Simulation of x-ray burst from NIF target

We present the code written for interpretation of x-ray spectrograms from NIF experiments. This code follows prescribed thermodynamic scenario expected for three zones of a target. While advancing along the time, the code computes spectral power radiated by the target, a sequence of spectrograms (frames) at required times, time-integrated spectrogram.

I. Advantages of the code

A. The code is written for a mix of 2 - 4 chemical elements or isotopes. 1-3 of them are isotopes of light elements (H, …, Ne). The last one is a much-heavier dopant for x-ray spectroscopy (e.g. Ge, Kr). For each spatial zone, a user can choose another ratio of the elements, including a time-dependent ratio for simulation of mass transfer.

B. We derived and use expression for the lowering of ionization energy of ions in plasmas of any chemical composition.

C. The code simulates radiation of plasmas with any prescribed distribution of free electrons over energy, $f(\varepsilon_e, t)$. The possibility of choosing arbitrary $f(\varepsilon_e, t)$ enables (i) analysis of plasma response to the laser irradiation and/or generation of electron beam, (ii) comparison of spectrograms (frames) computed with different $f(\varepsilon_e, t)$.

D. The code does not assume any type of equilibrium, therefore remains correct for arbitrarily fast increase/decrease in parameters and $f(\varepsilon_e, t)$. Moreover, present non-CRE code can show the time required for plasma relaxation to CRE at any constant parameters of interest.

E. The code can be converted in non-CRE post-processor of hydrodynamic simulations. This post-processor will compute spectral power radiated from the target, a sequence of spectrograms (frames) at requested times, time-integrated spectrogram.

II. The model and the code

We model the target using N > 2 identical spheric bright sources (**BS**s) randomly distributed in spheric **core** surrounded by plasma **capsule**. Within each of these **zones** plasma in uniform. Radius of BS is denoted $\mathbf{R_1}$, radius of the core $\mathbf{R_2 \gg R_1}$. The capsule is spheric layer with inner radius R_2 , outer radius R_3. All zones affect each other by **radiation**. Upper limit on N is defined by requirement of long mean distance between BSs; here we require typical size of the core volume per one BS, $R_2 (4\pi/3N)^{1/3}$, bigger than $10\, R_1$; this gives

$$\mathbf{N < (4\pi/3)\,[R_2/(10\,R_1)]^3}\ . \qquad \text{(II. 1)}$$

Each zone contains 1-3 isotopes of light chemical elements (e.g., any 1-3 of H, D, T, He, …, Ne) and one chemical element for spectroscopy at the photon energy hν » 1 keV (e.g. Kr, Ge). This element is **denoted X**. Diagnostic at hν » 1 keV restricts the electron temperature of interest, $T_{e,b}\,(t)$, to

$$\mathbf{T_{e,b}\,(t) \gg 100\ eV}\ , \qquad \text{(II. 2)}$$

subscript $\boldsymbol{b}$ **= 1, 2, 3** denotes BSs, core, capsule, respectively. Each of these three zones is characterized with **time-dependent**

(i) **ion number densities** (e.g. $n_{D,b}$, $n_{He,b}$, $n_{C,b}$, $n_{X,b}$). The units are [cm^{-3}]. A user can replace D, He, C with H, T or isotopes of other light elements, as explained in Section IV.

(ii) **distribution f_b of free electrons over their energy** ε_e [eV]. The code has no restrictions on $f_b(\varepsilon_e)$, except normalization to the under-shape area = 1 and units [eV^{-1}]. Function $f_b(\varepsilon_e)$ is prescribed in "*function EED(eeV)*" in the source file **Code2.for**. The possibility of using arbitrary $f_b(\varepsilon_e, t)$ is unique advantage of present code (*see point C in page 1*). For this advantage, transitions caused by electron-ion collisions are given **by cross-**

sections (*not by commonly used maxwellian rates*). The cross-sections are computed using Flexible Atomic Code (FAC) **[1]**. In demo version of the code, function $f_b(\varepsilon_e, t)$ consists of maxwellian and beam parts:

$$f_b(\varepsilon_e) = (1 - \xi_b)\, f_{\mathrm{Maxw}}(\varepsilon_e, T_{e,b}) + \xi_b\, f_{\mathrm{beam}}(\varepsilon_e, \varepsilon_{e,c,b}, \varepsilon_{e,w,b}) \quad [\mathrm{eV}^{-1}] \qquad \text{(II. 3)}$$

where $f_{\mathrm{Maxw}}(\varepsilon_e, T_{e,b})$ is Maxwell distribution at $T_{e,b}$; parameter ξ_b **is the beam part** of local number density of free electrons; density; $f_{\mathrm{beam}}(\varepsilon_e, \ldots)$ is the shape of electron beam. In demo version of the code this shape is rectangular; $\varepsilon_{e,c,b}$, $\varepsilon_{e,w,b}$ [eV] are central energy and the width of the e-beam. Functions f_{Maxw} and f_{beam} are each normalized to the under-shape area = 1. Rutherford cross-section of elastic e-e collisions ~ V_{ee}^{-4} **[2]**, therefore high-energy e-beam [that with $(\varepsilon_{e,c,b} - \varepsilon_{e,w,b}/2) \gg T_{e,b}$] does not interact with Maxwell electrons, therefore, two parts of $f_b(\varepsilon_e)$ don't mix; here V_{ee} is the velocity of relative motion of e-beam electrons vs electrons of Maxwell distribution.

