

DICEBOX

VERSION 1.0

User Manual

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Preface

The code DICEBOX is intended to simulate γ decay of excited nucleus from a region of high level density where individual levels are not well known but still resolved. The code was written by František Bečvář in late 90's of 20th century [3]. The main feature of the code is the possibility to treat correctly expected fluctuations of transition intensities and actual number of levels. The code allows to check influence of these fluctuations that might be important, for a few examples see Refs. [17, 16, 21]. The present version of the code, prepared mainly by Milan Krtička and Stanislav Valenta, is a modification of the original one. The present version of the code allows simulation of γ cascades from individual well-resolved initial states (resonances) and from (off resonance) thermal neutron capture. Detailed description of the main features of the code can be found below in this manual and in Ref. [17].

DICEBOX falls in the category of GNU General Public License software. Please read the release conditions in Appendix A. Although we have invested a lot of effort in the validation of our code, we will not make the mistake to guarantee perfection. Therefore, in exchange for the free use of DICEBOX: If you find any errors, or in general have any comments, corrections, extensions, questions or advice, we would like to hear about it. You can reach us at milan.krticka@mff.cuni.cz. The webpage for DICEBOX is <https://www-nds.iaea.org/CRP-photonuclear/>.

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In addition to the GNU GPL terms we have a few requests:

- When DICEBOX is used for your reports, publications, etc., please make a proper reference to the code. The present version of the code is described in: M. Krtička, F. Bečvář, S. Valenta, Nucl. Instr. Methods A *in preparation*. The original version of the code was described in: F. Bečvář, Nucl. Instr. Methods A **417**, 434 (1998).
- Please inform us about, or send, extensions you have built into DICEBOX. Of course, proper credit will be given to the authors of such extensions in future versions of the code.
- Please send us a copy/preprint of reports and publications in which DICEBOX is used. This will help us to maintain the DICEBOX related bibliography.

1 Installation and getting started

1.1 DICEBOX package

The entire DICEBOX package can be downloaded from <https://www-nds.iaea.org/CRP-photonuclear/> web page. The package consists of the DICEBOX fortran77 source code, `dicebox_v1.0.for`, this User Manual and a few examples, which are described in Sec. 7 of this manual. Required disk space is very small, only a few MBytes. However, some space is usually needed for storing outputs of the code. An output file with list of 100,000 cascades can easily reach several tens of MBytes.

1.2 Installation

The installation of DICEBOX is very simple. Just compile the source file `dicebox_v1.0.for` with any fortran77 or fortran90 compiler. For instance, the simplest way of compilation using the standard gfortran compiler can be made by typing `gfortran dicebox_v1.0.for`. There is no need for any external libraries or files.

Several different compilers have been tested including `gfortran` (version 5.2.1) on Ubuntu, (version 4.8.1.) on Windows, (version 6.3.0) on Mac High Sierra, `Lahey/Fujitsu Fortran95` (version 5.50e) on Windows, (version L6.20e) on Red Hat and `Intel Fortran` on Windows compilers. If any other warning or error occurs during the compilation, please, let us know.

During testing the code with the `Intel Fortran` Windows compiler we have realized that to run the code with `LMODE=1` option, see Sec. 5.1, a “Stack Reserve Size” must be set to a value at least about 10,000,000. An order of magnitude lower (standard) value is enough for any other input values.

1.3 Running the code

To run the code just type the name of the executable file produced from the compilation. The code requires input files but they are not used as parameters as their names are fixed. When running the code all input files must be present in the same directory as the executable file. The input file `DICE_EV.DAT` must be present in all cases. If variable `IVER` is set to 2 in the input file `DICE_EV.DAT`, the input file `RES_PAR.DAT` is also required; for details see Secs. 5.1 and 5.2.

Depending on adopted models of photon strength functions – values of variables `NOPT1`, `NOPTM1`, `NOPT2` in `DICE_EV.DAT` input file – and level density – value of variable `NOPTDE` in `DICE_EV.DAT` input file, some additional files (`PSFE1.DAT`, `PSFM1.DAT`, `PSFE2.DAT`, `LDTAB.DAT`) might be required, see Secs. 5.3 and 5.4 (and perhaps also Sec. 6) for details.

1.4 Verification

The success of the compilation can be tested using examples described in Sec. 7 of this manual. Running the code with provided input files should produce exactly the same output files as stored in corresponding example directory as even the random number generator used in the code is incorporated in the package and it starts from the seeds listed in the input file `DICE_EV.DAT`. The only possible difference (on the fifth or so valid digit) can appear in a few numbers given in `DICE.PRO` output file that correspond to averages and square root of the variance of several calculated quantities. This is

a result of the use of single precision form during calculation of these numbers. As the single precision is used also for storing energies of levels, the level energies in files `EVENTS.Ssss.Rrrr` might also differ by 0.00001 MeV.

2 General comments on the code

2.1 Time requirements

Exact time for getting results strongly depends not only on the CPU speed but also on the simulated nucleus. Typical simulation of 10^5 cascades from a nucleus in the rare-earth region starting at initial excitation energy near the neutron separation energy S_n needs about 10 – 20 minutes. Substantial amount of time is spent on the calculation of internal conversion coefficients at the moment. Additional time (about 10 minutes) is required for preparation of the level scheme for each nuclear supra-realization, see Sec. 3, if `LMODE=1` option is used in the input file `DICE.EV.DAT`, see Sec. 5.1. Simulation of the decay of nuclei with lower number of levels is much faster.

2.2 Comment on code version

The present version of the code allows simulation of γ cascades from individual resonances and from (of resonance) thermal neutron capture. Another treatment of initial state would be possible but it is usually unique for a given reaction and requires a knowledge of the energy dependence of the flux of incident particles and the probability for production of initial levels with different spins and parities. These cases are not treated in the available version of the code.

The present version uses only one thread (CPU). Parallelism is possible and it would allow much faster production of results for different nuclear realizations, see Sec. 3, as the code could run on several CPUs. We hope that parallel version of the code will be available soon.

2.3 Use of COMMON blocks

Values of many variables are transferred among different functions and subroutines via “old-style” `COMMON` blocks in this fortran77 code. The variable names of each `COMMON` block are exactly the same in all occurrences of the given block in different functions and subroutines.

3 Algorithm

3.1 Assumptions

The assumptions of the algorithm of the modeling are based on the validity of the Statistical Model of nucleus and on other simplifying assumptions:

- The levels of the product nucleus are a result of discretization of some an *a priori* known level-density formula.
- Partial radiation widths for different initial and/or final states are statistically independent and uncorrelated.
- Below certain excitation energy E_{crit} a *complete level scheme* is known.
- In a general case, when mixing of various multipolarities is allowed by selection rules, the partial radiation width $\Gamma_{\alpha\gamma\beta}$ for a transition $\alpha \rightarrow \alpha'$, initializing at level α with excitation energy E_α in the interval $E_{\alpha_c} > E_\alpha > E_{\text{crit}}$, E_{α_c} being the initial cascade energy, that often corresponds to the neutron separation energy S_n , is assumed to be a random quantity whose value is given by

$$\Gamma_{\alpha\gamma\alpha'} = (1 + \alpha_{IC}) \sum_{XL} y_{\alpha\alpha'XL}^2 (E_\alpha - E_{\alpha'})^{2L+1} \frac{f^{(XL)}(E_\alpha - E_{\alpha'}, E_{\alpha'})}{\rho(E_\alpha, J_\alpha, \pi_\alpha)}. \quad (1)$$

Here, $f^{(XL)}$ is the photon strength function (PSF) for transition type X ($\equiv E$ for electric and $\equiv M$ for magnetic transitions) and multipolarity L , and $\rho(E_\alpha, J_\alpha, \pi_\alpha)$ is the nuclear level density (NLD) at initial excitation energy E_α for levels with spin J_α and parity π_α . The summation is, in principle, assumed over all allowed XL values for which the contribution is not negligible. In reality, with the exception of transitions below E_{crit} only $E1$, $M1$, and $E2$ transitions are considered at the moment. The quantities $y_{\alpha\beta XL}$ are random values drawn independently from the normal distribution with a zero mean and a unit variance, $y_{\alpha\beta XL} \in \mathcal{N}(0, 1)$. This distribution forces individual transition intensities to fluctuate according to the χ^2 distribution with one degree of freedom which is in nuclear physics also known as the Porter-Thomas (PT) distribution [18].

The coefficient α_{IC} gives the contribution of the internal electron conversion. Partial radiation width $\Gamma_{\alpha\gamma\alpha'}$ thus consists of two parts – one describes the probability for photon emission and the other part the additional conversion electron emission probability. The latter one is uniquely determined by γ -ray energy $E_\gamma = E_\alpha - E_{\alpha'}$ and multipolarity make up of the transition.

If the quantity $f^{(XL)}$ depends only on γ ray energy $E_\gamma = E_\alpha - E_{\alpha'}$ and is completely independent of any other quantity, it follows the so-called Brink hypothesis [7]. The hypothesis was originally formulated for the Giant Electric Dipole Resonance $E1$ transitions but it is often assumed to be valid also for other transition types and excitation modes. Many PSFs models proposed in the past obey the hypothesis but some of them introduce additional dependence of $f^{(XL)}$ on excitation energy of initial and/or final levels, which is indicated in the second parameter of $f^{(XL)}$ in Eq. (1).

The intensity distribution of transitions follows the PT distribution only from a well-separated initial level. Fluctuation of primary transition intensities in thermal neutron (off-resonance) capture, that can also be simulated with the present version of the code, do not necessarily obey the PT distribution but the distribution given by Eqs. (6) and (8), see Sec. 3.4. This distribution is correctly enough taken into account if IVER=2 in input file DICE_EV.DAT, see Sec. 5.1.

3.2 Concept of nuclear realizations and supra-realizations

Following these assumptions, levels in a simulated nucleus can be obtained from a random discretization of the adopted NLD formula. Partial radiation widths $\Gamma_{\alpha\gamma\alpha'}$ responsible for transition intensities between all pairs of these levels can then be drawn from the PT distribution (or distribution given by Eqs. (6) and (8)) around the expectation value governed by PSFs. In a typical case of a rare-earth deformed nucleus this set is represented by $10^{10} - 10^{13}$ partial radiation widths up to the neutron separation energy. There exist virtually infinite number of different possible realizations of these quantities for a single nucleus with a chosen NLD and PSFs models.

In some cases – typically when studying decay of individual neutron resonances – one might probe decay of several different initial states with almost the same energy in the same nucleus. To take into account different sources of fluctuations in such a case, we introduce here two terms: *nuclear realization* and *nuclear supra-realization*, see also [17].

The nuclear realization (NR) stands for the simulated system of all levels, including level positions and their decay probabilities. Different initial states with (almost) the same excitation energy (neutron resonances) will have different decay probabilities only for primary transitions. So, we define nuclear supra-realization (NSR) as a set of all nuclear realizations that have identical levels below the initial state and differ only in decay properties of initial state. Different neutron resonances would then correspond to different NRs within a NSR, see Ref. [17]. No transitions between different initial states are assumed in this approach – this assumption is fully justified. Within this concept there exist virtually infinite number of NRs within each nuclear supra-realization, whose number is also virtually infinite even for a fixed NLD and PSFs model. One of the simulated NRs is identical with the set of levels and partial radiations widths in a real nucleus. It is believed that such a NR can be obtained only with NLD and PSFs models what are close to reality.

3.3 Algorithm of the Method

Electromagnetic cascades resulting from a decay of a well-defined single initial state or from the initial state formed in the thermal neutron capture are generated within the above-mentioned assumptions using the following algorithm based on the Monte Carlo method, see also Ref. [17]:

1. The level density $\rho(E, J, \pi)$ is discretized to yield energies E_α , spins J_α and parities π_α of all levels α between the critical energy E_{crit} and the initial energy of the cascade E_{α_c} .

To do that the excitation energy between E_{crit} and E_{α_c} is divided into N_B intervals (given by the value of variable NBIN in DICE_EV.DAT file, see Sec. 5.1). Using one of the level density formulas, mentioned in Sec. 6.1, the actual number of levels

expected in each interval is obtained. In our statistical approach, the number of simulated levels can fluctuate around expectation values according to a statistical distribution. Several different approaches for obtaining the actual number of levels are available, see Ref. [17]. Three of them allow fluctuations of the actual simulated levels: Poisson (LMODE=0 in DICE_EV.DAT) and Wigner (LMODE=2) distributions of nearest-neighbor level spacing are at our disposal together with a distribution based on predictions of the theory of Gaussian Orthogonal Ensembles (GOE) (LMODE=1) which expects long-range correlations in level positions. There are also two additional approaches that do not involve any fluctuation in the number of simulated levels: The sequence of positions of levels is prepared under the assumption that the nearest neighbor spacing does not fluctuate (LMODE=-1 in DICE_EV.DAT), and an approach (LMODE=-2) in which the number of levels in each interval is calculated as a rounded value of the expectation number of levels. The last option serves mainly for some checks and is not recommended to be used for simulations of physically relevant cases.

As follows from the GOE theory, the nearest-neighbor spacing between levels in the statistical region is described with a high precision by the Wigner distribution. This distribution seems to be fully consistent with observations from neutron resonances in heavy nuclei. However, in the low-energy region this distribution may be violated and the level spacing could be better described by the Poisson distribution. Since the Poisson distribution produces larger fluctuations of numbers of levels in a fixed energy interval than the Wigner distribution or prediction from GOE do, estimates of fluctuations with the Poisson distribution may be slightly conservative/higher.

2. To each level α with excitation energy $E_{\alpha_c} > E_{\alpha} > E_{\text{crit}}$ a generator seed ζ_{α} is ascribed, see Fig. 1. For correct functioning of the algorithm it is crucial that these seeds are ascribed to individual generated levels randomly. The process of generating all partial radiation widths $\Gamma_{\alpha\gamma\alpha'}$ for a fixed level α is initialized only after the generator of random numbers is preset using the seed ζ_{α} . This implies that each time when a full set of partial radiation widths for a given decaying level α is needed, the *same* set of values of $\Gamma_{\alpha\gamma\alpha'}$ is prepared. As seeds ζ_{α} are available for all levels α with $E_{\alpha_c} > E_{\alpha} > E_{\text{crit}}$, a set of partial widths $\Gamma_{\alpha\gamma\alpha'}$ is *latently* known for all possible pairs of levels $\{\alpha\alpha'\}$. Seeds ζ_{α} thus predict uniquely the outcome of generating partial radiation widths. They represent a key element of the algorithm together with the deterministic character of the random number generators that allows generation of a definite sequence from a given seed.
3. The seed ζ_{α_c} is ascribed also to the capturing state. If states with two different spins contribute to the thermal neutron capture, independent seeds ζ_{α_c} are ascribed to both of them. Thermal neutron capture is simulated with the option IVER=1 or 2.
4. A full set of partial widths $\Gamma_{\alpha_c\gamma\alpha'}$ for transitions $\alpha_c \rightarrow \alpha'$, leading from the initial state α_c to all possible levels α' , $E_{\alpha'} < E_{\alpha_c}$, is generated. Prior this procedure the random number generator is preset using the seed ζ_{α_c} , attributed to the initial state of given J and π .

Further, total radiation width of the initial state α_c

$$\Gamma_{\alpha_c\gamma} = \sum_{\alpha'} \Gamma_{\alpha_c\gamma\alpha'} \quad (2)$$

is calculated. A set of branching intensities $I_{\alpha\alpha'}$ for all the transitions initiating at the initial state α_c are then obtained as

$$I_{\alpha_c\alpha'} = \Gamma_{\alpha_c\gamma\alpha'} / \Gamma_{\alpha_c\gamma}. \quad (3)$$

These branching intensities, that satisfy a normalization condition

$$\sum_{\alpha'} I_{\alpha_c\alpha'} = 1, \quad (4)$$

are then stored (for both initial spins if the decay following thermal neutron capture is simulated). If there is a contribution of initial states with two different spins to the thermal neutron capture, the set is obtained for both spins.

