Code for deriving parameters of x-brightest volumes in z-pinch plasma of any chemical composition with any distribution of free electrons

X-ray images of z-pinch plasma show high nonuniformity in brightness. We present the code for deriving parameters of x-brightest volumes (XBVs) of this plasma. The code follows thermodynamic scenario that **user expects** for three zones of XBV. While advancing along scenario, the code computes contribution of one XBV to the radiated spectral power, signals of PCDs, spectrograms taken at requested times. **User may** compare these results to experimental data (divided by number of observed XBVs) and **improve his scenario** until satisfied with the comparison, thus obtaining an estimate of thermodynamic parameters in typical XBV.

I. Advantages of the code

A. The code simulates radiation of plasmas of **any chemical composition**, e.g. plasma of stainless steel (Fe, Cr, Ni, Mn); in particular, the code rigorously computes group shapes of merged spectral lines of all species. The merging affects widths and ratios of spectral lines, as well as probabilities of photoinduced transitions.

B. **Users can prescribe a distribution of free electrons over energy** $f(\varepsilon_e, t)$. This option enables (i) analysis of plasma response on generation of electron beam, (ii) comparison of spectrograms computed with different $f(\varepsilon_e, t)$, e.g. Maxwellian vs other solutions of Boltzmann equation.

C. We don't assume any type of equilibrium in plasma; therefore, **the code remains correct in case of quick changes in thermodynamic parameters and in $f(\varepsilon_e, t)$.** Moreover, the code may be used for computation of time required for relaxation of ion level populations (thus ionization composition and radiation as well) to equilibrium.

D. We derived and are using implicit expression for **continuum lowering** in plasmas of arbitrary chemical composition.

II. The model and the code

The code is written for deriving parameters of **x-bright volums (XBVs) in on-axis z-pinch plasma**. Model of XBV is as follows: N > 2 identical spheric bright sources (**BS**s) are randomly distributed in spheric **core** surrounded by **halo**. Radius of BS is R_1, radius of the core $R_2 \gg R_1$. The halo is spheric layer of inner radius R_2, outer radius R_3. In each of these three **zones** plasma is uniform. Zones affect each other by **radiation**. Parameters of zones change in time according to scenario **prescribed** in file *Params2.inp*. We limited N, R_1 by requement of long mean distance between BSs that allows to neglect interaction between them; namely, we require linear size of core volume per BS at least 10x longer than R_1, i.e.

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

One of advantages of present code is accurate treatment of plasmas composed of **a few chemical elements,** e.g. plasmas of alloys or gas mixes. **User can choose** chemical composition following explanation in Section IV.

Diagnostics at hν > 1 keV restricts the electron temperature to

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

subscript b = **1, 2, 3** denotes BS, core, halo, respectively. Each of these zones is characterized with time-dependent

(i) **ion number densities** $n_{a,b}(t)$; the units are [cm^{-3}]; a = 1, 2, 3, 4 is serial number of chemical elements in database of the code.

(ii) **distribution f_b of free electrons over their energy ε_e.**
No restrictions on $f_b(\varepsilon_e, t)$ except normalization to under-shape area = 1. Units of ε_e and f_b are [eV] and [eV^{-1}], respectively. **User may prescribe** any $f_b(\varepsilon_e, t)$ in "*function EED*" in the source file. The possibility of choosing $f_b(\varepsilon_e, t)$ is substantial

advantage of present code. In particular, this option enables simulations and analysis of spectra radiated by plasma with electron beam(s) and/or plasma subjected to laser radiation. For this option, transitions are characterized **by cross-sections** (not by commonly used maxwellian rates). For computation of the cross-sections we used Flexible Atomic Code **[1]**. In demo version of present code, function $f_b(\varepsilon_e, t)$ consists of maxwellian and beam parts:

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

where $f_{\mathrm{Maxw}}(\varepsilon_e, T_{e,b})$ is Maxwell distribution corresponding to $T_{e,b}(t)$; parameter $\xi_b(t)$ is the beam part of local number density of free electrons; $f_{\mathrm{beam}}(\varepsilon_e, \ldots)$ is the shape of electron beam. In demo version of the code this shape is rectangular; $\varepsilon_{e,c,b}(t)$, $\varepsilon_{e,w,b}(t)$ are central energy and width of e-beam. Functions f_{Maxw}, f_{beam} are each normalized to the under-shape area = 1. Rutherford cross-section of elastic e-e collisions $\sim \varepsilon_e^{-2}$ **[2]**, therefore interaction between high-energy e-beam [*that with* $(\varepsilon_{e,c,b} - \varepsilon_{e,w,b}/2) \gg T_{e,b}$] and maxwellian electrons is negligible, therefore two terms of (II.3) don't mix.

(iii) **mean absolute velocity of 3D motion of ions** $u_{3D,b}$. This parameter characterizes distribution of ion velocity in two simultaneous motions that are thermal motion of individual ions and their collective hydro motion in zone b; besides these two motions, $u_{3D,1}$ includes relative motion of BSs in the core.

- **Time dependence** of R_b, $n_{a,b}$, $T_{e,b}$, $u_{3D,.b}$, ξ_b, $\varepsilon_{e,c,b}$, $\varepsilon_{e,w,b}$ **must be prescribed** in file "*Params2.inp*".
- XBVs are observed in on-axis plasma, therefore **radial motion of XBVs (**thus Doppler shift of spectral lines**) are negligible**.

- For each chemical element atomic database of the code **must** include nuclei, H-like, He-like, Li-like ions and **can** include ionization stages below Li-like; all ionization stages must follow in one sequence (no missing stages) down to a stage which has the ionization energy of its ground state, $I_{a,q} < 1$ keV; here q denotes ionization stage. We omit lower q because at $T_{e,b} > 100$ eV their population is negligible. More info on database and instruction for replacement are given in Section IV.
- **Density of free electrons in zone *b*** is given by the equation of plasma neutrality

$$n_{e,b} = \Sigma_a \, Z_{a,b} \, n_{a,b} \qquad \text{(II. 4)}$$

where $Z_{a,b}$ is the mean charge of ions of chemical element a in zone b,

$$n_b = \Sigma_a \, n_{a,b}$$

is the number density of ions in zone b. Computed $Z_{a,b}$ depend on database of energy levels, method of computation of inelastic cross-sections, model of the lowering of continuum in plasma.

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

$$\Sigma_l \, n_{a,b,l} = n_{a,b}. \qquad \text{(II. 5)}$$

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

$$dn_{a,b,l}/dt = \Sigma_{l' \neq l} \, W_{l',l} \, n_{a,b,l'} - n_{a,b,l} \Sigma_{l' \neq l} \, W_{l,l'}. \qquad \text{(II. 6)}$$

On each step in time, the code integrates system (II.6) separately for each a,b but accounts radiation transfer between zones, *see below*. Function $W_{l',l}$ is the probability of $l' \rightarrow l$ transition due to all types (of transitions) possible for this pair. The code chooses them from

ionization, three-body recombination, excitation, deexcitation (*all caused by impacts of free electrons*), spontaneous and photoinduced radiative transitions (spectral lines and radiative recombination), photoionization, photoexcitation, photodeexcitation, autoionization, dielectronic recombination.

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

Due to differential eqs. (II.6) present code has big advantage over widely used CRE codes because CRE codes, by definition, assume $dn_{a,b,l}/dt = 0$, thus simplify system (II.6) to the algebraic equations, that means immediate relaxation of each $n_{a,b,l}$ to instant parameters of plasma. Computations show that this assumption is often wrong; namely, level populations depend on the entire scenario chosen for the period $t_0 \rightarrow t$. The code can used for determination of time, t_{CRE}, needed for relaxation of $n_{a,b,l}(t)$ to their CRE values at parameters of interest, *for details see the last paragraph in Section VI*. Comparison of results obtained for CRE plasmas vs results of non-equilibrium computations isn't included in the manual.

