The 4th Non-LTE Code Comparison Workshop

December 12-16, 2005

Universidad de Las Palmas de Gran Canaria,

Las Palmas de Gran Canaria, Spain

UNIVERSIDAD DE LAS PALMAS
DE GRAN CANARIA

Submission of Calculations

This document is intended to define the particulars of the workshop submissions. In the sections below we will define the case problems, the comparison quantities which we require and the detailed format of the data files that we will be expecting. The case problems are of two types: steady-state and time-dependent. These problems are completely defined by a specification of the *electron temperature* and *electron density*. For the time-dependent cases these quantities are provided as a time history. With the large number of case studies included in these two categories we have avoided additional variations on the general NLTE problem, i.e., we strongly suggest that there be no consideration of plasma non-uniformity, boundary effects, or heavy-particle interactions.

An http server will be set up shortly to serve our needs for this, and an email containing the relevant details will be distributed among the potential participants. The submission files are to be uploaded to the server `ftp.nist.gov`, directory `/incoming`. Please use an anonymous login. The uploaded files are not shown in the directory list although they are there. To reduce the server load and accelerate upload, it would be most convenient if the contributor(s) created an archive file containing all the individual result files. Submissions employing any modern data compression techniques (e.g., `zip/gzip/bzip2/arj/lha/rar`) along with the Unix `tar` archiving utility will be accepted. Also, please inform Yuri Ralchenko (email: *yuri.ralchenko@nist.gov*) when new files are uploaded. An example submission file will be provided on the http server for comparisons.

Timeline:

1. Early July – web server is set up
2. October 15 – submission deadline
3. December 12 – workshop opens
4. December 16 – workshop adjourns

I. STATEMENT OF STEADY-STATE CASES

We have selected a number of atoms to consider, and for each atom we are requesting results on a grid of electron temperatures and electron densities. In the following, temperatures are given in eV and particle densities in cm^{-3}.

The following problems have been established for the steady-state cases:

Element	Case ID	Total # of Points	Parameter	Grid	# of Points
Detailed NLTE case (proposed at NLTE-3); comparison with the benchmark theoretical results					
Carbon	C	16	T_e	3, 5, 7, 10	4
			N_e	10^{13}, 10^{15}, 10^{17}, 10^{19}	4
The same case (almost) as in NLTE-3; non-Maxwellian; **test the progress since NLTE-3**					
Argon	Ar	24	T_e	50, 100, 300, 600	4
			N_e	10^{12}, 10^{18}, 10^{23}	3
			T_2	10^4 (10 keV)	
			% of T_2 in N_e	0 and 10%	2
Astrophysical photoionization case; Planckian radiation field					
Iron	Fe	25	T_e	15, 30, 60, 150, 300	5
			N_e	10^7	1
			T_{rad}	15, 50	2
			U_x	0, 0.1, 10	3
			Spectrum	10-1000 eV, ΔE = 1 eV (for T_e = 30 and 150 eV only)	991
EUV lithography; includes optically thick case; spectrum emission; exp. data available					
Tin	Sn	50	T_e	20, 25, 30, 35, 40	5
			N_e	10^{18}, 5×10^{18}, 10^{19}, 5×10^{19}, 10^{21}	5
			Opacity	**r** = **0** and **0.1** mm; **L** = 5**r**	2
			Spectrum	**100−180** Å, $\Delta\lambda$ = **0.02** Å	4001
				Spectrum for N_e = 5×10^{18} only	
Radiation power loss case					
Xenon	Xe	27	T_e	10, 20, 50, 100, 200, 500, 1000, 2000, 5000	9
			N_e	10^{14}, 10^{18}, 10^{22}	3
Comparison with experimental data; Planckian radiation field					
Gold	Au	48	T_e	400, 870, 1400, 2000, 2500, 5000	6
			N_e	3×10^{20}, 10^{21}, 3×10^{21}, 10^{22}	4
			T_{rad}	0, 175	2
			Spectrum	**2.8−4.4** Å, $\Delta\lambda$ = **0.001** Å	1601

Table I. Steady-state case definitions.

The grid of plasma temperatures and densities is given in Table I. If your calculation requires an ion temperature, then you should assume it is identical to the electron temperature.

Each calculation will be referenced by a case name, which is to be given in the submission data file (as described further below). The case name is constructed by appending a suffix to the Case_ID shown in the preceding table. *Note that the rules for suffix generation are different from the previous workshops.* The suffix consists of two or more digits corresponding to the order of parameters in Table I. Correspondingly, the Carbon case with T_e = 5 eV and $N_e = 10^{19}$ cm^{-3} will be referred to as **C24**: 5 eV is the second temperature in the list of T_e, and 10^{19} cm^{-3} is the fourth density. For the Ar case, the third digit in the case name is 1 for 0% of hot electrons and 2 for 10% of hot electrons. Another example: for the Fe photoionization, the case of T_e = 15 eV, T_{rad} = 50 eV, and U_x = 10, will be referred to as **Fe1123**. Finally, for the Sn cases the third digit in the case name will be **1** or **2** for r = 0 or 0.1 mm, respectively.

In case of argon calculations, 10% of the hot electrons means 10% of the total electron density given by N_e. Thus, for instance, for $N_e = 10^{18}$ cm^{-3} the density of hot electrons would be 10^{17} cm^{-3} while the density of the bulk thermal electrons would be 9×10^{17} cm^{-3}. The hot electrons are to be presented as a second Maxwellian with the temperature of 10,000 eV (10 keV).

In the Fe photoionization case representing a new type of problems in this series of meetings, the intensity of Planckian radiation field is characterized by the dimensionless parameter U_X. It is defined by the following relation:

$$U_X = \frac{F_X}{c\,N_e},$$

where F_X is the flux of photons (in photons/cm^2/s) above 100 eV. Obviously, the ratio F_X/c is just the density of photons with hν > 100 eV. Perhaps a parameter, representing flux of photons of all energies rather than only hν > 100 eV, would look more attractive to those who are less familiar with astrophysical photoionization calculations; yet we decided to follow the standard terminology.

