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Improving PIC-DSMC Simulations of RF Plasmas via Event Splitting

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Talk outline

- **Motivation**
- **PIC-DSMC overview**
  - Variable-weight DSMC
  - Event splitting
  - Overview of cross-sections
- **Numerical results**
  - 0-D
    - Xenon
    - Helium
  - 1-D
    - Helium
- **Conclusions**

Introduction / Motivation

- Cannot apply fluid-based models in rarefied regimes without losing accuracy of modelling
- Particle-based methods (PIC-DSMC) are subject to stochastic noise
- This can affect accuracy of modelling of
  - Ionization
  - CEX collisions
  - Scattering events relevant to plume impingement, air-breathing EP intake design
  - Transient processes in general

- Thus, aim of current work is to present a method for **improved modelling** of **low-probability processes** within PIC-DSMC, apply to several benchmark problems to show benefits of method

DSMC

Basic ideas:

- Model (rarefied) gas by simulating motion of large number of computational particles
- Each particle represents $F_{num} = const$ real-life molecules
- Separate convection, collision and acceleration steps
- Collisions performed stochastically
- NTC/MF/Bernoulli trial collision schemes: cost linear in number of particles (e.g., $F^*_{num} = F_{num}/10$→10x more particles→10x increase in cost)

References:

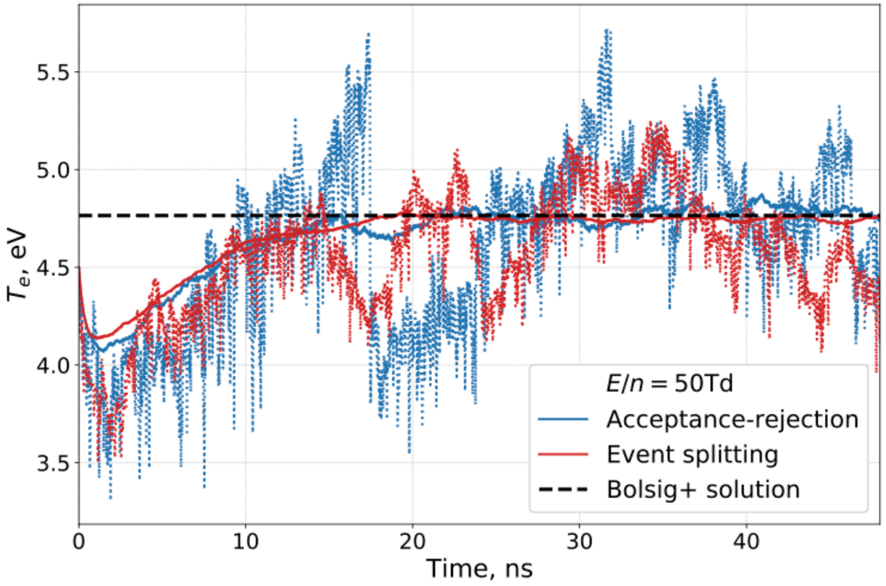
- G. A. Bird, Molecular gas dynamics and the direct simulation of gas flows, 1994
- M. S. Ivanov, S. V. Rogasinsky, Russian Journal of numerical analysis, 1988
- S. K. Stefanov, SIAM Journ. Sci. Comp., 2011

DSMC issues

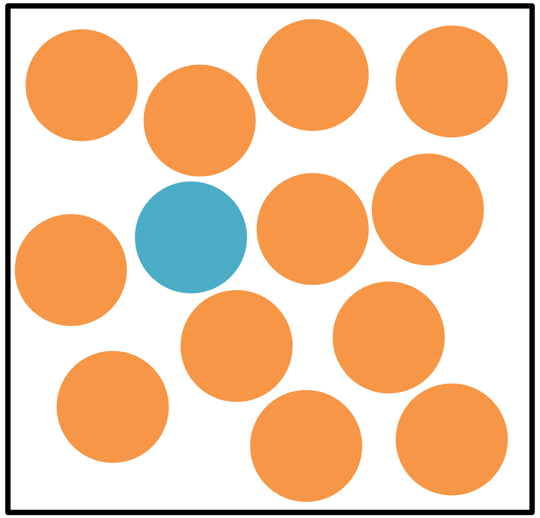
Stochasticity-related (aka "noise"):
- Low-speed flows
- Transient flows
- Coupling with CFD
- Particle-in-Cell (affects field solver)

Fixed F_{num}-related (hard to resolve trace populations):
- Trace chemical species
- Excited internal states
- High-velocity distribution function tails

PIC-DSMC simulations can have **(almost) all** of the above!



Oblapenko et al., Journ. Comp. Phys., 2022



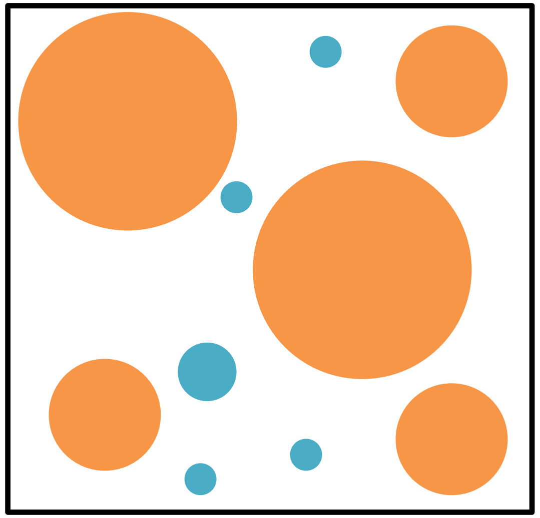
Variable weight DSMC

Idea: solve fixed F_{num}-related problems by allowing computational particles to represent **arbitrary** amounts of real-life particles

Resolves (mostly) issue of capturing trace populations

But new problems arise:

- Particles need to be split during collisions, which leads to growth in number of particles
- Controlling particle counts requires either conserving energy "on average" or particle merging
- Particle merging incurs additional computational cost, distorts velocity distribution function



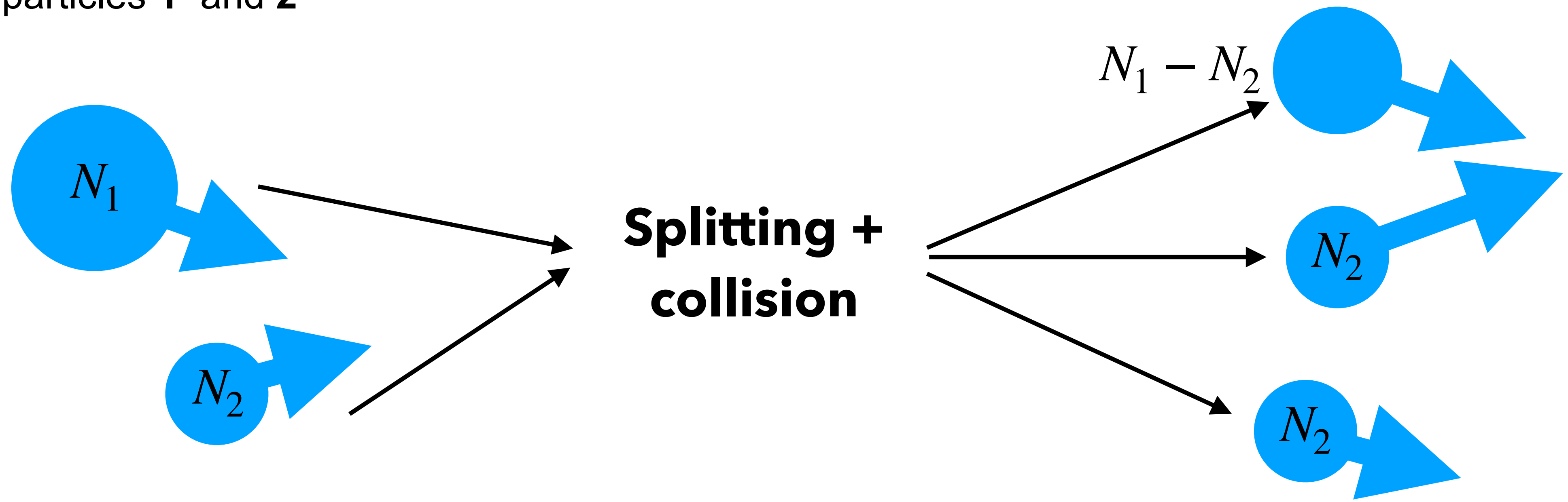
References:

- I. D. Boyd, Journ. Thermophys. Heat Transf., 1996
- S. Rjasanow, W. Wagner, Journ. Comp. Phys., 1996
- S. J. Araki, R. S. Martin, Phys. Plasmas, 2020

Particle splitting schematic

If particle **1** represents N_1 molecules, particle **2** represents N_2 molecules (and $N_1 > N_2$), then during collisions only N_2 molecules actually collide

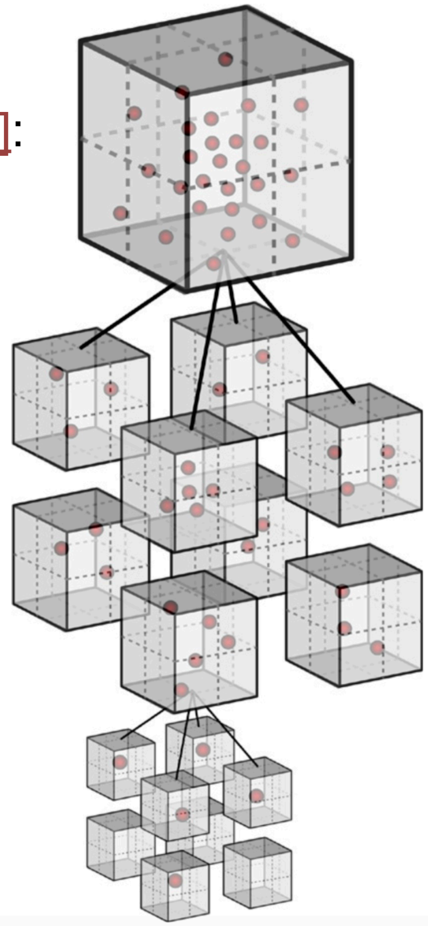
Have to split particle **1** into two particles **1'** and **1"** with weights N_2, $N_1 - N_2$, collide particles **1'** and **2**



Merging schematic

One of the (many) possible approaches
Octree merging [R. Martin, J.-L. Cambier, Journ. Comp. Phys., 2016]:

- Divide velocity space into octants
- Subdivide octants based on number density inside
- In each suboctant, can replace N (>2) particles with 2 particles (need 2 particles for conservation)
- Continue subdivision until target # of particles is reached
- Cost is $\mathcal{O}(n)$ (depends on particle sorting algorithm)



R. Martin, J.-L. Cambier, Journ. Comp. Phys., 2016

Event splitting

Outline

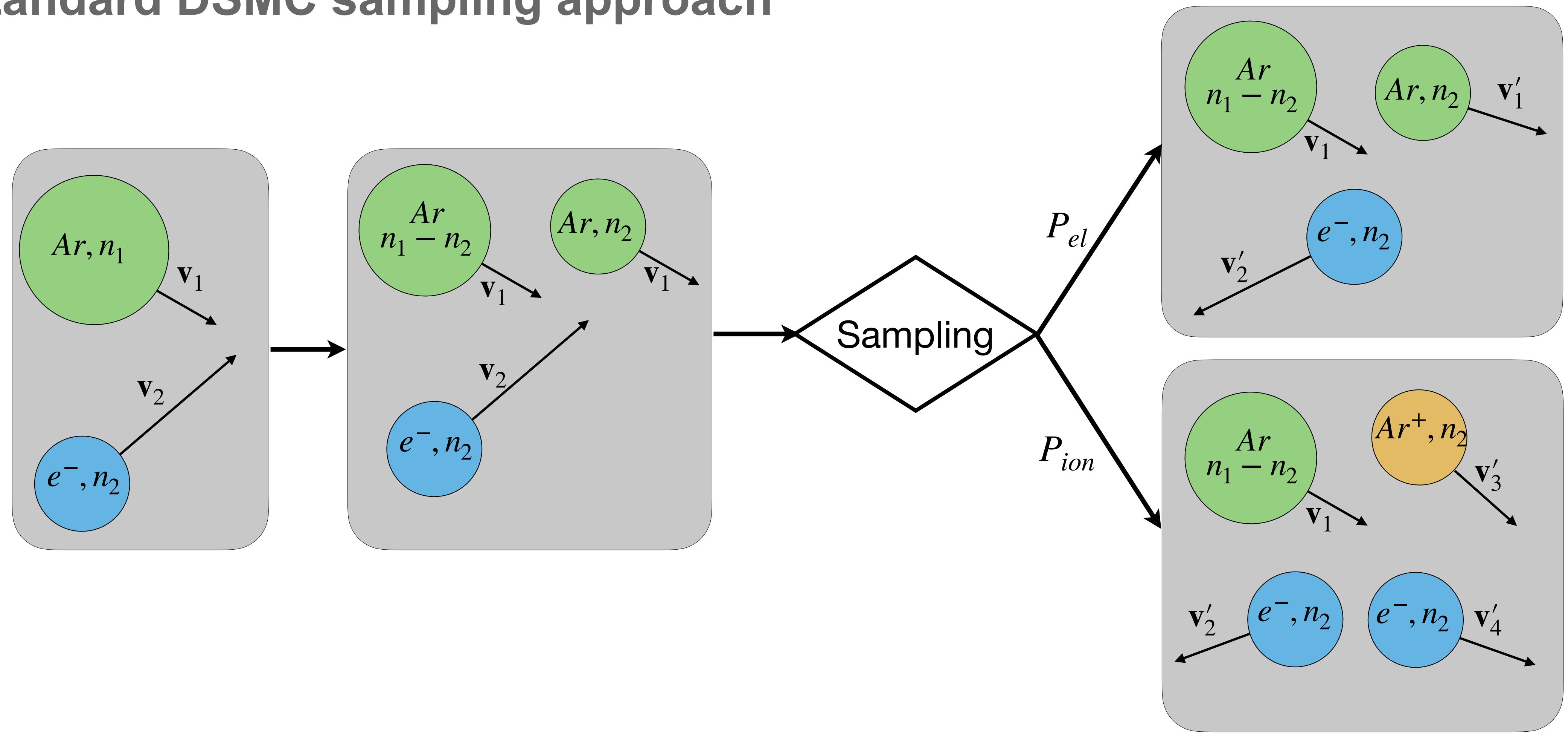
- Suppose we have N_p possible processes that can occur during a collision (e.g. elastic collision, ionization reaction, vibrational transition, etc.), and the corresponding probabilities are $\{p_i\}_{i=1}^{N_p}$
- Standard DSMC “all-or-nothing” approach: sample process type based on $\{p_i\}_{i=1}^{N_p}$ and model **only** that collision process
- But we’re doing particle splitting anyway, so what if we split particles proportionally to $\{p_i\}_{i=1}^{N_p}$ and simulate **all** possible collision outcomes?

