

CALENDF-2010 : USER MANUAL

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RAPPORT CEA-R-6277 – Jean-Christophe SUBLET, Pierre RIBON, Mireille COSTE-DELCLAUX

«Manuel d'utilisation de CALENDF - 2010»

Résumé - Le code CALENDF-2010 est une révision en Fortran-95 du code diffusé en 1994, 2001 puis 2005 avec une amélioration de sa "qualité" et de ses modalités d'utilisation. Destiné au calcul et au traitement des sections efficaces neutroniques multigroupes, il est largement basé sur l'utilisation de la quadrature de GAUSS. Ses principales fonctionnalités sont les suivantes: calcul de tables de probabilité basées sur les moments et calcul de sections effectives; regroupement de sections efficaces ponctuelles, de tables de probabilité et de sections effectives; condensation de tables de probabilité; mélange de tables de probabilité pour différents isotopes; interpolation de tables de probabilité; calcul de tables de probabilité basées sur les sections effectives; calcul de sections effectives à partir de tables de probabilité; comparaison de sections effectives; reconstruction de sections efficaces ponctuelles continues dans tout le domaine énergétique et calcul de la transmission moyenne à travers des échantillons de différentes épaisseurs. Le manuel d'utilisation de CALENDF, après avoir rappelé les principales fonctionnalités du code, présente de façon exhaustive les données relatives à chacune et commente les sorties associées. En annexe, il fournit les procédures d'installation sur les différents calculateurs, des cas-tests standard ainsi qu'une comparaison des performances des différents ordinateurs sur lesquels le code a été porté et qualifié.

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Abstract

CALENDF-2010 represents a Fortran-95 update of the 1994, 2001 then 2005 code distribution with emphasise on programming quality and standards, physics and usage improvements. Devised to process multigroup cross-sections it relies on Gauss quadrature mathematical principle and strength. The followings processes can be handled by the code: moment probability table and effective cross-section calculation; pointwise cross section, probability table and effective cross-section regrouping; probability table condensation; probability table mix for several isotopes; probability table interpolation; effective cross section based probability table calculations; probability table calculations from effective cross-sections; cross-section comparison, complete energy pointwise cross-section processing and thickness dependent averaged transmission sample calculation. The CALENDF user manual, after having listed all principal code functions, describes sequentially each of them and gives comments on their associated output streams. Installation procedures, test cases and running time platform comparisons are given in the appendix.

Résumé

Le code CALENDF-2010 est une révision en Fortran-95 du code diffusé en 1994, 2001 puis 2005 avec une amélioration de sa "qualité" et de ses modalités d'utilisation. Destiné au calcul et au traitement des sections efficaces neutroniques multigroupes, il est largement basé sur l'utilisation de la quadrature de GAUSS. Ses principales fonctionnalités sont les suivantes: calcul de tables de probabilité basées sur les moments et calcul de sections effectives; regroupement de sections efficaces ponctuelles, de tables de probabilité et de sections effectives; condensation de tables de probabilité; mélange de tables de probabilité pour différents isotopes; interpolation de tables de probabilité; calcul de tables de probabilité basées sur les sections effectives; calcul de sections effectives à partir de tables de probabilité; comparaison de sections effectives; reconstruction de sections efficaces ponctuelles continues dans tout le domaine énergétique et calcul de la transmission moyenne à travers des échantillons de différentes épaisseurs. Le manuel d'utilisation de CALENDF, après avoir rappelé les principales fonctionnalités du code, présente de façon exhaustive les données relatives à chacune et commente les sorties associées. En annexe, il fournit les procédures d'installation sur les différents calculateurs, des cas-tests standard ainsi qu'une comparaison des performances des différents ordinateurs sur lesquels le code a été porté et qualifié.

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1 INTRODUCTION

In the 60's, Levitt ¹⁾ proposed the denomination "probability table" for a natural discretisation of cross section data to describe the resolved resonance energy range. Simultaneously, the "sub-group method" was proposed by Nikolaev ²⁾, based on a different definition of the probability tables. Since then several different approaches have been put forward ^{3,4)}. The Ribon approach ⁵⁾, based on Gauss quadrature as a probability table definition and relying on their mathematical principle and strength, has now been used for nearly 25 years. In order to justify this approach, several aspects of the different table methodology are discussed while their accuracy, the calculational methods, efficiency, possible interpretation and manipulation are weighted.

This probability table (PT) approach has been introduced, exploited in both resolved (RRR) and unresolved (URR) resonance ranges, and programmed in the code CALENDF. The 2010 version of the code has been significantly revised in order to improve both its quality and clarity by adopting 90/95 Fortran standard while strengthening its physics. The step from a research tool to a reliable code system has now been attained, suitably documented, verified and QA'd. The main features of the code are described and exemplified. They include not only cross section processing but also some physical controls, particularly in the resonance parameter ranges, resolved and unresolved.

Although probability tables, used as a tool, certainly enhance classical neutronic calculational methods, they are not, even nowadays, in common use in industry or utility bodies because they demand dense data storage and interpretation methods. Their main interest is that, in the unresolved resonance range, they uniquely complement pointwise Monte Carlo treatment. However, in the resolved resonance range, the energy dependent information is embedded within each group, which can be summarized as the statistical hypothesis. This assumption is more physically acceptable for high-energy applications, fast spectrum systems notably; however probability tables have been proved to be most useful in accounting for all self-shielding effects in more thermal neutron environments. The present conditions of probability table usage and precincts are determined.

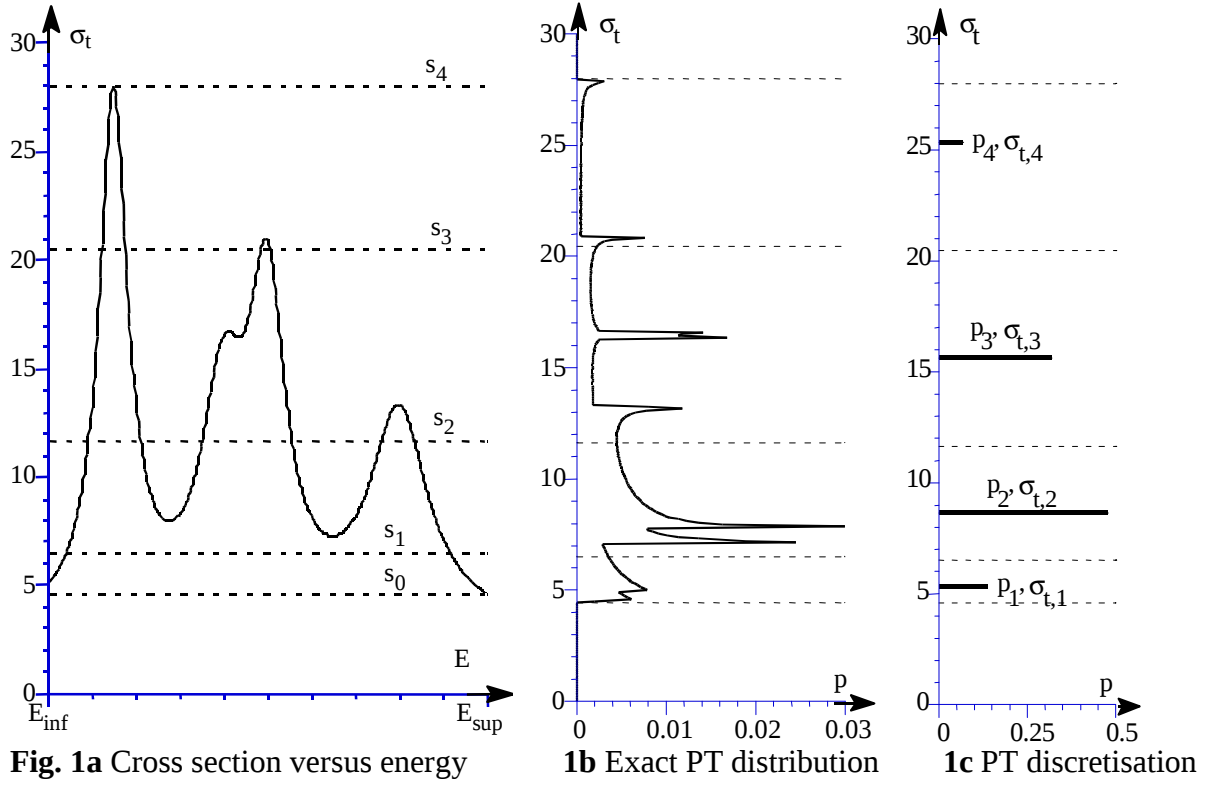
The principle of all probability tables is to describe the cross section, within a group, by a set of discrete values:

$$p_i, \sigma_{t,i}, [\sigma_{x,i}, x=\text{elastic, inelastic, fission, absorption...}] \text{ with } i=1 \text{ to } N$$

As the partial cross sections $\sigma_{x,i}$ always appear linearly in neutronic applications, to each step (N) of the total cross section $\sigma_{t,i}$ only one value of each partial can be associated.

1.1 Gauss Quadrature and PT-Moment

A probability distribution is exactly defined by its infinite moment sequence. A PT-Mt is formed of N doublets $(p_i, \sigma_i, i=1, N)$ exactly describing a sever sequence of 2N moments of the $\sigma_i(E)$ distribution. Such a probability table is a Gauss quadrature and as such will benefit from their entire mathematical settings⁷⁾.



The only degree of freedom is in the choice of moments for which a default is proposed in CALENDF, dependant on the table order, and associated to the required accuracy.

$$\frac{1}{G} \int_{E_{\text{inf}}}^{E_{\text{sup}}} \sigma_t^n(E) dE = \int_{\sigma_{\text{min}}}^{\sigma_{\text{max}}} p(\sigma_t) \sigma_t^n d\sigma_t = \sum_{i=1}^{i=N} p_i \sigma_{t,i}^n \text{ with } G = E_{\text{sup}} - E_{\text{inf}}. \quad (1)$$

Each one of the components of Equation (1) is illustrated in Fig. 1a, b and c. Equation (1) must be satisfied for $2N$ values of n . Due to orthogonal polynomial properties this set of $2N$ equations always has one solution, the roots $\sigma_{t,i}$ being real, over the range of σ_t , and the probabilities p_i being always positive.

1.2 Calculational methods

The moments having been computed, the probability table is established from the following relation:

$$\begin{aligned} I(z) &= \int \frac{p(x)}{1-zx} dx = \underbrace{M_0 + M_1 z + M_2 z^2 + \dots + M_{2N-1} z^{2N-1}}_{2N \text{ moments}} + R_{2N} z^{2N} \\ &= \frac{b_0 + b_1 z + b_2 z^2 + \dots + b_{N-1} z^{N-1}}{\underbrace{1 + a_1 z + a_2 z^2 + \dots + a_N z^N}_{Q_{N,N-1} = \text{PADE approximant}}} + R'_{2N} z^{2N} \\ &= \frac{b_0 + b_1 z + \dots + b_{N-1} z^{N-1}}{\prod_{i=1}^N (1 - zx_i)} + R'_{2N} z^{2N} = \sum_i \underbrace{\frac{p_i}{1 - zx_i}}_{p_i, x_i = \text{quad. table}} + R'_{2N} z^{2N} \end{aligned} \quad (2)$$

The second line is the Padé approximant that introduces an approximate description of higher moment order. Partial cross section steps obey the following equation:

$$P_n = \frac{1}{G} \int_G \sigma_t^n(E) \sigma_x(E) dE \equiv \sum_{i=1}^{i=n} p_i \sigma_{t,i}^n \sigma_{x,i} \quad (3)$$

Equation (3) must be satisfied for N values of n. The consistency between total and partials is obtained by a suitable choice of the indices n values. In the absence of mathematical background there is no reason why an individual partial cross section steps cannot be slightly negative, and sometimes this is the case. However, the effective cross section reconstructed from the sum of the steps values is always positive.

The moments taken into account are not only from 0 to 2N-1 for the total, but negative moments are also introduced in order to obtain a better numerical description of the excitation function troughs or dips (opposed to peaks) of the cross-sections. CALENDF standard choice ranges from 1-N to N for total cross section, and (1-N)/2 to (N-1)/2 for the partials.

Within the resonance range the cross sections are calculated from the resonance parameters described in the ENDF file using different formalisms. A slightly modified multi-level Breit and Wigner formalism is implemented by CALENDF in this energy range allowing the pointwise cross sections to be calculated.

1.3 Unresolved resonance range

The basic idea is to generate random ladders of resonances. The treatment of these ladders is then the same as that of the RRR (except, for the treatment of external or far-off resonance). For each group, or several groups in the case of fine structure, an energy range is defined, taking into account both the nuclear properties of the nuclei and the neutronic requirements (accuracy and grid). By default, in CALENDF, the energies are taken from a sequence of eigenvalues of a random matrix. A stratified algorithm, improved by an antithetic method, creates the partial widths⁶.

In the URR range CALENDF applies the "statistical hypothesis" based on the fact that the resonances can be statistically described.

1.4 Effective cross section and moment

The effective cross section can be calculated from either the pointwise cross section or the probability table as follows:

$$\sigma_{x,eff,quad.}(\sigma_d) = \frac{\sum_{i=1}^{i=N} \frac{p_i \sigma_{x,i}}{\sigma_{t,i} + \sigma_d}}{\sum_{i=1}^{i=N} \frac{p_i}{\sigma_{t,i} + \sigma_d}} \quad (4)$$

When the dilution is infinite this formula becomes:

$$\sigma_{x,eff,quad.} = \sum_{i=1}^{i=N} p_i \sigma_{x,i} \quad (5)$$

This equation represents the first order moment. CALENDF will compute the relative and absolute differences that could exist between the calculated effective cross sections (computed

from the PT and the pointwise data) in order to ascertain the calculational choice made. Those differences are usually well below the reconstruction accuracy required.

1.5 CALENDF specifics

The CALENDF Nuclear Data Processing System is used to convert the evaluation defining the cross-sections in ENDF format (i.e. the point-wise cross-sections and/or the resonance parameters, both resolved and unresolved) into forms useful for applications. Those forms used to describe neutron cross-section fluctuations correspond to "cross-section probability tables" (CSPT), based on Gauss quadratures and effective cross-sections.

The code accesses the data stored in MF-2 (resonance parameters) and MF-3 (point wise cross-sections) of the ENDF-5 or 6 data file provided as input, ignoring all other MF. Ladders of resonance parameters are generated into some energy 'zones' in the unresolved range, which are then treated as the resolved range. Checks of the consistency of the evaluated data are performed and messages emitted.

Within the resonance range the cross-sections are calculated from the resonance parameters described in the ENDF file using different formalisms. A slightly modified multi-level Breit and Wigner formalism (Multi Niveau Breit et Wigner MNBW $\neq$ MLBW) is applied by CALENDF in this energy range allowing the pointwise cross-sections to be calculated.

In the Unresolved Resonance Range (URR) the basic idea is to generate random ladders of resonances. The treatment of these ladders is then the same as that of the Resolved Resonance Range (RRR), except, for the treatment of external or far-off resonances. For each group, or several groups in case of fine structure, an energy range is defined, taking into account both the nuclear properties of the nuclei and the neutronic requirements (accuracy and grid). By default, in CALENDF, the energies are taken from a sequence of eigenvalues of a random matrix. A stratified algorithm, improved by an antithetic method, creates the partial widths. In the URR range CALENDF applies the "statistical hypothesis" based on the fact that the resonances can be statistically described.

The basic interpolation mode is a cubic one, based over 4 points, which requires a careful checking (and eventual introduction of new energy points) of the ENDF raw data (MF-3). An important point is that CALENDF will need MF-3 MT-1 (the total cross-section) present in the evaluated file. MF-2 is thoroughly checked and interpreted if felt necessary. All the MT numbers recognised by the code in MF-3 will be "cubicized", the different interpolation laws given are interpreted and the cross-section - energy grids are treated with a cubic interpolation:

$$y = P_n(x) \text{ with polynomial order } n \leq 3$$

$$y = a + bx + cx^2 + dx^3$$

It is assumed that the indicated formulae are applicable to interpolate between x_i and x_{i+1} taking into account x_{i-1} and x_{i+2} .