The Sn case includes optically thick plasma cases represented by a uniform cylinder of radius 0.1 mm and length 0.5 mm. The spectrum (energy from a unit area per unit time per unit wavelength) is requested for two directions, i.e., radial and axial (see Fig. 1).

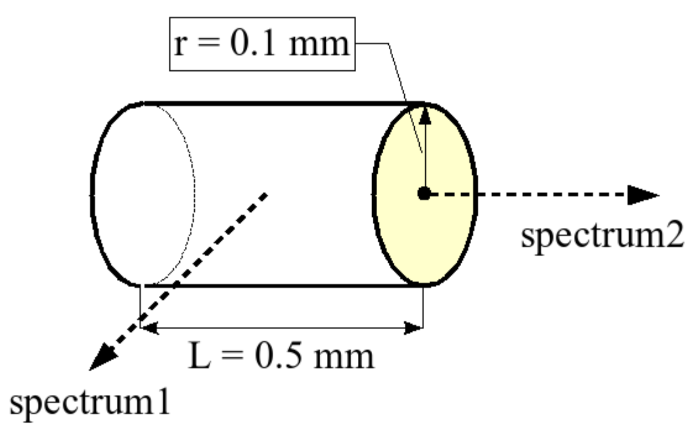

Fig 1. Schematics of spectra calculation for the Sn case.

The quantities to be computed for each case are described below. The Fe, Sn, and Au cases additionally require *calculation of emission spectra*.

In all the above cases, the calculations are to be solved in steady-state, at the specified electron densities and temperatures. For the cases with no T_{rad} the radiation field should be zero − only spontaneous radiative decays and radiative recombination shall be included – while for the Fe and Au cases we request the photoinduced processes (photoionization, photoexcitation, stimulated emission, etc.) to be added as well.

For both steady-state and time-dependent cases the submissions file should be named as **<case>.<contributor_name>.<code_name>**, so that Dr. A. Einstein's calculations for one of the hot-electron cases in Argon with his code GTOE would be in the file `ar212.einstein.gtoe` (case insensitive).

JUSTIFICATIONS OF THE STEADY-STATE CASES

C

This simple system showed noticeable difference at NLTE-3, thus we would like to explore in detail the region where non-LTE behavior is most prominent. It was also decided at NLTE-3 that carbon would serve as a benchmark case with a "complete" *generated* model. The LANL group is to produce very detailed results based on fine-structure level calculations that should greatly facilitate comparisons.

Ar

Argon represents the only case with non-Maxwellian electrons. We added one lower temperature and removed one high temperature. The primary idea is to compare progress since NLTE-3.

Fe

The iron case is derived from photoionized astrophysical plasmas. We hope it would not only help bring aboard more participants from astrophysics but also test codes originally developed for high-density plasmas in low-density conditions.

Sn

This case is motivated by the development of EUV sources for lithography. Although there are experimental data for both lower and upper densities, we will mainly concentrate on the former. Spectra synthesis is requested only for one data point where experimental data is available. Also this case includes optically thick plasma calculations.

Xe

Here we ask for a new parameter to be calculated, i.e., radiative power losses. In addition, as xenon is used in numerous, diverse plasma devices it is beneficial to study its kinetics over a large range of temperatures and densities.

Au

The Au cases were the most controversial at NLTE-3. Moreover, there are strong experimental efforts to study non-LTE kinetics of Au plasmas. We will compare theoretical results with the recently measured data.

II. STATEMENT OF TIME-DEPENDENT CASES

Unlike previous Workshops, the time-dependent simulations (three cases) are restricted to one element only, i.e., Argon. The T_e and N_e histories are chosen to have as many interesting features revealed as possible, and are not related to any particular experiment. The electron temperature history is the same for all cases, while the density varies significantly, from 10^{12} cm^{-3} (TD-Ar1) to almost 10^{25} cm^{-3} (TD-Ar3).

For all time-dependent cases the time grid is linear (total of 100 steps) starting from t = 0. The exact time grids as well as the electron temperature and density histories for each case are provided in the Appendix. The calculated data for all parameters, with the exception of levels, are to be provided at each time step. The level data are to be produced at every 10th step (e.g., for TD-Ar2, at $t = 10^{-10}$ s, $t = 2\times10^{-10}$ s, ..., $t = 10^{-9}$ s).

The plots of electron temperature and density vs. time are shown in Fig. 1, and the time histories are given in the Appendix. At time t = 0, all population is in the ground state of Ar II in all cases.

Case	Initial Condition	# Output Times	Output Δ	Stop Time
TD-Ar1	Ar II ground state	101	10^{-3} s	10^{-1} s
TD-Ar2	Ar II ground state	101	10^{-11} s	10^{-9} s
TD-Ar3	Ar II ground state	101	10^{-15} s	10^{-13} s

Table II. Summary of parameters for time-dependent calculations.

