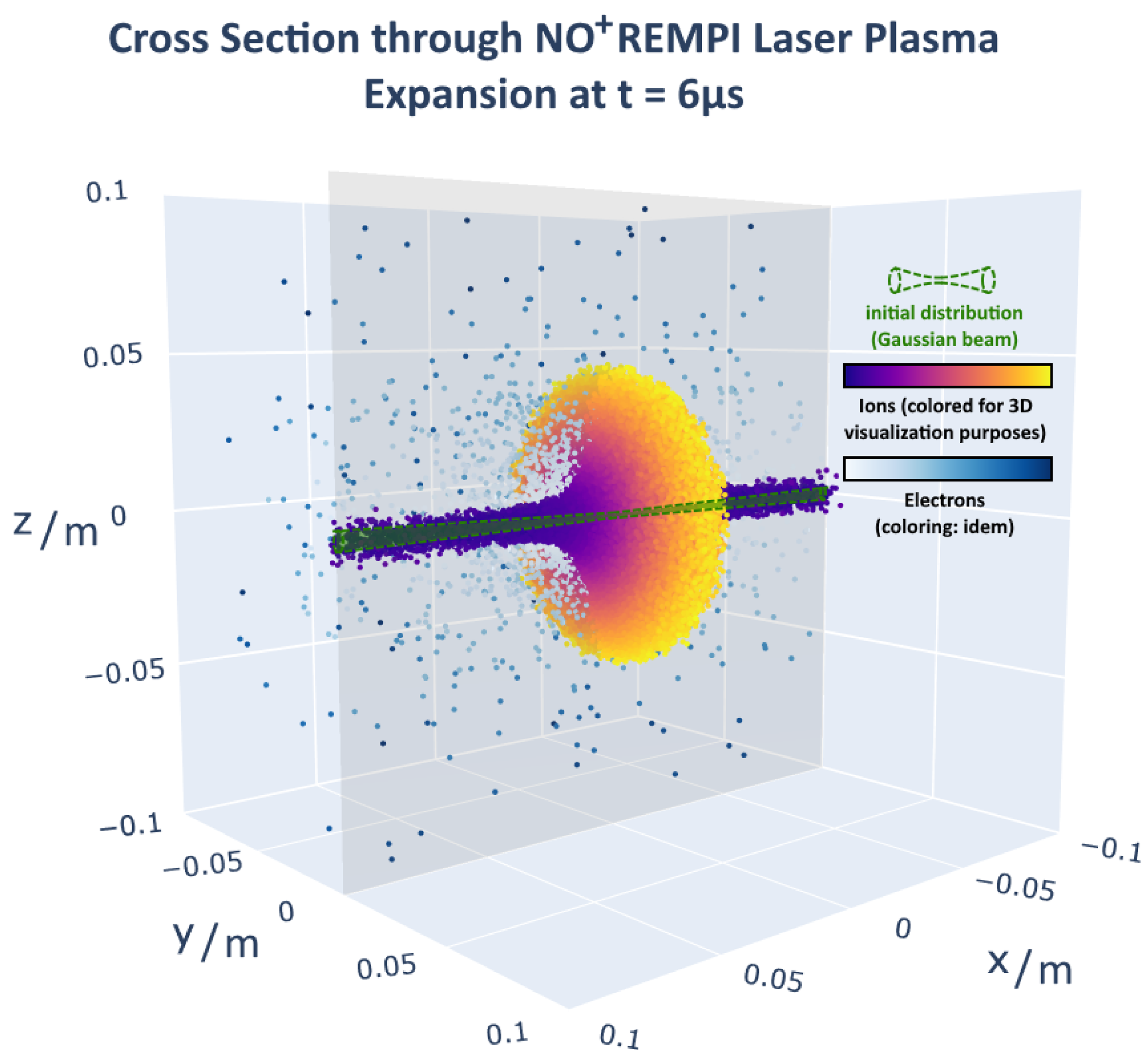

Figure 4: 3D cross section through the expansion of the Gaussian beam distribution in **IDSimF**

The appearance of a fast ion "front" effectively outrunning the plasma bulk is a known phenomenon for the expansion of transient plasmas into vacuum.[3]

