Modeling Collisional Ionization Using a Modified Binary-Encounter-Bethe Model in the Particle-in-Cell Code OSIRIS

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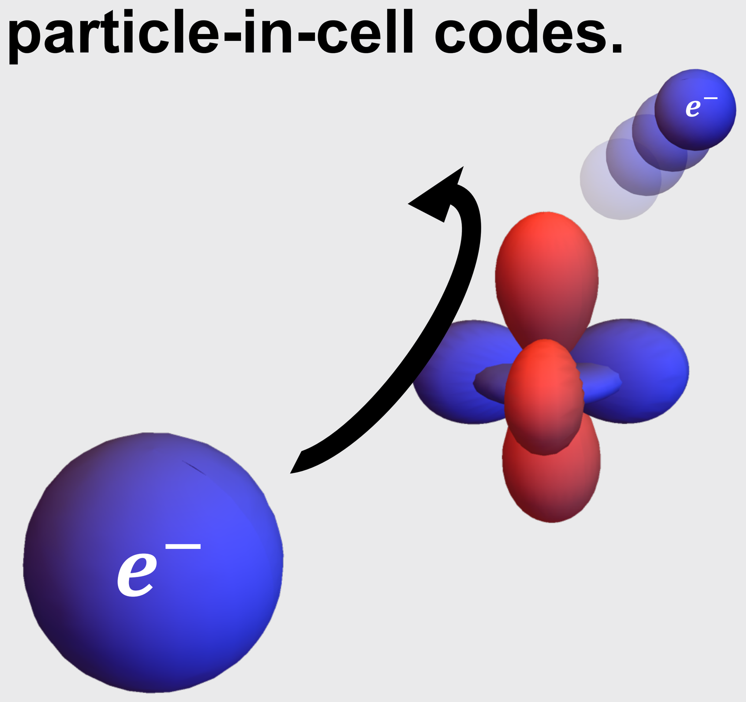
Introduction

Collisional ionization physics has become necessary to a proper understanding of plasma dynamics in a variety of situations, so it is has become important to develop and implement computational models that accurately depict the complex atomic physics of these interactions.

We have implemented a collisional ionization routine in the particle-in-cell code OSIRIS that draws on examples and advancements from other particle-in-cell codes.



Cross Section Calculations

We calculate cross sections using the modified binary-encounter-Bethe model presented by Guerra et al. [1].

$$\sigma_{n\ell j} = \frac{4\pi a_0^2 \alpha^4 N_{n\ell j}}{(\beta_t^2 + \chi_{n\ell j}\beta_b^2)2b'}\left\{\frac{1}{2}\left[\ln\left(\frac{\beta_t^2}{1-\beta_t^2}\right) - \beta_t^2 - \ln(2b')\right]\left(1-\frac{1}{t^2}\right) + 1 - \frac{1}{t} - \frac{\ln t}{t+1}\frac{1+2t'}{(1+t'/2)^2} + \frac{b'^2}{(1+t'/2)^2}\frac{t-1}{2}\right\}$$

$$\chi_{n\ell j} = \left(\frac{C_{n\ell j}}{B}\right)2R$$

A key ingredient for this calculation is the binding energy of each electron. For this, we use data collected in [2].

$$C_{n\ell j} = 0.3\frac{Z^2_{\mathrm{eff},n\ell j}}{2n^2} + 0.7\frac{Z^2_{\mathrm{eff},n'\ell' j'}}{2n'^2}$$

