Code Comparison for Sn LPP

October 26, 2021

Submission of Calculations

This document is intended to define the particulars of the workshop submissions. In the sections below we will define the test problems, the comparison quantities which we require and the detailed format of the data files that we will be expecting. The test problems include a set of zero-dimensional cases focused on the atomic kinetics of tin, a time-independent one-dimensional problem for tin radiation transport with an optional time-dependent evolution, and a time-dependent one-dimensional problem involving laser absorption in a tin plasma.

The zero-dimensional atomic kinetics cases are completely defined by a specification of the electron temperature, electron density, and radiation temperature. 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, and that the ion temperature is the same as the electron temperature.

The webpage of the meeting is at https://www.euvlitho.com/. The submission files for Problems 1, 2a and 2b are to be sent to Yuri Ralchenko. Please contact him at yuri.ralchenko@nist.gov for instructions for on submitting these files. Submission files for Problem 3 should be emailed to vivek.bakshi@euvlitho.com. 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 code as part of the file names (e.g. cretin_Sn132.tgz).

Timeline:

October 17 – submission deadline
October 26 – workshop

TEST PROBLEM 1 – ATOMIC KINETICS

These cases are designed to investigate the atomic kinetics of Sn under conditions relevant for EUV production. They are steady-state cases specified by electron temperature, mass density, and radiation temperature. The radiation field for each case should be a Planckian at the given radiation temperature. Ion temperatures should be taken as identical to electron temperatures.

Requested output quantities include gross plasma parameters, the charge state distribution, information on level populations and rates, and emission and absorption coefficients over a specified radiation wavelength range. The number and distribution of wavelengths over this range is not specified, and can be chosen by the participant for each submission to provide adequate resolution of the resulting spectral features.

Note that since the cases are now specified for a given mass density, some of the output quantities are now requested per gram of material rather than per cm^3. Quantities and units which have changed from the previous workshop are listed in red.

The case material temperatures (in eV), mass densities (in g/cm^3), and radiation temperatures (in eV) are given in the following table:

T_e	10, 15, 20 , 25 , 30 , 35 , 40 , 45 , 50
ρ	0.0002 , 0.002 , 0.02
T_r	0 , 20 , 40

SUBMISSION FILE DESCRIPTION – ATOMIC KINETICS

Each 0D 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 **Sn**. The suffix consists of three digits, with the first corresponding to the electron temperature, the second to the mass density, and the third to the radiation temperature. Thus the case with T_e = 30 eV, ρ = 0.0002 g/cm^3 , and T_r = 20 eV will be referred to as **Sn512**.

The submissions file should be named as **<case>.<code_name>**, so that calculations with the code WAG for one of the cases would be in the file `sn312.wag` (case insensitive).

The submissions file for this problem has been patterned after that used by the NLTE Code Comparison Workshops. The data requested here is a subset of the data requested for those files with the sole exception of the integrated spectra under the **`purity`** keyword. Codes are now encouraged to submit a full NLTE workshop file, plus the integrated spectra, as we will have use of the same database to manage the data during the workshop. Note that the units of the spectra and a few other quantities are different than those used for the NLTE workshop.

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 the next section, 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. 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. The exact definitions of the quantities requested, including units, are given later in this document.

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.

> The *initial section* provides general problem identification information. This section begins with the keyword `data`. The keywords after `data` may appear in any order.
>
> The *second section* gives overall quantities describing the plasma population and energy distribution. This section begins with the keyword `summary_quantities`. The keywords after `summary_quantities` may appear in any order.
>
> 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`. 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.

