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REVIEW OF THE NLTE KINETICS CODE WORKSHOP†

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Abstract—The first workshop to compare the output from Non-LTE kinetics codes using a standardized set of problems is reviewed. The background for the workshop is discussed and the planning is briefly outlined. The participation and general constraints for the workshop are given. Next the defined cases and a motivation for each case is presented. Some results from the workshop are shown which indicate both the utility of the workshop and some of the difficulties faced by those involved in NLTE kinetics modeling. Plans for the next workshop are discussed in the conclusion. © 1997 Published by Elsevier Science Ltd. All rights reserved

1. INTRODUCTION

The capability to accurately predict atomic level populations in plasmas not in local thermodynamic equilibrium LTE (NLTE) is central to the ability to understand and diagnose their radiative properties. NLTE plasmas constitute the majority of plasmas formed in laboratory studies related to hot dense matter and of interest to fusion, and consequently the diagnostic potential of the radiative properties is vast. In fact diagnostics of these plasmas is one of the primary driving forces in the study of the radiative properties of hot dense matter. As such it is important to provide a method and forum in which the calculations can be benchmarked against each other and against well characterized experiments. In the quest to provide NLTE code benchmarking we have devised a series of test cases as a first step towards a comprehensive cross-code comparison.

The method used to compare the codes was derived from the format developed by the Opacity Code Workshops which have provided insight into the problem areas of LTE opacity codes. Here a set of problems is agreed upon and then a call for participation is made. The basis for participation is simply that if you submit a case you can participate. Thus, there is a heavy emphasis on those working actively in the field. The results are further restricted from distribution so that no one can use the results to promote individual interests. The original submission of the cases is open to revision after the meeting so that the information learned can be incorporated into the codes. The results are then resubmitted and the entire complement of results is collated into a compendium for use by the participants.

The schedule for developing the comparison cases and the detailed meeting formats was fairly compressed. In November 1994 a group was formed at the Radiative Properties of Hot Dense Matter meeting and a plan was initiated to set up a workshop on NLTE kinetics. Then in April 1995 a set of cases was proposed, and by December of that year agreement was reached. A call for contributions was sent out in January of 1996 indicating that the deadline for submissions was June. The workshop took place at NIST in Gaithersburg, MD under the auspices of Dr W. Wiese and with the active support of Dr S. Bodner of the Naval Research Laboratory in Washington D.C.

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Table 1. The definition of the five steady state cases giving the atomic element, the case name, which is used in Table 3 for identification, the total number of points in the grid, the grid of temperatures and densities and finally the number of points in the temperature and density arrays

Element	Case	Total number	Grid	Number in temperature and density arrays
Carbon	C–SS	18	Te: 5, 10, 20, 40, 60, 80	6
			Ne: 10^{16}, 10^{20}, 10^{22}	3
Aluminum	Al–SS	18	Te: 50, 100, 200, 400, 600, 800	6
			Ne: 10^{20}, 10^{22}, 10^{23}	3
Argon	Ar–SS	16	Te: 675, 900, 1500, 2200	4
			Ne: 10^{12}, 3×10^{14}, 10^{18}, 10^{21}	4
Germanium	Ge–SS	27	Te: 150, 200, 250, 300, 350, 400, 450, 500, 600	9
			Ne: 10^{17}, 10^{20}, 3×10^{22}	3
Gold	Au–SS	6	Te: 800, 1200, 1600, 2000, 2400, 2800	6
			Ne: 10^{20}	1

2. DEFINITION OF THE CASES

A set of simple, well-defined cases were selected to ascertain that, at least for simple cases, the existing codes were in agreement. More difficult cases would be considered in the following workshops. It was decided to have two types of calculation, steady-state and time-dependent. For the steady-state cases, we provided a grid of temperatures and densities at which the calculations would be performed. For the time-dependent cases we provided the time histories of the temperature and density to define the problems. Since there were a large number of case studies included in these two categories, it was considered excessive to study further variations on the solution of the kinetics equations, e.g. including radiation transport.

In Table 1 the first three cases are considered "K shell" tests which implies that our interest lies in examining the opening of the K shell: the plasma conditions should produce ions primarily in the beryllium-like to helium-like range. The next case, for germanium, is an "L shell" test and should cover the transition from sodium-like to beryllium-like ions, with an emphasis on the neon-like ion. The intent here is to study both the opening of the L shell, and to examine the spread of the charge state distribution. Finally, the Au case is a nickel-like case and will provide insight into our capabilities when the 3d orbitals come into play. Moreover the Ge and Au cases have obvious association to x-ray lasing.

The temperature and density ranges for the steady-state cases were chosen to stress those regimes where previous experimental and theoretical interest lies. Thus, we attempted to pick cases that would have a reasonable level of participation and chance of success.