(iii) **mean absolute velocity of ions in collective** (i.e., non-thermal) **motion**, $u_{3D,b}$. The $u_{3D,1}$ includes motion of BSs in the core.

- **Time dependence** of R_b, $n_{D,b}$, $n_{He,b}$, $n_{C,b}$, $n_{X,b}$, $T_{e,b}$, $u_{3D,b}$, ξ_b, $\varepsilon_{e,c,b}$, $\varepsilon_{e,w,b}$ is prescribed in file **Params2.inp**.
- High density in compressed target results in sub-ps equilibration between $T_{e,b}$ and ion temperature $T_{i,b}$ **[3,4]**, therefore in the code

$$T_{i,b} = T_{e,b} \; . \qquad \text{(II. 4)}$$

- At at $T_{e,b} \gg 100$ eV (II.2) atoms of **D, He, C are ionized to nuclei**.
- **Density of free electrons** $n_{e,b}$ is given by plasma neutrality:

$$n_{e,b} = Z_{D,b}\, n_{D,b} + Z_{He,b}\, n_{He,b} + Z_{C,b}\, n_{C,b} + Z_{X,b}\, n_{X,b} \qquad \text{(II. 5)}$$

where $Z_{D,b}$, $Z_{He,b}$, $Z_{C,b}$ are nuclear charges of three light isotopes; user can replace D, He, C with H, T or isotopes of other light elements. $Z_{X,b}$ is the mean charge of ions of X in zone b. Computed $Z_{X,b}$ depends on the (i) database of energy levels, (ii) method of computation of inelastic cross-sections, (iii) assumptions on the lowering of ionization energy in plasma.

The database of X **must** include nucleus, H-like, He-like, Li-like ions and **can** include ionization stages below Li-like; these stages must follow in one sequence (no missing stages) down to the stage with the ground state ionization energy < 1 keV. We omit lower stages because at $T_{e,b} \gg 100$ eV (II. 2) their population is negligible. Total number of the energy levels in the database of X (sum over ionization stages)

$$l_{\max} < 2300. \qquad \text{(II. 6)}$$

More info on the database and instruction for replacement are given in Section IV.

Let $n_{b,l}$ denote the number density of X-ions on energy level l in zone b. Sum over the levels

$$\Sigma_l \, n_{b,l} = n_{X,b}. \quad [\text{cm}^{-3}] \qquad \text{(II. 7)}$$

Functions $n_{b,l}(t)$ are computed by integration of the system of $l_{\max}$ rate equations of the level-population kinetics **[5-7]**

$$dn_{b,l}/dt = \Sigma_{l' \neq l} \, W_{l',l} \, n_{b,l'} - n_{b,l} \, \Sigma_{l' \neq l} \, W_{l,l'} \qquad \text{(II. 8)}$$

where $W_{l',l}$ is the probability of $l' \rightarrow l$ transition due to spontaneous radiative decay, spontaneous radiative recombination, autoionization, dielectronic capture, photoionization, photoinduced recombination, photoexcitation, photodeexcitation, ionization, excitation and deexcitation by electron impact, three-body recombination.

Computation of probabilities of the photoinduced transitions requires **space- direction- average spectral intensity of radiation in each zone, $J_{\nu,b}(t)$**. This intensity includes irradiation of zone b by other zones, thus $J_{\nu,b}(t)$ depends on parameters of **all zones**. In the code, the units of $J_{\nu,b}$ are [W/eV/sr/cm^2].

Differential eqs. (II.8) give big advantage vs widely used **CRE codes** because CRE codes, by definition, assume $dn_{b,l}/dt = 0$ thus simplify eqs. (II.8) to algebraic equations, that means immediate relaxation of $n_{b,l}(t)$ to this-t thermodynamic parameters and $J_{\nu,b}(t)$. Computations show that **the assumption of CRE is often wrong**, namely, correct $n_{b,l}(t)$ depend on a history of parameters in the period from t_0 to t. Comparing $n_{k,\ell}(t)$ given by eqs. (II.8) to those in CRE, a user can see an error caused by the assumption of CRE for scenario that he prescribed in file **Params2.inp**. Moreover, present code can be used for determination of time, t_{CRE}, required for relaxation of $n_{b,l}(t)$ to their CRE values at parameters of interest, *see the last paragraph of Section IV*.

The code integrates equations (II. 8) by the 4$^{\mathrm{th}}$ order Runge-Kutta method using **NAG D02EAF subroutine**. On each step in time, the integration of eqs. (II. 8) for all zones is followed by computation of $J_{\nu,b}(t)$ in each zone. In the code, at t_0 all ions of X are on one energy level chosen in file **Params1.inp** (*same level for all zones*). Other levels are given $n_{b,l}(t_0) = 0$. Radiation and inelastic collisions distribute ions over all energy levels thus creating $n_{b,l}(t)$, $J_{\nu,b}(t)$ according to chosen thermodynamic scenario. Each zone is back-lighted by other zones, therefore in each zone $J_{\nu,b}(t)$, $n_{b,l}(t)$ depend on scenarios chosen for **all** zones.