5. If the spin of the initial state α_c is not unique (IVER=1 or 2) in the off-resonance (thermal) s -wave neutron capture, the spin of initial state α_c is chosen. The contribution of both allowed spins to the thermal neutron capture can either be set manually (via variable CAPFR(1) in combination with IVER=1 in DICE_EV.DAT) or deduced from known energies and neutron and total radiation widths of resonances participating at the specified (thermal) neutron energy (IVER=2 in DICE_EV.DAT).
6. A level to which the initial state α_c decays is determined with help of a random number, say s_1 , yielded by another random number generator that generates random numbers from a uniform distribution on the interval $(0, 1]$. The Monte Carlo based choice of such final state, α_1 , follows from the requirement that

$$\sum_{\alpha'=1}^{\alpha_1-1} I_{\alpha_c\alpha'} < s_1 \leq \sum_{\alpha'=1}^{\alpha_1} I_{\alpha_c\alpha'}. \quad (5)$$

7. If excitation energy E_{α_1} of level α_1 is greater than E_{crit} , analogously to item 4 the partial radiation widths $\Gamma_{\alpha_1\gamma\alpha'}$ for a full set of transitions $\alpha_1 \rightarrow \alpha'$, leading from the level α_1 to all levels α' with $E_{\alpha'} < E_{\alpha_1}$, are generated together with total radiation width $\Gamma_{\alpha_1\gamma}$ and all branching intensities $I_{\alpha_1\alpha'}$. Prior this process the random number generator is preset using the corresponding seed ζ_{α_1} . As mentioned in Sec. 3.1, if E_{α_1} falls bellow E_{crit} , branching intensities $I_{\alpha_1\alpha'}$ are deduced exclusively from input data given in the file DICE_EV.DAT. By generating a random number s_2 and using branching intensities $I_{\alpha_1\alpha'}$, a second intermediate level, α_2 , to which the level α_1 decays, is chosen.
8. The simulation procedure, outlined in the the previous item, continues up to the moment when n -th step of the cascade reaches the ground (or isomeric) state. In the example in Fig. 1 the ground state is reached by the 4th step. Whenever the ground state is reached, all data characterizing a single cascade decay are available: energies E_{α_i} , spins I_{α_i} and parities π_{α_i} of all hit levels, as well as the transition types XL , transition multipolarity mixing ratios δ , and information whether the transition is irradiated via γ or conversion electron. Total radiation width $\Gamma_{\alpha\gamma}$ is also available for all levels above E_{crit} . All these parameters are at disposal for modeling a quantity of interest, for instance a γ -ray spectrum, multiplicity distribution, etc.

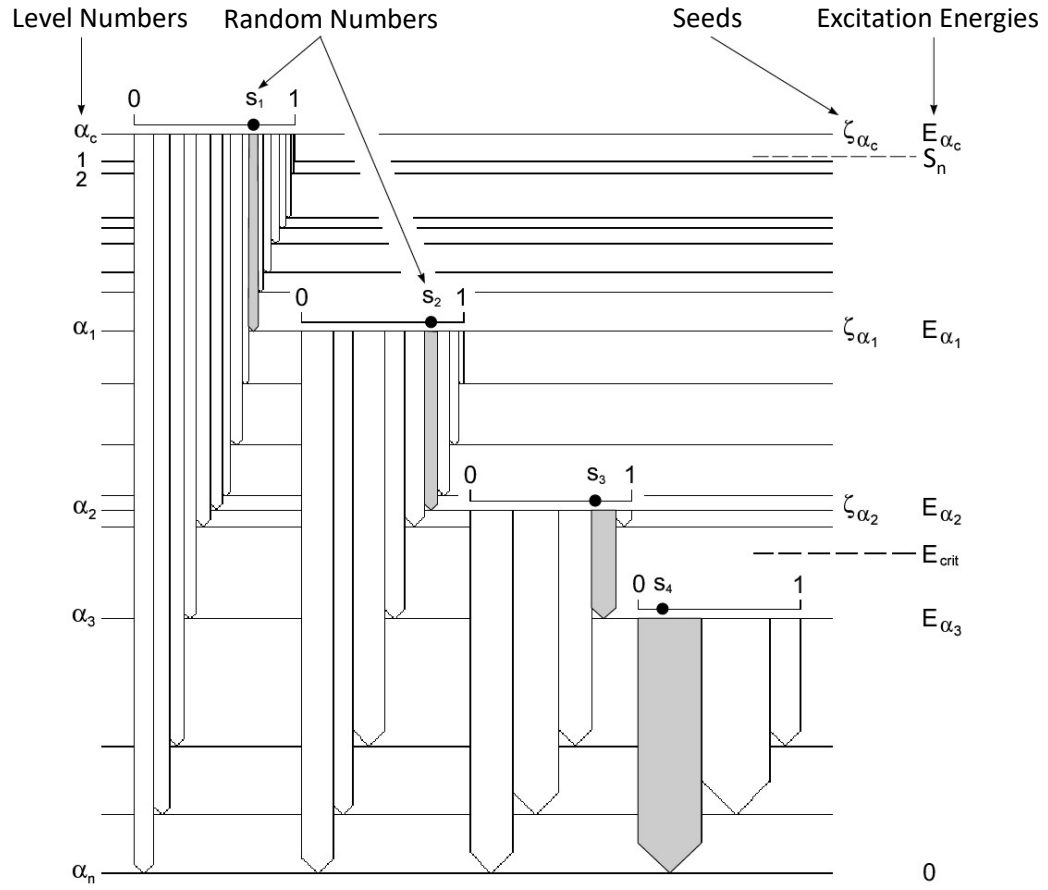


Figure 1: Schematic description of simulation of cascade process within a nuclear realization.

9. The procedure described in items 6-8 is to be repeated many times until satisfactory statistical accuracy of a modeled quantity of interest is achieved within a given nuclear realization. The number of cascades that should be simulated to reach a reasonable statistical accuracy of the estimate of the quantity of interest is discussed in [17] and typically reaches at least $10^5 - 10^6$.
10. To assess the role of the Porter-Thomas fluctuations of primary intensities within a NR, the algorithm described in items 3-9 is to be, at least in some cases, repeated several times. Depending on the character of the quantity of interest it might be sufficient to use only one nuclear realization within each nuclear supra-realization. However, nature of many quantities of interest requires at least a check of the behavior of different nuclear realizations within a nuclear supra-realization. The recommended number of simulated NRs is discussed in Ref. [17].
11. Finally, to assess also the role of the PT fluctuations of intensities of secondary transitions below initial state(s) and fluctuations due to the random discretization of the NLD used in different nuclear supra-realizations on the quantity of interest, the algorithm described in items 1-10 is to be repeated several times. Recommendations related to the number of simulated NSRs are again discussed in Ref. [17].

3.4 Intensity distribution from thermal neutron capture

Individual $\Gamma_{\alpha\gamma\alpha'}$ are expected to follow the PT distribution only for decays from well-resolved initial states. The distribution from the off-resonance capture can deviate from the (standard) PT distribution as wave functions from more states (neutron resonances in the case of thermal neutron capture which is discussed below) can contribute to the capture.

Let us consider transitions with a fixed multipolarity, i.e. with the same expectation value of $\Gamma_{\lambda\gamma\alpha'}$, to a single final state α' from a set of initial states (neutron resonances) λ having the same spin and parity. Assume further that the widths $\Gamma_{\lambda\gamma\alpha'}$ of these transitions are random variables that follow the PT distribution and that all the partial radiative widths of the initial states are uncorrelated. Now let several neutron resonances contribute to the thermal neutron capture cross section at neutron energy E_n . The intensity I_γ for the transition to a final state α' is

$$\begin{aligned}
I_\gamma &\approx \left| \sum_{\lambda} \frac{(\Gamma_{\lambda n} \Gamma_{\lambda\gamma\alpha'})^{\frac{1}{2}}}{(E_{\lambda} - E_n) + \frac{1}{2}i\Gamma_{\lambda}} \right|^2 = \\
&= \left| \sum_{\lambda} \frac{\Gamma_{\lambda n}^{\frac{1}{2}}}{(E_{\lambda} - E_n)^2 + \frac{1}{4}\Gamma_{\lambda}^2} [(E_{\lambda} - E_n) - \frac{1}{2}i\Gamma_{\lambda}] \Gamma_{\lambda\gamma\alpha'}^{\frac{1}{2}} \right|^2 = \\
&= \left| \sum_{\lambda} \frac{(E_{\lambda} - E_n) \Gamma_{\lambda n}^{\frac{1}{2}}}{(E_{\lambda} - E_n)^2 + \frac{1}{4}\Gamma_{\lambda}^2} \Gamma_{\lambda\gamma\alpha'}^{\frac{1}{2}} \right|^2 + \left| \sum_{\lambda} \frac{\Gamma_{\lambda}}{2} \frac{\Gamma_{\lambda n}^{\frac{1}{2}}}{(E_{\lambda} - E_n)^2 + \frac{1}{4}\Gamma_{\lambda}^2} \Gamma_{\lambda\gamma\alpha'}^{\frac{1}{2}} \right|^2. \quad (6)
\end{aligned}$$

Here, E_{λ} , $\Gamma_{\lambda n}$, and Γ_{λ} are the resonance energy, neutron width and total resonance width, which is – in the case that only elastic neutron scattering and radiative neutron

capture are possible – given by

$$\Gamma_\lambda = \Gamma_{\lambda_n} + \Gamma_{\lambda\gamma} = \Gamma_{\lambda_n} + \sum_{\alpha'} \Gamma_{\lambda\gamma\alpha'}. \quad (7)$$

The assumed PT distribution of widths $\Gamma_{\lambda\gamma\alpha'}$ is equivalent to the assumption that $\Gamma_{\lambda\gamma\alpha'}^{1/2}$ are random variables from normal distributions and zero means. Hence, the form of Eq. (6) implies that I_γ can be rewritten as

$$I_\gamma \approx f_{\alpha'}^2 + g_{\alpha'}^2 \quad (8)$$

where $f_{\alpha'}$ and $g_{\alpha'}$ are normally distributed, generally correlated, random variables with zero means.

Let us comment here on a few specific cases. If (i) $f_{\alpha'}^2 \gg g_{\alpha'}^2$ (or equivalently $E_\lambda - E_n \gg \Gamma_{\lambda}/2$) for all resonances or (ii) $f_{\alpha'}$ and $g_{\alpha'}$ are completely correlated – such a situation happens when one resonance makes the dominant contribution to both $f_{\alpha'}$ and $g_{\alpha'}$ – the intensities satisfy the PT distribution. On the other hand if (iii) $f_{\alpha'}^2 \approx g_{\alpha'}^2$ and $f_{\alpha'}$ and $g_{\alpha'}$ are independent the intensity distribution will be a χ^2 distribution with 2 degrees of freedom, i.e. the exponential distribution; this could happen if a weak resonance (with small Γ_{λ_n}) near the thermal neutron energy E_n dominates $g_{\alpha'}$ and strong resonances (with high Γ_{λ_n}) farther from E_n dominate $f_{\alpha'}$.

For all isotopes with target spin $J_T \neq 0$, two spin states can contribute to the thermal neutron capture cross section. Since the amplitudes for these two initial spins do not add coherently, the transition intensity is equal to the sum of two intensities, each of which satisfying Eq. (8). Thus, depending on the relative magnitudes of the two initial spin components, for most isotopes – corresponding to above-discussed cases (i) and (ii) – the distribution of intensities of the observed γ -ray lines following thermal neutron capture should be between χ^2 distribution with one and two degrees of freedom. However, in the extreme situation where resonances of both spins satisfy the conditions of case (iii), the distribution would be a χ^2 distribution with four degrees of freedom. The distribution given by Eq. (6) is used in simulations provided that IVER=2 in the DICE.EV.DAT input file.

3.5 Internal conversion coefficients

Internal conversion coefficients (ICCs) describe a probability, that the electromagnetic decay of a level does not proceed via emission of a photon but via a conversion electron. In this process the energy available for the electromagnetic transition is directly transferred to an electron on any atom orbit or converted to an electron-positron pair.

The conversion is usually described by the coefficient α_{IC} that gives the fraction of probability that the transition happens via the ICC instead of a photon emission. Total radiation width $\Gamma_{\alpha\gamma\alpha'}$ of an electromagnetic transition between levels α and α' can then be expressed as

$$\Gamma_{\alpha\gamma\alpha'} = 1 + \frac{\Gamma_{\alpha\gamma\alpha'}^{(e)}}{\Gamma_{\alpha\gamma\alpha'}^{(\gamma)}} \equiv 1 + \alpha_{IC}. \quad (9)$$

Here $\Gamma_{\alpha\gamma\alpha'}^{(e)}$ and $\Gamma_{\alpha\gamma\alpha'}^{(\gamma)}$ give the partial width (probability) for emission of an electron and a photon, respectively. If we restrict to one transition type and multipolarity XL ,

$\Gamma_{\alpha\gamma\alpha'}^{(\gamma,XL)}$ is given by, see also Eq. (1):

$$\Gamma_{\alpha\gamma\alpha'}^{(\gamma,XL)} = y_{\alpha\alpha'XL}^2 (E_\alpha - E_{\alpha'})^{2L+1} \frac{f^{(XL)}(E_\alpha - E_{\alpha'})}{\rho(E_\alpha, J_\alpha, \pi_\alpha)}. \quad (10)$$

The value of the coefficient α_{IC} for a transition with mixed multipolarity, i.e. $M1$ and $E2$ in our case, is

$$\alpha_{IC} = \frac{\alpha_{IC}(M1) + \delta^2 \alpha_{IC}(E2)}{1 + \delta^2} \quad (11)$$

where δ stands for the multipole mixing ratio

$$\delta^2 = \Gamma_{\alpha\gamma\alpha'}^{(\gamma,M1)} / \Gamma_{\alpha\gamma\alpha'}^{(\gamma,E2)}. \quad (12)$$

Total ICC can be expressed as

$$\alpha_{IC} = \alpha_{IC}^K + \alpha_{IC}^L + \alpha_{IC}^M + \dots + \alpha_{IC}^{ee} \quad (13)$$

where α_{IC}^X gives the probability for the conversion on the atomic shell X and α_{IC}^{ee} the probability for creation of an electron-positron pair. The present version of the code distinguishes electrons from K shell, i.e. α_{IC}^K , from other electrons. In reality, for some applications it might be more important to distinguish the emission of electron via electron-positron conversion than via the K -shell ICC. This is, in principle, possible if the tables corresponding to the K -shell electrons in the input file `DICE_EV.DAT` are replaced with the tables relevant for the electron-positron conversion.

A table of values of α_{IC}^X is a part of the input file `DICE_EV.DAT` and actual value of the coefficient α_{IC} is calculated via interpolating these values. If the energy of the transition is smaller than the first energy given in the input file, the α_{IC} corresponding to the first listed energy is used.