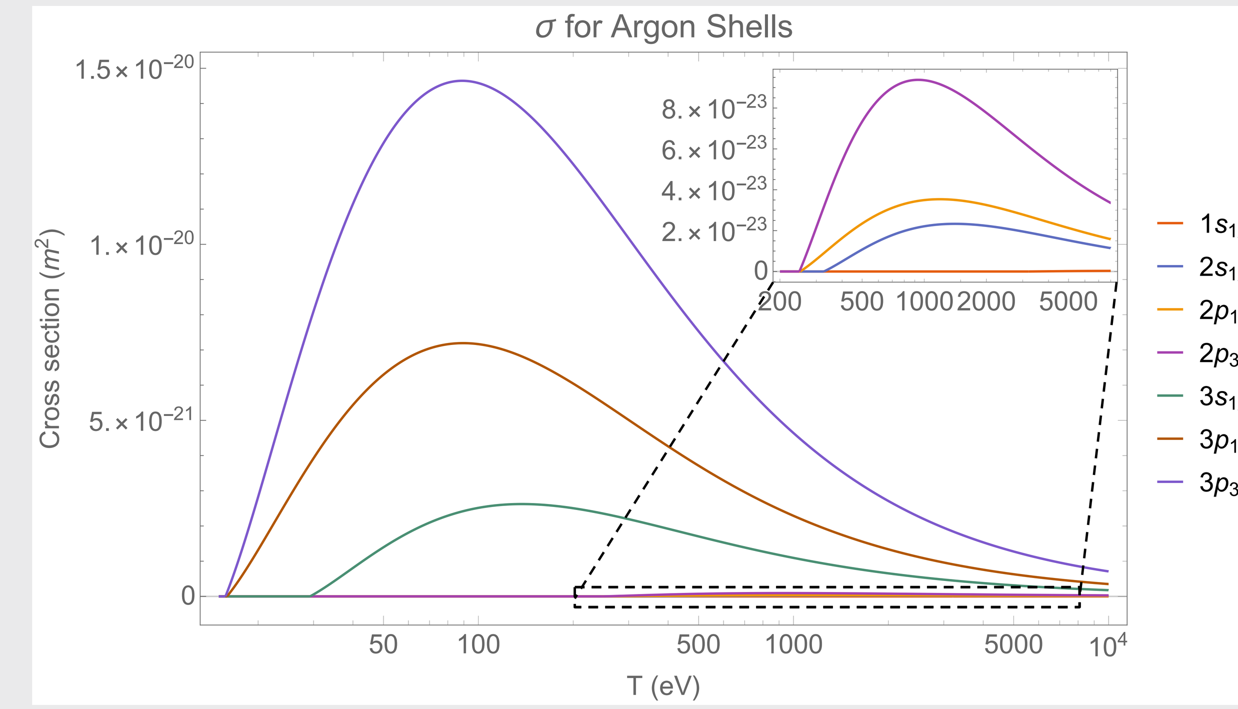
The effective nuclear charge is also required. For each electron shell, there might exist other electrons that shield the charge of the nucleus, creating an effective charge binding the electron to the atom. For this, we use the compiled data presented in [3,4].

Assumptions in Calculations:

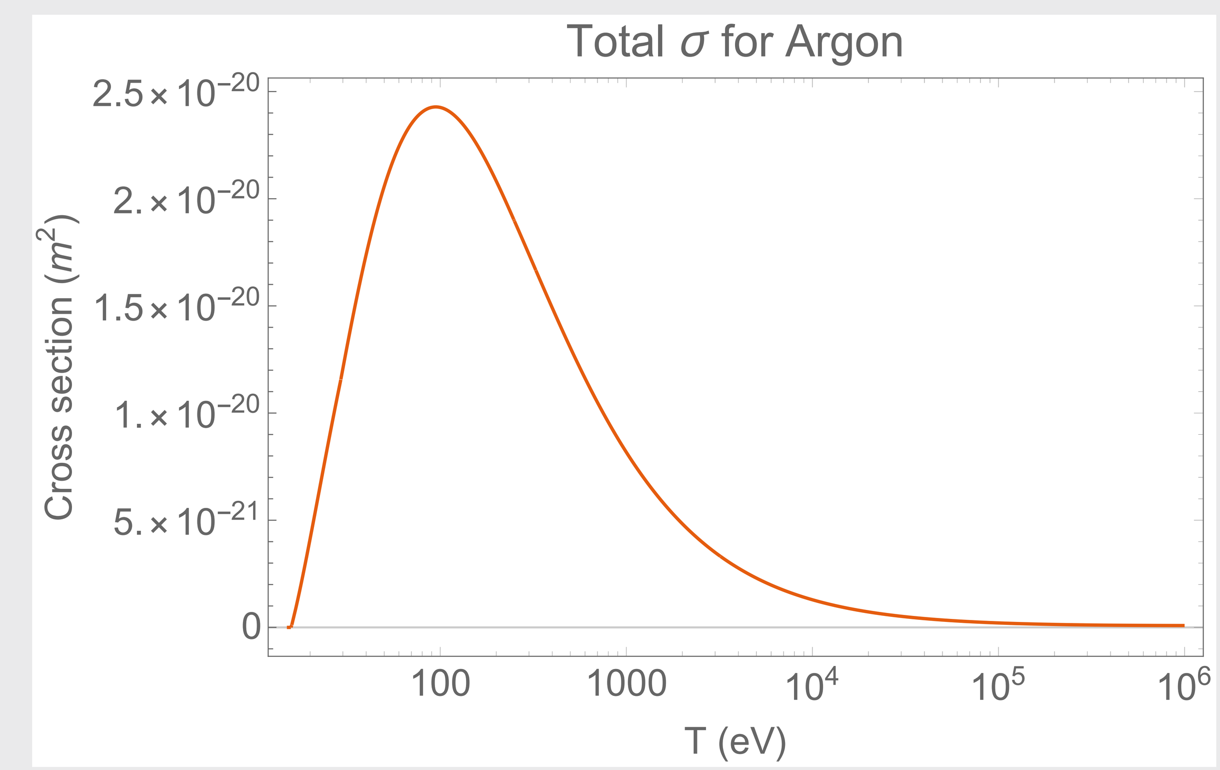
- Electrons are ionized from outermost electrons to innermost.
- Only one electron can be ionized per event.

$$t = \frac{T}{B} \quad t' = \frac{T}{m_e c^2} \quad \beta_t^2 = 1 - \frac{1}{(1+t')^2}$$

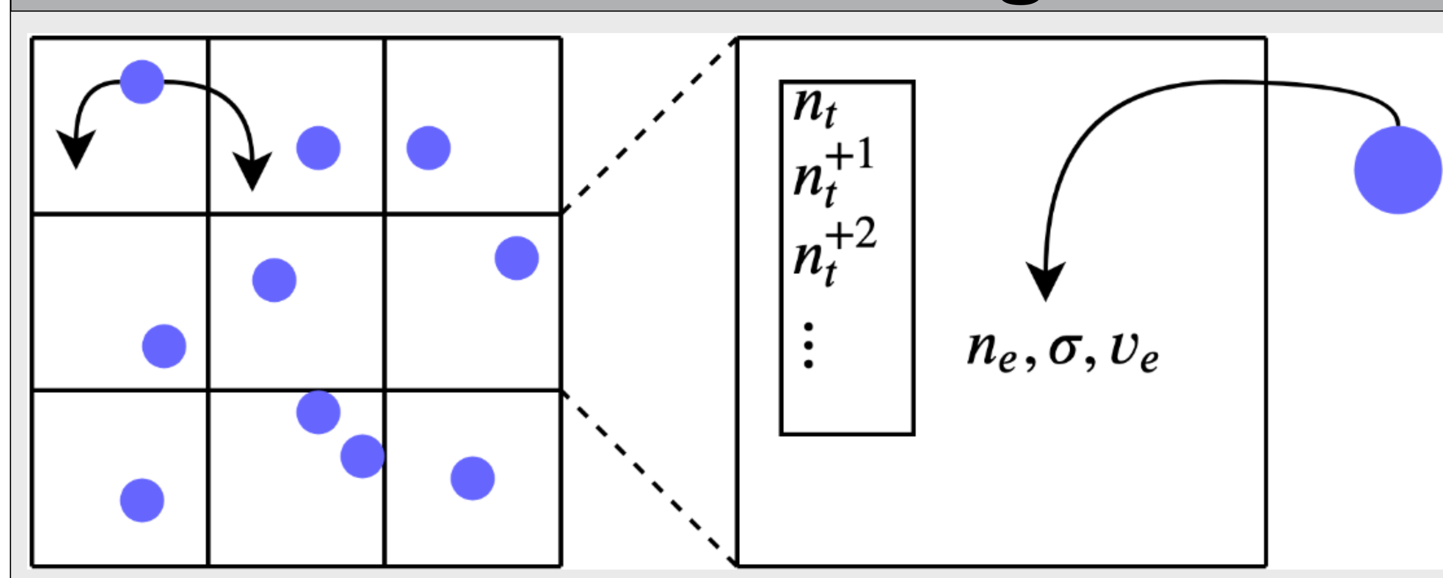
$$b' = \frac{B}{m_e c^2} \quad \beta_b^2 = 1 - \frac{1}{(1+b')^2}$$