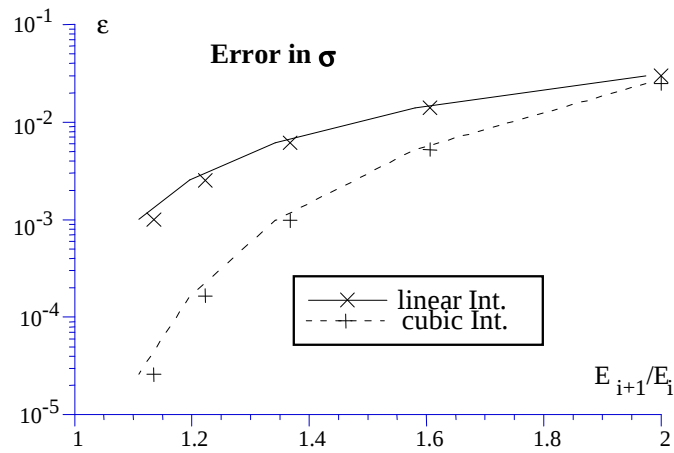


Fig 2 Cubic and linear interpolation errors

There is a precision advantage, depicted in Fig.2, when favouring a cubic polynomial interpolation against a linear one, particularly when a lot of fine resonance structures cohabit forcing the energy grid to be fine.

On the subject, and in order to illustrate differences between linear and cubic interpolation, one needs to remark that:

- When interpolating in-between points when the concavity is directed upward a linear interpolation will always over estimate the area. A cubic interpolation will lead to an area less than the former.
- When interpolating in-between points when the concavity is directed downward a linear interpolation will always under estimate the area. A cubic interpolation does not systematically lead to such an under-estimation, also its area will be greater than the former.

This to say that, particularly when the slope of the cross-section changes rapidly and the raw description has not been particularly well inputted in the parameter file, such different approaches could lead to group data discrepancies due to different reconstruction processes and not to any other processes.

As specified in the ENDF-6 Format manual ⁸⁾ the energy mesh for the total cross-section must be a union of all energy meshes used for the partial cross-sections. However, this rule has been regularly ignored in some evaluations, CALENDF will add the partials energy points within the meshes of the total and print a diagnostic. New energy points could also be added if necessary to satisfy the reconstruction criteria.

CALENDF Doppler broadens all cross-sections, assuming that they have structures. This feature contrasts with other processing systems and may generate differences when comparing group data, particularly in the first group of threshold channels. Such a feature affects the threshold itself as well.

1.6 CALENDF features

Cross-section probability tables allow various data handling processes to be performed once they have been calculated. These include isotopic smearing, condensation, interpolation and order reduction. Those data manipulation processes are made extremely efficient and strict, in terms of physical meaning and easy to perform which is due to the very explicit format of the probability tables.

Those operations all assume the statistical hypothesis and tend to be more exact at high energy, although for the Pu^{239} evaluation this limit is as low as a few hundred eV. The statistical hypothesis, in neutronic terms this time, implies a replacement of $\tau(E)$ by its mean value $\bar{\tau}$ and could be considered like a generalization of the narrow resonance hypothesis where $\tau(E)$ is replaced by a constant.

Point-wise cross-sections (CS) are calculated on pre-defined energy zones for every group. These energy zones are generally discontinuous (except in the branch SIGTTEUM, or in case of very fine groups) and they can be recorded on request.

Effective cross-section (SEFF) can be, on request, calculated from the point-wise cross-section as well and recorded. Effective cross-sections can also be rapidly calculated from the probability tables for any dilution.

Cross-section probability tables (CSPT), based on Gauss quadratures, are computed for every group. From these ladders effective cross-sections can be generated.

The use of the branches REGROUTP, REGROUSF and REGROUCS are often necessary to bind the resulting data CSPT, SEFF and CS. Their systematic use is recommended.

CALENDF (the main branch) can deal with evaluations describing several isotopes, the treatment of CSPT by REGROUTP is then rigorous, but the treatment of SEFF and CS is meaningless as there is no correct theory to amalgamate several isotopes.

In the unresolved resonance range (URR) several random samples of resonances can be generated to describe the same energy range, REGROUTP and REGROUSF provide an exact merging, but REGROUCS is meaningless (there is no meaning in averaging several random pointwise CS describing the same energy range).

CALENDF also allows utilitarian operations on these CSPT, such as the calculation of effective cross-sections, the comparison of sets of effective CS, the calculation of the neutron transmission of some samples.

CALENDF can process PENDF data, but then of course, does not provide a better description of the cross-sections in the unresolved energy range, nor allow a probability table calculation in this range if only averaged cross-sections are provided (unless the pointwise data file comes from the output containing the cross-sections (NFCS output) performed by CALENDF.

CALENDF evaluation processing can induce negative values of the probability table steps for the three following reasons:

1. If the evaluation and the processing are correct, no negative values of the σ_t steps (nor of the probabilities) should exist. However, small negative values of some partial cross-sections steps, associated to small probabilities, may occur for perfectly legitimate mathematical reasons.
2. The evaluation itself can induce negative values. For instance, the presence of negative pointwise cross-section in the unresolved resonance range (URR), inserted in order to correct averaged resonance parameters overestimation can lead to such a default. Furthermore, some doubtful evaluation still remains in some data libraries.
3. One must recognise, however, that CALENDF itself can occasionally produce negative values. A modification of the accuracy indice, IPRECI, generally improves the results.

Total negative steps are suppressed, if they exist. Partial negative steps are of no consequences and by default are preserved by the code. However, users are given the possibility to remove all negative values by using CALENDF or LECRITP keyword LPSPPPOS. The accuracy of the data will then be slightly decreased.

In some evaluation, in the Resolve Resonance Range the radiation widths could have been set to zero, in those cases the code will automatically set them to 10^{-6} when the Reich Moore approximation is used.

2 Use of CALENDF

Details of CALENDF and differences in running CALENDF on different platforms are discussed in Appendix A. This section concentrates on the information that a user must know prior to using CALENDF and on introducing the code words and their sequences that instruct CALENDF to carry out various types of calculation. The code is modular and is split into several branches, each of them being able to perform a set of well-defined tasks and processing:

cfmod.f	Module subroutines.
mcalendf.f	Main program.
spgbr.f	Branching subroutines
spgdop.f	Doppler subroutines
spgintg.f	Numerical subroutines
spglec.f	Read-Write subroutines
spgmat.f	Mathematical subroutines
spgnew.f	Recently added subroutines
spgsh.f	CALENDF branching subroutines
spgsig.f	Cross-section subroutines
spgsvc.f	Service subroutines
spgtps.f	Effective cross-section and probability table subroutines

3 Main Input

The input file constructed by a user consists of a sequence of code words that falls into different categories.

The code words are described in the following sections. The code words are shown in **BOLD** type with details of the various parameters that accompany some of them shown in an *ITALIC* font. Default values are assumed if the optional code word is not used and are enclosed in angle brackets < >. Optional code words are shown **underlined**. User parameter choices are described enclosed in angle bracket.

Many of the code words consist of several characters, of which only the upper case ones (as shown in this manual) are read, so abbreviations may be used if wished. All the input is "free format", the user may include as many blanks (white space), on the same line, between the words and the parameters as desired so that the file is readable and easily understood.

One or more commentary text line could begin the input file, afterward the input stream is continuous until the code word "end" Any type of characters can be added (comments, descriptions) once the code word and parameters sequences have been typed.

3.1 DIMENSIONAL OPTIONS

NORMAX and *NDILMX* are dimensions used by several branches, and can be currently modified by user. There is no limit to *NDILMX*, numerical accuracy may limit *NOR*, the order of the probability tables, to around 16 but greater values of *NORMAX* are probably useless.

All the other dimensions defined hereafter are only used in *CALENDF* and *SIGTTEUM*. They have been adapted so that all presently available evaluations could be processed by *CALENDF-2010*. However, future evaluations may oblige the users to modify these dimensions in order to process them appropriately.

MODIFDIM "word*6"

<i>NORMAX</i>	<11>	max. order of the probability tables
<i>NDILMX</i>	<16>	max. number of dilutions
<i>NISOMX</i>	<9>	max. number of isotopes described by the evaluation
<i>NPPRMX</i>	<30>	max. number of resolved resonance populations (including each isotope, energy range, orbital momentum, spin)
<i>NZORMX</i>	<11>	max. number of sub-ranges (or zones) describing the Resolved Resonance Range (RRR) in the evaluation
<i>NPPUMX</i>	<46>	max. number of unresolved resonance populations (isotope, orbital momentum, spin)
<i>NPEUMX</i>	<140>	max. number of energies used to define the average resonance parameters in the URR of the evaluation
<i>NPOPMX</i>	<12>	max. number of populations (orbital momentum, spin) for a given isotope (for the URR)
<i>NMODMX</i>	<13>	max. number of interpolation modes describing a raw cross-section in the evaluation

3.2 PARTIAL CROSS-SECTIONS GROUPING

In the present 2010 version CALENDF regroups the many partial cross-sections into 5 macro-partials stored into MTREFD(1:5) and identified by a MT number, inspired from ENDF-102 [1] and used by simulation codes. This grouping, defined in MTREP(1:20,1:5), is verified when probability tables and cross-sections are processed and can easily be modified. A maximum of 20 partial cross sections can be grouped together. The default sequences are:

MTREFD(1:5) <2 101 18 4 15> the partial grouped CS are identified (if they exist) by these 5 numbers

MTREFD(1) = MT-2, the elastic scattering cross-section

MTREFD(2) = MT-102 + MT-103 + ..., any process without outgoing neutron

MTREFD(3) = MT-18, the fission total

MTREFD(4) = MT-4 + MT-22 + ..., any process emitting one neutron only, except elastic

MTREFD(5) = MT-5 + MT-11 + ..., any process emitting several neutrons, except fission

The programmed grouping is given by:

MTREP(1:20,1) <2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0>

MTREP(1:20,2) <102 103 104 105 106 107 108 109 111 112 113 114 115 116 0 0 0 0 0 0>

MTREP(1:20,3) <18 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0>

MTREP(1:20,4) <4 22 23 28 29 32 33 34 35 36 44 45 0 0 0 0 0 0 0 0>

MTREP(1:20,5) <5 11 16 17 24 25 30 37 41 42 0 0 0 0 0 0 0 0 0 0>

MODIFCSGRP *"word*6"*

MTREFD <2 101 18 4 15 >

MODIFCSGRP *"word*5"*

MTREP <IX> one of the five MTREFD indices
 <20 values MT's array>

3.3 CALENDF

Reads an ENDF evaluation

Reconstructs pointwise cross sections

Computes effective cross sections and probability tables

CALENDF

MODIFOPT "word*7"

LCORSCT <.TRUE.> by default, the elastic scattering cross-section is the difference between the total CS and the sum of the partial CS other than the scattering.

<.FALSE.> the total cross-sections is the sum of the partial CS.

NCASUNR <1 1 1 4 9 16> by default, number of random sampling for each of the six IPRECI calculational accuracy indices 1, 2, 3, 4, 5, 6. However, if the group structure is considered as fine, 1 sampling is enough.

LFORMRF <.TRUE.> by default, the formalism used to calculate the RRR is free, i.e. determined by CALENDF from the numerous values of the resonance parameters

<.FALSE.> the formalism is the formalism recommended by the evaluator.

LFORMUR <.TRUE.> by default, the formalism used to calculate the URR is free, i.e. chosen by CALENDF against the numerous values of the resonance parameters

<.FALSE.> the user chooses the formalism:

LFORMUR <.FALSE.> IFORMUR

-if IFORMUR=1 SLBW

-if IFORMUR=2 MLBW

-if IFORMUR=3 BWMN

-if IFORMUR=4 RM

DISTLAW "word*6" three possible laws for resonance parameter distributions (every partial width distribution being a χ^2 law), only one of these three options may be active at any time:

-by default, word = LVPSTR, the energies are the eigenvalues of a random matrix and the width distributions are stratified, no bias, reduced variance.

-if word = LVPAL, the energies are the eigenvalues of a random matrix and the width distributions are simply randomly distributed; corresponds to the actual distribution of parameters.

-if word = LWIGAL, the energies are distributed according to Wigner law, and the width distributions are simply randomly distributed, the simplest approximation.

LANTITH <.TRUE.> by default, if LVPSTR, impose an antithetic generation of the stratified neutron widths.

LNORMGN <.FALSE.> by default, if .TRUE., in the unresolved resonance range, normalize the averaged neutron widths to exactly the theoretical value deduced from the neutron density function, it reduces the error but introduces a bias for the effective cross-sections.

LPSTPOS <.TRUE.> by default, negative steps of the total cross section are suppressed, if present
<.FALSE.> negative steps of the total cross section are preserved

LPSPPOS <.FALSE.> by default, negative steps of all partial cross sections are preserved
<.TRUE.> negative steps of all partial cross sections are set to 1.000000-7 barn

ENERgies <enmin> <enmax> energy range, in eV. It is normalised to the nearest group bound of the selected group structure

MAILlage "word*4"

READ the group structure is read
<ign> group structure name (see §3-15)

SPECTre <nrange> nrange = number of energy zones
For each zone ira (ira = 1 to nrange)
<enzinf(ira)> lower energy bound
<alphaz(ira)> weighting spectra indice (see §3-15)

GENEre the group structure is generated
<nrange> number of energy zones
for each zones ira (ira = 1 to nrange)

<ngc(ira)> <alphaz(ira)> <etop(ira)>
ngc number of groups in the zone for ira
alphaz weighting spectrum indices
etop upper energy bound of the first group in the range IRA
etop has to correspond, within 10^{-6} , to the last energy defined by ira-1

if ngc > 0 : the code reads NGC values of lower energy bounds:

<eng(ig)> ngc values

if ngc < 0 : the code reads τ , the energy step for |ngc| groups:

< τ > defines the energy step which is calculated

if $\tau > 0$ the lethargy step is $1/\tau$: $\text{eng}(\text{ig}+1) = \text{eng}(\text{ig}) \exp^{-1/\tau}$

if $\tau < 0$ the energy step is τ : $\text{eng}(\text{ig}+1) = \text{eng}(\text{ig}) + \tau$

N.B.: when $\text{ngc}(\text{ira}) > 0$ (grid given) it is possible to introduce energy points greater than the maximum of the range ($> \text{etop}(\text{ira})$). This allows the introduction of spurious energies points within the regular, previously calculated energy grid.

TEFF <teff> effective temperature, in Kelvin

NDIL <ndil> number of dilutions
If ndil > 0
<sdil(idil)> dilution values, ndil times

NFEV <unit for endf/b>
<material number to be processed>
<file name> file name in single quote on UNIX

SORTies

NFCS <nfc> if $\neq 0$ unit for pointwise data <file name>

NFPR <nfpr> if $\neq 0$ unit for the sets of group-resonance parameters <file name>

NFTC <nftc> if $\neq 0$ unit for pointwise and collision density data for each dilution
<file name>

NFSFRL <nfsfrl> if $\neq 0$ unit for effective cross-section and fine structure flux with exact slowing-down
<file name>

NFSF <nfsf> if $\neq 0$ unit for directly calculated effective cross-section with a Bondarenko flux.
<file name>

NFSFTP <nfsftp> if $\neq 0$ unit for PT calculated effective cross-section for each zones, prior to regrouping
<file name>

NFTP <nftp> if $\neq 0$ unit for probability tables
<file name>

IPRECI <ipreci> calculational accuracy indices (see §3-15)

NIMP <nimp> output dump indices on unit 6 (see §3-15)

<ncar> number of characters per output line on unit 6

Nota Bene: in a CALENDF group the weighting spectra is unique. Different weighting spectra can be introduced within a group by using the CONDENTP codeword. The energies boundaries given for a chosen weighting spectrum are adjusted to the closest group boundaries.

3.4 REGROUCS, REGROUPR, REGROUSF, REGROUTP

The use of these four branches is generally required after a CALENDF call:

- if NFCS $\neq$ 0 then REGROUCS
- if NFPR $\neq$ 0 then REGROUPR
- if NFTC, NFSFRL, NFSFTP $\neq$ 0 then REGROUSF
- if NFTP $\neq$ 0 then REGROUTP

Their aim is to mix, collapse or merge data belonging to the same group, but appearing in different tables of the CALENDF output. This is because the group covers several energy ranges of the evaluation, because CALENDF creates several computational zones, because there are several random samples in the unresolved energy range, because there are several isotopes in the evaluation.