SUBMISSION FILE FORMAT

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

```
data                    <user comment... >
case                    <case_id>
code                    <name>


summary_quantities
plasma                  <Te>  <Ne> <ρ> <Tr>
zbar                    <zbar>
m2                      <2nd central moment>
m3                      <3rd central moment>
emat                    <energy density>
dedt                    <specific heat>
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

The spectral information will be given in this same text file, following the information above. Note that all spectra are requested on a wavelength grid in format:

purity	**<P_{band}>**	**<P_{tot}>**	**< P_{frac} >**
spectrum	<case>	**<count>**	
< λ1 >	**< η1 >**		
< λ2>	**< η2 >**		
.....			
< λN>	**< ηN >**		
absorption	<case>	**<$count_1$>**	
< λ1>	**< α1 >**		
< λ2>	**< α2 >**		
.....			
< λN>	**< αN >**		

where wavelengths are in nm, emission coefficients η are in erg/s/cm^3/nm/ster and absorption coefficients α are in 1/cm.

DEFINITIONS OF REQUESTED QUANTITIES

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

`data`	Calculation identifier and user comment line. Comment should be limited to this one line only and might include the contributor's name, institution, the version of the code, and the date at which calculation was run or any other relevant information.
`case`	All calculations will have a case identification of the form `Sn312` or the like (see problem description).
`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.

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 and radiation temperatures are in units of eV. The electron density is in units of cm^{-3}. The mass density is in units of g/cm^3.
`zbar`	Average charge of the plasma.
`m2`	Second central moment of the charge state distribution.
`m3`	Third central moment of the charge state distribution.
`emat`	Energy density of the plasma. Units: **erg/g**.
`dedt`	Specific heat of the plasma. Units: **erg/eV/g**.
`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: $erg/cm^3/sec$.

The **central moments** are defined as:

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

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 **energy density** of the plasma includes both the kinetic energy of the free particles (electrons and ions) plus the internal energy of the bound electrons, with the internal energy E_{int} being the sum of level populations, n_j, multiplied by their energy value, E_j:

$$E = \left\{ \frac{3}{2}\left(n_e + n_i\right)kT + \sum_j E_j n_j \right\} \Big/ \rho$$

The energy reference for the internal energy 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 may need zero point shifts. Units are erg/g.

The **specific heat** is the derivative with respect to temperature of the energy density of the plasma, taken at fixed mass density. Units are erg/eV/g. 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.

For **power loss**, the total is the most important quantity, so that if one does not separate different contributions, then it would suffice to have zeros in fields other than **<P$_{total}$>**.

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:

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

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 population flux out** of this level. 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}>**.

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

<f_Θ_{collBB}> The *fractional* contribution of electron collision excitation/de-excitation processes to **<Θ_{tot}>**.

<f_$\Theta_{photoBB}$> 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_$\Theta_{photoBF}$> 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:

`purity` The integrated spectral emission: bandpass, total, spectral purity
Units: **erg/sec/cm^3** and **none**.

For **purity**, the first two values requested are the emission integrated over the **13.15 - 13.85** nm bandpass, and over the total spectral range of 5-20 nm, while the spectral purity is defined as the ratio of these two quantities. The units here are not particularly relevant, but using the same units as for **power loss** gives an indication of how much emission is not included in the spectral range of 5-20 nm. Note that we are using a bandpass of ~5% for this workshop rather than the usual 2% bandpass to obtain more meaningful comparisons between codes.

`spectrum`	caseID	count	
	column 1:		wavelength (nm),
	column 2:		emissivity (erg/s/cm^3/nm/ster);
`absorption`	caseID	count	
	column 1:		wavelength (nm),
	column 2:		absorption coefficient (cm^{-1});

Example of a spectrum section:

```
Purity        1.000e+20     1.000e+21     1.000e-01

spectrum      Sn512         1501
5.000         5.000e+18
5.010         5.100e+18
…             …
20.000        2.000e+18
```

