SAND2021-12218C

Sandia National Laboratories

Effect of dynamic particle reweighting on plasma swarm parameters in the particle-in-cell code Aleph

ALEPH
Advanced Plasma Transport & Kinetics

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74th Annual Gaseous Electronics Conference

Virtual Meeting

October 5th, 2021

U.S. DEPARTMENT OF ENERGY | NNSA

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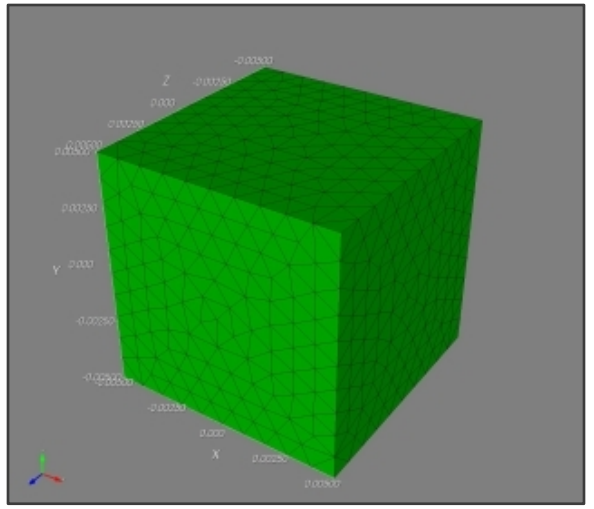
Aleph Collision Benchmarking

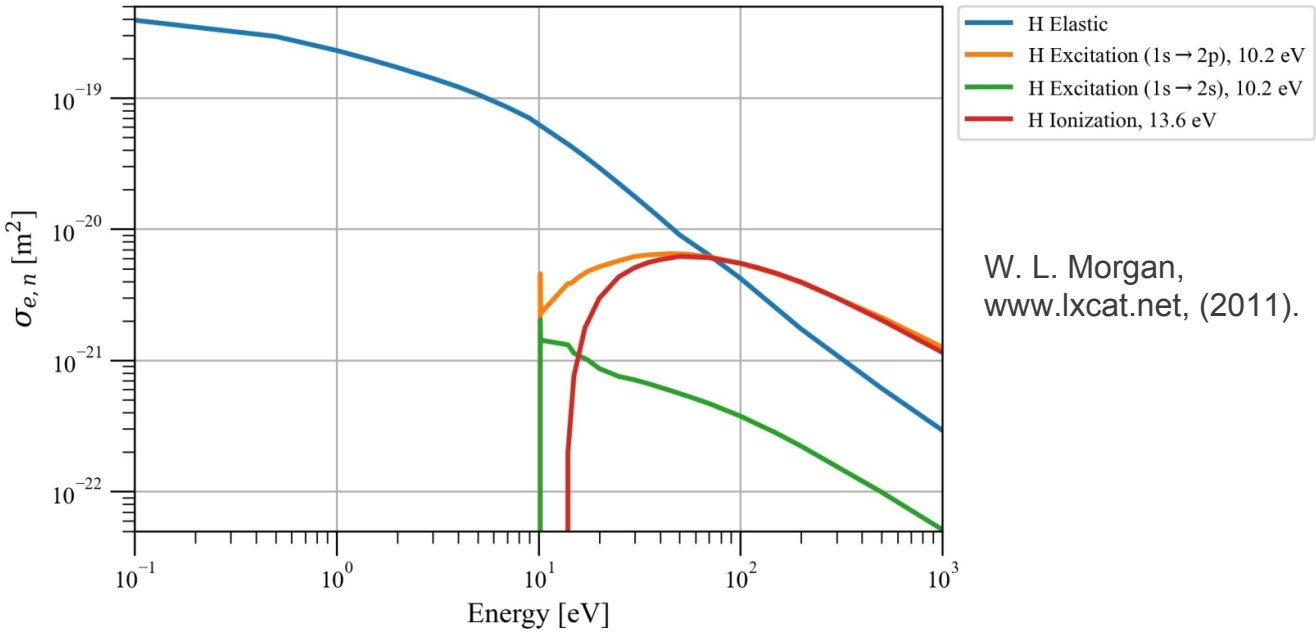
- Aleph is an unstructured particle-in-cell (PIC)/direct simulation Monte-Carlo (DSMC) code for simulating low-temperature plasmas developed at Sandia National Laboratories
- Combines various computational algorithms to model plasma systems
  - Velocity Verlet particle stepper
  - Discontinuous Galerkin finite element potential field solver
  - Coupled thermo-electric surface emission
  - Particle-particle interactions/plasma chemistry (DSMC)
- Utilized only the particle-particle interactions to test DSMC capabilities when applying Aleph's particle reweighting algorithm
- Results benchmarked against Bolsig+, a widely used Boltzmann equation solver

