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A Hybrid Model for Multiscale Laser Plasma Simulations with Detailed Collisional Physics

*AFOSR Plasma and Electroenergetics Review Meeting
13-15 June 2017*

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Outline



- **Goals**
- **Review of Past Work**
- **Argon Collisional-Radiative; comparison of reduction mechanisms**
- **Non-Maxwellian CR**

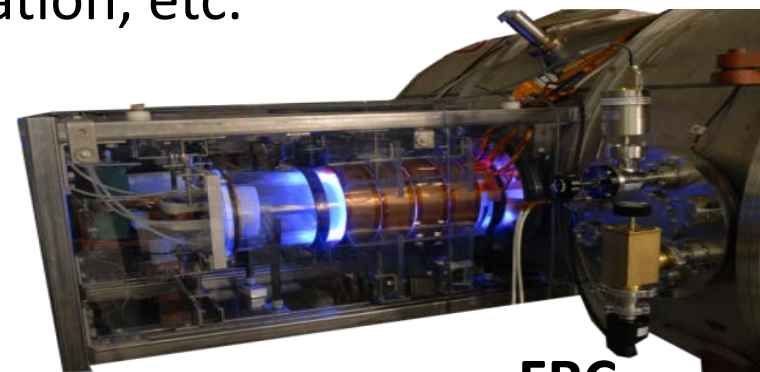


Goals

- Utilize hybridization techniques to produce accurate and efficient plasma simulations that spans many orders of magnitude in both space and time.
- Capture complex physics: excitation/ionization, transport, radiation, etc.
- Consistent collision operator across different levels of fidelity.

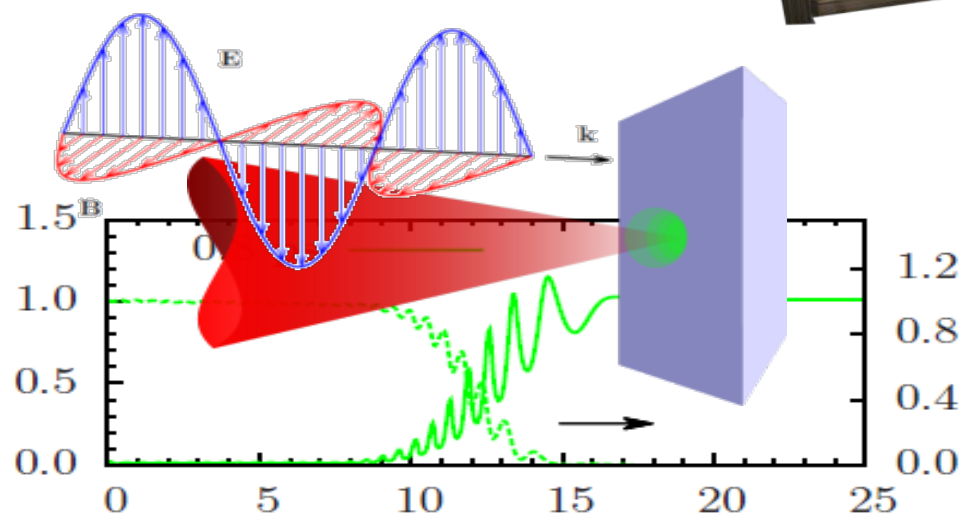
Current Focus:

- Generalization of collisional-radiative kinetics with level grouping
- General Hybridization techniques
- Focus on each solver before hybridization
- Special attention to low density low energy conditions



FRC

Laser Plasma Interaction





Summary of Past Work

Maxwellian Inelastic Collisions

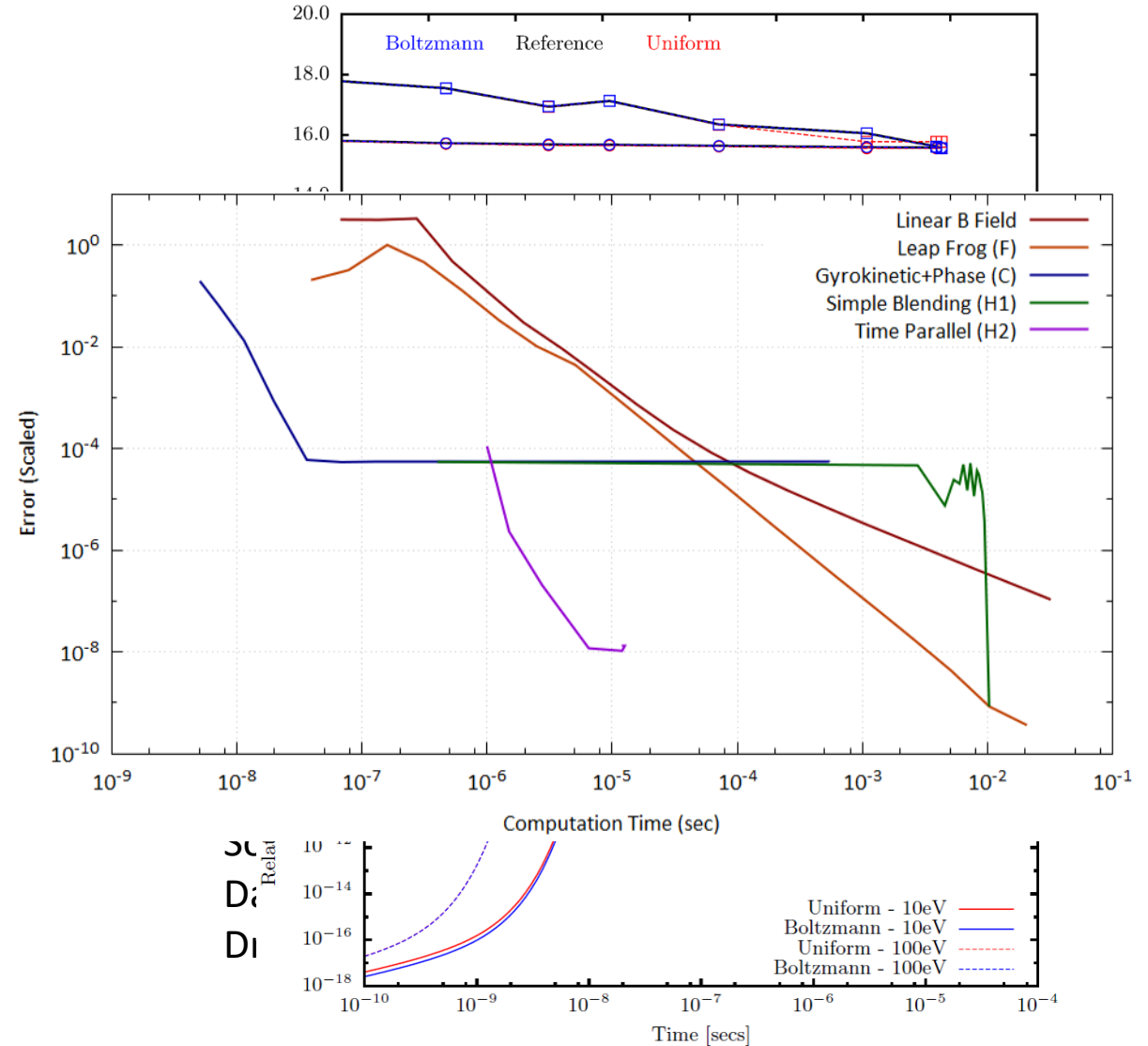
- Detailed CR model for multiple ionization stages
- Validation against experimental data
- Nonequilibrium radiation transport: coupling with a collisional-radiative model
- Inelastic collisions in a MF plasma: enhanced thermochemical kinetics.

