The 13th Non-LTE Code Comparison Workshop

November 4-7, 2025

Institut Henri Poincare
Paris, France

Last update: Oct 10, 2025

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. To most directly compare kinetics codes, most cases are completely defined by a specification of the electron temperature, electron density, and (possibly) a radiation field. These cases are zero-dimensional and do not admit the possibility of plasma non-uniformity or boundary effects. For cases with a non-zero plasma size, the specified electron density is the spatially-averaged value (appropriate for use in a zero-dimensional calculation). In all cases, we assume that the plasma is electrically neutral, with the electron density and ion density connected through the condition of charge neutrality. Generally, there is no consideration of heavy-particle interactions.

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. The submission files should have the name of the codes and the contributor as the parts of the file names (e.g., nomad_ralchenko_case1.tgz). Please contact Yuri Ralchenko (email: *yralchen@umd.edu*) for information on file uploads when ready to submit.

Timeline:

1. **October 7 – submission deadline**
2. October 28 – online database available
3. November 4 – workshop opens
4. November 7 – workshop adjourns

I. STATEMENT OF CASES

We have selected several elements for cases that are inspired by ongoing or future experiments. Steady-state cases are specified by plasma temperature and density. Ion temperatures should be taken as identical to electron temperatures. In the following, temperatures and energies are given in eV, particle densities in cm^{-3}, mass density in g/cm^{-3}, radius in cm.

Element	Case ID	# of cases	Parameter	Grid		
Carbon	TDC	3	**T_e**	**1, 10, 100**		
			N_e	**10^{18}**		
			Time steps	**$t_0=0$, $t_1=10^{-12}$, $t_i=t_{i-1}*1.2$ ($i\leq80$)**		
			Initial condition	All population is in C^{6+}		
			Emission	**Range (eV)**	**Resolution (eV)**	**# of points**
			Spectrum (even **$i \geq 2$**, 40 spectra)	250-500	$\Delta\varepsilon = 0.025$	10001
Argon	TDAr	3	**T_e**	**10, 50, 250**		
			N_e	**2×10^{21}**		
			Time steps	**$t_0=0$, $t_1=10^{-15}$, $t_i=t_{i-1}*1.2$ ($i\leq80$)**		
			Initial condition	All population is in Ar^{18+}		
			Emission	**Range (eV)**	**Resolution (eV)**	**# of points**
			Spectrum (even **$i \geq 2$**, 40 spectra)	3000-5000	$\Delta\varepsilon = 0.2$	10001
Copper	Cu	18	**T_e**	**10, 30, 100**		
			ρ	**1, 8.96, 20**		
			f_2 (T_2=10 keV)	**10^{-4}**		
			Planckian at 3550 eV	**10^{-8}**		
			Emission	**Range (eV)**	**Resolution (eV)**	**# of points**
			Spectrum	8000-10000	$\Delta\varepsilon = 0.25$	8001
Krypton	Kr	8	**T_e**	**3000, 5000**		
			N_i	**3×10^{21}, 3×10^{22}**		
			Radius	**0, 10^{-4}**		
			Emission	**Range (eV)**	**Resolution (eV)**	**# of points**
			Spectrum	12000-18000	$\Delta\varepsilon = 1$	6001
Comment: spectrum to include also separate contributions from H- to B-like ions (more below)						
Xenon	Xe	3	**T_e**	**1000, 3000, 5000**		
			N_e	**10^{14}**		
			Emission	**Range (eV)**	**Resolution (eV)**	**# of points**
			Spectrum	3400-8400	$\Delta\varepsilon = 0.5$	10001

II. JUSTIFICATION OF CASES AND DETAILS

Each calculation shown in the preceding table will be referenced by a case name, which is to be given in the submission data file (described further below). The case name is constructed by appending a suffix to the Case_ID from the table. The suffix consists of between one and three digits. For instance, the Kr case for 5000 eV / 3×10^{21}cm^{-3} / 10^{-4} cm will be referred to as **Kr212**. Similarly, Ar case for 50 eV will be **TDAr2**. The Cu cases will have three-digit suffices – the third digit will be 1 for hot electrons or 2 for the diluted radiation field, e.g., **Cu211**.

The submissions file should be named as **<case>.<contributor_name>.<code_name>**, so that Dr. A. Einstein's calculations with his code GToE for one of the cases would be in the file `kr212.einstein.gtoe` (case insensitive).