4 Structure of the code

4.1 Simplified structure of the code

Simplified, strongly restricted structure of the code reads:

```
! initialization of variables
CALL READ_EV('DICE_EV.DAT')
DO 55 NUC=1,NSREAL
  CALL LEVELS (...)
  CALL GERMS(IR2)
  CALL READ_INT('DICE_EV.DAT')
  DO IRL = 1, NRL
    IF (IPRIM.EQ.1) THEN
      IF (NLINC.GT.1) CALL READ_AGAIN('DICE_EV.DAT')
    ENDIF
    DO ILINC=1,NLINC
      CALL WIDTHS(...)
    ENDDO ! more sophisticated if primaries known

    DO 5 IEV=1,NEVENTS
      CALL ONESTEP(...)
      DO WHILE (EFI.GT.0.)
        CALL WIDTHS(...)
        CALL ONESTEP(...)
      ENDDO !WHILE EFI
      IF (ISWWR.EQ.1) CALL DO_IT(STEPS)
    5  CONTINUE
    ! updating output files
  ENDDO
55 CONTINUE
```

Parameters of the subroutines and functions were removed in this list.

4.2 Description of the most important functions and subroutines

The most important functions and subroutines are now listed together with their short description. The parameters are kept in this list. The order of subroutines and functions in this list is partially arbitrary.

General subroutines:

```
SUBROUTINE LEVELS(SPC,IR)
SUBROUTINE GERMS(IR)
SUBROUTINE WIDTHS (MODE,IPIN,SPIN,IBIN,ILIN,
  TOTCON,STCON,GACON,ISCON,TOTDIS,STDIS,GADIS,ISDIS)
SUBROUTINE ONESTEP
  (MODE,IPIN,SPIN,IBIN,ILIN,TOTCON,STCON,GACON,ISCON,TOTDIS,
  STDIS,GADIS,ISDIS,IPFI,SPFI,IBFI,ILFI,DMIX2,SIGN,IR,IRX)
```

- Subroutine **LEVELS**: Individual levels are created in the corresponding nuclear supra-realization based on the NLD model and chosen fluctuation properties.
- Subroutine **GERMS**: Seeds ζ_α , see Sec. 3.3, are assigned to all individual levels.
- Subroutine **WIDTHS**: Partial radiation widths for all individual transitions from an initial level are calculated according to Eq. (1) (or Eq. (8) for primary transitions from thermal neutron capture).
- Subroutine **ONESTEP**: Selection of the final level in a particular decay step is made.

Manipulation with input/output files:

```

SUBROUTINE READ_EV(NAME)
SUBROUTINE READ_INT(NAME)
SUBROUTINE READ_AGAIN(NAME)
SUBROUTINE READ_RES_PAR(NAME,En,SPINt)
SUBROUTINE OPEN_IT (INR)
SUBROUTINE DO_IT (NSTEP)
SUBROUTINE CLOSE_IT
SUBROUTINE WRITE_PARAMS(NAME)

```

- Subroutine **READ_EV**: All the information from the input file **DICE_EV.DAT** and if needed also from other input files is read.
- Subroutine **READ_INT**: Intensities of secondary transitions from levels below E_{crit} are read from **DICE_EV.DAT** file. Uncertainties in these intensities are used to generate different branching ratios in different nuclear supra-realizations.
- Subroutine **READ_AGAIN**: Intensities of primary transitions are read for each nuclear realization from **DICE_EV.DAT**. This subroutine is invoked only if the capturing energy is off an isolated resonance, i.e. capturing state spin is not unique and if intensities of primary transitions to levels below E_{crit} are known (**IPRIM=1**). Different ratios of intensities from resonances with different spins can thus be formed in different nuclear realizations.
- Subroutine **READ_RES_PAR**: Neutron resonance parameters are read from the input file **RES_PAR.DAT**. This subroutine is called only if **IVER=2**.
- Subroutine **OPEN_IT**: The output file **EVENTS.Ssss.Rrrr** (for given realization *rrr* and supra-realization *sss*) is opened for writing information on individual cascades.
- Subroutine **DO_IT**: Required information on the simulated cascade is written down to the output file **EVENTS.Ssss.Rrrr**.
- Subroutine **CLOSE_IT**: The output file **EVENTS.Ssss.Rrrr**, containing information on individual cascades, is closed.
- Subroutine **WRITE_PARAMS**: The subroutine writes basic information about models and used parameters to the output **DICE.PRO** file. Additional information on total radiation width of capturing state and populations of levels below E_{crit} also appears in the output file **DICE.PRO** but it is not written by this subroutine.

Functions related to level density and photon strength functions:

FUNCTION DENSITY(EEXC,SPIN,IPAR)

FUNCTION SGAMMA(EGAM,EINI,ITYP)

- Function DENSITY: The level density at given excitation energy for levels with given spin and parity is calculated.
- Function SGAMMA: Expectation value of the quantity $f^{(XL)} E_\gamma^{2L+1}$ for given E_γ (and excitation energy) is calculated. Several different functions can be called from this function.

Main auxiliary functions:

FUNCTION ALPH_TOT (EI,SPI,IPI,EF,SPF,IPF,DMISQ,NEN,ELEN,CONV)

FUNCTION AICC(ETRA,TABEN,TABICC,MAEL,MUL,N)

FUNCTION ITYPE(SPIN,IPIN,SPFI,IPFI)

FUNCTION RANO(ir)

FUNCTION NPOISS(IR,AM)

FUNCTION GAUSS(IR)

FUNCTION SEEDS(MODE,SP,IP,IL,IB)

- Function ALPH_TOT: The value of the electron conversion coefficient α_{IC} for the individual transition is calculated.
- Function AICC: The function is called from function ALPH_TOT and calculates the value of conversion coefficient α_{IC} for specified transition multipolarity via interpolation of the values listed in the table in the input file DICE_EV.DAT. A cubic interpolation in logarithmic scale is made using two higher and two lower E_γ values from the table.
- Function ITYPE: Determination of transition type – $E1$, $M1$ or $E2$.
- Function RANO: “Pseudo-random” generator of random numbers from a Uniform distribution on the $(0, 1]$ interval.
- Function NPOISS: Generation of a random number from the Poisson distribution.
- Function GAUSS: Generation of a random number from the Gaussian distribution.
- Function SEEDS: The function returns the value of the seed ζ_α .

5 Structure of Input and Output Data

5.1 Input File DICE_EV.DAT

A full set of READ statements of the subroutine DICE_EV for input from ASCII file DICE_EV.DAT is listed below. By this set a required file structure is uniquely given. As evident from this list, the exact structure of the input file DICE_EV.DAT depends on the value of variable IVER.

```
      READ (5,100) TITLE1
      READ (5,100) TITLE2
      READ (5,100) TITLE3
100  FORMAT (A80)
      READ (5,*)
      READ (5,*) IVER, IPRIM
      READ (5,*)
      READ (5,*) ISWWR, ISWBN, ISWEL, ISWSP, ISWPA, ISWIC, ISWMX, ISWWI, ISWLS
      READ (5,*)
      READ (5,*) NBIN, (IRINIT(I,1), I=1,4)
      READ (5,*)
      READ (5,*) NOPTFL, NOPTE1, NOPTM1, NOPTE2, NOPTDE, LMODE, LDENP
      READ (5,*)
      READ (5,*) NSREAL, NEVENTS, NRL
      READ (5,*)
      READ (5,*) NGIGE
      READ (5,*) (ER(I), W0(I), SIG(I), I=1, NCIGE)
      READ (5,*)
      READ (5,*) NGIGM
      READ (5,*) (ERM(I), W0(I), SIGM(I), I=1, NCIGM)
      READ (5,*)
      READ (5,*) NGIGE2
      READ (5,*) (ERE(I), WE0(I), SIGE(I), I=1, NCIGE2)
      READ (5,*)
      READ (5,*) DEG, DMG, QEL
      READ (5,*)
      READ (5,*) FERMC, EKO, EGZERO
      READ (5,*)
      READ (5,*) (PAR_E1(I), I=1,3)
      READ (5,*)
      READ (5,*) (PAR_M1(I), I=1,3)
      READ (5,*)
      READ (5,*) ASHELL, EONE, TEMPER, EZERO, AMASS, ZNUM, PAIRING
      READ (5,*)
      READ (5,*) ASHELL09, EONE09, TEMPER09, EZERO09, PAIRING09
      READ (5,*)
      READ (5,*) DENPC, (DENPEN(I), I=1,3)
      READ (5,*)
      READ (5,*) DENLO, DENHI, (DENPAR(I), I=1,4)
      READ (5,*)
```

```

IF (IVER.EQ.0) THEN
  READ (5,*) BN,SPINCS,IPINC
ELSEIF (IVER.EQ.1) THEN
  READ (5,*) BN,SPINT,IPINC,CAPFR(1)
ELSEIF (IVER.EQ.2) THEN
  READ (5,*) BN,SPINT,IPINC, En
  NAME_RES = 'RES_PAR.DAT'
  CALL READ_RES_PAR(NAME_RES,En,SPINT)
ENDIF
READ (5,*)
READ (5,*) XRAYK,XRAYL
READ (5,*) NMU
READ (5,*) NENT
READ (5,*) (ELENK(K),K=1,NENT)
READ (5,*) (((CONVT(ITY,MU,K),MU=1,NMU),ITY=0,1)K=1,NENT)
READ (5,*) NENK
READ (5,*) (ELENK(K),K=1,NENK)
READ (5,*) (((CONVK(ITY,MU,K),MU=1,NMU),ITY=0,1)K=1,NENK)
READ (5,*)
READ (5,*) ECRIT
READ (5,*)
READ (5,*) FACTNRM
READ (5,*)
READ (5,*) NUMLEV
DO I=1,NUMLEV
  IF (IVER.EQ.0) THEN
    READ (5,*) ENRG,SPFI,IPFI,DENUM(I)
  ELSE
    READ (5,*) ENRG,SPFI,IPFI,DENUM(I),PRIM,ERRPRIM
  ENDIF
  IF (DENUM(I).GT.0)
    DO K=1, DENUM(I)
      READ (5,*) (ENRGF(K),SAL(K),ERRSAL(K),DESP(K),IPAR(K),
*          DMIX(K),ALPHA(K),K=1,DENUM(I))
    ENDDO
  ENDIF
ENDDO

```

The meaning of individual variables involved in these READ statements is as follows:

Global variables:

TITLE1 thru TITLE3 – CHARACTER*80 variables filled with arbitrary text information.

These three variables are not used in the the rest of the code.

IVER – the INTEGER switch specifying the capturing state properties. The value IVER=0 allows simulations of γ cascades starting from a well isolated level at initial energy given by variable BN with specific spin and parity given by variables SPINCS and

IPINC, respectively. This option typically describes a decay of individual (neutron) resonances.

Values IVER=1 and 2 allow to simulate cascades from initial energy which does not necessarily correspond to an individual state. This typically corresponds to the thermal neutron capture. However, non-zero values of IVER can be, in principle, used in a broader variety of cases.

The value IVER=1 allows simulation of decay of states at energy variable BN with specified contribution of two initial spins (that differ in J by unity and has the same parity). The fluctuation of intensities of primary transitions is governed by the PT fluctuation from each resonance spin in this case. The choice of initial states with the same parity that differ in J by unity corresponds exactly to the situation happening in the thermal neutron capture.

The value IVER=2 then simulates the decay of “initial state” which is formed by contribution from several s -wave neutron resonances. Parameters of the contributing resonances are specified in input file RES_PAR.DAT. Fluctuations of primary transitions are not exactly governed by the Porter-Thomas distribution in this case but they follow the distribution given by Eq. (6).

It is important to note again that the structure of the input file DICE_EV.DAT related to properties of capturing state – see the list of READ statements starting with IF (IVER.EQ.0) THEN – depend on the value of IVER; see also the corresponding section of the description of the structure of this input file below (Specification of initial state).

IPRIM – the INTEGER switch specifying treatment of primary transitions to levels below excitation energy E_{crit} (variable ECRIT). The value IPRIM=0 means that intensities of these primary transitions are unknown. This is a typical situation when individual initial states (resonances) are the subject of decay. All individual primary transitions are then calculated using Eq. (1).

If IPRIM=1, the intensities of primary transitions (per decay) to levels below excitation energy E_{crit} are assumed to be known and are read via variable PRIM. Intensities of primary transitions (in units per neutron capture) to low-lying levels below E_{crit} are often known in thermal neutron capture.

ISWWR – the INTEGER switch that controls the writing of information on each cascade. Selecting ISWWR=1 the files EVENTS.Ssss.Rrrr, containing information about cascades, are produced. For all other cases the files are not created. Here, symbols sss and rrr stand for the three-digit integer numbers specifying the nuclear supra-realization and nuclear realization, respectively. Standard choice for many applications should be ISWWR=1. The choice ISWWR \neq 1 makes values of the following switches, ISWBN, ..., ISWWI, unimportant as information on individual cascades is not written.

ISWBN – the INTEGER switch that controls the mode of writing the output files EVENTS.Ssss.Rrrr.

The value ISWBN=0 selects the ASCII mode, while for ISWBN=1 these files are produced in the UNFORMATTED mode. The latter possibility can save some disc space but the exact file format then depends on the operating system and used FORTRAN compilers.

- ISWEL – the INTEGER switch. Selecting ISWEL=1 the information on energies of levels populated in individual cascades is included in the output files `EVENTS.Ssss.Rrrr`, while use of ISWEL \neq 1 disables writing this information.
- ISWSP – the INTEGER switch. Selecting ISWSP=1 the information on spins of levels populated in individual cascades is included in the output files `EVENTS.Ssss.Rrrr`, while use of ISWSP \neq 1 disables writing this information.
- ISWPA – the INTEGER switch. Selecting ISWPA=1 the information on parities of levels populated in individual cascades is included in the output files `EVENTS.Ssss.Rrrr`, while use of ISWPA \neq 1 disables writing this information.
- ISWIC – the INTEGER switch. Selecting ISWIC=1 the information about the type of emitted particle (γ or conversion electron) in individual cascade steps is included in the output files `EVENTS.Ssss.Rrrr`, while use of ISWIC=0 disables writing this information; see Sec. 5.5 for more details.
- ISWMX – the INTEGER switch. Selecting ISWMX=1 the information on multipolarity mixing ratios δ for individual cascade steps is included in the output files `EVENTS.Ssss.Rrrr`, while use of ISWMX \neq 1 disables writing this information.
- ISWWI – the INTEGER switch. Selecting ISWWI=1 the information on total radiation widths of levels populated in individual cascades is included in the output files `EVENTS.Ssss.Rrrr`, while use of ISWWI \neq 1 disables writing this information. Total radiation width is set to zero if the decaying level is below E_{crit} .
- ISWLS – the INTEGER switch that controls writing of information on all levels generated in individual nuclear supra-realizations. Selecting ISWLS=1 the files `LEVELS.sss`, containing information about all levels in the supra-realization `sss` are produced. For all other values of ISWLS the files are not created; see Sec. 5.7 for more details.
- NBIN – the INTEGER number N_B of bins used for discretization of level density above E_{crit} , see item 1 of Sec. 3.3. The bin width can be obtained as $(\text{BN-ECRIT})/\text{NBIN}$. The maximum allowed number is 700 at the moment. This maximum allowed number is given by the variable MAXBIN. The recommended value of NBIN partly depends on the way how individual levels are generated, i.e. on the value of LMODE, see discussion of influence of results for different approaches for generating individual levels in Ref. [17]. In general, the recommended value is to have a bin width of about 10 – 20 keV in heavy nuclei.
- IRINIT(I,1)-IRINIT(I,4) – INTEGER*4 initial seeds of 4 independently running random generators used in the code. These seeds are used to generate sets of four seeds for each nuclear realization. The seeds IRINIT(I=1,.) are responsible for discretization of level-density formula and generation of individual levels within individual nuclear supra-realizations, the seeds IRINIT(I=2,.) govern random generating of all widths $\Gamma_{\alpha\gamma\alpha'}$ via seeds ζ_α , see Sec. 3.3, while IRINIT(I=3,.) serve for generating individual cascades. The last seeds set, IRINIT(I=4,.) is used for generating multipole mixing ratios δ .
- NSREAL – the INTEGER variable specifying the number of simulated nuclear supra-realizations. The maximum allowed number is 999 at the moment.