Goal: Examine how Aleph's reweighting algorithm impacts swarm parameters

Simulation Parameters

- Particles randomly distributed throughout mesh
- Particle positions are fixed; velocities evolve due to collisions
- Electron-neutral interaction cross-sections from the Morgan database were used for testing
- Adaptive timestep used with condition $dt\frac{v_{th}}{\lambda_{mfp}} < 0.1$
- Mesh element size: $\frac{dl}{\lambda_{mpf}} \sim 0.01$
- Initial densities
  - $n_{n0} = 2.4 \times 10^{20}\ \mathrm{m}^{-3}$
  - $n_e = n_i = 2.4 \times 10^{15}\ \mathrm{m}^{-3}$
- Initial temperatures
  - $T_n = T_i = 0.026\ \mathrm{eV}$
  - $T_e = 0\ \mathrm{eV}$
- Reduced electric field: $E/n_0 = 100\ \mathrm{Td}$



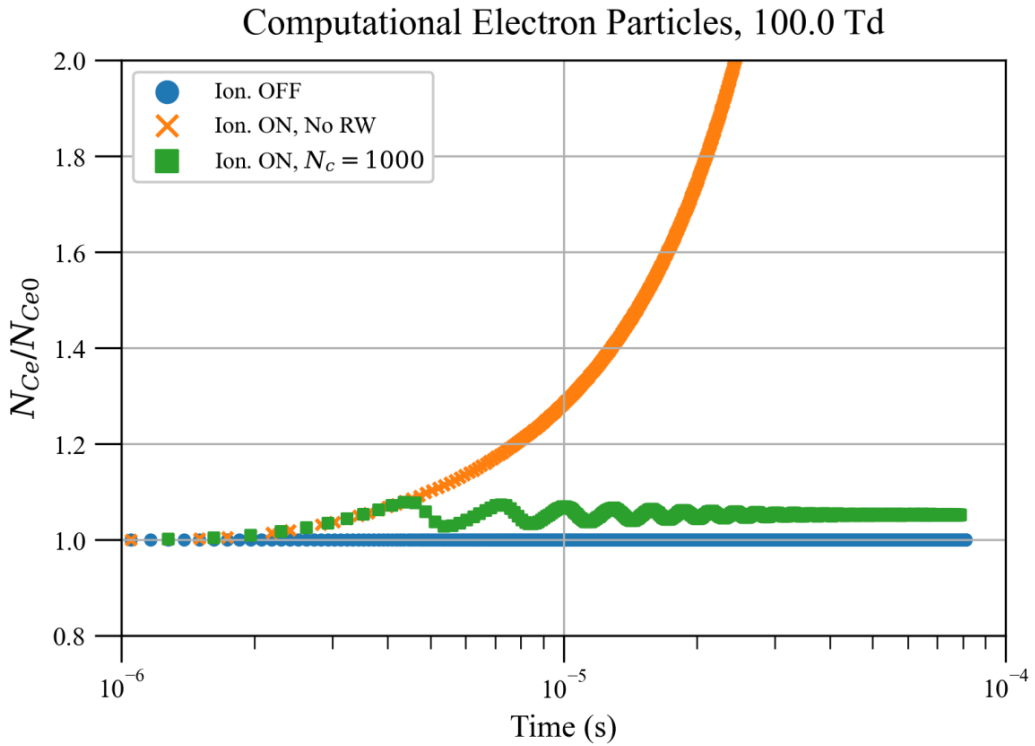


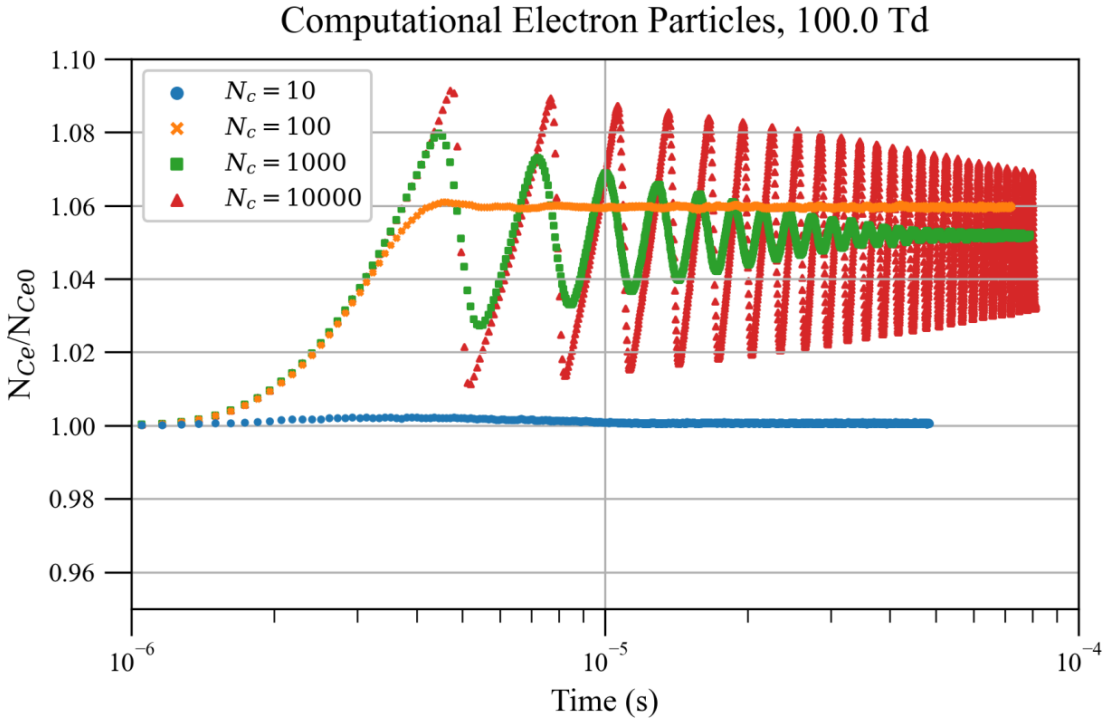
W. L. Morgan, www.lxcat.net, (2011).

Computational Electron Particles

- Aleph is capable of dynamically adjusting the weight of computational particles within an element to maintain a fixed count N_c (reweighting)
- When including electron impact ionization, the number of electrons can grow exponentially
- Reweighting maintains a particle count within some specified bounds which improves the computational efficiency

Case	Run Time (64 cores)
$N_c = 10$	2 min, 53 sec
$N_c = 100$	28 min, 55 sec
$N_c = 1{,}000$	15 hrs., 10 min, 15 sec
$N_c = 10{,}000$	20 hrs., 49 min, 23 sec* (288 cores)





Computational Electron Particles Weights

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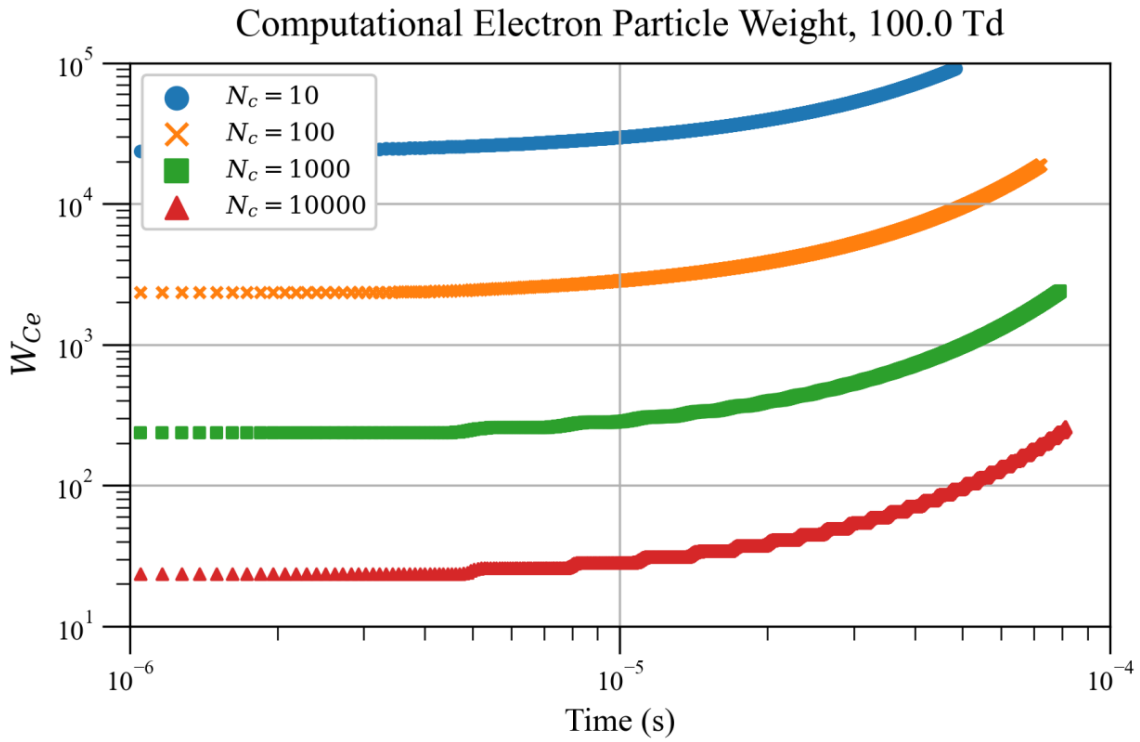

