Code Comparison for Sn LPP

November 3, 2020

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 looking at laser absorption in a simple plasma, and an optional time-dependent one-dimensional problem involving laser absorption in a hydrogen plasma.

The zero-dimensional atomic kinetics cases are completely defined by a specification of the electron temperature and electron density. 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 are to be email 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_Sn22.tgz).

Timeline:

October 28 – submission deadline
November 3 – workshop

I. TEST PROBLEM DESCRIPTION – 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 solely by electron temperature and density, with no extant radiation field. Ion temperatures should be taken as identical to electron temperatures.

Requested output quantities include gross plasma parameters, the charge state distribution, 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.

The case temperatures and electron densities are given in the follow tables, along with case IDs:

ID	1	2	3	4	5	6	7
$\mathbf{T_e}$	10	15	20	25	30	35	40
$\mathbf{N_e}$	10^{19}						

ID	8	9	10	11	12	13	14	15	16
$\mathbf{T_e}$	20	25	30	35	40	45	50	55	60
$\mathbf{N_e}$	10^{20}								

ID	17	18	19	20	21	22	23	24	25
$\mathbf{T_e}$	20	25	30	35	40	45	50	55	60
$\mathbf{N_e}$	10^{21}								

II. SUBMISSION FILE DESCRIPTION – ATOMIC KINETICS

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 welcome to submit a full NLTE workshop file, with the addition of the integrated spectra, but note that the units of the spectra and a few other quantities are different.

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 4 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 `plasma`. The keywords after `plasma` 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.
>
> Finally, the *fourth section* contains calculated spectral characteristics.

III. SUBMISSION FILE FORMAT

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

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


plasma              <Te>  <Ne>
zbar                <zbar>
eint                <internal_energy>
ploss               <Pbb>  <Pbf>  <Pff>  <Ptotal>