NRL – the **INTEGER** variable specifying the number of simulated nuclear realizations within each nuclear realization. The maximum allowed number is 999 at the moment.

For many applications, it might be reasonable to use $\text{NRL}=1$. In general, for obtaining meaningful results on fluctuations, the product of values of **NSREAL** and **NRL** should equal at least to several tens. For detailed discussion of the recommended number of simulated nuclear realizations see Ref. [17].

NEVENTS – the **INTEGER** number of generated cascades in each nuclear realization. The recommended value is, in general, at least around 10^5 . However, it is recommended to check Ref. [17] for more detailed discussion of this number.

Specification of initial state:

BN – the **REAL** energy of initial state expressed in units of MeV. In the case of the simulation of the radiative neutron capture it should correspond to the sum of the neutron separation energy and the energy of incident neutron.

IPINC – the **INTEGER** parameter characterizing the parity of the capturing state. Values $\text{IPINC}=0$ and 1 correspond to the positive and the negative parity, respectively. If the spin of the target nucleus is specified instead of the spin of the initial state ($\text{IVER}>0$), it is always assumed that the parity of the initial state is the same as the parity of the target nucleus.

SPINCS – the **REAL** spin of the initial state of the cascade J (which often corresponds to the spin of an individual resonance). This variable is used only if $\text{IVER}=0$; the variable **SPINT** is used for other values of **IVER**. If J is a half-integer number its value should be given in the form 0.5, 1.5, etc.

SPINT – the **REAL** spin of the target nucleus J_T (for s -wave neutron capture). This variable is used only if $\text{IVER}=1$ or 2. Spins of the two initial states in thermal neutron capture (J) then correspond to $J_T \pm 1/2$ (or $J_T + 1/2$ if $J_T = 0$). If J_T is a half-integer number its value should be given in the form 0.5, 1.5, etc.

En – the **REAL** energy of incoming neutrons in eV. This variable is used only with $\text{IVER}=2$ value, typically for the simulation of thermal neutron capture where $E_n \simeq 0.025$ eV.

CAPFR(1) – the **REAL** variable which is used only for $\text{IVER}=1$, i.e. for off-resonance (thermal neutron) capture where two possible spins with $J = J_T \pm 1/2$ contribute (if $J_T > 0$); the value of J_T is stored in variable **SPINT**. Value of **CAPFR(1)** defines the fraction of captures on resonances with lower of the two possible spins, i.e. those with $J = J_T - 1/2$. If $J_T = 0$, the **CAPFR(1)** is set automatically to 1.0 in the code which means that all decays start from $J = 1/2$ initial state.

Setting **CAPFR(1)=0.0** and **1.0** the captures exclusively via $J = J_T + 1/2$ and $J = J_T - 1/2$ states are chosen, respectively. These choices are equivalent to use of $\text{IVER}=0$ with the selected value of the resonance spin J . In reality, use of values **CAPFR(1)>0.999** and **CAPFR(1)<0.001** in the input file leads to use of values **CAPFR(1)=1.0** and **CAPFR(1)<0.0** in the code, respectively.

Parameters related to the photon strength functions:

NOPTFL – the INTEGER switch controlling the fluctuations of individual partial radiation widths. For NOPTFL=0 fluctuations of partial radiation widths are disabled, while in case of NOPTFL=1 these quantities fluctuate according to Porter-Thomas distribution. It is to be noted that if IVER=2, the fluctuations of primary transitions are not governed exactly by Porter-Thomas distribution but by a distribution given by Eq. (6).

NOPT1 – the INTEGER option serving for the choice of the $E1$ PSF $f^{(E1)}(E_\gamma, .)$. List of individual options can be found in Sec. 6.2.

NOPTM1 – the INTEGER option serving for the choice of the $M1$ PSF $f^{(M1)}(E_\gamma)$. List of individual options can be found in Sec. 6.3.

NOPT2 – the INTEGER option serving for the choice of the $E2$ PSF $f^{(E2)}(E_\gamma)$. List of individual options can be found in Sec. 6.4.

NGIGE – the INTEGER number of resonance $E1$ terms (usually corresponding to the Giant Electric Dipole Resonance) of the sum on the right-hand sides of several equations in Sec. 6.2; see description of individual models in that section. The resonance terms are not used in all the models. If they are not used, this number can be arbitrary but must in any case correspond to the number of lines with resonance parameters explained just below. Maximum value of NGIGE is 5 at the moment.

ER(5), W0(5) and SIG(5) – the REAL parameters E_{Gi} , Γ_{Gi} and σ_{Gi} specified in Sec. 6.2, respectively. Values of ER(I) and W0(I) are to be given in units of MeV; values of the maximum peak cross section SIG(I) then in units of mb.

NGIGM – the INTEGER number of resonance $M1$ terms of the sum on the right-hand sides of equations in Sec. 6.3; see description of individual models in that section. The resonance terms are not used in all the models. If they are not used, this number can be arbitrary but must in any case correspond to the number of lines with resonance parameters explained just below. Maximum value of NGIGM is 5 at the moment.

ERM(5), WM0(5) and SIGM(5) – the REAL parameters E_{Mi} , Γ_{Mi} and σ_{Mi} specified in Sec. 6.3, respectively. Values of ERM(I) and WM0(I) are to be given in units of MeV; values of the maximum peak cross section SIGM(I) then in units of mb.

NCIGE2 – the INTEGER number of resonance $E2$ terms of the sum on the right-hand sides of equations in Sec. 6.4. The resonance terms are not used in all the models. If they are not used, this number can be arbitrary but must in any case correspond to the number of lines with resonance parameters explained just below. Maximum value of NCIGE2 is 5 at the moment.

ERE(5), WE0(5) and SIGE(5) – the REAL parameters E_{Ei} , Γ_{Ei} and σ_{Ei} specified in Sec. 6.4, respectively. Values of ERE(I) and WE0(I) are to be given in units of MeV; values of the maximum peak cross section SIGE(I) then in units of mb.

DEG – the REAL parameter k_{E1} , expressed in units of MeV^{-3} , used in a few $E1$ PSF models, see Sec. 6.2. If this parameter is not used in the selected $E1$ PSF model, its value can be arbitrary.

DMG – the REAL parameter k_{M1} , expressed in units of MeV^{-3} , used in a few $M1$ PSF models, see Sec. 6.3. If this parameter is not used in the selected $M1$ PSF model, its value can be arbitrary.

QEL – the REAL parameter k_{E2} , expressed in units of MeV^{-5} , used in a few $E2$ PSF models, see Sec. 6.4. If this parameter is not used in the selected $E2$ PSF model, its value can be arbitrary.

FERMC – the dimensionless REAL parameter F_K , introduced in Eq. (30), see Sec. 6.2.

EKO, **EGZERO** – the REAL parameters k_0 and E_γ^0 introduced in Eq. (32), see Sec. 6.2, respectively. The parameter k_0 is dimensionless, while E_γ^0 is expressed in units of MeV.

PAIRING – the REAL parameter E_P , expressed in units of MeV, introduced in Eq. (33), see Sec. 6.3.

PAR_E1(3), – REAL parameters used in some models of $E1$ PSF. The exact meaning of these parameters differs among different $f^{(E1)}$ models, see description of individual models in Sec. 6.2.

PAR_M1(3), – REAL parameters used in some models of $M1$ PSF. The exact meaning of these parameters differs among different $f^{(M1)}$ models, see description of individual models in Sec. 6.3.

Parameters related to nuclear level density:

NOPTDE – the INTEGER option whose value determines the level density formula to be used. Individual options are specified in Sec. 6.1.

LMODE – the INTEGER switch fixing the fluctuation in the actual number of levels of the same spin and parity in individual nuclear supra-realizations. These fluctuations are closely related to the distribution of spacings between neighboring levels of same spin and parity.

In case of **LMODE=0** these fluctuations are assumed to follow Poisson distribution, while **LMODE=1** uses the prediction of level positions based on the predictions of random matrix theory, specifically of Gaussian Orthogonal Ensemble (GOE). The GOE predicts Wigner distribution of the nearest-neighbor spacings and long-range correlation in positions of individual levels. It is also possible to use **LMODE=2**, which takes into account Wigner distribution of nearest-neighbor spacings but no long-range correlations, **LMODE=-1** that switches completely off all the fluctuations of nearest-neighbor spacings, or **LMODE=-2** where the number of levels in each of N_B bins is calculated as a rounded value of the expectation number of levels in the bin. The number of levels in individual bins will be the same in all nuclear supra-realizations for **LMODE=-1** and **LMODE=-2**. The option **LMODE=-2** was added mainly for checks and is not recommended to be used. For expected differences among different approaches see discussion in Ref. [17].

LDENP – the INTEGER switch whose value specifies a use of parity dependence of the level density formula at excitation energies above E_{crit} . Using **LDENP=0**, no parity dependence is assumed, i.e. there is the same number of levels of both parities

in the whole energy range above E_{crit} . Selecting **LDENP=1** the parity dependence proposed by Al-Quraishi [1] and given by Eq. (27) is used, see Sec. 6.1.2. Finally, the value **LDENP=2** allows to use the excitation-energy dependence given by Eq. (27) but with the parameters defined by users, see Eq. (27) and Sec. 6.1.2.

ASHELL, **EONE**, **TEMPER** and **EZERO** - the **REAL** parameters a , E_1 , T and E_0 , respectively, as used in some of NLD models specified in Sec. 6.1.1. Parameters **EZERO**, **EONE** and **TEMPER** are assumed to be expressed in units of MeV, while **ASHELL** in MeV^{-1} . For parameters used in NLD models corresponding to **NOPTDE=8** and **9**, see next item.

ASHELL09, **EONE09**, **TEMPER09**, **EZERO09**, and **PAIRING09** - the **REAL** parameters a , E_1 , T , E_0 , and P_{09} respectively, as used in level density models **NOPTDE = 8** and **9** introduced in Sec. 6.1.1. Parameters **EZERO09**, **EONE09**, **TEMPER09** and **PAIRING09** are assumed to be expressed in units of MeV, while **ASHELL09** in MeV^{-1} .

Please, note that parameters a , E_1 , T and E_0 appear two times in the input file. However, their values (stored in variables explained in this and previous item) are used in different level density models. Both sets are used in the input file to avoid retyping them if different level density models (different values of the option **NOPTDE**) are used.

AMASS – the **REAL** mass number (number of nucleons) A of the compound nucleus.

ZNUM – the **REAL** proton number Z of the compound nucleus.

DENPC and **DENPEN(3)** – the **REAL** variables C_π and $F_\pi^{(i)}$, $i = 1, 2, 3$, respectively, as defined in Eqs. (27) and (28) in Sec. 6.1.2. These variables are used for calculation of the level density for each parity if option **LDENP=2** is chosen. Variable C_π is given in units of MeV^{-1} , $F_\pi^{(1)}$ and $F_\pi^{(2)}$ in MeV and $F_\pi^{(3)}$ is dimensionless. If **LDENP=0** or **LDENP=1**, these coefficients can be arbitrary as they are not used in simulations.

DENLO, **DENHI** – the **REAL** energies E_L and E_H used in some level density models specified in Sec. 6.1.1, including relatively standard models under options **NOPTDE=8** and **9**.

DENPAR(4) – the **REAL** coefficients $D_p^{(i)}$, $i = 1, \dots, 4$ used if **NOPTDE=2** or **3**, see Sec. 6.1.1.

Parameters related to discrete levels below E_{crit} :

ECRIT – the **REAL** critical energy E_{crit} , expressed in MeV. Statistical approach is applied to generate levels and transition intensities at excitation energies $E > E_{\text{crit}}$ while for levels below E_{crit} all the information is to be taken from available literature data. The value of E_{crit} should be chosen to assure that the level scheme –including level energies, spins and parities as well as branching ratios – is complete below this energy (in the relevant spin/parity window).

FACTNRM – the **REAL** dimensionless scaling factor of primary intensities to levels below E_{crit} if these intensities are known. The value of this factor is used only with the **IPRIM=1** switch. If the code runs with **IPRIM=0**, the value of this factor can be arbitrary.

This factor was build into the code only for user's comfort – using this factor it is not necessary to recalculate intensity of each primary transition (variable PRIM) available in literature to absolute values per neutron capture used by the code. One can only copy the intensities from literature, which are often not expressed in units per one capture, to the input file and the absolute intensities in units per neutron capture can then be obtained for all the transitions at the same time. The absolute intensity of the primary transition per neutron capture is given by the product of variables FACTNRM and PRIM; see also text related to variable PRIM.

NUMLEV – the INTEGER number of all levels below E_{crit} , including the ground state. The maximum permissible value is 99 at the moment. In addition, it is not allowed to have more than 30 levels with the same spin and parity below E_{crit} .

ENRG(99), SPFI(99), IPFI(99) and DENUM(99) – the variables referring to the individual levels below E_{crit} . Variables IPFI and DENUM are INTEGER, while remaining ones are REAL ones. Elements ENRG(I), SPFI(I), IPFI(I) and DENUM(I) represent the excitation energy in MeV, spin, parity and the number of depopulating transitions of the level. If the SPFI(I) is a half-integer number its value should be given in the form 0.5, 1.5, etc. The number of de-exciting transitions of a given level (variable DENUM) must be smaller or equal to 20.

Values IPFI(I)=0 and 1 represent positive and negative parities, respectively. Values of ENRG(I) should be listed in increasing order.

PRIM(99) and ERRPRIM(99) – intensities and their uncertainties, respectively, of primary transitions feeding individual levels below E_{crit} . These variables are read only if IPRIM=1 and can be given in “arbitrary” units. The absolute intensity of primary transitions per neutron capture, that is used by the code, is given by the product of variables FACTNRM and PRIM. If values of PRIM are given in intensities per neutron capture, the value of FACTNRM has to be equal to unity. If uncertainties are unknown, it is strongly recommended to use 0.0 value for them. In fact, values of ERRPRIM are not used in the present version of the code.

ENRGF, DESP, IPAR, SAL, ERRSAL, ALPHA and DMIX – variables referring to each depopulating transition of a given initial level with energy ENRG(I). The variable IPAR is INTEGER, while the remaining ones are REAL.

Variables ENRGF, DESP, IPAR, SAL, ERRSAL, ALPHA and DMIX stand for the excitation energy of a final level in MeV, its spin and parity, the dimensionless depopulating intensity and its error, the value of internal conversion coefficient α_{IC} , see Eq. (1) and Sec. 3.5, and the values of multipole mixing ratio δ (in the Rose-Brink convention), respectively. The convention for parity IPAR is identical with that for the variable IPFI. If DESP is a half-integer number its value should be given in the form 0.5, 1.5, etc.

The number of lines with the set of these variables for each initial level has to be equal to the value of variable DENUM. It is recommended to have individual lines corresponding to de-exciting transitions of the level with initial energy ENRG ordered increasingly in energy ENRGF.

Branching intensities SAL can be given in arbitrary units. However, all these intensities must be positive, i.e. higher than zero. The errors of the intensities of

secondary transitions `ERRSAL(I)` are used for calculation of branching intensities in individual nuclear supra-realizations. If `ERRSAL(I)=0.0` for all transitions de-exciting the level with energy `ENRG`, the branching intensities are the same for all nuclear supra-realizations.