Densities $n_{k,\ell}(t)$ obtained by integration of eq. (II. 8) are used, in particular, for computation of the absorption coefficient corrected for stimulated emission, $k_\nu'(t)$, and emissivity, $\varepsilon_\nu(t)$, both needed for integration of the equation of radiation transfer (ERT). In the code, units of $k_\nu'(t)$ and $\varepsilon_\nu(t)$ are [cm^{-1}] and [W/eV/sr/cm^{-3}], respectively. The emissivity is caused by bound-bound, free-bound, free-free transitions; $k_\nu'(t)$, is caused by bound-bound, bound-free, free-free transitions.

In computations of the bound-bound part of ε_ν, k_ν' each spectral line is given Voigt shape with Gaussian part defined by Doppler broadening (thus function of $T_{i,b}$, $u_{3D,b}$), Lorentzian part defined by Stark effect or by the uncertainty principle (a bigger one of these two). For the uncertainty principle, a life time of an energy level is computed in Baranger' approach **[6]**. In computations of Stark effect we follow Ref. **[8]** and later improvements **[9]**. Contribution of each mechanism of the line broadening is shown in files "…**LineInfo.dat**", *see Section IV for details*.

$J_{\nu,b}$ is approximated by solution of ERT along typical line of sight (LOS) to a representative point (RP) of zone b. This solution is similar to that along **hot LOS** in Section III. Function $J_{\nu,b}$ in each zone and contributions of all zones are shown in file **EffSpIns.dat**.

Lowering of the ionization energy of ion A^{q+} is denoted $\Delta I_{q,b}$ and is taken in the Ion Sphere approach. In Appendix we show that for plasma of **any chemical composition** (here, X+C+He+D)

$$\Delta I_{q,b} = 2(q+1)\, I_H\, \alpha_0/\alpha_{q,b}\,, \qquad \text{(II. 9)}$$

where I_H = 13.606 eV is Rydberg energy, $\alpha_0 = 0.52918 \times 10^{-8}$ cm is Bohr radius,

$$\alpha_{q,b} = [3q/(4\pi n_{e,b})]^{1/3} \qquad \text{(II. 10)}$$

is radius of the ion sphere of A^{q+}.

III. Radiation from the target

In computations of the target radiation **towards a detector** we use two groups of LOSs, each at certain distance from central LOS (that through $r = 0$). The first group traverses capsule, core, capsule. We call this group **hot LOSs**. If no capsule, no BSs, then spectral power radiated by the core-only target is

$$P_{\nu,2} = \pi R_2^2 \, I_{\nu,2} \quad [\text{W/eV/sr}] \qquad \text{(III.1)}$$

where πR_2^2 is the largest plane cross-section of the core,

$$I_{\nu,2} = (\varepsilon_{\nu,2}/\kappa'_{\nu,2}) \cdot [1 - \exp(-\kappa'_{\nu,2} L_2)] \quad [\text{W/eV/sr/cm}^2]; \qquad \text{(III.2)}$$

is the spectral intensity of radiation on the exit of hot LOS (solution of ERT); L_2 is the path of this LOS through the core. For **optically thin core** (that with $\kappa'_{\nu,2} R_2 \ll 1$) expressions (III.1), (III.2) give

$$P_{\nu,2,\,\text{thin}} = \pi R_2^2 \, \varepsilon_{\nu,2} \, L_2 \, . \qquad \text{(III.3)}$$

On the other hand, exact result is

$$P_{\nu,2,\,\text{thin exact}} = \varepsilon_{\nu,2} \, V_2 \qquad \text{(III.4)}$$

where

$$V_2 = 4\pi R_2^3/3 \qquad \text{(III.5)}$$

is volume of the core. Equality (III.3) = (III.4) gives

$$L_2 = 4R_2/3 \, , \qquad \text{(III.6)}$$

then a distance of hot LOS from central (through $r = 0$) LOS is

$$d_2 = [R_2^2 - (L_2/2)^2]^{1/2} = 5^{1/2} R_2/3 \approx \mathbf{0.7454\ R_2} \, . \qquad \text{(III.7)}$$

Let us consider a random distribution of **N identical BSs** within $r < R_2$; no core, no capsule. BSs of $R_1 \ll R_2$ don't shade each other, thus the **power from N BSs** towards a detector is

$$P_{\nu,N} = N \pi R_1^2 \, I_{\nu,1} \quad [\text{W/eV/sr}] \qquad \text{(III.8)}$$

where $I_{\nu,1}$ is spectral intensity of radiation of **one** BS. For $I_{\nu,1}$ ERT gives expression similar to (III.2) except subscript 1 instead of 2, i.e.