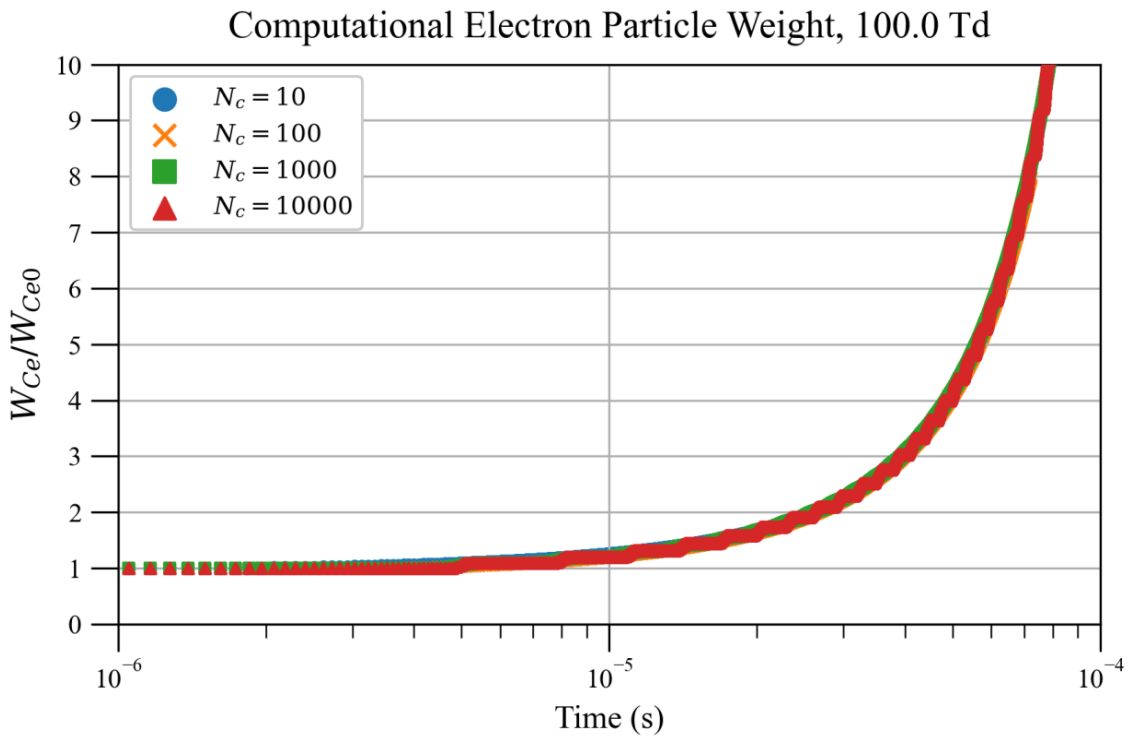

Electron Density

- While reweighting limits the number of computational particles, Aleph maintains the proper exponential growth of real particles
- Increasing the target count of particles per element helps increase the accuracy of the simulation but at the cost of computational resources and time