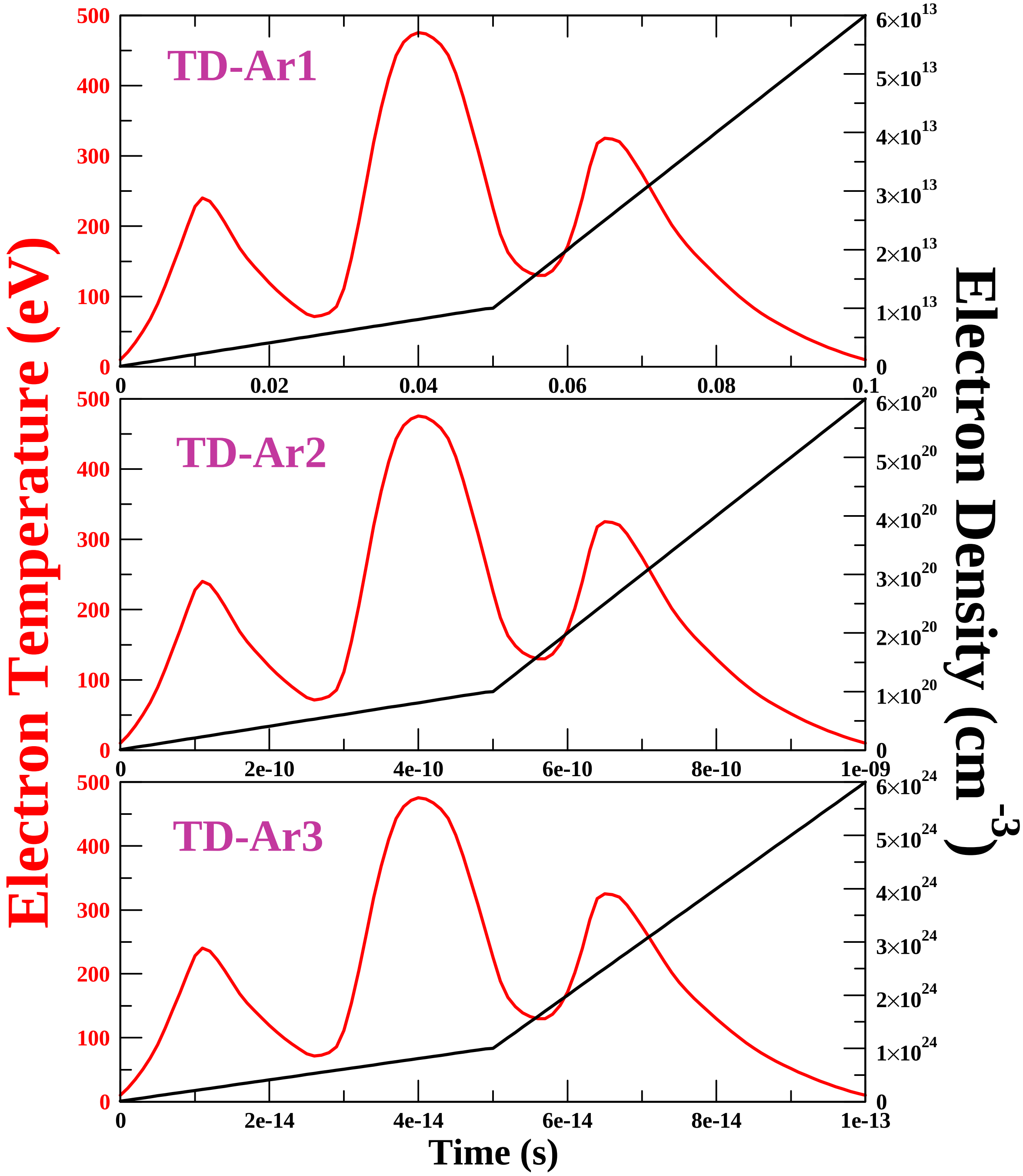

Fig 2. Time history of plasma parameters for the TD-Ar cases.

III. SUBMISSION FILE DESCRIPTION

We are asking for a fairly large amount of information. To simplify the specification for the contributors we have adopted a keyword approach within the submissions file. In this approach, all quantities are space delimited. In Section V, we give a schematic of the file format. For clarity we will use the `courier` font to indicate the keywords (the actual submissions should be unformatted plain ASCII text). The user-supplied data that are problem-dependent are indicated by a **bold-face** parameter name in brackets (e.g., <**pop_frac**>). We anticipate that not all information will be provided by every user. However, since the information is space delimited, and not fixed in a particular column, then *some* value must be given for each field. The best default value is to put a zero. The longer records, such as the `ion` and `elev` lines, may continue over several lines at the contributor's discretion. Do not break a line in the middle of a keyword or a number. Blank lines may be used anywhere within the file to make the text more readable. While some of the names we use suggest integer quantities, please use decimal values if appropriate to your calculation. For floating point numbers an `e11.4` format is generally adequate although for level energies a high accuracy may be necessary. The exact definitions of the quantities requested, including units, are given in Section V.

The submissions file is structured in 5 sections. These sections are identified by keywords. In some cases, an integer follows the section keyword to indicate the number of records which follow for that section. Some codes will not be able to provide information for every section. Thus, an entire section may be omitted. If all information is provided, then there will be a certain amount of redundancy. This redundancy is intentional and has at least two uses. First, it can be used to detect errors in the file formatting. Second, it is often possible to compute overall quantities more accurately internal to the kinetics code than by post-processing the results.

The *initial section* provides general problem identification information. This section begins with the keyword `data`.

The *sections 2-4* constitute a set of output data that is to be generated at each time step for the time-dependent problems. Naturally, only one such set should be produced for the steady-state cases.

> The *second section* gives overall quantities describing the plasma population and energy distribution. This section is signaled by the keyword `summary_quantities`. Note there are no spaces in the keywords.
>
> The *third section* gives information by ionization stage. This section is signaled by the keyword `ion_stages`. Within this section, information for each ionization stage begins with the keyword `ion`. As mentioned above, multiple lines may be used if desired (we intentionally used multiple lines in the schematic file listing below to improve its readability). Important note: we use <**Nbound**>, the number of bound electrons, *not* the ion stage charge, to label the ion stages.
>
> The *fourth section* gives information by energy level (keyword `energy_levels`). Since many codes employ some form of continuum lowering and/or moving calculational windows, we require that energy level definitions be provided for every case. The shell occupation numbers (<**occK**>, <**occL**> etc.) as defined for each `elev` record will be used to compare codes for the cross-over from a ladder-like de-excitation regime to one which is in Saha-Boltzmann equilibrium with the continuum.

Finally, the *fifth section* contains spectra intensities, either for a prescribed spectral range (steady-state) or for some specific lines (time-dependent).

A relational database tool will be used to manage the data during the course of the workshop. To simplify the data access, the database layout will parallel the file formats specified here.