In addition to the steady-state cases three time-dependent case were selected and are indicated in Table 2. The first case, for carbon, is motivated by the advent of short pulse lasers where it has been proposed that various mechanisms can lead to extremely rapid ionization. This hypothetically leads to a plasma containing fully-stripped ions, but with a plasma temperature and density appropriate for a more recombined state. This is intended as an interesting test of both recombination rates and the high-lying level structure of the kinetics model. For this case the ion number density and temperature are fixed for the entire duration of the evolution at 10^{19} cm^{-3} and 2 eV respectively.

The latter two cases may be of more obvious origin. The aluminum exploding foil case is essentially a case for a region near the outer boundary of a laser heated foil, i.e. an exploding

Table 2. The definition of the three time-dependent cases giving the atomic element and case name, which is used in Table 3 for identification, the increment in time whether a multiplier for each step specified as log or linear, the start and stop time, and finally the description of the case.

Case	Initial condition	Time increment	Start	Stop	Case description
TD–C	Fully stripped	0.2690 (log)	0.1 ps	0.1 ns	Recombination laser
TD–Al	LTE	0.2174 (log)	5.0 ps	1.5 ns	Exploding foil
TD–Ar	LTE	20.0 ps (linear)	20.0 ps	2.0 ns	ICF implosion core

foil. The final time-dependent case is for the implosion of a hydrogen plasma containing an argon impurity. The atomic density of argon is one part in a thousand of the hydrogen. The specified plasma time history represents the central portion of the imploded core, where there is a long lead time before the shock gets to the central region at which time the plasma rapidly undergoes compression and heating.

3. CONTRIBUTIONS

The contributions were forwarded to an FTP site and use was made of an on-line WWW-based analysis package.[1] The number of contributions was substantial and given the rather short time indicates the strong interest. In Table 3 we present a list of the codes represented and the cases that were submitted from each code. The identification of the cases can be made with reference to Tables 1 and 2. As one would expect the aluminum case, which in some sense is the oldest of the laser plasma spectroscopy experiments, had the largest number of contributions with the germanium time-dependent x-ray laser case following close behind. Not too surprisingly the Au case had few submissions, which is clearly due to the fact that it is only recently that detailed NLTE kinetics codes have been capable of addressing the high Z problem.

4. RESULTS

The results of the workshop were quite illuminating as the cases, although selected to be straightforward, proved to be sufficient to challenge the participants. In all cases compared there was no case that showed strong agreement amongst the ensemble of submissions. Thus, the utility of the workshop was borne out by the obvious lack of agreement for these well-defined cases. Three particular examples of the comparisons are shown below. First we will show the results for the time dependent carbon recombination, it dramatically illustrates the role of high principal quantum number (PQN) states in the recombination process.

In Fig. 1 we show the average ionization stage, $\bar{z}$, as a function of time in nanoseconds. The different curves show the different contribution. In the spirit of the workshop we do not label the curves. We may nonetheless discuss the general features of this case. First, note that at early

Table 3. The set of submitted cases. The first column gives the code name and the top row indicates the case as defined in Tables 1 and 2. An x in the table indicates that there was a submission for that case from the code.

Code	C-ss	C-td	Al-ss	Al-td	Ar-ss	Ar-td	Ge-ss	Au-ss
Crad			x		x		x	
Dick	x	x	x	x	x			
Fine	x	x						x
Fly	x	x	x	x	x	x		
IonCowan	x		x		x		x	
IonFnl			x	x				
IonFnlInt			x	x			x	
IonMeyer			x	x				
IonMeyerInt			x	x			x	
IonRelac			x	x			x	
IonRelacInt			x	x			x	
Lasix	x		x	x			x	
M3r			x	x				
Mcuta							x	x
Mcxsn							x	x
McxsnNoDR								x
Med103							x	
Miccron	x		x					
Nebula	x		x		x		x	x
Nimp	x	x	x	x		x	x	x
Nomad	x	x	x	x	x	x		
Scroll			x				x	x
Transpec	x	x	x	x	x	x	x	x
TranspecH			x					
TranspecK	x	x	x	x	x	x		
Uwnlte	x	x	x	x	x	x		

