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

*AFOSR Plasma and Electroenergetics Review Meeting
29-30 November 2016*



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Outline

- **Goals**
- **Review of Past Work**
- **Argon Collisional-Radiative Complexity Reduction Validation**
- **Non-Maxwellian CR**
- **Phase-accurate Multiscale Particle Push**



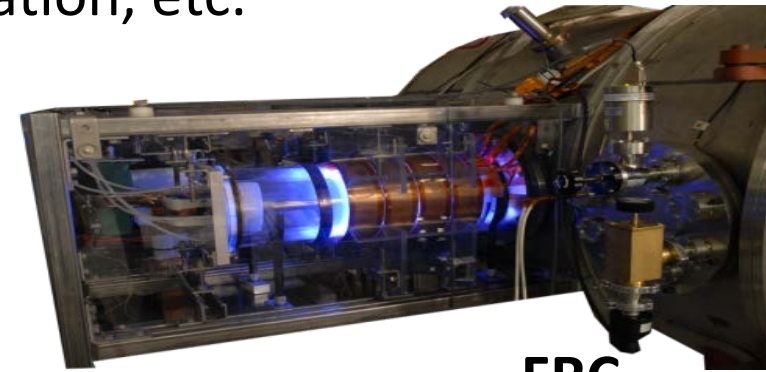
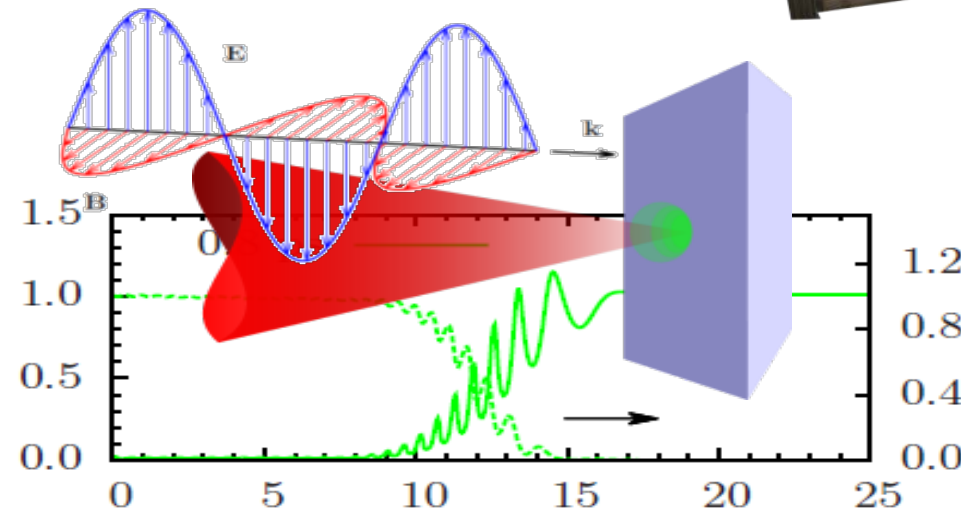
Goals

- 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

Laser Plasma Interaction



FRC



RQRS M&S Group



- **Government**

- Dr. David Bilyeu (LPI, in-space Chem)
- Dr. Justin Koo (Flight Support, Group Lead)
- Dr. Rob Martin (FRC)

- **Onsite Contractors (ERC inc.)**

- Richard Abrantes (Grad Student, LPI)
- Dr. Jun Araki (Flight Support, PIC)
- Dr. Carl Lederman (LPI)
- Dr. Michelle Scharfe (Flight Support)
- Dr. Eder Sousa (FRC)
- Jonathan Tran (Grad Student, Implicit PIC)

- **Summer Students**

- Astrid Raisanen
 - PhD UofM; Vlasov HET
- Daniel Crews
 - M.S. Washington; Collisionless Shock for V&V
- Kari Kawashima
 - B.S. UCLA; SM/MURF beta tester

- **Previous**

- Dr. Hai Le (LPI; now at Livermore)
- Dr. Artan Qerushi (FRC now at Lockheed)



Summary of Past Work

Maxwellian Inelastic Collisions

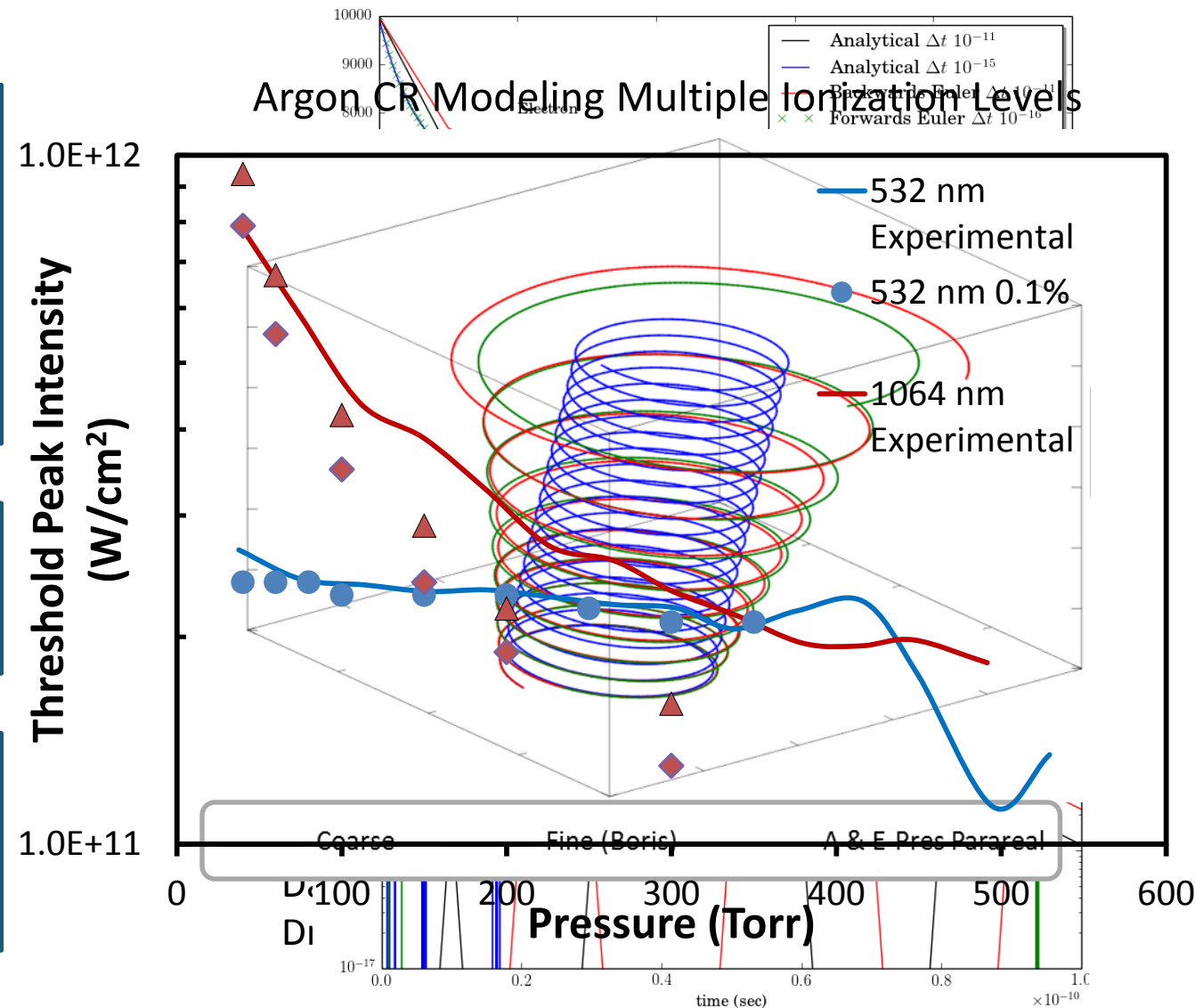
- Detailed CR model for multiple ionization stages
- Validation against experimental data
- Nonequilibrium radiation transport: coupling with a collisional-radiative model
- Inelastic collisions in a MF plasma: enhanced thermochemical kinetics.