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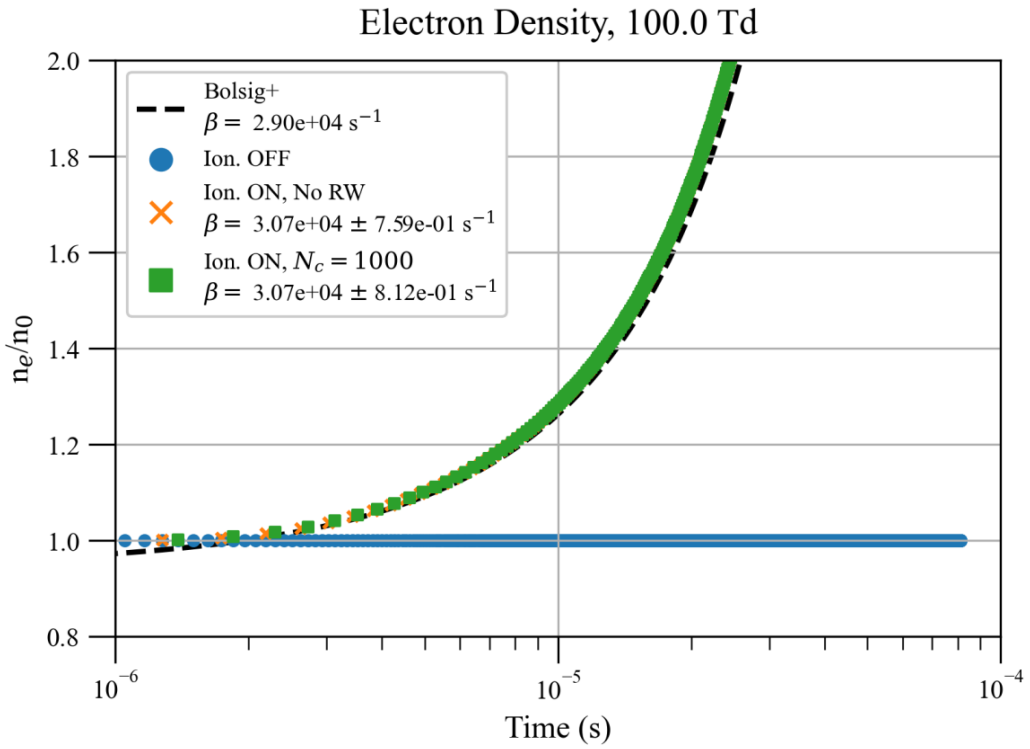