This is what we call “**event splitting**” (similar reasoning also be applied to boundary conditions and scattering)

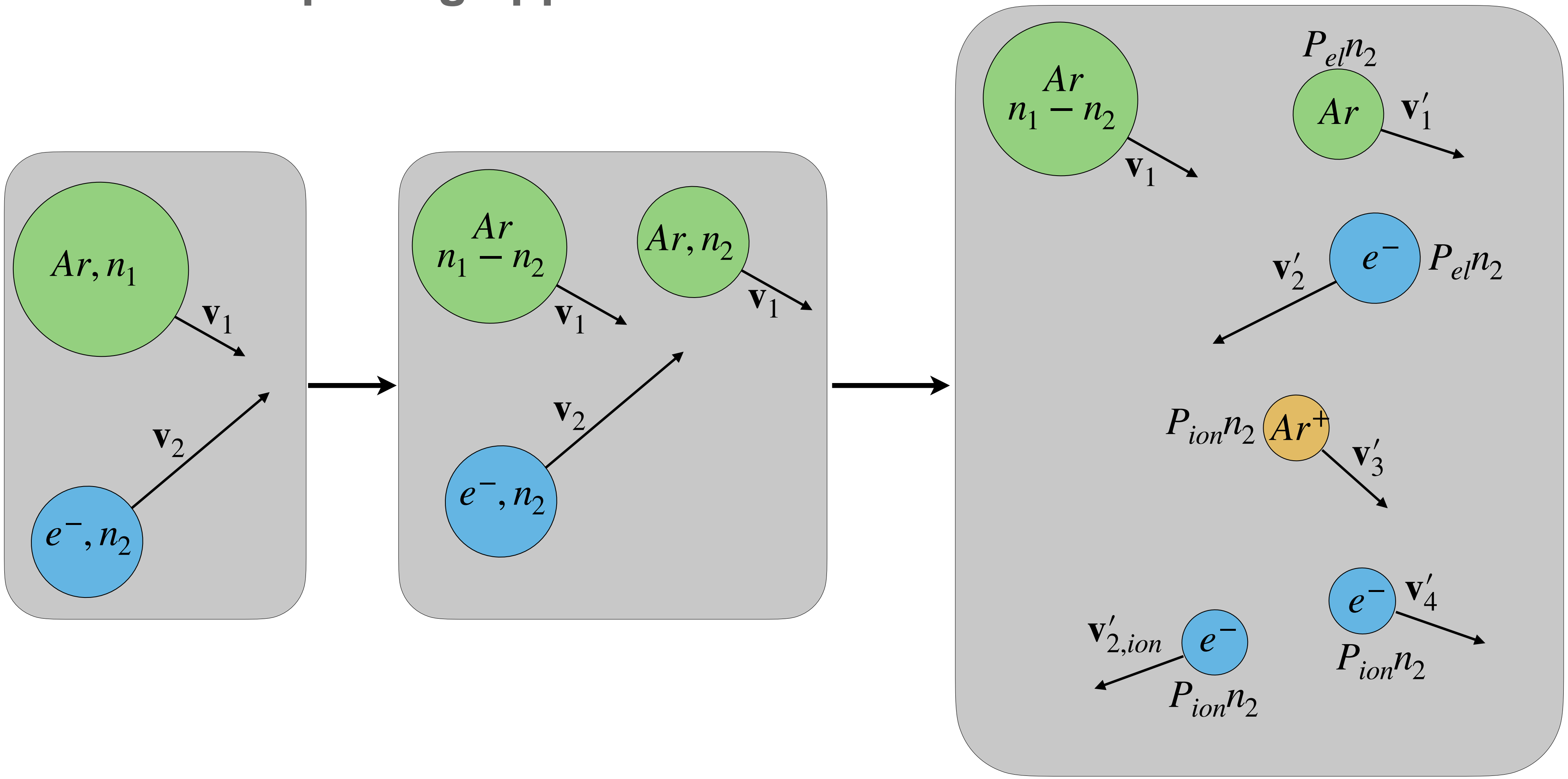
References:

- G. Oblapenko et al., Journ. Comp. Phys., 2022
- G. Oblapenko et al., Scitech 2022 Proceedings, 2022

Standard DSMC sampling approach



New DSMC event splitting approach



Event splitting motivation

Why do event splitting?

- Improve simulation of low-probability processes
- Reduce need for particle cloning, since we create more particles during a collision step

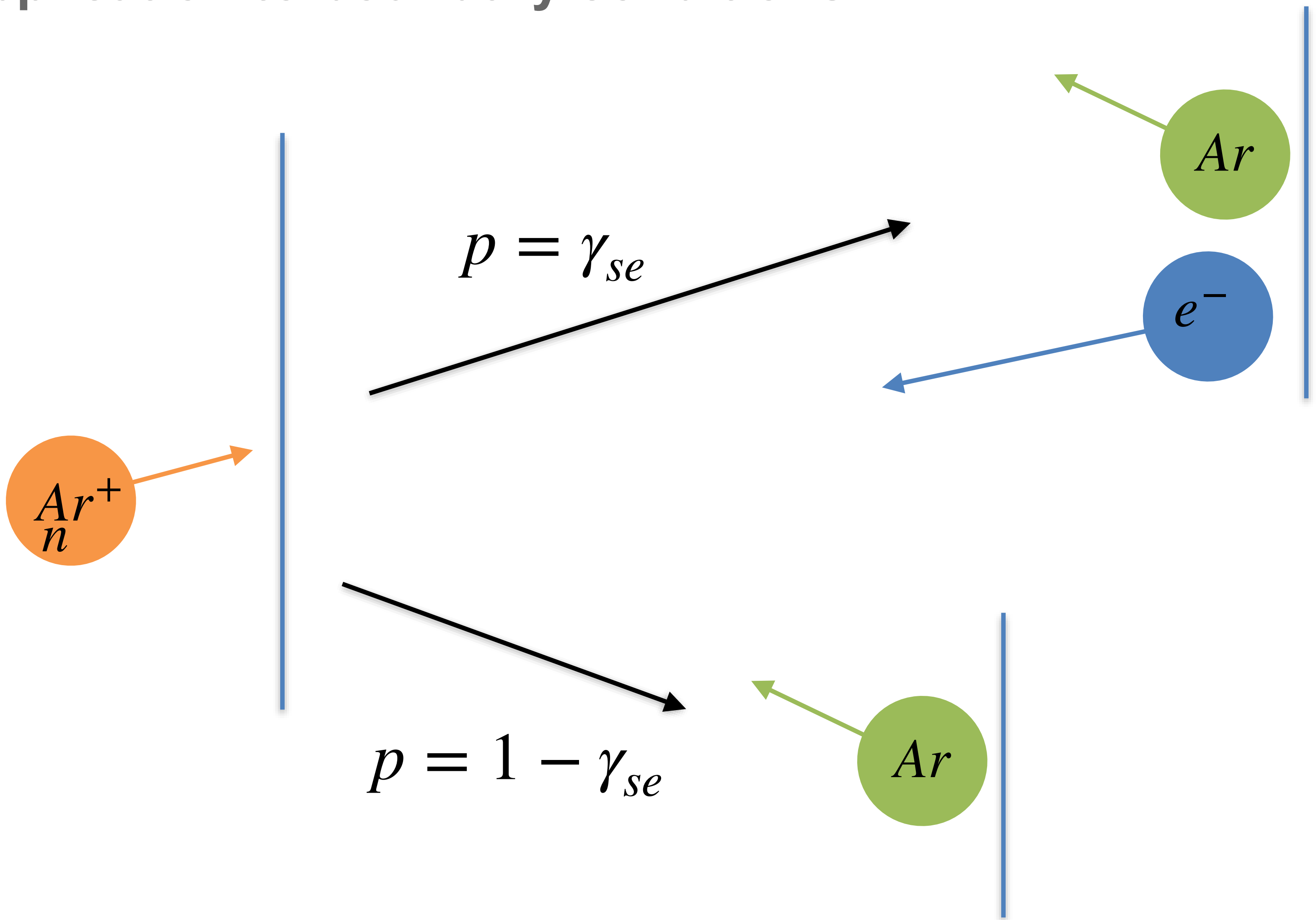
Possible cons of the event splitting approach?