1. Time-dependent C and Ar
TD-C (recombination from a bare ion) was at the very first NLTE workshop back in 1996 so we'd like to see the level of agreement reached since ~30 years ago. Nowadays the Beyond-EUV (or Blue-X) lithography researchers also discuss such recombination from bare nuclei for production of strong emission in Ly-α. As mentioned above, all population at time t=0 should be in the bare ion.

2. Steady-state Cu
K-shell fluorescence lines in transition metals are increasingly being considered as diagnostics for warm, near-solid-density plasmas created in implosions, compression experiments, and at X-ray free electron lasers. Line shifts and broadening due to ionization and density effects are of particular interest.

3. Steady-state Kr
This case follows up the optically-thin case for Kr from the previous workshop. In the present case, optical depths for the He-like resonance line will be on the order of 20-200. We hope to explore the competing effects of opacity and Stark broadening on the spectra and kinetics.

4. Steady-state Xe
L-shell Xe lines are planned to be used for diagnostics of magnetic fusion devices. However, M-shell W lines are also in the same spectral region which may hamper this diagnostics. While W spectroscopy has already been extensively explored at NLTE workshops, Xe has not been studied for some time.

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 IV, 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 *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 calculated spectral characteristics.

A relational database tool will be used to manage the data during the course of the workshop.

If necessary, additional clarification 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_S_coll> <f_S_photo> <f_S_auto>
                                <α_tot>  <f_α_coll> <f_α_photo> <f_α_auto>
...

ion                             <N_bound> <pop_frac> <nouter>
                                <S_tot> <f_S_coll> <f_S_photo> <f_S_auto>
                                <α_tot> <f_α_coll> <f_α_photo> <f_α_auto>