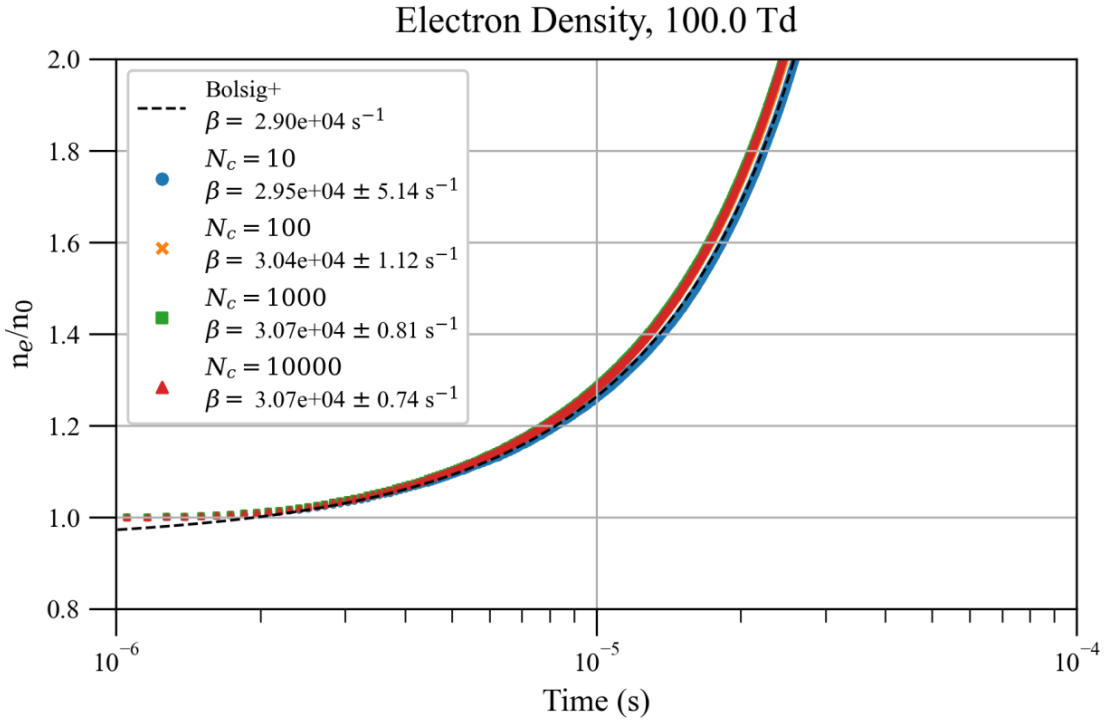
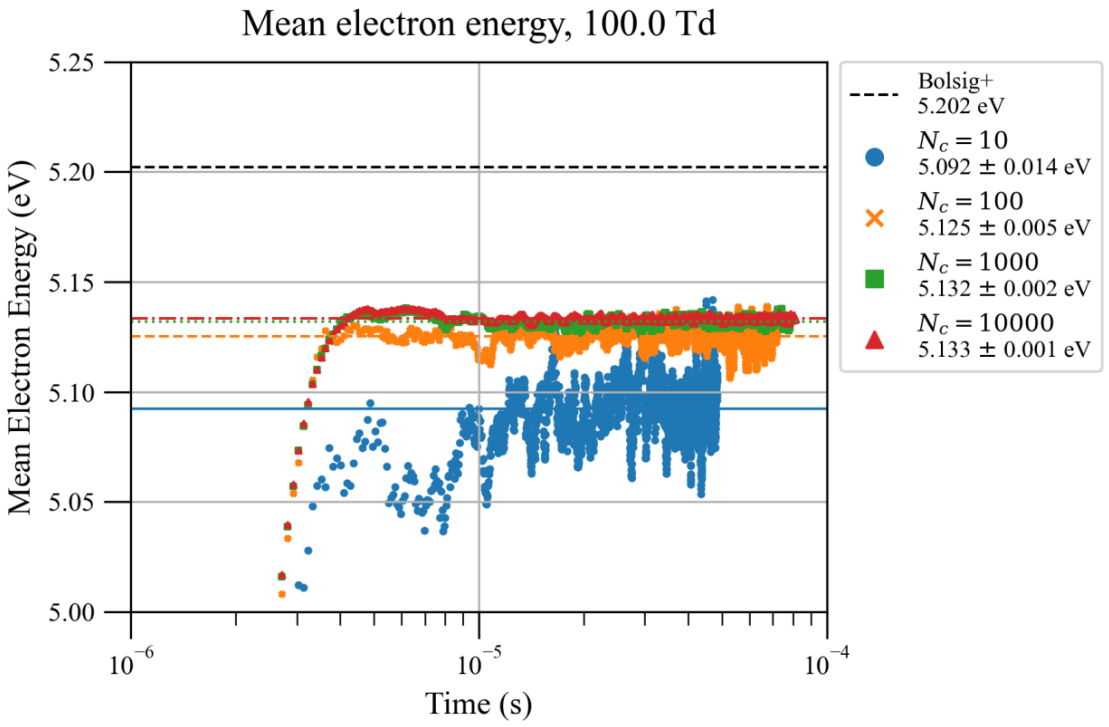
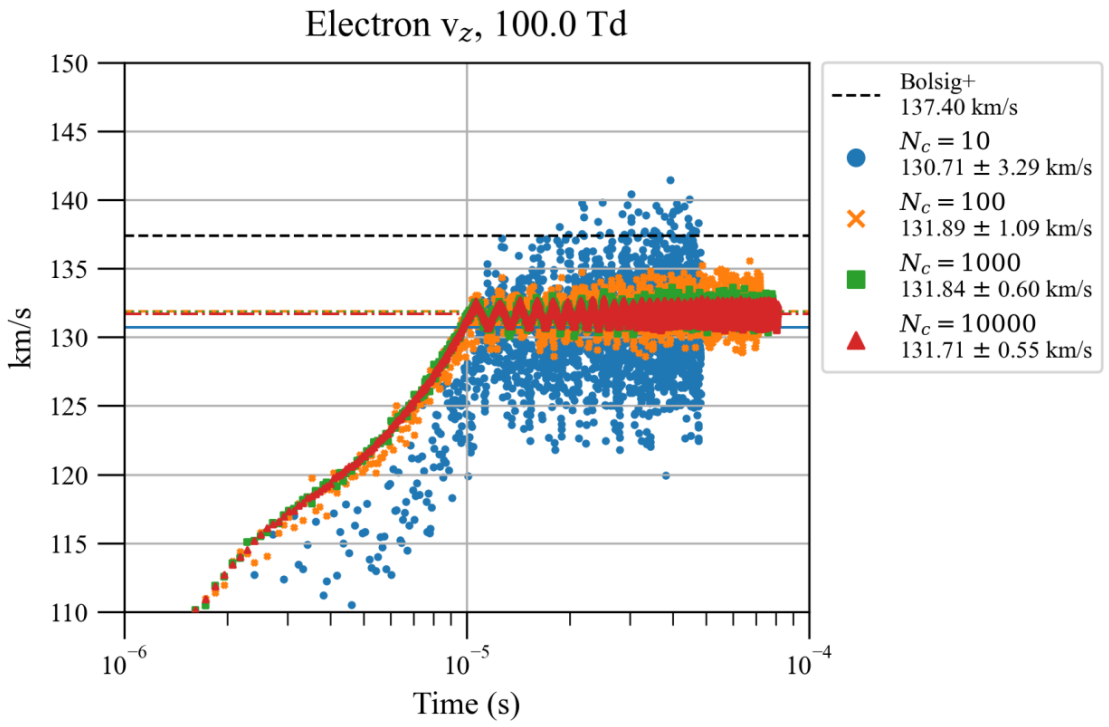