- Increased computational cost
  1. Need to simulate N_p scattering events for each collision instead of 1

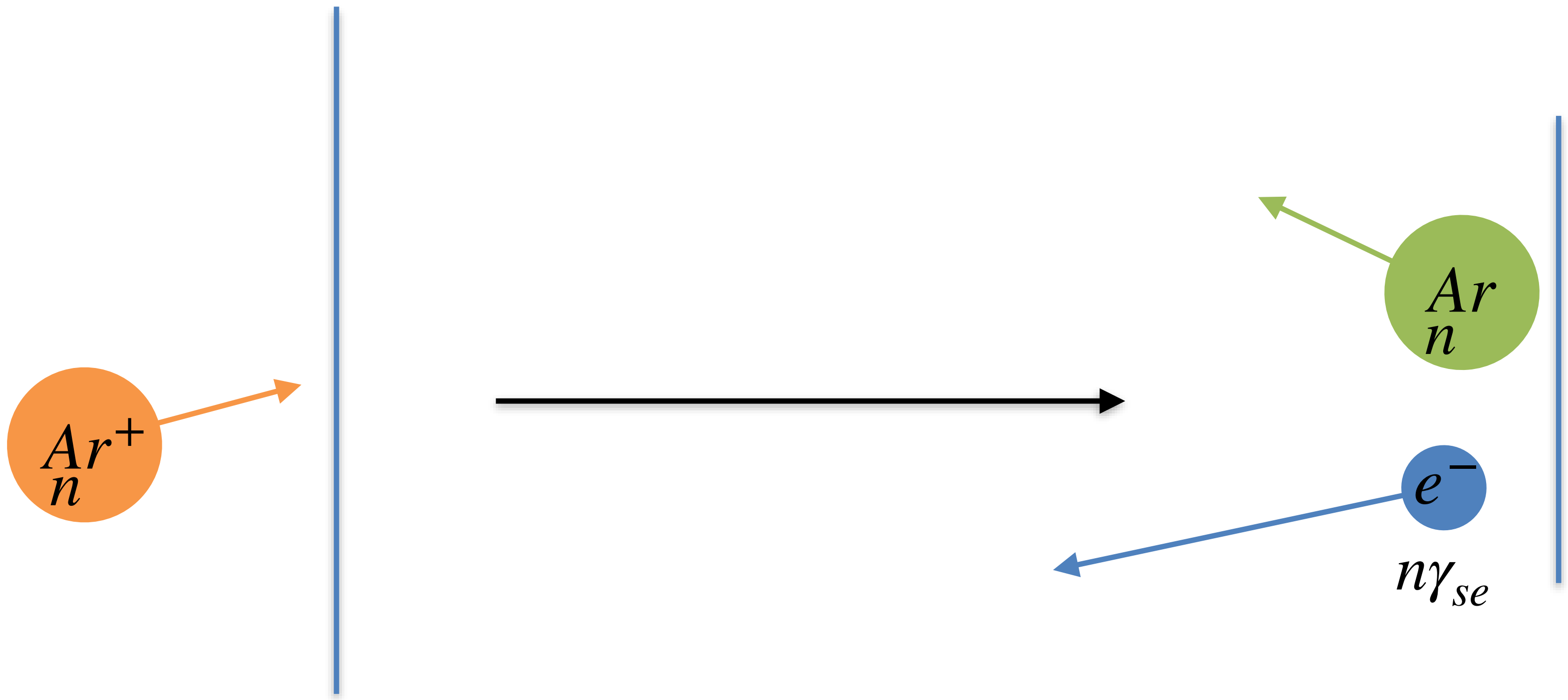
     Example: $Ar - e^-$ collisions with electronic excitation:
     31 excitation reactions + ionization + elastic scattering = 33 processes!

  2. More particles produced → more frequent merging required (also causes distortion in VDF)
     Explored in more detail for excitation reactions in [Oblapenko et al., Scitech 2022 Proceedings, 2022]

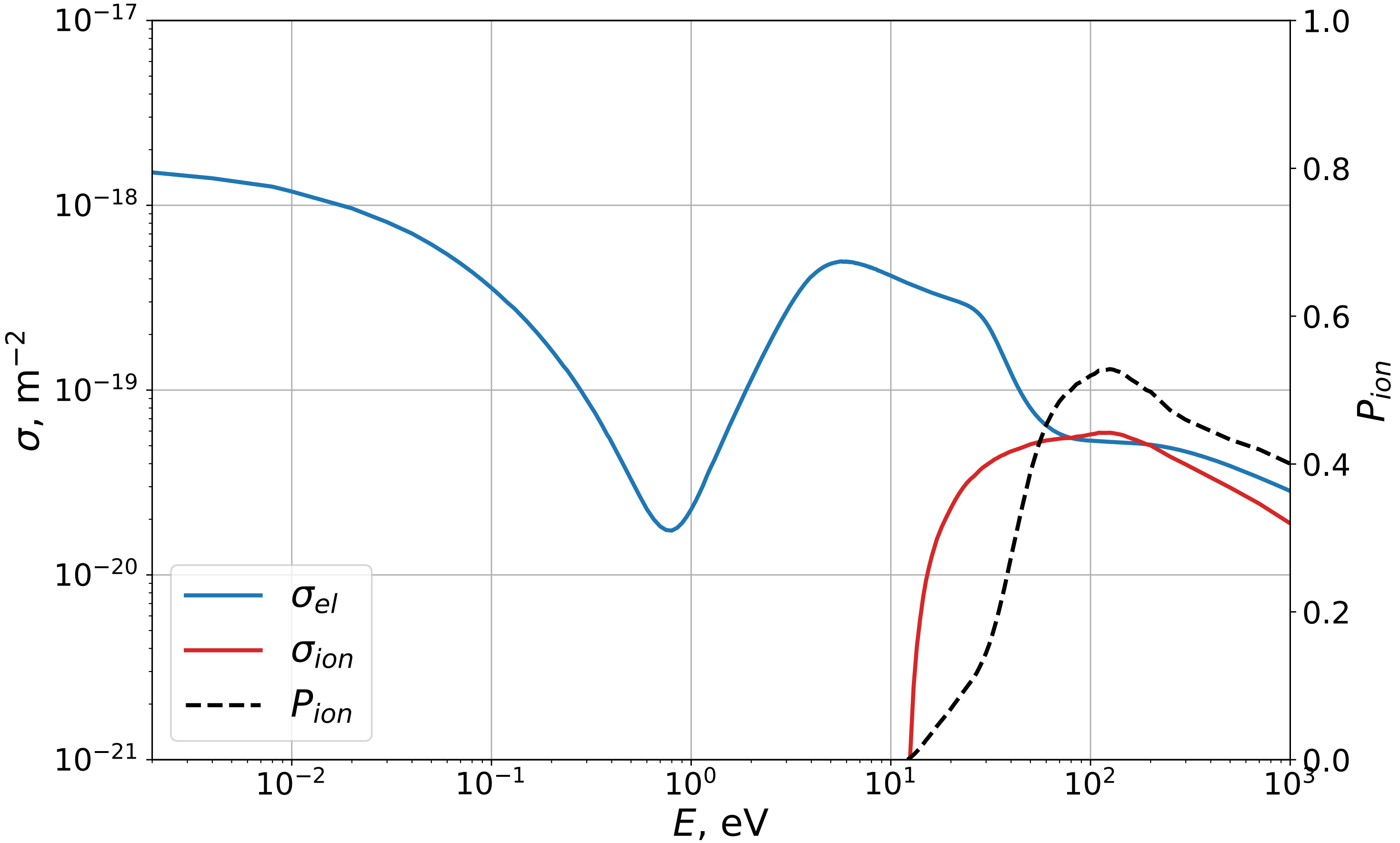
Example of application to boundary conditions