$$I_{\nu,1} = (\varepsilon_{\nu,1}/\kappa'_{\nu,1}) \cdot [1 - \exp(-\kappa'_{\nu,1} \cdot 4R_1/3)]. \qquad \text{(III.9)}$$

If **no empty zones**, spectral intensity of radiation from capsule to the core along **hot LOSs**

$$I_{\nu,\,cap/cor} = (\varepsilon_{\nu,3}/\kappa'_{\nu,3}) \cdot [1 - \exp(-\kappa'_{\nu,3} L_3)]\,; \qquad \text{(III.10)}$$

here L_3 is the LOS path in capsule

$$L_3 = (R_3^2 - d_2^2)^{1/2} - L_2/2\,. \qquad \text{(III.11)}$$

In the core, intensity (III.10) is attenuated by core+BSs and is increased due to their emission, thus spectral intensity on the interface from the core to the capsule

$$I_{\nu,\,cor/cap} = I_{\nu,\,cap/cor} \cdot \exp[-\kappa'_{\nu,2} L_2 - \kappa'_{\nu,1} \cdot (4R_1/3) \cdot W_{BS}] + I_{\nu,2} + I_{\nu,1} W_{BS}\,. \qquad \text{(III.12)}$$

Here W_{BS} is the probability that hot LOS traverses a BS; such event can happen only with a BS which has center closer than R_1 to the LOS, i.e. has the center inside volume $V_{LOS} = L_2 \pi R_1^2$. If N BSs are randomly distributed in the core of volume $V_2 = 4\pi R_2^3/3$, then the probability to find at least one BS in V_{LOS} is

$$W_{BS} = N V_{LOS}/V_2 = N(R_1/R_2)^2\,, \qquad \text{(III.13)}$$

remember $R_1 \ll R_2$. On the exit from capsule towards detector, radiation intensity along hot LOS

$$I_{\nu,\,\textbf{hot out}} = I_{\nu,\,cor/cap} \cdot \exp(-\kappa'_{\nu,3} L_3) + I_{\nu,\,cap/cor}\,, \qquad \text{(III.14)}$$

Thus the power towards detector due to **the hot LOSs**

$$\mathbf{P_{\nu,\,hL}} = \pi R_2^2 \cdot I_{\nu,\,\textbf{hot out}}\ \text{[W/eV/sr]}. \qquad \text{(III.15)}$$

The second group of towards-detector LOSs traverses capsule only. We call them **cold LOSs**. Let them go at distance

$$d_{cL} = (R_2 + R_3)/2 \qquad \text{(III.16)}$$

from the central towards-detector LOS, then their path in capsule is

$$\ell_{cL} = 2\,(R_3^2 - d_{cL}^2)^{1/2}\ , \qquad \text{(III.17)}$$

spectral intensity of radiation on the exit of cold LOS

$$I_{\nu,cL} = (\varepsilon_{\nu,3}/\kappa'_{\nu,3}) \cdot [1 - \exp(-\kappa'_{\nu,3}\,\ell_{cL})]\ \text{[W/eV/sr/cm}^2\text{]}. \qquad \text{(III.18)}$$

LOSs at $d \approx R_3$ are much shorter than ℓ_{cL}, LOSs at $d \approx R_2$ are longer than ℓ_{cL}; therefore I express the power radiated due to the cold LOSs via their ***effective*** *cross-section*

$$A_{cL} = 2\pi d_{cL}\, w_{cL}\ , \qquad \text{(III.19)}$$

here $w_{cL} < (R_3 - R_2)$ is the "*effective width*" of radial belt seen to the detector. **Spectral power** through A_{cL} **towards the detector**

$$\mathbf{P_{\nu,\,cL}} = 2\pi d_{cL}\, w_{cL}\, I_{\nu,\,cL} \quad \text{[W/eV/sr]}. \qquad \text{(III.20)}$$

We derive w_{cL} from the optically-thin limit ($\kappa'_{\nu,3}\,\ell_{cL} \ll 1$) of the capsule radiation (**empty core, no BSs**); in other words, from the equality between $(P_{\nu,\,hL} + P_{\nu,\,cL})$ and exact $\varepsilon_{\nu,3}\,V_{capsule}$, i.e. from equation

$$\varepsilon_{\nu,3}\,4\pi(R_3^3 - R_2^3)/3 = 2\pi d_{cL}\, w_{cL}\, \varepsilon_{\nu,3}\,\ell_{cL} + \pi R_2^2\, 2\varepsilon_{\nu,3}\, L_3\ .$$

This equation gives

$$w_{cL} = [2\,(R_3^3 - R_2^3)/3 - R_2^2\, L_3]\,/\,(d_{cL}\,\ell_{cL}). \qquad \text{(III.21)}$$

For $R_3 \gg R_2$ expression (II.21) gives

$$w_{cL} = 4R_3/3^{3/2} \approx 0.77\, R_3\ ;$$

for $(R_3 - R_2) \ll R_2$ expression (II.21) gives

$$w_{cL} \approx R_3^{1/2}(R_3 - R_2)^{1/2}/4.$$

While following along scenario, the code computes up to eigth **absolutely calibrated spectrograms** at times requested in file **Params2.inp**. Requested spectral intervals and instrumental broadening must be given in file **Params1.inp** using three coefficients (quadratic function of photon energy). Computed spectrograms will be printed in file **Frames.dat** in units [J/keV/sr] that means **the radiation yield from the target during one frame**. Duration of the frame must be given in file **Params2.inp**. The last column of file **Frames.dat** displays the energy [J/keV/sr] radiated by the target during entire computation (from t_0 till "StopTime"). More comments and explanations are given in the next Section. Note: scenario given in file **Params2.inp** of the demo package does not correspond to simulation of any NIF shot.

