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An Event Splitting Collision Scheme for PIC-DSMC Simulations

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DSMC

Basic ideas:

- Model gas by simulating motion of large number of 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: <u>cost linear in number of particles</u>

  (e.g., $F^*_{num} = F_{num}/10 \rightarrow$ 10x more particles $\rightarrow$ 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

Standard DSMC issues

Issues:

- Stochasticity-related (noise $\propto 1/\sqrt{N_p}$):
  - Low-speed flows
  - Transient flows
  - Coupling with CFD
- Fixed F_{num}-related (hard to resolve trace populations):
  - Trace chemical species
  - Excited internal states
  - High-velocity distribution function tails

Variable weight DSMC

What happens if each particle can represent a <u>different</u> number of molecules/atoms/electrons?

Pros:

- Alleviates the issue of capturing trace species
- Improves resolution of the tails (particles have lower computational weights)

Cons:

- Either we forego exact conservation (conservation “on average” instead) or we have to split particles during collisions
- Particle splitting→growth of the number of particles→need to merge particles

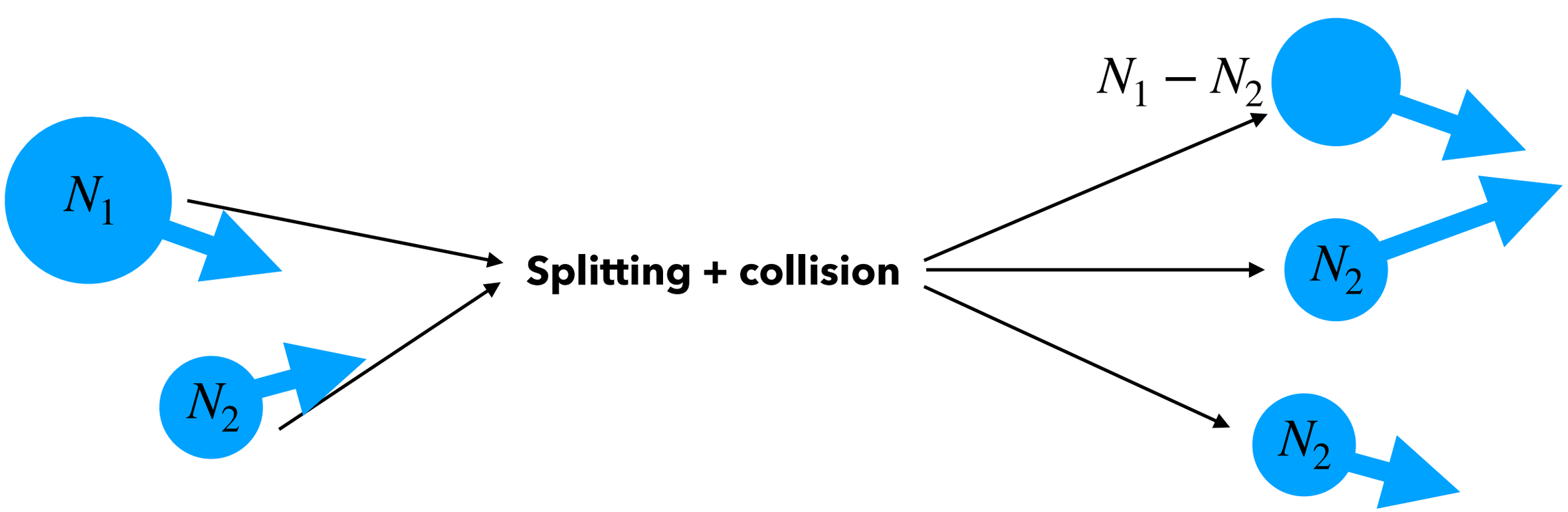
References:

- 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

Variable weight DSMC

Splitting during collisions (same species colliding):

- 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

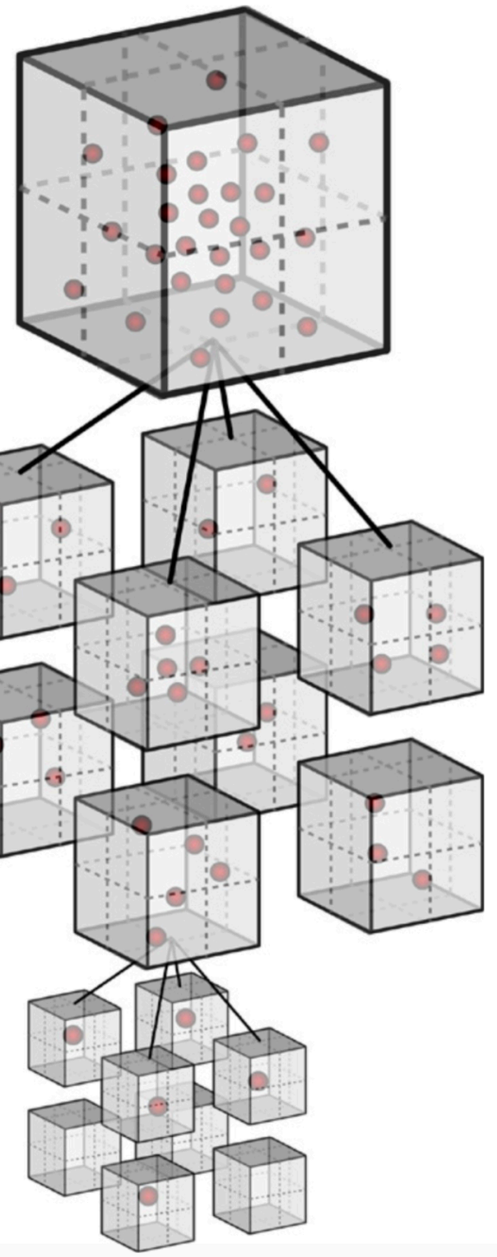


Particle merging

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 mass 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 $\mathcal{O}(n \log n_{c,max})$



