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# Tabular Cross Section File Generation and Utilization Techniques

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# TABULAR CROSS SECTION FILE GENERATION AND UTILIZATION TECHNIQUES

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Criteria of importance to the generation of linear cross section tabulations are presented. Algorithms for reducing or thinning such tables within a desired accuracy criterion and the implementation of paging techniques for efficient utilization of large data tables are reviewed.

(Cross sections, tables, pre-processing, relative error, linearization, thinning, paging.)

## Introduction

For many applications it is necessary to reduce the ENDF/B data files into a tabular form with a linear functional variation specified between the data points. Such tabular data bases are presently in use at a number of national laboratories.

Tabular representation of the files greatly simplifies the requirements for computer programs utilizing such data. The straight forward task of displaying a cross section, which may require a rather expensive resonance calculation when the base ENDF/B file is used as the starting point, is reduced to a simple table look-up and interpolation problem for tabular files. Great reductions in computing time can be realized in various codes (such as the point Monte Carlo Code REP[1]) which have been designed to do repetitive cross section calculations at a large number of energies.

When generated at a temperature of $0^0K$ data tables can be easily Doppler broadened to any desired temperature using numerical kernel broadening techniques.[2] Numerical broadening has the advantage of not being restricted to the "resonance range" and not ignoring the contribution of the "smooth" background correction terms which in fact often exhibit considerable structure. These advantages become particularly significant in the case of high temperature or CTR applications and for light materials for which no explicit resonance parameters are given on the ENDF/B file.

The generation and use of such tabular files requires a number of special considerations: Tabular files are generated within a specified controlled accuracy criterion. (The accuracy is defined as the fractional deviation from the "true" value which would be obtained from the ENDF/B file.) Thus at any stage the upper bound on the processing error is known.

The accuracy criterion must be selected in a manner that will insure the adequacy of the tabular files in the widest range of applications yet result in the smallest number of points. Typically tables with 10000 to 40000 points per reaction type are generated when major isotopes are reconstructed at $0^0K$ with an accuracy of .1%. As the experimental resolution is improved and the unresolved resonance range is further reduced[3] files with 150000 to 200000 points should be expected.

| Percent Accuracy | Number of points in the tabulation of the Total cross section | | |
|---|---|---|---|
| | U-238 | U-233 | Fe |
| 0.5 | 33644 | 2873 | |
| 1.0 | 12253 | 889 | 4215 |
| 2.0 | 5792 | 577 | 3834 |
| 5.0 | 6674 | 344 | 3100 |

Table I. Dependence of table size on accuracy

Such high accuracy files should be considered as a master data base and need to be generated only once. For many applications data with considerably lower accuracy may be sufficient. Thinning techniques are used to reduce the size of the tables depending on the required accuracy. Doppler broadened tables should be thinned even if the accuracy is the same because the smoothing effect of the Doppler process results in fewer points being required to represent a function within the same accuracy.

Finally special paging techniques for utilizing tabular data files a section (or page) at a time should be incorporated into codes operating on this data base since even with a virtual core capability it is often more efficient to have control over the amount of data brought in core at any one time.

Points to be considered during the generation, thinning and paging of tabular data files are discussed in the following sections.

| Temperature °K | Number of points necessary to represent the U-238 total cross section within 1% (ENDF/B-IV Data) |
|---|---|
| 0 | 12253 |
| 293 | 6819 |
| 1000 | 5050 |

Table II. Smoothing effect of the Doppler process.

## Generation

The major consideration in generating tabular data files is the selection of a proper convergence or accuracy criterion. When reducing ENDF/B files into a linearized tabular form two problems are encountered:

a) Conversion of cross section data which is already in tabular form but may have a logarithmic or semilogarithmic functional dependence between the tabulated points into a linear tabulation (Linearization)

b) Processing of data given in parametric form (e.g. resonance range data) into tables with an energy grid selected in a manner to insure the fewest number of points for a desired accuracy.

Both of these problems can be considered as approximating a function $f(E)$ defined for all $E$, by another $\bar{f}(E)$ such that:

$\bar{f}(E_i) \equiv f(E_i)$ at the tabulated points $E_i$, and the deviation of $\bar{f}(E)$ in areas between the tabulated points is less than a specified accuracy criterion.

For inherently positive functions such as a cross section the convergence between tabulated points should be determined on the basis of the fractional difference

i.e. $|f(E) - \bar{f}(E)| < \varepsilon f(E)$, as opposed to the absolute difference $|f(E) - \bar{f}(E)| < \varepsilon$.

Criteria based on the fractional difference are consistent with uncertainties in the experimental data and result in a more uniform distribution of data points in low as well as high cross section areas.

A numerical "interval halving" algorithm incorporated into the code RESEND[4] and compatible with the fractional difference criterion has been found well suited for the generation of tabular files in the resonance range as well as for the linearization of already tabular ENDF/B data files. This algorithm consists of the following steps:

a) A set of initial energy "node points" is selected. For tabular data, nodes are located at the edges of nonlinear interpolation ranges. For resonance data nodes are set at the peaks of resonances and mid-points between the peaks.

b) The exact cross section f(E) is calculated at the node points and $\bar{f}(E)$ is set equal to f(E).

c) The value of the approximate function $\bar{f}(E)$ at the mid-point between two nodes is obtained by linear interpolation and compared with the exact value f(E) at the same point. If the fractional difference at the mid-point is larger than the desired convergence criterion the mid-point is defined to be a new node and the process repeated in the halved interval. When a difference smaller than the convergence criterion is reached the interval is assumed to have converged and the process is repeated between the next set of nodes.

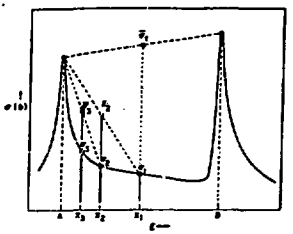

Figure 1. Generation of Energy Grid in Program RESEND.