IV. The input files, module, library

Atomic database of high-Z dopant consists of files "**QSs.inp**", "**AIw.inp**", "**Exc.inp**", "**Inz.inp**". In the demo package of files, the dopant is Krypton. To change the dopant, the database must be replaced by similar files **printed in the format of the above four files**. Database of the dopant **must** include nuclei, H-like ions, He-like, Li-like ions and **can** include ions of 1-34 spectroscopic symbols (SpSs) below Li-like; all SpSs must follow in one sequence (no missing SpSs). Total number of energy levels in a database of dopant must be less than 2300. Changes in a database require changes in parameters nXE, FSS, HSS, Nnu, NST, NSTm, HSSm, nFAI introduced and explained in the module "**mo1code2.for**".

In the demo package of files, "**QSs.inp**" is the file of atomic data of Kr ions in the last eight charge states, i.e., N-like to nucleus. Lines 3-9 give the number of non-autoionizing energy levels (ELs), the number of autoionizing (AI) ELs, ionization energies (computed with FAC **[1]**).

Lines from 12 till the end of the file give info on each EL included in the database of dopant. In these lines:

first group of columns gives configuration of electron shells,
column "g0" gives the degeneracy of EL,
column "E(eV)" gives the energy of EL (relative to the ground state),
column "#" gives serial number of EL among ELs of same-charge ions;
AI ELs are placed below nucleus; they are given
negative serial numbers,
column "##" gives serial number of EL in the full list of ELs of the dopant.

In the demo package of files, "**AIw.inp**" is the file of autoionization (AI) probabilities of ELs of Kr. The probabilities are computed with FAC **[1]**.

Column 1, 2 give spectroscopic symbol (SpS) and serial number of AI EL.
Columns 3,4 give SpS and serial number of final (after AI) EL.
Column "WAI" gives the probability of AI in units [s^{-1}].
Column DE(eV) gives the difference [eV] between energies of initial and final ELs prior to the lowering of continuum.

In the demo package of files, "**Exc.inp**" is the file of electron impact excitation cross sections of ELs of Kr. The cross-sections are computed with FAC. Column 1 gives SpS of an ion. Column 2 gives serial number of initial (lower) EL in the list of ELs of this SpS. Column 3 gives serial number of final (upper) EL in this list. Column 4 gives the number of formula used for interpolation of the cross section points computed with FAC, see *function "SigExc(eeV)"* in the file "**Code2.for**". Columns 5 - 10 give coefficients for this interpolation formula. Sign "-" in column 11 is a **mark**; it marks a computation with FAC. Absolute value in column 11 is the absorption oscillator strength for this transition.

In the demo package of files, "**Inz.inp**" is the file of electron impact ionization cross-sections of Kr. Column 1 gives SpS of an ion. Column 2 gives serial number of EL to be ionized (the number among ELs of this SpS). Columns 3, 4 display similar info on EL obtained due to the ionization. Columns 5 - 9 display coefficients of formula used for interpolation of cross-section points given by FAC, see *function "SigInz(eeV)"* in the file "**Code2.for**". Columns 10 – 13 displays coefficients of formula used for interpolation of computed points of the photoionization cross-sections, see *function "SigPhi(hv)"* in the file "**Code2.for**". The last column gives the difference between energies [eV] of initial and final ELs prior to the lowering of continuum.

Files "**QSsC.inp**", "**QSsHe.inp**" "**QSsH.inp**" show atomic data on C, He, H. User can replace H, He, C with D, T or any isotopes of other light elements (up to Ne). If any zone contains less than three light elements, then one or two can be given low ion number density in this zone. At T_e of interest, ions of light chemical elements are stripped to nuclei, therefore for light elements we use 2-state databases which consist of nuclei and ground state of H-like ion. This state is required by the structure of the code, but remains empty (for light elements). No ionization of this state, no recombination to it.

Files "**Params0.inp**", "**Params1.inp**", "**Params2.inp**" give parameters of simulation. These files must be filled in by a user. Each parameter is explaned on the right side of a same line. Note: Sample scenario given in file **Params2.inp** of the demo package does not correspond to simulation of any of the NIF shots.

File **"Naglib.lib"** is a small part of NAG library. This part contains (i) subroutine **D02EAF** which integrates the system of ordinary differential equations by the 4th order Runge-Kutta method, (ii) definite integral **D01AH.**

Module "**mo1ode2.for**" gives parameters of atomic databases, some parameters of computation, shows the size of arrays, explains the meaning of parameters.