If the value of the conversion coefficient α_{IC} is for a given transition unknown from previous experiments, it is recommended to use `ALPHA=0.0`. In such a case, the α_{IC} is calculated in the code using information on E_γ and δ (variable `DMIX`), see Eq. (11).

Energy of the same level below E_{crit} often appears several times in the input data – as `ENRG` and then possibly several times as `ENRGF`. It is important to note that energies of the same level at different places in the input file has to differ by less than 0.00001 MeV!

Data needed for internal conversion coefficients calculation:

`XRAYK`, `XRAYL` – the `REAL` electron binding energy (in MeV) for K and L shells in atoms containing the nuclei of interest. In reality, these energies are not used for calculation of any quantity in the present version of the code. So, they can be arbitrary at the moment.

`NMU` – the `INTEGER` parameter, representing the highest multipolarity, L , for which the electron internal conversion coefficients (ICCs) are tabulated. The maximum permissible value is 5. Conversion coefficients α_{IC} can be obtained from the BRICC database [12] up to $L = 5$.

`NENT` – the `INTEGER` parameter, representing the number of transition energies for which total ICCs α_{IC} are tabulated just below in the input file, see variables `ELENT` and `CONVT`. The maximum permissible value of `NENT` is 50 at the moment.

`ELENT(50)` – the `REAL` array of transition energies (in units of MeV) for which the values of total ICC α_{IC} are stored in the array `CONVT`. The energies should be listed in the increasing order. The lowest energy should be smaller (or at least very similar) to a width of each bin given by `(BN-ECRIT)/NBIN`.

`CONVT(0:1,5,50)` – the `REAL` array, whose elements carry values of total ICCs coefficients α_{IC} . For definition of the coefficient see Sec. 3.5. The element `CONVT(ITY,MU,K)`, occurring in the above-shown set of `READ` statements, represents the ICC for the type of radiation `ITY`, the multipolarity `MU` and the transition energy `ELENT(K)`. Here, `ITY=0` and `ITY=1` correspond to electric and magnetic type of radiation, respectively. The value `MU=1` stands for the dipole radiation ($L = 1$), `MU=2` for the quadrupole radiation ($L = 2$), etc.

`NENK` – the `INTEGER` parameter, representing the number of transition energies for which K -shell ICCs are tabulated just below in the input file, see variables `ELENK` and `CONVK`. The maximum permissible value of `NENK` is 50 at the moment.

`ELENK(50)` – the `REAL` array of transition energies (in MeV) for which the values of K -shell ICC α_{IC}^K are stored in the array `CONVK`. The energies should be listed in the increasing order.

`CONVK(0:1,5,50)` – the REAL array, whose elements carry values of K-shell ICCs coefficients α_{IC}^K . For definition of the coefficient see Sec. 3.5. The element `CONVK(ITY,MU,K)`, occurring in the above-shown set of READ statements, represents the ICC for the type of radiation ITY, the multipolarity MU and the transition energy ELENK(K). Here, ITY=0 and ITY=1 correspond to electric and magnetic type of radiation, respectively. The value MU=1 stands for the dipole radiation ($L = 1$), MU=2 for the quadrupole radiation ($L = 2$), etc.

General remarks to the input data:

- All energies in the input data, with the exception of the neutron energy (variable `En`), should be given in units of MeV! This requirement was each time noticed in the above-given description of the variables.
- Energy of a discrete level can occurs several times (as `ENRG` and `ENRGF` variables) in the input data. For correct functioning of the code it is important that numerical representation of this energy is in all these cases *identical*. More precisely their values must differ by less than 0.00001 MeV.
- Further, energies of any pair of different levels should differ by more than 0.00001 MeV.

5.2 Input File RES_PAR.DAT

This input file is required only if option `IVER = 2` is used in `DICE_EV.DAT` file. In such a case it is assumed that the initial state comes from *s*-wave neutron capture. Contribution of neighboring resonances at the neutron energy E_n (variable `En`) is calculated and the fluctuation properties of primary transitions are determined using Eq. (6). This distribution might differ from the Porter-Thomas one used in all other cases.

Parameters of (significantly) contributing resonances must then be specified in the input file `RES_PAR.DAT`. A full set of READ statements of the subroutine `RES_PAR`, that reads this ASCII input file, is listed here. By this set a required file structure is again uniquely given.

```

READ(6,*)
READ(6,*) NRES(1)
DO 1=1,NRES(1)
  READ(6,*) ERES(1,1),GRED(1,1),GGAM(1,1)
ENDDO
IF (SPINt.NE.0.) THEN
  READ(6,*)
  READ(6,*) NRES(2)
  DO 1=1,NRES(2)
    READ(6,*) ERES(1,2),GRED(1,2),GGAM(1,2)
  ENDDO
ENDIF

```

The meaning of individual variables is:

NRES(2) – the INTEGER numbers of neutron resonances that significantly contribute to the capture cross section. NRES(1) serves for the resonances with spin $J = J_T - 0.5$, while NRES(2) for the resonances with spin $J = J_T + 0.5$; value of J_T is stored in variable SPINT. At least two resonances of each contributing spin are required, i.e. $\text{NRES(I)} \geq 2$!

ERES(50,2), GRED(50,2), GGAM(50,2) – the REAL energies, “reduced neutron widths” and total radiation widths of the neutron resonances contributing to the neutron capture, respectively. The energy is expressed in eV, while the two remaining quantities in meV. The quantity $2g\Gamma_n^{(0)}$ is assumed here to be the reduced neutron width instead of “pure” reduced neutron width $\Gamma_n^{(0)}$. Thy symbol g stands here for the spin factor. The reason for using $2g\Gamma_n^{(0)}$ instead of $\Gamma_n^{(0)}$ is that the former quantity is often listed in literature.

In reality, if the contribution of one resonance spin to the capture cross section at the specified neutron energy is below 10^{-3} , the spin of initial level for all cascades is set to the other possible capturing spin.

5.3 Input Files PSFE1.DAT, PSFM1.DAT, PSFE2.DAT

These input files are required only if the value of the corresponding switch NOPTE1, NOPTM1 or NOPTE2, specifying the $E1$, $M1$ or $E2$ PSF models, respectively, equals to a value between 11 and 15. If this is the case, the file for given transition type ($E1$, $M1$ or $E2$) is read in subroutine READ_EV. These values of switches indicate that (at least of a part of) the PSF of a given type is assumed to be given in tabulated form. The following sequence of the READ statements is called:

```

      READ(5,*)
      READ(5,*) NPSF(n)
      READ(5,*)
      DO IEN = 1, NPSF(n)
         READ(5,*) TABENPSF(n,IEN),TABPSF(n,IEN)
      ENDDO

```

The meaning of individual variables is:

NPSF(n) – the INTEGER number of lines with data on PSFs. The value of $n = 1, 2$ or 3 stands for $E1$, $M1$, and $E2$ transitions, respectively. Only data for one value of n are read in one file, i.e. NPSF(1) is read in the file PSFE1.DAT, NPSF(2) is read in the file PSFM1.DAT, and NPSF(3) is read in the file PSFE2.DAT.

TABENPSF(3,400) – the REAL E_γ energies in MeV which the tabulated PSFs are given for. All energies must be positive (i.e. not even equal to zero) and the individual lines must be ordered from the lowest to the highest γ -ray energy.

TABPSF(3,400) – the REAL values of PSFs in units of MeV^{-3} corresponding to the γ energy specified in TABENPSF.

It should be noted again that the corresponding file is read only if the switch NOPTE1, NOPTM1 or NOPTE2 equals to a value between 11 and 15.

5.4 Input File LDTAB.DAT

This input file is required only if NOPTDE=11. The level density is assumed to be given in the tabular form for each spin and parity of levels. If this is the case, the file is read in subroutine READ_EV. The following sequence of the READ statements is called:

```
      READ(5,*)
      READ(5,*) NLD, SPACRES,SPINi,IPINi,corAlpLD,corDelLD
      READ(5,*)
      DO IEN = 1, NLD
        READ(5,*) TABENLD(IEN),DUMMY,DUMMY,DUMMY,DUMMY,
*              (TABLD(IEN,J,0),J=0,MAXJC)
      ENDDO
      READ(5,*)
      DO IEN = 1, NLD
        READ(5,*) TABENLD(IEN),DUMMY,DUMMY,DUMMY,DUMMY,
*              (TABLD(IEN,J,1),J=0,MAXJC)
      ENDDO
```

The meaning of individual variables is:

NLD – the INTEGER number of excitation energies the level density is tabulated for.

SPACRES – the REAL value of the *s*-wave resonance spacing in units of MeV. In reality, this variable is not used in the present version of the code. So, its value can be arbitrary.

SPINi and IPINi – the REAL spin and INTEGER parity of the capturing state for neutron capture. These values are supposed to be the same as those of variables SPINt and IPINt in DICE_EV.DAT input file. However, also these variables are not used in the present version of the code. So, their values can be arbitrary.

TABENLD(270) – the REAL excitation energies in MeV for which the tabulated level density is given. All energies must be positive (i.e. not even equal to zero) and the individual lines should be ordered from the lowest to the highest excitation energy.

TABLD(270,0:49,0:1) – the REAL values of level density in units of MeV^{-1} corresponding to the excitation energy specified in TABENLD, spin *J* (second parameter) and parity specified in the last parameter of the array. The convention of parity is the same as for other parity values in the code, i.e. 0 and 1 for positive and negative parity, respectively.

Each line corresponds to given energy and parity and values for all spins must be given. Used form of the level-density table corresponds to that available in the RIPL database [5] for the “HFB Total Level Densities”. Corresponding parts of the table available in RIPL can thus be used in LDTAB.DAT input file. Level densities for positive and negative parity levels are read in the two parts of the file.

In the case of odd nucleus with half-integer spin values the integer part of the spin corresponds to the second parameter of the TABLD array. In other words, TABLD(.,0,.) stores information on levels with $J = 1/2$ and TABLD(.,49,.) on levels with $J = 99/2$.

DUMMY – the REAL variable that is not used in the code. The presence of this variable is motivated by the structure of the table in just mentioned level density in RIPL database.

corAlpLD and corDeLLD – the REAL variables used for renormalization of data given in the input file LD TAB.DAT, see Eq. (26).

5.5 Output Files EVENTS.Ssss.Rrrr

These files store information on individual γ cascades from different nuclear realizations *rrr* and supra-realizations *sss*, see Sec. 3.1. The files are created if ISWWR=1. The symbols *sss* and *rrr* are three-digit integers of the form FORMAT(I3.3). Depending on the choice of the switch ISWBN, these files are written either in the ASCII format or as UNFORMATTED files. Each file consists of N_{ev} (variable NEVENTS) portions of data on individual cascades. The structure of these portions is given by the following set of WRITE commands:

```

      IF (ISWBN.EQ.0) THEN
        WRITE (12,100) SPQQ(0),IPQQ(0),NSTEP,ELQQ(0)
        IF (ISWEL.EQ.1) WRITE (12,200) (ELQQ(J),J=1,NSTEP)
        IF (ISWSP.EQ.1) WRITE (12,300) (SPQQ(J),J=1,NSTEP)
        IF (ISWPA.EQ.1) WRITE (12,400) (IPQQ(J),J=1,NSTEP)
        IF (ISWIC.EQ.1) WRITE (12,400) (ICQQ(J),J=1,NSTEP)
        IF (ISWMX.EQ.1) WRITE (12,500) (DMQQ(J),J=1,NSTEP)
        IF (ISWWI.EQ.1) WRITE (12,500) (WIQQ(J),J=1,NSTEP)
      ELSE
        WRITE (12) SPQQ(0),IPQQ(0),NSTEP,ELQQ(0)
        IF (ISWEL.EQ.1) WRITE (12) (ELQQ(J),J=1,NSTEP)
        IF (ISWSP.EQ.1) WRITE (12) (SPQQ(J),J=1,NSTEP)
        IF (ISWPA.EQ.1) WRITE (12) (IPQQ(J),J=1,NSTEP)
        IF (ISWIC.EQ.1) WRITE (12) (ICQQ(J),J=1,NSTEP)
        IF (ISWMX.EQ.1) WRITE (12) (DMQQ(J),J=1,NSTEP)
        IF (ISWWI.EQ.1) WRITE (12) (WIQQ(J),J=1,NSTEP)
      ENDIF
100  FORMAT (F5.1,I3,I5,F11.5)
200  FORMAT (2X,8F11.5)
300  FORMAT (2X,8F11.1)
400  FORMAT (2X,8I11)
500  FORMAT (2X,8E11.3)

```

This set of WRITE statements shows that the actual structure of the output file depends on values of several switches described in the part related to global variables in the input file DICE_EV.DAT. If all relevant switches are set to 1, the structure of each portion is as follows:

1st record contains the REAL spin of the capturing state (variable SPQQ(0)), the INTEGER parity of the capturing state (variable IPQQ(0)), the INTEGER number of steps l of a cascade (variable NSTEP) and the REAL energy of capturing state in MeV (variable ELQQ(0)).

2nd record contains l **REAL** values of energies of all levels hit during the cascade (variable **ELQQ(J)**). These energies are given in units of MeV.

3rd record lists l **REAL** values of spins of all levels hit during the cascade (variable **SPQQ(J)**). If the spins are half-integer numbers their value is 0.5, 1.5, etc.

4th record consists of l **INTEGER** values representing parities of all levels hit during the cascade (variable **IPQQ(J)**). Values 0 and 1 belong to positive and negative parity, respectively.

5th record is formed by l **INTEGER** values representing the type of radiation emitted in individual cascade steps (variable **ICQQ(J)**). Values 0 correspond to γ rays, while positive values to conversion electrons. The present version differentiates electrons originating from ICC on the K shell (**ICQQ(J)=1**) from all other electrons (**ICQQ(J)=2**). The latter electrons might come from any of L , M , ... shells as well as from the conversion to the electron-positron pair.

6th record refers to l **REAL** values of multipolarity mixing ratios δ for the individual cascade steps (variable **DMQQ(J)**).

7th record gives l **REAL** values of total radiation widths $\Gamma_{\alpha\gamma}$ of individual decaying levels (variable **WIQQ(J)**). The first value corresponds to the total radiation width of the initial state of the decay. These widths are given in units of MeV. The value of $\Gamma_{\alpha\gamma}$ is set to zero for levels below E_{crit} .

5.6 Output file DICE.PRO

This file lists some additional information on simulated cascades and is formed by following parts:

- The beginning of the file summarizes the most important input data (related to the PSFs and level density). The meaning of each variable should be evident from the text description in the file.
- The value of total radiation width of the capturing state, $\Gamma_{\alpha\gamma}$, (variable **RADW**) is printed together with its square root of variance obtained from simulations of different nuclear realizations.
- The number of cascades that do not reach the ground state of the nucleus is given. These are cascades ending at a level which has no possibility to decay. Such a level can occur below E_{crit} if the number of de-exciting transitions **DENUM=0** or, in principle, also above E_{crit} if no level reachable via $E1$, $M1$ or $E2$ transitions is available at lower excitation energy. The latter case can be avoided if there is sufficiently wide range of spins of levels below E_{crit} in the **DICE_EV.DAT** input file. Listed number gives total number of such cascades in all nuclear realizations. Information, whether such an “isomeric” state appeared in one or more nuclear realizations is not provided at the moment.
- The list of simulated level populations per a cascade (the average and the square root of the variance) based on populations in individual nuclear realizations is given for each level below E_{crit} . Energies (in MeV) of individual levels (in the second

column) together with their spins and parities (in the last two columns) are also listed.

