Applied and Computational Mathematics | RWTH AACHEN UNIVERSITY

# Bachelor/Project Thesis

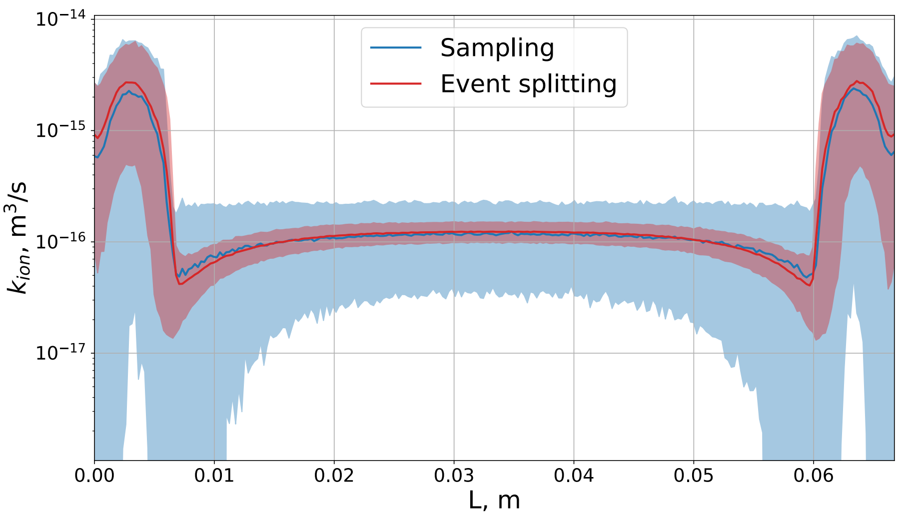
## Moment-preserving particle merging algorithms

## Motivation

Rarefied flows play a crucial role in numerous industrial applications and research areas, from nano-scale devices and semiconductor manufacturing to spacecraft re-entry, satellite design, and planetary science.
Standard computational fluid dynamics methods are unsuitable for simulation of such flows, and other approaches, such as the particle-based Direct Simulation Monte Carlo (DSMC) method [1], need to be applied. In this work we wish to improve certain aspects of the DSMC method pertaining to the control of the number of particles in a simulation.

## DSMC

New versions of the DSMC method [2,3] allow for great flexibility in terms of modelling of various physical processes occurring in gases, such as ionization. However in these formulations of the method, the particle count increases exponentially unless somehow controlled. This periodic reduction in the particle count is referred to as particle merging and it decreases the quality of the simulation, as information is inevitably lost. New particle merging algorithms aim to minimize this negative impact of merging [4], but have not been well investigated in terms of stability and computational efficiency.




Example of a DSMC simulation of a radio-frequency plasma: use of a new collision scheme [3] ("Event splitting") leads to a significant reduction in the uncertainty in the simulation, but requires improved merging algorithms.

## Task

The core task is to study the properties of the newly proposed merging scheme [4], as well as modify it to improve its numerical stability and accuracy. These modifications are to be implemented in the open-source `Merzbild.jl` code (github.com/merzbild/Merzbild.jl), a modular DSMC code written entirely in Julia.

## Outcomes

A successful thesis will lead to a joint publication in one of the major journals in the field (e.g. Journal of Computational Physics, Journal of Scientific Computing). You will also contribute to an open-source project, as well as learn the fundamentals of DSMC simulations.

## Your profile

- Interest in applied mathematics and simulation tools
- Code development experience
- Good grades in relevant subjects

## Contact information

Sounds interesting? Drop me an e-mail!
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## References

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2. Araki, S. J., & Martin, R. S. (2020). Interspecies fractional collisions. Physics of Plasmas, 27(3). DOI: 10.1063/1.5143145
3. Oblapenko, G., Goldstein, D., Varghese, P., & Moore, C. (2022). Hedging direct simulation Monte Carlo bets via event splitting. Journal of Computational Physics, 466, 111390. DOI: 10.1016/j.jcp.2022.111390
4. Oblapenko, G. (2024). A Non-Negative Least Squares-based Approach for Moment-Preserving Particle Merging. arXiv preprint arXiv:2412.12354. DOI: 10.48550/arXiv.2412.12354