V. The output files

Files **"BSinfo.dat", "CoreInfo.dat", "CapInfo.dat"** display (i) parameters of plasma in each zone on each step in time, according to the scenario prescribed in file **Params2.inp**; (ii) some of computed parameters of plasma.

Column 1 shows time [ps] ,
column 2 shows outer radius of zone [μm],
column 3 shows T_e [keV] in the zone,
column 4 shows u_{3D} [cm/s] **/10^7** in the zone,
column 5 shows $n_{e,b}$ [cm^{-3}] in the zone,
column 6 shows mean (over chemical elements) ion charge in the zone,
columns 7-10 show mean ion charge of each chemical element in the zone,
columns 11-14 show the number density of ions [cm^{-3}]of each chemical element in the zone,
column "bp" shows parameter ξ_b that is the part ($0 \le \xi_b \le 1$) of beam electrons in $n_{e,b}$, see (II.3),
columns "bcKeV" and "bwKeV" show central energy [keV] and width [keV] of electron beam in the zone, see (II.3).

File **"LineList.dat"** is the list of spectral lines which satisfy all three of the following: (i) line center, $h\nu_c$, is in the interval $[h\nu_{min} , h\nu_{max}]$, (ii) absorption oscillator strength f_{lu} > "f_{lu}Min", (iii) Einstein coefficient A_{ul} > "A_{ul}Min". Parameters $h\nu_{min}$, $h\nu_{max}$, "f_{lu}Min", "A_{ul}Min" are given in **Params1.inp** .

1st column displays chemical element (here Kr, i.e. parameter "XE" = 1),
2nd column displays spectroscopic symbol of the ion,
3rd column displays the energy of photons, $h\nu_c$ [eV],
4th column displays the wavelength of the line, λ_c [A],
5th column displays A_{ul} [s^{-1}],
6th column displays serial number of upper level in file "**QSs.inp**",
7th column displays electron configuration of this level,
the 8th column displays serial number of lower level in file "**QSs.inp**",
the 9th column displays electron configuration of this level,

the 10^{th} column displays the absorption oscillator strength, f_{lu}.

Files "**BSsLineInfo.dat**", "**CorLineInfo.dat**", "**CapLneInfo.dat**' display info on contribution of each broadening mechanism to the widths of spectral lines in BSs, core, capsule, respectively. These files (and the computations) include only spectral lines which satisfy all three of the following: (i) line center, $h\nu_c$, is in the interval $[h\nu_{min}, h\nu_{max}]$, (ii) absorption oscillator strength f_{lu} > "f_{lu}Min", (iii) Einstein coefficient A_{ul} > "A_{ul}Min". Parameters $h\nu_{min}$, $h\nu_{max}$, "f_{lu}Min", "A_{ul}Min" are given in file **Params1.inp**.

Column "hvCeV" displays $h\nu_c$ [keV],
column "XE" displays chemical element which radiated the line
(now it shows "1" that means "the dopant"),
column "SS" displays spectroscopic symbol of ion which radiated this line,
column "Lambda" displays the line-center wavelength (in Angstroms),
two columns "Upper" display serial number and electron configuration
of the upper level of this line,
two columns "Lower" display serial number and the electron configuration
of the lower level of this line,
column "viaTi" displays contribution of thermal broadening to the
FWHM [eV] of Voigt shape of the line in k_ν', ε_ν; i.e.,
FWHM [eV] of thermal part of Gaussian part of Voigt FWHM;
column "via3D" displays contribution of hydro (collective) broadening to
FWHM [eV] of Voigt shape of the line in k_ν', ε_ν; i.e.,
FWHM [eV] of hydro part of Gaussian part of Voigt FWHM;
column "Baranger" displays the lower limit for Lorentzian part of
FWHM [eV] of Voigt shape of the line in k_ν', ε_ν;
this limit is caused by the uncertainty principle;
column "Lorentz" displays FWHM [eV] of Lorentzian caused by either the
uncertainty principle or Stark effect (a bigger one of these two);
column "Voigt" displays FWHM [eV] of Voigh shape of the line in k_ν', ε_ν;
column "PopUpper" displays population of the upper level: $n_{b,Up}/n_{X,b}$,
column "flu" displays the absorption oscillator strength f_{lu}.

In file **"Frames.dat"** the 1st column displays the energy of photons [keV], columns 2-9 display the energy [J/keV/sr] radiated by the target during one frame. All frames are of equal duration "FrL" [s]. This duration and central time [s] of each frame, "FrP(#)" must be given in file "**Params2.inp**". Parameter "StopTime" [s] allows to stop a computation after needed number (say, A) frames. For this purpose, "StopTime" must be > {FrP(A) + FrL/2 +10ps}. Mean spectral power of radiation from the target during a frame $P_\nu(t) = Y_\nu(t)/FrL$ [W/keV/sr]. The 10th column displays the energy [J/keV/sr] radiated by the target during entire computation (from t_0 till "StopTime").