Electron Mean Energy and Drift Velocity

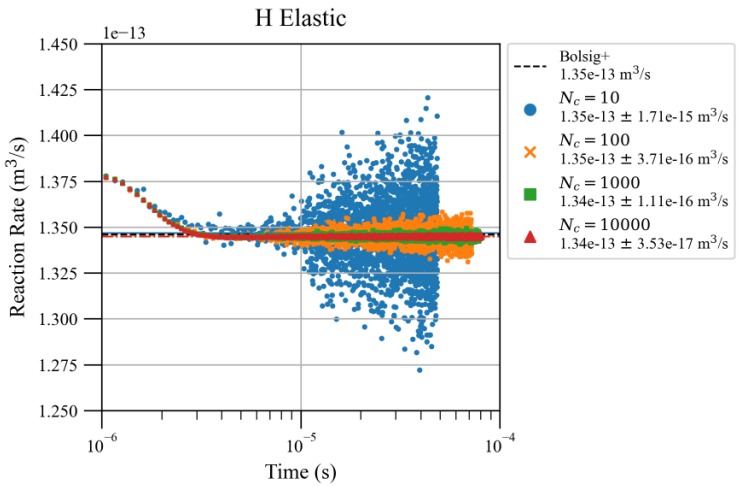
- Aleph results for swarm parameters converge with increasing computational particle count
- Results differ from Bolsig+ values by only a few percent (~1-5%)
- Reweighting reduces time variance of swarm parameters but at the cost of computational time and resources