It is recommended to always use them. It may not be always necessary, in case of a fine group treatment of a pointwise energy range for instance or of pointwise data. However, their usage does not penalise the processing and they just copy the data from the input to the output file.

REGROUPR

NFPR	<nfpr> <file name>	unit for resonances parameters table input
NFPRR	<nfppr> <file name>	unit for resonances parameters table output
NIMP	<nimp> <ncar>	output dump indices on unit 6 (see §3-15) number of characters per output line on unit 6

Regroups resonances parameters tables computed on all the zones

REGROUTP

NFTP	<nftp> <file name>	unit for probability table input
NFTPR	<nftpr> <file name>	unit for probability table output
NIMP	<nimp> <ncar>	output dump indices on unit 6 (see §3-15) number of characters per output line on unit 6

Regroups probability tables computed on several zones of a singular energy group. In particular if the energy domain changes, if a mixture of isotopes occurs or if several sampling have been made.

REGROUSF

NFSF	<nfsf> <file name>	unit for effective cross-section input
NFSFR	<nfsfr> <file name>	unit for effective cross-section output
NIMP	<nimp> <ncar>	output dump indices on unit 6 (see §3-15) number of characters per output line on unit 6

Regroups effective cross-sections computed on several zones of a singular energy group for just one isotope. In particular if the energy domain changes or if several sampling have been made. REGROUSF has no sense in the case of several isotopes in the same evaluation, for there is no strong theoretical background to calculate the merging of the effective cross-sections for several isotopes.

REGROUCS

NFCS	<nfsf> <file name>	unit for pointwise cross-section input
NFCSR	<nfsfr> <file name>	unit for pointwise cross-section output
NIMP	<nimp> <ncar>	output dump indices on unit 6 (see §3-15) number of characters per output line on unit 6

Regroups pointwise cross-sections computed on several zones of a singular energy group for just one isotope and one sampling. REGROUCS cannot calculate the merging of several isotopes in the same evaluation, (which may be defined over different energy zones). If there are several random samples (MCASUNR #1), it just takes into account the first sample.

3.5 CONDENTP

Condenses a probability table given in a fine group structure to a coarser one, with common boundaries.

CONDENTP

MODIFOPT

LPSTPOS <.TRUE.> by default, negative steps of the total cross section are suppressed, if present
 <.FALSE.> negative steps of the total cross section are preserved

LSPPOS <.FALSE.> by default, negative steps of all partial cross sections are preserved
 <.TRUE.> negative steps of all partial cross sections are set to 1.000000-7 barn

ENERgies <enmin> <enmax> energy range, in eV. It is normalised to the nearest group bound of the selected group structure

MAILLage "word*4"

READ the group structure is read
<ign> group structure name (see §3-15)

SPECTre <nrange> nrange = number of energy zones
For each zone ira (ira = 1 to nrange)
<enzinf(ira)> lower energy bound
<alphaz(ira)> weighting spectra indice (see §3-15)

GENEre the group structure is generated
<nrange > number of energy zones
for each zones ira (ira = 1 to nrange)

<ngc(ira)> <alphaz(ira)> <etop(ira)>
ngc number of groups in the zone for ira
alphaz weighting spectrum indices
etop upper energy bound of the first group in the range IRA
 etop has to correspond, within 10^{-6} , to the last energy defined by ira-1

if ngc>0 : the code reads NGC values of lower energy bounds:
 <eng(ig)> ngc values

if ngc<0 : the code reads τ , the energy step for |ngc| groups:
 < τ > defines the energy step which is calculated
 if $\tau > 0$ the lethargy step is $1/\tau$: $\text{eng(ig+1)} = \text{eng(ig)} \exp^{-1/\tau}$

if $\tau < 0$ the energy step is τ : $\text{eng}(\text{ig}+1) = \text{eng}(\text{ig}) + \tau$

N.B.: when $\text{ngc}(\text{ira}) > 0$ (grid given) it is possible to introduce energy points greater than the maximum of the range ($> \text{etop}(\text{ira})$). This allows the introduction of spurious energies points within the regular, previously calculated energy grid.

NDIL $\langle \text{ndil} \rangle$ number of dilutions
 If $\text{ndil} > 0$
 $\langle \text{sdil}(\text{idil}) \rangle$ dilution values, ndil times

NFTPD $\langle \text{unit} \rangle$ for the PT to be condensed
 $\langle \text{file name} \rangle$ file name of this PT

SORTies

NFSFC $\langle \text{nfsfc} \rangle$ if $\neq 0$ unit for calculated effective cross-sections
 $\langle \text{file name} \rangle$

NFTPC $\langle \text{nftpc} \rangle$ if $\neq 0$ unit for collapsed probability table
 $\langle \text{file name} \rangle$

IPRECI $\langle \text{ipreci} \rangle$ calculational accuracy indices

NIMP $\langle \text{nimp} \rangle$ output dump indices on unit 6 (see §3-15)
 $\langle \text{ncar} \rangle$ number of characters per output line on unit 6

Nota Bene: in a CONTENTP group the weighting spectra can vary. The energies boundaries given for a chosen weighting spectrum are adjusted to the closest group boundaries of the inputted group structure.

3.6 MIXISOTP

Smear, mixes several isotopic probability tables together that have to be defined on the same grid.

MIXISOTP

ENERgies	<i><enmin></i> <i><enmax></i> energy range, in eV
NISO	<i><niso></i> number of isotopes to be mixed described by their probability tables
AISO	relative isotopic atomic percentage <i><aiso(iiso)></i> niso times
NFTP	unit for the probability table input file <i><nftp></i> <i><file name></i> niso times
NDIL	<i><ndil></i> number of dilutions If <i>ndil</i> > 0 <i><sdil(idil)></i> dilution values, <i>ndil</i> times
SORTies	
<i>NFSFM</i>	<i><nfsfm></i> if $\neq 0$ unit for calculated effective cross-sections <i><file name></i>
<i>NFTPM</i>	<i><nftpm></i> if $\neq 0$ unit for collapsed probability table <i><file name></i>
IPRECI	<i><ipreci></i> calculational accuracy indices (see §3-15)
NIMP	<i><nimp></i> output dump indices on unit 6 (see §3-15) <i><ncar></i> number of characters per output line on unit 6

3.7 INTERTP

Interpolates between probability tables following an interpolation variable T. T could represent the temperature for example.

INTERTP

ENERgies	<enmin> <enmax> energy range, in eV
NTP	<ntp> number of probability tables and interpolation variable T
NFTP	<nftp> unit <tnftp> file name ntp times
ABSC	<T(ntp)> values of the interpolation variable, ntp times
ILOINT	<iloint> interpolation laws = 1 interpolation in T = 2 interpolation in $\sqrt{T}$ = 3 interpolation in $T^{0.25}$ = 4 interpolation in Log(T)
NDIL	<ndil> number of dilutions If ndil > 0 <sdil(idil)> dilution values, ndil times
TINT	<tint> interpolation variable final value (i.e. output temperature)
SORTies	
<i>NFSFI</i>	<nfsf> if $\neq 0$ unit for calculated effective cross-sections <file name>
<i>NFTPI</i>	<nftp> if $\neq 0$ unit for the calculated probability table <file name>
IPRECI	<ipreci> calculational accuracy indices (see §3-15)
NIMP	<nimp> output dump indices on unit 6 (see §3-15) <ncar> number of characters per output line on unit 6

3.8 TPMQSEFF

Calculates probability tables from effective cross-sections or reaction rates.

TPMQSEFF

ENERgies	<i><enmin></i> <i><enmax></i>	energy range, in eV
NFSF	<i><nfsf></i> <i><file name></i>	unit for effective cross-section file name
NFTP	<i><nftp></i> <i><file name></i>	unit for probability tables output file name
LTAUR	logical variable <i><.TRUE.></i> <i><.FALSE.></i>	the probability tables are adjusted on the reaction rate by default, the probability tables are adjusted on the effective cross-section
IPRECI	<i><ipreci></i>	calculational accuracy indices (see §3-15)
NIMP	<i><nimp></i> <i><ncar></i>	output dump indices on unit 6 (see §3-15) number of characters per output line on unit 6

3.9 SEFFNRA

Calculates effective cross-sections from probability tables after regrouping.

SEFFNRA

ENERgies	<enmin> <enmax> energy range, in eV
NFTP	<nftp> unit for probability table <file name>
NFSFTP	<nfsftp> unit for effective cross-section output <file name>
NDIL	<ndil> number of dilutions If ndil > 0 <sdil(idil)> dilution values, ndil times
NIMP	<nimp> output dump indices on unit 6 (see §3-15) <ncar> number of characters per output line on unit 6

3.10 REDUORTP

Reduces the order of a probability table. Allows to bias the table: the tables calculated by CALENDF are always "normal", i.e. of order IOR=1-NOR to NOR.

REDUORTP allows, as an option, to bias the reduced table:

- by describing mainly the negative moments (useful for small background cross sections or deep penetration)
- by describing mainly the positive moments (useful for large background cross sections or small penetration)

REDUORTP

ENERgies	<enmin> <enmax> energy range, in eV
NFTPD	<nftpd> if/=0 unit input probability table <file name>
MAXNOR	<maxnor> maximum order of the reduced probability table
MAXIorini	optional word; if absent : the reduced PT will be "normal" if present: <maxiorini> the reduced PT will describe the moments from MAXIORINI to MAXIORINI+2*NOR-1 or from MAXIORINI to MAXIORINI+NOR-1/2
NFTPR	<nftpr> unit for reduced probability table <file name>
IPRECI	<ipreci> calculational accuracy indices (see §3-15)
NIMP	<nimp> output dump indices on unit 6 (see §3-15) <ncar> number of characters per output line on unit 6

3.11 LECRICS, LECRISF, LECRITP

Read and write specific CALENDF branches

LECRICS

NFCSL	<nfcsl> unit for cross section input <file name>.
NFCSE	<nfcse> unit for cross section output <file name>
NFPEF	<nfpes> unit for pendf style cross section output <file name>
NIMP	<nimp> output dump indices on unit 6 (see §3-15) <ncar> number of characters per output line on unit 6

Read and write pointwise cross-section files

LECRISF

NFSFL	<nfsfl> unit for effective cross section input <file name>
NFSFE	<nfsfe> unit for effective cross section output <file name>
NFSFP	<nfsfp> unit for effective cross section output <dilution> <file name>
NIMP	<nimp> output dump indices on unit 6 (see §3-15) <ncar> number of characters per output line on unit 6

Read and write effective cross-section files

LECRITP

MODIFOPT “word*7”

LPSPPOS <.FALSE.> by default, negative steps of all partial cross sections are preserved
<.TRUE.> negative steps of all partial cross sections are set to 1.000000-7 barn

NFTPL	<nftpl> unit for probability tables input <file name>
NFTPE	<nftpe> unit for probability tables output <file name>

NIMP	<nimp>	output dump indices on unit 6 (see §3-15)
	<ncar>	number of characters per output line on unit 6

Read and write probability table files

3.12 COMPSF

Compares two different effective cross-section files. Computes the relative difference as the log of the cross-sections ratio and the absolute difference as the simple difference.

COMPSF

NFSF1	<nfsf1> if $\neq 0$ unit for effective cross-section input 1 <file name>
NFSF2	<nfsf2> if $\neq 0$ unit for effective cross-section input 2 <file name>
NFSFDR	<nfsfdr> if $\neq 0$ unit for relative difference output <file name>
NFSFDA	<nfsfda> if $\neq 0$ unit for absolute difference output <file name>
NIMP	<nimp> output dump indices on unit 6 (see §3-15) <ncar> number of characters per output line on unit 6

3.13 SIGTTEUM

Computes pointwise cross-section:

- in the resolved resonance range, on a grid created by the code (as CALENDF)
- in the unresolved resonance range, at the energies of definition of the average parameters. These cross-sections are the average values of the (infinite dilution) cross-sections, calculated from several random samples.

The pointwise cross-sections are taken into account over the whole energy range.

SIGTTEUM

ENERgies	<enmin> <enmax> energy range, in eV
TEFF	<teff> effective temperature, in Kelvin
NFEV	<unit for endf/b> <material number to be processed> <file name> file name in single quotes on UNIX
NFCS	<nfsf> unit for pointwise cross-section output <file name>
IPRECI	<ipreci> calculational accuracy indices (see §3-15)
NIMP	<nimp> output dump indices on unit 6 (see §3-15) <ncar> number of characters per output line on unit 6

The use of REGROUCS after SIGTTEUM is generally required.

3.14 TRANSMOY

Computes the averaged transmission of samples of different thickness in a neutron beam. A probability table resulting from a mixture of several isotopes describes the sample.

TRANSMOY

ENERgies	<enmin> <enmax> energy range, in eV	
NFTP	<nftp> unit for probability tables input <file name>	
NTHICK	<nthick> number of thickness If nthick > 0 <thick(nthick)> thickness values, nthick times	
NFTRM	<nfrm> unit for averaged transmission output <file name>	
NIMP	<nimp>	output dump indices on unit 6 (see §3-15)
	<ncar>	number of characters per output line on unit 6

3.15 INPUT variables

Options for input variables

ign	meaning
ECCO33	Ecco 33 groups structure
ECCO1968	Ecco 1968 groups structure
XMAS172	Xmas 172 groups structure
TRIP315	Tripoli 315 groups structure
VITJ175	Vitamin-J 175 groups structure
RED616	LLNL 616 groups structure
SCAL44	ORNL SCALE 44 groups structure
SCAL238	ORNL SCALE 238 groups structure

These group structures are hard coded with 7 digits accuracy (1.234567D+00)

ipreci	meaning
1	test case ($\sim 2.5 \cdot 10^{-2} = 2.5\%$ accuracy)
2	better case ($\sim 5 \cdot 10^{-3}$ accuracy)
3	for secondary isotope ($\sim 1 \cdot 10^{-3}$ accuracy)
4	for primary isotope ($\sim 2 \cdot 10^{-4}$ accuracy)
5	for $\sim 4 \cdot 10^{-5}$ accuracy
6	for $\sim 8 \cdot 10^{-6}$ accuracy

The CALENDF results accuracy is governed by only one parameter: **ipreci**. This parameter controls:

- The point wise grid created to describe the resonance region. The target accuracy resulting from a numerical integration is: $0.125 \times 0.2^{\text{ipreci}}$
- The number of random samples generated in every zone of the unresolved resonance regions governed by NCASUNR:
 - Default = 1 for ipreci = 1, 2 or 3,
 - = 4 for ipreci = 4,
 - = 9 for ipreci = 5,
 - = 16 for ipreci = 6
- The order NOR of the probability tables.

nimp	meaning
0	only diagnostics
1	some intermediary results
2	intermediary, physicist
3	intermediary, debug mode

4	only for numerical checks
ncar	meaning
“number”	number of possible characters per line
alphaz	define the weighting spectrum for each group :
< 10	alpha(ig) = alphaz (i.e. -1 => 1/E, 0 => constant) $\Phi(E) = E^{\text{alpha(ig)}}$
> 10	alpha(ig) = mean slop of $\Phi(E)$ in the group width:
$10 < \text{alphaz} < 1.0 \cdot 10^6$	alphaz = maxwellian spectrum temperature (in Kelvin) $\Phi(E) = E \cdot e^{-E/k \cdot \text{alphaz}}$
$1.10^6 < \text{alphaz} < 1.10^7$	alphaz = fission spectrum temperature (in eV) $\Phi(E) = \sqrt{E} \cdot e^{-E/\text{alphaz}}$
alphaz > 1.10^7	alphaz = fusion spectrum mean energy $\Phi(E) = e^{-0.0002 \cdot (\sqrt{E} - \sqrt{\text{alphaz}})^2}$

The weighting spectrum is constant within a group (i.e. the energy bounds of alphaz are adjusted on the nearest group bounds), except in CONDENTP, which allows several groups with weights defined by two spectra to be collapsed.

4 CALENDF output format

4.1 Output Files

The following rules are available for all the output files of CALENDF.

A positive output unit number will generate ASCII coding while a negative unit number will lead to binary coding.