Files "**BSemiAbso.dat**", "**CoreEmiAbso.dat.dat**", "**CapEmiAbso.dat**" display plasma emissivity ε_ν [W/cm^3/sr] and plasma absorption coefficient corrected for induced emission k_ν' [cm^{-1}] in BSs, core, capsule, respectively, at t = "tiInf" given in file "**Params2.inp**".

Column "hvKeV" displays the photon energy [keV].

Columns 2 - 4 display three parts of plasma emissivity [W/cm^3/sr]:
free-bound (i.e. due to the radiative recombination),
bound-bound (i.e. due to radiation in spectral lines),
free-free (i.e. due to radiation of free electrons);

Column 5 displays full ε_ν [W/cm^3/sr] that is a sum of the above three parts.

Columns 6 - 8 display three parts of k_ν' [cm^{-1}]:
bound-free (i.e. due to photoionization),
bound-bound (i.e. absorption in spectral lines),
free-free (due to absorption by free electrons),

Column 9 displays full k_ν' [cm^{-1}] that is a sum of the above three parts.

Files "**PIR_BS.dat**", "**PIR_Core.dat**", "**PIR_Cap.dat**" display info on the lowering of continuum in BSs, core, capsule, respectively.

Columns 1-4 display time [ps], $T_{e,b}$ [keV], $n_{e,b}$ [cm^{-3}], $n_{X,b}$ [cm^{-3}],

columns 5-11 relate to ions of Kr in N-like to H-like ionization stages.
These columns display the ratio of the ground state ionization energy in plasma to a similar energy for the ion in vacuum. The lowering of the ionization energy in plasma

is taken in the Ion Sphere approach, see (II. 9).

For ions in vacuum, the ionization energy from the ground state is shown in the last column of lines 3-9 of file **QSs.inp**.

File **"EffSpIns.dat"** displays $J_{\nu,b}(t)$ [GW/keV/sr/cm^2] that is space- direction-average spectral intensity of radiation in representative points (RP) of all zones at t = "tiInf" given in file "**Params2.inp**". Also shown is the contribution of each zone to $J_{\nu,b}(t)$. The columns display as follows:

Column "hvKeV": photon energy [keV] .

Column "BS": $J_{\nu,BS}$ in RP of BS.

Column "Exte1": contribution of capsule+core to $J_{\nu,BS}$, i.e. spectral intensity of capsule+core radiation towards typical BS, attenuated in BS on the path to its RP.

Column "Self1": contribution of BS itself to $J_{\nu,BS}$.

Column "Core": $J_{\nu,Core}$ in RP of the core.

Column "Exte2bs": contribution of BSs to $J_{\nu,Core}$, i.e. spectral intensity of radiation of BSs towards RP of the core, attenuated in the core on the path to its RP.

Column "Exte2cap": contribution of capsule to $J_{\nu,Core}$, i.e. spectral intensity of capsule radiation towards RP of the core, attenuated in the core on the path to its RP.

Column "SelfCo": contribution of the core to $J_{\nu,Core}$.

Column "Capsule": $J_{\nu,Cap}$ in RP of capsule.

Column "Exte3co": contribution of the core to $J_{\nu,Cap}$, i.e. spectral intensity of the core radiation towards RP of capsule, attenuated in the capsule on the path to its RP.

Column "SelfCap": contribution of the capsule to $J_{\nu,Cap}$.

Column "abRbs": $\kappa'_{\nu,1} \cdot R_1$

Column "abRcore": $\kappa'_{\nu,2} \cdot R_2$

Column "abR3mR2": $\kappa'_{\nu,3} \cdot (R_3 - R_2)$.

Column "CapFromBSs": contribution of BSs to $J_{\nu,Cap}$, i.e. spectral intensity of radiation of all BSs towards RP of capsule, attenuated in the core+capsule on the path to RP of capsule.

First column of files "**ZpopsBS.dat**", "**ZpopsCore.dat**", "**ZpopsCap.dat**" displays time [ps] along the scenario.

Columns 2-4 display $T_{e,b}$ [keV], $n_{e,b}$ [cm^{-3}], $n_{Kr,b}$ [cm^{-3}] in BSs, core, capsule, respectively;

columns 5-12 display population of the last 8 ionization stages of Kr; sum over the stages = 1.

If a user wants to know time, t_{CRE}, required for plasma relaxation to CRE at certain parameters, he must prescribe these parameters to **all zones** of scenario (file **Params2.inp**) for sufficiently long time. Then files **ZpopsBS.dat**, **ZpopsCore.dat**, **ZpopsCap.dat** will show population of last ionization stages as a function of time on the way to CRE. The longest time is required for equilibration of population of nuclei (the last column), therefore the population of nuclei is most reasonable for determination of t_{CRE}. User can define t_{CRE} according to his own criterion, e.g., "t_{CRE} is the time at which population of nucleus differs from CRE value by less than 1%" or "…. by less than 0.01%", etc.

Appendix. Ionization energy of ion A^{q+} in plasma of arbitrary chemical composition

Widely used models of the reduction of ionization energy in plasma (continuum lowering), $\Delta I_{q,b}$, such as Debye-Hűckel, Ion Sphere, Stewart-Pyatt **[4, 6, 10]** ignore a few fundamental effects **[11]**. On the other hand, no closed-form expression to account these effects; therefore here we use the Ion Sphere model that we modified for plasmas of complex chemical composition.

