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

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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
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

Argon CR Modeling Multiple Ionization Levels

- Threshold Peak Intensity (W/cm²)
- Pressure (Torr)

Graph shows comparison between Analytical and Experimental data for 532 nm and 1064 nm.
**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

\[
\left( \frac{df_e(\varepsilon,t)}{dt} \right)_{\text{coll,ex/dex}} = - \sum_{m>n} N_{n} \left( f_e(\varepsilon) \right) \left( \sqrt{\frac{2e_0}{m_e}} \right) \sigma_{(m|n)}^{e,\uparrow} (\varepsilon_0)
\]

\[
+ \sum_{m>n} N_{m} \left( f_e(\varepsilon_1) \right) \left( \sqrt{\frac{2e_1}{m_e}} \right) \sigma_{(n|m)}^{e,\downarrow} (\varepsilon_1)
\]

\[
+ \sum_{m<n} N_{m} \left( f_e(\varepsilon_1) \right) \left( \sqrt{\frac{2e_1}{m_e}} \right) \sigma_{(n|m)}^{e,\downarrow} (\varepsilon_1)
\]

\[
- \sum_{m>n} N_{n} \left( f_e(\varepsilon_0) \right) \left( \sqrt{\frac{2e_0}{m_e}} \right) \sigma_{(m|n)}^{e,\downarrow} (\varepsilon_0)
\]

\[
\left( \frac{dN_{n}(t)}{dt} \right)_{\text{coll,ex/dex}} = - \sum_{m>n} N_{n} \int_{\varepsilon_0}^{\varepsilon_1} \left( f_e(\varepsilon) \right) \left( \sqrt{\frac{2e_0}{m_e}} \right) \sigma_{(m|n)}^{e,\uparrow} (\varepsilon_0) d\varepsilon_0
\]

\[
+ \sum_{m>n} N_{m} \int_{\varepsilon_1}^{\varepsilon_0} \left( f_e(\varepsilon_1) \right) \left( \sqrt{\frac{2e_1}{m_e}} \right) \sigma_{(n|m)}^{e,\uparrow} (\varepsilon_1) d\varepsilon_0
\]

\[
+ \sum_{m<n} N_{m} \int_{\varepsilon_1}^{\varepsilon_0} \left( f_e(\varepsilon_1) \right) \left( \sqrt{\frac{2e_1}{m_e}} \right) \sigma_{(n|m)}^{e,\uparrow} (\varepsilon_1) d\varepsilon_0
\]

\[
- \sum_{m<n} N_{n} \int_{\varepsilon_0}^{\varepsilon_1} \left( f_e(\varepsilon_0) \right) \left( \sqrt{\frac{2e_0}{m_e}} \right) \sigma_{(m|n)}^{e,\downarrow} (\varepsilon_0) d\varepsilon_0
\]
CR Governing Equations cont.

\[ \frac{dn_n^{+k}}{dt} = \]

\[ = - \sum_{m>n} \alpha^{+k,e}_{(m|n)} N_e N_{k+n} + \sum_{m>n} \beta^{+k,e}_{(n|m)} N_e N_{k,m} + \sum_{m>n} A^{+k}_{(n|m)} N_{k,m} \]

\[ + \sum_{m<n} \alpha^{+k,e}_{(n|m)} N_e N_{k,m} - \sum_{m<n} \beta^{+k,e}_{(m|n)} N_e N_{k,n} - \sum_{m<n} A^{+k}_{(m|n)} N_{k,n} \]

\[ - \sum_j \alpha^{+k,e}_{(+,j|n)} N_e N_{k+n,j} + \sum_j \beta^{+k,e}_{(n,+j)} N_{e+(k+1),j} N_e \]

\[ \alpha^{e}_{(m|n)} = \int_{E_{nm}}^{\infty} \sigma_{nm}^{e}(\epsilon) v_e f(v_e) dv_e \]

\[ \beta^{e}_{(n|m)} = \frac{n^2}{m^2} e^{+x_{nm}} \alpha(n|m) \]

\[ A(n|m) = \left( \frac{8 \pi^2 e^2}{m_e c^3} \right) \frac{g_n}{g_m} f_{nm} \]

*Previous included

- **Current Assumptions**
  - Electron dominated collisions
  - \( \delta \) function for ion distribution
  - Maxwellian electrons

- **Current Model Includes**
  - Multiple ionization levels
  - Excitation/de-excitation
  - Ionization/recombination
  - Multi-photon ionization and inverse Bermsstrahlung
  - Radiation losses via, Bound-Bound and Bound-Free
CR Grouping Techniques