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

Event splitting

Outline

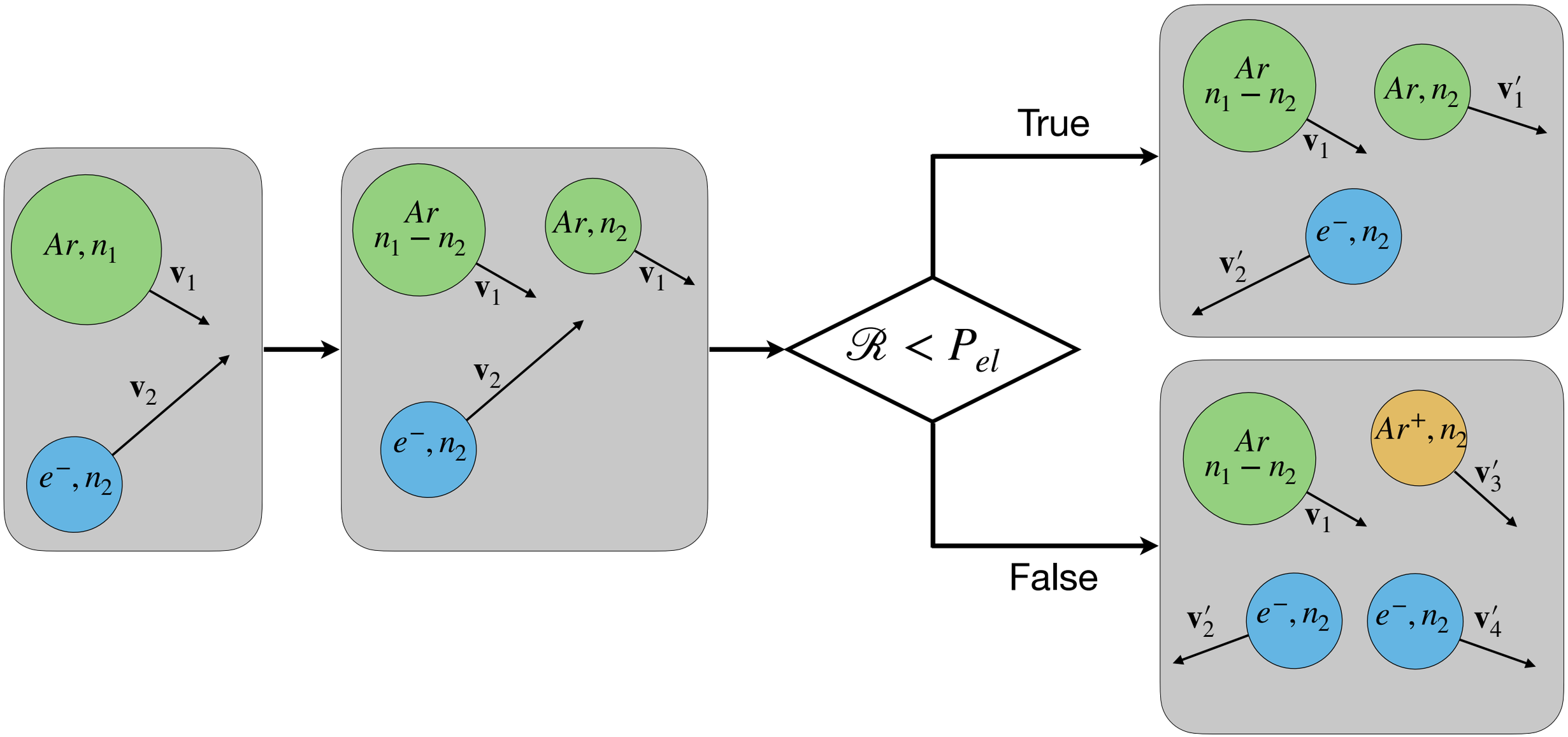
- Suppose we have N_p possible processes that can occur during a collision (e.g. elastic collision, ionization reaction, vibrational transition, etc.), and the corresponding probabilities are $\{p_i\}_{i=1}^{N_p}$
- Standard DSMC "all-or-nothing" approach: sample process type based on $\{p_i\}_{i=1}^{N_p}$ 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)