Example of application to boundary conditions

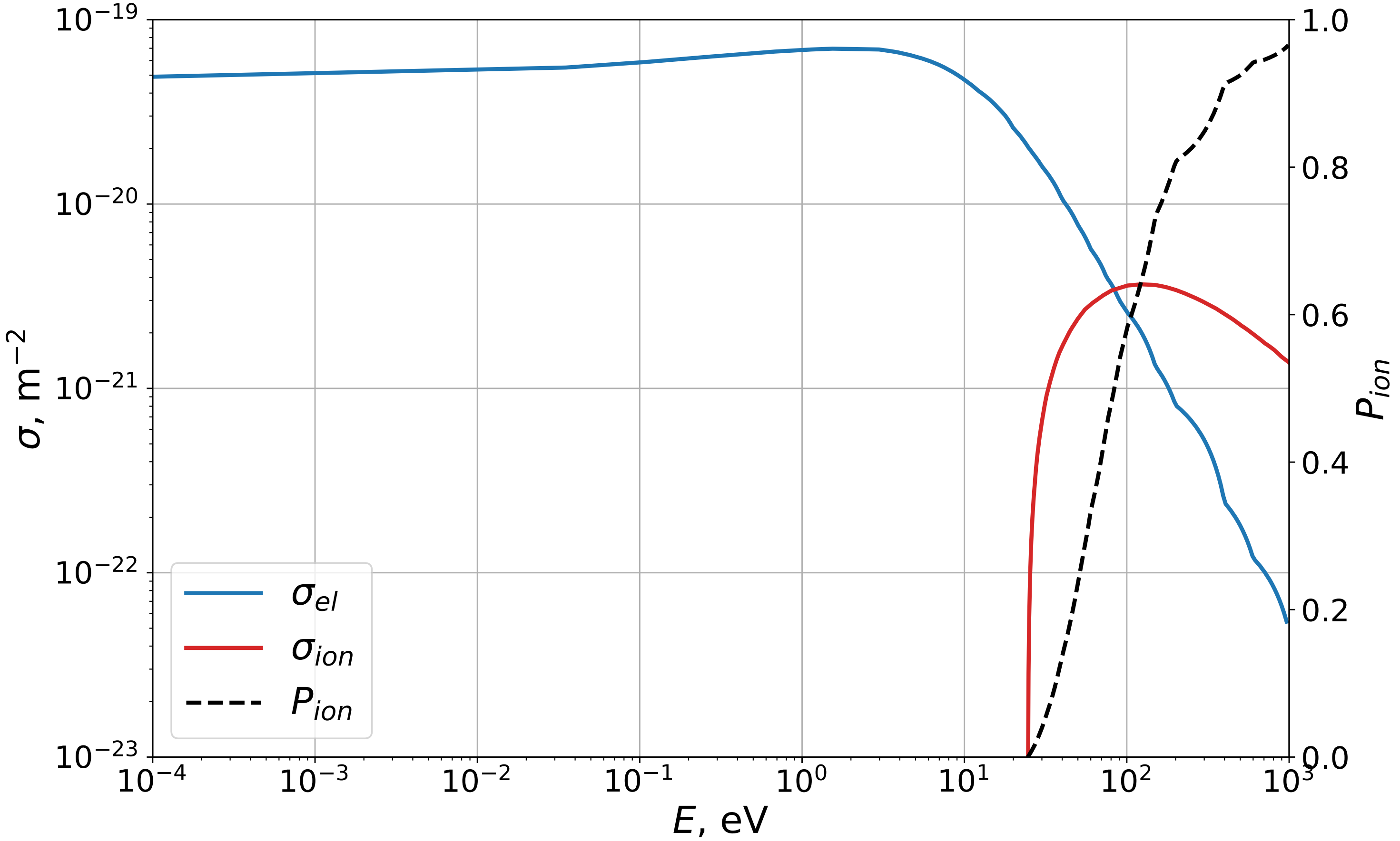


Electron-neutral collision cross-sections (xenon)



COP dataset for elastic scattering: R. McEachran, A. Stauffer, Eur. Phys. J. D, 2014-2015
Hayashi dataset for ionization: M. Hayashi, Technical Report
Scattering model: Okhrimovskyy et al., Phys. Rev. E, 2002

Electron-neutral collision cross-sections (helium)