ion_stages          <count>
                        <Nbound>  <pop_frac>
                        <Nbound>  <pop_frac>
...
```

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              <Pband>      <Ptot>       < Pfrac >      [ λmin   λmax ]

spectrum            <count>
< λ1 >              < η1 >
< λ2>               < η2 >
...........
< λN>               < ηN >

absorption          <count1>
< 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.

IV. 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 `Sn12` or the like (see Section I).

`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 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.

`zbar` Average charge of the plasma.

`eint` Specific internal energy of the atom.

`ploss` The radiative power losses: bound-bound, bound-free, free-free, and total. Units: **erg/sec/cm^3**.

The **specific internal energy** is the sum of level populations, n_j, multiplied by their energy value, E_j:

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

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 may need zero point shifts. Units are ergs/cm^3.

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

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.

In *section 4*, 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**.

[Optional] : minimum / maximum bandpass limits
Units: **nm**

For **purity**, the first two values requested are the emission integrated over the bandpass, 13.365-13.635 nm, and the total spectral range, 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. The relevant bandpass for the atomic data used for a submission may be different than that designated here. If so, the minimum and maximum limits of the bandpass can be listed after the spectral purity.

`spectrum`
column 1: wavelength (nm),
column 2: emissivity (erg/s/cm^3/nm/ster);

`absorption`
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      1501
5.000         5.000e+18
5.010         5.100e+18
…             …
20.000        2.000e+18


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

V. TEST PROBLEM DESCRIPTION – 1D LASER ABSORPTION

This steady-state setup is designed to investigate laser absorption in a well-defined plasma. The plasma parameters - temperature, density, <Z> - are specified and do not change in time. Laser interaction with the plasma should be modeled with inverse bremsstrahlung absorption only.

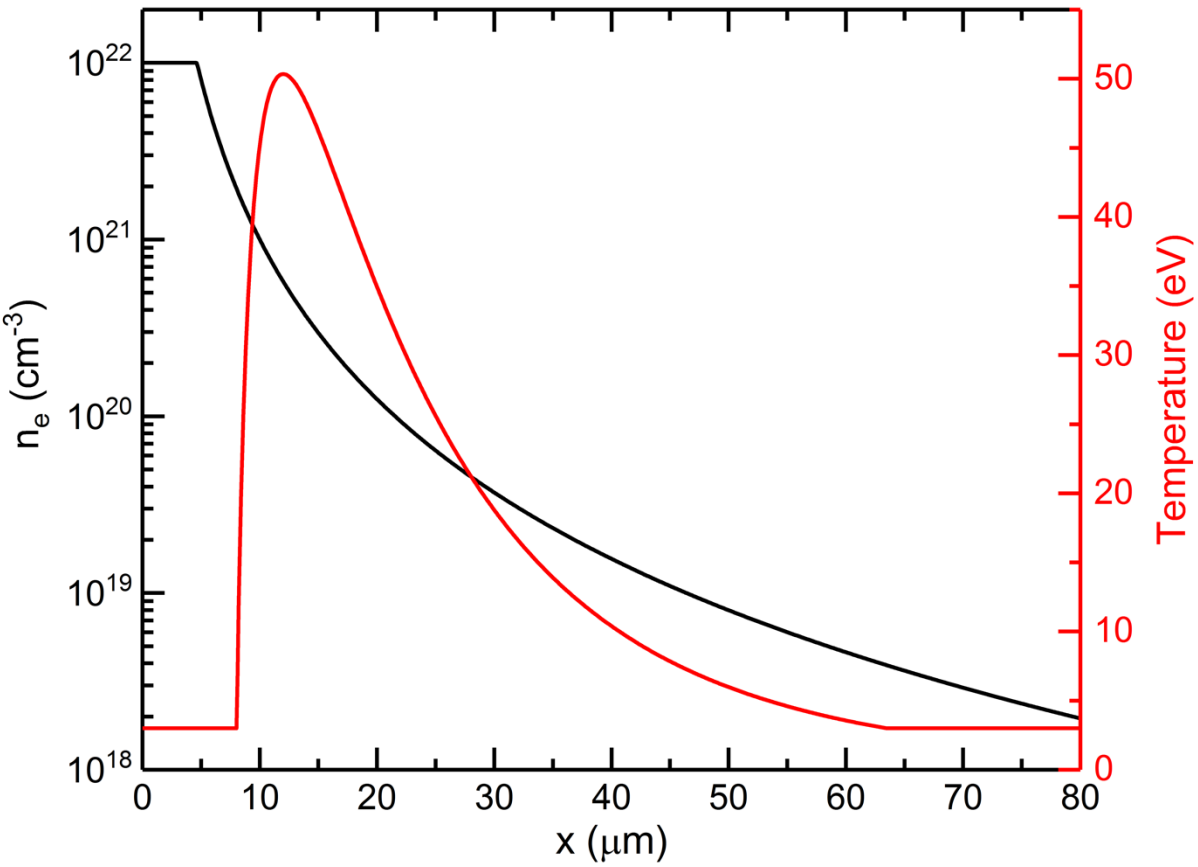
The plasma geometry is one-dimensional planar geometry, with the computational domain defined over $x \in [0.\,, 300.]$ μm.

The temperature and number density of the plasma are given by

$$N_e = \min\left(10^{22}, \frac{10^{24}}{x^3}\right) cm^{-3}$$

$$T_e = \max\left[3, 93\, y \exp(-y^{1/2})\right] eV \quad , \quad y = \max(0, x-8)$$

where x is measured in μm. The figure below illustrates these profiles (out to x = 80 μm).



The plasma consists of fully-ionized hydrogen, so the given number density specifies both the electron and ion densities. If it is not possible to specify the conditions and ionization state separately for a code, the number density can be taken to specify the density of atomic hydrogen with the ionization obtained under LTE conditions.

The spatial mesh to be used consists of 20000 equally-spaced zones over the computational domain.

The laser is incident at x = 300 μm with normal incidence. The incident laser power for all cases is 10^{11} W/cm^2.

The two cases defined here differ only in the laser wavelength:

case 1 : laser wavelength = 1.064 μm (Nd:YAG)
case 2 : laser wavelength = 10.6 μm (CO_2)

Requested output quantities include spatial profiles of the laser power deposited (per unit length) into the plasma, and the laser power density.

VI. 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`.

The *third section* gives spatial profiles related to laser absorption. This section begins with the keyword `laser`.

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

laser         <count>
< x1 >              < E1 >        < I1 >        [ < I1+ > ]
< x2 >              < E2 >        < I2 >        [ < I2+ > ]
...........
< xN>               < EN >        < IN >        [ < IN+ > ]
```

