

# CALENDF

## CALENDF-2001 : a short presentation and some problems

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NJOY

What does CALENDF do ?

|         |  |  |
|---------|--|--|
| CALENDF | <p>Generates sets of res. par. in the URR<br/>Treat this URR as the RRR<br/>Calculates Probability Tables<br/>Data handling with these PT :<br/>-group collapse,<br/>-interpolation (temperature,...)<br/>-mixture of nuclei<br/>-calculate sigma-eff(dil)</p> | <p>Processes angular and energy distributions<br/>Kerma<br/>Thermalisation (Sab)<br/>gamma production<br/>covariances<br/>.....<br/>(also PT ==&gt; module PURR)</p> |
|         |  | <p>Computes pointwise c.s. in the RRR<br/>Broaden pointwise c.s.<br/>Computes group sigma-eff(dil) for the whole E-range (but differs in the URR)</p>                |

But uses different methods even for the common purposes.

Choice of two basic methods:

**1- CUBIC INTERPOLATION:** it's the basic mode of interpolation, i.e. polynomial over 4 points

Interest: computing time; wider mesh.

Example: numerical integration of functions defined over a non-constant mesh (test of linear, cubic and 5th degree interpolation)

==> General recommendation: degree of the polynomial =  $-\log_{10}(\text{accuracy})$

Comparison of the number of points and of the computing time required by a linear and a cubic interpolation algorithms to obtain a given accuracy:

| accuracy | relative number of points | relative computing time |
|----------|---------------------------|-------------------------|
| 10**-3   | 2 to 3                    | 4 to 5                  |
| 10**-5   | 3 to 7                    | 10 to 15                |

But:

-careful check of pointwise data in order to avoid erroneous interpolation by cubic (generally unphysical description of  $\sigma(E)$ , numerous in evaluations though "... should avoid sharp features such as triangles or steps ... because such features cannot be realistically Doppler broadened" (ENDF-102, 3.3.1)

-the energy mesh has to be predetermined.

## 2- PADE APPROXIMANTS and GAUSS QUADRATURE.

**2-1 Their link:** moments, orthogonal polynomials, Pade approximants and Gauss quadrature are closely related. To establish the quadrature table ( $p_i, x_i$ ) of:

$$I(z) = \int \frac{p(x)}{1-zx} dx = \sum_i \frac{p_i}{1-zx_i}$$

we successively write:

$$\begin{aligned} I(z) &= \int \frac{p(x)}{1-zx} dx = \int p(x) \left( 1 + zx + z^2x^2 + \dots + z^{2N-2}x^{2N-2} + z^{2N-1}x^{2N-1} + z^{2N}x^{2N} + \dots \right) dx \\ &= \underbrace{M_0 + M_1z + M_2z^2 + \dots + M_{2N-2}z^{2N-2} + M_{2N-1}z^{2N-1} + R_{2N}z^{2N}}_{2N \text{ moments}} \\ &= \frac{b_0 + b_1z + b_2z^2 + \dots + b_{N-1}z^{N-1}}{1 + a_1z + a_2z^2 + \dots + a_Nz^N} + R'_{2N}z^{2N} \\ &\quad \underbrace{Q_{N,N-1} = \text{PADE approximant}} \\ &= \frac{b_0 + b_1z + b_2z^2 + \dots + b_{N-1}z^{N-1}}{z^N \left( a_N + a_{N-1} \frac{1}{z} + \dots + a_1 \frac{1}{z^{N-1}} + \dots + a_N \frac{1}{z^N} \right)} + R'_{2N}z^{2N} \\ &\quad \underbrace{P_N \left( \frac{1}{z} \right) = \text{orth. pol. } p(x) \implies \text{roots} = x_i} \\ &= \frac{b_0 + b_1z + b_2z^2 + \dots + b_{N-1}z^{N-1}}{\prod_{i=1}^N (1-zx_i)} + R'_{2N}z^{2N} \\ &= \underbrace{\sum_i \frac{p_i}{1-zx_i}}_{p_i, x_i = \text{Gauss quad. table}} + R'_{2N}z^{2N} \end{aligned}$$

**2-2 PADE approximants:** to calculate functions:

- for Doppler broadening by the Gaussian kernel  $\implies$  functions  $\psi, \chi$
- for exponential integral

**2-3 GAUSS quadrature:** to calculate integrals, convolutions:

- for Doppler broadening: can describe any Doppler-broadening model;
- to describe the resolution function of a experimental setup; it results from the convolution of several contributions:  $\mathcal{R} = R_1 * R_2 * R_3 * \dots$  (\* = convolution)
- to describe the total cross section within an energy group  $\implies$  c.s. probability tables

**3 - CROSS SECTIONS PROBABILITY TABLES:** set of

$$\left[ p_i, \sigma_{t,i}, \sigma_{s,i}, \sigma_{c,i}, \sigma_{f,i}, \dots \right] \quad i = 1 \implies N$$

Several approach; the two extremes (the oldest):

- L. B. LEVITT (1971)  $\implies$  gave the name; the range of cross section is regularly divided (or Log ( $\sigma$ )), and  $p_i$  is the relative presence of  $\sigma(E)$  within the subrange  $i$ .  
 $\implies$  Provides physical tables, but lengthy and cumbersome: up to 70 steps;

- M. N. NICOLAEV et al. (1970)  $\implies$  the sub-group method; the P.T. is established in order to fit at best the effective cross sections:

$$\sum_k \left( \sigma_{x,\text{eff}}(\sigma_{d,k}) - \sum_i \frac{p_i \sigma_{x,i}}{\sigma_{t,i} + \sigma_{d,k}} \right)^2 \quad \text{minimum}$$

- $\implies$  up to 5 steps, but it's sometimes difficult to obtain a physical table.