If necessary, extra clarifications regarding the submission format will be provided at the Workshop's web site.

IV. SUBMISSION FILE FORMAT

The text that follows is a schematic of a submissions file:

```
data                <user comment... >
case                <case_id>
code                <name>
atom                <name>  <Znuc>
calctime            <CPU>  <human>


summary_quantities
plasma              <Te>  <Ne>
time                <time>
zbar                <zbar>
m2                  <2nd central moment>
m3                  <3rd central moment>
eint                <internal_energy>
deintdt             <dE_int/dT_e>
pfn                 <partition_fn>
nmax_eff            <n_value>
ploss               <P_bb>  <P_bf>  <P_ff>  <P_total>



ion_stages          <count>
ion                 <Nbound>  <pop_frac>     <nouter>
                    <S_tot>      <f_Scoll>   <f_Sphoto>      <f_Sauto>
                    <αtot>       <f_αcoll>   <f_αphoto>      <f_αauto>
...

ion                 <Nbound>  <pop_frac>  <nouter>
                    <S_tot>      <f_Scoll>   <f_Sphoto>      <f_Sauto>
                    <αtot>       <f_αcoll>   <f_αphoto>      <f_αauto>


energy_levels       <count>
elev       <Nbound>      <level1>      <stwt>  <energy>  <population>
           <Γtot>   <f_ΓcollBB> <f_ΓphotoBB> <f_ΓcollBF>  <f_ΓphotoBF> <f_Γauto>
           <occK>   <occL>      <occM>   ...  <nouter>
...

elev       <Nbound> <levelN>  <stwt>  <energy>  <population>
           <Γtot>   <f_ΓcollBB> <f_ΓphotoBB> <f_ΓcollBF>  <f_ΓphotoBF> <f_Γauto>
           <occK>   <occL>      <occM>   ...  <nouter>
…
…
```

```
summary_quantities
plasma          <Te> <Ne>
time            <time>
…

ion_stages      <count>
…

energy_levels   <count>
…


summary_quantities
plasma          <Te> <Ne>
time            <time>
…

ion_stages      <count>
…

energy_levels   <count>
…
```

The energy levels are to be provided for all steady state cases. As for the TD cases, the complete data for energy levels are requested *only at every 10th time step*; for instance, for the TD-Ar2 case those are t = 1×10^{-10}, 2×10^{-10}...10^{-9} s.

Spectrum Output

For the cases where we request spectra, the output format is different for the Fe case and Sn and Au cases. The spectral information will be given in this same text file, following the information above. The Fe spectrum will be in the format:

spectrum **Fe**		**<count>**		
<energy1>	**<ε_{bb}1>**	**<ε_{bf}1>**	**<ε_{ff}1>**	**<ε_{tot}1>**
<energy2>	**<ε_{bb}2>**	**<ε_{bf}2>**	**<ε_{ff}2>**	**<ε_{tot}2>**
....				
<energyN>	**<ε_{bb}N>**	**<ε_{bf}N>**	**<ε_{ff}N>**	**< ε_{tot}N>**

where energy1 = 10, energy2 = 20..., energy991 = 1000.

For the Sn cases the output will be in a similar format with wavelengths in place of energies:

spectrum **Sn1 (or Sn2)**		**<count>**		
<wavelength1>	**<ε_{bb}1>**	**<ε_{bf}1>**	**<ε_{ff}1>**	**<ε_{tot}1>**
<wavelength2>	**<ε_{bb}2>**	**<ε_{bf}2>**	**<ε_{ff}2>**	**<ε_{tot}2>**
....				
<wavelengthN>	**<ε_{bb}N>**	**<ε_{bf}N>**	**<ε_{ff}N>**	**< ε_{tot}N>**

with wavelengths in Ångstroms in place of energies in eV, and the same for the Au case:

spectrum	**Au**	**<count>**		
<wavelength1>	**<ε_{bb}1>**	**<ε_{bf}1>**	**<ε_{ff}1>**	**<ε_{tot}1>**
<wavelength2>	**<ε_{bb}2>**	**<ε_{bf}2>**	**<ε_{ff}2>**	**<ε_{tot}2>**
....				
<wavelengthN>	**<ε_{bb}N>**	**<ε_{bf}N>**	**<ε_{ff}N>**	**< ε_{tot}N>**

The meaning of parameters **ε** is different for different cases and is discussed in detail below.

V. DEFINITIONS OF REQUESTED QUANTITIES

Before proceeding to a detailed description of the requested quantities, we would like to comment on the ion density. In absence of heavy-particle interactions, the influence of ion density would mostly be exposed through the ionization potential lowering. To provide a (almost) unique description of N_i, for all but the `Fe` case the electron and ion densities are to be related via the plasma neutrality condition, i.e., $N_i = N_e/Z$. For the `Fe` astrophysical case, we accept that the iron ion density is $N_i = 10^{-5} \cdot N_e$, i.e., $N_i(\mathrm{Fe}) = 10^2$ cm^{-3}.

In *section 1*, the identification section, the following quantities are requested:

`data`	Calculation identifier and user comment line. Comment should be limited to this one line only and should include the contributor's name, institution, the version of the code, and the date at which calculation was run. This can be invaluable in maintaining order in large number of submissions.
`case`	All steady-state and time-dependent calculations will have a case identification of the form `Au11`, `C24` or the like (see Section I). These identifiers are assigned in the section below where the specific calculations are called out.
`code`	An identifier for each contributor's code which may be chosen by the contributors. For convenience in post-processing and tabulation the names should not be excessively long. The names will be used in all tables and graphs of comparisons, and must be the same from case to case.
`atom`	Identifies the atom under study. The field <**name**> is a convenience for the contributor. In many cases, calculations are driven by atomic data found in a file. The file <**name**> may be used to specify that name. The field <**Znuc**> is the nuclear charge of the atom.
`calctime`	Provides information on the CPU time (computer) and total time (human) spent on calculation of this particular case.