VII. 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 `LaserSS1` for a laser wavelength of 1.064 μm and `LaserSS2` 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})
[optional]	column 4:	α : absorption coefficient (cm^{-1})
[optional]	column 5:	Λ : e-i Coulomb logarithm
[optional]	column 6:	**Cv** : specific heat ($ergs/eV/cm^3$)
[optional]	column 7:	**P** : radiative power loss ($ergs/s/cm^3$)

The positions to be used when reporting results is the upper boundary of that spatial zone, e.g. the first zone from 0 - 0.015 μm should be reported at $x = 0.015$.

The quantities requested in columns 4-7 are optional. 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 specific heat and radiative power loss are of more interest in the time-dependent test problem, but are described here along with the other quantities in this section.

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

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

	column 1:	x : position (in μm)
	column 2:	E : deposited power (W/cm^3)
	column 3:	I : total laser power density (W/cm^2)
[optional]	column 4:	I+ : laser power density for reflected ray (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. As an option, the power density in the reflected ray can be listed separately in column 4.

Example of a profiles section:

```
profiles      20000
0.015         3.000e+00    1.000e+22    5.000e+06    2.0
0.030         3.000e+00    1.100e+22    5.000e+06    2.0
…             …
300.0         3.000e+00    3.704e+16    2.000e-04    2.0
```

Example of a laser section:

```
laser         20000
0.015         0.000e+00    0.000e+00
0.030         0.000e+00    0.000e+00
…             …
300.0         2.000e+02    1.200e+18
```

Optional format with ***I*** and ***I+***

```
laser         20000
0.015         0.000e+00    0.000e+00    0.000e+00
0.030         0.000e+00    0.000e+00    0.000e+00
…             …
300.0         2.000e+02    1.200e+18    2.000e+17
```

VIII. BONUS PROBLEM DESCRIPTION – TIME-DEPENDENT LASER ABSORPTION

This setup is designed to investigate the evolution of a simple plasma due to laser absorption. The initial plasma temperature and density are specified. The intention here is to combine the physics of the previous two problems with a minimal amount of other physics. 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 hydrogen.

The plasma composition, geometry and computational mesh are identical to those used for the steady-state laser absorption test problem. The density specification is also the same, but specifies the number density of hydrogen atoms, and this quantity remains fixed throughout the time evolution. The initial temperature is set to T = 1 eV everywhere in the computational domain.

The submissions file for these cases is very similar to those for the steady-state laser absorption cases. The same information is requested, but spatial profiles are requested for a number of different times, with the time appearing as an additional field on the keyword line.

Changes from the steady-state requested quantities:

`case` All calculations for this problem should use case identification `LaserTD1` for a laser wavelength of 1.064 μm and `LaserTD2` for a laser wavelength of 10.6 μm.

`time` problem time (ns)

The temporal extent of this problem for the 1.064 μm wavelength is $t \in [0.,1.]$ ns, with the incident laser power fixed at 10^{11} W/cm^2 throughout this interval. Spatial profiles are requested at intervals of 0.1 ns, at times given by

t = [0., 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0] ns

The evolution for the 10.6 μm wavelength occurs faster, so the corresponding temporal extent for this case is $t \in [0.,0.1]$ ns, with profiles requested at intervals of 0.01 ns, at times given by

t = [0., 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.1] ns

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 >       [ < I1+ > ]
< x2 >            < E2 >       < I2 >       [ < I2+ > ]
...........
< xN>             < EN >       < IN >       [ < 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 >       [ < I1+ > ]
< x2 >            < E2 >       < I2 >       [ < I2+ > ]
...........
< xN>             < EN >       < IN >       [ < 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 >       [ < I1+ > ]
< x2 >            < E2 >       < I2 >       [ < I2+ > ]
...........
< xN>             < EN >       < IN >       [ < IN+ > ]
```