Multiscale Hybridization

- A time-parallel/multiscale method with energy preservation

Analytical BGK

- Conservative even for large mass ratios
- Conservation are independent of collisional frequencies





Collisional Radiative (CR) Overview

Updates

- Expanded complexity reduction to include multiple ionization levels
- Adaptive integration technique -> fixes rate calculation for higher electron temperature
- Investigate grouping sensitivity
- Linked with LANL database for Argon cross sections and atomic level information
- Algorithms not hard coded for Argon.

Levels of Complexity

- Full rates (LANL)
- Cutoff nearly ionized levels
- Grouping Strategies
 - Uniform
 - Boltzmann
 - QSS (Boltzmann and Planck equilibrium)
- Group Selection
 - Electron configuration (no splitting information)
 - Highly excited states
 - Analysis of full run
 - Numerical optimization



CR Governing Equations

$$\begin{aligned} \left(\frac{df_e(\varepsilon, t)}{dt} \right)_{\text{coll, ex/dex}} = & - \sum_{m>n} N_n(f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}} \right) \sigma_{(m|n)}^{e,\uparrow}(\varepsilon_0) \\ & + \sum_{m>n} N_m(f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}} \right) \sigma_{(n|m)}^{e,\downarrow}(\varepsilon_1) \\ & + \sum_{m<n} N_m(f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}} \right) \sigma_{(n|m)}^{e,\uparrow}(\varepsilon_1) \\ & - \sum_{m>n} N_n(f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}} \right) \sigma_{(m|n)}^{e,\downarrow}(\varepsilon_0) \end{aligned}$$

$$\begin{aligned} \left(\frac{df_e(\varepsilon, t)}{dt} \right)_{\text{coll, i/r}} = & - \sum_n N_n(f_e(\varepsilon)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}} \right) \sigma_{(+|n)}^{e,\uparrow}(\varepsilon_0) \\ & + N_+ \int_{\varepsilon_1} \int_{\varepsilon_2} (f_e(\varepsilon_1))(f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}} \right) \left(\sqrt{\frac{2\varepsilon_2}{m_e}} \right) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n|+)}^{e,\downarrow}(\varepsilon_1, \varepsilon_2; \varepsilon_0) \right) d\varepsilon_1 d\varepsilon_2 \\ & - N_+(f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_2}{m_e}} \right) \int_{\varepsilon_0} \int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}} \right) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n|+)}^{e,\downarrow}(\varepsilon_1, \varepsilon_2; \varepsilon_0) \right) d\varepsilon_1 d\varepsilon_0 \\ & + \sum_n N_n \int_{\varepsilon_1} \int_{\varepsilon_0} \left(\sqrt{\frac{2\varepsilon_0}{m_e}} \right) (f_e(\varepsilon_0)) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(+|n)}^{e,\uparrow}(\varepsilon_2; \varepsilon_0, \varepsilon_1) \right) d\varepsilon_0 d\varepsilon_1 \end{aligned}$$

$$\begin{aligned} \left(\frac{dN_n(t)}{dt} \right)_{\text{coll, ex/dex}} = & - \sum_{m>n} N_n \int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}} \right) \sigma_{(m|n)}^{e,\uparrow}(\varepsilon_0) d\varepsilon_0 \\ & + \sum_{m>n} N_m \int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}} \right) \sigma_{(n|m)}^{e,\downarrow}(\varepsilon_1) d\varepsilon_1 \\ & + \sum_{m<n} N_m \int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}} \right) \sigma_{(n|m)}^{e,\uparrow}(\varepsilon_1) d\varepsilon_1 \\ & - \sum_{m<n} N_n \int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}} \right) \sigma_{(m|n)}^{e,\downarrow}(\varepsilon_0) d\varepsilon_0 \end{aligned}$$

$$\begin{aligned} \left(\frac{dN_n(t)}{dt} \right)_{\text{coll, i/r}} = & - N_n \int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}} \right) \sigma_{(+|n)}^{e,\uparrow}(\varepsilon_0) d\varepsilon_0 \\ & + N_+ \int_{\varepsilon_0} \int_{\varepsilon_1} \int_{\varepsilon_2} (f_e(\varepsilon_1))(f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}} \right) \left(\sqrt{\frac{2\varepsilon_2}{m_e}} \right) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n|+)}^{e,\downarrow}(\varepsilon_1, \varepsilon_2; \varepsilon_0) \right) d\varepsilon_1 d\varepsilon_2 \end{aligned}$$



CR Governing Equations cont.