The code integrates system (II.6) by the 4th order Runge-Kutta method using *D02EAF* subroutine of NAG library. Zones affect each other by radiation, therefore a computation of $J_{\nu,b}(t)$ for each b requires $n_{a,b,l}(t)$ of all chemical elements in all zones.

At t_0 the code loads all ions of a on one energy level ***to be chosen*** *in file "Params1.inp"*. In demo package of files, this level is $1s^2$ of He-like ion for each a in each zone; other levels are given

initial population $n_{a,,b,l} = 0$. In a few time steps, inelastic collisions and radiation populate each level. Spectral intensity of radiation in a zone, $J_{\nu,b}(t)$, is due to all zones, therefore pair $J_{\nu,b}(t)$, $n_{b,l}(t)$ depends on scenarios chosen for **all zones**.

Thus obtained $n_{a,b,l}(t)$ are used in solution of the equation of radiation transfer (**ERT**) along lines of sight (**LOS**s) directed towards detectors, see expressions (III.15), (III.20) below. In demo version, the code computes a sequence of eigth frames of radiation emitted by one x-bright spheric region. Duration of a frame **to be chosen** in file "*Params1.inp*"; timing of the frames **to be prescribed** in file "*Params2.inp*".

In the model, we approximate $J_{\nu,b}$ with solution of the ERT along typical LOS towards a representative point (**RP**) of zone b. RPs of BS, core are chosen at half-mass distance from their centers, RP of halo is chosen at $r = (R_3 + R_2)/2$. Integration along typical LOS towards a RP is similar to the integration along **hot LOS** explained in Section III. Function $J_{\nu,b}$ in each zone and contribution of each to each zone are shown in file "*EffSpIns.dat*".

Lowering of the ionization energy of ion A^{q+} is denoted $\Delta I_{a,q,b}$ and is taken in the Ion Sphere approach. In Appendix we show that in neutral plasma

$$\Delta I_{a,q,b} = 2(q+1) I_H \zeta_0/\zeta_{q,b}, \qquad \text{(II.7)}$$

where $I_H = 13.606$ eV is the Rydberg energy, $\zeta_0 = 0.52918 \times 10^{-8}$ cm is Bohr radius, $\zeta_{q,b} = [3q/(4\pi n_{e,b})]^{1/3}$ is radius of ion sphere of A^{q+}.

III. Radiation from one x-bright volume (XBV)

Plasma emissivity $\varepsilon_{\nu,b}$ is due to bound-bound, free-bound, free-free transitions of electrons. Absorption coefficient corrected for stimulated emission $\kappa'_{\nu,b}$ is due to bound-bound, bound-free, free-free transitions. In the code, units of $\varepsilon_{\nu,b}$, $\kappa'_{\nu,b}$ are [W/eV/cm^3/sr] and [cm^{-1}], respectively. In the bound-bound part of $\varepsilon_{\nu,b}$, $\kappa'_{\nu,b}$ each spectral line is given **voigt shape** with **gaussian part of the width** defined by Doppler broadening (thus by $u_{3D,b}$), **lorentzian part of the width** defined by bigger of two: Stark effect or the uncertainty principle. In computations of Stark width we follow Refs. **[8,9]**. For the uncertainty principle, life time of a level is taken in Baranger' approach **[6]**. Gaussian and lorentzian parts of the width of each line in three zones are shown in three files *"...LineInfo.dat"*.

Radiation towards a detector is computed using two groups of parallel towards-detector LOSs, each group at known distance from the center of core ($r = 0$). First group traverses the core; we call them **hot LOSs**. Their distanse from $r = 0$ is defined as follows: if no halo, no BSs, then spectral power radiated by the core alone is

$$P_{\nu,2} = \pi R_2^2 \, I_{\nu,2} \qquad \text{(III.1)}$$

where πR_2^2 is the plane area seen to far detector,

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

is spectral intensity of radiation on the exit of hot LOS from plasma, L_2 is the path of this LOS in the core. In the code, units of spectral intensity and power are [W/eV/sr/cm^2], [W/eV/sr], respectively.