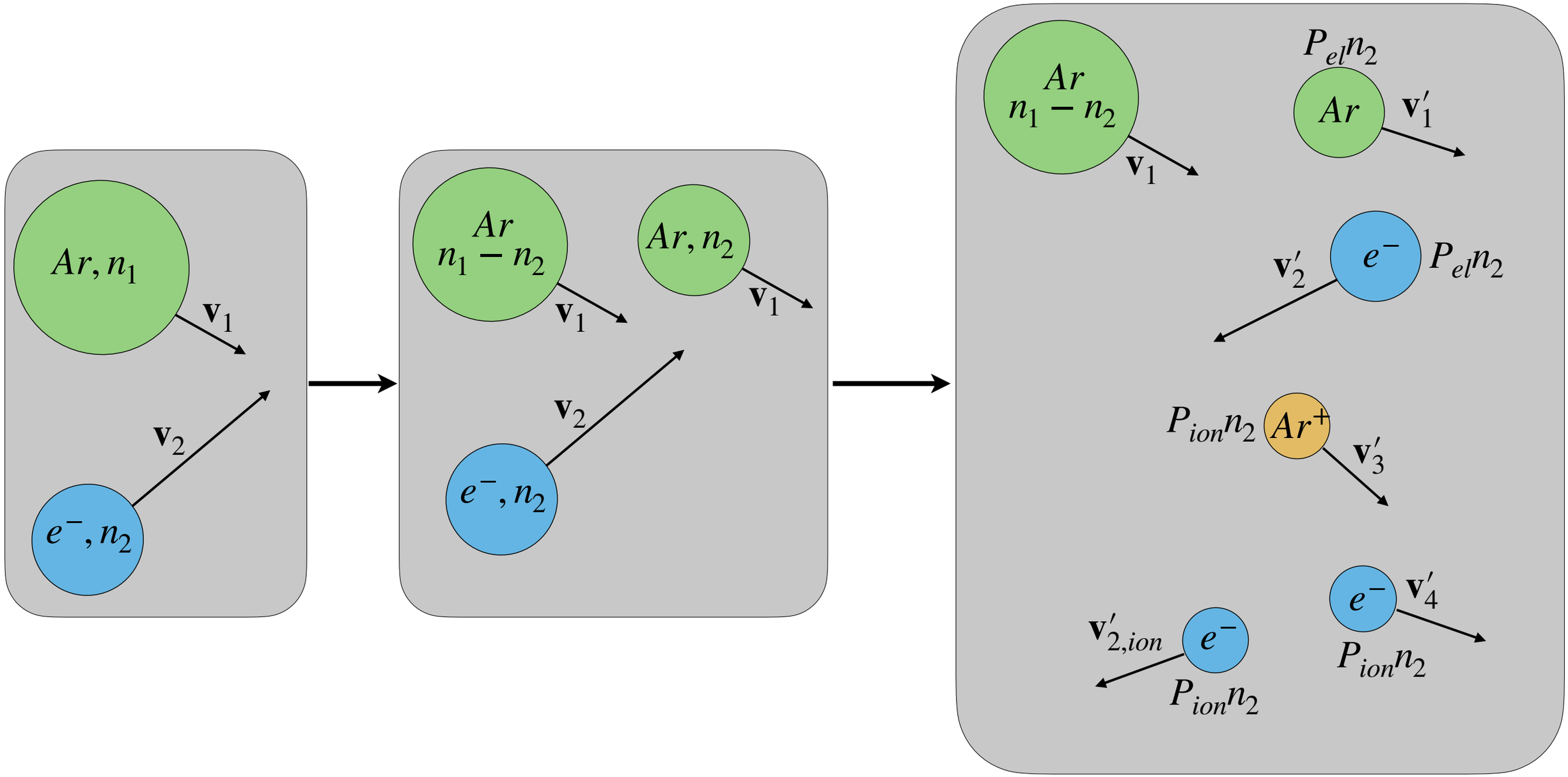
References:

- G. Oblapenko et al., submitted to Journ. Comp. Phys., 2021
- G. Oblapenko et al., Scitech 2021 Proceedings, 2021

Standard (all-or-nothing) DSMC approach



Event splitting approach



Event splitting

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
  2. More particles produced→more frequent merging required

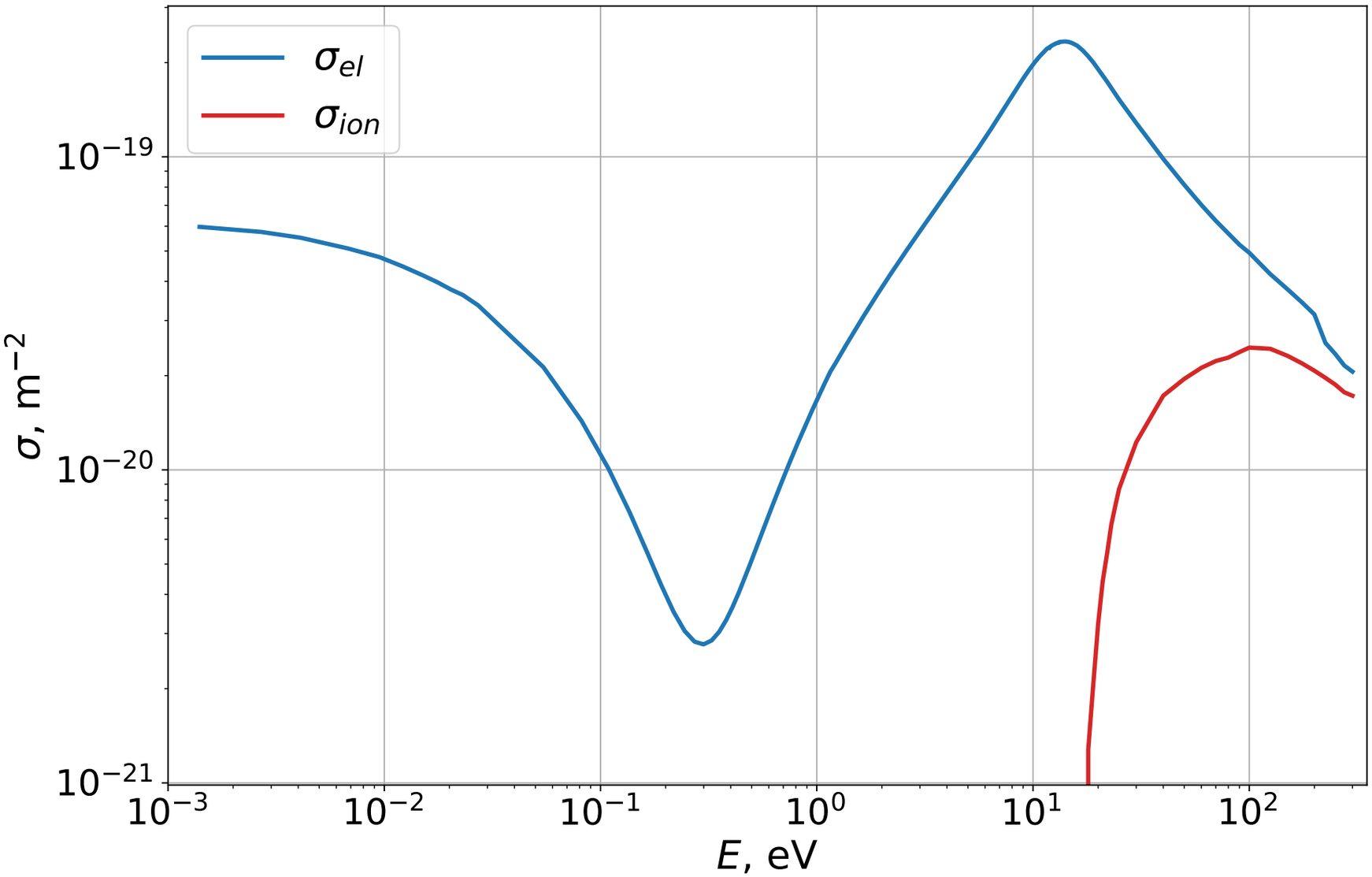
Possible workarounds/cost reduction measures:

- Perform splitting based not on specific processes, but on process groups: e.g., don't split based on all vibrational transition reactions, but based on total probability of a vibrational transition occurring, choose specific transition using the standard DSMC approach

Numerical results: 0D

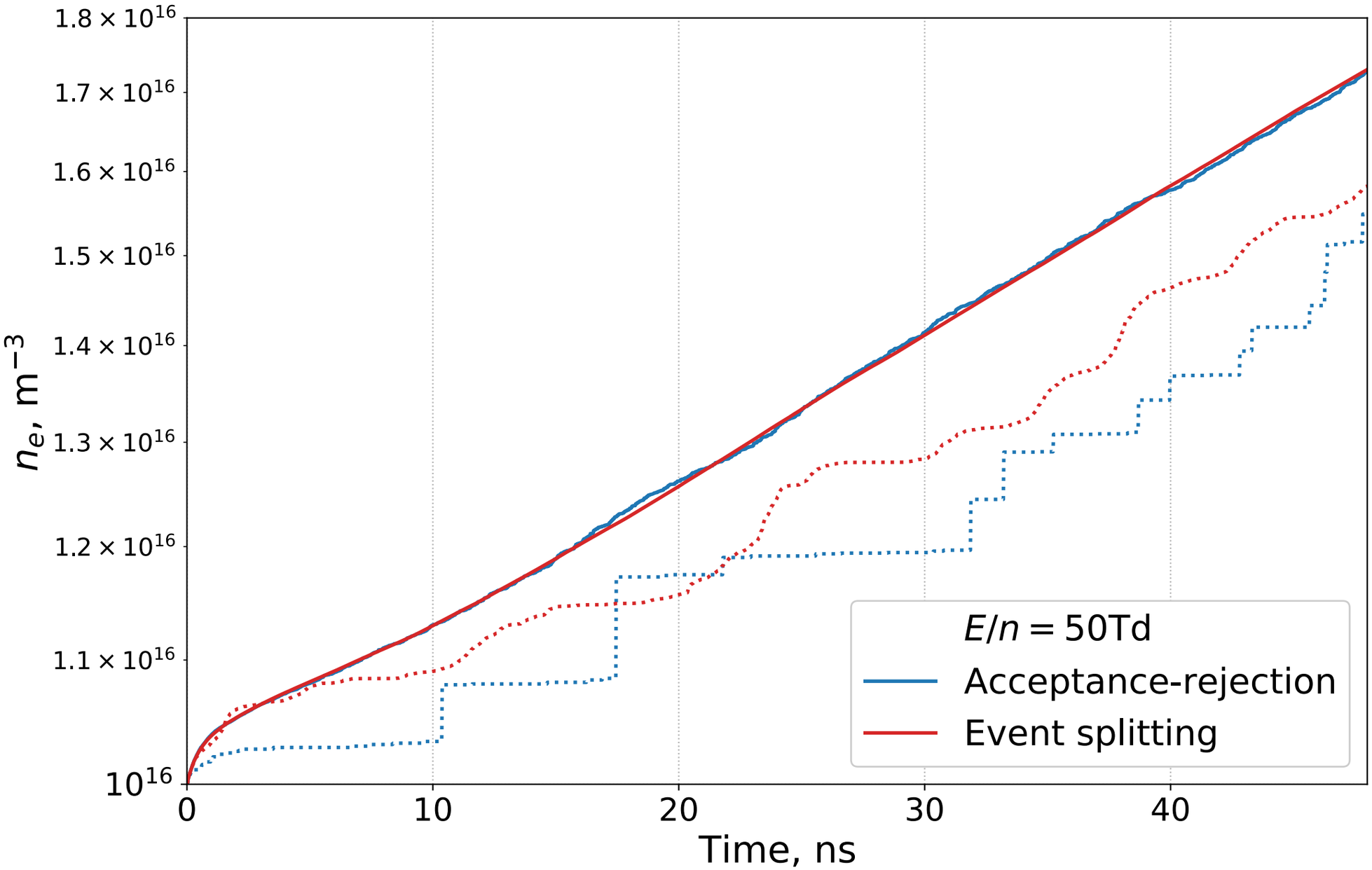
- $Ar/Ar^{+}/e^{-}$ mixture, initialized with small molar fraction of ions and electrons
- Accelerated by a constant electric field
- After initial transient period, gas reaches quasi-steady state (characterized by constant ionization rate coefficient)
- Steady-state dependent only on value of reduced electric field, processes considered, and their cross-sections
- Considered electron-argon collision processes:
  - Elastic scattering
  - Electron-impact ionization
- Can gather statistics for the instantaneous ionization rate coefficient
- Can compare to Bolsig+ solver