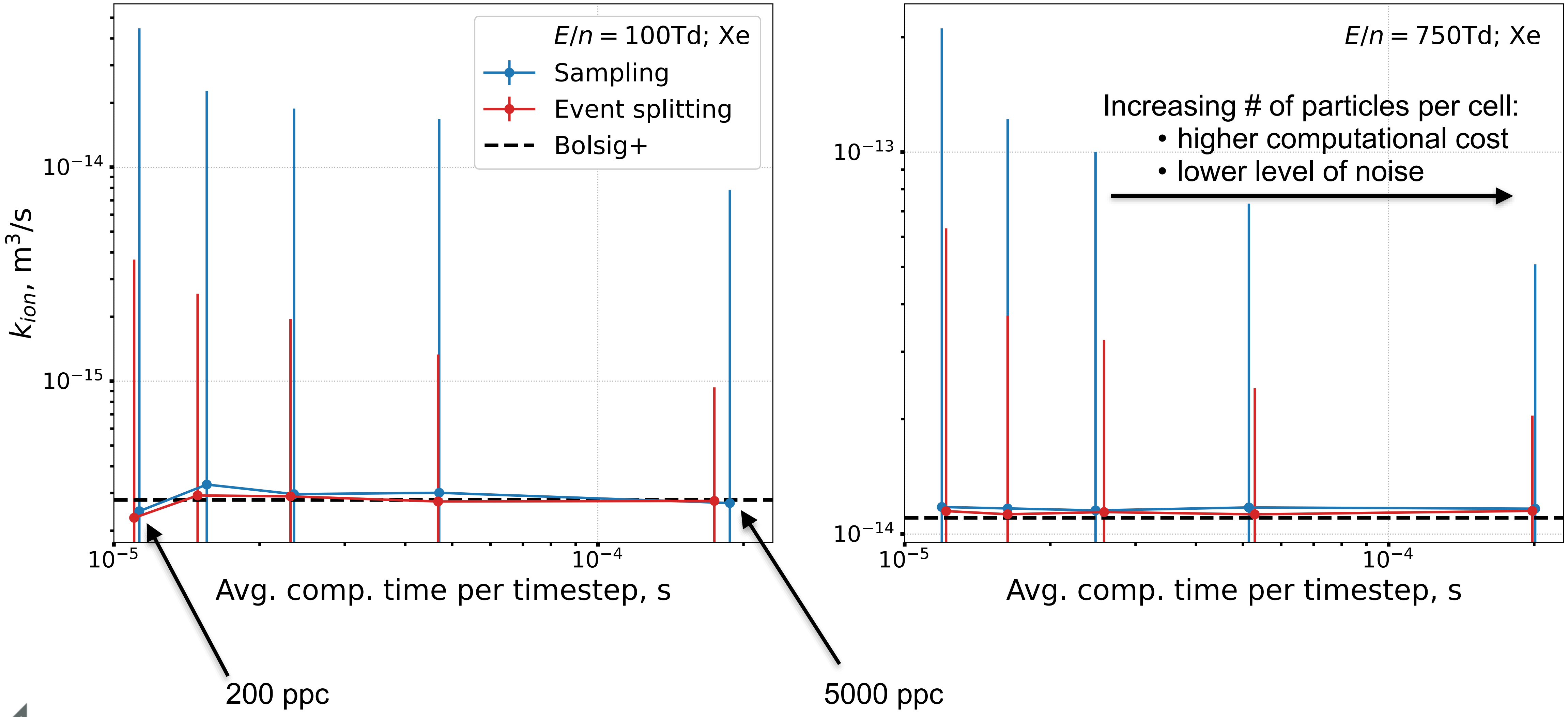


Biagi dataset: L. Alves et al., J. Phys. D: Appl. Phys, 2013
Scattering model: isotropic

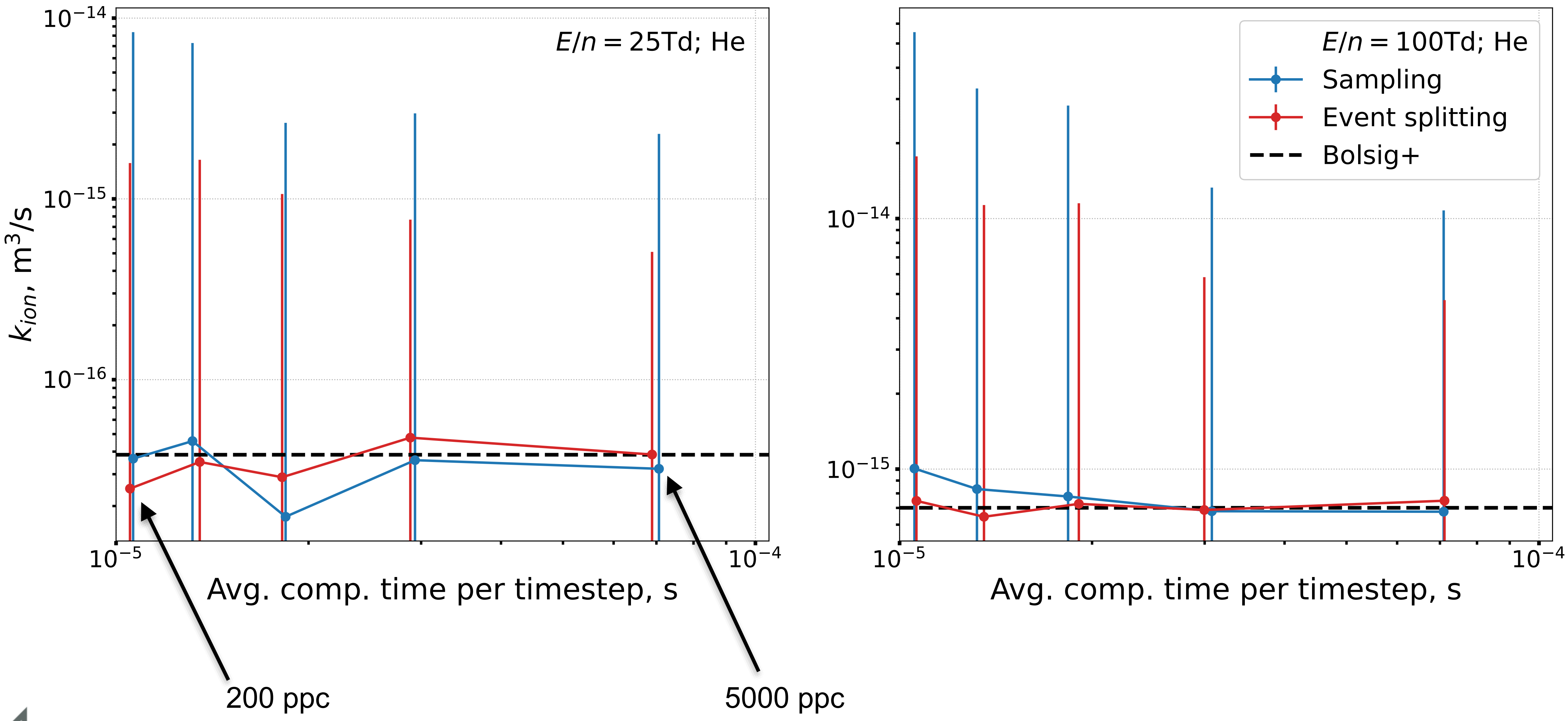
0-D test cases

- $Xe/Xe^{+}/e^{-}$ or $He/He^{+}/e^{-}$ mixture, initialized with small population of ions and electrons
- Accelerated by a constant electric field
- After initial transient period, gas reaches quasi-steady state (characterized by constant ionization rate coefficient)
- Steady-state dependent only on
  1. Value of reduced electric field (E/N)
  2. Processes considered
  3. Cross-sections
- Can gather statistics for the instantaneous ionization rate coefficient
- Can compare to Bolsig+ solver