For **optically thin core** (that with $\kappa'_{\nu,2}\, R_2 \ll 1$) expressions (III.1), (III.2) result in

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

On the other hand, exact result is

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

where

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

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

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

then the distance of hot LOS from $r = 0$ 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 halo. BSs of $R_1 \ll R_2$ don't shade each other, thus the **power from N BSs** towards a detector is

$$P_{\nu,N} = N \pi R_1^2\, I_{\nu,1} \qquad \text{(III.8)}$$

where $I_{\nu,1}$ is intensity of radiation of **one** BS. This intensity is given by expression similar to (III.2) except subscript 2 instead of 1, 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 **all zones are active**, then spectral intensity of radiation from halo to the core along hot LOSs

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

here L_3 is the path of hot LOS through halo

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

In the core, intensity (III.10) is attenuated by core+BSs but increased due to emission of core+BSs, thus spectral intensity on the interface from the core to the halo in towards-detector direction

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

Here W_{BS} is the probability to traverse a BS; such event can happen only with BSs which have center closer than R_1 to the LOS, i.e. 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 halo towards detector, intensity of radiation along hot LOS

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

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

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

The second group of towards-detector LOSs traverses halo only. We call this group **cold LOSs**. Let them pass at distance

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

from $r = 0$; cold LOS path in halo

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

spectral intensity of radiation on the exit of cold LOS

$$I_{\nu,cL} = (\varepsilon_{\nu,3}/\kappa'_{\nu,3}) \cdot \left[1 - \exp\left(-\kappa'_{\nu,3}\,\ell_{cL}\right)\right]. \qquad \text{(III.18)}$$

Towards-detector LOSs at $d \approx R_3$ are much shorter than ℓ_{cL}, LOSs at $d \approx R_2$ are longer than ℓ_{cL}; therefore we express **the power**

radiated along cold LOSs using their ***effective*** *area* on a plane normal to the LOSs

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

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

$$\mathbf{P_{\nu,\ cL}} = 2\pi d_{cL} w_{cL} I_{\nu,cL} \ . \qquad \text{(III.20)}$$

We derive w_{cL} from optically-thin limit (here, $\kappa'_{\nu,3}\, \ell_{cL} \ll 1$) of halo radiation (*empty core, no BSs*), i.e from equality of ($P_{\nu,\,hL} + P_{\nu,\,cL}$) to exact value $\varepsilon_{\nu,3} V_{halo}$:

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

that results in

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

For $R_3 \gg R_2$ expression (III.21) results in

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

for $(R_3 - R_2) \ll R_2$ expression (III.21) results in

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

Spectral power radiated by XBV ($P_{\nu,\,hL} + P_{\nu,\,cL}$) is used in computation of spectrograms and signals of PCDs. For compatison to TREX frames the spectral power **should be multiplied** by spectral response of particular TREX. In computation of PCD signals we used spectral response of diamond PCDs with kapton filters of 5-, 10-, 40-mils thickness (used in Z shot 1520), *see explanations to output files in Section VI*.

IV. Input files

Atomic database of demo version of the code consists of files

"QSsFe.inp", "QSsCr.inp", "QSsNi.inp", "QSsMn.inp",
"InzFe.inp", "InzCr.inp", "InzNi.inp", "InzMn.inp",
"AIwFe.inp", "AIwCr.inp", "AIwNi.inp", "AIwMn.inp",
"ExcFe.inp", "ExcCr.inp", "ExcNi.inp", "ExcMn.inp".

This set of files corresponds to chemical composition of stainless steel **[13]**. **For plasma of another composition**, these 16 files must be replaced by similar ones prepared **in format of present files**, see *details in the next four paragraphs.* For each chemical element, the database **must** include info on nuclei, H-like, He-like, Li-like ions and **can** include ions of spectroscopic symbols (SpSs) below Li-like; all SpSs must follow in one sequence (no missing SpSs). **Changes in the database** require changes in parameters nXE, FSS, HSS, Nnu, NST, NSTm, HSSm, nFAI introduced and explained in module "*mo1code3.for*".