Electron-neutral cross-sections



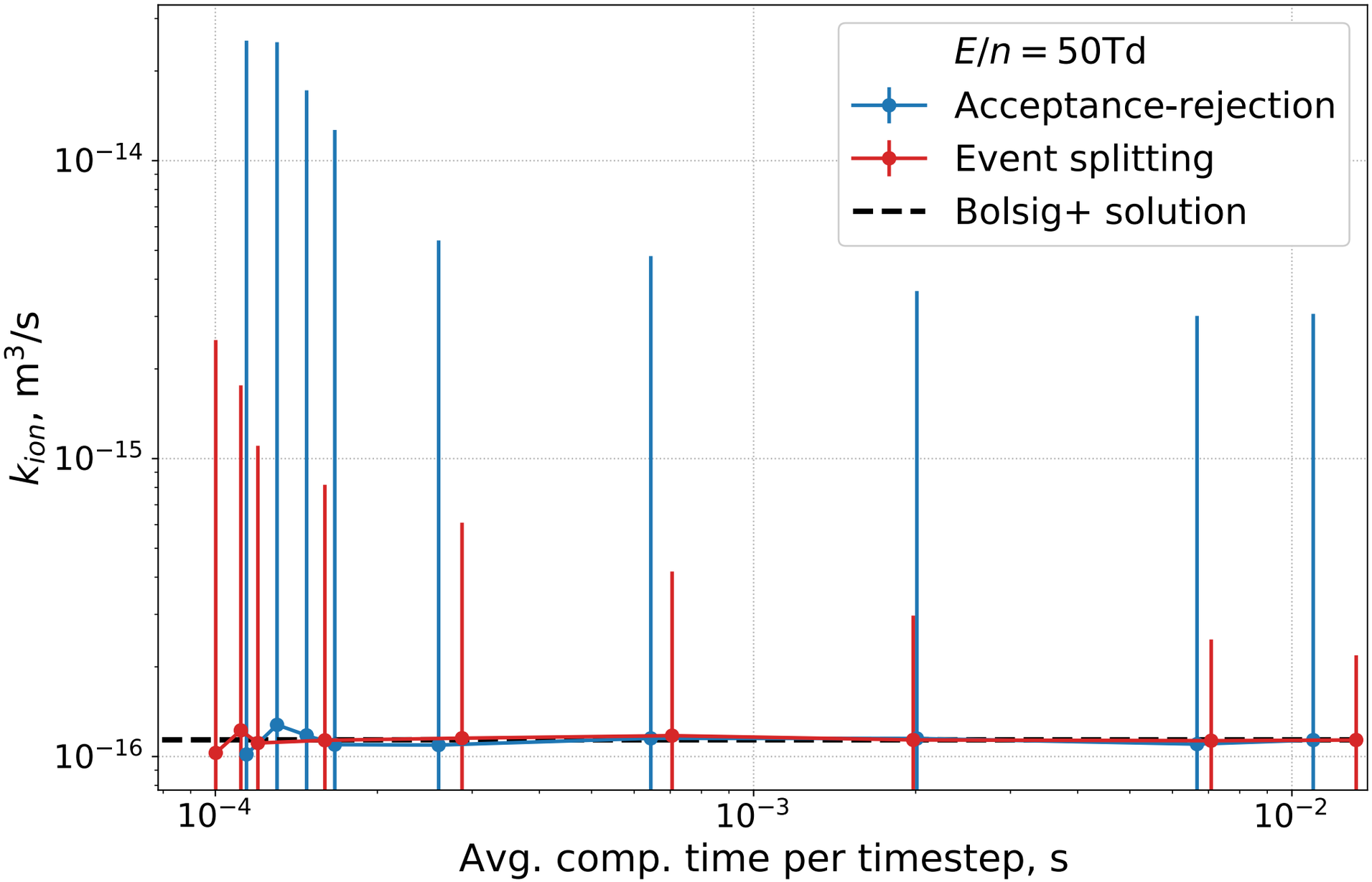
- Tabular data from the BSR model [L. Pitchford et al., J. Phys. D, 2013]
- Anisotropic scattering model from [Okhrimovskyy et al., Phys. Rev. E, 2002]

