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Implementation of a Particle-in-Cell based space charge solver and electron chemistry model in an open simulation Framework (IDSimF)

Maja Hammelrath*, Walter Wißdorf, Thorsten Benter
*hammelrath@uni-wuppertal.de

Introduction

Particle-In-Cell (PIC) is a numerical technique used to model the motion of charged particles in self-consistent electromagnetic or electrostatic fields. It is a grid based method wherein discrete simulation particles move through continuous space, whereas properties such as potential or electric field are determined only at the grid nodes and need to be extrapolated to the positions of the particles.

Simulated particles generally encounter and interact with other particles, both neutral and charged. Collision and reaction models serve to determine the occurrence and effects of such interactions on the particle trajectories.

Methods

IDSimF
The Ion Dynamics Simulation Framework (IDSimF) is an open-source software written in C++, containing various models and modules for the simulation of ion trajectories. It provides different simulation applications, each its own C++ program representing a different experimental setup [1]. All simulations shown here were performed using IDSimF.

SailFFish
The open-source FFT-Poisson solver SailFFish is integrated with IDSimF to solve the Poisson equation on a rectangular grid with regular grid spacing in order to determine the electric potential at the grid nodes [2].

The Particle-in-Cell solver

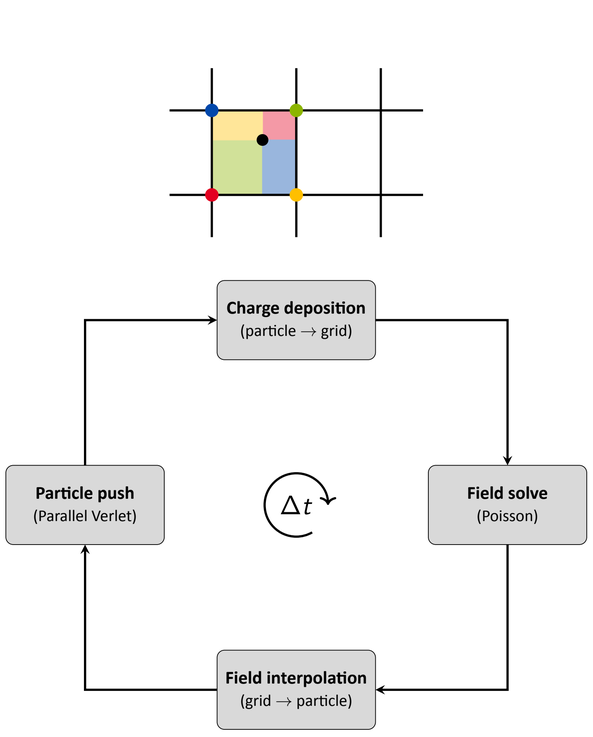

Figure 1: PIC simulation cycle showing charge deposition, field solve, field interpolation, and particle push.

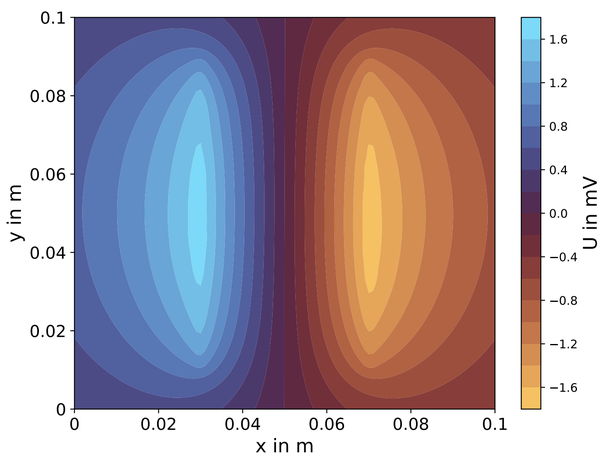

Figure 2: Contour plot showing the potential distribution induced by two groups of opposing charges (50k each) placed opposite of each other.

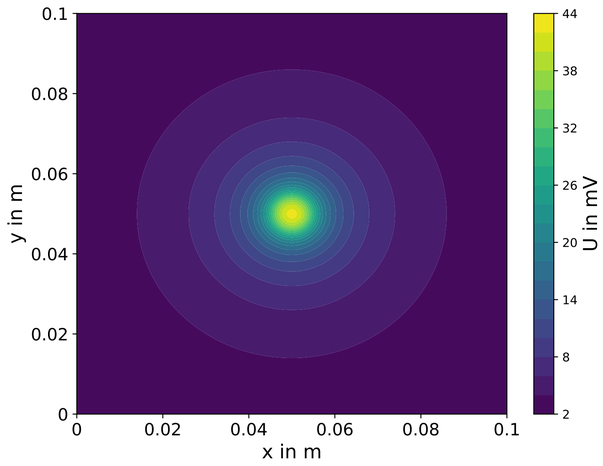

Figure 3: Contour plot showing the potential distribution induced by one group of 100k charges placed in a sphere at the center of the domain.