In demo version of the code, files *"QSsFe.inp", "QSsCr.inp", "QSsNi.inp", "QSsMn.inp"* give info on energy levels (ELs) of the last five charge states, i.e. Be-like to nucleus of Fe, Cr, Ni, Mn, respectively. Lines 3-6 give the number of non-autoionizing ELs, the number of autoionizing (AI) ELs, ionization energies (computed with Flexible Atomic Code **[1]**). Lines from 9 till the end of each file give info on each EL:

columns 1,2 give electron configuration of EL,
column 3 gives the degeneracy of EL,
column 4 gives its energy above the ground state of thi ion,
column 6 gives serial number of EL among ELs of same-charge ions
Note: in this column AI ELs are placed below nucleus;
for convenience of programming, AI ELs given numbers > 200;
column 7 gives serial number of EL in the full list of ELs of this chemical element (CE).

In demo version of the code, files *"AIwFe.inp", "AIwCr.inp", "AIwNi.inp", "AIwMn.inp"* give autoionization (AI) probabilities of energy levels (ELs) of Fe, Cr, Ni, Mn, respectively. The probabilities are computed using Flexible Atomic Code (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.
Column DE gives the difference [eV] between energies of initial and final ELs prior to the lowering of continuum.

In demo version of the code, files *"ExcFe.inp", "ExcCr.inp", "ExcNi.inp", "ExcMn.in"* give cross-sections of excitation of ELs by electron impact. The cross-sections are computed using 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 cross-section computed with FAC, see *function "SigExc(eeV)"* in the code. 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 of this transition.

In demo version of the code, files *"InzFe.inp", "InzCr.inp", "InzNi.inp", "InzMn.inp"* give cross-sections of ionization of Els by electron impact. The cross-sections are computed with FAC. Column 1 gives SpS of an ion. Column 2 gives serial number of EL to be ionized (*the number in the list of ELs of this SpS*). Columns 3, 4 display similar info on EL obtained due to the ionization. Columns 5 - 8 display coefficients of formula used for interpolation of computed cross-section, see *function "SigInz(eeV)"* in the source file. Column 9 isn't used in present version. Columns 10 – 13 displays coefficients of formula used for interpolation of computed photoionization cross-sections, see *function "SigPhi(hv)"* in the source file. The last column gives the difference between energies [eV] of initial and final ELs prior to the lowering of continuum.

Files "*Respo5milKapPCD.inp*",
"*Respo10miKapPCD.inp*",
"*Respo40miKapPCD.inp*"
present spectral response of diamond PCDs with kapton filters of 5-, 10-, 40-mils thickness (those used in Z shot 1520). The 1st column gives the photon energy [eV], the 2nd column gives the response of PCD. $0 \le$ response ≤ 1. **User can replace** these three files with spectral response of his PCDs. In this case, he **must change** integers "np5kap", "np10ka", "np40ka" in module "*mo1code3.for*". Thesee three integers show the number of *hv* points in each of these three input files.

Files "*Params1.inp*", "*Params2.inp*" **must be filled in by user**. These files give parameters of computation, explanations and/or comments on each parameter. File *Params2.inp* prescribes ion number density $n_{a,b}$ only for a = 1; ion number density of other chemical elements (a = 2, 3, 4) is calculated in subroutine "*Scenario"* based on known quantitative composition of plasma. If less than four elements in plasma, e.g. two, than a = 3, 4 must be given negliginle $n_{a,b}$. In demo version of the code we consider plasma of stainless steel, thus prescribe $n_{a,b}$ of iron, $n_{Fe,b}(t)$. Ion number density of Cr, Ni, Mn is calculated in subroutine "*Scenario"* based on known percents of mass in composition of stainless steel **[13]**. Note: thermodynamic scenario given in file *Params2.inp* does not correspond to any experiment.