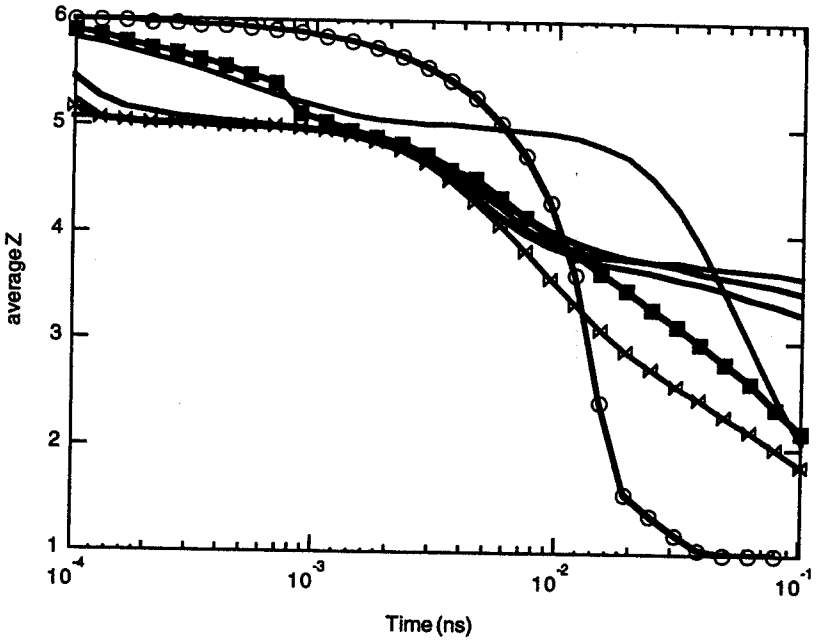

Fig. 1. The time history of the average ion stage, $\bar{z}$, vs time in nanoseconds for all the cases submitted. The initial state is such that the average z is 6. Extremely rapid recombination occurs on time scales smaller than 100 fs for those codes which include principle quantum numbers up to $n = 10$ in their kinetics model.

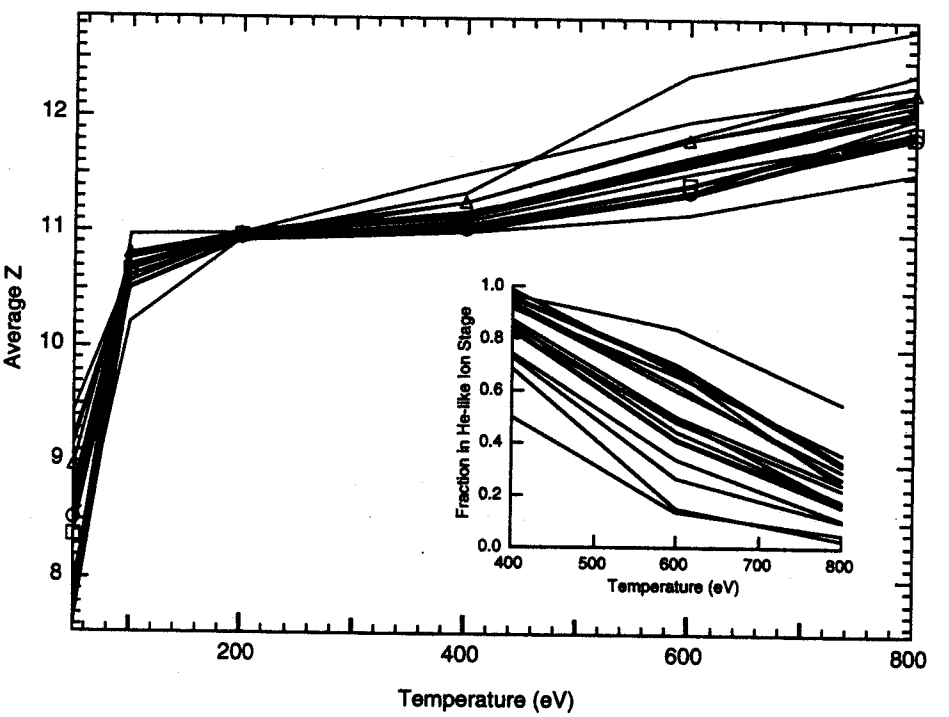

Fig. 2. The time history of the average ion stage vs temperature in eV for all the cases submitted for Al, at an electron density of 10^{20} cm^{-1}. The mean charge state of He-like at $\bar{z} = 11$ is preferentially populated due to the large closed shell ionization potential. In terms of a more physical quantity, we show in the inset the fraction of the total population that is in the He-like ion stage as a function of temperature.

time the recombination, which was initially specified to be in a single ion stage, that is, the fully stripped state yielding an initial $\bar{z}$ of 6, has three different groupings. These groups are related to the number of high PQN states in the hydrogenic ion. The slowest to recombine have the fewest; the group that clusters around a $\bar{z}$ of 5 has levels up to PQN = 10. Further, the calculations all move toward the hydrogenic ion by 3×10^{-3} ns, after which the curves separate again. It is interesting to note that the calculations with the most states in the ion stages below Li-like fall rapidly toward neutral, while the remainder essentially have a bottleneck, as the population does not recombine into the ion stages that are treated with few levels. Thus at both early and late times it is essential to have a fairly complete level description to obtain the correct ionization history.