An output unit number greater than 100 generates “E” formatted result: 1.123456E+01

An output unit number less than 100l generates “F” formatted results: 1.123456+1

4.2 Examples

Example of an NFTP (.tp) output corresponding to Hf¹⁷⁸ probability tables in Xmas 172 groups format prior to REGROUTP. One remark is that group 37 has been sub-divided into three zones by the code.

```
tables de probabilite pour 72-HF-178 NAIG+          DIST-xxxx
IPRECI = 4 → ~0.0002 accuracy
ZA= 72178. MAT=7237 TEFF= 300.0 172 groupes de 1.0000E-5 a 1.9640E+7 IPRECI=4
Group 1 NOR = Table order NPAR = number of partial
IG 1 ENG=1.733253E+7 1.964033E+7 NOR= 2 I= -1 NPAR=4 KP= 2 101 4 15 0
  4.094861-1 5.513532+0 3.182873+0 4.079314-3 4.225357-1 1.904044+0
  5.905139-1 5.604854+0 3.246516+0 3.155175-3 4.421208-1 1.913062+0
Probability Total Elastic Absorption Inelastic N,xN
      2          101          4          15
.....
NOR = table order NPAR = number of partial
IG 37 ENG=5.000000E+4 5.516564E+4 NOR= 1 I= 0 NPAR=2 KP= 2 101 0 0 0
  1.000000+0 1.166758+1 1.142097+1 2.466165-1
IG 37 ENG=4.520382E+4 5.000000E+4 NOR=11 I=-10 NPAR=2 KP= 2 101 0 0 0
  3.433220-4 7.618463-1 6.215518-1 1.402945-1
  2.235189-3 1.028660+0 8.354195-1 1.932406-1
  7.939953-3 1.508435+0 1.345200+0 1.632347-1
  2.825066-2 2.712981+0 2.538652+0 1.743293-1
  1.023008-1 4.865225+0 4.682912+0 1.823134-1
  3.539862-1 8.156930+0 7.956202+0 2.007281-1
  3.240754-1 1.240664+1 1.212878+1 2.778589-1
  1.180622-1 2.025037+1 1.988871+1 3.616566-1
  4.545310-2 3.112827+1 3.074876+1 3.795007-1
  1.523489-2 4.232851+1 4.195875+1 3.697636-1
  2.118302-3 5.168061+1 5.111961+1 5.610059-1
IG 37 ENG=4.086771E+4 4.520382E+4 NOR=11 I=-10 NPAR=2 KP= 2 101 0 0 0
  3.881368-4 6.555958-1 5.343885-1 1.212072-1
  1.285089-3 8.387795-1 7.196014-1 1.191781-1
  6.364072-3 1.349498+0 1.216702+0 1.327956-1
  2.541038-2 2.347179+0 2.136141+0 2.110377-1
  9.061974-2 4.395784+0 4.217302+0 1.784828-1
  3.422754-1 7.891743+0 7.706997+0 1.847458-1
  3.521294-1 1.237046+1 1.208213+1 2.883303-1
  1.182076-1 2.089486+1 2.049793+1 3.969330-1
  4.568197-2 3.277071+1 3.241213+1 3.585716-1
  1.576334-2 4.467187+1 4.423119+1 4.406813-1
  1.874864-3 5.518622+1 5.493299+1 2.532238-1
.....
```

I = first negative moment

IG 171	ENG=3.000000E-3	5.000000E-3	NOR= 2	I= -1	NPAR=2	KP= 2 101	0	0	0
5.072824-1	2.033169+2	4.554983+0	1.987619+2						
4.927176-1	2.349110+2	4.586717+0	2.303243+2						

Group 172 **with table order = 8 and 2 partials**

IG 172	ENG=1.000010E-5	3.000000E-3	NOR= 8	I= -7	NPAR=2	KP= 2 101	0	0	0
4.790513-2	2.605929+2	4.608785+0	2.559841+2						
1.107177-1	3.258078+2	4.680370+0	3.211274+2						
1.662634-1	4.829956+2	4.914168+0	4.780815+2						
1.981846-1	8.160701+2	5.695631+0	8.103745+2						
1.902789-1	1.431781+3	7.800669+0	1.423980+3						
1.496186-1	2.335819+3	1.150792+1	2.324312+3						
9.609510-2	3.319366+3	1.579922+1	3.303567+3						
4.093668-2	4.036773+3	1.900039+1	4.017772+3						

Example of an NFTPR (.tpr) output corresponding to Hf¹⁷⁸ probability tables in Xmas 172 format after REGROUP. The probability tables from the sub-groups of Xmas group 37 have now been re-grouped.

```

tables de probabilite pour 72-HF-178 NAIG+          DIST-xxxx
ZA= 72178. MAT=7237 TEFF= 300.0 172 groupes de 1.0000E-5 a 1.9640E+7 IPRECI=4
IG   1 ENG=1.733253E+7 1.964033E+7 NOR= 2 I= -1 NPAR=4 KP=  2 101  4 15  0
4.094861-1 5.513532+0 3.182873+0 4.079314-3 4.225357-1 1.904044+0
5.905139-1 5.604854+0 3.246516+0 3.155175-3 4.421208-1 1.913062+0
IG   2 ENG=1.491825E+7 1.733253E+7 NOR= 2 I= -1 NPAR=4 KP=  2 101  4 15  0
2.643676-1 5.597086+0 3.183352+0 1.396993-3 4.846315-1 1.927705+0
7.356324-1 5.635838+0 3.247459+0 2.193585-3 4.653467-1 1.920838+0

.....

IG   37 ENG=4.086771E+4 5.516564E+4 NOR=10 I= -9 NPAR=2 KP=  2 101  0  0  0
1.817951-4 6.660090-1 5.466607-1 1.193480-1
1.020717-3 8.935837-1 7.481450-1 1.454390-1
6.100122-3 1.459432+0 1.297162+0 1.622696-1
2.992847-2 2.912367+0 2.720470+0 1.918979-1
1.605709-1 6.196353+0 6.019160+0 1.771922-1
6.324775-1 1.111158+1 1.086710+1 2.444874-1
1.192779-1 1.821346+1 1.784775+1 3.657134-1
3.747613-2 3.054167+1 3.017495+1 3.667078-1
1.171656-2 4.322708+1 4.281148+1 4.155950-1
1.249877-3 5.405850+1 5.368656+1 3.719273-1
Probability      Total      Elastic      Absorption

.....

IG  172 ENG=1.000010E-5 3.000000E-3 NOR= 8 I= -7 NPAR=2 KP=  2 101  0  0  0
4.790513-2 2.605929+2 4.608785+0 2.559841+2
1.107177-1 3.258078+2 4.680370+0 3.211274+2
1.662634-1 4.829956+2 4.914168+0 4.780815+2
1.981846-1 8.160701+2 5.695631+0 8.103745+2
1.902789-1 1.431781+3 7.800669+0 1.423980+3
1.496186-1 2.335819+3 1.150792+1 2.324312+3
9.609510-2 3.319366+3 1.579922+1 3.303567+3
4.093668-2 4.036773+3 1.900039+1 4.017772+3

```

Example of an NFSF (.sf) output corresponding to Hf¹⁷⁸ directly calculated effective cross section in Xmas 172 groups format prior to REGROUSF. Remark that group 37 has been sub-divided into three zones by the code.

```
s. effectives (direct) for 72-HF-178 NAIG+ DIST-xxxx
ZA= 72178. MAT=7237 TEFF= 300.0 172 gr. de 1.0000E-5 a 1.9640E+7 IP=4 NDIL= 3
SDIL= 1.0000 100.00 1.00000E+10 Dilutions in barns
IG 1 ENG=1.733253E+7 1.964033E+7 NK= 1 NOR= 0 NPAR=4 KP= 2 101 4 15 0
SMOY= 5.567459+0 3.220455+0 3.533597-3 4.341010-1 1.909369+0
      Total Elastic Absorption Inelastic (N,XN)
SEF(0)= 5.567151+0 5.567440+0 5.567459+0
SEF(1)= 3.220240+0 3.220442+0 3.220455+0
SEF(2)= 3.536712-3 3.533790-3 3.533597-3
SEF(3)= 4.340350-1 4.340969-1 4.341010-1
SEF(4)= 1.909339+0 1.909367+0 1.909369+0
IG 2 ENG=1.491825E+7 1.733253E+7 NK= 1 NOR= 0 NPAR=4 KP= 2 101 4 15 0
SMOY= 5.625593+0 3.230511+0 1.982992-3 4.704450-1 1.922653+0
SEF(0)= 5.625549+0 5.625590+0 5.625593+0
SEF(1)= 3.230438+0 3.230507+0 3.230511+0
SEF(2)= 1.982083-3 1.982935-3 1.982992-3
SEF(3)= 4.704670-1 4.704464-1 4.704450-1
SEF(4)= 1.922661+0 1.922654+0 1.922653+0

.....

IG 37 ENG=5.000000E+4 5.516564E+4 NK= 1 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 1.166758+1 1.142097+1 2.466165-1 (Continuum)
SEF(0)= 1.166712+1 1.166753+1 1.166758+1
SEF(1)= 1.142051+1 1.142092+1 1.142097+1
SEF(2)= 2.466081-1 2.466156-1 2.466165-1
IG 37 ENG=4.520382E+4 5.000000E+4 NK= 4 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 1.205705+1 1.180382+1 2.532232-1 (URR, 1st zone)
EPSMOY= 2.194043-1 2.186461-1 8.100010-4 Standard deviation
SEF(0)= 9.055990+0 1.161169+1 1.205705+1 effective cross section (total)
EPSEFF= 2.941875-1 2.187865-1 2.194043-1 Standard deviation
SEF(1)= 8.830609+0 1.136219+1 1.180382+1 effective cross section (elastic)
EPSEFF= 2.904991-1 2.179013-1 2.186461-1 Standard deviation
SEF(2)= 2.253812-1 2.495000-1 2.532232-1 effective cross section (absorption)
EPSEFF= 4.127730-3 8.975879-4 8.100010-4 Standard deviation
IG 37 ENG=4.086771E+4 4.520382E+4 NK= 4 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 1.229967+1 1.204160+1 2.580676-1 (URR, 2nd zone)
EPSMOY= 1.054639-1 1.063011-1 9.614032-4 4 random samples per zones
SEF(0)= 9.004422+0 1.179915+1 1.229967+1 3 zones in group 37
EPSEFF= 1.035748-1 9.955265-2 1.054639-1
SEF(1)= 8.778806+0 1.154539+1 1.204160+1
EPSEFF= 1.054210-1 1.005223-1 1.063011-1
SEF(2)= 2.256161-1 2.537609-1 2.580676-1
EPSEFF= 2.354784-3 1.160998-3 9.614032-4

.....

IG 171 ENG=3.000000E-3 5.000000E-3 NK= 1 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 2.188839+2 4.570619+0 2.143133+2 infinite dilute cross section
SEF(0)= 2.177516+2 2.181033+2 2.188839+2
SEF(1)= 4.569482+0 4.569839+0 4.570619+0
SEF(2)= 2.131822+2 2.135335+2 2.143133+2
IG 172 ENG=1.000010E-5 3.000000E-3 NK= 1 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 1.396740+3 8.186960+0 1.388553+3
SEF(0)= 7.431022+2 7.944199+2 1.396740+3
SEF(1)= 5.894722+0 6.055967+0 8.186959+0
SEF(2)= 7.372074+2 7.883639+2 1.388553+3
```