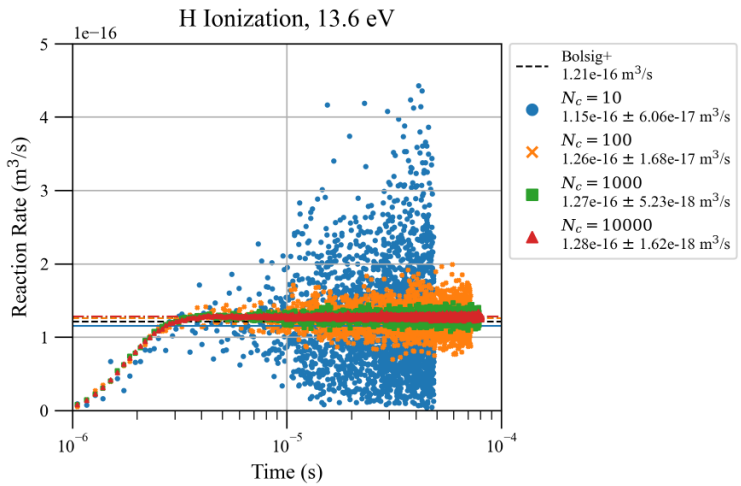


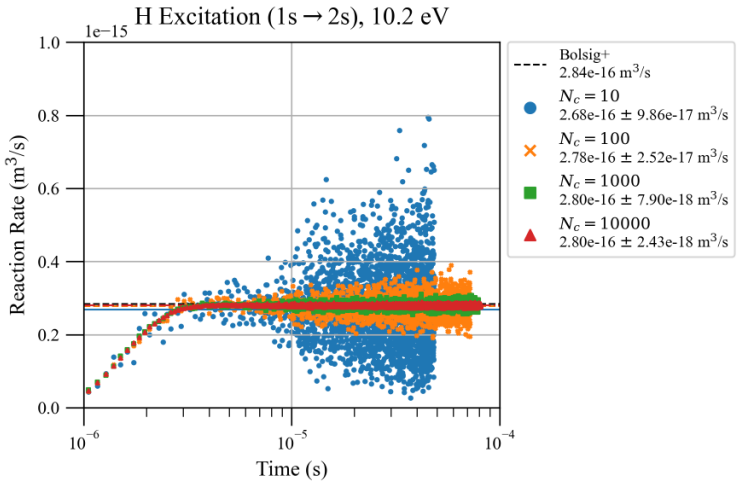


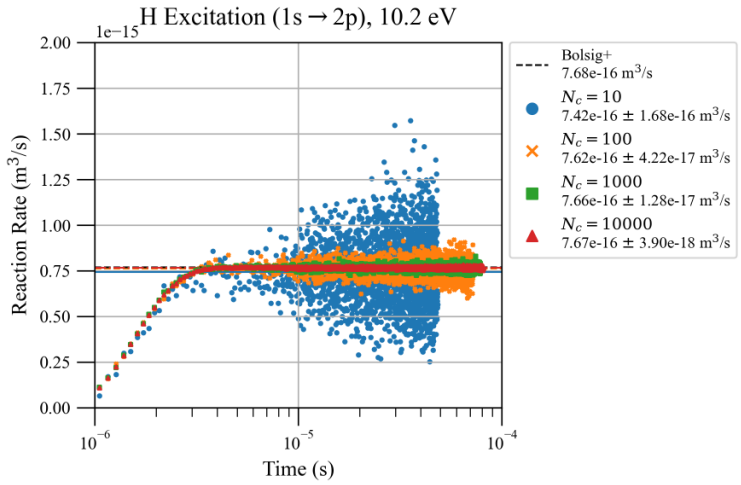
Electron-neutral Interaction Rates

- Reaction rates from Aleph are found to converge towards the Bolsig+ results
- The average ionization rate for low particle counts ($N_c = 10$) is skewed lower than other cases
- Difference in reaction rate from Aleph is typically less than 2% from Bolsig+