```
absorption    Sn512         1501
5.000         2.000e+01
5.010         2.100e+01
…             …
20.000        2.000e+02
```

TEST PROBLEM 2a – 1D STEADY-STATE RADIATION TRANSPORT

This steady-state problem is designed to investigate radiation transport through a uniform sphere of Sn plasma. The plasma temperature (for both electrons and ions) is set to **25 eV**, while the mass density, sphere radius, and problem ID are specified in the following table:

ID	SSR1	SSR2	SSR3	SSR4
ρ	0.0002 g/cm^3	0.0002 g/cm^3	0.02 g/cm^3	0.02 g/cm^3
R	100.0 μm	1000. μm	1. μm	10. μm

The goal of this problem is to obtain a self-consistent radiation field and material properties throughout the sphere under the assumption of steady-state NLTE conditions with the boundary condition that radiation escapes freely from the surface of the sphere.

Requested output quantities include gross plasma parameters, the charge state distribution, and emission and absorption coefficients plus the radiated power distribution over the specified wavelength range of 5-20 nm. Spectral data over this range should be submitted at 301 wavelengths, equally spaced at a resolution of 0.05 nm. Information on radiation or radiative properties outside this range is not requested, and these wavelengths can be chosen by the participant.

SUBMISSION FILE DESCRIPTION – RADIATION TRANSPORT

The submission files for test problems 2a and 2b are largely a subset of the submission file for test problem 1, and any of these quantities may be included. Additional quantities in the `summary_quantities` section for each data set identify the spatial position and time, and the radiation flux is requested as an additional in the `spectrum` section. The recommended submission set is described below.

Multiple submission files are to be used for each case, with each file corresponding to a spatial position *r*. Output is requested at the following 11 positions:

r/R = [0., 0.33, 0.55, 0.70, 0.80, 0.88, 0.92, 0.95, 0.975, 0.99, 1.0]

These positions do not specify the spatial zoning to be used, but should provide sufficient spatial resolution to determine zoning if desired.

The case names are defined in the above table for Case_ID **SSR**.

Results are requested in a separate submission file for each of the zones identified above. The submissions file should be named as **<case>.<zone #>.<code_name>**, so that calculations with the code WAG for the case defined as SSR2 would be in the files `SSR2.N.wag`, where N is an integer varying from 1 to 11.

DEFINITIONS OF REQUESTED QUANTITIES

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

`data`	Calculation identifier and user comment line. Comment should be limited to this one line only and might include the contributor's name, institution, the version of the code, and the date at which calculation was run or any other relevant information.
`case`	All calculations will have a case identification of the form SSR2 or the like (see problem description).
`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.

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 and radiation temperatures are in units of eV. The electron density is in units of cm^{-3}. The mass density is in units of g/cm^3. The radiation temperature is optional, and should measure the energy density of the radiation $E_{rad} = aT_r^4$.
`time`	Problem time in units of ns (ignored if steady-state).
`r`	Data position in units of μm (ignored if 0D).
`zbar`	Average charge of the plasma.
`m2`	Second central moment of the charge state distribution.
`m3`	Third central moment of the charge state distribution.
`emat`	Energy density of the plasma.
`dedt`	Specific heat of the plasma.
`pfn`	Partition function of the atom.
`nmax_eff`	For this calculation, the principal quantum number of the outermost electron in any bound state.
`ploss`	The radiative power losses: bound-bound, bound-free, free-free, and total. Units: **erg/sec/cm^3**.

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.

Section 4, the `energy_levels` section, is not requested for these cases.

In *section 5*, the `spectrum` section, the data requested are summarized below:

`purity` The integrated spectral power: bandpass, total, spectral purity
Units: **erg/sec** and **none**.

For `purity`, the first two values requested are the spectral power integrated over the 13.15-13.85 nm bandpass, and over the total spectral range of 5-20 nm, while the spectral purity is defined as the ratio of these two quantities. The spectral power, P_ν, requested in `power` and integrated over wavelength in `purity`, is defined as the net flux at position r integrated over the spherical area at that position. At the outermost radius, this gives the total power radiated by the sphere.

$$P_\nu = 4\pi r^2 F_\nu \ , \ F_\nu = \oint \hat{\mathbf{n}} \bullet \hat{\Omega}\, I_\nu(\theta,\phi)\, d\Omega$$

`spectrum`	case	count	
	column 1:		wavelength (nm),
	column 2:		emissivity (erg/s/cm^3/nm/ster);
`absorption`	case	count	
	column 1:		wavelength (nm),
	column 2:		absorption coefficient (cm^{-1});
`power`	case	count	