0-D results, electron number density



- Dotted lines: 100 particles/species
- Filled lines: 30000 particles/species

0-D results, error and cost

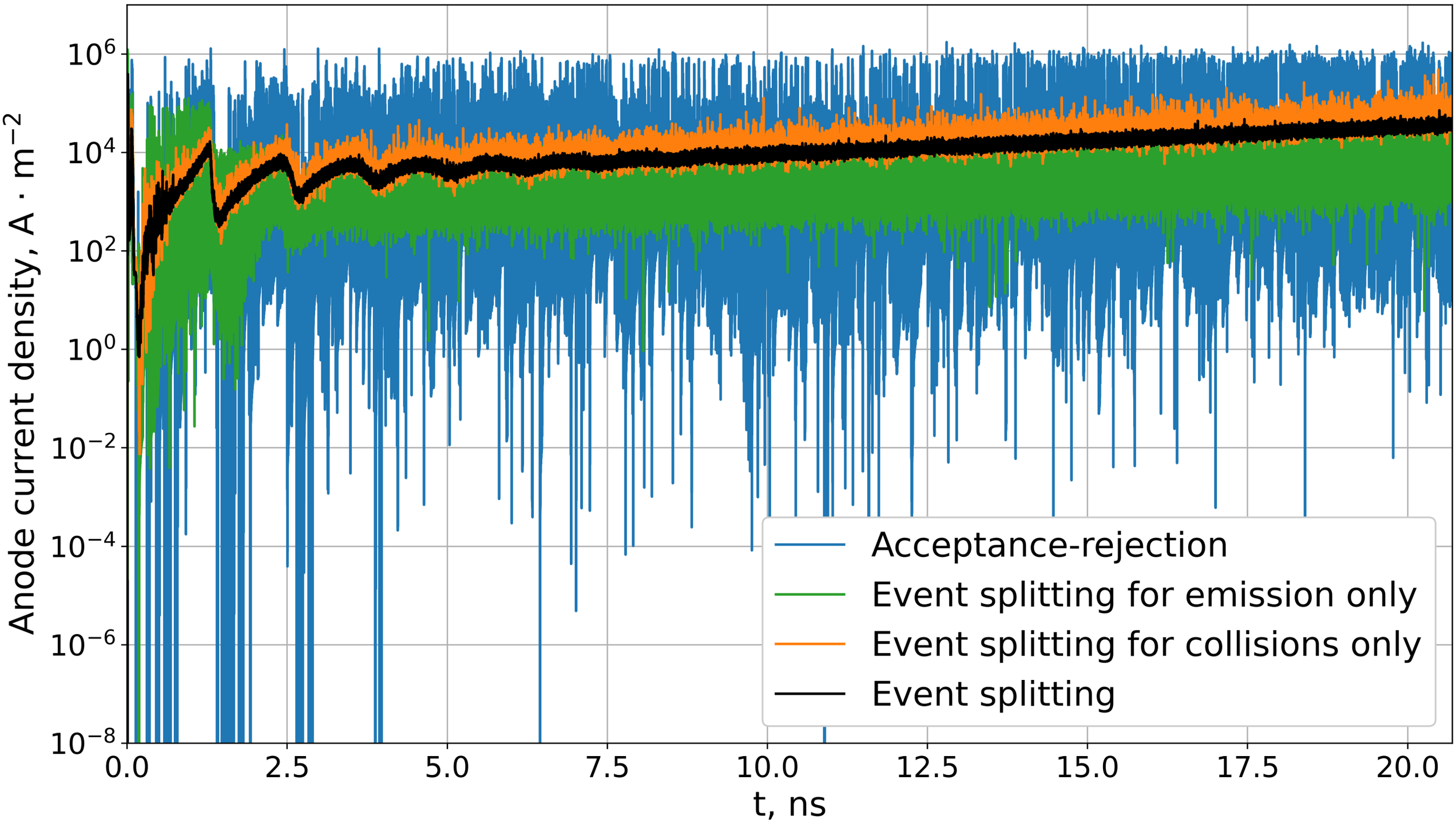


- Computational cost similar, but significant reduction in noise!