0-D test case: Xenon



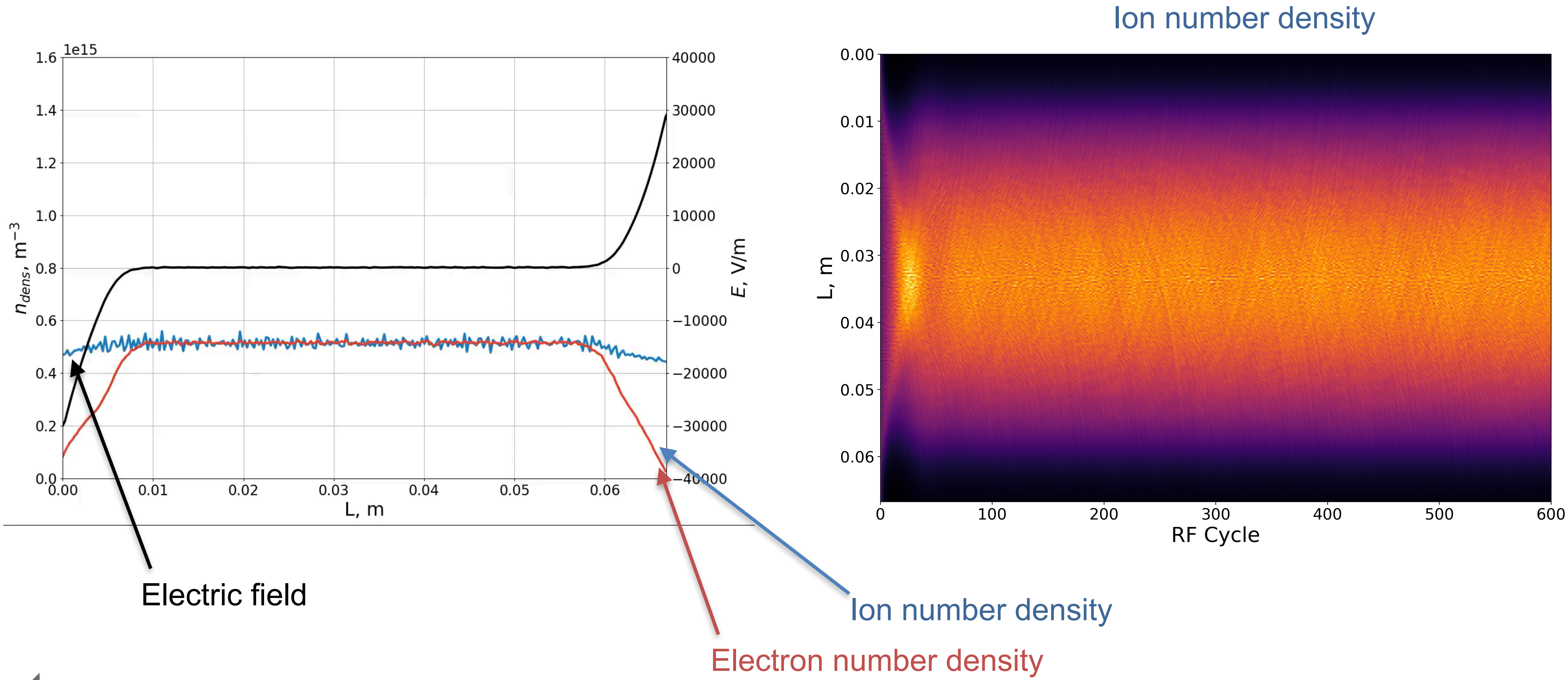
0-D test case: Helium



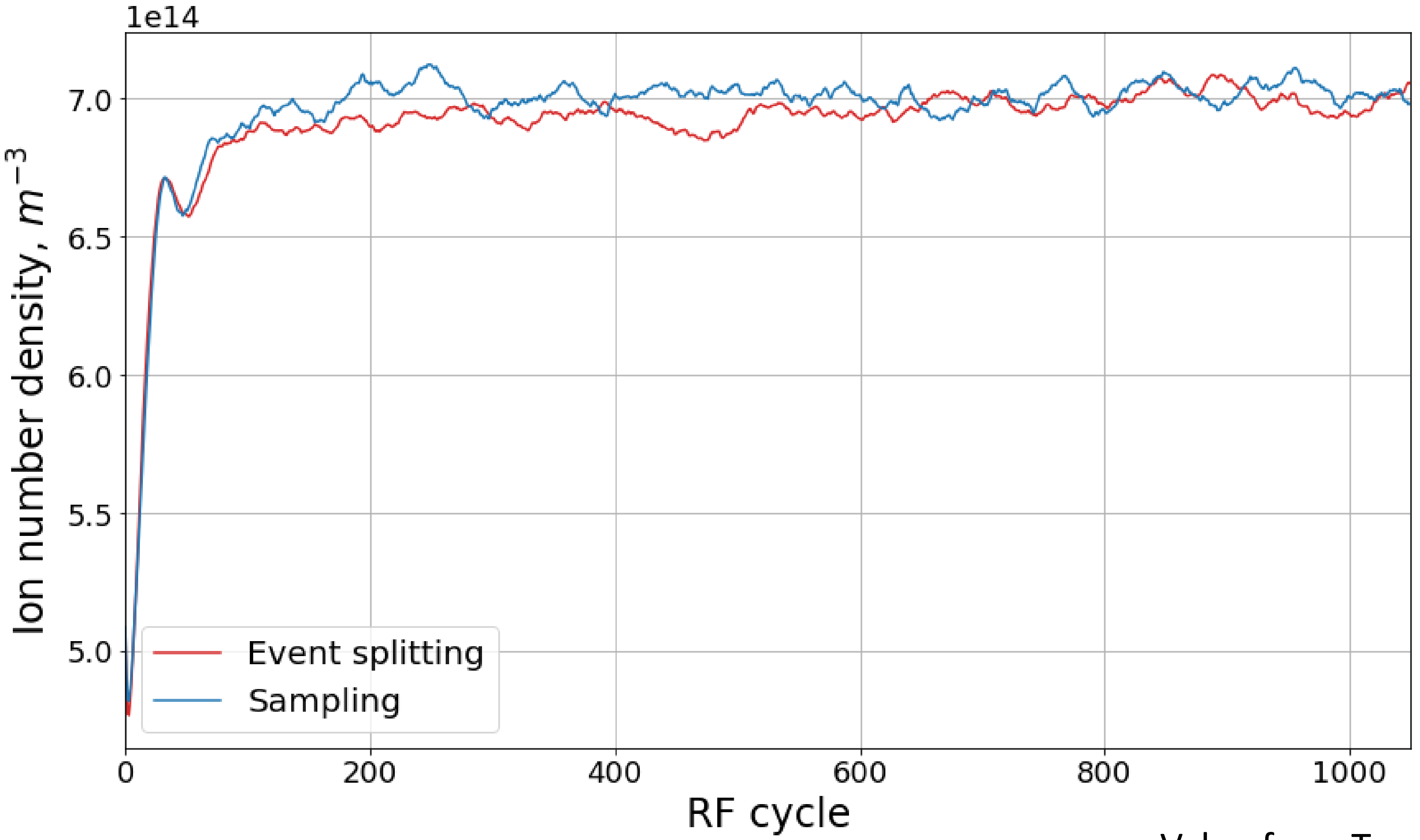
1-D test case

- Helium CCRF plasma
- Based on case 2 from set of benchmark cases by Turner et al. [M.M. Turner et al., Phys Plasmas, 2013]
- 13.56 MHz frequency, 200 V voltage, 13.3 Pa pressure
- 6.7 cm domain, 256 cells, 800 timesteps per RF cycle; cycle-averaged quantities
- **Main QOI: Cycle-averaged** k_{ion}
- Particles per cell (approximately): varied from 55 to 550
- Not considered:
  - Excitation reactions
  - Neutral-ion collisions