Multiscale Hybridization

- A time-parallel/multiscale method with energy preservation

Boltzmann – Uniform Grouping comparison

- Boltzmann is more accurate when compared to electron configuration





Collisional Radiative (CR) Overview

Updates

- Investigated Quasi-Steady-State
- Investigated single temperature Boltzmann grouping
- Reintroduced radiation sources
- Investigate grouping sensitivity
- Linked with LANL database for Argon cross sections and atomic level information
- Algorithms not hard coded for Argon.
- Adaptive time steps

Kinetics

- Electron-Impact Rates:
 - Excitation \leftrightarrow De-excitation
 - Ionization \leftrightarrow Three-body Recombination
- Radiation (Planckian)
 - Photoexcitation \leftrightarrow Stimulated + Spontaneous Emission
 - Photoionization \leftrightarrow Stimulated Radiative Recombination



CR Grouping Techniques

Quasi Stead-State (QSS)

- Assumes fast kinetics between states within an ion distribution
- Assumes longer diffusion/decay times than excited state lifetimes
- Does not conserve mass of excited states

$$\frac{DN_1^{+k}}{Dt} = R_n^{+k} - F_n^{+k} N_n^{+k}$$

$$\frac{DN_1^{+k}}{Dt} = 0 \text{ for } n > 1$$

Boltzmann Grouping

- Conserves number density
- Preserves energy in groups through group temperature description
- Consistent with Boltzmann equilibrium.

Conserved Variable:

$$N_{n_0} \& N'_n = \frac{N_{n_0}}{g_{n_0}} \sum_{i \in n} g_i e^{-\Delta E_i / T_n}$$

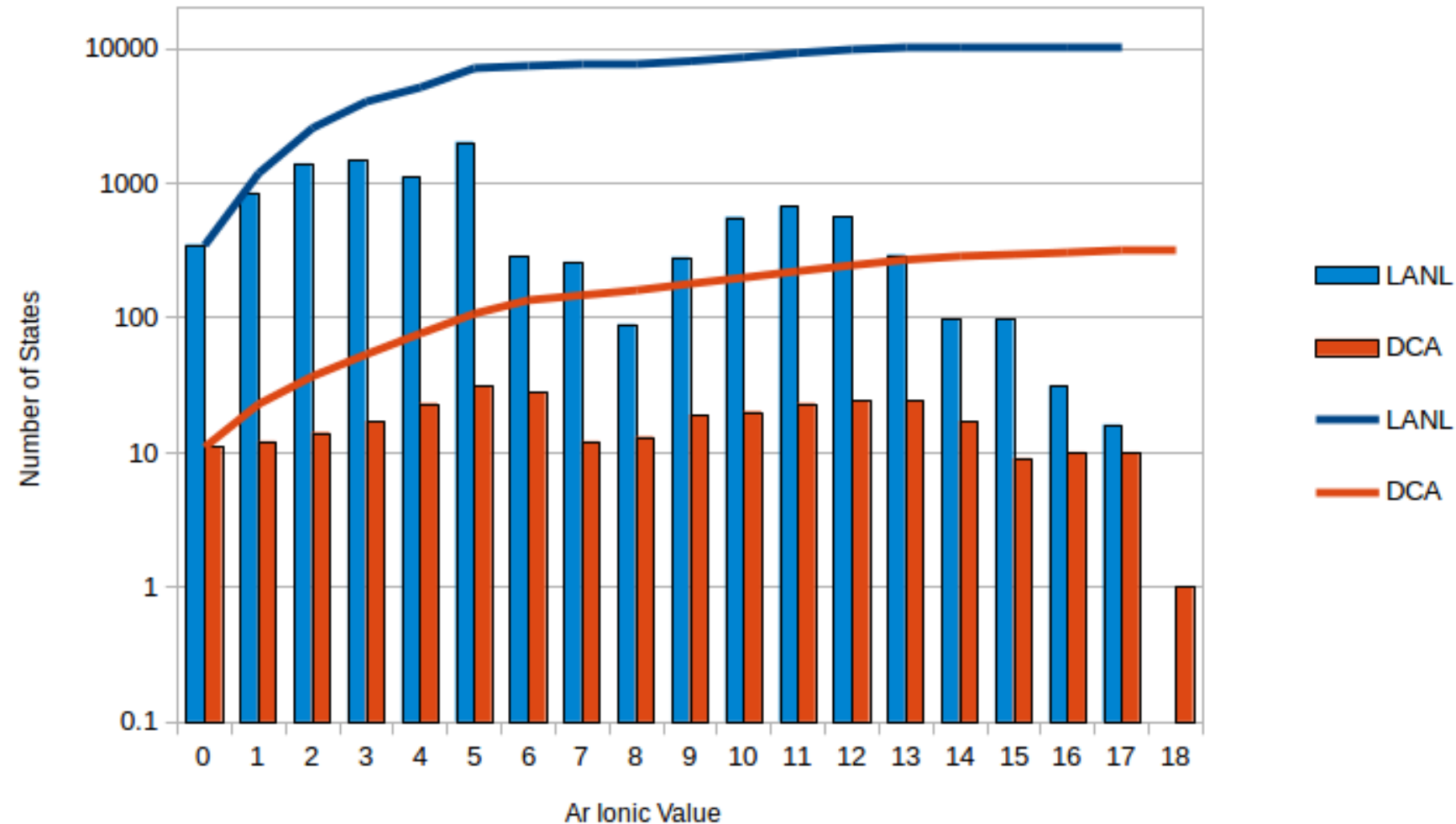
Effective rate:

$$\tilde{\alpha}(m'|n') = \sum_{i \in n} \frac{g_i e^{-\Delta E_i / T_n}}{Z'_n} \sum_{j \in m'} \alpha(j|i)$$



Complexity Reduction for Argon

- Prevalent in numerous applications, i.e. electric propulsion, LPI, etc.
- Extracted atomic data sets from Los Alamos Natl. Lab (LANL) database for all 18 iso-sequences of argon
- Detail level of atomic data is LS-coupling. Reduced the data to detailed configuration-averaged (DCA). Previously known as electron configuration





Argon CR Test Cases



Isothermal Heating

- Comparison between DCA, QSS, and single Boltzmann grouping
- Single Boltzmann grouping applies grouping to whole ionic distribution
 - “Worst case” scenario for accuracy
- Most comparable formulation to QSS