Numerical results: 1D

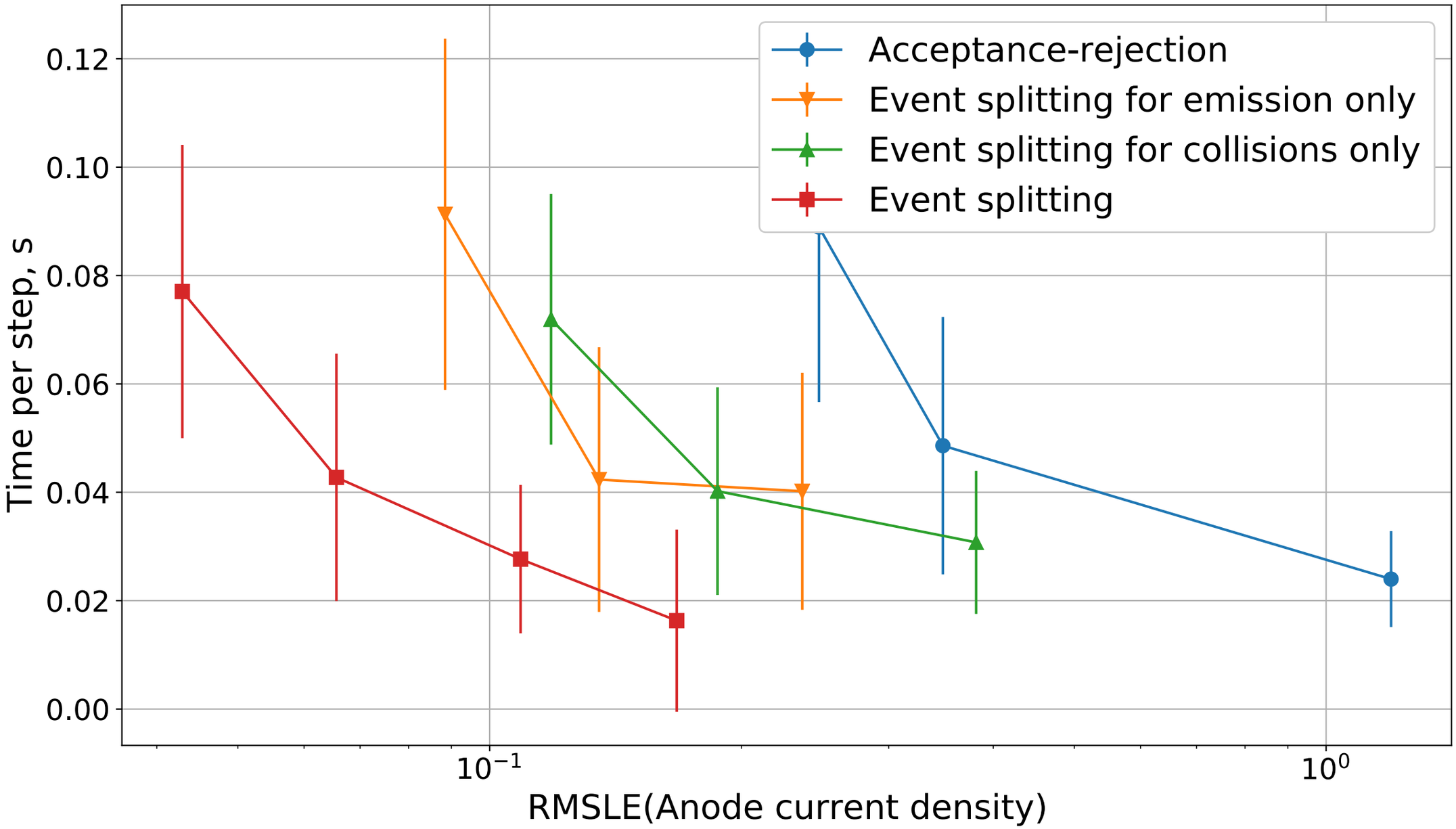
- Argon-filled gap, $pd = 0.3$ Torr·cm
- Constant voltage drop across gap: 450V
- Cell closest to cathode seeded with small fraction of ions and electrons
- Boundary conditions
  - Electrons absorbed at boundaries
  - Ions neutralized at anode
  - Ions hitting cathode emit an electron with probability $\gamma_{se} = 0.1$
- Electrons accelerated across gap cause ionization→produced ions create more electrons at cathode→breakdown at sufficiently high enough voltage
- Breakdown characterized by exponential rise in current density at anode
- Event splitting can be performed for
  - Electron-neutral collisions
  - Ions hitting cathode
  - Both collisions and emission

Numerical results: 1D



- Initial oscillation frequency $\nu \propto 1/$(time for ion to cross gap)