Example of an NFSFR (.sfdr) output corresponding to Hf¹⁷⁸ directly calculated effective cross section in Xmas 172 groups format after REGROUSF. The effective cross-sections from the sub-groups of Xmas group 37 have now been re-grouped.

```
s. effectives (direct) for 72-HF-178 NAIG+          DIST-xxxx
ZA= 72178. MAT=7237 TEFF= 300.0 172 GR. DE 1.0000E-5 a 1.9640E+7 IP=4 NDIL= 3
SDIL= 1.0000      100.00      1.00000E+10
IG 1 ENG=1.733253E+7 1.964033E+7 NK= 1 NOR= 0 NPAR=4 KP= 2 101 4 15 0
SMOY= 5.567459+0 3.220455+0 3.533597-3 4.341010-1 1.909369+0
SEF(0)= 5.567151+0 5.567440+0 5.567459+0
SEF(1)= 3.220240+0 3.220442+0 3.220455+0
SEF(2)= 3.536712-3 3.533790-3 3.533597-3
SEF(3)= 4.340350-1 4.340969-1 4.341010-1
SEF(4)= 1.909339+0 1.909367+0 1.909369+0
IG 2 ENG=1.491825E+7 1.733253E+7 NK= 1 NOR= 0 NPAR=4 KP= 2 101 4 15 0
SMOY= 5.625593+0 3.230511+0 1.982992-3 4.704450-1 1.922653+0
SEF(0)= 5.625549+0 5.625590+0 5.625593+0
SEF(1)= 3.230438+0 3.230507+0 3.230511+0
SEF(2)= 1.982083-3 1.982935-3 1.982992-3
SEF(3)= 4.704670-1 4.704464-1 4.704450-1
SEF(4)= 1.922661+0 1.922654+0 1.922653+0

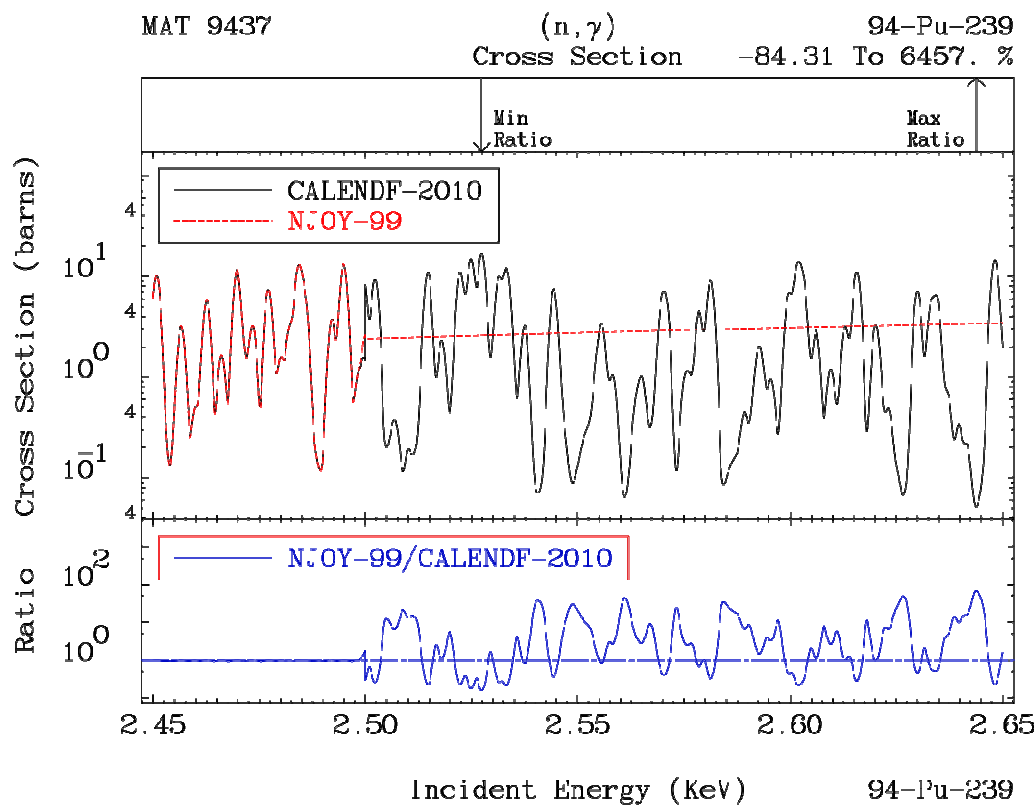
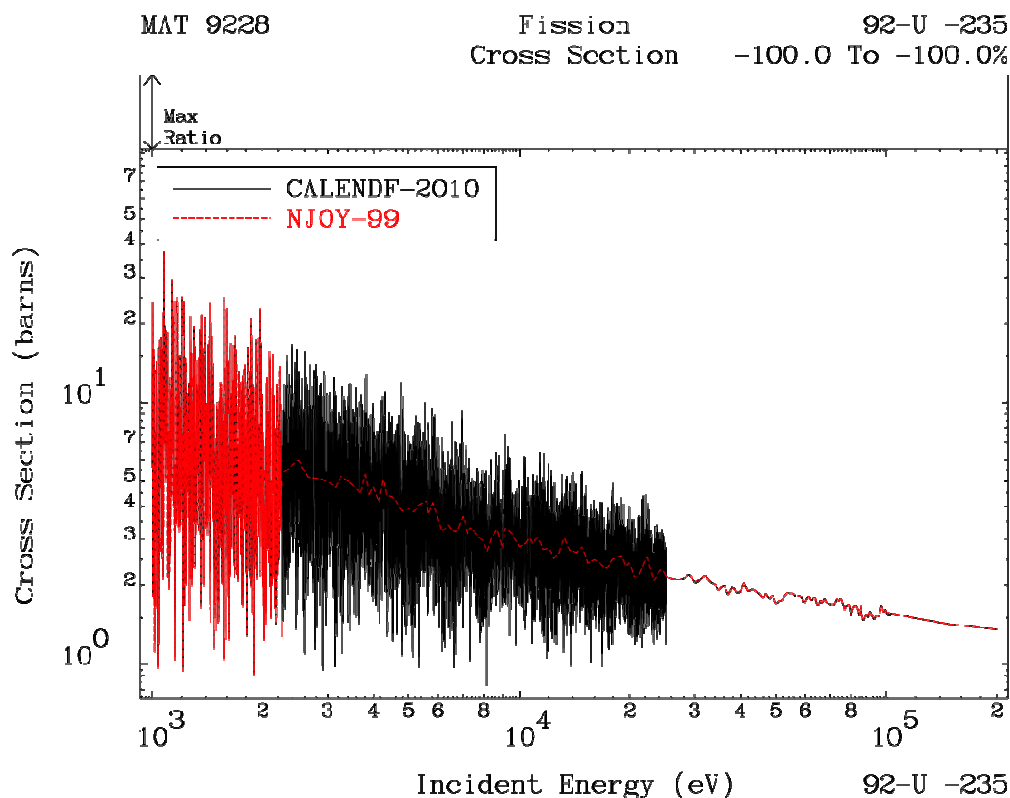
*****

IG 37 ENG=4.086771E+4 5.516564E+4 NK= 4 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 1.201096+1 1.175828+1 2.526864-1 infinite dilute cross section
EPSMOY= 8.182794-2 8.172096-2 4.225719-4 standard deviation
SEF(0)= 9.898621+0 1.169300+1 1.201096+1
EPSEFF= 1.047461-1 8.079674-2 8.182794-2
SEF(1)= 9.666170+0 1.144302+1 1.175828+1
EPSEFF= 1.037859-1 8.066198-2 8.172096-2
SEF(2)= 2.324502-1 2.499868-1 2.526864-1
EPSEFF= 1.595166-3 4.932675-4 4.225719-4

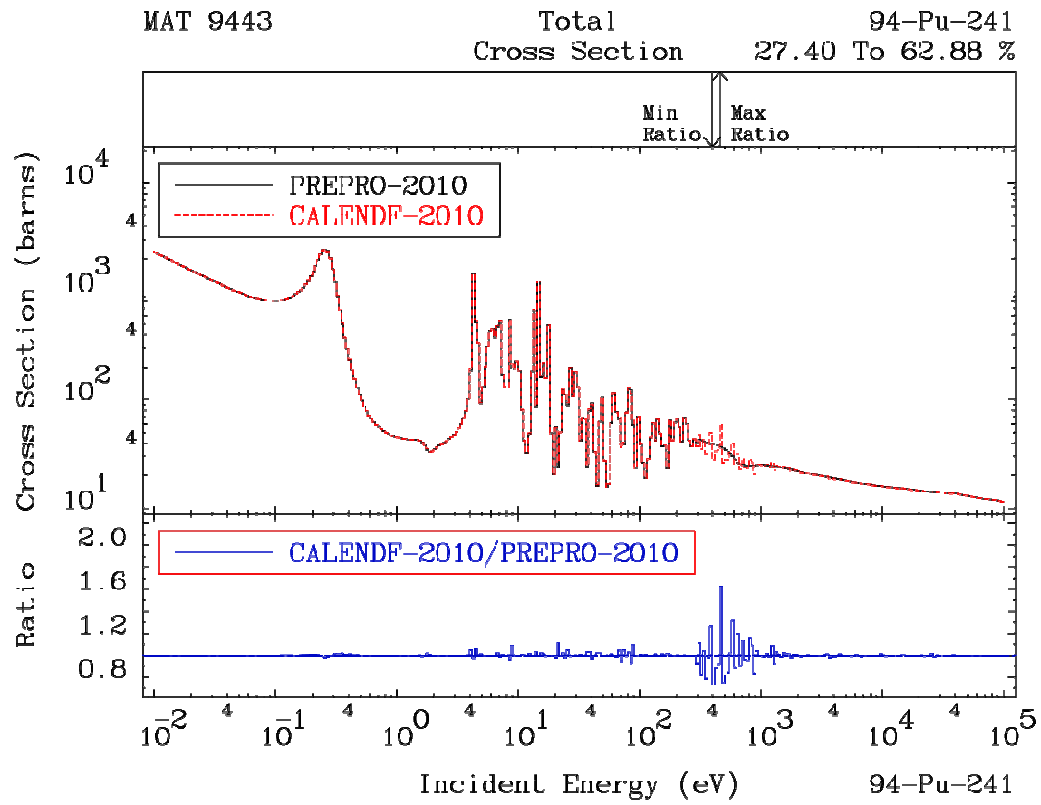
*****

IG 171 ENG=3.000000E-3 5.000000E-3 NK= 1 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 2.188839+2 4.570619+0 2.143133+2
SEF(0)= 2.177516+2 2.181033+2 2.188839+2
SEF(1)= 4.569482+0 4.569839+0 4.570619+0
SEF(2)= 2.131822+2 2.135335+2 2.143133+2
IG 172 ENG=1.000010E-5 3.000000E-3 NK= 1 NOR= 0 NPAR=2 KP= 2 101 0 0 0
SMOY= 1.396740+3 8.186960+0 1.388553+3
SEF(0)= 7.431022+2 7.944199+2 1.396740+3
SEF(1)= 5.894722+0 6.055967+0 8.186959+0
SEF(2)= 7.372074+2 7.883639+2 1.388553+3
```

Linearly interpolated pointwise cross section produced from resonance parameters. One should notice the statically generated resonances produced by CALENDF in the URR of this Pu-239 evaluation.



Groupwise infinitely dilute cross section set.



5 Appendix A Code installation

This appendix explains how to install CALENDF on various computer systems. CALENDF is currently available on those computer platforms:

- Intel 32, 64 running Window XP, 7
- Intel 64, AMD 64 running Linux
- Unix workstation (Oracle, Apple, IBM, ..)

The CALENDF code package is available on different media although the Fortran code itself could be loaded on less than 1.44 Mbytes. It will require around 300 Mbytes of free disk space on the workstation on which it will be installed, and this includes all the input data files and test cases results.

Operating system under which the code has been executed

- Oracle Solaris 11 and Studio 12 Fortran 90/95 compiler
- Apple OSX 10.6 and Intel ifort 11, gfortran 4.5, g95 compilers
- Ubuntu 10, Fedora 13 linux and gfortran 4.5 compiler
- Windows XP, 7 and gfortran 4.5, Lahey 6 compilers

README files are supplied that details the installation and the QA procedures as well as the necessary adaptations required for use on the different Operating System and compiler tandem.

README files follows:

Multi-platforms installation

The CALENDF code package, including diverse utility programs and interfaces is available through the Nuclear Data Centre.

It requires a minimum of 300 Mbytes of free disk space on the machine On which it shall be installed on.

The disk contains the following files:

/Calendf-2010	The CALENDF directory
README	This file
/Src	Source code directory
README	Execution instruction (NEEDS TO BE READ)
Makefile	The file needed to compile CALENDF and create the executable xcalendf
Makeliste	c-shell make (>&) output
*.f	Calendf source code
xcalendf	Calendf executable (OsX 10.6)
system dependent sub-directories	
/OsX	Apple intel
/Oracle	Oracle Solaris Sparc
/Linux	Ubuntu 10, Fedora 13
/Windows	Microsoft Window XP, 7

/QAcad	Directory containing test cases
Runtest in****	Unix script to run all test cases CALENDF input data
/Docs	Directory containing the documentation and User Manuals in Acrobat PDF format.
/Util	Directory containing utility codes
/gecco	Ecco library interface
/merge	Merge NJOY-GENDF and probability tables (MF-50)

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6 Appendix B Standard test cases

The following input files constitute the set of standard test cases and participate in the code QA processes. This set covers the code words and is supplied to users to enable them to confirm that a new installation is working correctly. Unix and Windows CALENDF input file differ only concerning filenames input convention:

- Unix ➔ './filename'
- Windows ➔ .\filename

inal27

```
CALENDF
MODIFOPT LCOR SCT .FALSE.
MODIFOPT LFORMRF .FALSE.
ENERgies 1.0E-5 20.0E+6
MAILLage READ
XMAS172
SPECTre (borne inferieure, ALPHA)
1 zones
0. -1.
TEFF 293.6
NDIL 5
1. 10. 100. 1000. 1.0E+10
NFEV 9 1325 './jeff30n1325_2.asc'
SORTies
NFSFRL 0 './al27.sfr'
NFSF 12 './al27.sf'
NFSFTP 11 './al27.sft'
NFTP 10 './al27.tp'
IPRECI 4
NIMP 0 80
REGROUTP
NFTP 10 './al27.tp'
NFTPR 17 './al27.tpr'
NIMP 0 80
REGROUSF
NFSF 12 './al27.sf'
NFSFR 13 './al27.sfdr'
NIMP 0 80
REGROUSF
NFSF 11 './al27.sft'
NFSFR 14 './al27.sftr'
NIMP 0 80
COMPSF
NFSF1 13 './al27.sfdr'
NFSF2 14 './al27.sftr'
NFSFDR 20 './al27.err'
NFSFDA 21 './al27.era'
NIMP 0 80
END
```

inb10

```
CALENDF
MODIFOPT LCORSCT .FALSE.
ENERGIES 1.0E-5 20.0E+6
MAILLAGE READ
XMAS172
SPECTRE
1 zone
0. -1.
TEFF 300.
NDIL 5
1. 10. 100. 1000. 1.0E+10
NFEV 9 525 './jeff30n525_1.asc'
SORTIES
  NFSFRL 0 './b10.sfr'
  NFSF 12 './b10.sf'
  NFSFTP 11 './b10.sft'
  NFTP 10 './b10.tp'
IPRECI 4
NIMP 0 80
REGROUTP
  NFTP 10 './b10.tp'
  NFTP 17 './b10.tpr'
NIMP 0 80
REGROUSF
  NFSF 12 './b10.sf'
  NFSFR 13 './b10.sfdr'
NIMP 0 80
REGROUSF
  NFSF 11 './b10.sft'
  NFSFR 14 './b10.sftr'
NIMP 0 80
COMPSF
  NFSF1 13 './b10.sfdr'
  NFSF2 14 './b10.sftr'
  NFSFDR 20 './b10.err'
  NFSFDA 21 './b10.era'
NIMP 0 80
END
```

inb10a

```

CALENDF
ENERGIES 100000. 1.
MAILLAGE GENERE
2 zones
-7284 -1. 19640330.0
480
147 293. 5.043477
298500. 297200. 82500. 79500. 28500. 27000.
4.918953 4.797503 4.679053 4.563526 4.450853 4.340961 4.233782 4.129250
4.000000 3.927860 3.830880 3.736300 3.644050 3.554080 3.466330 3.380750
3.300000 3.217630 3.137330 3.059020 2.983490 2.909830 2.837990 2.767920
2.720000 2.659320 2.600000 2.550000 2.485030 2.421710 2.382370 2.360000
2.300270 2.242050 2.185310 2.130000 2.100000 2.059610 2.020000 1.974490
1.930000 1.884460 1.855390 1.840000 1.797000 1.755000 1.711970 1.670000
1.629510 1.590000 1.544340 1.500000 1.475000 1.440000 1.404560 1.370000
1.337500 1.300000 1.267080 1.235000 1.202060 1.170000 1.150000 1.123000
1.110000 1.097000 1.080000 1.071000 1.045000 1.035000 1.020000 0.996000
0.986000 0.972000 0.950000 0.930000 0.910000 0.876425 0.860000 0.850000
0.819450 0.790000 0.780000 0.741550 0.705000 0.682560 0.653150 0.625000
0.595280 0.566960 0.540000 0.531580 0.519620 0.500000 0.485000 0.467010
0.449680 0.433000 0.413990 0.400000 0.391000 0.369930 0.350000 0.334660
0.320000 0.314500 0.300000 0.280000 0.263510 0.248000 0.233580 0.220000
0.209140 0.198810 0.189000 0.180000 0.169710 0.160000 0.153030 0.146370
0.140000 0.134000 0.115000 0.100000 0.095000 0.080000 0.077000 0.067000
0.058000 0.050000 0.042000 0.035000 0.030000 0.025000 0.020000 0.015000
0.010000 0.006900 0.005000 0.003000 1.000010-5
TEFF 300.
NDIL 1
1.0E+10
NFEV 9 525 './jeff30n525_1.asc'
SORTIES
NFSFRL 0 './b10a.sfr'
NFTP 10 './b10a.tp'
IPRECI 3
NIMP 0 80
END

Calculates from 1.eV to 100.Kev with two weighting spectrums
7284 groups with lethargy width of 1/480 and 1/E weighting
The energy boundaries are calculated from E= 1.964033E+07
147 groups with the low energy group boundaries read and a
maxwellian spectrum with T = 293 K.
The six energies 298500. 297200. 82500. 79500. 28500. 27000
are inserted above 5.043477 eV (= 19640330. * exp(-7284/480))
Thus only 141 groups will be present below this energy
N.B. In that case REGROUTP is not necessary, this evaluation does not
contain any resonance range.

```

infe56

```
CALENDF
  MODIFOPT LCORSCT .FALSE.
  ENERGIES 1.0E-5 20.0E+6
  MAILLAGE READ
  XMAS172
  SPECTRE
  1 zone
  0. -1.
  TEFF 300.
  NDIL 1
  1.0E+10
  NFEV 9 2631 './jeff30n2631_2.asc'
  SORTIES
    NFSFRL 0 './fe56.sfr'
    NFSF 12 './fe56.sf'
    NFSFTP 11 './fe56.sft'
    NFTP 10 './fe56.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './fe56.tp'
    NFTP 17 './fe56.tpr'
  NIMP 0 80
  REGROUSF
    NFSF 12 './fe56.sf'
    NFSFR 13 './fe56.sfdr'
  NIMP 0 80
  REGROUSF
    NFSF 11 './fe56.sft'
    NFSFR 14 './fe56.sftr'
  NIMP 0 80
  COMPSF
    NFSF1 13 './fe56.sfdr'
    NFSF2 14 './fe56.sftr'
    NFSFDR 20 './fe56.err'
    NFSFDA 21 './fe56.era'
  NIMP 0 80
END
```

inhf178

```
CALENDF
  MODIFOPT LSCORSCOT .FALSE.
  ENERGIES 1.0E-5 20.0E+6
  MAILLAGE READ
  XMAS172
  SPECTRE
  1
  0. -1.
  TEFF 300.
  NDIL 6
  0.1 1. 10. 100. 1000. 1.0E+10
  NFEV 9 7237 './jeff30n7237_1.asc'
  SORTIES
    NFSFRL 0 './hf178.sfs'
    NFSF 12 './hf178.sf'
    NFSFTP 0 './hf178.sft'
    NFTP 10 './hf178.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './hf178.tp'
    NFTP 17 './hf178.tpr'
  NIMP 0 80
  REGROUSF
    NFSF 12 './hf178.sf'
    NFSFR 13 './hf178.sfr'
  NIMP 0 80
  SEFFNRA
    ENERGIES 0. 2.E+7
    NFTP 17 './hf178.tpr'
    NFSFTP 18 './hf178.sft'
  NDIL 6
  0.1 1. 10. 100. 1000. 1.0E+10
  NIMP 0 80
  COMPSF
    NFSF1 13 './hf178.sfr'
    NFSF2 18 './hf178.sft'
    NFSFDR 20 './hf178.err'
    NFSFDA 21 './hf178.era'
  NIMP 0 80
END
```

inhf178a

```
CALENDF
  MODIFOPT LCORSCT .FALSE.
  ENERGIES 1.0E-5 6.9E-03
  MAILLAGE READ
  XMAS172
  SPECTRE
  1
  0. -1.
  TEFF 300.
  NDIL 1
  1.0E+10
  NFEV 9 7237 './jeff30n7237_1.asc'
  SORTIES
    NFCS 14 './hf178a.cs'
    NFSFRL 0 './hf178a.sfr'
    NFSF 0 './hf178a.sf'
    NFSFTP 0 './hf178a.sft'
    NFTP 10 './hf178a.tp'
  IPRECI 4
  NIMP 0 80
END
```