Irradiated System

- Implemented radiation source terms for the DCA case with Planckian field (i.e. black body radiation)
- Required addition of electron energy equation
- Uses tabulated cross sections to calculate photo-ionization rates (more flexible than analytical)

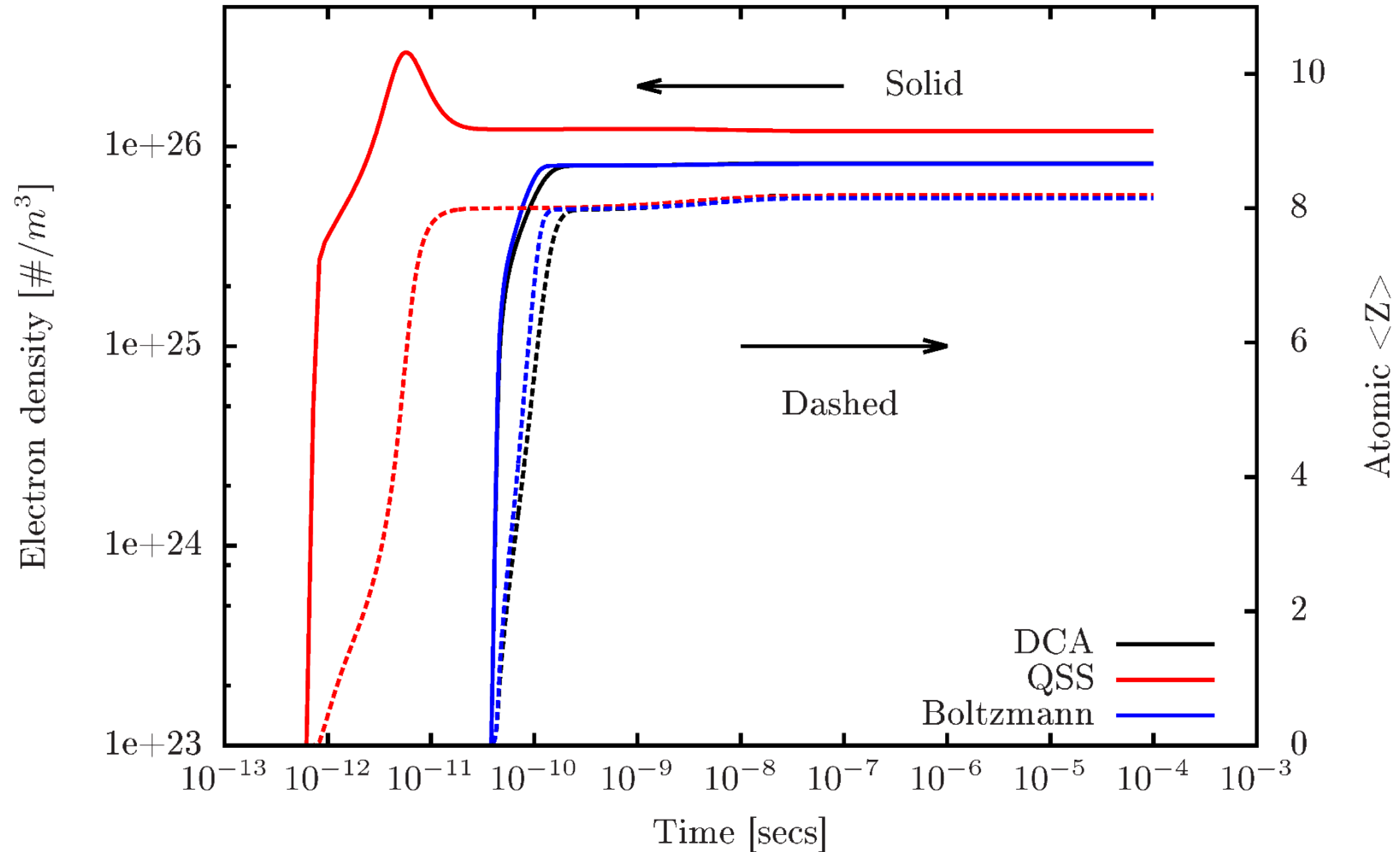


Test Case: Isothermal Heating



Conditions

- **Heavy ions:**
 - 10^{25} m^{-3}
- **Initial electron density**
 - 10^{10} m^{-3}
- **Fixed electron temperature**
 - 50 eV