File "*Naglib.lib*" is the part of NAG library, namely, (i) subroutine D02EAF which integrates the system of ordinary differential equations by the 4th order Runge-Kutta method, (ii) definite integral D01AH that we use in computations of transition rates.

Module "*mo1code3.for*" (i) defines size of arrays, gives parameters of database and computations,
(ii) explains the meaning of each parameter.

V. Info on display

On each step in time (denoted "*tstep*" in the source file), the code displays initial instant, t_i, of this *tstep*, parameters of each zone at $t = t_i$, namely, serial nunber of zone (b = 1, 2, 3 for BS, core, halo, respectively), outer radius of zone [cm], electron temperature [eV], mean absolute velocity of 3D motion of ions [cm/s], electron density [cm^{-3}], mean charge of ions of Fe, Cr, Ni, Mn.

Central time of k-th frame is denoted *FrP(k)*, duration of each frame is *FrL,* both given in file *Params2.inp*. If t_i is within k-th frame, i.e.

$$(FrP(k) - FrL/2) \le t_i < (FrP(k) + FrL/2), \qquad (V.1)$$

the k-th spectrogram is computed as spectral energy collected during k-th frame:

$$\mathrm{FrY}_\nu(k) = \sum_{j=1}^{jmax} tstep \cdot [\mathrm{P}_{\nu,\,hL}(t_i) + \mathrm{P}_{\nu,\,cL}(t_i)]; \qquad (V.2)$$

here j_{max} is the number of time steps during k-th frame, integer j counts these steps. In the code, *tstep* is constant, FrL is equal for all frames, therefore j_{max} is also equal for all frames. Restriction $tstep \le \mathrm{FrL}/10$ (see 3rd line in file *Params2.inp*) results in $j_{max} \ge 10$. The units of $\mathrm{FrY}(k)$ are [J/eV/sr]. In file *Frames.dat* the units are [J/keV/sr]. Spectral power radiated towards detector, $[\mathrm{P}_{\nu,\,hL}(t_i) + \mathrm{P}_{\nu,\,cL}(t_i)]$, is given by expressions (III.15), (III.20).

During each frame, i.e. for t_i that satisfies inequality (V.1), the code displays k, j.

VI. The output files

Files *"BSinfo.dat", "CoreInfo.dat", "HaloInfo.dat"* display parameters of plasma in each zone of XBV as functions of time [ns], namely: outer radius [cm], electron temperature [eV], mean absolute velocity [cm/s] of ions in their thermal+hydro motions inside a zone, number density of free electrons [cm^{-3}], mean ion charge "Z_{bar}", mean charge of ions of each chemical element, number density of ions of each chemical element [cm^{-3}]. Files *"...info.dat"* are convenient for graphic display of these parameters.

File "*LineList.dat*" is the list of spectral lines which have (i) their centers, $h\nu_c$, within 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* .
In file *LineList.dat*:

the 1st column displays serial number of chemical element,
the 2nd column displays spectroscopic symbol of the ion,
the 3rd column displays central energy of the line, $h\nu_c$ [eV],
the 4th column displays the wavelength of the line, λ_c [A],
the 5th column displays A_{ul} [s^{-1}],
the 6th column displays serial number of upper level (in file *QSs….inp*),
columns 7,8 displays electron configuration of this level,
the 9th column displays serial number of lower level (in *QSs….inp*),
columns 10,11 display electron configuration of this level,
the 12th column displays f_{lu}.