The next example is one density value from the aluminum steady-state case. In Fig. 2 we show the average ionization stage, $\bar{z}$, for Al vs temperature in eV at an electron density of 10^{20} cm^{-1}. The curves for all the submissions are in rough agreement in the central temperature region as the ionization balance moves to the He-like ground state. As this ion has a substantially larger ionization potential than the Li-like stage, due to the closed shell, the codes show a small variation in mean ion stage until 600 eV. It is important to understand that the agreement between 200 and 400 eV is only an agreement on the average. To understand what this means in practice, we show in an inset in Fig. 2 the He-like fraction of the total number density vs temperature. Here we observe that the agreement on the $\bar{z}$ seen in Fig. 2 is not carried over to the number density in the He-like ion stage and indeed there is wide disagreement at, for example, 400 eV. Note that the variation in calculated He-like fraction at 400 eV is a factor of 2. This spread in the calculations becomes even more substantial at higher temperatures. The causes for this will require a detailed study that is yet to be performed, but we note that even for this case which should be well understood there is much room for improvement.

In the final example we show the results from the comparison of the gold steady-state case. The fact that detailed kinetics models now can attack problems having the complexity of the M-shell gold case is impressive. The contributions for this case came from both detailed configuration and average atom type codes. In Fig. 3 we have the mean ionization stage vs temperature

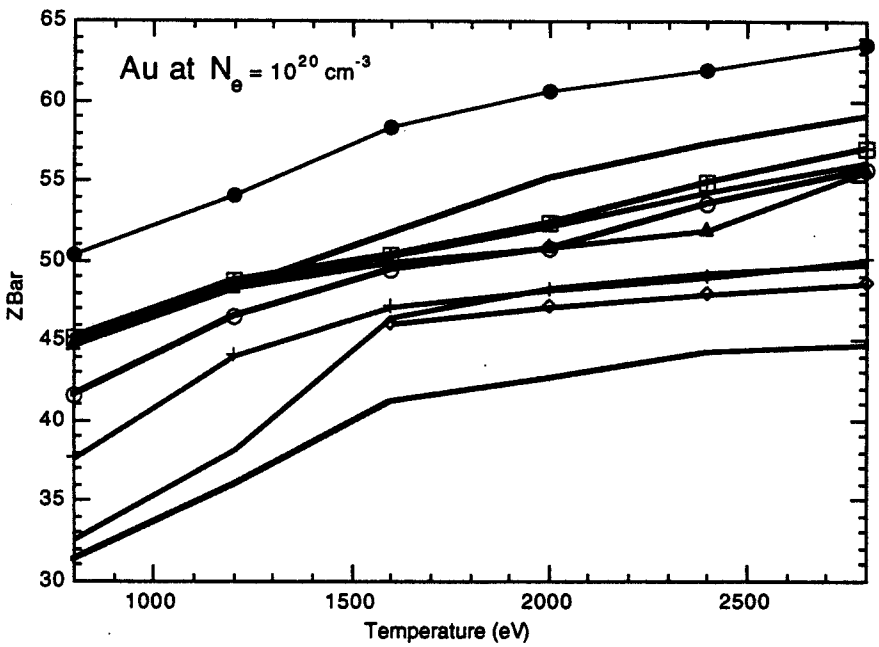

Fig. 3. The time history of the average ion stage vs temperature in eV for all the cases submitted for Au at an electron density of 10^{20} cm^{-3}. For reference we point out that the mean charge state of Ni-like Au is 50. The disagreement amongst the submissions is fairly uniform across the temperature range. The largest part of the discrepancy appears to be attributable to the method for including autoionizing states and their effects on the kinetics.

at the fixed electron density of $10^{20}\,cm^{-1}$. While there is progress in being able to address these problems, work is indeed needed, as there is a broad range of results for this case.

5. CONCLUSIONS AND COMMENTS

The NLTE Kinetics Code workshop succeeded in bringing together a large number of individuals involved in the kinetics modeling and development of codes for that purpose. We were at the outset concerned that the level of the problems should not be too simple as to obviate any need for comparison, nor too difficult to overly restrict participation. In retrospect, trying to keep the cases as simple as possible proved important as it shows us, as witnessed by the lack of agreement, the depth of the problems we face.

The relatively simple problems which were addressed nonetheless provided a significant amount of information and understanding for the participants. From this point, the participants have the option to re-submit their calculations to allow the incorporation of those things learned. Based on their final submissions, the summary document of the workshop will be sent out.

There will be another workshop in the spring of 1998 with a call for contributions and suggestions being made well in advance. We are also working on a set of interactive tools to allow the participants to perform analysis and comparisons in an interactive manner using a distributed data base access.

REFERENCES

1. Y. Ralchenko, Software for kinetics code analysis, see the website http://plasma-gate.weizmann.ac.IL/FsfAPP.html.