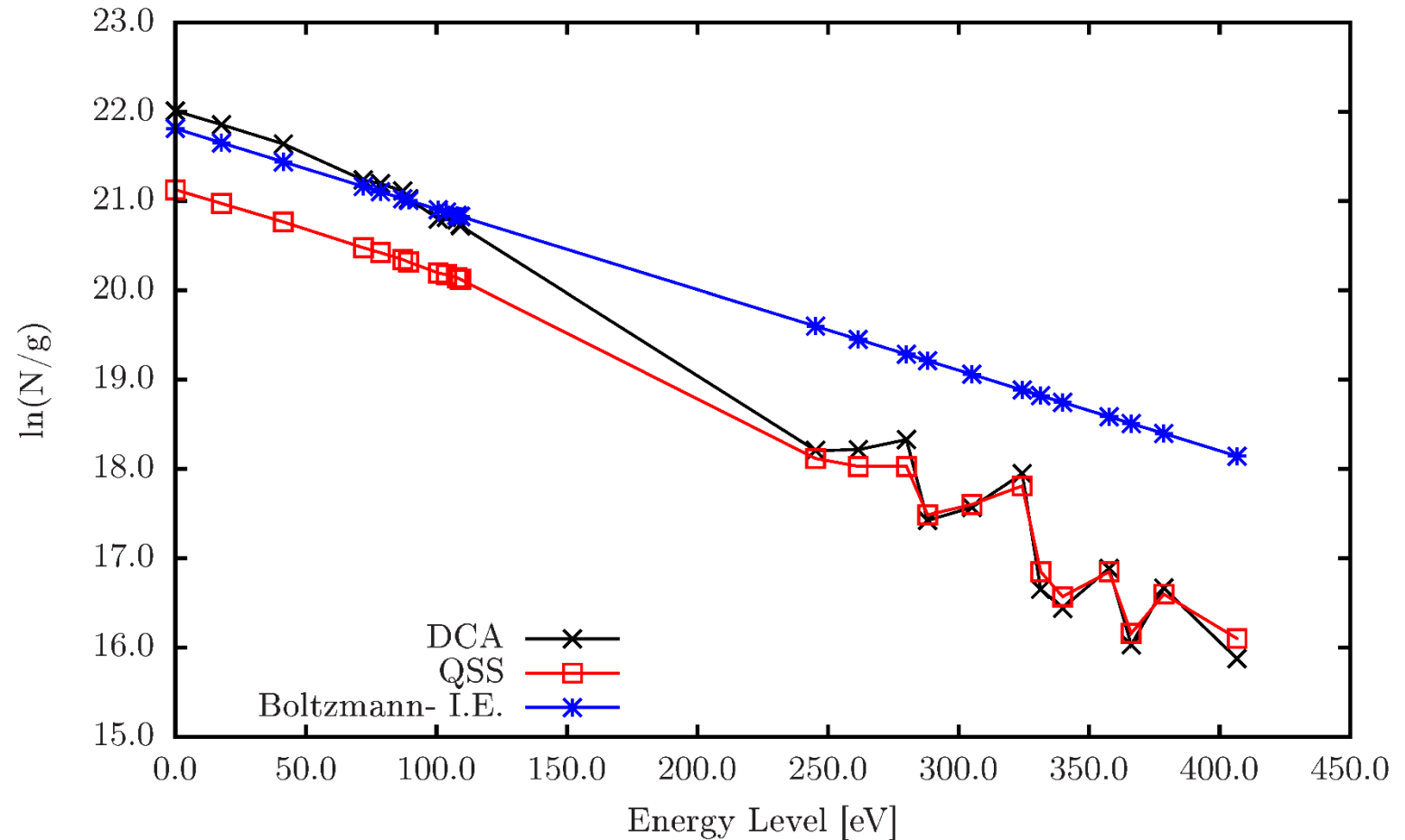




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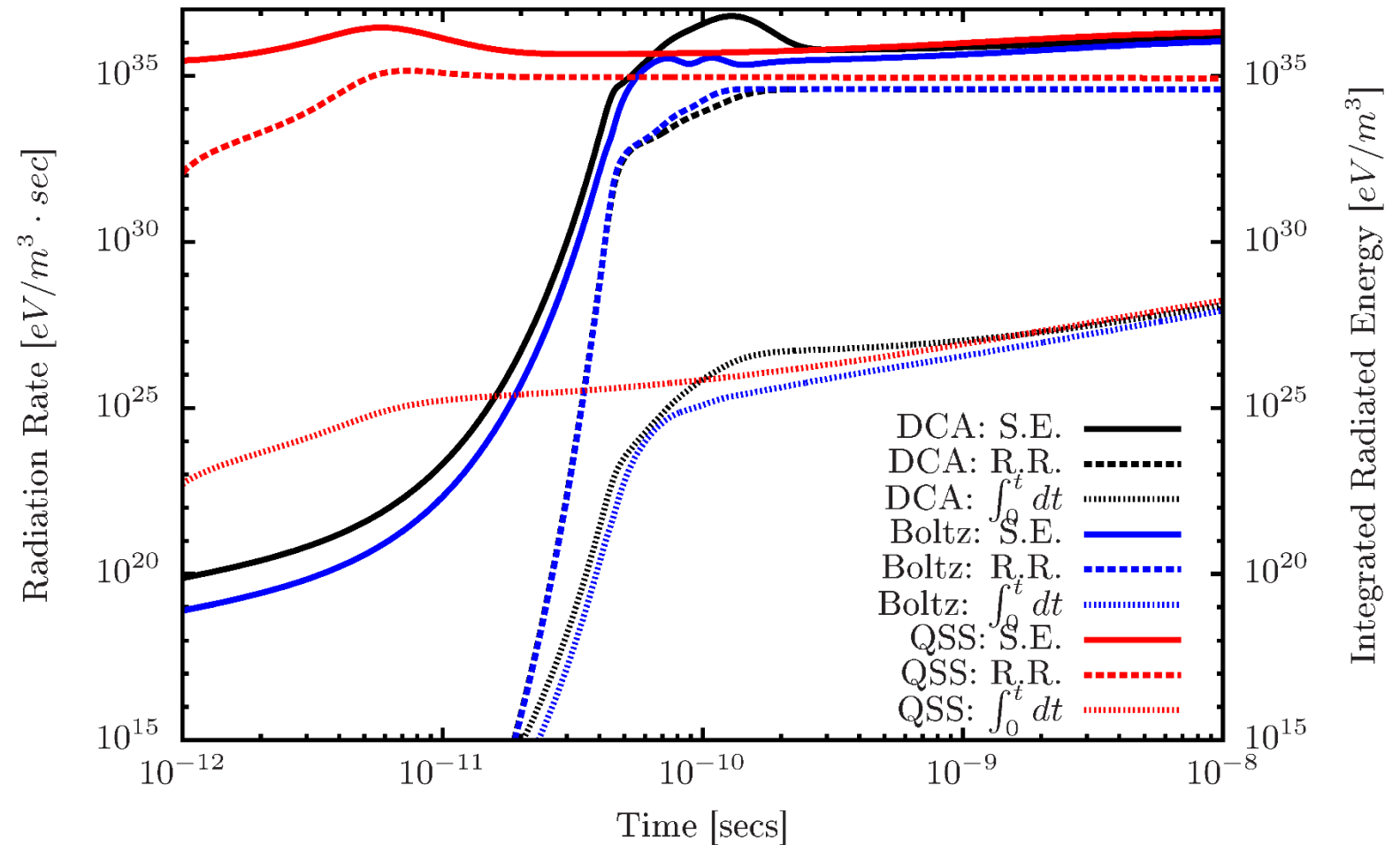