Files "*BSsLineInfo.dat*", "*CorLineInfo.dat*", "*HalLineInfo.dat*' display info on FWHM [eV] of spectral lines in corresponding zones. These files include only spectral lines which have (i) centers, $h\nu_c$, within 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 $h\nu_{min}$, $h\nu_{max}$, $f_{lu}Min$, $A_{ul}Min$ to be chosen in file *Params1.inp* .
In *files "...LineInfo.dat*":

column "hvCeV" displays $h\nu_c$ [keV],

column “XE” displays serial number of chemical element,
column “SpS” displays spectroscopic symbol of radiating ion,
column “Lambda” displays the line-center wavelength [A],
three columns “Upper” display serial number and electron configuration of upper level of this line,
three columns “Lower” display serial number and electron configuration of lower level of this line,
column “Gauss” displays FWHM of Gaussian distribution caused by u_{3D},
column “Baranger” displays FWHM of Lorentzian caused by uncertainty principle (in Baranger’ approach **[6]),**
column “Lorentz” displays FWHM of Lorentzian caused by either the uncertainty principle or Stark effect (bigger of two),
column “Voigt” displays FWHM of Voigh shape of the line,
column “PopUpper” displays population of the upper level, $n_{a,b,Up}/n_{a,b}$,
column “flu” displays the absorption oscillator strength f_{lu}.

File “*Frames.dat*” displays spectrograms taken in each frame. Spectral edges of the frames and instrumental resolution **to be given** in file *Params1.inp*. Timing and duration of the frames **to be given** in file *Params2.inp*. All frames are of equal duration “FrL” [ns]. In this file:
the 1st column gives the energy of photons [keV],
columns 2-9 display the radiation yield $Y_\nu(t)$ [J/eV/sr] gained due to one x-bright volume (XBV) during each of the eight frames,
the last column gives the radiation yield $Y_\nu(t)$ [J/eV/sr] gained due to one XBV during entire time of the computation.
For compatison to TREX frames the spectral power **should be multiplied** by spectral response of the TREX.

Files “*BSemiAbso.dat*”, “*CoreEmiAbso.dat*”, “*HaloEmiAbso.dat*” display plasma emissivity [W/eV/cm^3/sr] and plasma absorption coefficient corrected for stimulated emission [cm^{-1}] at t = “tiInf” given in file *Params2.inp*.
Column “hvKeV” displays full array of the photon energy points [keV].
Columns 2 - 5 display plasma emissivity: free-bound (due to radiative recombination), bound-bound (due to spectral lines),

free-free (that is radiation of free electrons),
total (i.e. the sum of these three).

Columns 6 - 9 display plasma absorption coefficient corrected for stimulated emission: bound-free (i.e. due to photoionization),
bound-bound (that is absorption in spectral lines),
free-free (that is absorption by free electrons),
total (i.e. the sum of these three).

Files "*PIR_Fe_BS.dat*", "*PIR_Fe_Core.dat*", "*PIR_Fe_Halo.dat*" display time along scenario [ns], $T_{e,b}$ [keV], $n_{e,b}$ [cm^{-3}], $n_{Fe,b}$ [cm^{-3}], ratio of the ground state ionization energy in plasma to its table value (*that for single ion*). Lowering of the ionization energy (the lowering of continuum) in plasma is taken in the Ion Sphere approach, see (II.7).

File "*EffSpIns.dat*" displays $J_{\nu,b}$ (t) [W/eV/sr/cm^2] that is space- direction-average spectral intensity of radiation in representative point (RP) of each zone at t = "tiInf" given in file "*Params2.inp*". Also shown is the contribution of each zone to $J_{\nu,b}$ (t).

Column "hvEV": photon energy [eV] .
Column "BS": $J_{\nu,BS}$ in RP of BS.
Column "SelfBS": contribution of BS itself to $J_{\nu,BS}$.
Column "ExteToBS": contribution of halo+core to $J_{\nu,BS}$, i.e. spectral intensity of halo+core radiation towards RP of BS, attenuated in BS on the path to the RP.
Column "Core": $J_{\nu,Core}$ in RP of the core.
Column "SelfCore": contribution of the core to $J_{\nu,Core}$.
Column "BSsToCor": contribution of BSs to $J_{\nu,Core}$, i.e. spectral intensity of radiation of N BSs towards RP of the core, attenuated in the core on the path to its RP.
Column "HaloToCor": contribution of halo to $J_{\nu,Core}$, i.e. spectral intensity of halo radiation towards RP of the core, attenuated in the core on the path to its RP.
Column "Halo": $J_{\nu,Halo}$ in RP of the halo.
Column "SelfHalo": contribution of the halo to $J_{\nu,Halo}$.