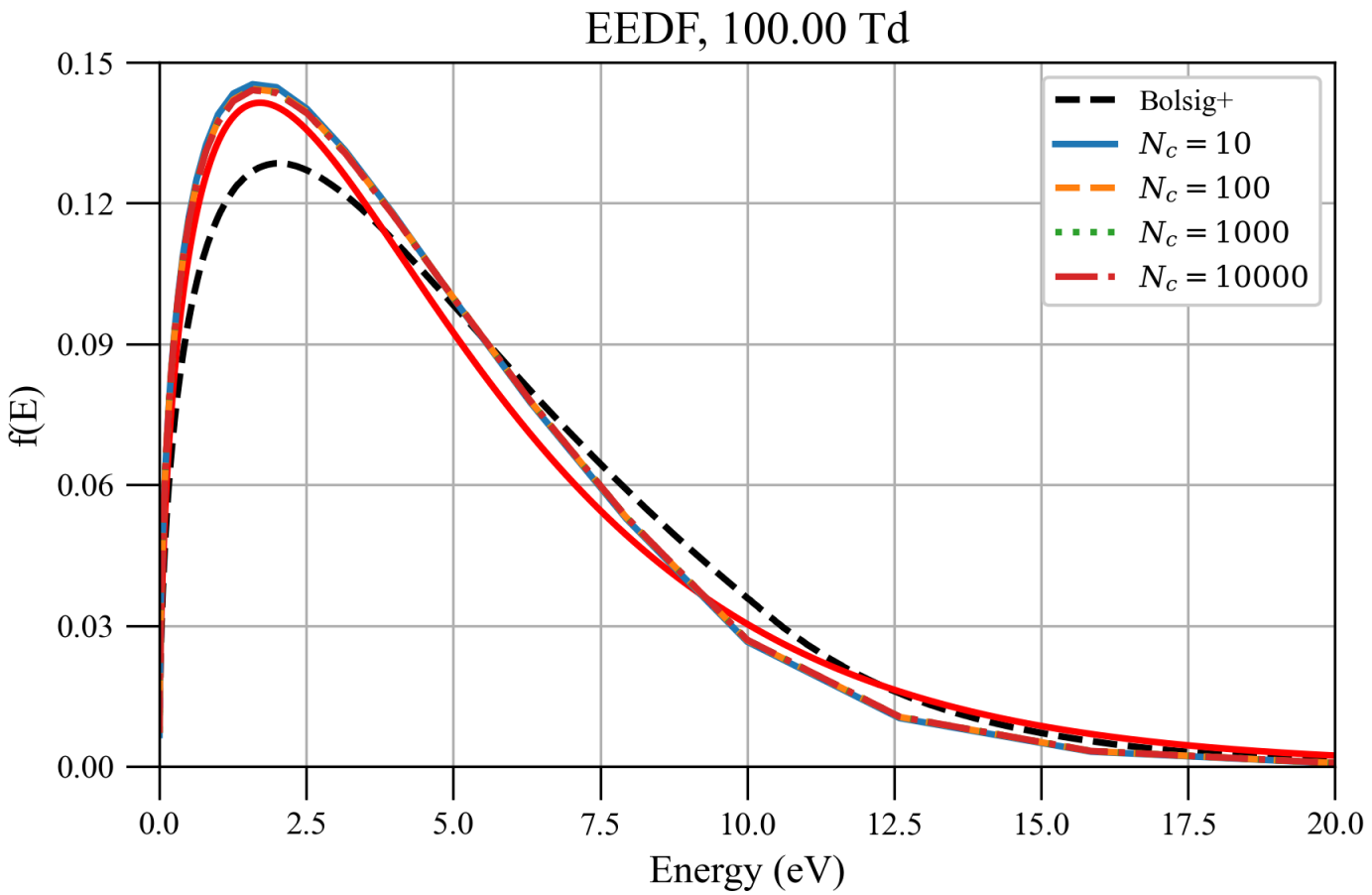




Electron Energy Distribution Function

- Aleph also capable of outputting particle histograms
- Electron energy distributions show that Aleph results are very nearly Maxwellian (red, solid line)
  - $k_B T_e = 3.423$ eV
- Particle energy distributions are not dependent on the particle weight

$$f(E) = 2\sqrt{\frac{E}{\pi}}\left(\frac{1}{k_B T}\right)^{\frac{3}{2}} \exp\left(-\frac{E}{k_B T}\right)$$



Conclusions

- Aleph is a robust PIC/DSMC code for modeling low-temperature plasmas
- Dynamic particle reweighting allows Aleph to modify the weight of computational particles on a per-element basis
- Using particle reweighting to maintain lower computational particle counts drastically decreases computational expense while only slightly increasing time variance of parameters
- Aleph results typically differ from Bolsig+ by only a few percent indicating that the DSMC algorithm is correctly handling particle interactions
- Average plasma swarm parameters are not affected by using higher particle weighting

Funding Acknowledgements

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Thank you for your time and attention!

Questions?