1-D test case: ion density, electric field

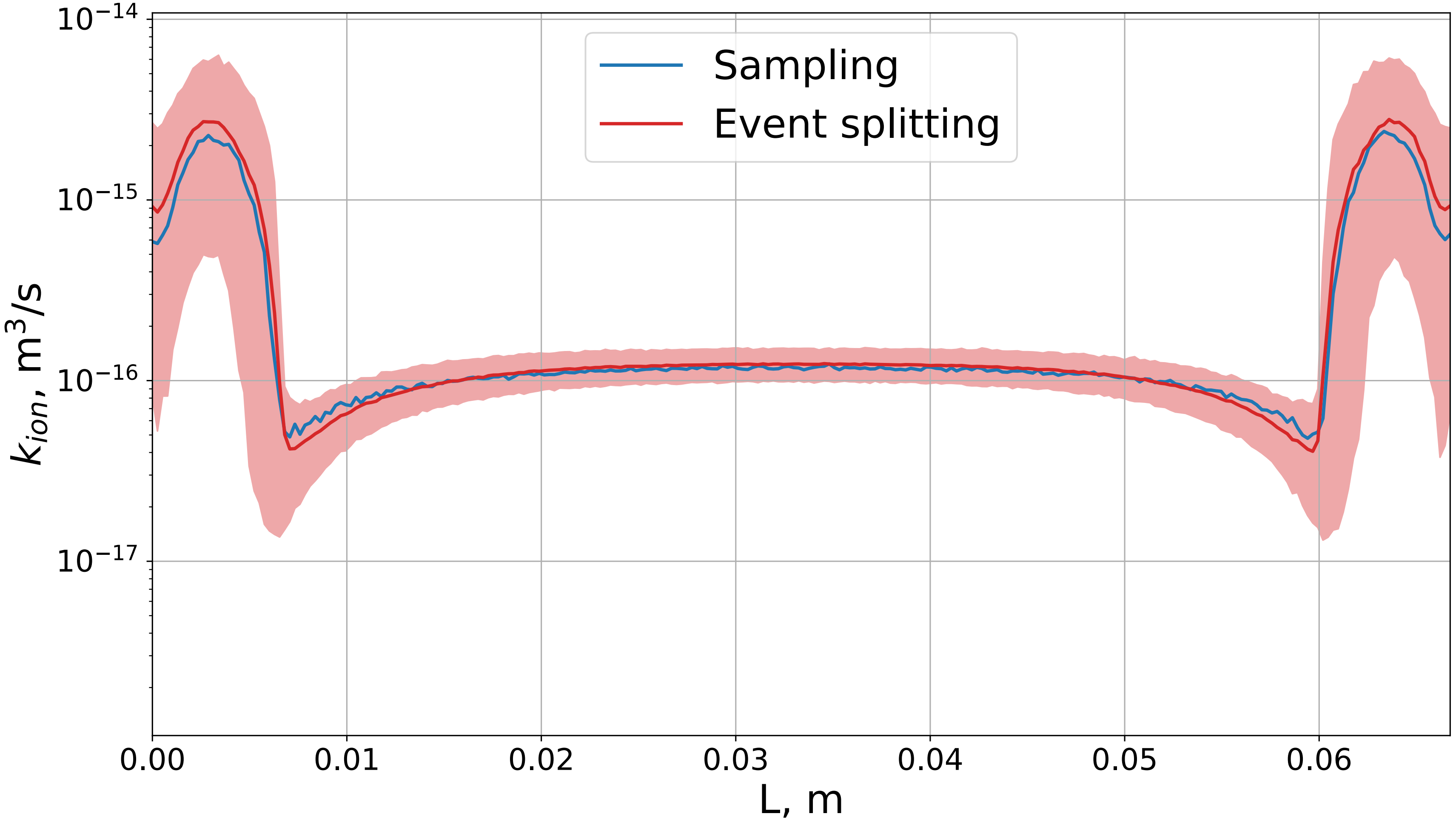


1-D test case: total ion number density



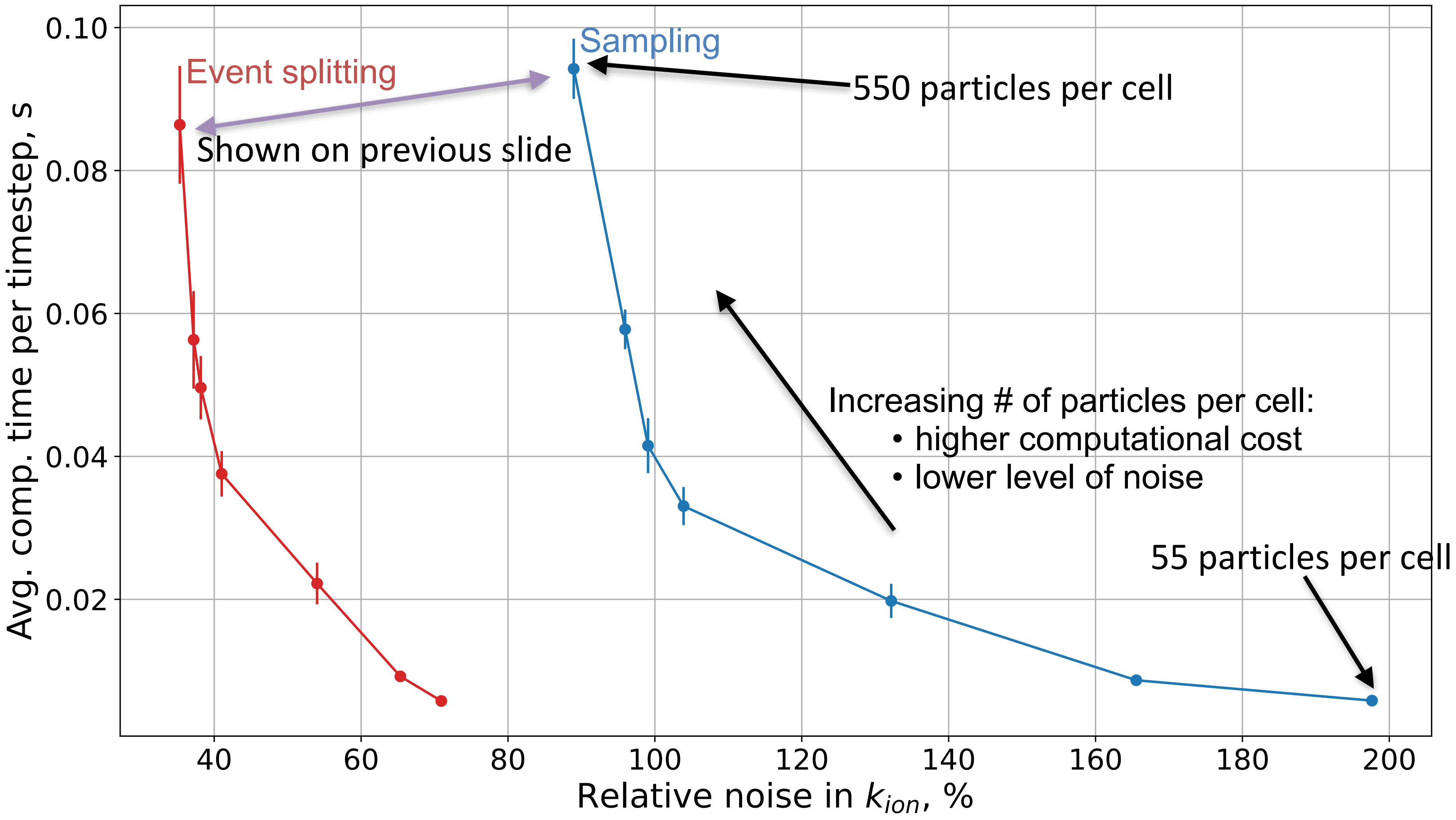
Value from Turner et al.: $8.28 \cdot 10^{14}$

1-D test case: ionization rate coefficient



- **Significant reduction in noise** throughout whole domain
- **Computational cost not affected!**

1-D test case: error in ionization rate coefficient



Conclusions

- Recently developed **event splitting scheme** tested for xenon and helium plasmas
- Shows significant **improvement** over standard DSMC collision scheme in **xenon**
- 1-D simulations of CCRF helium plasma show **2.5-fold reduction of noise** in ionization rate coefficient for same level of computational cost
- **Planned extensions**:
  - CEX collisions
  - Scattering events

Acknowledgements

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