In plasmas, each free electron moves in collective electric field of surrounding ions (of different charge and mass) and free electrons. This collective field chaotizes trajectories of free electrons. In neutral uniform

plasma the chaotization of trjectories results in uniform distribution of free electrons even on a scale if ion-ion distances; then **the mean volume per free electron**

$$V_{e,b} \approx 1/n_{e,b}.$$

Due to plasma neutrality, mean number of free electrons crossing the ion sphere of A^{q+} at any time is approximately q, thus the volume of ion sphere in zone b

$$V_{q.b} \approx qV_{e,b} \approx q/n_{e,b}, \qquad (A.1)$$

then radius of ion sphere

$$\alpha_{q.b} \approx [3V_{q.b}/4\pi]^{1/3} \approx \mathbf{[3q/(4\pi n_{e,b})]^{1/3}}. \qquad (A.2)$$

For example, radius of the ion sphere of H-like ion Kr^{+35} is 3.3x bigger than radius of the ion sphere of D^+.

If ion A^{q+} isn't surrounding by electrons and ions (i.e., it is a **solitary A^{q+} in vacuum)**, then it can be treated as a point-like $A^{(q+1)+}$ with one electron bound in potential

$$U(r) = - e\,(q+1)/r\,. \qquad (A.3)$$

Removal of this electron from r to infinity (i.e. ionization of A^{q+}) requires the ionization energy

$$I_{q.b} = eU(\infty) - eU(r) = 0 + e^2(q+1)/r\,. \qquad (A.4)$$

In neutral plasma, q free electrons traversing an ion sphere, weaken potential (A.3) so that on the edge of this sphere (i.e. on interface between two ion spheres) bound electron does not belong to any of them, thus became free; its ionization from $r = \alpha_{q,b}$ does not require energy. In comparison to a solitary ion [*see* (A.4) *at* $r = \alpha_{q.b}$] the ionization energy became lower by $e^2(q+1)/\alpha_{q.b}$; in other words, the lowering of ionization energy in plasma

$$\mathbf{\Delta I_{q,b}} \approx e^2(q+1)/\alpha_{q,b} = \mathbf{2\,(q+1)\,I_H\,\alpha_0/\alpha_{q,b}}\,. \qquad (A.5)$$

Here we used known relation $2I_H = e^2/\alpha_0$ where α_0 is Bohr radius.

Expression (A.5) is derived for neutral plasma of **arbitrary** chemical composition with **any** distribution of ions over ionization stages. In the limit of identical ions (*i.e., **all** ions are* A^{q+}) expression (A.5) exceeds by factor $4/3$ known result obtained for this limit*. Numeric factor ~ 1 depends on

particular model, *see discussion in Ref.* **[6]**. Comparison of predicted $\Delta I_{q,b}$ to experimental data does not prove any model because all predictions (i) differ by less than factor 2, *see Figs.1,2 in Ref.* **[12]**, (ii) differ in dependence on plasma density and temperature which in experiments are t, $\boldsymbol{r}$-dependent and their estimates have wide error bars.

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* See expressions (7.42), (7.43) in Ref. **[6]** and (10.12) in Ref. **[3]**.

References

[1] M. F. Gu, Flexible Atomic Code, *Can. J. Phys.* ***8****, 5, (2008)*.

[2] L. D. Landau and E. M. Lifshitz, Mechanics, *Elsevier, 2005.*

[3] S. Atzeni and J. Meyer-ter-Vehn, The Physics of Inertial Fusion, *Oxford University Press, 2009.*

[4] Ya. B. Zel'dovich, Yu. P. Raizer, Physics of Shock Waves and High-Temperature Hydrodynamics Phenomena, *Academic Press, New York, 1967.*

[5] D. Mihalas, B. Weibel-Mihalas, Foundations of Radiation Hydrodynamics, *Dover Publications, Inc, New York, 1999.*

[6] H.R. Griem, Principles of Plasma Spectroscopy, *Cambridge University Press, Cambridge, 1997.*

[7] V. I. Fisher, D. V. Fisher, and Y. Maron. Radiation transport and density effects in non-equilibrium plasmas. *High Energy Density Phys.* ***3****, 283 (2007).*

[8] E. Stambulchik and Y. Maron, Quasicontiguous frequency-fluctuation model for calculation of hydrogen and hydrogen-like Stark-broadened line shapes in plasmas. *Phys. Rev. E* ***87****, 053108 (2013).*

[9] E. Stambulchik, private communication.

[10] R. P. Drake, High-Energy-Density Physics, *Springer-Verlag, Berlin, Heidelberg, 2006.*

[11] G. Röpke et al., Ionization potential depression and Pauli blocking in degenerate plasmas at extreme densities. *Phys. R*ev. E **99**, 033201 (2019).

[12] B. J. B. Crowley, Continuum lowering – A new perspective. *High Energy Density Phys.* ***13****, 84 (2014).*