As has already been explained above, the group of sections `summary_quantities`, `ion_stages` and `energy_levels` (on every 10th step) repeats for each time step for the time-dependent cases.

In *section 2*, the `summary_quantities` section, the following items are requested:

`plasma`	This record specifies the plasma conditions used in this calculation. The electron temperature is in units of eV. The electron density is in units of cm^{-3}. For time-dependent cases both T_e and N_e may be arbitrary.
`time`	The output time for time-dependent cases or arbitrary value (e.g., zero) for steady-state cases.
`zbar`	The average charge of the plasma.
`m2`	The second central moment of the charge state distribution.

`m3`	The third central moment of the charge state distribution.
`eint`	The specific internal energy of the atom.
`deintdt`	The "specific heat" of the atom.
`pfn`	The "partition function" of the atom.
`nmax_eff`	For this calculation, the principal quantum number of the outermost electron in any bound state. We will be interested in sensitivity of comparison quantities to the highest bound states accounted for by the model. This quantity will also be used as a measure of continuum lowering.
`ploss`	The radiative power losses: bound-bound, bound-free, free-free, and total. Units: erg/sec/cm^3.

The **central moments** are defined as:

$$m_N = \sum_j y_j \left(q_j - \overline{Z}\right)^N ,$$

where y_j is the fractional population of ion stage j, q_j is the ion charge, and $\overline{Z}$ is the average charge.

The **specific internal energy** is the sum of level populations, n_j, multiplied by their energy value, E_j, divided by the total ion density N_i:

$$E_{\mathrm{int}} = \sum_j \frac{E_j n_j}{N_i} .$$

The energy reference is the ground state of the neutral atom. We recognize that a kinetics model may not include all ionization stages of the atom – the ground state of the most neutral ion is the most reasonable substitute. For intercomparisons, this quantity will likely need zero point shifts. Units are eV/atom.

The **specific heat** is the derivative with respect to electron temperature of the specific internal energy of the atom. Units are eV/atom/eV. If computed by finite difference, the step size is to be chosen by the contributor.

The **partition function** is defined as the classical partition function:

$$Q = \sum_j g_j \exp\left(-E_j / T_e\right),$$

where g_j is the statistical weight of level j and E_j is the energy of the level, with respect to the ground state of the most neutral ion.

The **power loss** output is *generally* requested only for Xe, but it would be welcome for other cases too. The total power loss is the most important quantity, so that if one has difficulties separating different contributions, then it would suffice to have zeros in fields other than **<P$_{\mathrm{total}}$>**.

Note that many of the "thermodynamic" quantities are intentionally sensitive to continuum lowering models. Quantities possibly affected are <**eint**>, <**deintdt**>, and <**pfn**>. If your continuum lowering model alters the energy levels or statistical weights, please include these effects in the appropriate "thermodynamic" quantities.

High-lying bound states can be included in the population kinetics in a variety of ways. The field `nmax_eff` is intended to give information on the highest-lying bound state, which is affecting the calculation of the populations. It is thus an "effective" principal quantum number. If a code includes a level, which accounts for more than one *n* value, then for this field we recommend giving the *largest* value that is being modeled.

In *section 3*, the `ion_stages` section, the following quantities are requested:

<Nbound> The number of bound electrons in this ionization stage.
<pop_frac> The fraction of atoms in this ionization stage. Sum over all ions should benormalized to unity.
<nouter> The principal quantum number of the outermost electron for any state in this ion stage.
<S_{tot}> The total ionization rate out of this ion stage, averaged over all initial states in this ion stage (weighted by the fractional populations of the initial states), and summed over all final states. This quantity is further summed over all ionization processes.
<f_S_{coll}> The fractional contribution of electron collisional ionization processes to <**S_{tot}**>**.**
<f_S_{photo}> The fractional contribution of photo-ionization processes to **S_{tot}**>**.**
<f_S_{auto}> The fractional contribution of auto-ionization processes to <**S_{tot}**>.
<α_{tot}> The total recombination rate out of this ion stage, averaged over all initial states in this ion stage (weighted by the fractional populations of the initial states), and summed over all final states. This quantity is further summed over all recombination processes.
<f_α_{coll}> The fractional contribution of three-body recombination to the total <α_{tot}>.
<f_α_{photo}> The fractional contribution of radiative-recombination to the total <α_{tot}>.
<f_α_{auto}> The fractional contribution of dielectronic capture processes to the total <α_{tot}>.

We note that the total ionization and recombination rates are rates, and not rate coefficients. It is also important to be precise about the direction of these total rates. <**S_{tot}**> is the total rate *out* of the indicated ion. Similarly, **<**α_{tot}> is the total rate out of the indicated ion, that is, *into* the less ionized ion.

The definitions of **S_{tot}** and α_{tot} are best clarified through an example. Consider a three-ion stage problem consisting of levels in Li-like, He-like, and H-like ions. For the He-like ion, **S_{tot}** is the sum of all ionization rates *out* of He-like, weighted by the appropriate He-like initial state populations, and summed over all final states in the H-like ion. The averaging over initial states is completed by dividing the above sum by the total population of the He-like ion. **α_{tot}** for the He-like ion is the sum of all recombination rates out of He-like, weighted by the appropriate He-like initial state populations, and summed over all final states in the Li-like ion. The averaging over initial states is completed by dividing the above sum by the total population of the He-like ion. With these definitions, we can define a set of ionization rate equations. In the case of the He-like ion, we write:

$$\frac{dn(He)}{dt} = \alpha_{tot}(H)n(H) - [\alpha_{tot}(He) + S_{tot}(He)]n(He) + S_{tot}(Li)n(Li).$$

Our primary interest is the collisional radiative modeling of highly-charged ions and so we have not requested detailed information for contributions due to other processes, such as charge-exchange and heavy ion collisions. Units of **<S_{tot}>** and **<α_{tot}>** are 1/sec.