- **Current Assumptions**

- Electron dominated collisions
- δ function for ion distribution
- Maxwellian electrons

- **Current Model Includes**

- Multiple ionization levels
- Excitation/de-excitation
- Ionization/recombination
- Multi-photon ionization and inverse Bremsstrahlung
- Radiation losses via, Bound-Bound and Bound-Free

*previous included

$$\begin{aligned} \frac{dn_n^{+k}}{dt} = & - \sum_{m>n} \alpha_{(m|n)}^{+k,e} N_e N_{+k,n} + \sum_{m>n} \beta_{(n|m)}^{+k,e} N_e N_{+k,m} + \sum_{m>n} A_{(n|m)}^{+k} N_{+k,m} \\ & + \sum_{m<n} \alpha_{(n|m)}^{+k,e} N_e N_{+k,m} - \sum_{m<n} \beta_{(m|n)}^{+k,e} N_e N_{+k,n} - \sum_{m<n} A_{(m|n)}^{+k} N_{+k,n} \\ & - \sum_j \alpha_{(+,j|n)}^{+k,e} N_e N_{+k,n} + \sum_j \beta_{(n|+,j)}^{+k,e} N_{+(k+1),j} N_e^2 \\ & \alpha_{(m|n)}^e = \int_{E_{nm}}^{\infty} \sigma_{nm}^e(\varepsilon) v_e f(v_e) dv_e \\ & \beta_{(n|m)}^e = \frac{n^2}{m^2} e^{+x_{nm}} \alpha_{(m|n)} \quad A_{(n|m)} = \left(\frac{8\pi^2 e^2}{m_e c^3} \right) \frac{g_n}{g_m} f_{nm} \end{aligned}$$



CR Grouping Techniques

Uniform

- Solely conserves number density
- Weights each level according to level degeneracy within group

Conserved Variable:

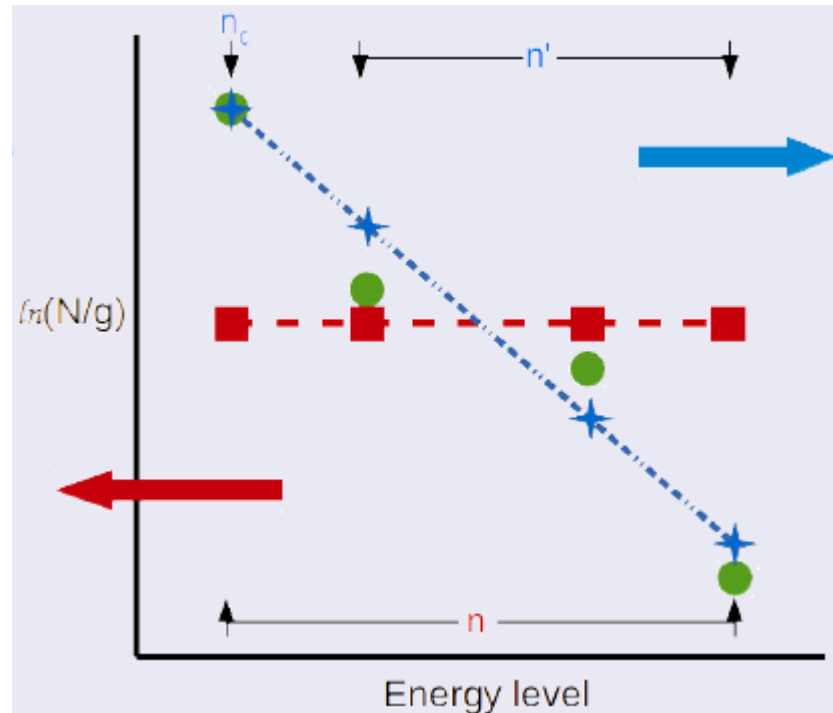
$$\tilde{N}_n = \sum_{i \in n} N_i$$

Effective rate:

$$\tilde{\alpha}(m|n) = \sum_{i \in n} \frac{g_i}{g_n} \sum_{j \in m} \alpha(j|i)$$

$$\frac{dN_n}{dt} = N_e \left[\sum_{m>n} \alpha_{(m|n)} N_n + \sum_{m<n} \beta_{(m|n)} N_n \right] + \dots$$

$$\frac{d\tilde{N}_n}{dt} = N_e \tilde{N}_n \left[\sum_{m>n} \tilde{\alpha}_{(m|n)} + \sum_{m<n} \tilde{\beta}_{(m|n)} \right] + \dots$$



Boltzmann

- Conserves number density
- Preserves energy in groups through group temperature description

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:

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



Complexity Reduction for Argon

Full Lines (LANL)

