Reduction of Collisional-Radiative Models for Transient Atomic Plasmas

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Introduction

Laser-plasma interactions (LPI) is a growing field abound with many complex processes unique to each LPI application's operating regime. Focusing on the atomic kinetics of LPI, acceleration/reduction techniques must be used, if one is to couple a collisional-radiative (CR) model to other time-dependent physical models to thoroughly investigate an LPI system. A recently-developed CR model using the Los Alamos National Laboratory (LANL) argon data set was extended to include a complexity reduction technique developed by Le et al.[1,2] The technique allows for the acceleration of CR codes, especially when considering a large number of atomic states. Three stable techniques discussed here include uniform grouping, the quasi-steady-state, or QSS, solution, and the newly-developed Boltzmann grouping method. In an attempt to relieve the computational burden placed on solving a full laser-produced plasma simulation, these reduction methods are compared against full, isothermal argon simulations. Preliminary results and error analysis shown here will provide insight into the use of the reduction technique for future laser-plasma simulations.

Collisional-Radiative Model

Collisional excitation $\leftrightarrow$ Collisional deexcitation

$$Ar_i^{+k} + e^-(\varepsilon_1) \leftrightarrow Ar_j^{+k} + e^-(\varepsilon_2)$$

Collisional ionization $\leftrightarrow$ 3-body recombination

$$Ar_i^{+k} + e^-(\varepsilon_1) \leftrightarrow Ar_j^{+(k+1)} + e^-(\varepsilon_2) + e^-(\varepsilon_3)$$

Bound-bound radiative transition

$$Ar_i^{+k} + h\nu \leftarrow Ar_j^{+k}$$

Bound-free radiative transition

$$Ar_i^{+k} + h\nu \leftarrow Ar_j^{+(k+1)} + e^-(\varepsilon_1)$$

Ordinary Differential Equation Solver

Backward Euler:

- $\Rightarrow$ Appropriate solver for chemical equations because of system stiffness
- $\Rightarrow$ Stiffness due to large separations in timescales, such as *collisional timescale vs. radiation timescale* or *highly-excited states' kinetics vs. low-lying levels' kinetics*

For Quasi-Steady-State (QSS):

- $\Rightarrow$ ODE solver is applied only to each ion's ground state, while enforcing quasi-neutrality
- $\Rightarrow$ Upper states are known immediately if one assumes fast excitation kinetics, for given ionic ground states, electron density, and electron temperature

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Complexity Reduction Techniques

Uniform Grouping

- Solely conserves number density
- Equivalent to infinite group temperatures in Boltzmann method

Conserved variable:

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

Level distribution:

$$N_i = \frac{g_i}{g_n} \mathcal{N}_n$$

Effective rate:

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

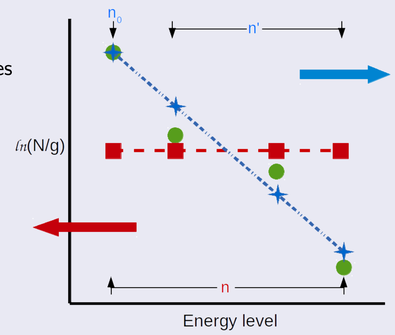


Figure: Sample grouping distributions

Boltzmann Grouping

- Conserves number density and energy
- Groups characterized by a temperature

Conserved variables:

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

Level distribution:

$$N_i = \frac{\mathcal{N}'_n}{\mathcal{Z}'_n} g_i e^{-\Delta E_i / T_n}$$

Effective rate:

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

Simulation Parametrization

Initial Conditions (2 Cases)

- $\Rightarrow$ Type: Isothermal Heating
- $\Rightarrow$ Electron Temperature: 10 eV & 100 eV
- $\Rightarrow$ Electron Density: 10^6 m^3
- $\Rightarrow$ Atomic Density: 10^{20} m^3
- $\Rightarrow$ Atomic Temperature: $3.5 \cdot 10^{-2}$ eV ($\sim 400K$)

Assumptions:

- $\Rightarrow$ Boltzmann equilibrium for each Ar ion
- $\Rightarrow$ Prime electrons distributed across Ar II

Argon Data Set

Table: Level assignment into isolation/groups

	Lvl	Grp		Lvl	Grp		Lvl	Grp
I	2	1 (9)	VII	2	1 (26)	XIII	5	2 (19)
II	4	1 (8)	VIII	2	1 (10)	XIV	6	2 (18)
III	2	1 (12)	IX	2	1 (11)	XV	5	2 (12)
IV	2	1 (15)	X	3	4 (16)	XVI	2	2 (7)
V	2	1 (21)	XI	4	3 (16)	XVII	10	0
VI	2	1 (29)	XII	4	3 (19)	XVIII	10	0

- $\Rightarrow$ Obtained level and cross sectional argon data from LANL
- $\Rightarrow$ Best application of the complexity reduction for accuracy uses a mix of groups and levels