- The list of simulated level side-feedings is given analogously to the previous item. The displayed side-feedings are understood to be given by the difference between the sum of depopulating intensities and the sum of all those populating intensities of a given “discrete” level, that belong to transition from level with energies below E_{crit} . It means that direct feeding of a level via primary transition is incorporated into the side-feeding at the moment.

5.7 Output file LEVELS.sss

These files are produced only if the switch ISWLS=1 and provide information on all levels simulated in individual nuclear supra-realizations *sss* that is given by a three-digit INTEGER number in the FORMAT(I3.3) form.

Each line of the ASCII output file corresponds to one simulated level with given excitation energy E (REAL value in MeV), spin J (REAL number) and parity π (INTEGER number). The values of $\pi = 0$ and 1 correspond to positive and negative parity levels, respectively. The levels are ordered according to J and π . For given J^π the levels are then ordered decreasingly with their excitation energy.

5.8 Output files PSF_GS.DAT and PSF_INI.DAT

These two output files give a table with the PSFs values used in simulations in the step of 50 keV. The first column corresponds to the transition energy E_γ in MeV and the next three columns list the corresponding PSF values for $E1$, $M1$, and $E2$ transitions (in units of $\text{MeV}^{-(2L+1)}$), respectively.

If the PSFs follow the Brink hypothesis, the two files are identical. However, if the Brink hypothesis is violated, they differ. The file PSF_GS.DAT lists the PSFs for transitions to the ground state (or PSFs for photoexcitation from the ground state) while the file PSF_INI.DAT lists the PSFs corresponding to transitions starting at the initial energy of the cascade.

6 Adopted models

This section lists different options for level density and PSFs that are available in the code via different values of the corresponding switches.

The parameters used in the formulas in this section are often identified with corresponding variable names used in the input files described in Sec. 5. This correspondence is indicated via “ X (variable **XNAME**)”, where X stands for the parameter name used in formulas and **XNAME** for the variable name used in Sec. 5.

Some values of the options are omitted in the lists of individual models. These omitted values correspond usually to some test models that were used in the code in the past.

6.1 Level Density Models

The level density ρ can be factorized as

$$\rho(E, J, \pi) = f(\pi)f(J)\rho(E), \quad (14)$$

where the three factors on the right hand side of the equation stand for dependence on parity π , spin J and excitation energy E , respectively.

Two switches govern the behavior of level density. The switch **NOPTDE** is responsible for dependence of level density on excitation energy and spin, i.e. factors $\rho(E)$ and $f(J)$ from Eq. (14), see Sec. 6.1.1 while the switch **LDENP** is used for description of the parity dependence $f(\pi)$, see Sec. 6.1.2. It is to be noted that any level density model is used only at excitation energies $E > E_{\text{crit}}$; all the information on levels for $E \leq E_{\text{crit}}$ is taken from the input file **DICE_EV.DAT**.

6.1.1 Energy and spin dependence – parameter **NOPTDE**

The present version of **DICEBOX** code offers the following possibilities for the choice of the level density ρ as a function of excitation energy E , spin J .

- **NOPTDE=0** – the Constant-Temperature (CT) level-density model in the form given by von Egidy *et al.* [24, 4]

$$\rho(E, J, \pi) = f(J)f(\pi) \frac{1}{T} e^{(E-E_0)/T}, \quad (15)$$

where the parameters T (variable **TEMPER**) and E_0 (variable **EZERO**) are, respectively, the nuclear temperature and the back-shift.

The factor $f(J)$ represents a probability that a level has a spin J . Following Ref. [8] it is expected to have the form

$$f(J) = \frac{2J+1}{2\sigma^2} e^{-(J+\frac{1}{2})^2/2\sigma^2}, \quad (16)$$

where σ is a spin cut-off parameter [8]. In the parametrization of CTF from [24, 4], a semi-empirical prescription for σ is used

$$\sigma = 0.98 A^{0.29}, \quad (17)$$

where A (variable **AMASS**) is a mass number.

- **NOPTDE=1** – the Back-Shifted Fermi Gas (BSFG) model in the form given by von Egidy *at al.* in their article published in 1988 [24]

$$\rho(E, J, \pi) = f(J)f(\pi) \frac{e^{2\sqrt{a(E-E_1)}}}{12\sqrt{2}\sigma a^{1/4}(E-E_1)^{5/4}} \quad (18)$$

The quantity a (variable **ASHELL**) is the conventional shell-model level-density parameter, while E_1 (variable **EONE**) is another back shift.

Calculating level density according to BSFG parametrization from [24], the factor σ is assumed to be

$$\sigma^2 = 0.0888 A^{2/3} a^{1/2} (E - E_1)^{1/2}. \quad (19)$$

- **NOPTDE=2** – the energy and spin dependence of ρ given by Eqs. (18) and (19) is multiplied by a factor f_{mult} for excitation energies E in the range $E_L < E < E_H$:

$$f_{\text{mult}} = D_p^{(1)} + D_p^{(2)} E + D_p^{(3)} E^2 + D_p^{(4)} E^3. \quad (20)$$

The factor f_{mult} is equal to 1 for $E < E_L$ and $E > E_H$, where values of E_L and E_H are given by variables **DENLO** and **DENHI**, respectively.

- **NOPTDE=3** – the energy and spin dependence of ρ given by Eqs. (15)-(17) is multiplied by a factor f_{mult} from Eq. (20) for excitation energies E in the range $E_L < E < E_H$. The factor f_{mult} is equal to 1 for $E < E_L$ and $E > E_H$ as in the case of **NOPTDE=2**.
- **NOPTDE=6** – the BSFG model with the same energy dependence of ρ as in **NOPTDE=1**, see Eq. (14), but with the spin cut-off factor σ given by von Egidy and Bucurescu in their paper from 2005 [4]

$$\sigma^2 = 0.0146 A^{5/3} \left(1 + \frac{\sqrt{1 + 4a(E - E_1)}}{2a} \right). \quad (21)$$

The a and E_1 parameters in this model are again given by variables **ASHELL** and **EONE** in the input file **DICE_EV.DAT**.

- **NOPTDE=8** – the CT model with the same energy dependence of ρ as for **NOPTDE=0**, see Eq. (15), but with the spin factor $f(J)$ as proposed in von Egidy and Bucurescu in their work from 2009 [23]

$$f(J) = f_s \frac{2J+1}{2\sigma^2} e^{-(J+\frac{1}{2})^2/2\sigma^2}, \quad (22)$$

with

$$\sigma^2 = 0.391 A^{0.675} (E - 0.5P_{09})^{0.312}. \quad (23)$$

Parameters of T , E_0 , P_{09} and A in this model correspond to variables **TEMPER09**, **EZERO09**, **PAIRING09** and **AMASS** in the input file, respectively.

The factor $f_s = 1$ for odd-odd and odd-mass nuclei. For even-even mass nuclei, f_s depends on excitation energy E and describes the observed staggering in the number of levels with even and odd spins at low excitation energy:

$$\begin{aligned} f_s &= 1.0 + 0.227(1.0 - x_s) && \text{for even positive } J \\ f_s &= 1.0 - 0.227(1.0 - x_s) && \text{for odd } J \\ f_s &= 1.0 + 1.02(1.0 - x_s) && \text{for } J = 0. \end{aligned} \quad (24)$$

The value of $x_s = 0$ and 1 for excitation energy $E < E_L$ and $E > E_H$, respectively, and in the region $E_L < E < E_H$ it is expressed as

$$x_s = \frac{E - E_L}{E_H - E_L}. \quad (25)$$

Energies E_L and E_H correspond to variables `DENLO` and `DENHI` in the input file `DICE.EV.DAT`, respectively.

This treatment of x_s allows to have the level density with the staggering proposed in [23] at low excitation energies but no staggering at high excitation energies. In reality, there is no prescription for behavior of x_s with excitation energy in Ref. [23]. However, dying out of the staggering with excitation energy has been proposed in calculations from [2] and we adopted one possible form of this behavior. It is expected that in well-deformed rare-earth nuclei the staggering is completely gone at excitation energies near 4 MeV.

- **NOPTDE=9** – the BSFG model with the same energy dependence as for **NOPTDE=1** and **NOPTDE=6** but with the spin factor $f(J)$ as proposed in von Egidy and Bucurescu in Ref. [23] and given by Eqs. (22-25); see the text related to **NOPTDE=8**.

Parameters of a and E_1 in this model are given by variables `ASHELL09` and `EONE09` in the input file `DICE.EV.DAT`, respectively.

- **NOPTDE=11** – the level density in a tabulated form as a function of E , J , and π . The values are read from the file `LDTAB.DAT`. The structure of this input file is described in Sec. 5.4. The tabulated values obtained with calculations based on the HFB approach can be obtained from RIPL3 database.

In reality, (calculated) tabulated values ρ_{tab} do not necessarily reproduce the number of levels at low excitation energies and/or spacing of neutron resonances. A renormalization of tabulated data was proposed in Ref. [9] to get the renormalized NLD ρ_{ren} :

$$\rho_{\text{ren}}(E, J, \pi) = \rho_{\text{tab}}(E - \delta_R, J, \pi) e^{\alpha_R \sqrt{E - \delta_R}}. \quad (26)$$

The two parameters α_R and δ_R are stored in variables `corAlpLD` and `corDelLD`, respectively.

The renormalized NLD ρ_{ren} is then used in simulations. Use of $\alpha_R = 0$ and $\delta_R = 0$ makes $\rho_{\text{tab}} = \rho_{\text{ren}}$.

6.1.2 Parity dependence – parameter `LMODE`

This subsection deals with the parity dependence factor $f(\pi)$ from Eq. (14) that is fully independent of the level density dependence on excitation energy E and spin J .

A parity dependence can be applied to all NLD models described above in Sec. 6.1.1 with the exception of **NOPTDE=11**, where the parity dependence is implicitly present in the tabulated values. Treatment of parity dependence is governed by the value of the option `LDENP`:

- **LDENP=0** – no parity asymmetry is considered for levels above E_{crit} . In other words, $f(\pi) = 0.5$ for both parities. This is the standard option if no parity dependence is expected.

- **LDENP=1** – the parity dependence as proposed by Al-Quraishi *et al.* [1] is used:

$$f(\pi = +) \equiv \frac{\rho(+)}{\rho(+) + \rho(-)} = \frac{1}{2} \left(1 \pm \frac{1}{1 + \exp(C_\pi(E - \Delta_\pi))} \right). \quad (27)$$

Here, Δ_π is a “shift” in excitation energy that determines position of change from “parity-dependent” to “parity-independent” regime of level density and C_π (variable DENPC) is a parameter that characterizes the “derivative of this change”. The sign $+$ or $-$ depends on the dominant parity of levels at the lowest excitation energies. Specifically, parity of five lowest levels (including the ground state) as given in DICE_EV.DAT input file is checked. If the number of positive-parity levels exceeds the number of negative-parity levels, the sign “ $+$ ” is used in Eq. (27). If the number of negative-parity levels exceeds the number of positive-parity levels, the sign “ $-$ ” is used in Eq. (27). For negative-parity level density $f(\pi = -) = 1 - f(\pi = +)$. The value of $f(\pi) = 1/2$ is reached at high excitation energies.

In reality, with the option LDENP=1 the value of parameter Δ_π as suggested in Ref. [1] is used. The parameter C_π (variable DENPPC) is to be set manually; the value $C_\pi = 3 \text{ MeV}^{-1}$ was proposed in [1].

- **LDENP=2** – the same parity dependence as in the case of LDENP=1 is used, see Eq. (27), but the parameter Δ_π is calculated from parameters in the input file as

$$\Delta_\pi = F_\pi^{(1)} + \frac{F_\pi^{(2)}}{A F_\pi^{(3)}}. \quad (28)$$

The values of parameters A and $F_\pi^{(I)}$ are stored in variables AMASS and DENPEN(I), respectively.

6.2 E1 PSF Models

Selection of the E1 PSF model is made via switch NOPTE1. The following models are available:

- **NOPTE1=0** – The single-particle (SP) model in which the E1 PSF is an E_γ -independent constant, $f^{(E1)} = k_{E1}$. The value of the constant is given by variable DEG in input file DICE_EV.DAT.
- **NOPTE1=1** – Standard Lorentzian (SLO) shape of the E1 PSF, sometimes also called Axel-Brink model:

$$f_{\text{SLO}}^{(E1)}(E_\gamma) = \frac{1}{3(\pi\hbar c)^2} \sum_{i=1}^n \frac{\sigma_{G_i} E_\gamma \Gamma_{G_i}^2}{(E_\gamma^2 - E_{G_i}^2)^2 + E_\gamma^2 \Gamma_{G_i}^2}. \quad (29)$$

where, parameters E_{G_i} , Γ_{G_i} and σ_{G_i} correspond to the energy, width and cross section at the maximum of the i^{th} assumed resonance, respectively. The values of these parameters are given by variables ER(i), W0(i) and SIG(i) in the input file DICE_EV.DAT in units of MeV, MeV and mb, respectively. Although the SLO shape of the Giant Electric Dipole Resonance is usually given by one or two resonance terms, the allowed number of resonances in the code is $n = 5$.

- **NOPT1=3** – Usually used form of the Enhanced Generalized Lorentzian (EGLO) model proposed as a generalization of the GLO model (see **NOPT1=5**) for deformed nuclei by Kopecky *et al.* [14]. The $E1$ PSF in this model is given by

$$f_{\text{EGLO}}^{(E1)}(E_\gamma, T) = \sum_{i=1}^n \frac{\sigma_{G_i} \Gamma_{G_i}}{3(\pi\hbar c)^2} \left[\mathcal{A}(E_\gamma, T) + \frac{F_K \Gamma_{G_i}^k(E_\gamma = 0, T)}{E_{G_i}^3} \right], \quad (30)$$

$$\mathcal{A}(E_\gamma, T) = \frac{E_\gamma \Gamma_{G_i}^k(E_\gamma, T)}{(E_\gamma^2 - E_{G_i}^2)^2 + (E_\gamma \Gamma_{G_i}^k(E_\gamma, T))^2}. \quad (31)$$

Parameter F_K (variable **FERMC**) was suggested to be about 0.7 in [11, 5], and the temperature-dependent width $\Gamma_{G_i}^k(E_\gamma, T)$ is given by

$$\Gamma_{G_i}^k(E_\gamma, T) = \Gamma_{G_i} \frac{E_\gamma^2 + 4\pi^2 T^2}{E_{G_i}^2} \left[k_0 + (1 - k_0) \frac{E_\gamma - E_\gamma^0}{E_{G_i} - E_\gamma^0} \right], \quad (32)$$

with the temperature

$$T = T(E_f) \equiv \sqrt{(E_f - E_P)/a} = \sqrt{(E_i - E_\gamma - E_P)/a}, \quad (33)$$

where E_i and E_f are excitation energies of the initial and the final level in the decay and $T = 0$ if the argument of the square root in Eq. (33) is negative. The parameter a is the usual shell-model level density parameter (variable **ASHELL**) and E_P is the pairing energy (variable **PAIRING**). Parameters k_0 (variable **EKO**) and E_γ^0 (variable **EGZERO**) were discussed in [14, 5]. Ref. [14] suggested $E_\gamma^0 = 4.5$ MeV and the value of the parameter k_0 depending on the level-density formula. Analysis of spectra from neutron resonances indicates that k_0 could reach values in the range $\approx 2 - 4$ in well-deformed rare-earth nuclei, see e.g. Ref. [15, 21].

Please note that the shape of $f^{(E1)}$ depends on the excitation energy of initial/final level via Eq. (33) in this model.