- Based on quantum calculations with corrections for low temperature

NIST Cutoff

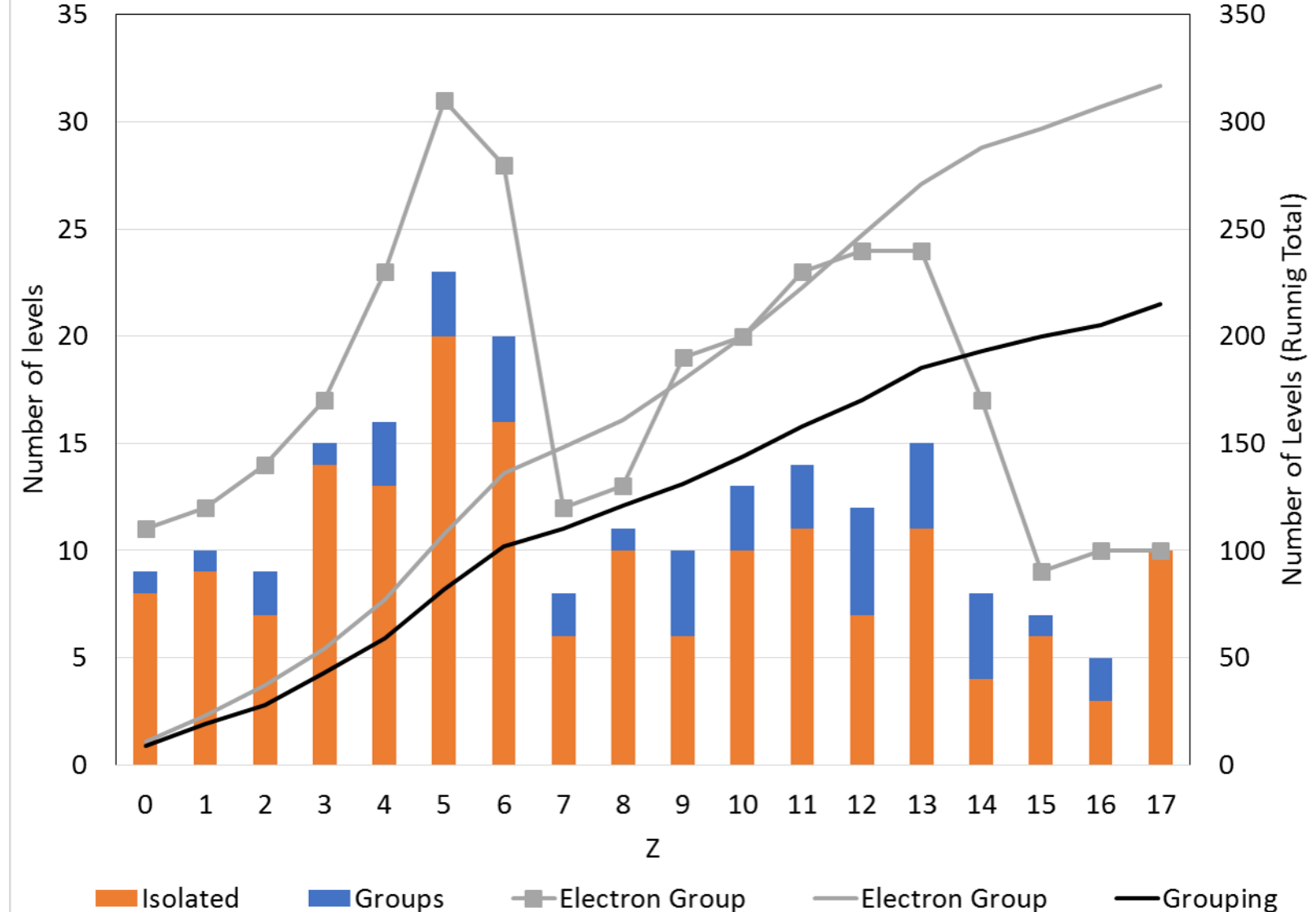
- Starts with LANL and assumes higher excited states are ionized
- Cutoff experimentally determined
- 2-3x reduction

Electron Configuration

- Groups based on electron configuration
- Uses uniform grouping
- 10-15x reduction over NIST

Grouping

- Boltzmann or Uniform grouping
- Saves 20-30% over Electron Splitting
- Case by case basis





Argon Level Grouping Isothermal Test Setup



Simulation Setup

- Pressure: 4.22 Torr (5.55×10^{-3} atm)
- Ion Temperature: 0.035 eV
- Atomic Density: 10^{20} 1/m³
- Ionization fraction: 10^{-13}
- Electron Temperature: 10 & 100 eV
- $t = [0, 10^6]$ seconds

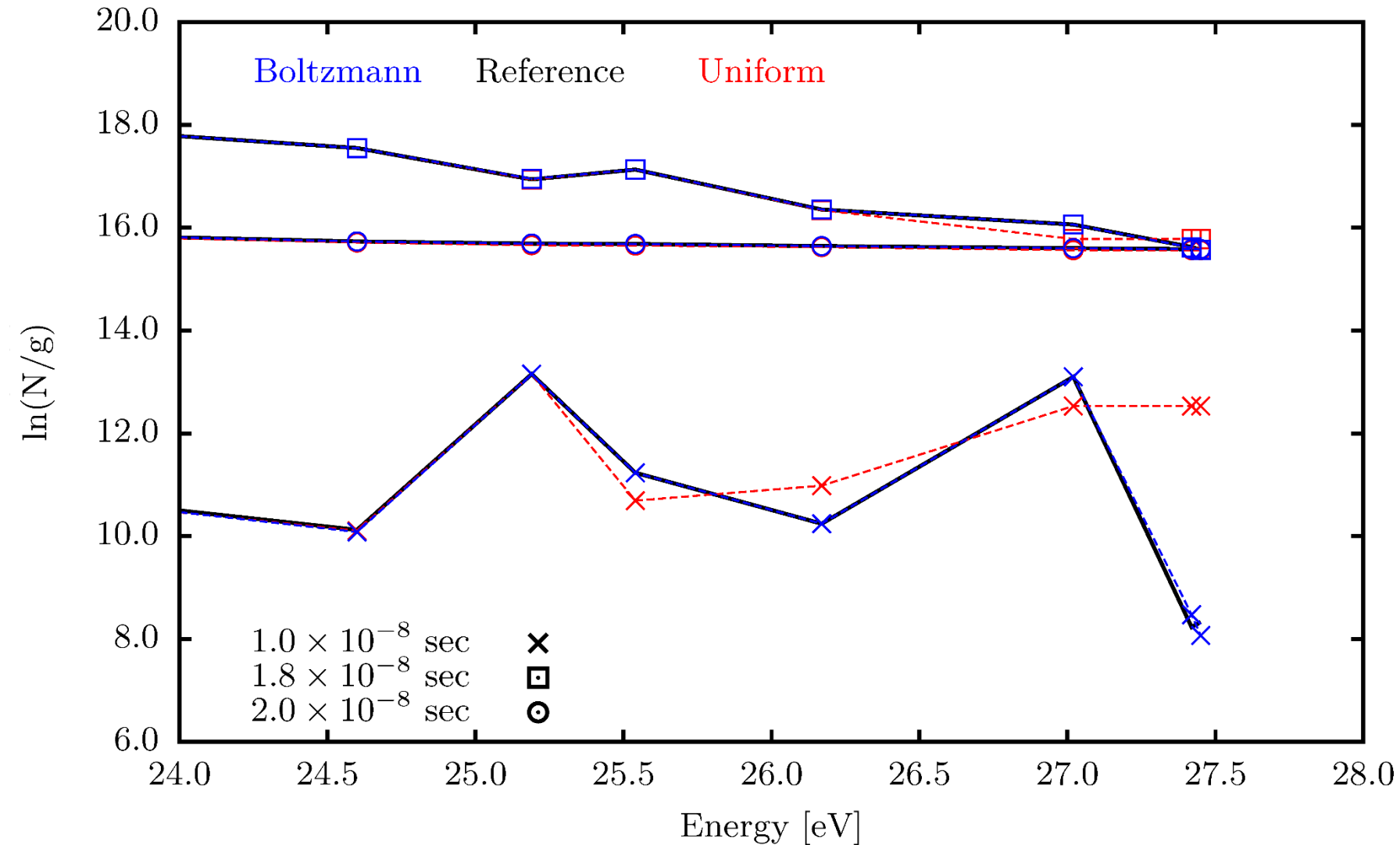
Groupings

- NIST cutoff with electron grouping
- NIST cutoff with electron grouping and Boltzmann grouping
- NIST cutoff with electron grouping and Uniform grouping