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

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

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

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

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

Note: for convenience of using Origin, zero is replaced with 1.e-24

Files "*ZpopsFe_BS.dat*", "*ZpopsFe_Core.dat*", "*ZpopsFe_Halo.dat*" display population of the last five ionization stages of **iron.** Sum over the stages = 1. Columns of these three files display time along the scenario [ns], $T_{e,b}$ [keV], $n_{e,b}$ [cm^{-3}], $n_{Fe,b}$ [cm^{-3}], population of Be-like, Li-like, He-like, H-like ions of iron, nuclei of iron.

In file "*PCDs.dat*" the 1st column gives time [ns] along scenario, next three columns give contribution of one XBV to the radiation power [W] to be shown by three absolutely calibrated diamond PCDs with kapton filters of 5-, 10-, 40-mils thickness (*in demo version of present code we used info known for PCDs used in Z shot 1520*). The last column gives the power [W] radiated by one XBV (no filters).

File "*PCDrespo.dat*" gives spectral response of diamond PCDs with kapton filters of 5-, 10-, 40-mils thickness (here PCDs used in Z shot 1520). The 1st column shows the photon energy [eV]. Columns 2 – 4 show spectral response of the PCDs in the interval ["hvMin" , "hvMax"]. $0 \le$ response ≤ 1. Output file "*PCDrespo.dat*" differs from input files "*Respo5milKapPCD. inp", "Respo10miKapPCD.inp", "Respo40miKapPCD.inp"* by number of hν points. In "*PCDrespo.dat*" the hν points are those of present computation, the response (columns 2-4) is calculated by interpolation between points of the input files.

If user wants to estimate time, t_{CRE}, required for plasma relaxation to CRE at certain parameters, he must prescribe these (constant) parameters to **all zones** (in file *Params2.inp*) and run the code with short time step, "*tstep*". Frames converge with $t \to t_{CRE}$. The computation should be repeated with 2x, 4x, 8x, ... shorter *tstep*, until dependence of t_{CRE} on *tstep* becomes negligible. Keep in mind that t_{CRE} is depends on (i) initial distribution of ions over energy levels, (ii) database of levels and cross-sections.

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

Widely used simple models of continuum lowering in plasma $\Delta I_{a,q,b}$ 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 that accounts these effects; therefore we have chosen the Ion Sphere model but modified it for plasmas of complex chemical composition.

In plasmas, each free electron moves in collective electric field of other free electrons and ions of different charge and mass. This rapidly-changing collective field complicates trajectories of free electrons. In neutral uniform plasma it results in uniform distribution of free electrons; then **the mean volume per free electron**

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

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

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

then the ion sphere radius

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

If ion A^{q+} is **solitary)**, then it can be treated as a point-like $A^{(q+1)+}$ with one electron bound in potential

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

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

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

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

$$\boldsymbol{\Delta I_{a,q,b} \approx e^2(q+1)/\zeta_{q,b} = 2\,(q+1)\,I_H\,\zeta_0/\zeta_{q,b}}\,. \qquad \text{(A.5)}$$

Here we used known relation $2I_H = e^2/\zeta_0$ where ζ_0 is Bohr radius.

Derived $\Delta I_{a,q,b}$ depends on the ion charge and electron density but does not depend on chemical and ionization composition of plasma, therefore expression (A.5) does not differ (*except factor* $^4/_3$) from result known for identical ions*; numeric factor ~1 is model-dependent, *see discussion in Ref.* **[6]**. Comparison of predicted $\Delta I_{q,b}$ to experimental data does not prove any model because their results (i) differ by less than factor 2, *see e.g. Figs 1, 2 in Ref.* **[12]**, (ii) differ in dependence on plasma density and temperature which in experiments are t, $\boldsymbol{r}$-dependent and have wide error bars.

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

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