In *section 4*, the `energy_levels` section, the following quantities are requested:

<Nbound>	Identifies the ionization stage to which this energy level belongs. As always, this quantity is the number of bound electrons in the level.
<level>	A sequential level number within this ionization stage. This index begins at 1 within each ionization stage for use as a label in model comparisons. The ground state of each ion stage will be identified by locating the state of lowest energy within the ion stage.
<stwt>	The statistical weight of this energy level.
<energy>	The energy of the level relative to the overall model. Ionization potentials will be obtained by subtraction of successive ground state energies. Units are in eV. The overall energy reference is the ground state of the most neutral ion in the problem.
<population>	The **normalized** ion density of this level. *Sum of all level populations over all ions is unity*.
<Γ_{tot}>	The **total** destruction rate of this level. This is the absolute value of the corresponding term in the rate matrix diagonal. Units are 1/sec.
<f_Γ_{collBB}>	The *fractional* contribution of electron collision excitation/de-excitation processes to **<Γ_{tot}>**.
<f_$\Gamma_{photoBB}$>	The *fractional* contribution of bound-bound radiation processes to **<Γ_{tot}>**.
<f_Γ_{collBF}>	The *fractional* contribution of electron collision ionization-recombination processes to **<Γ_{tot}>**.
<f_$\Gamma_{photoBF}$>	The *fractional* contribution of photo-ionization-recombination to **<Γ_{tot}>**.
<f_Γ_{auto}>	The *fractional* contribution of auto-ionization/dielectronic recombination processes to **<Γ_{tot}>**.
<occK>	Occupation number: for this energy level, the number of electrons in the K shell. Users of configuration interaction codes might wish to use the dominant configuration to assign this value.
<occL>	The number of electrons in the L shell.
…	
<nouter>	The principal quantum number of the outermost electron in that energy level.

The shell occupation numbers (**<occK>**, **<occL>**, etc.) could be variable in number for each code, plasma condition, and energy level. Contributors are not constrained on this point: they may specify as many shells as necessary, and as relevant to their calculational approach. The final entry for this energy level record should be the principal quantum number of the outermost electron in that level. In the case of highly-excited levels, the shell occupation numbers may be simplified by only specifying the core, <**Nbound>**-1, electrons. In this case the field <**nouter>** will be used to set the location of the remaining electron. We will be using the values given in this section to compute some of the quantities given in section 2 for consistency checks.

In *section 5*, the `spectrum` section, the data requested and the format vary slightly for different cases and are summarized below:

Fe

x-axis:	energy (in eV),
emissivity units:	erg/cm^3/sec/eV;

Au

x-axis:	wavelength (in Å),
emissivity units:	erg/cm^3/sec/Å;

Sn

x-axis:	wavelength (in Å),
emissivity units:	erg/cm^2/sec/Å;

As one can see, emissivity for Fe and Au is requested *per unit volume* while for the Sn case it is requested *per unit area*. The required data are bound-bound **<ε_{bb}**>, free-bound **<ε_{fb}**>, free-free **<ε_{ff}>** and total **<ε_{tot}>** emissivities. The field <**count**> specifies the number of *(energy/wavelengths, emissivities)* rows which follow.

Please note also that for the Sn case, we ask for **two** spectra that are distinguished by adding 1 or 2 next to “Sn” for the radial and axial spectra, respectively.

Finally, the line broadening should be natural+Doppler for all optically thin cases.

APPENDIX. TIME HISTORIES FOR TIME-DEPENDENT CASES

TD-Ar1

Time (s)	T_e (eV)	N_e (cm^{-3})
0.0E+00	10.00	1.0E+11
1.0E-03	21.04	3.0E+11
2.0E-03	34.66	5.0E+11
3.0E-03	50.29	7.0E+11
4.0E-03	67.97	9.0E+11
5.0E-03	89.48	1.1E+12
6.0E-03	115.24	1.3E+12
7.0E-03	142.56	1.5E+12
8.0E-03	170.26	1.7E+12
9.0E-03	200.29	1.9E+12
1.0E-02	228.10	2.1E+12
1.1E-02	240.28	2.3E+12
1.2E-02	235.33	2.5E+12
1.3E-02	221.61	2.7E+12
1.4E-02	205.51	2.9E+12
1.5E-02	186.96	3.1E+12
1.6E-02	168.89	3.3E+12
1.7E-02	154.48	3.5E+12
1.8E-02	142.23	3.7E+12
1.9E-02	130.48	3.9E+12
2.0E-02	119.31	4.1E+12
2.1E-02	108.83	4.3E+12
2.2E-02	99.25	4.5E+12
2.3E-02	90.49	4.7E+12
2.4E-02	82.45	4.9E+12
2.5E-02	75.01	5.1E+12
2.6E-02	71.45	5.3E+12
2.7E-02	72.87	5.5E+12
2.8E-02	76.45	5.7E+12
2.9E-02	85.67	5.9E+12
3.0E-02	111.30	6.1E+12
3.1E-02	154.21	6.3E+12
3.2E-02	205.84	6.5E+12
3.3E-02	263.00	6.7E+12

Time (s)	T_e (eV)	N_e (cm^{-3})
3.4E-02	319.16	6.9E+12
3.5E-02	368.26	7.1E+12
3.6E-02	410.12	7.3E+12
3.7E-02	442.76	7.5E+12
3.8E-02	461.75	7.7E+12
3.9E-02	471.37	7.9E+12
4.0E-02	475.60	8.1E+12
4.1E-02	473.70	8.3E+12
4.2E-02	467.50	8.5E+12
4.3E-02	458.18	8.7E+12
4.4E-02	443.36	8.9E+12
4.5E-02	417.54	9.1E+12
4.6E-02	383.82	9.3E+12
4.7E-02	346.80	9.5E+12
4.8E-02	308.39	9.7E+12
4.9E-02	267.20	9.9E+12
5.0E-02	225.76	1.0E+13
5.1E-02	188.47	1.1E+13
5.2E-02	163.10	1.2E+13
5.3E-02	148.45	1.3E+13
5.4E-02	139.00	1.4E+13
5.5E-02	133.19	1.5E+13
5.6E-02	129.90	1.6E+13
5.7E-02	129.81	1.7E+13
5.8E-02	136.82	1.8E+13
5.9E-02	150.42	1.9E+13
6.0E-02	171.37	2.0E+13
6.1E-02	201.66	2.1E+13
6.2E-02	239.88	2.2E+13
6.3E-02	284.73	2.3E+13
6.4E-02	317.78	2.4E+13
6.5E-02	325.09	2.5E+13
6.6E-02	324.15	2.6E+13
6.7E-02	320.14	2.7E+13
6.8E-02	307.63	2.8E+13
6.9E-02	291.27	2.9E+13
7.0E-02	274.23	3.0E+13
7.1E-02	256.34	3.1E+13