$$\sigma_{Tot} = \sum \sigma_{n\ell j} \Downarrow$$



Integration into Particle-in-Cell Codes



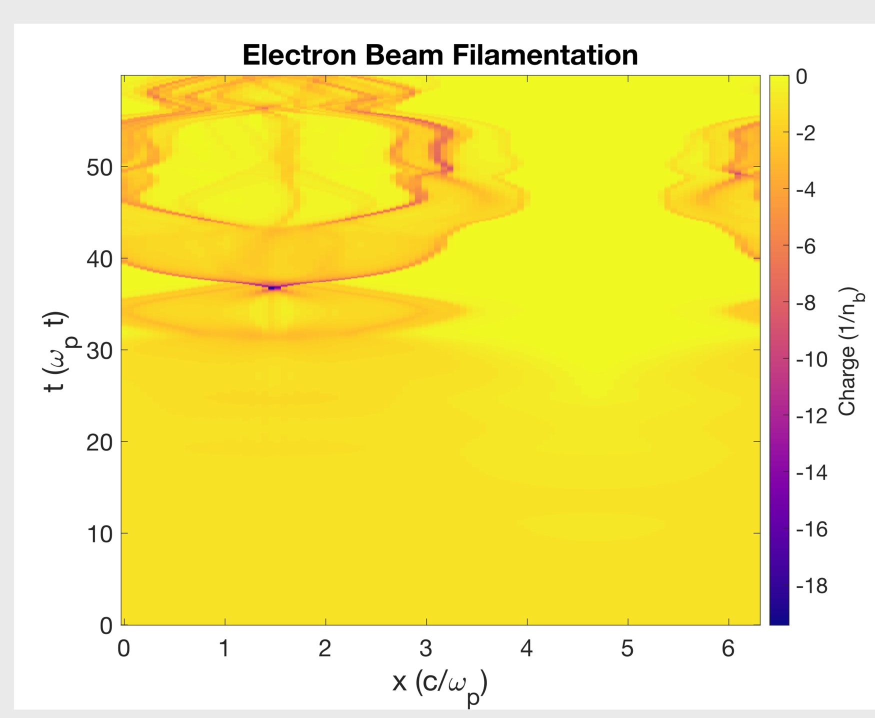
$$\frac{dn_t}{dt} = n_e n_t \langle \sigma v_e \rangle$$