	column 1:		wavelength (nm),
	column 2:		radiated power (erg/s/nm);

TEST PROBLEM 2b – 1D TIME-DEPENDENT RADIATION TRANSPORT

This time-dependent problem is designed to investigate radiative cooling of a uniform sphere of Sn plasma. The plasma temperature (for both electrons and ions) is initially set to **50 eV**, while the mass density, sphere radius, and problem ID are specified in the following table, which is the same as the table from Problem 2a with the addition of a timescale Δt:

ID	TDR1	TDR2	TDR3	TDR4
ρ	0.0002 g/cm^3	0.0002 g/cm^3	0.02 g/cm^3	0.02 g/cm^3
R	100.0 μm	1000. μm	1. μm	10. μm
Δt	1.0 ns	1.0 ns	0.5 ns	0.5 ns

The goal of this problem is to obtain a self-consistent radiation field, plasma temperature and material properties throughout the sphere as a function of time as the plasma cools over the time interval Δt. The initial values are obtained in the same manner as Problem 2a, but with a higher temperature. The initial radiation field should be calculated as consistent with material properties under the assumption of steady-state NLTE conditions, while the time evolution will use radiation transfer and time-dependent atomic kinetics. Hydrodynamics and thermal conduction are not included, so the plasma cools radiatively with radiation escaping through the surface of the sphere. Electron and ion temperatures are assumed to be closely coupled and always have the same values.

The submission files for this problem are the same as for Problem 2a, but output in each file is requested at times (equal or close to)

t = [0., 0.05, 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1.0] Δt

The case names are defined in the above table for Case_ID **TDR**.

The case name is constructed with the designated ID from the above table, so that calculations with the code WAG for the case defined as TDR2 would be in the files `TDR2.N.wag`, where N is an integer varying from 1 through 11.

TEST PROBLEM 3 – 1D TIME-DEPENDENT LASER ABSORPTION

This time-dependent problem is designed to investigate the evolution of a Sn plasma due to laser absorption. The initial plasma temperature and mass density are specified, with the ionization obtained under the assumption of LTE. The plasma can gain energy through laser absorption and lose energy by radiating, while the plasma temperature and ionization change. Laser interaction with the plasma should be modeled with inverse bremsstrahlung absorption only. Hydrodynamics, thermal conduction and radiation transport are not to be included in these calculations. Radiated energy is immediately lost from the system. The electron and ion temperatures are assumed to be the same at all times, i.e. the electron-ion coupling is assumed to be very large. The electron number density is obtained by evolving the ionization balance in time using NLTE atomic kinetics of the Sn.

The three cases defined here differ in the laser wavelength:

case 1 : λ = 1.064 μm (Nd:YAG)
case 2 : λ = 1.88 μm (Th)
case 3 : λ = 10.6 μm (CO_2)

The plasma geometry is one-dimensional planar geometry, with the computational domain defined over $x \in [0. , X]$, where X is given in the table defining the case parameters. The spatial mesh to be used consists of 100 equally-spaced zones over the computational domain. The mass density ρ varies with position as

$$\rho = \rho_0 \left(1 - \frac{x}{X} \right)^2$$

The laser is incident at x = X at normal incidence. The incident laser power P is constant over the problem duration of Δt.

The following table contains the parameters defining the problem for each case. The initial temperature for all cases is T = 10 eV. The case_ID is TDL.

ID	TDL1	TDL2	TDL3
λ	1.064 μm	1.88 μm	10.6 μm
ρ_0	0.03 g/cm^3	0.01 g/cm^3	0.0003 g/cm^3
X	10. μm	100. μm	1000. μm
P	5x10^{10} W/cm^2	5x10^{10} W/cm^2	10^{10} W/cm^2
Δt	0.4 ns	0.4 ns	4.0 ns

The case name is constructed using the designated ID from the above table, so that calculations for the case defined as TDL2 with the code WAG would be in the file `TDL2.wag`.

Requested output quantities include spatial profiles of the laser power deposited (per unit length) into the plasma, and plasma quantities such as temperature and ionization as a function of space and time.

SUBMISSION FILE DESCRIPTION – LASER ABSORPTION

This submissions file is structured in 3 sections, identified by keywords. The 2nd and 3rd sections contain the input and output spatial profiles, formatted as 3 or more columns.

> The *initial section* provides general problem identification information. This section begins with the keyword `data`. The keywords after `data` may appear in any order.
>
> The *second section* gives spatial profiles of plasma properties. This section begins with the keyword `profiles`, followed by **count**, the number of spatial points, and **time**, the problem time in ns.
>
> The *third section* gives spatial profiles related to laser absorption. This section begins with the keyword `laser`, also followed by **count** and **time**.

SUBMISSION FILE FORMAT – LASER ABSORPTION

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