Inhf000

```
CALENDF
MODIFOPT LCORSCT .FALSE.
MODIFOPT NCAS 1 2 1 4 9 16
ENERGIES 1.0E-5 20.0E+6
MAILLAGE READ
XMAS172
SPECTRE
1
0. -1.
TEFF 300.
NDIL 6
0.1 1. 10. 100. 1000. 1.0E+10
NFEV 9 7200 './jeff30n7200_1.asc'
SORTIES
NFSFRL 0 './hf000.sfs'
NFSF 12 './hf000.sf'
NFSFTP 0 './hf000.sft'
NFTP 10 './hf000.tp'
IPRECI 4
NIMP 0 80
REGROUTP
NFTP 10 './hf000.tp'
NFTPR 17 './hf000.tpr'
NIMP 0 80
REGROUSEF
NFSF 12 './hf000.sf'
NFSFR 13 './hf000.sfr'
NIMP 0 80
SEFFNRA
ENERGIES 0. 2.E+7
NFTP 17 './hf000.tpr'
NFSFTP 18 './hf000.sft'
NDIL 6
0.1 1. 10. 100. 1000. 1.0E+10
NIMP 0 80
COMPSF
NFSF1 13 './hf000.sfr'
NFSF2 18 './hf000.sft'
NFSFDR 20 './hf000.err'
NFSFDA 21 './hf000.era'
NIMP 0 80
END
```

inpu239

```
CALENDF
MODIFOPT LSCORST .FALSE.
ENERGIES 1.0E-5 20.0E+6
MAILLAGE READ
XMAS172
SPECTRE
1
0. -1.
TEFF 300.
NDIL 1
1.0E+10
NFEV 9 9437 './jeff30n9437_1.asc'
SORTIES
  NFSFRL 0 './pu239.sfr'
  NFSF 12 './pu239.sf'
  NFSFTP 11 './pu239.sft'
  NFTP 10 './pu239.tp'
  IPRECI 4
  NIMP 0 80
REGROUTP
  NFTP 10 './pu239.tp'
  NFTP 17 './pu239.tpr'
  NIMP 0 80
REGROUSF
  NFSF 12 './pu239.sf'
  NFSFR 13 './pu239.sfdr'
  NIMP 0 80
REGROUSF
  NFSF 11 './pu239.sft'
  NFSFR 14 './pu239.sftr'
  NIMP 0 80
COMPSF
  NFSF1 13 './pu239.sfdr'
  NFSF2 14 './pu239.sftr'
  NFSFDR 20 './pu239.err'
  NFSFDA 21 './pu239.era'
  NIMP 0 80
END
```

inpu239a

```
CALENDF
MODIFOPT NCASUNR 1 1 1 2 9 16
ENERGIES 5.0E+6 6.0E+6
MAILLAGE READ
ECC01968
SPECTRE
3 zones
1.32E+6 1.29E+6
0.1 -1
0. 293.
TEFF 293.
NDIL 1
1.0E+10
NFEV 9 9437 './jeff30n9437_1.asc'
SORTIES
NFCS 14 './pu239a.cs'
NFSFRL 0 './pu239a.sfr'
NFSF 0 './pu239a.sf'
NFSFTP 0 './pu239a.sft'
NFTP 10 './pu239a.tp'
IPRECI 4
NIMP 0 80
END
```

inpu239b

```
CALENDF
MODIFOPT NCASUNR 1 1 1 2 9 16
ENERGIES 5.0E+6 6.0E+6
MAILLAGE READ
ECC01968
SPECTRE
3 zones
1.32E+6 1.29E+6
0.1 -1
0. 293.
TEFF 2500.
NDIL 1
1.0E+10
NFEV 9 9437 './jeff30n9437_1.asc'
SORTIES
NFCS 14 './pu239b.cs'
NFSFRL 0 './pu239b.sfr'
NFSF 0 './pu239b.sf'
NFSFTP 0 './pu239b.sft'
NFTP 10 './pu239b.tp'
IPRECI 4
NIMP 0 80
END
```

inpu239c

```
CALENDF                      PT of Pu9;
ENERGIES 10000. 0.00001
MAILLAGE READ
XMAS172
SPECTRE
  1 zones
    0.    -0.
TEFF 300.
NDIL 0
NFEV 9 9437 './jeff30n9437_1.asc'
SORTIES
  NFTP 10 './pu239c.tp'
  IPRECI 4
  NIMP 0 80
REGROUTP
  NFTP 10 './pu239c.tp'
  NFTP 11 './pu239c.tpr'
  NIMP 0 80
CALENDF                      PT of Pu40;
ENERGIES 10000. 0.00001
MAILLAGE READ
XMAS172
SPECTRE
  1 zones
    0.    -0.
TEFF 300.
NDIL 0
NFEV 9 9440 './jeff30n9440_2.asc'
SORTIES
  NFTP 10 './pu240c.tp'
  IPRECI 4
  NIMP 0 80
REGROUTP
  NFTP 10 './pu240c.tp'
  NFTP 12 './pu240c.tpr'
  NIMP 0 80
CALENDF                      PT of Pu42;
ENERGIES 10000. 0.00001
MAILLAGE READ
XMAS172
SPECTRE
  1 zones
    0.    -0.
TEFF 300.
NDIL 0
NFEV 9 9446 './jeff30n9446_2.asc'
SORTIES
  NFTP 10 './pu242c.tp'
  IPRECI 4
  NIMP 0 80
REGROUTP
  NFTP 10 './pu242c.tp'
  NFTP 13 './pu242c.tpr'
  NIMP 0 80
MIXISOTP mixture for n(i)/n(total) = 0.175 0.625 0.2
ENERGIES 10000. 0.
NISO 3
  AISO 0.175 0.625 0.2
  NFTP 11 './pu239c.tpr'
```

```

NFTPD 12 './pu240c.tpr'
NFTPD 13 './pu242c.tpr'
NDIL 0
NFSFM 0 text
NFTPM 17 './pumc.tp'
IPRECI 4
NIMP 0 80
TRANSMOY      transmission for n = 0.001  0.0004  0.0001 at/b
ENERGIES 10000. 0.00001
NFTP 17 './pumc.tp'
NTHICK 3
      0.001  0.0004  0.0001
NFTRM 18 './pumc.trm'
NIMP 0 80
END

Calculates Pu9, Pu40 et Pu42 mixture transmission
Mixture with 0.175 0.625 0.2
Average transmission for n = 0.001  0.0004  0.0001 at/b

```

inpu239d

```

CALENDF
  ENERgies 1.0E-5  30.0E+6
  MAIlIage GENERe
    3 zones
    17      1.32E+6  26511672.1
22255409.3  19640329.76  17332530.179  14918246.976  13840306.460
11618342.427  10000000.00000  8187307.53078  6703200.46036  6065306.59713
  5488116.36094  4493289.6411  3678794.41171  3011942.11912  2465969.63942
  2231301.60148  2018965.17995
    125      -1.      2018965.17995
1652988.88222  1353352.83237  1224564.28253  1108031.58362  1002588.43723
  907179.53289  820849.98624  608100.62625  550232.20056  497870.68368
  450492.02394  407622.03978  301973.83422  273237.22447  247235.26470
  183156.38889  122773.39903  111089.96538  82297.47049  67379.46999
  55165.64421  40867.71438  36978.63716  29282.99695  27394.44819
  24787.52177  16615.57273  15034.39193  11137.75148  9118.81966
  7465.85808  5530.84370  5004.51433  3526.62165  3354.62628
  2248.67324  2034.68369  1507.33075  1433.81736  1234.09804
  1010.39402  914.24231  748.51830  677.28736  453.99930
  371.70319  304.32483  203.99503  148.62539  136.74196
  91.66088  75.67357  67.90405  55.59513  51.57802
  48.25160  45.51744  40.16900  37.26653  33.72015
  30.51126  27.60773  24.98050  22.60329  19.45484
  15.92827  13.70959  11.22446  9.90555  9.18981
  8.31529  7.52398  6.16012  5.34643  5.04348
  4.12925  4.00000  3.38075  3.30000  2.76792
  2.72000  2.60000  2.55000  2.36000  2.13000
  2.10000  2.02000  1.93000  1.84000  1.75500
  1.67000  1.59000  1.50000  1.47500  1.44000
  1.37000  1.33750  1.30000  1.23500  1.17000
  1.15000  1.12300  1.11000  1.09700  1.07100
  1.04500  1.03500  1.02000  0.99600  0.98600
  0.97200  0.95000  0.93000  0.91000  0.86000
  0.85000  0.79000  0.78000  0.70500  0.62500
  0.54000  0.50000  0.48500  0.43300  0.40000
    32      293.16      0.40000
  0.39100  0.35000  0.32000  0.31450  0.30000
  0.28000  0.24800  0.22000  0.18900  0.18000
  0.16000  0.14000  0.13400  0.11500  0.10000
  0.09500  0.08000  0.07700  0.06700  0.05800
  0.05000  0.04200  0.03500  0.03000  0.02500
  0.02000  0.01500  0.01000  0.00690  0.00500
  0.00300  0.00011
TEFF 300.
NDIL 1
1.0E+10
NFEV 9 9437 './jeff30n9437_3.asc'
NFEV 9 9437 './jeff30n9437_3.asc'
SORTies
  NFSFRL 0 './pu23d.sfr'
  NFSF 12 './pu23d.sf'
  NFSFTP 11 './pu23d.sft'
  NFTP 10 './pu23d.tp'
IPRECI 4
NIMP 0 80
REGROUTP
  NFTP 10 './pu23d.tp'
  NFTP 17 './pu23d.tpr'
NIMP 0 80
REGROUSF
  NFSF 12 './pu23d.sf'
  NFSFR 13 './pu23d.sfdr'
NIMP 0 80
REGROUSF
  NFSF 11 './pu23d.sft'

```

```
NFSFR 14 './pu23d.sftr'  
NIMP 0 80  
COMPSF  
NFSF1 13 './pu23d.sfdr'  
NFSF2 14 './pu23d.sftr'  
NFSFDR 20 './pu23d.err'  
NFSFDA 21 './pu23d.era'  
NIMP 0 80  
END
```

inpu240

```
CALENDF
  MODIFOPT LCCORSCT .FALSE.
  MODIFOPT LFORMRF .FALSE.
  ENERGies 1.0E-5 20.0E+6
  MAILlage READ
  XMAS172
  SPECTre (borne inferieure, ALPHA)
  1 zones
  0. -1.
  TEFF 293.6
  NDIL 1
  1.0E+10
  NFEV 9 9440 './jeff30n9440_3.asc'
  SORTies
    NFSFRL 0 './pu240.sfr'
    NFSF 12 './pu240.sf'
    NFSFTP 11 './pu240.sft'
    NFTP 10 './pu240.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './pu240.tp'
    NFTP 17 './pu240.tpr'
  NIMP 0 80
  REGROUSF
    NFSF 12 './pu240.sf'
    NFSFR 13 './pu240.sfdr'
  NIMP 0 80
  REGROUSF
    NFSF 11 './pu240.sft'
    NFSFR 14 './pu240.sftr'
  NIMP 0 80
  COMPSF
    NFSF1 13 './pu240.sfdr'
    NFSF2 14 './pu240.sftr'
    NFSFDR 20 './pu240.err'
    NFSFDA 21 './pu240.era'
  NIMP 0 80
END
```

inpu240a

```

CALENDF
MODIFOPT LCORSCT .FALSE.
MODIFOPT LFORMRF .FALSE.
ENERGIES 1.0E-5 20.0E6
MAILLAGE GENERE 11277
5
-4572 -1. 19640329.8
480.
-3744 -1. 1433.81736
1920.
-1320 -1. 203.99503
960.
-1116 -1. 51.578022
480.
525 -1. 5.0434766
5.012346 4.981215 4.950084 4.918953 4.888590 4.858228 4.827866 4.797503
4.767891 4.738278 4.708666 4.679053 4.650171 4.621290 4.592408 4.563526
4.535358 4.507190 4.479021 4.450853 4.423380 4.395907 4.368434 4.340961
4.314166 4.287372 4.260577 4.233782 4.207649 4.181516 4.155383 4.129250
4.103400 4.077550 4.051700 4.025850 4.000000 3.975950 3.951900 3.927860
3.903615 3.879370 3.855125 3.830880 3.807235 3.783590 3.759945 3.736300
3.713238 3.690175 3.667113 3.644050 3.621557 3.599065 3.576572 3.554080
3.532143 3.510205 3.488268 3.466330 3.444935 3.423540 3.402145 3.380750
3.360563 3.340375 3.320188 3.300000 3.279408 3.258815 3.238223 3.217630
3.197555 3.177480 3.157405 3.137330 3.117753 3.098175 3.078598 3.059020
3.040138 3.021255 3.002373 2.983490 2.965075 2.946660 2.928245 2.909830
2.891870 2.873910 2.855950 2.837990 2.820473 2.802955 2.785438 2.767920
2.751947 2.735973 2.720000 2.704830 2.689660 2.674490 2.659320 2.644490
2.629660 2.614830 2.600000 2.583333 2.566666 2.550000 2.533758 2.517515
2.501272 2.485030 2.469200 2.453370 2.437540 2.421710 2.405897 2.395483
2.382370 2.371185 2.360000 2.345067 2.330135 2.315202 2.300270 2.285715
2.271160 2.256605 2.242050 2.227865 2.213680 2.199495 2.185310 2.171483
2.157655 2.143828 2.130000 2.120000 2.110000 2.100000 2.086537 2.073073
2.059610 2.049708 2.039805 2.029903 2.020000 2.008623 1.997245 1.985868
1.974490 1.963368 1.952245 1.941123 1.930000 1.918615 1.907230 1.895845
1.884460 1.874770 1.865080 1.855390 1.847695 1.840000 1.829250 1.818500
1.807750 1.797000 1.786500 1.776000 1.765500 1.755000 1.744243 1.733485
1.722728 1.711970 1.701478 1.690985 1.680493 1.670000 1.659878 1.649755
1.639633 1.629510 1.619633 1.609755 1.599878 1.590000 1.578585 1.567170
1.555755 1.544340 1.533255 1.522170 1.511085 1.500000 1.491667 1.483333
1.475000 1.466250 1.457500 1.448750 1.440000 1.431140 1.422280 1.413420
1.404560 1.395920 1.387280 1.378640 1.370000 1.361875 1.353750 1.345625
1.337500 1.328125 1.318750 1.309375 1.300000 1.291770 1.283540 1.275310
1.267080 1.259060 1.251040 1.243020 1.235000 1.226765 1.218530 1.210295
1.202060 1.194045 1.186030 1.178015 1.170000 1.165000 1.160000 1.155000
1.150000 1.143250 1.136500 1.129750 1.123000 1.118667 1.114333 1.110000
1.105667 1.101333 1.097000 1.091333 1.085667 1.080000 1.075500 1.071000
1.065800 1.060600 1.055400 1.050200 1.045000 1.040000 1.035000 1.030000
1.025000 1.020000 1.014000 1.008000 1.002000 .996000 .991000 .986000
.981333 .976667 .972000 .966500 .961000 .955500 .950000 .945000 .940000 .935000
.930000 .925000 .920000 .915000 .910000 .903285 .896570 .889854 .883139 .876425
.870950 .865475 .860000 .855000 .850000 .842363 .834725 .827088 .819450 .812088
.804725 .797363 .790000 .785000 .780000 .770388 .760775 .751163 .741550 .732413
.723275 .714137 .705000 .697520 .690040 .682560 .675207 .667855 .660502 .653150
.646113 .639075 .632038 .625000 .617570 .610140 .602710 .595280 .588200 .581120
.574040 .566960 .560220 .553480 .546740 .540000 .535790 .531580 .527593 .523607
.519620 .514715 .509810 .504905 .500000 .496250 .492500 .488750 .485000 .480503
.476005 .471508 .467010 .462678 .458345 .454013 .449680 .445510 .441340 .437170
.433000 .428248 .423495 .418743 .413990 .409327 .404663 .400000 .395500 .391000
.385733 .380465 .375198 .369930 .364948 .359965 .354983 .350000 .346165 .342330
.338495 .334660 .330995 .327330 .323665 .320000 .317250 .314500 .310875 .307250
.303625 .300000 .295000 .290000 .285000 .280000 .275877 .271755 .267633 .263510
.259633 .255755 .251878 .248000 .244395 .240790 .237185 .233580 .230185 .226790
.223395 .220000 .217285 .214570 .211855 .209140 .206557 .203975 .201392 .198810
.196358 .193905 .191453 .189000 .186750 .184500 .182250 .180000 .177428 .174855
.172283 .169710 .167283 .164855 .162428 .160000 .157677 .155353 .153030 .150810
.148590 .146370 .144247 .142123 .140000 .138000 .136000 .134000 .130200 .126400
.122600 .118800 .115000 .111250 .107500 .103750 .100000 .097500 .095000 .091250
.087500 .083750 .080000 .077000 .074500 .072000 .069500 .067000 .064750 .062500
.060250 .058000 .056000 .054000 .052000 .050000 .048000 .046000 .044000 .042000
.040250 .038500 .036750 .035000 .033750 .032500 .031250 .030000 .028750 .027500
.026250 .025000 .023750 .022500 .021250 .020000 .018750 .017500 .016250 .015000
.013750 .012500 .011250 .010000 .008967 .007934 .006900 .006500 .006000 .005500
.005000 .004500 .004000 .003500 .003000 .002300 .001700 .001300 .001000 .000800
.000500 .000110 .00001000010
TEFF 293.16
NDIL 0
NFEV 9 9440 './jeff31tn9440_3.asc'
SORTIES
NFTP 10 './pu240a.tp'
IPRECI 4
NIMP 0 90
REGROUTP