Data Analysis

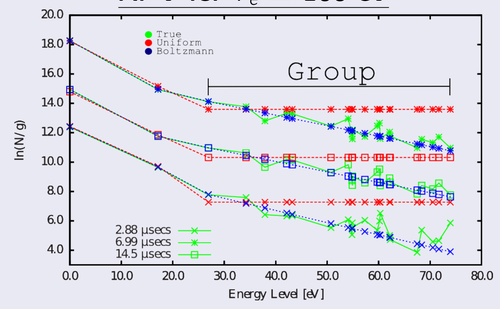
- $\Rightarrow$ Comparisons through Boltzmann plots will qualitatively show how well the reduction strategies, QSS, Uniform, and Boltzmann, capture the true solution
- $\Rightarrow$ Impact on coupling will be easily observed on macroscopic variables, particularly the electron density and radiated energy

Note:

- Current CR model applies a Maxwellian EEDF for rate calculations

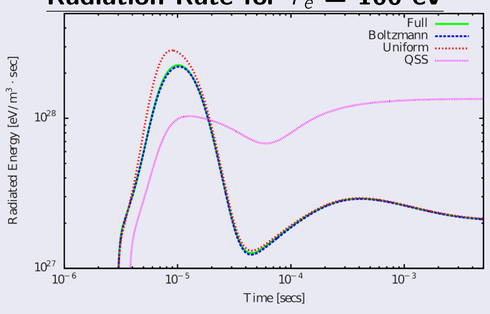
Atomic State Distribution (ASD) Profile and Electron Density Evolution

Ar V for $T_e = 100$ eV



- $\Rightarrow$ Isothermal heating populates the Ar V distribution and diminishes as higher ionic stages are populated
- $\Rightarrow$ Boltzmann strategy is better able to capture the true solution's profile during the transient stage
- $\Rightarrow$ Uniform method overestimates the excited states by orders of magnitude; as the Ar V distribution begins to diminish, penalties can be subtly observed in the lower-lying levels
- $\Rightarrow$ Both schemes accurately capture the electron density rates; however, the orders of magnitude difference for excited states leads to erroneous radiation solutions (shown right)

Radiation Rate for $T_e = 100$ eV



- $\Rightarrow$ During the transient times, uniform solution overestimates the radiation rate by almost twice as much; Boltzmann lies directly on top of the true solution for entire duration
- $\Rightarrow$ Well-known that QSS inaccurately captures electron density for high temperatures, which causes the radiation mismatch during the transient and steady-state times
- $\Rightarrow$ Implicates Boltzmann as being the better reduction model than QSS or uniform, if one considers coupling to the radiation transport equation

Method Acceleration and Accuracy

Wall Clock Time of Each Run

Grouping	10 eV	100 eV	1000 eV
True	81.8 s	81.71 s	81.80 s
Uniform	5.17 s	5.13 s	5.17 s
Boltzmann	19.14 s	19.10 s	18.16 s
QSS	13.75 s	14.01 s	13.51 s

- $\Rightarrow$ Timing is consistent for each grouping scheme across temperatures (and also for various densities)
- $\Rightarrow$ Boltzmann grouping requires iterating on group temperatures to obtain fitted profile between base level and excited subgroup; QSS requires Gaussian elimination for all ions' excited states

Radiation Rate Error at Peak

Grouping	10 eV	100 eV	1000 eV
Uniform	73.7 %	21.6 %	37.7 %
Boltzmann	0.30 %	2.37 %	4.86 %
QSS	68.4 %	56.1 %	58.7 %

- $\Rightarrow$ Uniform errors stem from inaccurate capture of excited states while QSS errors stem from density mismatching between integration timestepping and Gaussian elimination
- $\Rightarrow$ Possible that Boltzmann error may converge to uniform at higher temperature. Note that uniform is the limit of an infinite group temperature for Boltzmann formulation

Summary and Prospective Objectives

- $\Rightarrow$ Boltzmann better captures the true solution's distribution compared to QSS and uniform, with implications for coupling due to errors seen in macroscopic variables electron density and radiated energy
- $\Rightarrow$ Reduction in stiffness and speedups are present with Boltzmann relative to the true solution. Slower than uniform likely because of temperature iterations.

- $\Rightarrow$ Inclusion of irradiation terms (photoexcitation and photoionization)
- $\Rightarrow$ Line identification and width assignments in conjunction with experimental spectra that uses a discharge setup
- $\Rightarrow$ Port the reduction mechanism into a time-dependent fluid solver to simulate and validate an argon shock
- $\Rightarrow$ Radiation transport extension to the CR model, along with fluid solver

References

[1] Le, Karagozian, Cambier, PoP 20:12, (2013)
[2] Argon Atomic Data Sets. https://www-amdis.iaea.org/LANL/argon/
[3] Kapper and Cambier, J. of App. Phys., 109:113308 (2011)