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Incorporating Radiation Transport into Particle-Based Plasma Simulations

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Abstract

In an effort to expand modern Particle-in-Cell (PIC) plasma simulations, a method for including radiation transport is examined. Here, discrete photons are emitted from excited state species with a state-dependent wavelength [1]. This self-produced emission from the plasma is broadened according to natural and Doppler line widths resulting in a broadened emission profile and emitted isotropically. By directly tracking the velocities of the excited species that emit radiation, the Doppler shift is easily found and the expensive convolution calculation for the Voigt profile is avoided. Discrete photon particles also have the advantage of being easily coupled to an existing collision routine such as Direct Simulation Monte Carlo (DSMC) or Monte Carlo Collision (MCC). Simulations of a helium discharge demonstrate the effectiveness of this method for determining non-equilibrium emission spectra and incorporating energy-dependent photo-processes (e.g. photo-emission, photo-ionization) [2,3].

Implementation

- Photons are modeled as discrete particles and are pushed independently through the simulation.
- The wavelength of each photon is chosen corresponding to a Voigt distribution.

Natural Line Broadening

$$L(\lambda,\Delta\lambda_L) = \frac{\left(\frac{\Delta\lambda_L}{2}\right)^2}{\left(\lambda-\lambda_0\right)^2 - \left(\frac{\Delta\lambda_L}{2}\right)^2}$$

Doppler Line Broadening

$$G(\lambda,\Delta\lambda_D) = \sqrt{\frac{4\ln(2)}{\pi}}\frac{1}{\Delta\lambda_D}e^{-4\ln(2)\left(\frac{\lambda-\lambda_0}{\Delta\lambda_D}\right)^2}$$

Voigt Distribution

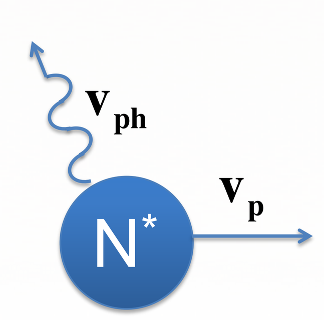
$$g(\lambda,\Delta\lambda_D,\Delta\lambda_L) = \int_{-\infty}^{\infty} G(\lambda',\Delta\lambda_D)L(\lambda-\lambda',\Delta\lambda_L)\,d\lambda'$$

(1) Determine if an excited particle radiates via the equation $R < 1 - e^{-\Delta t/\tau}$

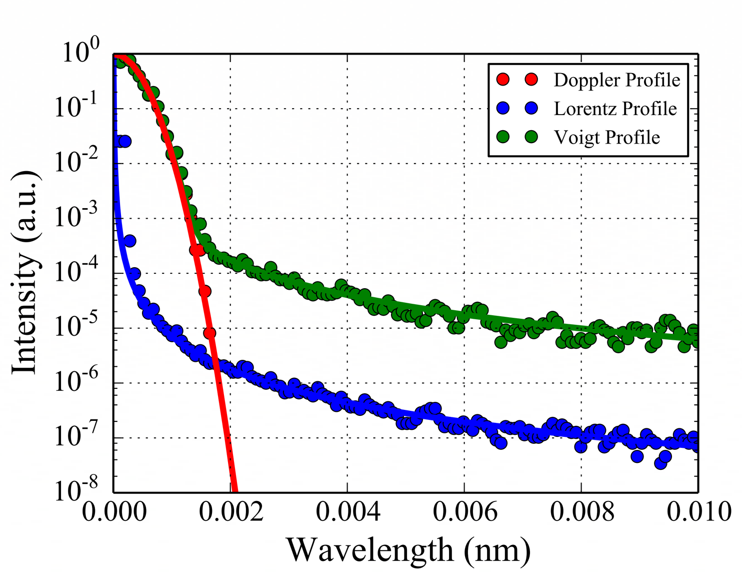
(2) Choose wavelength from inverse transform of the CDF of Lorentz Distribution $\lambda_s = \tan((r-0.5)\pi)\Delta\lambda_L + \lambda_0$

(3) Determine the vector for photon propagation (chosen isotropically), $\mathbf{v}_{ph}$ and the vector of the emitting particle, $\mathbf{v}_p$.