```

```

NFTP 10 './pu240a.tp'
NFTPR 15 './pu240a.tpr'
NIMP 0 90
CONDENTP
ENERGIES 1.0E-5 20.0E6
MAILLAGE READ
ECC033
SPECTRE
6 zones
11.E+6 15.E+6
600000. 2.E+6
500000. 1.
300000. 0.
4. -1.
0. 290.
NDIL 4
1. 10. 100. 1.E+10
NFTPD 15 './pu240a.tpr'
SORTIES
NFSFC 16 './pu240a.sfc'
NFTPC 17 './pu240a.tpc'
IPRECI 4
NIMP 0 90
LECRITP
MODIFOPT LPSPPOS .TRUE.
NFTPR 15 './pu240a.tpr'
NFTPP 18 './pu240a.tpp'
NIMP 1 90
CONDENTP
ENERGIES 1.0E-5 20.0E6
MAILLAGE READ
ECC033
SPECTRE
6 zones
11.E+6 15.E+6
600000. 2.E+6
500000. 1.
300000. 0.
4. -1.
0. 290.
NDIL 4
1. 10. 100. 1.E+10
NFTPD 15 './pu240a.tpr'
SORTIES
NFSFC 20 './pu240a.sfx'
NFTPC 21 './pu240a.tpx'
IPRECI 4
NIMP 1 90
END

```

inpu240b

```
CALENDF
  MODIFOPT LCORSCT .FALSE.
  MODIFOPT LFORMRF .FALSE.
  MODIFOPT LPSPPOS .TRUE.
  ENERGies 1.0E-5 20.0E+6
  MAILlage READ
  XMAS172
  SPECTre (borne inferieure, ALPHA)
  1 zones
  0. -1.
  TEFF 293.6
  NDIL 1
  1.0E+10
  NFEV 9 9440 './jeff31tn9440_3.asc'
  SORTies
    NFSFRL 0 './pu240b.sfr'
    NFSF 12 './pu240b.sf'
    NFSFTP 11 './pu240b.sft'
    NFTP 10 './pu240b.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './pu240b.tp'
    NFTP 17 './pu240b.tpr'
  NIMP 0 80
  REGROUSF
    NFSF 12 './pu240b.sf'
    NFSFR 13 './pu240b.sfdr'
  NIMP 0 80
  REGROUSF
    NFSF 11 './pu240b.sft'
    NFSFR 14 './pu240b.sftr'
  NIMP 0 80
  COMPSF
    NFSF1 13 './pu240b.sfdr'
    NFSF2 14 './pu240b.sftr'
    NFSFDR 20 './pu240b.err'
    NFSFDA 21 './pu240b.era'
  NIMP 0 80
END
```

inpu240c

```
CALENDF
  MODIFOPT LCORSCT .FALSE.
  MODIFOPT LFORMRF .FALSE.
  ENERGies 1.0E-5 20.0E+6
  MAILlage READ
  XMAS172
  SPECTre (borne inferieure, ALPHA)
  1 zones
  0. -1.
  TEFF 293.6
  NDIL 1
  1.0E+10
  NFEV 9 9440 './jeff31tn9440_3.asc'
  SORTies
    NFSFRL 0 './pu240c1.sfr'
    NFSF 12 './pu240c1.sf'
    NFSFTP 11 './pu240c1.sft'
    NFTP 10 './pu240c1.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './pu240c1.tp'
    NFTP 17 './pu240c1.tpr'
  NIMP 0 80
  REGROUSF
    NFSF 12 './pu240c1.sf'
    NFSFR 13 './pu240c1.sfdr'
  NIMP 0 80
  REGROUSF
    NFSF 11 './pu240c1.sft'
    NFSFR 14 './pu240c1.sftr'
  NIMP 0 80
  COMPSF
    NFSF1 13 './pu240c1.sfdr'
    NFSF2 14 './pu240c1.sftr'
    NFSFDR 20 './pu240c1.err'
    NFSFDA 21 './pu240c1.era'
  NIMP 0 80
END
```

inpu240d

```
CALENDF
  MODIFOPT LCORSCT .FALSE.
  MODIFOPT LFORMRF .FALSE.
  ENERGies 1.0E-5 20.0E+6
  MAILlage READ
  XMAS172
  SPECTre (borne inferieure, ALPHA)
  1 zones
  0. -1.
  TEFF 293.6
  NDIL 1
  1.0E+10
  NFEV 9 9440 './jeff31tn9440_3.asc'
  SORTies
    NFSFRL 0 './pu240d.sfr'
    NFSF 12 './pu240d.sf'
    NFSFTP 11 './pu240d.sft'
    NFTP 10 './pu240d.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './pu240d.tp'
    NFTP 17 './pu240d.tpr'
    NIMP 0 80
  LECRITP
    MODIFOPT LPSPPOS .TRUE.
    NFTP 17 './pu240d.tpr'
    NFTP 18 './pu240d.tpp'
    NIMP 0 80
  REGROUSF
    NFSF 12 './pu240d.sf'
    NFSFR 13 './pu240d.sfdr'
    NIMP 0 80
  REGROUSF
    NFSF 11 './pu240d.sft'
    NFSFR 14 './pu240d.sftr'
    NIMP 0 80
  COMPSF
    NFSF1 13 './pu240d.sfdr'
    NFSF2 14 './pu240d.sftr'
    NFSFDR 20 './pu240d.err'
    NFSFDA 21 './pu240d.era'
    NIMP 0 80
  END
```

inpu240e

```
CALENDF
MODIFOPT LCORSCT .FALSE.
MODIFOPT LFORMRF .FALSE.
ENERgies 1.0E-5 20.0E+6
MAILIage READ
XMAS172
SPECTre (borne inferieure, ALPHA)
1 zones
0. -1.
TEFF 293.6
NDIL 1
1.0E+10
NFEV 9 9440 './jeff31pu240p.asc'
SORTies
NFSFRL 0 './pu240e.sfr'
NFSF 12 './pu240e.sf'
NFSFTP 11 './pu240e.sft'
NFTP 10 './pu240e.tp'
IPRECI 4
NIMP 0 80
REGROUTP
NFTP 10 './pu240e.tp'
NFTPR 17 './pu240e.tpr'
NIMP 0 80
REGROUSF
NFSF 12 './pu240e.sf'
NFSFR 13 './pu240e.sfdr'
NIMP 0 80
REGROUSF
NFSF 11 './pu240e.sft'
NFSFR 14 './pu240e.sftr'
NIMP 0 80
COMPSF
NFSF1 13 './pu240e.sfdr'
NFSF2 14 './pu240e.sftr'
NFSFDR 20 './pu240e.err'
NFSFDA 21 './pu240e.era'
NIMP 0 80
END
```

inpu240f

```
CALENDF
  MODIFOPT LPSPPOS .TRUE.
  MODIFOPT LPSTPOS .TRUE.
  ENERGIES 1.0E-5 20.0E6
  MAILLAGE READ
  XMAS172
  SPECTRE
    3 zones
    500000. 1000000.
    0.5 -1.
    0. 310.
  TEFF 300.
  NDIL 5
0. 1. 10. 100. 1.E+7
  NFEV 9 9440 './jeff31tn9440_3.asc'
  SORTIES
    NFSF 12 './pu240f.sf'
    NFSFTP 11 './pu240f.sft'
    NFTP 10 './pu240f.tp'
  IPRECI 4
  NIMP 1 80
  REGROUTP
    NFTP 10 './pu240f.tp'
    NFTP 13 './pu240f.tpr'
    NIMP 0 90
  LECRITP
    MODIFOPT LPSPPOS .TRUE.
    NFTP 13 './pu240f.tpr'
    NFTP 117 './pu240f.tpp'
    NIMP 1 90
END
```

inpu241

```
CALENDF
  MODIFOPT LCCORSCT .FALSE.
  ENERGIES 1.0E-5 20.0E+6
  MAILLAGE READ
  XMAS172
  SPECTRE
  1
  0.      -1.
  TEFF 300.
  NDIL 1
  1.0E+10
  NFEV 9 9443 './jeff30n9443_2.asc'
  SORTIES
    NFSFRL 0 './pu241.sfr'
    NFSF 12 './pu241.sf'
    NFSFTP 11 './pu241.sft'
    NFTP 10 './pu241.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './pu241.tp'
    NFTP 17 './pu241.tpr'
  NIMP 0 80
  REGROUSF
    NFSF 12 './pu241.sf'
    NFSFR 13 './pu241.sfdr'
  NIMP 0 80
  REGROUSF
    NFSF 11 './pu241.sft'
    NFSFR 14 './pu241.sftr'
  NIMP 0 80
  COMPSF
    NFSF1 13 './pu241.sfdr'
    NFSF2 14 './pu241.sftr'
    NFSFDR 20 './pu241.err'
    NFSFDA 21 './pu241.era'
  NIMP 0 80
END
```

inu238

```
CALENDF
  MODIFOPT LCOR SCT .FALSE.
  ENERGIES 1.0E-5 20.0E+6
  MAILLAGE READ
  XMAS172
  SPECTRE
  1
  0. -1.
  TEFF 300.
  NDIL 1
  1.0E+10
  NFEV 9 9237 './jeff30n9237_2.asc'
  SORTIES
    NFSFRL 0 './u238.sfr'
    NFSF 12 './u238.sf'
    NFSFTP 11 './u238.sft'
    NFTP 10 './u238.tp'
  IPRECI 4
  NIMP 0 80
  REGROUTP
    NFTP 10 './u238.tp'
    NFTP 17 './u238.tpr'
  NIMP 0 80
  REGROUSEF
    NFSF 12 './u238.sf'
    NFSFR 13 './u238.sfdr'
  NIMP 0 80
  REGROUSEF
    NFSF 11 './u238.sft'
    NFSFR 14 './u238.sftr'
  NIMP 0 80
  COMPSF
    NFSF1 13 './u238.sfdr'
    NFSF2 14 './u238.sftr'
    NFSFDR 20 './u238.err'
    NFSFDA 21 './u238.era'
  NIMP 0 80
END
```

inu238a

```
CALENDF
ENERGIES 20000000. .00001
MAILLAGE READ
XMAS172
SPECTRE
  4      zones
10000000. 15000000.
2000000.  1400000.
    0.25    -1.
    0.      293.16
TEFF 300.
NDIL 0
NFEV 9 9237 './jeff30n9237_2.asc'
SORTIES
  NFTP 10 './u238a.tp'
  IPRECI 4
  NIMP 0 80
REGROUTP
  NFTP 11 './u238a.tp'
  NFTP 12 './u238a.tpr'
  NIMP 0 80
END
```

Calculates from 1.E-5eV to 20.MeV with 4 weighting spectrums:

```
20. Mev > E > 10. MeV : fusion spectrum (T = 15 MeV)
  thus alphaz > 10**7
10. Mev > E > 2. MeV : fission spectrum (<E> = 1.4 MeV)
  thus 10**6 < alphaz < 10**7)
2. MeV > E > 0.25 eV : E**-1 spectrum
  thus alphaz < 10.
0.25 eV > E > .00001 : maxwellian spectrum (T = 293.16)
  thus 10. < alphaz < 10**6
```

inu238b

```

CALENDF
ENERGIES 4. 9000.
MAILLAGE GENERE
3 zones
15 1.32E+6 19640330.00000
17332530.39074 14918247.15894 13840306.62915
11618342.56943 10000000.00000 8187307.53078 6703200.46036 6065306.59713
5488116.36094 4493289.6411 3678794.41171 3011942.11912 2465969.63942
2231301.60148 2018965.17995
132 -0.95 2018965.17995
1652988.88222 1353352.83237 1224564.28253 1108031.58362 1002588.43723
907179.53289 820849.98624 608100.62625 550232.20056 497870.68368
450492.02394 407622.03978 301973.83422 273237.22447 247235.26470
183156.38889 122773.39903 111089.96538 82297.47049 67379.46999
55165.64421 40867.71438 36978.63716 29282.99695 27394.44819
24787.52177 16615.57273 15034.39193 11137.75148 9118.81966
7465.85808 5530.84370 5004.51433 3526.62165 3354.62628
2248.67324 2034.68369 1507.33075 1433.81736 1234.09804
1010.39402 914.24231 748.51830 677.28736 453.99930
371.70319 304.32483 203.99503 148.62539 136.74196
91.66088 75.67357 67.90405 55.59513 51.57802
48.25160 45.51744 40.16900 37.26653 33.72015
30.51126 27.60773 24.98050 22.60329 19.45484
15.92827 13.70959 11.22446 9.90555 9.18981
8.31529 7.52398 6.16012 5.34643 5.04348
4.12925 4.00000 3.38075 3.30000 2.76792
2.72000 2.60000 2.55000 2.36000 2.13000
2.10000 2.02000 1.93000 1.84000 1.75500
1.67000 1.59000 1.50000 1.47500 1.44000
1.37000 1.33750 1.30000 1.23500 1.17000
1.15000 1.12300 1.11000 1.09700 1.07100
1.04500 1.03500 1.02000 0.99600 0.98600
0.97200 0.95000 0.93000 0.91000 0.86000
0.85000 0.79000 0.78000 0.70500 0.62500
0.54000 0.50000 0.48500 0.43300 0.40000
0.39100 0.35000 0.32000 0.31450 0.30000
0.28000 0.24800
25 293.16 0.24800
0.22000 0.18900 0.18000 0.16000 0.14000
0.13400 0.11500 0.10000 0.09500 0.08000
0.07700 0.06700 0.05800 0.05000 0.04200
0.03500 0.03000 0.02500 0.02000 0.01500
0.01000 0.00690 0.00500 0.00300 0.00011
TEFF 300.
NDIL 1
1.0E+10
NFEV 9 9237 './jeff30n9237_2.asc'
SORTIES
NFSFRL 0 './u238b.sf1'
NFSF 12 './u238b.sf'
IPRECI 2
NIMP 0 80
END

```

Calculates from 4. to 9000. eV with 3 weighting spectrums:
 15 groups with lower boundaries read, fission spectrum $\langle E \rangle = 1.32E+6$ eV
 132 groups with lower boundaries read, $E^{*(-0.95)}$ spectrum
 25 groups with lower boundaries read, Maxwell spectrum $T = 293.16$ K

The upper energy bounds of each zones (2018965.18, 0.24800) should be equal to the last lower bound of the next one.