energy_levels           <count>
elev                            <N_bound> <level> <stwt> <energy> <population>
                                <Γ_tot> <f_Γ_collbb> <f_Γ_photobb> <f_Γ_collbf> <f_Γ_photobf> <f_Γ_auto>
                                <Θ_tot> <f_Θ_collbb> <f_Θ_photobb> <f_Θ_collbf> <f_Θ_photobf> <f_Θ_auto>
                                <occK> <occL> <occM>    ...          <nouter>
...
elev                            <N_bound> <level> <stwt> <energy> <population>
                                <Γ_tot> <f_Γ_collbb> <f_Γ_photobb> <f_Γ_collbf> <f_Γ_photobf> <f_Γ_auto>
                                <Θ_tot> <f_Θ_collbb> <f_Θ_photobb> <f_Θ_collbf> <f_Θ_photobf> <f_Θ_auto>
                                <occK> <occL> <occM>    ...          <nouter>
…
…
```

Spectrum Output

For the cases where we request spectra, the spectral information will be given in this same text file, following the information above. Note that all spectra are requested on an energy grid in format:

spectrum	**<case>**	**<count$_1$>**		
<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>**
. . . . .				
< energy N>	**<ε_{bb}N>**	**<ε_{bf}N>**	**<ε_{ff}N>**	**< ε_{tot}N>**

where energies are in eV and emission spectra **ε** for bound-bound (bb), bound-free (bf), and free-free (ff) transitions are in J/s/cm^3/eV for all cases except for Kr where same-type intensities in J/s/cm^2/eV are requested. The Kr cases should also have five extra columns with bb spectra for H-, He-, Li-, Be, and B-like ions (in that order left to right).

Importantly, the spectra for the time-dependent cases of C and Ar are requested only for the even values of the time index (excluding t=0), i.e., t_2, t_4… The ion/level data, however, should be provided for all times. This will unavoidably increase the file sizes but scp/sftp protocols can easily handle even multi-GB files.

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 description of N_i, for the cases other than Kr (see above) the electron and ion densities are to be related via the plasma neutrality condition, i.e., $N_i = N_e/Z$.

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 calculations will have a case identification of the form `Ge23` or the like (see Section III). 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.

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.
`time`	A value (e.g., zero) for steady-state cases.
`zbar`	Average charge of the plasma.
`m2`	Second central moment of the charge state distribution.
`m3`	Third central moment of the charge state distribution.
`eint`	Specific internal energy of the atom.

`pfn`	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: **J/s/cm^3**.

The **central moments** are defined as:

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

where y_j is the fractional population of ion stage j, q_j is the ion charge, and $\bar{Z}$ 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:

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

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 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$_{\text{total}}$**>.

Note that many of the "thermodynamic" quantities are intentionally sensitive to continuum lowering models. Quantities possibly affected are **<eint>** 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 be normalized to unity.

<nouter> The principal quantum number of the outermost electron for any state in this ion stage.

<S_{tot}> The total (effective) 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 (effective) 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 effective 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 effective rate out of the indicated ion into the more ionized ion. Similarly, <α_{tot}> is the total effective rate out of the indicated ion 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:

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

Units of **<S_{tot}>** and **<α_{tot}>** are 1/s.

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 population flux out** of this level. Units are 1/s.

<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}>**.

<Θ_{tot}> The **total population flux into** this level. For steady-state condition **<Θ_{tot}> = -<Γ_{tot}>.** Units are 1/s.

<**f_Θ$_{collBB}$**> The *fractional* contribution of electron collision excitation/de-excitation processes to <**Θ$_{tot}$**>.

<**f_Θ$_{photoBB}$**> The *fractional* contribution of bound-bound radiation processes to <**Θ$_{tot}$**>.

<**f_Θ$_{collBF}$**> The *fractional* contribution of electron collision ionization-recombination processes to <**Θ$_{tot}$**>.

<**f_Θ$_{photoBF}$**> The *fractional* contribution of photo-ionization-recombination to <**Θ$_{tot}$**>.

<**f_Θ$_{auto}$**> The *fractional* contribution of auto-ionization/dielectronic recombination processes to <**Θ$_{tot}$**>.

<**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.

Parameter **Γ** describes all processes originating from a particular level while **Θ** describes all processes ending on this level. The population flux is defined as a product of the population by the corresponding rate, so that, for instance, the total **Θ** for a level *i* is:

$$\Theta_i = \sum_j POP_j \times R_{ij},$$

where POP_j is the population of level *j* and R_{ij} is the rate of a physical process originating in level *j* and ending in level *i* (e.g., probability for a radiative transition from the upper level *j* into the lower level *i*).

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 are summarized below:

C, Ar, Cu, Xe

x-axis:	energy (in eV),
spectrum units:	J/s/cm^3/eV.

The spectra for the present optically thin cases are requested per unit volume.

Kr

x-axis:	energy (in eV),
spectrum units:	J/s/cm^2/eV.

The spectra for the optically thick Kr cases are requested per unit area.

The required data are bound-bound **<ε_{bb}>**, free-bound **<ε_{fb}>**, free-free **<ε_{ff}>** and total **<ε_{tot}>** spectra. The field <**count**> specifies the number of *(energy, spectra)* rows which follow.

The line broadening should be best-effort, especially for the Kr cases, including at least Doppler + natural broadening but also (if possible) collisional and Stark effects.

Example of a spectrum file for Kr (with extra columns for H-, He-… ions):

```
…
spectrum      Krl22         6001
12000         1.000e-15     1.000e-16     2.500e-15     3.600e-15     1.200e-15     …
12001         2.000e-15     2.000e-16     5.000e-15     7.200e-15     1.500e-15     …
…             …             …             …             …             …             …
18000         1.000e-15     1.000e-16     2.500e-15     3.600e-15     1.300e-15     …
```

For TD cases which require multiple spectra, the spectra should follow the corresponding ion/level data for specific times (parameter values below are completely arbitrary), for example:

```
……
plasma        2             1e18
time          0
…
spectrum      TDC2          10001
250.000       1.000e-15     1.000e-16     2.500e-15     3.600e-15
250.025       2.000e-15     2.000e-16     5.000e-15     7.200e-15
…             …             …             …             …
500.000       1.000e-15     1.000e-16     2.500e-15     3.600e-15
……
plasma        2             1e18
time          1.0e-12
…
<NO SPECTRUM FOR AN ODD TIME STEP>
……
plasma        2             1e18
time          1.2e-12
…
spectrum      TDC2          10001
250.000       1.000e-15     1.000e-16     2.500e-15     3.600e-15
250.025       2.000e-15     2.000e-16     5.000e-15     7.200e-15
…             …             …             …             …
500.000       1.000e-15     1.000e-16     2.500e-15     3.600e-15
……
```