Numerical results: 1D

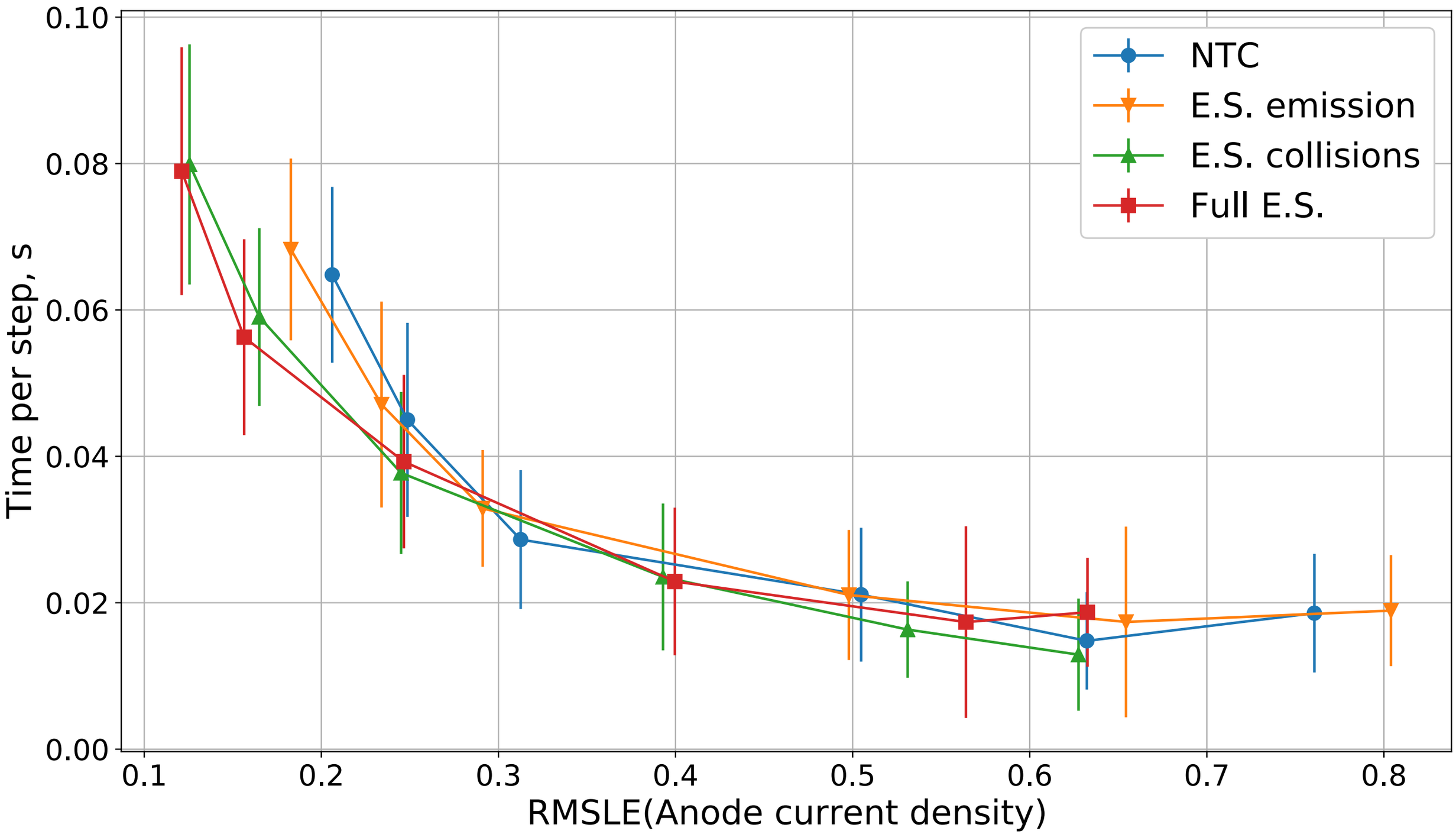


- Significant reduction in noise whilst maintaining similar computational cost

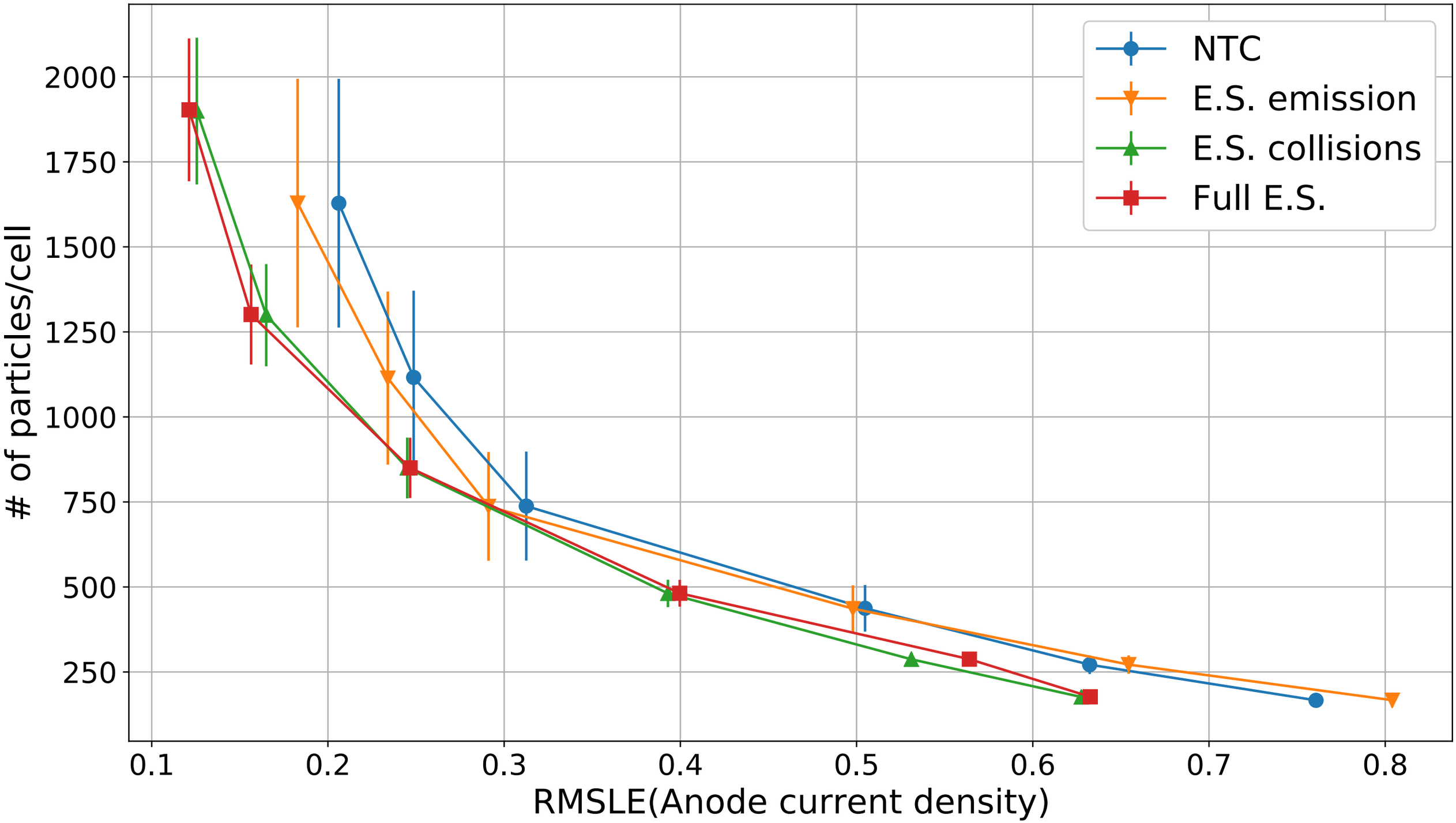
Numerical results: 1D, PIC-DSMC

- Argon-filled gap, $pd = 0.5$ Torr·cm
- Constant voltage drop across gap: 200V
- Fully coupled PIC-DSMC simulation
- Thomson's algorithm used for Poisson equation solver
- Velocity Verlet used for particle movement

Numerical results: 1D, PIC-DSMC



Numerical results: 1D, PIC-DSMC



Conclusions

- **New collision scheme** proposed for variable-weight DSMC simulations
- **Reduces variance** in modeling of low-probability processes
- For test case without a coupled PIC solver, provides **significant benefits in terms of computational cost-vs-noise**
- For test case with a couple PIC solver, provides **an advantage in terms of noise vs average number of particles per cell**
- **Further extensions** may include splitting on probability of grouped processes (i.e. electronic excitation), as well improvement of anisotropic scattering