N.B.: in that case REGROUSF is not necessary thus the computation concerns only the resolved energy range.

inu238c

```
CALENDF
ENERGIES 5500.    5800.
MAILLAGE GENERE
1
2      -1.    19640330.00000
5800.    5500.
TEFF 300.
NDIL 0
NFEV 9 9237 './jeff30n9237_2.asc'
SORTIES
      NFCS 15 './u238c.cs'
IPRECI 3
NIMP 3 80
END
```

Calculates from 5500. to 5800. eV
with 1 weighting spectrum
1 group with boundaries read
Pointwise cross sections output

inu238d

```
CALENDF
ENERGIES 100.    1100.
MAILLAGE GENERE
1 zone
-10    -0.    1100.0
-100.
TEFF 300.
NDIL 0
NFEV 9 9237 './jeff30n9237_2.asc'
SORTIES
      NFCS 15 './u238d.cs'
      NFSF 12 './u238d.sf'
IPRECI 3
NIMP 2 80
END
```

Calculate from 100. to 1100.eV with a flat
weighting
10 groups of calculated energy boundaries
with constant width of 100 eV
Pointwise and effective cross-sections
output

inu238e

```

CALENDF
MODIFOPT NCAS 1 1 1 3 9 16
ENERGIES 1.0E-05 20.0E+6
MAILLAGE GENERE 11232 groups, universal
5 zones
-4572 -1. 19640329.8
480.
-3744 -1. 1433.81736
1920.
-1320 -1. 203.99503
960.
-1116 -1. 51.578022
480.
524 -1. 5.0434766
5.012346 4.981215 4.950084 4.918953 4.888590 4.858228 4.827866 4.797503
4.767891 4.738278 4.708666 4.679053 4.650171 4.621290 4.592408 4.563526
4.535358 4.507190 4.479021 4.450853 4.423380 4.395907 4.368434 4.340961
4.314166 4.287372 4.260577 4.233782 4.207649 4.181516 4.155383 4.129250
4.103400 4.077550 4.051700 4.025850 4.000000 3.975950 3.951900 3.927860
3.903615 3.879370 3.855125 3.830880 3.807235 3.783590 3.759945 3.736300
3.713238 3.690175 3.667113 3.644050 3.621557 3.599065 3.576572 3.554080
3.532143 3.510205 3.488268 3.466330 3.444935 3.423540 3.402145 3.380750
3.360563 3.340375 3.320188 3.300000 3.279408 3.258815 3.238223 3.217630
3.197555 3.177480 3.157405 3.137330 3.117753 3.098175 3.078598 3.059020
3.040138 3.021255 3.002373 2.983490 2.965075 2.946660 2.928245 2.909830
2.891870 2.873910 2.855950 2.837990 2.820473 2.802955 2.785438 2.767920
2.751947 2.735973 2.720000 2.704830 2.689660 2.674490 2.659320 2.644490
2.629660 2.614830 2.600000 2.583333 2.566666 2.550000 2.533758 2.517515
2.501272 2.485030 2.469200 2.453370 2.437540 2.421710 2.405897 2.395483
2.382370 2.371185 2.360000 2.345067 2.330135 2.315202 2.300270 2.285715
2.271160 2.256605 2.242050 2.227865 2.213680 2.199495 2.185310 2.171483
2.157655 2.143828 2.130000 2.120000 2.110000 2.100000 2.086537 2.073073
2.059610 2.049708 2.039805 2.029903 2.020000 2.008623 1.997245 1.985868
1.974490 1.963368 1.952245 1.941123 1.930000 1.918615 1.907230 1.895845
1.884460 1.874770 1.865080 1.855390 1.847695 1.840000 1.829250 1.818500
1.807750 1.797000 1.786500 1.776000 1.765500 1.755000 1.744243 1.733485
1.722728 1.711970 1.701478 1.690985 1.680493 1.670000 1.659878 1.649755
1.639633 1.629510 1.619633 1.609755 1.599878 1.590000 1.578585 1.567170
1.555755 1.544340 1.533255 1.522170 1.511085 1.500000 1.491667 1.483333
1.475000 1.466250 1.457500 1.448750 1.440000 1.431140 1.422280 1.413420
1.404560 1.395920 1.387280 1.378640 1.370000 1.361875 1.353750 1.345625
1.337500 1.328125 1.318750 1.309375 1.300000 1.291770 1.283540 1.275310
1.267080 1.259060 1.251040 1.243020 1.235000 1.226765 1.218530 1.210295
1.202060 1.194045 1.186030 1.178015 1.170000 1.165000 1.160000 1.155000
1.150000 1.143250 1.136500 1.129750 1.123000 1.118667 1.114333 1.110000
1.105667 1.101333 1.097000 1.091333 1.085667 1.080000 1.075500 1.071000
1.065800 1.060600 1.055400 1.050200 1.045000 1.040000 1.035000 1.030000
1.025000 1.020000 1.014000 1.008000 1.002000 .996000 .991000 .986000
.981333 .976667 .972000 .966500 .961000 .955500 .950000 .945000
.940000 .935000 .930000 .925000 .920000 .915000 .910000 .903285
.896570 .889854 .883139 .876425 .870950 .865475 .860000 .855000
.850000 .842363 .834725 .827088 .819450 .812088 .804725 .797363
.790000 .785000 .780000 .770388 .760775 .751163 .741550 .732413
.723275 .714137 .705000 .697520 .690040 .682560 .675207 .667855
.660502 .653150 .646113 .639075 .632038 .625000 .617570 .610140
.602710 .595280 .588200 .581120 .574040 .566960 .560220 .553480
.546740 .540000 .535790 .531580 .527593 .523607 .519620 .514715
.509810 .504905 .500000 .496250 .492500 .488750 .485000 .480503
.476005 .471508 .467010 .462678 .458345 .454013 .449680 .445510
.441340 .437170 .433000 .428248 .423495 .418743 .413990 .409327
.404663 .400000 .395500 .391000 .385733 .380465 .375198 .369930
.364948 .359965 .354983 .350000 .346165 .342330 .338495 .334660
.330995 .327330 .323665 .320000 .317250 .314500 .310875 .307250
.303625 .300000 .295000 .290000 .285000 .280000 .275877 .271755
.267633 .263510 .259633 .255755 .251878 .248000 .244395 .240790
.237185 .233580 .230185 .226790 .223395 .220000 .217285 .214570
.211855 .209140 .206557 .203975 .201392 .198810 .196358 .193905
.191453 .189000 .186750 .184500 .182250 .180000 .177428 .174855
.172283 .169710 .167283 .164855 .162428 .160000 .157677 .155353
.153030 .150810 .148590 .146370 .144247 .142123 .140000 .138000
.136000 .134000 .130200 .126400 .122600 .118800 .115000 .111250
.107500 .103750 .100000 .097500 .095000 .091250 .087500 .083750

```

.080000	.077000	.074500	.072000	.069500	.067000	.064750	.062500
.060250	.058000	.056000	.054000	.052000	.050000	.048000	.046000
.044000	.042000	.040250	.038500	.036750	.035000	.033750	.032500
.031250	.030000	.028750	.027500	.026250	.025000	.023750	.022500
.021250	.020000	.018750	.017500	.016250	.015000	.013750	.012500
.011250	.010000	.008967	.007934	.006900	.006500	.006000	.005500
.005000	.004500	.004000	.003500	.003000	.002300	.001700	.001300
.001000	.000800	.000500	.000110				

TEFF 293.16
NDIL 6
0.1 1. 10. 100. 1000. 1.0E+10
NFEV 9 9237 './jeff30n9237_2.asc'
SORTIES
NFCFS 0 './u238e.sfr'
NFSF 12 './u238e.sf'
NFTP 10 './u238e.tp'
IPRECI 4
NIMP 0 80
REGROUTP
NFTP 10 './u238e.tp'
NFTPR 11 './u238e.tpr'
NIMP 0 80
REGROUSF
NFSF 12 './u238e.sf'
NFSFR 13 './u238e.sfr'
NIMP 0 80
SEFFNRA
ENERGIES 1.0E-5 20.0E+6
NFTP 11 './u238e.tpr'
NFSFTP 18 './u238e.sft'
NDIL 6
0.1 1. 10. 100. 1000. 1.0E+10
NIMP 0 80
COMPSF
NFSF1 13 './u238e.sft'
NFSF2 18 './u238e.sfr'
NFSFDR 20 './u238e.err'
NFSFDA 21 './u238e.era'
NIMP 0 80
END

inu238f

```
SIGTTEUM
  ENERGIES 4000000. 9000.
  TEFF 300.
  NFEV 9 9237 .\jeff30n9237_2.asc
  NFCS 10 .\u238f.cs
  IPRECI 1
  NIMP 0 80
REGROUCS
  NFCS 10 .\u238f.cs
  NFCSR 11 .\u238f.csr
  NIMP 0 80
LECRICS
  ENERGIES 0. 20000000.
  NFCSL 11 .\u238f.csr
  NFCSE 12 .\u238f.cse
  NIMP 0 80
END
```

inu239e

```
CALENDF
  MODIFOPT NCASUNR 1 1 1 1 1 16
  MODIFOPT LFORMRF .FALSE.
  ENERGIES 40000. 2000.
  MAILLAGE READ
    RED616
  SPECTRE
    1 zones
      0. -1.
  TEFF 293.
  NDIL 1
    10. 100. 1000. 1000000.
  NFEV 9 9437 './jeff30n9437_3.asc'
  SORTIES
    NFPR 11 './pu239e.pr'
    NFSF 12 './pu239e.sf'
  IPRECI 3
  NIMP 0 90
REGROUSF
  NFSF 13 './pu239e.sf'
  NFSFR 14 './pu239e.sfr'
  NIMP 0 90
REGROUPR
  NFPR 15 './pu239e.pr'
  NFPRR 16 './pu239e.prr'
  NIMP 4 90
LECRISF
  NFSFL 17 './pu239e.sfr'
  NFSFE 119 './pu239e.sfe'
  NFSFP 121 2 './pu239e10b.sfp'
  NIMP 0 90
END
```

inu239f

```
essai SIGTTEUM
SIGTTEUM
  ENERGIES 1.0E-3 2.0E+6
  TEFF 293.6
  NFEV 9 9437 './jeff30n9437_3.asc'
  NFCS 10 './pu239f.cs'
  IPRECI 4
  NIMP 0 95
LECRICS
  ENERGIES 1.0E-3 2.0E+6
  NFCSL 15 './pu239f.cs'
  NFCSE 16 './pu239f.cse'
  NFPEF 17 './pu239f.csp'
  NIMP 0 95
END
```

inW184

```
calcul test ecriture PENDF
CALENDF
  MODIFOPT NCASUNR 1 1 1 1 1 1
  ENERGIES 0. 20000000.
  MAILLAGE READ
    ECC01968
  SPECTRE
    1 zones
      0. 0.
  TEFF 300.
  NDIL 0
  NFEV 9 7437 'endfb70n7437_1.asc'
  SORTIES
    NFSF 0 './w184.sf'
    NFCS 14 './w184.cs'
  IPRECI 4
  NIMP 0 95
REGROUCS
  NFCS 14 './w184.cs'
  NFCSR 15 './w184.csr'
  NIMP 0 95
LECRICS
  ENERGIES 0. 2.E+7
  NFCSL 15 './w184.csr'
  NFCSE 16 './w184.cse'
  NFPEF 17 './w184.csp'
  NIMP 1 95
END
```

inPu241b

```
test cas CAD pour sorties ENDF
CALENDF
ENERGIES 0. 200000000.
  MAILLAGE READ
    RED616
  SPECTRE
    1 zones
      0. -1.
  TEFF 294.
  NDIL 5
    1. 10. 100. 1000. 1.E+8
  NFEV 9 9443 './ornlpu241.asc'
  SORTIES
    NFCS 10 './pu241b.cs'
    NFSF 12 './pu241b.sf'
  IPRECI 3
  NIMP 0 80
  REGROUSF
    NFSF 12 './pu241b.sf'
    NFSFR 13 './pu241b.sfr'
  NIMP 0 80
  REGROUCS
    NFCS 10 './pu241b.cs'
    NFCSR 17 './pu241b.csr'
  NIMP 0 80
  LECRICS
    ENERGIES 0. 200000000.
    NFCSL 17 './pu241b.csr'
    NFPEF 116 './pu241b.csp'
    NFCSE 118 './pu241b.cse'
    NIMP 1 100
  LECRISF
    NFSFL 13 './pu241b.sf'
    NFSFE 119 './pu241b.sfe'
    NFSFP 121 1 './pu241-1b.sfp'
    NIMP 0 100
  END
```

inPu240e

```
CALENDF
  MODIFOPT LCORSCT .FALSE.
  MODIFOPT LFORMRF .FALSE.
  ENERgies 1.0E-5    20.0E+6
  MAILlage READ
  XMAS172
  SPECTre (borne inferieure, ALPHA)
  1      zones
  0.      -1.
  TEFF 293.6
  NDIL 1
  1.0E+10
  NFEV 9 9440 './jeff31pu240p.asc'
  SORTies
    NFTP 10 './pu240e.tp'
  IPRECI 1
  NIMP 2 80
END
```

6.1 Timings

To give some idea of the relative speeds of the code system on various platforms the running times, in second, for some of the test cases (on a single processor with no optimisation) can be compared. All test cases will typically complete in less than 10 minutes.

	SunBlade 2500 Sparc 1.6 Ghz {a}	Intel Xeon 64 2.26 Ghz {b}	AMD 64 2.2 Ghz {c}
inal27	2.52	0.27	0.48
inb10	0.5	0.11	0.16
inb10a	1.9	0.19	0.30
infe56	15.3	1.33	2.66
inhf178	282.6	21.9	54.9
inhf178a	0.03	0.01	0.01
inpu239	384.7	63.8	72.9
inpu239a	0.08	0.02	0.03
inpu239b	0.07	0.02	0.03
inpu239c	341.1	41.0	70.7
inpu239d	377.5	64.0	73.0
inpu240	293.8	25.4	59.8
inpu240a	608.4	54.9	130.0
inpu240b	291.0	25.4	59.8
inpu240c	293.6	25.3	59.8
inpu240d	269.7	25.3	59.8
inpu240e	48.7	4.6	8.9
inpu240f	234.1	25.6	60.1
inpu241	195.6	21.3	38.3
inu238	342.4	38.8	91.0
inu238a	289.4	36.2	85.8
inu238b	26.4	3.9	10.0
inu238c	1.0	0.29	0.57
inu238d	4.6	0.7	1.8
inu238e	1413.7	157.4	341.6
inu238f	1.0	0.3	0.49

Time in Seconds

{a} Solaris 10 Sparc and Studio 10 Fortran 77/95 Compiler

{b} Apple OsX 10.6 and Intel ifort 11.1 Compiler

{c} Solaris 10 i86 and Studio 11 Fortran 77/95 Compiler

Fortran compiler FFLAGS for normal, full debugging and fast execution are provided for each compilers and platforms. Older Fortran 95 compiler releases, on all platforms, are also generally supported. On some platforms a factor of 3 to 5 time improvement can be achieved between normal and fast compilation executable test cases runs.

7 Reference

- 1) L. B. Levitt, "The probability table method for treating unresolved resonances in Monte-Carlo criticality calculations", Trans. Am. Nucl. Soc. 14, 648(1971).
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- 3) D. E. Cullen, "Application of the probability table method to multigroup calculations of neutron transport", Nucl. Sc. Eng. 55, 387-400 (1974).
- 4) D. E. Cullen, "Calculation of Probability Tables parameters to include intermediate resonance self-shielding", UCRL 79761, ANS Winter Meeting, San Francisco, (1977).
- 5) P. Ribon and J. M. Maillard, "Les tables de probabilité: Application des sections efficaces pour la neutronique", CEA internal report, (1986).
- 6) F. J. Dyson, "Statistical Theory of the Energy Levels of Complex Systems", J. Math. Phys., 3,140(1962); 3,157(1962); 3,160(1962).
- 7) P. Ribon, "CALENDF et les programmes associés - Notice Théorique", CEA internal report, (1995).
- 8) "ENDF-6 Formats Manual", Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII, Written by the Members of the Cross Sections Evaluation Working Group Last Revision Edited by M. Herman and A. Trkov, Report BNL-90365-2009, June 2009.

ÉDITÉ PAR
LA DIRECTION DES SYSTEMES
D'INFORMATION

CEA / SACLAY 91191 GIF-SUR-YVETTE CEDEX FRANCE