When generating tabular cross section files from resonance parameter data, the convergence test should be applied to each of the individual reaction types separately and not be limited to the total cross section, since variations in reaction types with a low cross section (e.g. interference dips in elastic scattering) tend to be washed out when contributions from other, larger reactions are added on.

For the process of linearization of data tables an algorithm based on the analytic determination of the location of the maximum in the absolute difference $|f(E) - \bar{f}(E)|$ has been developed and implemented in the code MINX.[5] However the interval halving technique is found to be preferable since it is dependent on the fractional error and is somewhat simpler and faster. An extension of the MINX algorithm to fractional errors has not been found to be practical.

## Thinning

The thinning procedure is logically equivalent to the process of linearization since one starts with a function f(E) which is given as a table of values and a linear interpolation law between the tabulated values, and one tries to determine a function $\tilde{f}(E)$, such that:

a) $\tilde{f}(E)$ is also a table of values and linear interpolation laws.

b) The fractional difference between the "exact" f(E) and the approximation $\tilde{f}(E)$ is less than some desired allowable error $\varepsilon$ for all energies.

i.e. $|f(E) - \bar{f}(E)| < \varepsilon f(E)$.

However an additional criterion is added:

c) The tabulated values of $\tilde{f}(E)$ must constitute the smallest possible sub set of the tabulated vales in f(E).

*Thus all values in the tabulation of f(E) that can be approximated (to within $\varepsilon$) by linear interpolation between adjacent points must be eliminated.*

The following multipoint algorithm has been developed for thinning data files.

a) The first and third point of a table are selected and a test is made to determine whether point number two can be approximated by linear interpolation between points 1 and 3.

b) If the test is successful the test interval is extended to include point 4 and again points 2 and 3 are tested to see whether they can be approximated by an interpolation between points 1 and 4.

c) Generalizing to N points, if the points 2, 3, . . . (N-1) can be approximated by interpolating between points 1 and N the algorithm proceeds to N + 1 points.

d) If any one (or more) of the points 2, 3, . . . (N-1) fail the interpolation test between points 1 and N the test interval has been extended too far. However since the previous test (with N-1 points) must have been successful for the algorithm to reach this far all the points between 1 and N-1 can be removed leaving only the end points 1 and N-1. The algorithm is repeated with points N-1, N and N + 1.

The multipoint algorithm is considerably different from the "three-point" thinning technique used in the earlier versions of the ENDF/B system routine CROP.[6]

The three point algorithm operates by discarding point 2 if it can be interpolated between the adjacent points 1 and 3 then proceeds to test point 3 by interpolating between points 1 and 4. If point 3 is rejected there remains no guarantee that point 2 which was rejected earlier can be obtained by interpolating between the remaining points 1 and 4. This method produces particularly erroneous results when thinning points located very closely on a slowly varying smooth curve. The multipoint thinning algorithm is not limited to linear tables but can be used with any interpolation law. A generalized version has been implemented in a revised subroutine CROP.

## Paging

Two types of paging can be considered.

### 1. Physical Paging

If one recognizes that only a section of a large data table will be used in a computation for a reasonable length of time a program may be initially designed to keep only a portion of the table (a page) core resident at any one time. For applications requiring each portion of a table only once (e.g. group averaging, Doppler broadening) this physical paging may consist of simply allowing for the reading of a table a section at a time. Applications using different portions of a table repeatedly may require the use of scratch files or logic to randomly access different sections of a table.

### 2. Logical Paging

Programs written without a paging capability can easily be converted to a logical form of paging with only minor coding modifications.

Removing the name of an array to be paged from all COMMON and DIMENSION statements is equivalent to replacing that array by a function. One only needs to add a function by the same name to determine which section of the data table the desired point is located in, load that section if not already resident in core and return the desired value from the table. Such logical paging has been incorporated in code CHECKER and some versions of ETOG-3[7] programs with a paging capability are not only more versatile but may actually be more economical to use. The size of a page should be selected depending on the type of computer environment the program is to be used in.

a) In single user batch type of an environment I/O operation should be minimized by making the pages as large as possible within the available core. As the program is expanded, the page size can be reduced to allow it to fit in the same core.

b) In a multi-user time slice environment page size is determined by the amount of data that can be used within a single time slice. Ideally the size of a page in a time sharing environment should be such that the program can be finished and ready to read the next page at the end of its time slice.

### 3. Page Overlap

For applications requiring the use of two or more adjacent table entries simultaneously it is necessary to structure the paging logic in such a manner that the last few points of a page are repeated at the beginning of the next page. The purpose of this overlap is to avoid the repeated reading of pages that would result when the program attempts to use points located in two adjacent pages.

## Conclusion

The methods described in this paper have been implemented into a number of computer programs. The programs given on Table III in combination supply all the software necessary for processing the ENDF/B data files into a linear tabulation at any desired temperature, or to a multigroup cross section form.

| Program | Function | Characteristics |
|---|---|---|
| Scope[8] | Displays ENDF/B and/or experimental data (e.g. EXFOR-200) | Thinning, Logical Paging |
| CHECKER[6] | Checks correctness of ENDF/B files | Logical Paging |
| RESEND[4] | Reconstructs pointwise ENDF/B data tables from Resonance parameter data | Physical Paging |
| LINEAR[9] | Linearizes point ENDF/B data | Linearizing, Thinning Physical Paging |
| SIGMA1[10] | Doppler broadens linearized tabular ENDF/B data | Thinning, Physical Paging |
| RCN[5] | System for the production of multi-group cross sections from ENDF/B data | Physical Paging |

Table III. List of programs utilizing tabular data files

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