Argon Level Grouping Isothermal Test

Electron Temperature 10 eV



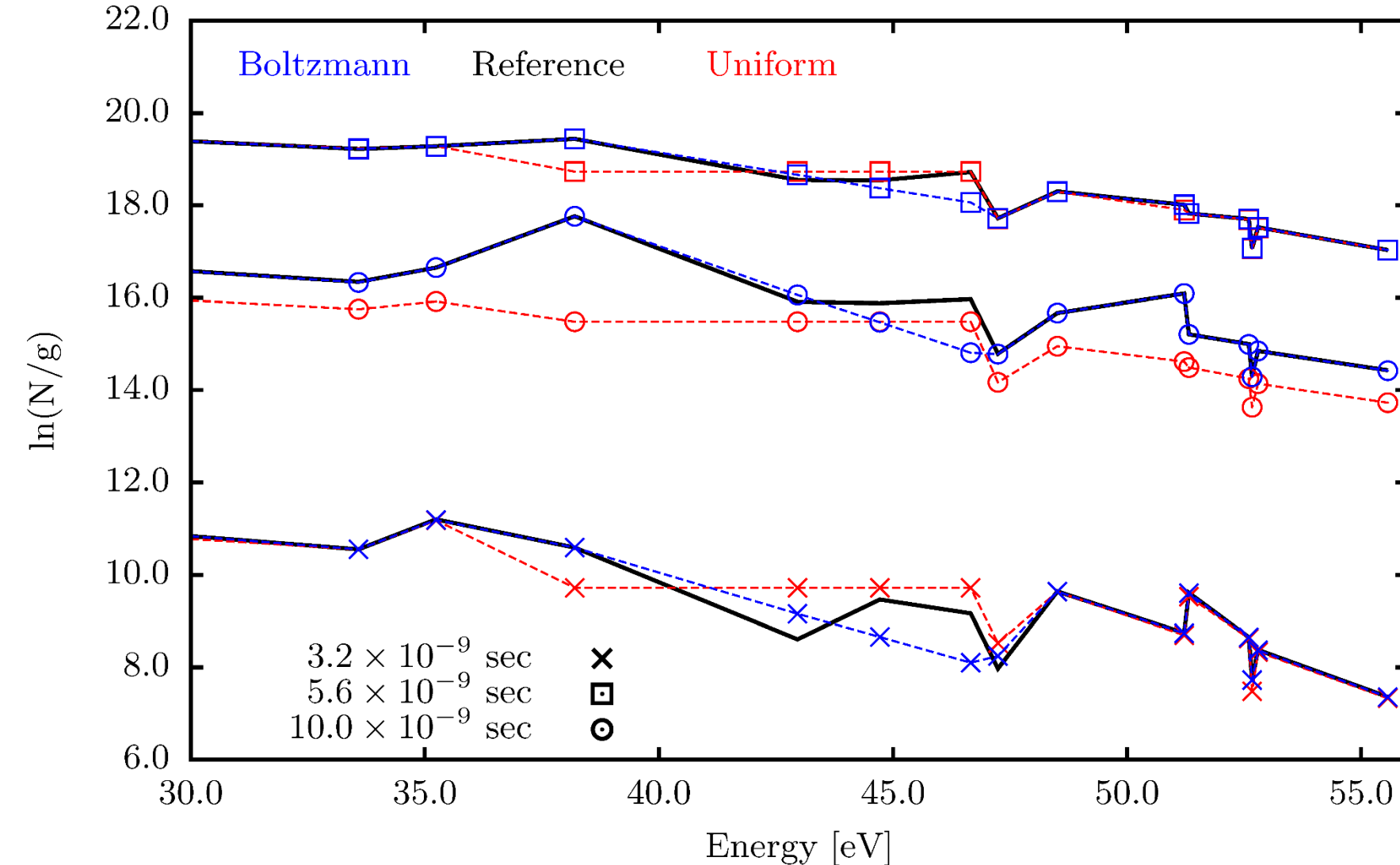
Argon +1
12 electron configurations
9 Isolates states
1 group with 3 states