- **NOPT1=4** – Model suggested in [11] by Kadenskij, Markushev and Furman, often called the KMF model:

$$f_{\text{KMF}}^{(E1)}(E_\gamma, T) = \frac{F_K}{3(\pi\hbar c)^2} \sum_{i=1}^n \frac{\sigma_{G_i} E_{G_i} \Gamma_{G_i} \Gamma_{G_i}^T(E_\gamma, T)}{(E_\gamma^2 - E_{G_i}^2)^2}, \quad (34)$$

with the T -dependent width

$$\Gamma_{G_i}^T(E_\gamma, T) = \Gamma_{G_i} \frac{E_\gamma^2 + 4\pi^2 T^2}{E_{G_i}^2} \quad (35)$$

The meaning of all parameters is the same as in the **NOPT1=3** option; temperature T is given by Eq. (33). Please note that the shape of $f^{(E1)}$ depends on the excitation energy of initial/final level via Eq. (33) in this model.

- **NOPT1=5** – Phenomenological Generalized Lorentzian (GLO) model proposed by Kopecky and Uhl in [13]:

$$f_{\text{GLO}}^{(E1)}(E_\gamma, T_f) = \frac{1}{3(\pi\hbar c)^2} \sum_{i=1}^n \sigma_{G_i} \Gamma_{G_i} \left[\frac{E_\gamma \Gamma_{G_i}^T(E_\gamma, T)}{(E_\gamma^2 - E_{G_i}^2)^2 + E_\gamma^2 \Gamma_{G_i}^{T^2}(E_\gamma, T)} + F_K \frac{4\pi^2 T^2 \Gamma_{G_i}^T}{E_{G_i}^5} \right]. \quad (36)$$

where $\Gamma_{G_i}^T(E_\gamma, T)$ is given by Eq. (35).

Please note that the shape of $f^{(E1)}$ depends on the excitation energy of initial/final level via Eq. (33) in this model. It should be stressed that there exist other formulations of the GLO model where $f^{(E1)}$ is not a function of excitation energy – the model is sometimes used with a fixed temperature or with the temperature defined as $T = \sqrt{(S_n - E_P)/a}$, where S_n is the neutron separation energy and E_P is an energy shift.

- **NOPTE1=6** – The Modified Generalized Lorentzian (MGLO) model as introduced in Ref. [15]. The functional form of this model is similar to the EGLO model, see **NOPTE1=3**, but in the MGLO model it is assumed that $k_0 \equiv 1$ in this second term of Eq. (30), so that the expression for the MGLO $E1$ PSF reads

$$f_{\text{MGLO}}^{(E1)}(E_\gamma, T) = \sum_{i=1}^2 \frac{\sigma_{G_i} \Gamma_{G_i}}{3(\pi\hbar c)^2} \left[\mathcal{A}(E_\gamma, T) + \frac{4\pi^2 F_K \Gamma_{G_i}^k T^2}{E_{G_i}^5} \right]. \quad (37)$$

The meaning of all variables is the same as in options **NOPTE1=1** and **NOPTE1=3**. Please note that the shape of $f^{(E1)}$ depends on the excitation energy of initial/final level via Eq. (33) in this model.

The change of the PSF with respect to **NOPTE1=3** leads to significant suppression of the “low-energy enhancement” of the PSF for transitions to excited states.

- **NOPTE1=7** – The SMLO form of the $E1$ PSF, which is given by [20]

$$f_{\text{SMLO}}^{(E1)}(E_\gamma) = \frac{1}{3(\pi\hbar c)^2} \frac{1}{1 - \exp(-E_\gamma/T)} \sum_{i=1}^n \frac{\sigma_{G_i} E_\gamma \Gamma_{G_i} \Gamma_{G_i}^S(E_\gamma, T)}{(E_\gamma^2 - E_{G_i}^2)^2 + E_\gamma^2 \Gamma_{G_i}^{S2}(E_\gamma, T)}. \quad (38)$$

where

$$\Gamma_{G_i}^S(E_\gamma, T) = \Gamma_{G_i} \frac{E_\gamma E_{G_i} + 4\pi^2 T^2}{E_{G_i}^2}. \quad (39)$$

and

$$T = \sqrt{(E_i - E_\gamma)/A * 10} = \sqrt{E_f/A * 10}. \quad (40)$$

where E_i and E_f are excitation energies of the initial and the final level in the decay, respectively. Please note that the shape of $f^{(E1)}$ depends on the excitation energy of initial/final level via temperature T in this model.

- **NOPTE1=11** - The $E1$ PSF is given in a tabulated form as a function of E_γ , $f_{\text{tab}}^{(E1)}(E_\gamma)$. The values of $f_{\text{tab}}^{(E1)}(E_\gamma)$ are read from the file **PSFE1.DAT**. The structure of this input file is described in Sec. 5.3. Exact validity of the Brink hypothesis is assumed in this model. The value of $f^{(E1)}(E_\gamma)$ for a specific energy is obtained from interpolation using two points for lower and two for higher E_γ .
- **NOPTE1=12** – The $E1$ PSF model is given by [10]

$$f^{(E1)}(E_\gamma, T) = f_{\text{tab}}^{(E1)}(E_\gamma) + \frac{E_i f_0^{(E1)}}{1 + \exp(E_\gamma - E_{\gamma E1}^{(E1)})} \quad (41)$$

where $f_{\text{tab}}^{(E1)}(E_\gamma)$ is the $E1$ PSF in the same tabulated form as in `NOPT1=11` option. Individual $f_{\text{tab}}^{(E1)}(E_\gamma)$ values are read from the input file `PSFE1.DAT`. The structure of this input file is described in Sec. 5.3. Further, $E_i = E_f + E_\gamma$ is the excitation energy of the decaying state and parameters $f_0^{(E1)}$ and $E_{\gamma E1}^{(E1)}$ are given by variables `PAR_E1(1)` and `PAR_E1(2)` of input file `DICE_EV.DAT`, respectively. The model introduces “phenomenological” low-energy E_γ enhancement in $E1$ PSF as a function of excitation energy; it thus partly violates the Brink hypothesis.

The product of E_i and $f_0^{(E1)}$ characterizes the $E1$ PSF limit at $E_\gamma = 0$ for given initial excitation energy E_i . As E_i is expressed in units of MeV, the units of $f_0^{(E1)}$ are MeV^{-4} . Parameter $E_{\gamma E1}^{(E1)}$ is then expressed in units of MeV and characterizes the region of E_γ energies which are affected by the low- E_γ enhancement.

- `NOPT1=42` – The $E1$ PSF model given by the KMF model, see option `NOPT1=4` above, multiplied by a dimensionless constant $C_1^{(E1)}$ (variable `PAR_E1(1)` in the `DICE_EV.DAT` input file):

$$f_{\text{KMF-REN}}^{(E1)}(E_\gamma, T) = C_1^{(E1)} f_{\text{KMF}}^{(E1)}(E_\gamma, T) = \frac{C_1^{(E1)} F_K}{3(\pi \hbar c)^2} \sum_{i=1}^n \frac{\sigma_{G_i} E_{G_i} \Gamma_{G_i} \Gamma_{G_i}^T(E_\gamma, T)}{(E_\gamma^2 - E_{G_i}^2)^2}, \quad (42)$$

with the T -dependent width given by Eq. (35) and temperature T by Eq. (33).

- `NOPT1=43` – The $E1$ PSF model given by the sum of the KMF-REN model, see `NOPT1=42` option, and a low-energy enhancement of exponential form:

$$f^{(E1)}(E_\gamma, T) = f_{\text{KMF-REN}}^{(E1)}(E_\gamma, T) + \frac{C_1^{(E1)} C_2^{(E1)} E_\gamma^{-C_3^{(E1)}}}{3(\pi \hbar c)^2} \quad (43)$$

Parameters describing the low-energy enhancement $C_i^{(E1)}$ are given by variables `PAR_E1(i)` in the input file `DICE_EV.DAT`. The constants $C_1^{(E1)}$ and $C_3^{(E1)}$ are dimensionless and the factor $C_2^{(E1)}$ is given in $\text{fm}^2 \cdot \text{MeV}^{-1}$.

6.3 $M1$ PSF Models

Selection of the $M1$ PSF model is made via switch `NOPTM1`. The following models are available:

- `NOPTM1=0` – The single-particle (SP) model in which the $M1$ PSF is an E_γ -independent constant, $f_{\text{SP}}^{(M1)} = k_{M1}$. The value of the constant is given by variable `DMG` in input file `DICE_EV.DAT`.
- `NOPTM1=1` – The Lorentzian PSF shape given by the same functional form as in Eq. (29) but with different parameters of individual resonances:

$$f_{\text{SLO}}^{(M1)}(E_\gamma) = \frac{1}{3(\pi \hbar c)^2} \sum_{i=1}^n \frac{\sigma_{M_i} E_\gamma \Gamma_{M_i}^2}{(E_\gamma^2 - E_{M_i}^2)^2 + E_\gamma^2 \Gamma_{M_i}^2}. \quad (44)$$

Parameters E_{M_i} , Γ_{M_i} and σ_{M_i} correspond to the energy, width and cross section at the maximum of the i^{th} assumed resonance, respectively. The values of these

parameters are given by variables `ERM(i)`, `WMO(i)` and `SIGM(i)` in the input file `DICE_EV.DAT` in units of MeV, MeV and mb, respectively. The allowed number of resonances in the code is $n = 5$.

This functional form of $f^{(M1)}$ is often used for description of the spin-flip as well as the scissors resonances. The model follows the Brink hypothesis.

- **NOPTM1=4** – The combination of the models given by `NOPTM1=0` and `NOPTM1=1`. The functional form of $f^{(M1)}(E_\gamma)$ can be expressed as:

$$f^{(M1)}(E_\gamma) = k_{M1} + f_{\text{SLO}}^{(M1)}(E_\gamma) = k_{M1} + \frac{1}{3(\pi\hbar c)^2} \sum_{i=1}^n \frac{\sigma_{M_i} E_\gamma \Gamma_{M_i}^2}{(E_\gamma^2 - E_{M_i}^2)^2 + E_\gamma^2 \Gamma_{M_i}^2}. \quad (45)$$

The meaning of all variables is the same as in `NOPTM1=0` and `NOPTM1=1` options.

In reality, the value of k_{M1} is assumed to be given by variable `DMG` only for energy of the final state of the decay $E_f = E_i - E_\gamma$ satisfying the relation $E_f \leq E_{\text{thr}}$ (variable `PAR_M1(1)`). For $E_f > E_{\text{thr}}$ it is assumed that $k_{M1} = 0$. It is thus recommended to use the value of variable `PAR_M1(1)` higher than the energy of initial state (variable `BN`).

- **NOPTM1=6** – The functional form of $f^{(M1)}(E_\gamma)$ is given by the sum of `NOPTM1=1` and an exponential background

$$f^{(M1)}(E_\gamma) = k_{M1} \exp(-E_\gamma/C_1^{(M1)}) + f_{\text{SLO}}^{(M1)}(E_\gamma) \quad (46)$$

where the constant $C_1^{(M1)}$ in units of MeV corresponds to the variable `PAR_M1(1)` in the `DICE_EV.DAT` file.

- **NOPTM1=11** – The $M1$ PSF is given in a tabulated form as a function of E_γ , $f_{\text{tab}}^{(M1)}(E_\gamma)$. The values of $f_{\text{tab}}^{(M1)}(E_\gamma)$ are read from the file `PSFM1.DAT`. The structure of this input file is described in Sec. 5.3. Exact validity of the Brink hypothesis is assumed in this model.
- **NOPTM1=12** – The $M1$ PSF model as proposed in Ref. [10]:

$$f^{(M1)} = f_{\text{tab}}^{(M1)} + f_0^{(M1)}(1.0 + \Delta^{(M1)} E_\gamma^3) \exp(-h_{\gamma M1}^{(M1)} E_\gamma) \quad (47)$$

where $f_{\text{tab}}^{(M1)}$ is the $M1$ PSF in the same tabulated form as in `NOPTM1=11` option. Individual $f_{\text{tab}}^{(M1)}$ values are read from the input file `PSFM1.DAT`. The structure of this input file is described in Sec. 5.3. Additional parameters f_0^{M1} , $h_{\gamma M1}^{(M1)}$, and $\Delta^{(M1)}$, given in units MeV^{-3} , MeV^{-1} and MeV^{-3} , then describe the behavior of a low- E_γ $M1$ PSF enhancement and correspond to variables `PAR_M1(1)`, `PAR_M1(2)` and `PAR_M1(3)` in `DICE_EV.DAT` input file, respectively. Exact validity of the Brink hypothesis is assumed in this model.

- **NOPTM1=21** – The $M1$ PSF model given by the Lorentzian $M1$ PSF model, see option `NOPTM1=1` above, multiplied by a dimensionless constant $C_1^{(M1)}$ (variable `PAR_M1(1)` in the input file `DICE_EV.DAT`):

$$f^{(M1)}(E_\gamma) = C_1^{(M1)} f_{\text{SLO}}^{(M1)}(E_\gamma). \quad (48)$$

- **NOPT1=22** – The $M1$ PSF model given by the sum of the model corresponding to the sum of the **NOPT1=21** option and an exponential low-energy enhancement:

$$f^{(M1)}(E_\gamma) = C_1^{(M1)} f_{\text{SLO}}^{(M1)}(E_\gamma) + \frac{C_1^{(M1)} C_2^{(M1)} E_\gamma^{-C_3^{(M1)}}}{3(\pi\hbar c)^2} \quad (49)$$

Parameters describing the low-energy enhancement $C_i^{(M1)}$ are given by variables **PAR.M1(i)** in the input file **DICE_EV.DAT**. The constants $C_1^{(M1)}$ and $C_3^{(M1)}$ are dimensionless and the factor $C_2^{(M1)}$ is given in $\text{fm}^2 \cdot \text{MeV}^{-1}$.

6.4 $E2$ PSF Models

Selection of the $E2$ PSF model is made via switch **NOPT2**. The following models are available:

- **NOPT2=0** – The single-particle (SP) model in which the $E2$ PSF is an E_γ -independent constant, $f^{(E2)} = k_{E2}$. The value of the constant is given by variable **QEL** in input file **DICE_EV.DAT**.
- **NOPT2=1** – The $E2$ PSF shape which is based on the Lorentzian shape of photoabsorption cross section

$$f^{(E2)}(E_\gamma) = \frac{1}{5(\pi\hbar c)^2} \frac{1}{E_\gamma} \sum_{i=1}^n \frac{\sigma_{E_i} \Gamma_{E_i}^2}{(E_\gamma^2 - E_{E_i}^2)^2 + E_\gamma^2 \Gamma_{E_i}^2}. \quad (50)$$

where, parameters E_{E_i} , Γ_{E_i} and σ_{E_i} correspond to the energy, width and cross section at the maximum of the i^{th} assumed resonance, respectively. The values of these parameters are given by variables **ERE(i)**, **WE0(i)** and **SIGE(i)** in the input file **DICE_EV.DAT** in units of MeV, MeV and mb, respectively. The allowed number of resonances in the code is $n = 5$.

The factor $1/E_\gamma$ appeared in Eq. (50) instead of E_γ in Eqs. (29) and Eq. (44) due to the relation between the average photoabsorption cross section (for absorption of a transition of type X and multipolarity L) $\sigma^{(XL)}(E_\gamma)$ and PSFs

$$f^{(XL)} = \frac{1}{(\pi\hbar c)^2} \frac{\sigma^{(XL)}(E_\gamma)}{(2L+1)E_\gamma^{2L-1}}. \quad (51)$$

As a consequence, the same form of the photoabsorption cross section for transitions of all multiplicities leads to different E_γ dependence of PSFs.