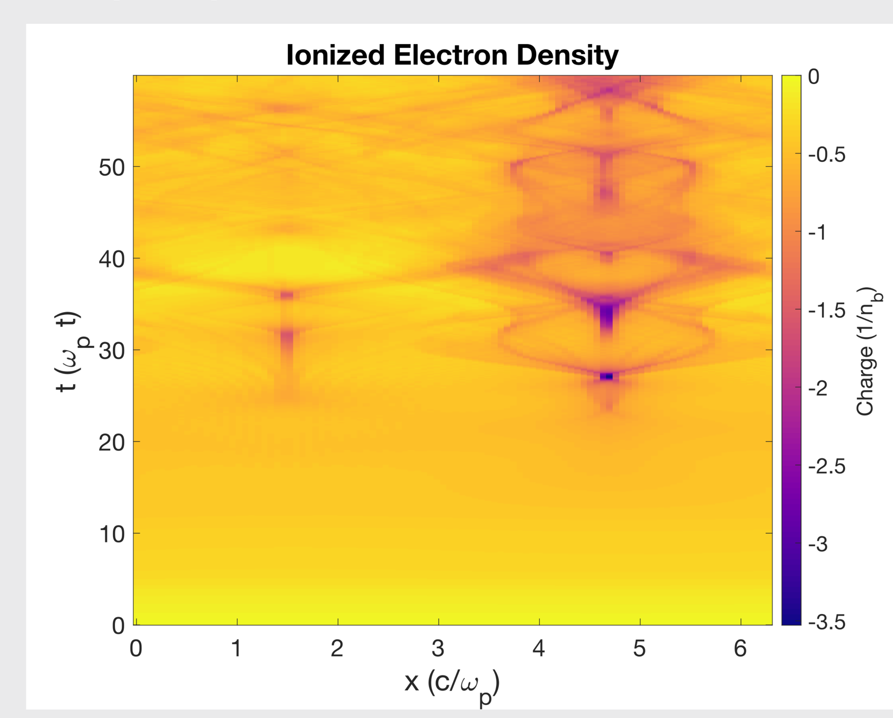
We use these cross section calculations to enable impact ionization capabilities in PIC codes, particularly within Osiris.

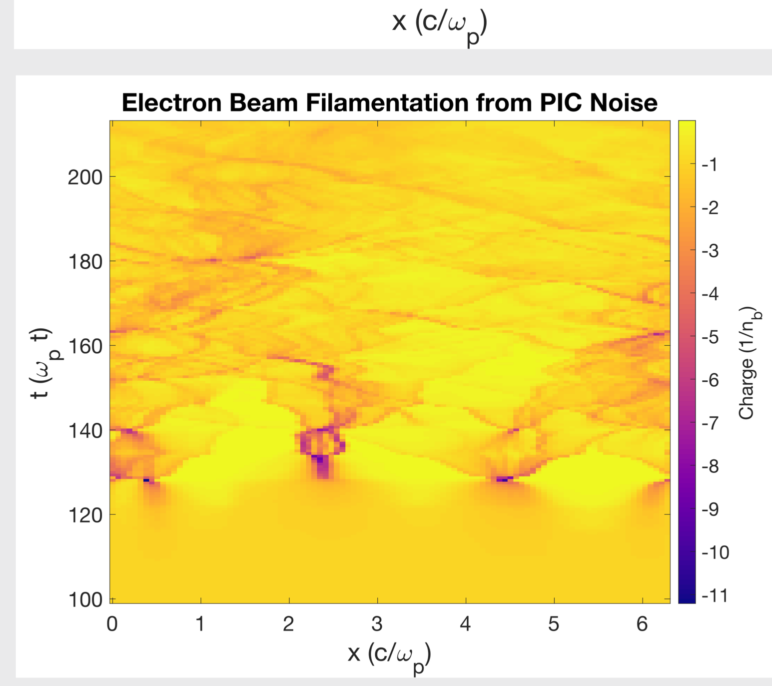
- During initialization, the cross sections are tabulated in a look-up table.
- Every PIC loop involves depositing n_e, v_e, σ onto the grid and then calculating the ionization rates for every ionization state.
- Ion densities are then advanced and new electrons injected into the simulation.

Test Case: e^- Beam Filamentation

- Electron beam ($\gamma = 10$) incident on neutral Nitrogen
- *Only* ionization mechanism is *impact ionization*
- Electron beam seeded with small (1%) sinusoidal perturbation







Species were at a ratio of $^{n_b}/_{n_t} = 7$ so that the electron densities were approximately equal when fully ionized.

This allowed for impact ionization to seed unstable growth of ionization events until the Nitrogen was completely ionized.

Future Work

Once Osiris supports multiple moving ion species, implement particle-particle ionization interactions proposed by F. Pérez et al. [Phy of Plasmas 19, 083104 (2012)], and determine whether ionization events occur using a similar formulation to C. P. Ridgers et al. [J of Comp Phy 260, 273 (2014)].

References and Support

[1] M. Guerra et al., Int J of Mass Spect 313, 1 (2012).
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