Uniform group propagates
errors to isolated states



Argon Level Grouping Isothermal Test

Electron Temperature 100 eV

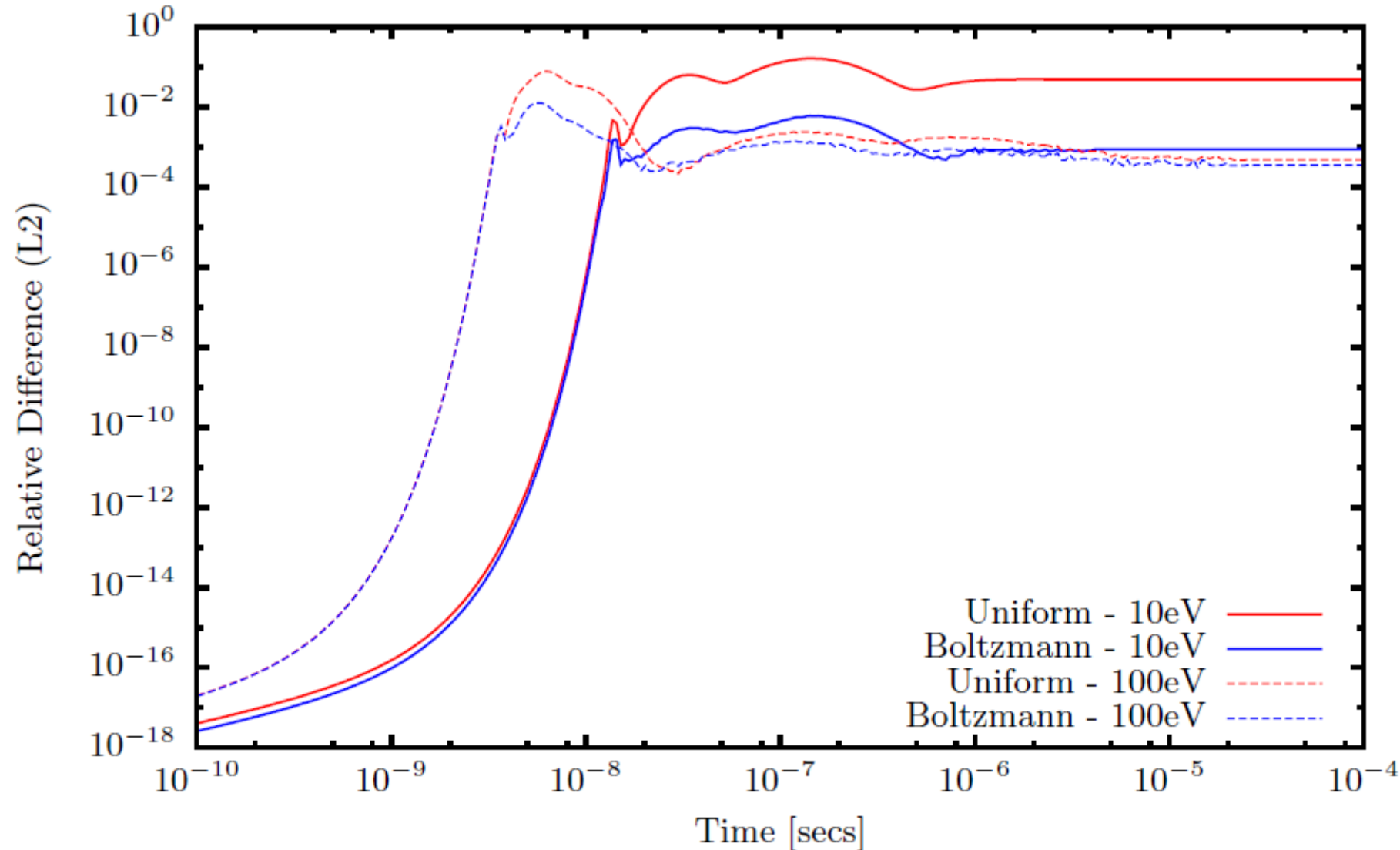


Argon +3
17 electron configurations
14 Isolates states
1 group with 3 states

Uniform groups propagates errors to isolated states



Argon Level Grouping Isothermal Test Error



ODE Solver tolerance
Relative error 1^{-4}
Absolute error 1
~1200 Radau5 time steps
dt increases exponentially

Solution improves if
either tolerance is
decreased but at the
expense of computational
time. E.g. relative error
 10^{-6} -> computational
time triples



Non-Maxwellian Electrons CR - Ions (Preliminary)



• Current Assumptions

- Electron dominated collisions
- Single ionization level
- Isotropic EEDF
- δ function for ion distribution

$$\left(\frac{dN_n(t)}{dt}\right)_{\text{coll,ex/dex}} = - \sum_{m>n} N_n \int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma_{(m|n)}^{e,\uparrow}(\varepsilon_0) d\varepsilon_0$$

$$+ \sum_{m>n} N_m \int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma_{(n|m)}^{e,\downarrow}(\varepsilon_1) d\varepsilon_1$$

$$+ \sum_{m<n} N_m \int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma_{(n|m)}^{e,\uparrow}(\varepsilon_1) d\varepsilon_1$$

$$- \sum_{m<n} N_n \int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma_{(m|n)}^{e,\downarrow}(\varepsilon_0) d\varepsilon_0$$

• Current Model Includes

- Elastic electron collisions
- Excitation/de-excitation
- Ionization/recombination

$$\left(\frac{dN_n(t)}{dt}\right)_{\text{coll,i/r}} =$$

$$- N_n \int_{\varepsilon_0} (f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma_{(+|n)}^{e,\uparrow}(\varepsilon_0) d\varepsilon_0$$

$$+ N_+ \int_{\varepsilon_0} \int_{\varepsilon_1} \int_{\varepsilon_2} (f_e(\varepsilon_1))(f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n|+)}^{e,\downarrow}(\varepsilon_1, \varepsilon_2; \varepsilon_0)\right) d\varepsilon_1 d\varepsilon_2$$



Non-Maxwellian Electrons CR - Electrons (Preliminary)



- **Current Assumptions**

- Electron dominated collisions
- Single ionization level
- Isotropic EEDF
- δ function for ion distribution

$$\left(\frac{df_e(\varepsilon, t)}{dt}\right)_{\text{coll, ex/dex}} = - \sum_{m>n} N_n(f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma_{(m|n)}^{e,\uparrow}(\varepsilon_0) \\ + \sum_{m>n} N_m(f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma_{(n|m)}^{e,\downarrow}(\varepsilon_1) \\ + \sum_{m<n} N_m(f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \sigma_{(n|m)}^{e,\uparrow}(\varepsilon_1) \\ - \sum_{m>n} N_n(f_e(\varepsilon_0)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma_{(m|n)}^{e,\downarrow}(\varepsilon_0)$$

- **Current Model Includes**

- Elastic electron collisions
- Excitation/de-excitation
- Ionization/recombination