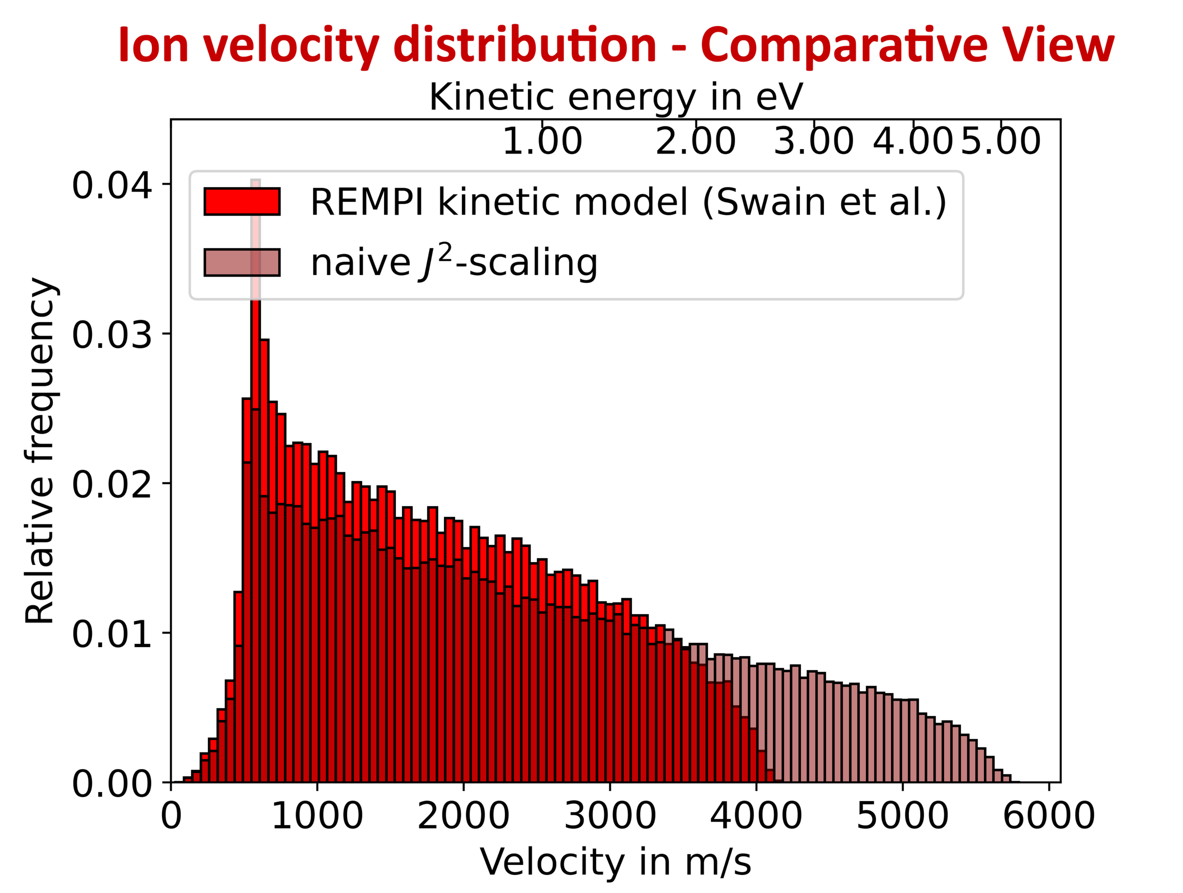

Figure 5: IEDFs for the same set of simulations (see left side)

Conclusion and Outlook

Modifications to the treecode enabled the simulation of bipolar charge distributions at reasonable computational cost. Spherically symmetric simulations in 1D and IDSimF yielded similar IEDFs at lower particle densities, while the Gaussian beam results deviated significantly from the 1D model, emphasizing the need for 3D modeling of more complex charge distributions. Inclusion of a kinetic model was necessary and successful at the experimental laser intensities.

Literature and COI Declaration

[1] IDSimF; Ion Dynamics Simulation Framework; https://idsimf.readthe- docs.io/en/latest/
[2] Swain, S. (1979). *A Simple Model for Multiphoton Ionisation*. *JPB*, *12*(19), 3201-3228.
[3] Crow, Auer & Allen (1975). *The Expansion of a Plasma into a Vacuum*. *JPP*, *14*(1), 65-76.

Financial support within the 14AMI project funded by the BMBF (16MEE0370) and the EU-CHIPS JU (101111948) is gratefully acknowledged. The author wishes to thank the Analytical Group of the Society of German Chemists (GdCh) for sponsoring the attendance of this conference.