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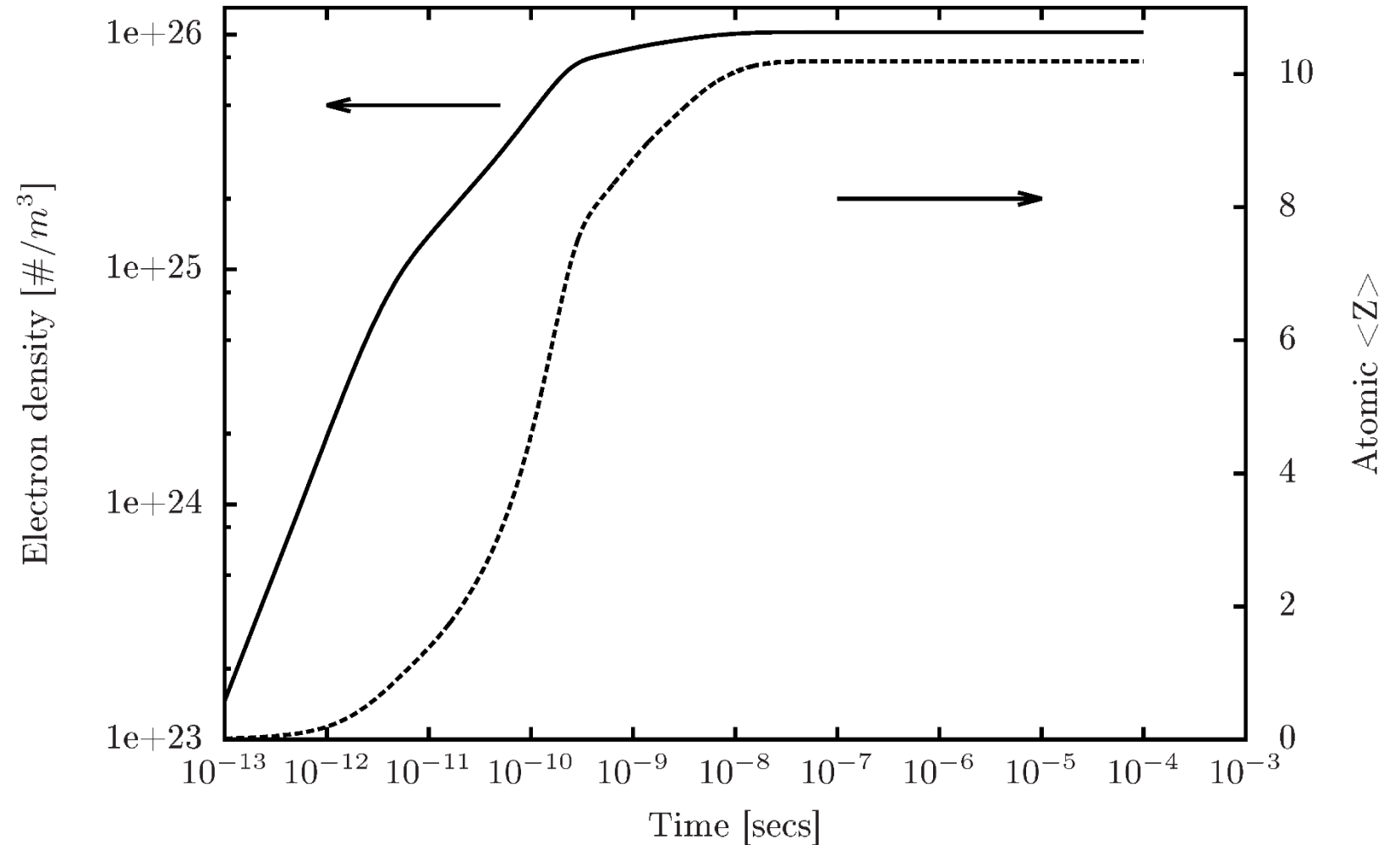




Test Case: Irradiated System

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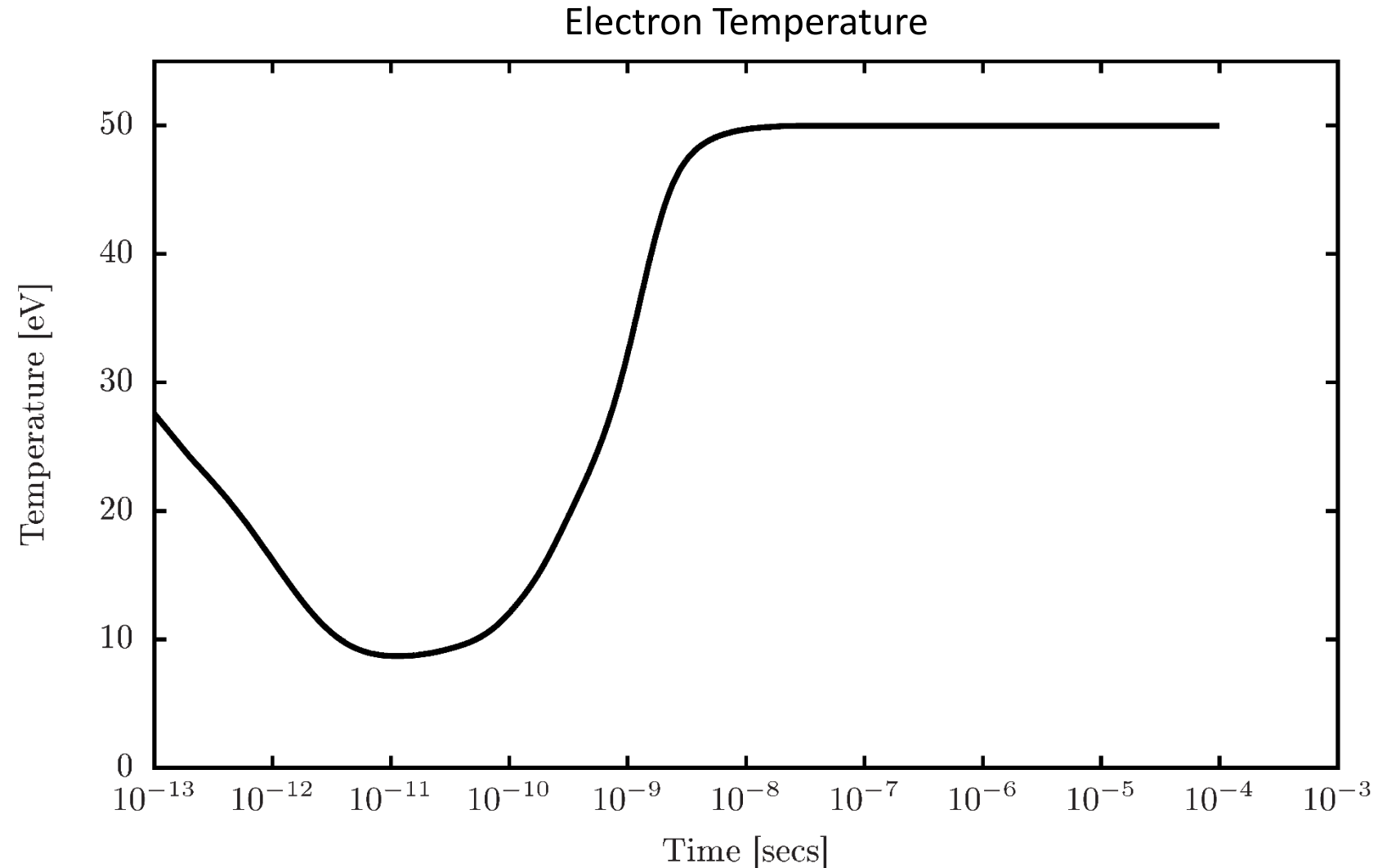