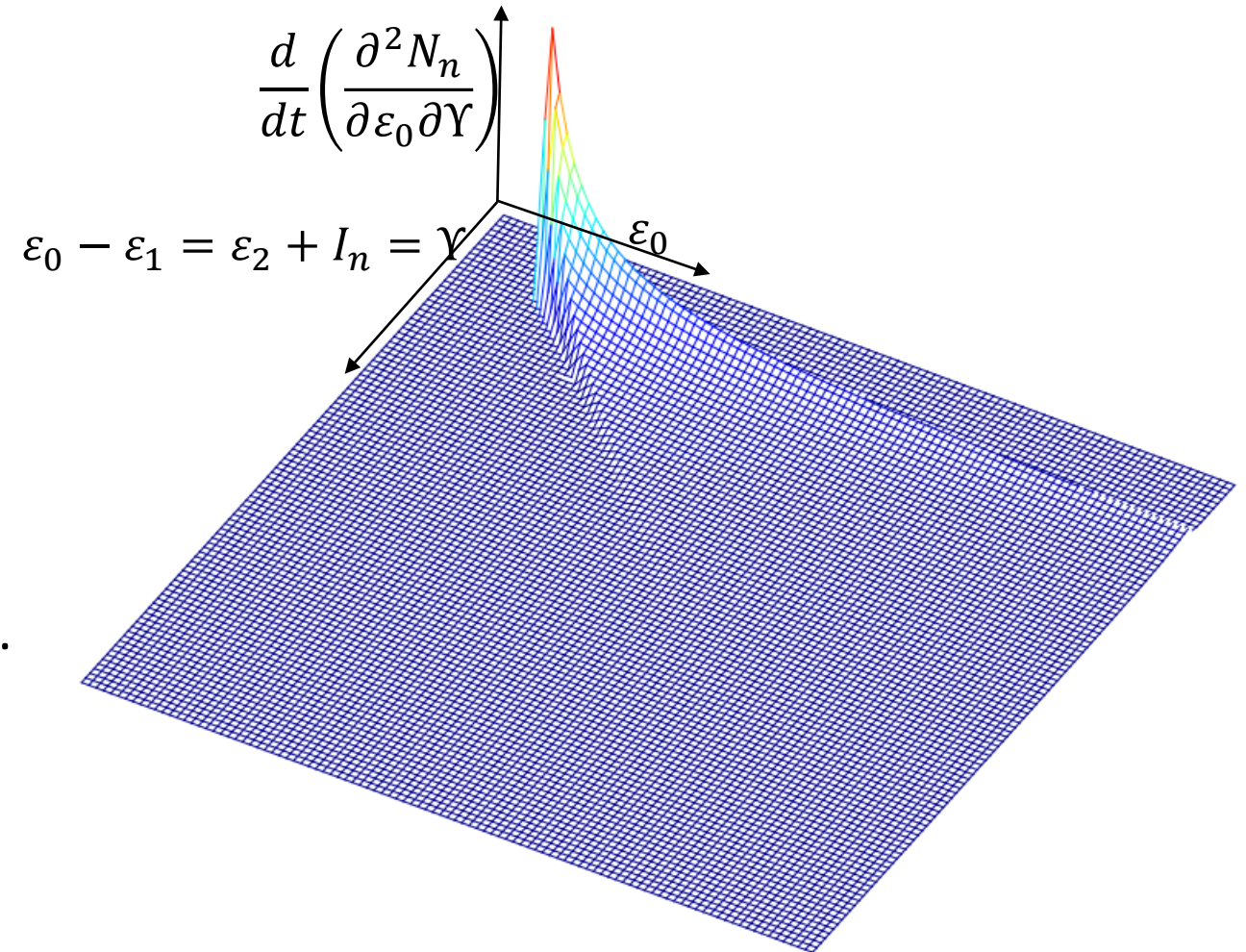
$$\left(\frac{df_e(\varepsilon, t)}{dt}\right)_{\text{coll, i/r}} = - \sum_n N_n(f_e(\varepsilon)) \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) \sigma_{(+|n)}^{e,\uparrow}(\varepsilon_0) \\ + N_+ \int_{\varepsilon_1} \int_{\varepsilon_2} (f_e(\varepsilon_1))(f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n|+)}^{e,\downarrow}(\varepsilon_1, \varepsilon_2; \varepsilon_0)\right) d\varepsilon_1 d\varepsilon_2 \\ - N_+ (f_e(\varepsilon_2)) \left(\sqrt{\frac{2\varepsilon_2}{m_e}}\right) \int_{\varepsilon_0} \int_{\varepsilon_1} (f_e(\varepsilon_1)) \left(\sqrt{\frac{2\varepsilon_1}{m_e}}\right) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n|+)}^{e,\downarrow}(\varepsilon_1, \varepsilon_2; \varepsilon_0)\right) d\varepsilon_1 d\varepsilon_0 \\ + \sum_n N_n \int_{\varepsilon_1} \int_{\varepsilon_0} \left(\sqrt{\frac{2\varepsilon_0}{m_e}}\right) (f_e(\varepsilon_0)) \left(\frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(+|n)}^{e,\uparrow}(\varepsilon_2; \varepsilon_0, \varepsilon_1)\right) d\varepsilon_0 d\varepsilon_1$$

$$\left(\frac{df_e(\varepsilon, t)}{dt}\right)_{\text{elastic}} = \nu_{ee}(F_e - f_e) + \nu_{ei}(F_{ei} - f_e)$$



Non-Maxwellian CR Numerical Challenges

- Long complex CR formulas
 - Stiff equations
 - Range of scales
 - Boundary conditions
 - Multi-dimensional integrations
-
- Hydrogen recombination example:
 - $e_0 + H_n \leftarrow e_1 + e_2 + H_+$
 - Energy equation in terms of the electron's kinetic energies, ε , and ionization energy I_n .
 - $\varepsilon_0 = \varepsilon_1 + \varepsilon_2 + I_n$
 - Evaluating the effect of recombination on a single species of hydrogen requires the evaluation of a 2D integral.