**Uniform**

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

Conserved Variable:
\[ \bar{N}_n = \sum_{i \in n} N_i \]

Effective rate:
\[ \tilde{\alpha}(m|n) = \sum_{i \in n} g_i \sum_{j \in m} \alpha(j|i) \]

\[
\frac{dN_n}{dt} = N_e \left[ \sum_{m>n} \alpha(m|n)N_n + \sum_{m<n} \beta(m|n)N_n \right] + \ldots
\]

**Boltzmann**

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

Conserved Variable:
\[ N_{n0} \& N'_n = \frac{N_{n0}}{g_{n0}} \sum_{i \in n} g_i e^{-\Delta E_i/T_n} \]

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

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
Simulation Setup

- Pressure: 4.22 Torr (5.55x10^{-3} atm)
- Ion Temperature: 0.035 eV
- Atomic Density: 10^{20} 1/m^3
- 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

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

- **Current Model Includes**
  - Elastic electron collisions
  - Excitation/de-excitation
  - Ionization/recombination

\[
\frac{dN_n(t)}{dt}_{\text{coll,ex/dex}} = - \sum_{m>n} N_n \int_{\varepsilon_0} f_e(\varepsilon_0) \left( \sqrt{\frac{2\varepsilon_0}{m_e}} \sigma_{(m|n)}^{e,\uparrow}(\varepsilon_0) \right) d\varepsilon_0 \\
+ \sum_{m>n} N_m \int_{\varepsilon_1} f_e(\varepsilon_1) \left( \sqrt{\frac{2\varepsilon_1}{m_e}} \sigma_{(n|m)}^{e,\downarrow}(\varepsilon_1) \right) d\varepsilon_1 \\
+ \sum_{m<n} N_m \int_{\varepsilon_1} f_e(\varepsilon_1) \left( \sqrt{\frac{2\varepsilon_1}{m_e}} \sigma_{(m|n)}^{e,\downarrow}(\varepsilon_1) \right) d\varepsilon_1 \\
- \sum_{m<n} N_n \int_{\varepsilon_0} f_e(\varepsilon_0) \left( \sqrt{\frac{2\varepsilon_0}{m_e}} \sigma_{(m|n)}^{e,\uparrow}(\varepsilon_0) \right) d\varepsilon_0
\]
Non-Maxwellian Electrons CR - Electrons
(Preliminary)

• Current Assumptions
  — Electron dominated collisions
  — Single ionization level
  — Isotropic EEDF
  — $\delta$ function for ion distribution

• Current Model Includes
  — Elastic electron collisions
  — Excitation/de-excitation
  — Ionization/recombination

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

\[
\left( \frac{df_e(\varepsilon,t)}{dt} \right)_{\text{coll,i/r}} =
\]

\[
-N_+ \int_{\varepsilon_1} \int_{\varepsilon_2} (f_e(\varepsilon_1)) (f_e(\varepsilon_2)) \left( \sqrt{\frac{2\varepsilon_1}{m_e}} \right) \left( \sqrt{\frac{2\varepsilon_2}{m_e}} \right) \left( \frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n+)}^{e,\uparrow}(\varepsilon_1, \varepsilon_2; \varepsilon_0) \right) d\varepsilon_1 d\varepsilon_2
\]

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

\[
+ \sum_n N_n \int_{\varepsilon_1} \int_{\varepsilon_0} (f_e(\varepsilon_0)) \left( \sqrt{\frac{2\varepsilon_0}{m_e}} \right) \left( \frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \sigma_{(n+)}^{e,\uparrow}(\varepsilon_2; \varepsilon_0, \varepsilon_1) \right) d\varepsilon_0 d\varepsilon_1
\]

\[
\left( \frac{df_e(\varepsilon,t)}{dt} \right)_{\text{elastic}} = \nu_{ee}(F_e - f_e) + \nu_{ei}(F_{ei} - f_e)
\]
Non-Maxwellian CR Numerical Challenges

- Long complex CR formulas
- Stiff equations
- Range of scales
- Boundary conditions
- Multi-dimensional integrations

- Hydrogen recombination example:
  - $e_0 + H_n \leftrightarrow e_1 + e_2 + H_+$
  - Energy equation in terms of the electron’s kinetic energies, $\varepsilon$, 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.

\[ \frac{d}{dt} \left( \frac{\partial^2 N_n}{\partial \varepsilon_0 \partial \Upsilon} \right) \]

\[ \varepsilon_0 - \varepsilon_1 = \varepsilon_2 + I_n = \Upsilon \]
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
- $h, \varepsilon, Q, & R$, are problem dependent

Simpler hybrid (H) method

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

More complex time parallel (TP) method

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