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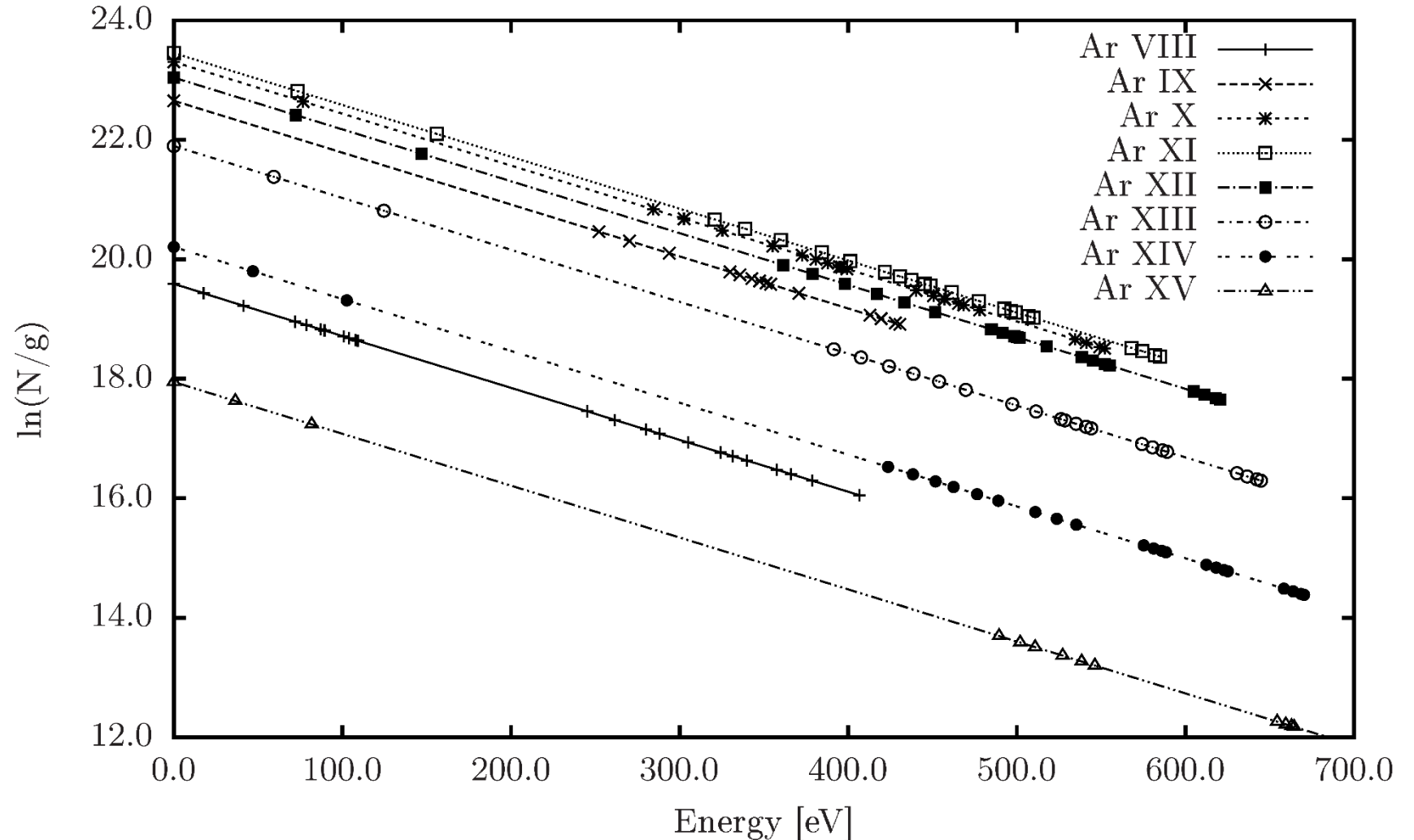




Test Case: Irradiated System

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Non-Maxwellian Inelastic Collision Modeling: Overview



- **Model inelastic and elastic collisions amongst electrons, hydrogen atoms, and ions while allowing non-Maxwellian electron energy distribution functions. (Excitation, De-excitation, Ionization, Recombination, the Fokker-Planck Equation, Bremsstrahlung, along with radiative transitions and many other processes in the future).**
- **Previous work on this task either assumed a Maxwellian electron distribution function OR involved a very simple collision model (BGK).**
- **The task objective is not the further development of these physical process, or even analytical approximations of them, but rather, an attempt to incorporate as much of the important physical process as possible with as little computational cost as possible.**
- **To that end, we are in the early processes of characterizing all the different types of relevant CR processes that occur, along with the assumptions on shape of the distribution functions, and determining the circumstances under which higher accuracy/higher computational cost models are necessary to fully implement.**



Non-Maxwellian Inelastic Collision Modelling



- ***Complex CR Formulas:***
 - Typical differential equations can be written on a single line where as these take pages to write out.
- ***Boundary conditions:***
 - Vlasov boundary conditions are a challenge. Additionally, each inelastic collision process has its own type of boundary condition in which a region can be drawn out where there is sufficient energy for that process to occur.
- ***Non-local interactions:***
 - Even for explicit methods with a small time step, updating the solution at a single location requires calculations with a dependence on every point being modeled.
- ***Incorporation of other non-trivial mathematical algorithms:***
 - Pre-computation of quantities required for propagation of the solution.



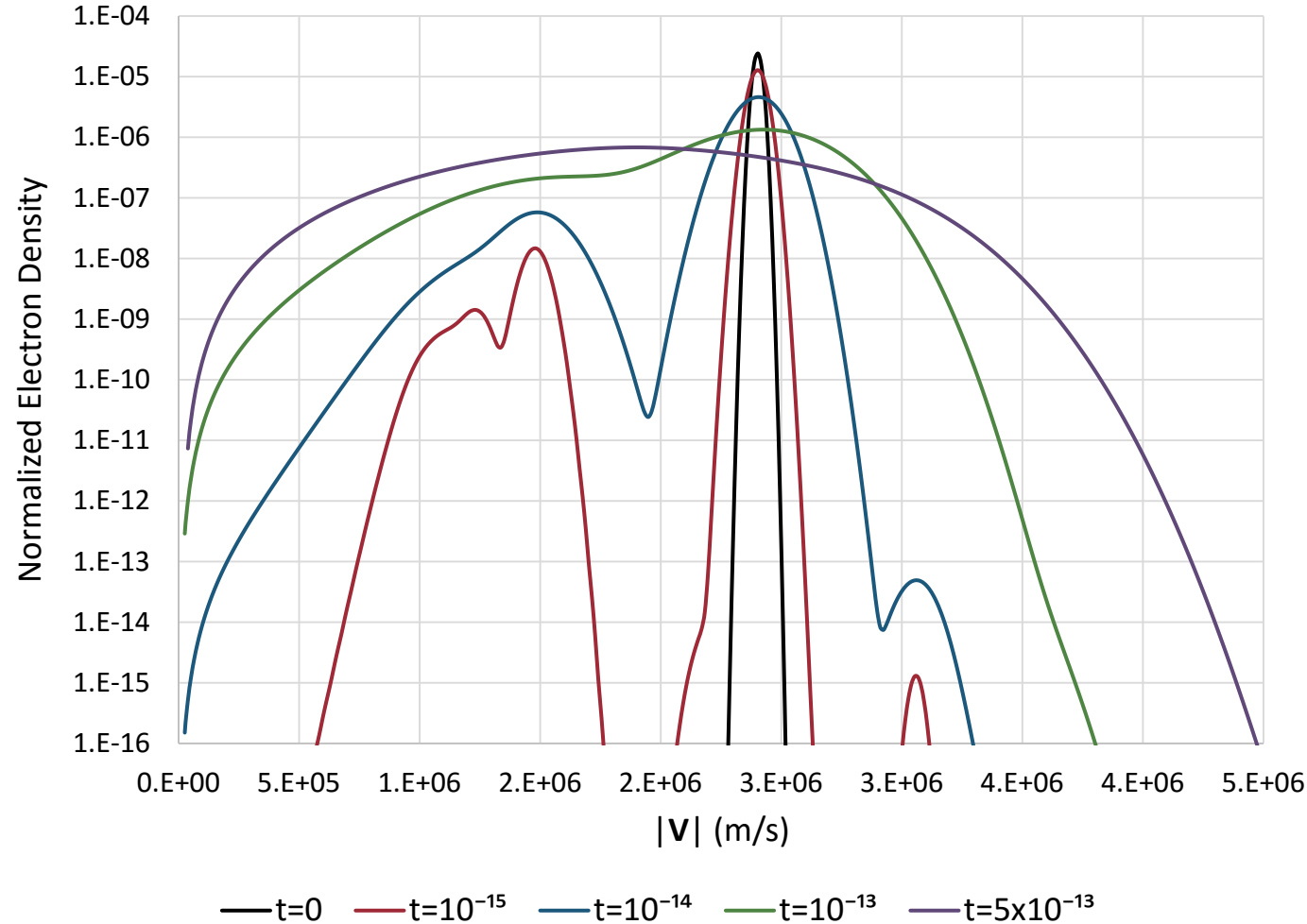
Non-Maxwellian Inelastic Collisions: Test Case Setup