Remark: clearly distinguish between  
 - "c. s. probability table" (a mode of description of nuclear data, a tool)  
 - "sub-group method" (a method to treat the transport, which avoid the introduction of the "equivalent c.s.")

-Our approach: a PT is a Gauss quadrature table for  $\sigma_t$ ; introduction of "partial moments":

$$\mathcal{M}_n = \frac{\int_{\Delta E} \sigma_t^n(E) dE}{\Delta E} = \int_G p(\sigma_t) \sigma_t^n d\sigma_t = \sum_i p_i \sigma_{t,i}^n$$

$$\mathcal{P}_{x,m} = \frac{\int_{\Delta E} \sigma_x(E) \sigma_t^m(E) dE}{\Delta E} = \iint_G \omega(\sigma_t, \sigma_x) \sigma_x \sigma_t^m d\sigma_t d\sigma_x = \sum_i p_i \sigma_{x,i} \sigma_{t,i}^m$$

==> strong mathematical background, efficient way of computation, allows handling of data, up to 11 or 13 steps for a very good accuracy, physical table for  $\sigma_t$ ;

==> but  $\sigma_x$  may be unphysical (cf. example); more important: as for all PT, statistical hypothesis

Example of P.T.: 238U, obtained from the collapse of fine groups:  $du=1/480$

#### 4 - CALENDF vs. EVALUATIONS: specifications and evolution

*Respect of "recommendations":*

##### 4-1 Interpolation in the Unresolved Resonance Region. (ENDF 102: 2.4.2)

"... the recommended procedure is to interpolate on the cross sections derived from the unresolved resonance parameters (URP) ... The energy grid should be fine enough..."

But also: if no "reasonable accuracy ... additional intermediate energy points.... compute the cross sections ... using parameter interpolation."

???

==> CALENDF interpolates the average resonance parameters, and calculates their mean value over the described energy range.

##### 4-2 Formalism in the Unresolved Resonance Region (ENDF 102: 2.4.16.2)

"... only the SLBW formalism is allowed in ENDF/B, for the reason that no significant multilevel effect can be demonstrated...."

Later on: "... the use of SLBW to construct resonance profiles in the unresolved region will result in the defects associated with this formalism... and is not recommended.... the SLBW scheme should be used only for constructing average cross sections..."

!!!!

As a fact the multilevel effects increase as  $\Gamma_x/D$  increases; as  $\Gamma_x$  increases with energy while D decreases, the multilevel effects are generally more important in the unresolved range than in the resolved.

==> CALENDF uses the suitable approximation (BWMN or RM if necessary).

##### 4-3 Approximation of formalism for resonance.

All the resonance parameters are R-matrix parameters<sup>1</sup> and the appropriate method for their processing (Reich-Moore method or another approximation) depends on these parameters and the required accuracy. The method specified by the evaluator may be a non-sense: the use of the Reich-Moore method to treat the p wave resonances of 238U for example; but the ENDF/B format does not allow different specification of the recommended approximation for the different orbital momentum.

==> in its default option CALENDF determines the suitable approximation whatever is the evaluator recommendation.

<sup>1</sup> Except the Adler-Adler parameters, not treated by CALENDF

#### 4-4 Energy mesh for pointwise cross sections. (ENDF 102: 3.4.1)

"... The ... energy mesh for the total cross section must be a union of all energy meshes used for the partial cross sections."

==> CALENDF strictly applied this prescription: any point of a partial cross section, which is not a point of the total cross section, is ignored.

Unfortunately NJOY does not apply this prescription, accepts such "wrong" points, and result may differ with CALENDF.

Remark: interpolation law: we should require that:

the interpolate of the sum = the sum of the interpolates

==> this is not possible when LOG(s) (int. mode 4 and 5)

==> which data has to be corrected?

*Unphysical data in evaluations:*

#### 4-5 Great faraway resolved resonances.

Example: very great resonances at -5 keV and 15 keV in 238U-JEF2.

Dilemma:

1) do evaluations have to adapt themselves to actual processing codes, even if this imply non-physical presentation of data?

2) or do evaluations have to describe at best the physics, and processing codes to adapt themselves?

*Needs for improvements of the ENDF-B format: easy improvements:*

#### 4-6 Number of degrees of freedom.

It is very likely that the actual distribution of partial widths is not exactly an integer, equal to the number of open channels; even for the neutron widths.

For 238U or 232Th,  $\Gamma_n$  is likely to be distributed according 1.1 to 1.2 degree of freedom; this would induced a 0.5 to 1% effect on the self-shielding for a 10 barns dilution.

==> as the AMU\* are real numbers in the evaluation, no format change would be needed.

#### 4-7 Great resolved resonances in the unresolved range.

It is always desirable to substitute an actual data (resonance) to a statistical information.

==> Without any change in the format it would be possible (for CALENDF at least) to substitute an actual great resonance to a random great resonance.

*Needs for improvements of the ENDF-B format: important modifications:*

Many possibilities, or requirements; just one example:

#### 4-8 Correct description of the subthreshold fission in the unresolved resonance range.

Case of 238U.

==> CALENDF: in the past the possibility to applied to some data the same self-shielding than for a major data was planned; but never actualized.

**CONCLUSION :** CALENDF-2001 is an informtic revision of CALENDF (Fortran 90, clarification of coding, and test of compilers). Several options, defined inside the code, have been made modifiable by external users.

Few routines have been improved: the energy mesh for a better description of high energy resonances, the linearisation (in fact, "cubitisation") of pointwise c.s.,.....

There are still a few branches which have to be tested: for example, there are now 2 methods of P.T. interpolation, they have to be compared in order to determine the best choice according the case.