```
data              <user comment... >
case              <case_id>
code              <name>


profiles      <count>          <time1>
< x1 >            < Te1 >      < Ne1 >      [ < α1 > ]     [ < Λ1 > ]     [ < Cv1 > ]     [ < P1 > ]
< x2 >            < Te2 >      < Ne2 >      [ < α2 > ]     [ < Λ2 > ]     [ < Cv2 > ]     [ < P2 > ]
...........
< xN>             < TeN >      < NeN >      [ < αN > ]     [ < ΛN > ]     [ < CvN > ]     [ < PN > ]

laser         <count>          <time1>
< x1 >            < E1 >       < I1 >|
< x2 >            < E2 >       < I2 >
...........
< xN>             < EN >       < IN >

profiles          <count>      <time2>
< x1 >            < Te1 >      < Ne1 >      [ < α1 > ]     [ < Λ1 > ]     [ < Cv1 > ]     [ < P1 > ]
< x2 >            < Te2 >      < Ne2 >      [ < α2 > ]     [ < Λ2 > ]     [ < Cv2 > ]     [ < P2 > ]
...........
< xN>             < TeN >      < NeN >      [ < αN > ]     [ < ΛN > ]     [ < CvN > ]     [ < PN > ]

laser             <count>      <time2>
< x1 >            < E1 >       < I1 >
```

```
< x2 >              < E2 >          < I2 >
...........
< xN>               < EN >          < IN >


                                    ...


profiles            <count>         <time11>
< x1 >              < Te1 >         < Ne1 >         [ < α1 > ]      [ < Λ1 > ]      [ < Cv1 > ]     [ < P1 > ]
< x2 >              < Te2 >         < Ne2 >         [ < α2 > ]      [ < Λ2 > ]      [ < Cv2 > ]     [ < P2 > ]
...........
< xN>               < TeN >         < NeN >         [ < αN > ]      [ < ΛN > ]      [ < CvN > ]     [ < PN > ]

laser               <count>         <time11>
< x1 >              < E1 >          < I1 >
< x2 >              < E2 >          < I2 >
...........
< xN>               < EN >          < IN >
```

DEFINITIONS OF REQUESTED QUANTITIES

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

`data`	Calculation identifier and user comment line. Comment should be limited to this one line only and might include the contributor's name, institution, the version of the code, and the date at which calculation was run or any other relevant information.
`case`	All calculations for this problem should use case identification TDL1 for a laser wavelength of 1.064 μm, TDL2 for a laser wavelength of 1.88 μm, and TDL3 for a laser wavelength of 10.6 μm.
`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.

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

column 1:	**x** : position (in μm)
column 2:	**T** : plasma temperature (eV)
column 3:	$\mathbf{N_e}$: electron density (cm^{-3})
column 4:	**α** : absorption coefficient (cm^{-1})
column 5:	**Λ** : e-i Coulomb logarithm
column 6:	$\mathbf{C_v}$: specific heat (erg/eV/g)
column 7:	**P** : radiative power loss (erg/g/s)

The positions to be used when reporting results is the upper boundary of that spatial zone, e.g. a first zone from 0 - 0.1 μm should be reported at $x = 0.1$.

The quantities requested in columns 4-7 are optional (but recommended). Since the data are interpreted according to the column number, any field which is omitted must have a placeholder (suggested: 0) if a later field is intended to be meaningful.

The quantity α in column 4 is the inverse bremsstrahlung absorption coefficient for the laser photons (*not* corrected for the index of refraction).

Spatial profiles are requested at times (equal or close to)

$t = [\ 0., 0.05, 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1.0]\ \Delta t$

In *section 3*, the following items are requested:

column 1:	x : position (in μm)
column 2:	E : deposited power (erg/g/s)
column 3:	I : total laser power density (W/cm^2)

The laser power density here is the laser intensity in the absence of the swelling factor, i.e. intensity x n^2 where n is the real part of the index of refraction. When reporting the laser power density profiles, a submission should list the *total* power density (incident + reflected rays) in column 3.

Example of a profiles section:

```
profiles      100          0.0
0.10          1.000e+01    6.000e+20    1.000e+04    2.0    3.000e+11    1.000e+03
0.20          1.000e+01    5.800e+20    1.000e+04    2.0    2.900e+11    0.990e+03
…             …
10.0          1.000e+01    0.000e+00    0.000e+00    2.0    0.000e+00    0.000e+00
```

Example of a laser section:

```
laser         100          0.0
0.1           1.000e+03    1.000e+09
0.2           1.000e+03    1.000e+09
…             …
10.0          1.000e-03    5.000e+10
```