- **NOPT2=11** - The $E2$ PSF is given in a tabulated form as a function of E_γ , $f_{\text{tab}}^{(E2)}(E_\gamma)$. The values of $f_{\text{tab}}^{(E2)}(E_\gamma)$ are read from the file **PSFE2.DAT**. The structure of this input file is described in Sec. 5.3. Exact validity of the Brink hypothesis is assumed in this model.

6.5 Adding new models

Users are welcome to add their own models of level density or PSFs. The function **DENSITY(...)** should be used to add new models of level density. New models of

photon strength functions should then be added to the function `SGAMMA(...)`. Please note that function `SGAMMA` does not calculate $f^{(XL)}$ but the product $f^{(XL)} E_\gamma^{2L+1}$.

If new variables are to be used in a user defined model, they should be added to the corresponding `COMMON` blocks. The `COMMON` block `/DEN/` is recommended to be used for variables related to level density, the `COMMON` blocks `PHOTO` or `DIPE1` for variables related to the strength functions. However, there should be sufficient number of available variables in the present version of input file `DICE_EV.DAT` that could be used for different parameters in the models; see variables `DENPC`, `DENPEN(3)` and `DENPAR(4)` for level density and `PAR_E1(3)`, `PAR_M1(3)`, `EK0`, `EGZERO` for PSFs.

One of the possible ways how to add a user-defined model is to exploit the options `NOPTLD=11`, `NOPT1=11`, `NOPTM1=11`, and `NOPT2=11`. In these cases the level density and/or PSF models can be added in the form of a table into the corresponding input file, see description of these options in Secs. 5.1 and 6. The description of the format of these input tables is given in Secs. 5.3 and 5.4. Any model of level density can be used with `NOPTDE=11`. The PSF models with the corresponding option equal to 11 are restricted to those that follow the Brink hypothesis. Use of these options does not require any changes of the `COMMON` blocks in the code.

7 Examples

A few examples of input files are attached to the present DICEBOX distribution. These examples can also be used for verification of successful compilation of the code. The number of nuclear supra-realizations (variable `NSREAL`), nuclear realizations (variable `NRL`) and cascades (variable `NEVENTS`) are small in these examples. These numbers are recommended to be used for the verification but must be changed for real use of the code; see recommendations for each number in description of these variables in the “Global variables” part of Sec. 5.1 and in Ref. [17]. As a rule of thumb, the number of cascades is recommended to be at least a few hundred thousands during the use of the code for realistic simulations.

In all the examples below we will assume that Porter-Thomas fluctuations of individual partial radiation widths are switched on, i.e. `NOPTFL=1`. At the same time, it is usually assumed that the actual number of levels in a given simulated bin fluctuates according to the Poisson distribution, i.e. the `LMODE=0` option is used.

7.1 Example 1:

Decay of 2^+ level (resonance) at neutron separation energy of ^{96}Mo

This is probably the most typical option for running the code. It corresponds to a decay of a well separated level with specified spin and parity at certain excitation energy. If this level is just above the neutron (proton) separation energy, we usually talk about neutron (proton) resonances. Intensities of primary transitions are usually unknown in these cases. Global switches governing the run of the code are thus set to:

```
* Switches governing the run of the code (IVER, IPRIM)
0 0
```

and the specification of the capturing state, that corresponds to a low-lying *s*-wave neutron resonance (with $J^\pi = 2^+$) originated from a neutron capture in ^{95}Mo target, is

```
# Neutron capturing states - Sn (MeV), J, Pi
9.1540 2.0 0
```

If one wants to write down all available information on the decay process (in the ASCII form) and also all the levels produced in individual nuclear supra-realizations, the switches governing the writing down the output files should be set to

```
* Switches governing writing (ISWR,ISWB,ISWEL,ISWSP,ISWPA,ISWIC,...)
1 0 1 1 1 1 1 1 1
```

The combination of the GLO *E1* PSF model (`NOPT1=5`) and a “composite *M1* PSF model” (`NOPTM1=4`) is used. The Giant quadrupole resonance model (`NOPT2=1`) is used for *E2* PSF together with the BSFG model from [4] (`NOPTDE=6`) with parity dependence at low excitation energies (`LDPDEP=2`). In this example parameters governing the parity dependence of the level density are given in:

```
* LD parameters for "parity-dependent" level density - PRC67, 015803
1.0 5.0 0.0 0.0
```

This model is based on results presented in Refs. [16, 19].

Critical energy, E_{crit} , is set to 2.79 MeV with 23 levels known below this excitation energy. The normalization factor for intensities can be ignored in this case as intensities of primary transitions to levels below E_{crit} are not considered. The factor can reach any value; it is set to 0.01 in the example file. In reality, intensities of primary transitions to levels below E_{crit} can be found in the input file but they are not read using the set of above-given options.

As the switch that governs writing of information on levels is on, files with levels generated in the code for each nuclear supra-realization (`LEVELS.sss`) are produced. Total number of levels generated levels (i.e. the number of levels below energy of initial state (variable BN) with $J = 0 - 49$ or $J = 1/2 - 99/2$) is about 10^5 .

7.2 Example 2:

Decay of 3^+ level(resonance) at neutron separation energy of ^{98}Mo using user defined models for PSFs and level density

This example, simulating a decay of a 3^+ level (a low-lying s -wave neutron resonance produced in the neutron capture in ^{97}Mo) at neutron separation energy of 8.6426 MeV in ^{98}Mo , shows how to use “user defined” models of the photon strength functions for $E1$ and $M1$ transitions and of the level density. Use of these “user defined” models is achieved with `NOPT1=11`, `NOPTM1=11` and `NOPTDE=11` options; in reality the values in the input files correspond to models based on the HFB calculations available via RIPL-3 database [5]. The corresponding input files – `PSFE1.DAT`, `PSFM1.DAT`, and `LDTAB.DAT` – are needed in this case, see Secs. 5.1, 5.3 and 5.4.

Fluctuation in the number of generated levels is in this case given by the `LMODE=2` option, i.e. the Wigner distribution of the nearest neighbor spacings without long-range correlations is used for producing levels in individual bins. Intensities of primary transitions to levels below E_{crit} are assumed to be unknown similarly to the previous example.

Using the global options

```
* Switches governing writing (ISWWR,ISWBN,ISWEL,ISWSP,ISWPA,ISWIC,...)
1  0  1  0  0  1  0  0  0
```

only information on the excitation energy of levels fed in each simulated decay and on the type of the emitted particle (γ or e^- due to electron conversion) is written down into the (ASCII) output files `EVENTS.Ssss.Rrrr`. The files `LEVELS.sss` are not created.

7.3 Example 3:

Decay of 2^- level (resonance) at neutron separation energy of ^{158}Gd with known intensities of primary transitions to low-lying levels

It might (although very rarely) happen that intensities of primary transitions from a well-separated initial level (neutron resonance) to levels below E_{crit} are known. If this is the case, the switches governing the run of the code should be set to:

```
* Switches governing the run of the code (IVER, IPRIM)
0  1
```

An example of this might be the decay of the first resonance in the $^{157}\text{Gd}(n,\gamma)$ reaction. The intensities of primary transitions to many levels are known as thermal neutron capture is really dominated by this resonance. Intensities of primary transitions measured in thermal neutron capture can thus be used.

Similarly to the previous example, only information on energy of levels hit in the decay and the type of the emitted particle (γ or e^-) is stored in the output files `EVENTS.Ssss.Rrrr`.

The KMF model (`NOPT1=4`) is used in this example for $E1$ PSF, while the $M1$ PSF is given by a composite model `NOPT1=4`. The resonance terms in this $M1$ PSF model correspond to a Lorentzian parametrization of the scissors mode – resonance near 3 MeV –, and the double-humped resonance description of the spin-flip mode – two resonances between 5 and 10 MeV. The SP model is used for $E2$ PSF (`NOPT2=0`) and the BSFG model from [4] (`NOPTLD=6`) with no parity dependence above E_{crit} for level density. This selection of parameters is based on results of [6, 22].

The combination of switches `IVER=0` and `IPRIM=1` can often be used also for simulation of decay from thermal neutron capture on nuclei with the target $J_T^\pi = 0^+$. In this case, only resonances with $J^\pi = 1/2^+$ contribute to thermal neutron capture. The only difference with respect to the choice of switches `IVER=2` and `IPRIM=1`, see Sec. 7.6, is the difference in fluctuation properties of primary transitions. However, the difference between the Porter-Thomas distribution – used for `IVER=0` – and the distribution obtained from all contributing resonances is for many nuclei very small.

7.4 Example 4:

Decay following thermal neutron capture in ^{195}Pt with known intensities of primary transitions and unknown neutron resonance parameters

Several neutron resonances usually contribute to the thermal neutron capture. Specification of their contribution can be made in two different ways. One way of the specification is described here and in Sec. 7.5, for the second possibility see Sec. 7.6.

This example describes a situation typical for odd- A target where two capturing spins may contribute to the neutron capture and the fraction of captures via individual initial spins are known. Specifically, the $J_T^\pi = 1/2^-$ ground state of ^{195}Pt can produce s -wave capture on resonances with $J^\pi = 0^-$ or 1^- . Experimental data on individual resonances indicate that about 3.2% of captures proceeds via 0^- while the rest via 1^- resonances. At the same time, intensities of primary transitions to levels below $E_{\text{crit}} = 1.8$ MeV are assumed to be known. As a result, the switches and variables governing the run of the code can be set to:

```
* Switches governing the run of the code (IVER, IPRIM)
1    1
# Neutron capturing state (Sn, J_T, pi_T, CAPFR(1))
7.9219  0.5  1  0.032
```

Here, the fraction of captures on the lower spin, $J^\pi \equiv J_T^\pi - 1/2 = 0^-$, is given by the variable `CAPFR(1)`. The fluctuation properties of primary transitions from the capturing state of given J^π obey the PT distribution with this choice of switches.

The $E1$ PSF is assumed to be given in a tabulated form (NOPTE1=11), $M1$ PSF is given by the SF resonance of Lorentzian shape (NOPTM1=1) and $E2$ PSF by the SP model (NOPTE2=0). The constant temperature formula from [4] is used for level density model (NOPTDE=0), no parity dependence is assumed above E_{crit} (LDPDEP=0). Information on energy of hit levels in the decay and its spin and parity is stored in the ASCII output files EVENTS.Ssss.Rrrr. Files with levels generated in individual nuclear supra-realizations are not produced.

In a general case, the fraction of the capturing state with lower spin can reach any value between 0.0 and 1.0. If the value CAPFR(1)=0.0 (1.0) was used, all decays would proceed via $J^\pi = 1^-$ (0^-) resonances. This situation, CAPFR(1)=0.0 or 1.0, is not rare and means that only resonances with one spin contribute to the (thermal neutron) capture. As the fluctuations of primary transitions follow the PT distribution for IVER=1, the following two choices of switches and variables in DICE.EV.DAT, which would simulate decay of $J^\pi = 1^-$ resonance, are equivalent:

1. * Switches governing the run of the code (IVER, IPRIM)


```

1      1
# Neutron capturing state (Sn, J_T, pi_T, CAPFR(1))
7.9219  0.5  1  0.0
```
2. * Switches governing the run of the code (IVER, IPRIM)


```

0      1
# Neutron capturing state (Sn, J_res, pi_res)
7.9219  1.0  1
```

The same situation would happen for a resonance decay from the s -wave neutron capture in even-even nucleus with target spin $J_T^\pi = 0^+$. In this case, any of the following choices can be used:

1. * Switches governing the run of the code (IVER, IPRIM)


```

1      1
# Neutron capturing state (Sn, J_T, pi_T, CAPFR(1))
6.500   0.0  0  1.0
```
2. * Switches governing the run of the code (IVER, IPRIM)


```

0      1
# Neutron capturing state (Sn, J_res, pi_res)
6.500   0.5  0
```

The energy of the initial level was (randomly) set to 6.5 MeV in this artificial example.

7.5 Example 5:

Decay following thermal neutron capture in ^{97}Mo with unknown intensities of primary transitions

It can happen that primary transitions to low-lying levels from the thermal neutron capture are unknown. This example describes this option using the decay of ^{98}Mo produced in $^{97}\text{Mo} (n, \gamma)$ reaction. General switches in this case are

```
* Switches governing the run of the code (IVER, IPRIM)
1 0
# Neutron capturing state
8.6426 2.5 0 0.0
```

This choice indicates that there is no contribution of 2^+ resonances to the thermal neutron capture and all γ decays thus start from $J^\pi = 3^+$ resonances. As already mentioned in the previous example, see Sec. 7.4, exactly the same treatment of the capturing state can be reached using

```
* Switches governing the run of the code (IVER, IPRIM)
0 0
# Neutron capturing state (Sn, J_res, pi_res)
8.6426 3.0 0
```

The PSFs models used in this example are the same as in Sec. 7.1. The level density model has a parity dependence and an even-odd spin staggering above E_{crit} . The parity dependence is indicated by LDPDEP=2 and the even-odd spin staggering is an inherent part of the level density model used. (The staggering is an integral part of the models NOPTDE=8 and 9 from [23], see Sec. 6.1.1.) The parity dependence is specified via:

```
* LD parameters for "parity-dependent" level density - PRC67, 015803
1.0 3.2 0.0 0.0
```

This setting corresponds to $C_\pi = 1.0 \text{ MeV}^{-1}$ and $\Delta_\pi = 3.2$ in Eq. (27). These parameters mean that the parity independence can be considered only above excitation energy of about 5 – 6 MeV.

The even-odd spin staggering of the model NOPTDE=9 is assumed to fade away with excitation energy, see description of the model in Sec. 6.1.1. The two energies describing this fading, E_L and E_H from Eq. (25) are the first two parameters on the line

```
* Auxiliary level density parameters (DENPL,DENPU,DENPA,DENPB,DENPC,DENPD)
2.0 5.0 0.0 0.0 0.0 0.0
```

Thus, the staggering completely disappears at excitation energy of 5 MeV.

7.6 Example 6:

Decay following thermal neutron capture on ^{95}Mo with specified resonance parameters

The second (and more precise) way to characterize the off-resonance s -wave neutron (thermal) capturing state is via specification of parameters of individual contributing resonances. Usually only a few neighbor resonances are important. The contribution of different resonances might modify the expected Porter-Thomas distribution of primary transition. In reality, such a modification is probably rather small in any actual nucleus. Let us assume that intensities of primary transition to levels below E_{crit} are known, i.e.

```
* Switches governing the run of the code (IVER, IPRIM)
2 1
```


The parameters of individual resonances are specified in the file `RES_PAR.DAT`, see Sec. 5.2, and there must be at least two resonances for each contributing spin. In our case this minimum value is reached for 2^+ resonances while four 3^+ resonances are specified. “Bound resonance” (with negative neutron energy) contributes to the capture in the case of $J^\pi = 3^+$.

Parameters describing the neutron capturing state read as:

```
# Neutron capturing states - Bn (MeV), J_T, Pi_T, En (eV)
9.1540 2.5 0 0.025
```

Here, the last value indicates that the contribution of each resonance to the neutron capture is calculated at neutron energy $E_n = 0.025$ eV. The fraction of captures via different spins can be checked in the `DICE.PRO` file – as indicated there, only resonances with $J^\pi = 3^+$ levels were simulated. In reality, the relative contribution of 2^+ resonances to the capture cross section is about 3×10^{-4} in this case. As indicated by the text in Sec. 5.2, such a small fraction (smaller than 10^{-3}) leads to use of all initial states with $J^\pi = 3^+$.

The PSFs and NLD models are almost the same as in the Example 7.1. The only difference is in the $E2$ PSF, where the SP model (`NOPT2=0`) is used instead of the Giant quadrupole resonance model.

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A Appendix A:

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