Time (s)	T_e (eV)	N_e (cm^{-3})
7.2E-02	237.60	3.2E+13
7.3E-02	219.09	3.3E+13
7.4E-02	201.97	3.4E+13
7.5E-02	186.91	3.5E+13
7.6E-02	173.62	3.6E+13
7.7E-02	161.68	3.7E+13
7.8E-02	150.69	3.8E+13
7.9E-02	140.23	3.9E+13
8.0E-02	129.94	4.0E+13
8.1E-02	119.82	4.1E+13
8.2E-02	110.01	4.2E+13
8.3E-02	100.61	4.3E+13
8.4E-02	91.76	4.4E+13
8.5E-02	83.59	4.5E+13
8.6E-02	76.20	4.6E+13
8.7E-02	69.61	4.7E+13
8.8E-02	63.37	4.8E+13
8.9E-02	57.42	4.9E+13
9.0E-02	51.76	5.0E+13
9.1E-02	46.38	5.1E+13
9.2E-02	41.28	5.2E+13
9.3E-02	36.45	5.3E+13
9.4E-02	31.89	5.4E+13
9.5E-02	27.59	5.5E+13
9.6E-02	23.53	5.6E+13
9.7E-02	19.66	5.7E+13
9.8E-02	16.06	5.8E+13
9.9E-02	12.81	5.9E+13
1.0E-01	10.00	6.0E+13

TD-Ar2

Time (s)	T_e (eV)	N_e (cm^{-3})
0.0E+00	10.00	1.0E+18
1.0E-11	21.04	3.0E+18
2.0E-11	34.66	5.0E+18

Time (s)	T_e (eV)	N_e (cm^{-3})
3.0E-11	50.29	7.0E+18
4.0E-11	67.97	9.0E+18
5.0E-11	89.48	1.1E+19
6.0E-11	115.24	1.3E+19
7.0E-11	142.56	1.5E+19
8.0E-11	170.26	1.7E+19
9.0E-11	200.29	1.9E+19
1.0E-10	228.10	2.1E+19
1.1E-10	240.28	2.3E+19
1.2E-10	235.33	2.5E+19
1.3E-10	221.61	2.7E+19
1.4E-10	205.51	2.9E+19
1.5E-10	186.96	3.1E+19
1.6E-10	168.89	3.3E+19
1.7E-10	154.48	3.5E+19
1.8E-10	142.23	3.7E+19
1.9E-10	130.48	3.9E+19
2.0E-10	119.31	4.1E+19
2.1E-10	108.83	4.3E+19
2.2E-10	99.25	4.5E+19
2.3E-10	90.49	4.7E+19
2.4E-10	82.45	4.9E+19
2.5E-10	75.01	5.1E+19
2.6E-10	71.45	5.3E+19
2.7E-10	72.87	5.5E+19
2.8E-10	76.45	5.7E+19
2.9E-10	85.67	5.9E+19
3.0E-10	111.30	6.1E+19
3.1E-10	154.21	6.3E+19
3.2E-10	205.84	6.5E+19
3.3E-10	263.00	6.7E+19
3.4E-10	319.16	6.9E+19
3.5E-10	368.26	7.1E+19
3.6E-10	410.12	7.3E+19
3.7E-10	442.76	7.5E+19
3.8E-10	461.75	7.7E+19
3.9E-10	471.37	7.9E+19
4.0E-10	475.60	8.1E+19

Time (s)	T_e (eV)	N_e (cm^{-3})
4.1E-10	473.70	8.3E+19
4.2E-10	467.50	8.5E+19
4.3E-10	458.18	8.7E+19
4.4E-10	443.36	8.9E+19
4.5E-10	417.54	9.1E+19
4.6E-10	383.82	9.3E+19
4.7E-10	346.80	9.5E+19
4.8E-10	308.39	9.7E+19
4.9E-10	267.20	9.9E+19
5.0E-10	225.76	1.0E+20
5.1E-10	188.47	1.1E+20
5.2E-10	163.10	1.2E+20
5.3E-10	148.45	1.3E+20
5.4E-10	139.00	1.4E+20
5.5E-10	133.19	1.5E+20
5.6E-10	129.90	1.6E+20
5.7E-10	129.81	1.7E+20
5.8E-10	136.82	1.8E+20
5.9E-10	150.42	1.9E+20
6.0E-10	171.37	2.0E+20
6.1E-10	201.66	2.1E+20
6.2E-10	239.88	2.2E+20
6.3E-10	284.73	2.3E+20
6.4E-10	317.78	2.4E+20
6.5E-10	325.09	2.5E+20
6.6E-10	324.15	2.6E+20
6.7E-10	320.14	2.7E+20
6.8E-10	307.63	2.8E+20
6.9E-10	291.27	2.9E+20
7.0E-10	274.23	3.0E+20
7.1E-10	256.34	3.1E+20
7.2E-10	237.60	3.2E+20
7.3E-10	219.09	3.3E+20
7.4E-10	201.97	3.4E+20
7.5E-10	186.91	3.5E+20
7.6E-10	173.62	3.6E+20
7.7E-10	161.68	3.7E+20
7.8E-10	150.69	3.8E+20