(4) The final wavelength is selected by $\lambda_f = \frac{(c + \hat{\mathbf{v}}_{ph}\cdot\mathbf{v}_p)\lambda_s}{c}$



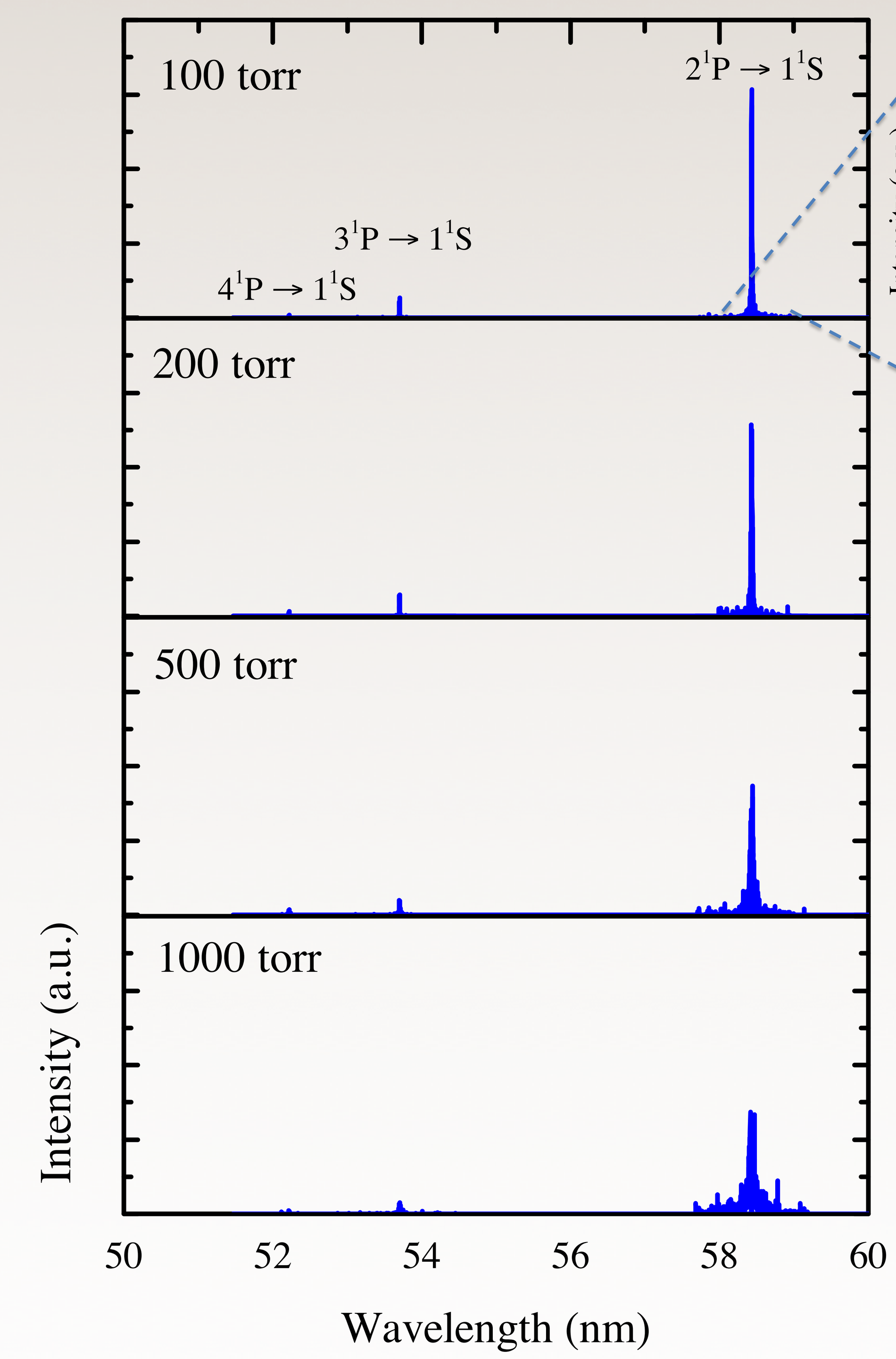
Verification

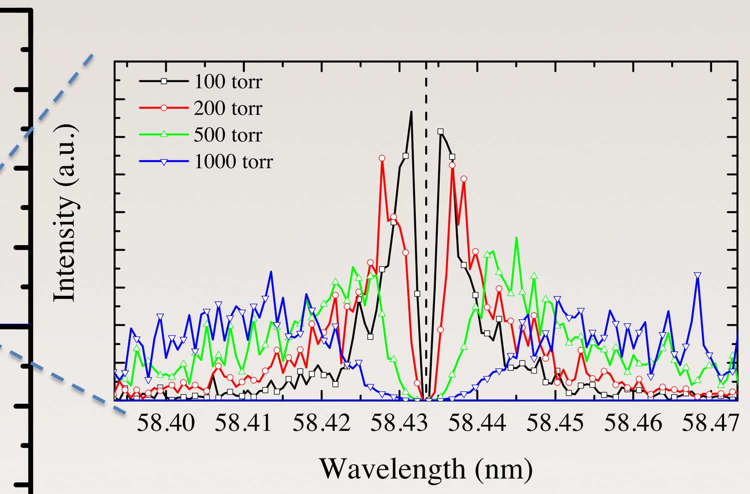


- Zero-dimensional simulation that represents the ground-state transition $2^1P \rightarrow 1^1S$ in helium gas centered at 58.4334 nm (no self-absorption included).
- Seed density of 10^{21} m^{-3} of the He 2^1P state into the simulation volume and record the wavelength of photons in the volume after some time.
- Histogram of the resulting wavelengths allows emission profile generation.
- Transition rate of 1.799 × 10^9 s^{-1}.
- Gas temperature (T_g) of 1500 K.
- Excellent agreement between simulation (solid circles) and theory (solid lines).