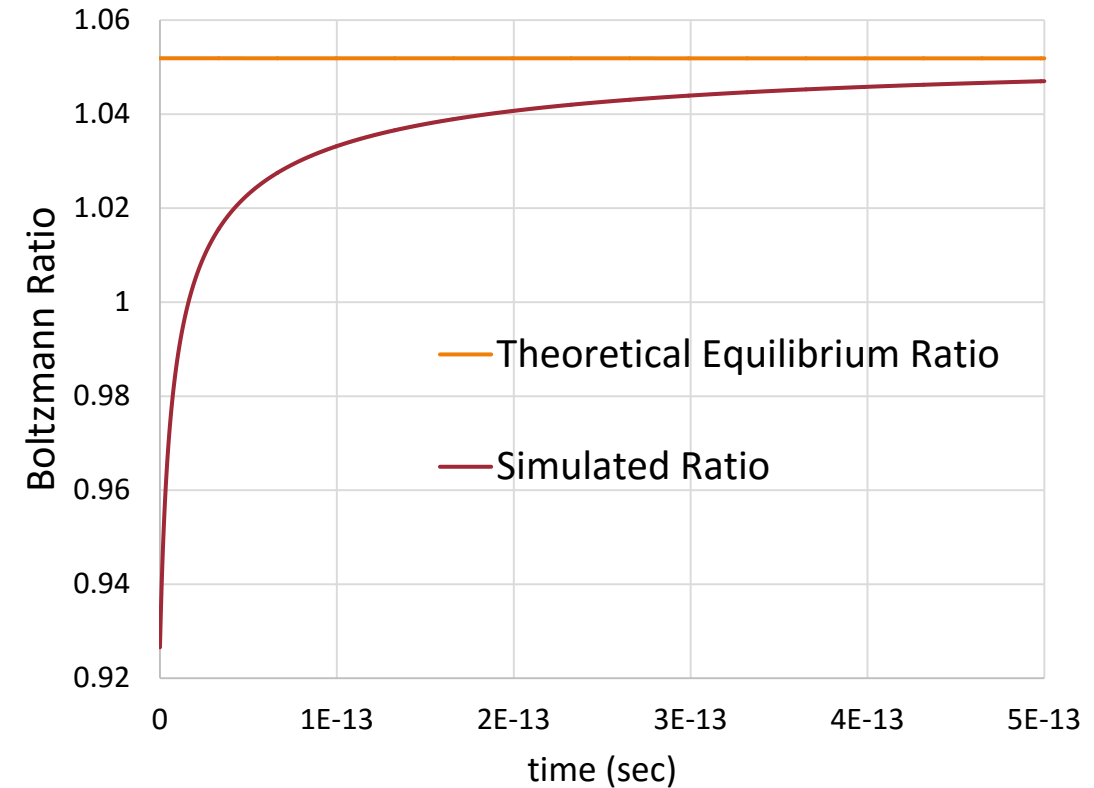
- **Atomic Hydrogen**
- **Electron impact excitation/de-excitation**
- **40 excited states**
- **Delta function for H, H⁺**
- **Photo-ionization (pre-process)**
 - 41 nm laser
 - 30 eV
- **Initial Conditions**
 - Atmospheric like conditions
 - H = $2.68 \times 10^{25} \text{ m}^{-3}$
 - H⁺, e = $4.06 \times 10^{21} \text{ m}^{-3}$
 - Te = 10.9eV



Non-Maxwellian Inelastic Collision Modeling: Laser Example (preliminary)



Boltzmann Ratio of two highest energy species (for the same simulation shown on the left)



Initial photo-ionization of hydrogen. Discrete changes in electron velocities from excitation/de-excitation and smoothing from the Fokker-Planck Equation



Non-Maxwellian Inelastic Collision Modeling : Limitations of Standard Numerical Methods



- ***Multiscale Hybridization:***
 - Standard explicit schemes may not perform adequately when modeling highly non-polynomial solutions and/or when the number of points employed to represent the solution is huge. An approach to improving performance is to fall back on a known low computational cost coarse solution approximation rather than a polynomial.
- ***Sobolev Regularization with Coordinate Transforms:***
 - Implicit schemes may be less than desirable when they require solving complicated non-linear equations where the repeated linear solves to be performed involve dense matrices. Previous work has shown this type of regularization to be an effective alternative to fully implicit methods for complex problems.
- ***Lagrangian-TV Regularization:***
 - Another type of regularization that may better allow for shocks and other specific solution features.



Regularization: Motivation

- ***Faster Linear Solves***
 - The matrices that arise from implementing the implicit schemes for the differential equations that we wish to solve are dense and ill conditioned. The matrices arising from the regularization are always sparse and well conditioned.
- ***Faster Development***
 - The differential equations are complex and an implicit method needs to incorporate all aspects of f (boundary conditions, convolutions, precomputing global variables, etc.) which can be a time consuming process.
- ***Vlasov Merging***
 - Lagrangian coordinates with frequent re-gridding/re-initialization (semi-Lagrangian) are a standard approach for modelling the Vlasov equation. Looking ahead to a Vlasov simulation with inelastic collisions and other non-linear processes, it may be desirable to have a single Lagrangian framework to model all these processes.
- ***Lagrangian-TV Regularization on $u(X)$ has a 'light touch'***
 - In the extreme case where the time step is small enough that no regularization is needed, the solution will not change at all.
- ***Two Step Regularization***
 - Even in cases where a smooth solution is sought, applying the TV-Regularization first ensures even a small amount of L^2 smoothing will bring the solution into a Sobolev space.