Time (s)	T_e (eV)	N_e (cm^{-3})
7.9E-10	140.23	3.9E+20
8.0E-10	129.94	4.0E+20
8.1E-10	119.82	4.1E+20
8.2E-10	110.01	4.2E+20
8.3E-10	100.61	4.3E+20
8.4E-10	91.76	4.4E+20
8.5E-10	83.59	4.5E+20
8.6E-10	76.20	4.6E+20
8.7E-10	69.61	4.7E+20
8.8E-10	63.37	4.8E+20
8.9E-10	57.42	4.9E+20
9.0E-10	51.76	5.0E+20
9.1E-10	46.38	5.1E+20
9.2E-10	41.28	5.2E+20
9.3E-10	36.45	5.3E+20
9.4E-10	31.89	5.4E+20
9.5E-10	27.59	5.5E+20
9.6E-10	23.53	5.6E+20
9.7E-10	19.66	5.7E+20
9.8E-10	16.06	5.8E+20
9.9E-10	12.81	5.9E+20
1.0E-01	10.00	6.0E+20

TD-Ar3

Time (s)	T_e (eV)	N_e (cm^{-3})
0.0E+00	10.00	1.0E+22
1.0E-15	21.04	3.0E+22
2.0E-15	34.66	5.0E+22
3.0E-15	50.29	7.0E+22
4.0E-15	67.97	9.0E+22
5.0E-15	89.48	1.1E+23
6.0E-15	115.24	1.3E+23
7.0E-15	142.56	1.5E+23
8.0E-15	170.26	1.7E+23
9.0E-15	200.29	1.9E+23
1.0E-14	228.10	2.1E+23

Time (s)	T_e (eV)	N_e (cm^{-3})
1.1E-14	240.28	2.3E+23
1.2E-14	235.33	2.5E+23
1.3E-14	221.61	2.7E+23
1.4E-14	205.51	2.9E+23
1.5E-14	186.96	3.1E+23
1.6E-14	168.89	3.3E+23
1.7E-14	154.48	3.5E+23
1.8E-14	142.23	3.7E+23
1.9E-14	130.48	3.9E+23
2.0E-14	119.31	4.1E+23
2.1E-14	108.83	4.3E+23
2.2E-14	99.25	4.5E+23
2.3E-14	90.49	4.7E+23
2.4E-14	82.45	4.9E+23
2.5E-14	75.01	5.1E+23
2.6E-14	71.45	5.3E+23
2.7E-14	72.87	5.5E+23
2.8E-14	76.45	5.7E+23
2.9E-14	85.67	5.9E+23
3.0E-14	111.30	6.1E+23
3.1E-14	154.21	6.3E+23
3.2E-14	205.84	6.5E+23
3.3E-14	263.00	6.7E+23
3.4E-14	319.16	6.9E+23
3.5E-14	368.26	7.1E+23
3.6E-14	410.12	7.3E+23
3.7E-14	442.76	7.5E+23
3.8E-14	461.75	7.7E+23
3.9E-14	471.37	7.9E+23
4.0E-14	475.60	8.1E+23
4.1E-14	473.70	8.3E+23
4.2E-14	467.50	8.5E+23
4.3E-14	458.18	8.7E+23
4.4E-14	443.36	8.9E+23
4.5E-14	417.54	9.1E+23
4.6E-14	383.82	9.3E+23
4.7E-14	346.80	9.5E+23
4.8E-14	308.39	9.7E+23

Time (s)	T_e (eV)	N_e (cm^{-3})
4.9E-14	267.20	9.9E+23
5.0E-14	225.76	1.0E+24
5.1E-14	188.47	1.1E+24
5.2E-14	163.10	1.2E+24
5.3E-14	148.45	1.3E+24
5.4E-14	139.00	1.4E+24
5.5E-14	133.19	1.5E+24
5.6E-14	129.90	1.6E+24
5.7E-14	129.81	1.7E+24
5.8E-14	136.82	1.8E+24
5.9E-14	150.42	1.9E+24
6.0E-14	171.37	2.0E+24
6.1E-14	201.66	2.1E+24
6.2E-14	239.88	2.2E+24
6.3E-14	284.73	2.3E+24
6.4E-14	317.78	2.4E+24
6.5E-14	325.09	2.5E+24
6.6E-14	324.15	2.6E+24
6.7E-14	320.14	2.7E+24
6.8E-14	307.63	2.8E+24
6.9E-14	291.27	2.9E+24
7.0E-14	274.23	3.0E+24
7.1E-14	256.34	3.1E+24
7.2E-14	237.60	3.2E+24
7.3E-14	219.09	3.3E+24
7.4E-14	201.97	3.4E+24
7.5E-14	186.91	3.5E+24
7.6E-14	173.62	3.6E+24
7.7E-14	161.68	3.7E+24
7.8E-14	150.69	3.8E+24
7.9E-14	140.23	3.9E+24
8.0E-14	129.94	4.0E+24
8.1E-14	119.82	4.1E+24
8.2E-14	110.01	4.2E+24
8.3E-14	100.61	4.3E+24
8.4E-14	91.76	4.4E+24
8.5E-14	83.59	4.5E+24
8.6E-14	76.20	4.6E+24

Time (s)	T_e (eV)	N_e (cm^{-3})
8.7E-14	69.61	4.7E+24
8.8E-14	63.37	4.8E+24
8.9E-14	57.42	4.9E+24
9.0E-14	51.76	5.0E+24
9.1E-14	46.38	5.1E+24
9.2E-14	41.28	5.2E+24
9.3E-14	36.45	5.3E+24
9.4E-14	31.89	5.4E+24
9.5E-14	27.59	5.5E+24
9.6E-14	23.53	5.6E+24
9.7E-14	19.66	5.7E+24
9.8E-14	16.06	5.8E+24
9.9E-14	12.81	5.9E+24
1.0E-13	10.00	6.0E+24