Hybridization Techniques

- Solve ODE/PDE with a coarse “C” solver and fine “F” solver
- Coarse propagates less information and is more computationally efficient
- Fine propagates more information and is more accurate
- User defined coarse error function $h(u), 0 \leq h \leq 1$
- when $h=0$ coarse is accurate
- Q compression operator
- R reconstruction operator
- $h, \epsilon, Q, \& R,$ are problem dependent

Simpler hybrid (H) method

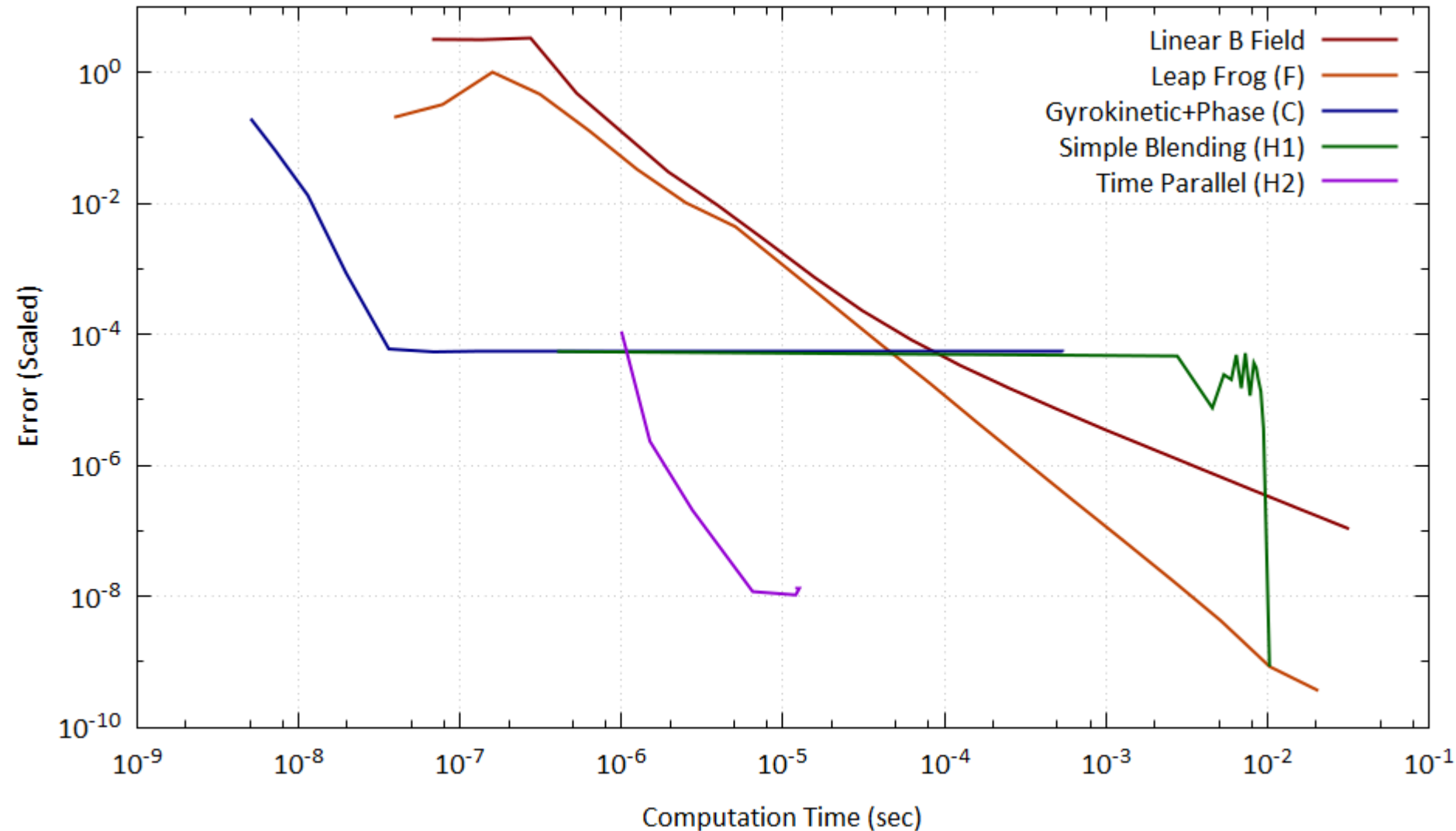
$$H1_{[t+dt,t]} = \begin{cases} C_{[t+dt,t]}(Q(\text{if needed})) & \text{if } h \leq \epsilon \\ F_{[t+dt,t]}(R(\text{if needed})) & \text{if } h > \epsilon \end{cases}$$

More complex time parallel (TP) method

$$H2_{[Jdt,0]}(u(0)) = \begin{cases} C_{[Jdt,0]}Q(u(0)) & \text{if } h \leq \epsilon \\ C_{[Jdt,0]}Q(u(0)) + \left(\sum_{j=0}^{j=J-1} RC_{[Jdt,(j+1)dt]}QF_{(j+1)dt,jdt}RC_{[jdt,0]}Q(u(0)) \right) & \text{if } \epsilon < h \leq \gamma \\ \left(\sum_{j=0}^{j=J-1} RC_{[Jdt,(j+1)dt]}C_{(j+1)dt,jdt}C_{[jdt,0]}Q(u(0)) \right) & \\ F_{[Jdt,0]}(u(0)) & \text{if } h > \gamma \end{cases}$$



Hybridization Charged Particle in Magnetic Mirror



$$B_x = -\frac{2Cxz^3}{a^4}$$
$$B_y = -\frac{2Cyz^3}{a^4}$$
$$B_z = C\left(1 - \frac{z^4}{a^4}\right)$$

Gyrokinetic + Phase and Time Parallel method are the most efficient

Simple blending could be more accurate as the problem approaches steady state

*Submitted to Journal



Summary



- **Collisional Radiative**

- Boltzmann grouping improves group representation over applied uniform distribution
- Minimization of error, which is expected to accumulate quickly during highly-transient durations, and acceleration of method makes Boltzmann reduction a strong case for future coupled simulations
- Adaptive integration allowed for faster simulations at larger electron temperatures
- Sensitive to selected groups
- Grouping reduces stiffness
- Robust solver capable of handling, T_e from 1 – 1,000 eV and 10^{16} - 10^{24} particles
- Initial work on non-Maxwellian CR has begun and early numerical issues have been addressed

- **Hybridization**

- Shows that hybridization technique can be more computational efficient than the schemes that comprise it



Future Work

- **Collisional Radiative Simulations**
 - Further comparisons between reduced mechanisms with QSS
 - Line identification and width assignments in conjunction with experimental spectra
 - Apply Boltzmann grouping to new CR Argon rates and test with 1D MHD Argon shock by Kapper, et.al. Future plans to extend to 2 and 3D MF
 - Rerun previous LPI test case with level grouping; laser source term, heavy-electron elastic collisions, and multi-electron energy correction and heavy energy equation (Te, Th)
- **Group selection through numerical analysis, optimization**
- **Hybridize Maxwellian CR with QSS**
- **Non-Maxwellian finite rate EEDF implementation**



Questions?