Regularization: General Background

- The standard approach to achieving stability of a numerical scheme is to write it in such a way that the propagation in time is implicitly defined. A pen and paper analysis of the scheme (like Von Neumann) is used to establish stability, which typically means that the function will remain in a Sobolev space.

- **Explicit:** $z_{n+1} = z_n + dtf(z_n)$ **Implicit:** $z_{n+1} = z_n + dtf(z_{n+1})$

- An alternative, somewhat more recent and less common approach is to keep a solution in a Sobolev space by simply directly incorporating that restriction into the numerical method:

$$y_{n+1} = \operatorname{argmin} \int (y - dtf(z_n))^2 dx + \int (\nabla y)^2 dx$$

$$z_{n+1} = z_n + y_{n+1} = z_n + (I - \Delta)^{-1}(dtf(z_n))$$

- While extremely simple, this approach has been shown effective for even very complex simulations.
- An alternative functional space to consider, most common in data processing but increasingly spreading into physics applications, is the following (with one L^2 term and one L^1 term):
 - $y_{n+1} = \operatorname{argmin} \int (y - dtf(z_n))^2 dx + \int |\nabla y| dx$
- And more recently, fast approaches to solving problems like this that do not rely on classical approaches (i.e. gradient descent and the Euler-Lagrange equation) have been developed.
- Regularization can be applied directly to a distribution $\varphi(x)$ (Eulerian) or to $u(X) = x$ (Lagrangian).

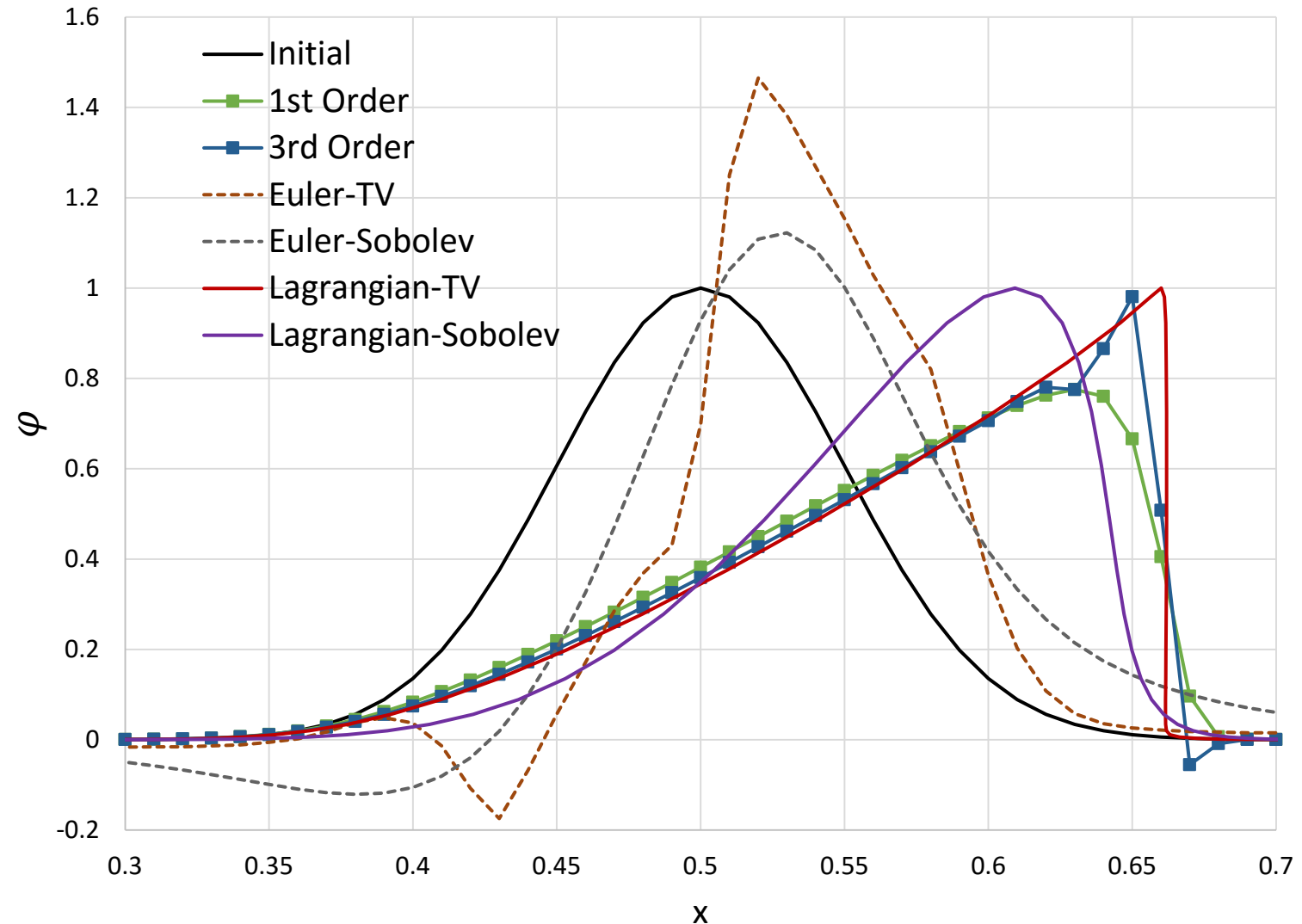


Lagrangian-TV Regularization: Burger's Equation Example



- The Lagrangian-TV regularization can produce an exact shock solution with no diffusion and no dispersion in a computationally efficient and straightforward manner.
- 1st and 3rd Order solutions provide accurate shock locations but have diffusion or dispersion errors
- Lagrangian-Sobolev does not get the correct shock location and has moderate diffusion errors
- Euler-TV and Euler-Sobolev does not obtain the correct shock location and has significant errors in its profile.

Inviscid Burger's Equation, $\varphi_t = \varphi\varphi_x$, solved with various schemes





Conclusion

- **Maxwellian CR**
 - Added QSS and single temperature Boltzmann grouping and compared with DCA results
 - Included radiation source term with Planckian field which is a stepping stone to radiation transport
- **Non-Maxwellian CR**
 - Demonstrated ability to capture non-Maxwellian EEDF effects on Zero-D LPI like simulation
 - Implemented the Fokker-Planck collision operator along with excitation/dexcitation
 - Ionization and recombination processes are near completion



Future Work

- **Maxwellian CR**
 - Affect of grouping on generated spectra
 - Automatic level-grouping (looking for collaborators!)
 - Coupling with fluid model for 1D simulations (high Mach Argon shock 1D LPI breakdown)
 - Use cFAC to generate atomic data for low- to mid-Z elements (up to Xenon)
 - Compare with other CR codes, e.g. FLYCHK
- **Non-Maxwellian CR**
 - Add Bremsstrahlung, along with radiative transitions
 - Move to 2V Fokker-Planck solver
 - Further implement regularization techniques to collisional modelling and compare against standard explicit and implicit schemes



Questions?