Helium Emission Spectra

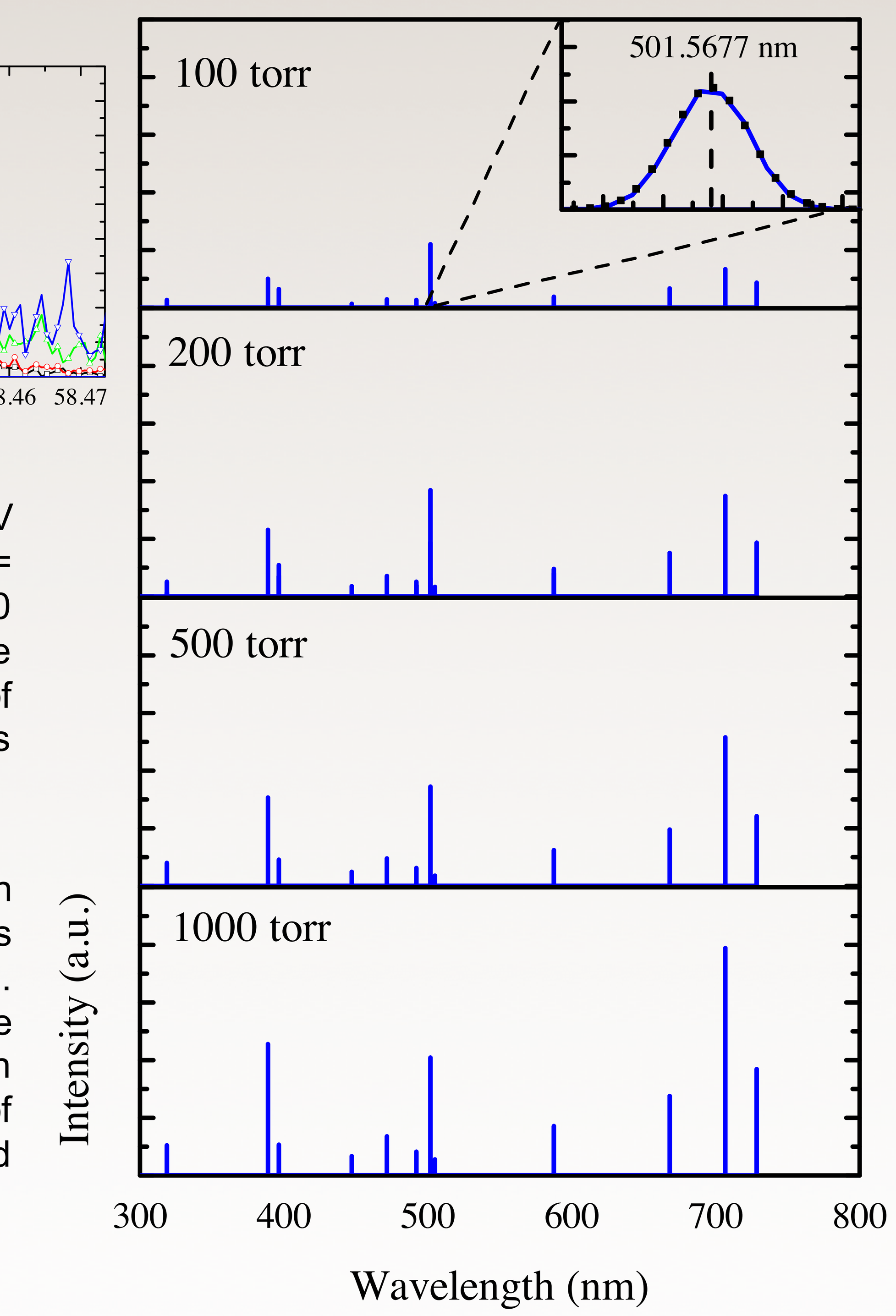
- One-dimensional Townsend discharge simulation in helium gas with a constant voltage applied to the anode.





Left and above: VUV emission spectra taken at t = 50 ns and integrated over 10 ns. Zoomed in image depicts the self-absorption of this transitions that is pressure dependent.

Right: UV-VIS emission spectra taken at t = 50 ns and integrated over 10 ns. Inset graph shows the theoretical Voigt emission profile (squares) on top of the kinetically simulated emission profile.



Conclusions

- A discrete photon approach is used that enables photons to be created from excited states with a wavelength corresponding to a Voigt distribution.
- Simulations in one dimension demonstrate the method's ability to simulate emission spectra as well as include self-absorption mechanisms that may be important for some plasma physics investigations [4].
- The method coupled with a kinetic code allows the simulation of non-equilibrium emission spectra and the inclusion of energy-dependent photo-processes into existing simulation frameworks.

References

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[2] A. Fierro, J. Stephens, S. Beeson, J. Dickens, A. Neuber, "Discrete Photon Implementation for Plasma Simulations," Physics of Plasmas, 23, 013506, 2016.

[3] A. Fierro, C. Moore, B. Scheiner, B. Yee, M. Hopkins, "Radiation Transport in Kinetic Simulations and the Influence of Photo-emission on Electron Current in Self-Sustaining Discharges," Journal of Physics D: Applied Physics, to be submitted, 2016.

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[5] Y. Ralchenko, R. Janeiv, T. Kato, D. Fursa, I. Bray, F. Heer, "Electron-impact Excitation and Ionization Cross Sections for Ground State and Excited Helium Atoms," Atomic Data and Nuclear Data Tables, 94, 603, 2008.

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