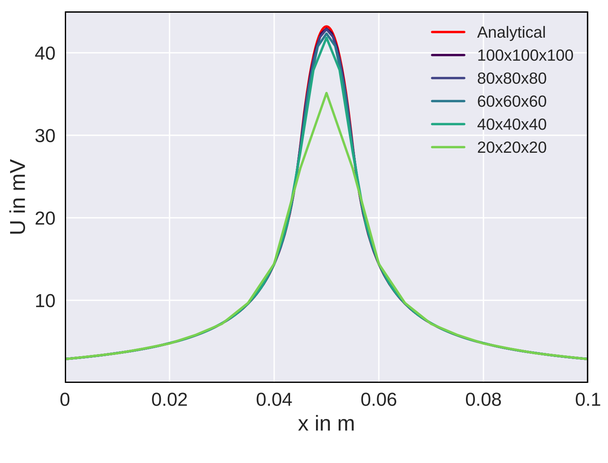

Figure 4: Potential contour for different grid resolutions compared to the analytical solution of a potential sphere.

- To validate the charge deposition and potential solution steps of the field solver, charged particles were placed in different arrangements in the simulation domain (single sphere and two opposing groups)
- The potential lines in the contour plots follow the expected distribution (potential sphere and pseudo plate capacitor) and can be further compared with the analytical solution of the field
- The accuracy of the solution provided by the solver is dependent on the grid resolution
- The lower the resolution, the higher the deviation from the analytical solution

Collisions between electrons and neutrals

- The probability P_i for a given electron reaction i to occur is approximated by [3]:

$$P_i = n_g v_e \sigma_i \Delta t \qquad (1)$$

n_g: neutral density
v_e: electron velocity
σ_i: cross section
Δt: time step length

- The probability is compared with a randomly drawn number (Monte-Carlo approach)
- Isotropic scattering of the incident electron is performed in the center-of-mass frame

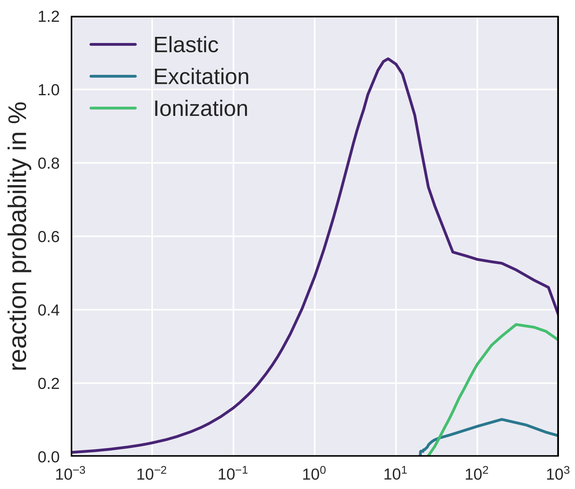

Figure 5: Reaction probability of electrons in helium at a pressure of 10 Pa and a time step length of 500 ns.

- The Townsend coefficient, i.e. a measure of how many new ion pairs an electron can create in a neutral gas, is acquired by counting the number of ionization events
- Simulated Townsend coefficients are compared with data obtained using BOLSIG+ [4]
- BOLSIG+ and simulation results correlate up to 400 Td but begin to deviate for higher fields

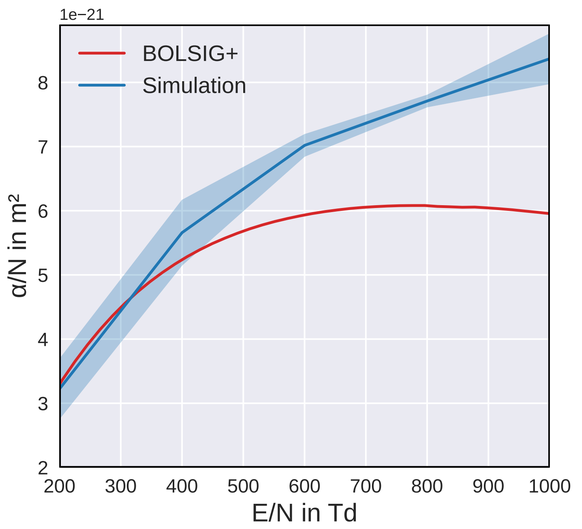

Figure 6: Townsend coefficient as a function of reduced electric field in helium at 10 Pa.

Conclusion

- The Particle-in-Cell solver generally yields the correct potentials for different particle distributions so long as the grid resolution is sufficient
- The Monte-Carlo electron collision model in IDSimF accurately reproduces BOLSIG+ Townsend coefficients for low to moderate reduced electric fields
- Caus of deviation at higher field strengths is not clear but indicates areas for further refinement and development

References

[1] M. Rajkovic et al., IDSimF: An Open-Source Framework for the Simulation of Molecular Ion Dynamics in Mass Spectrometry and Ion Mobility Spectrometry, Universität Wuppertal, 2024

[2] J. Saverin, SailFFish : A lightweight, parallelised fast poisson solver library, Technische Universität Berlin, 2023

[3] K. Nanbu, Probability Theory of Electron–Molecule, Ion–Molecule, Molecule–Molecule, and Coulomb Collisions for Particle Modeling of Materials Processing Plasmas and Gases, Tohoku University, 2000

[4] https://www.bolsig.laplace.univ-tlse.fr/index.html