



UNITED STATES
NUCLEAR REGULATORY COMMISSION

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January 4, 1996

MEMORANDUM TO: David L. Morrison, Director
Office of Nuclear Regulatory Research

FROM: Carl J. Paperiello, Director
Office of Nuclear Material Safety
and Safeguards *Carl J. Paperiello*

SUBJECT: REQUEST FOR ASSISTANCE IN DEVELOPING INDEPENDENT
CAPABILITIES FOR PROCESSING NUCLEAR CROSS-SECTION DATA

The Office of Nuclear Material Safety and Safeguards (NMSS) performs safety evaluations and safeguards reviews for the licensing and regulation of away-from-reactor nuclear material operations, including those for uranium enrichment, fuel fabrication, storage and transportation of fresh and spent fuel, and nuclear waste management. These evaluations and reviews frequently entail independent analyses to explore safety issues and corroborate analyses performed by licensees and applicants. This is in keeping with the Energy Reorganization Act of 1974, which mandates that the Commission have "an independent capability for developing and analyzing technical information in support of the licensing and regulatory process" (Legislative History, P.L. 93-438, p. 5548).

The Office of Nuclear Regulatory Research (RES) has supported the independent analysis capabilities of NMSS by assisting in the development of the SCALE computer code system at Oak Ridge National Laboratory (ORNL). Included in the SCALE system is a modular set of radiation transport and nuclear transmutation codes used by the NRC and its contractors, and often by industry, for calculating subcriticality safety margins as well as radiation source terms and shielded external dose rates. SCALE's radiation transport and transmutation codes, along with essentially all other such codes in the U.S., generally rely on libraries of nuclear cross-section data processed from a single data source, the Evaluated Nuclear Data File, Volume B (ENDF/B).

The fact that most nuclear analyses have a shared reliance on ENDF/B data has long led to concerns that any errors or deficiencies in the ENDF/B files will produce common-mode analysis errors, even when calculations are checked using otherwise independent codes and methods. There have indeed been numerous cases over the years in which anomalies appearing in the results of code benchmarking exercises were traced to serious errors or deficiencies in the ENDF/B data files. It is worth noting that in most such cases, the ENDF/B errors were discovered largely by chance, owing to peculiar circumstances in the benchmark problems themselves, and that the errors were found in data that had been in use for many years.

The current Version VI of ENDF/B, first released in 1990, features new formatting standards that have enabled the incorporation of updated and substantially improved data in many key areas. Unfortunately, however, only one processing code, the NJOY code, maintained at Los Alamos National

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Laboratory (LANL), has been revised to handle the new data formats. Moreover, recent attempts to use NJOY have exposed a series of code errors and deficiencies whose resolution has required extensive assistance from the code's sole remaining author, Dr. Robert MacFarlane of LANL. Shared dependence on NJOY processing of ENDF/B-VI data would thus appear to introduce further potential for common-mode analysis errors, and many such NJOY-produced errors have indeed been found, again largely by chance and often after extensive use of the processed data.

While benchmarking of NRC and industry codes against integral experiments remains indispensable as a means of determining and ensuring calculational accuracy (i.e., validation), it is clear that code-to-code benchmarks play an important role in helping span inevitable gaps in the experimental data base. Such code-to-code benchmarks might consist, for example, of checking industry or NRC results from the KENO or MORSE modules of SCALE against those from an independent code like MCNP. The elimination of common-mode analysis errors attributable to NJOY-processed ENDF/B cross-section data is particularly important to such benchmarking efforts.

Specific licensing or safety issues can be expected to arise in NMSS involving several analysis areas where nuclear cross-section data are used. These analysis areas include criticality safety, radiation shielding, and material safeguards assay. Foremost among these is criticality safety, an area that continues to receive heightened attention in the wake of events several years ago at two U.S. fuel cycle facilities. New criticality prevention issues are foreseen primarily in the enrichment, fabrication, and handling of new fuels in the 5-10% enrichment range, in the storage and transportation of highly enriched Naval fuels, in the down-blending of highly enriched uranium received from the former Soviet weapons program, and in the proposed use of burnup credit in calculating subcriticality margins for spent-fuel storage and transportation packages. Criticality safety is also beginning to play an increasing role in the waste management arena. Here, for example, the lack of applicable criticality data for many of the material mixtures arising in aged and degraded high-level waste forms will place particular importance on code-to-code benchmarks using high-quality cross-section data.

The initiative to establish upgraded and independent cross-section capabilities has arisen in part from experiences last year involving RES support for the Office of Nuclear Reactor Regulation (NRR). In the course of having ORNL provide NRR's vessel fluence program with new cross-section libraries based on ENDF/B-VI, RES's Division of Engineering Technology (RES/DET) encountered several NJOY code deficiencies requiring the assistance of Dr. MacFarlane at LANL. In response to RES/DET's difficulties with NJOY, a September 1994 conference call involving staff of RES/DET, ORNL, the Department of Energy (DOE), and the Defense Nuclear Agency (DNA) concluded that there was general interagency interest in having ORNL upgrade its AMPX suite of codes to provide an independent processing capability equivalent or superior to NJOY's. ORNL then prepared the attached white paper describing the current situation, the general nature of the work that would be needed, and the benefits that would accrue. With modest additional effort, the NRC's independence could be enhanced by having AMPX also process selected independent data found in the foreign counterparts of ENDF/B-VI.

Certain DOE- and DNA-sponsored portions of the work to upgrade AMPX were started earlier this year as tasks within larger ORNL projects and are now supported at a level totaling slightly less than one full-time equivalent staff member (FTE). Dr. Donald Carlson of my staff has reviewed DOE's and DNA's task descriptions and has estimated that timely completion of this and related work in a way that responds to the NRC's specific nuclear data needs, with due emphasis on particular nuclides over appropriate fast, epithermal, and thermal neutron energies and processing of foreign data files as well as ENDF/B-VI, will require RES support at a level of one additional FTE at ORNL for the next two to three years.

NMSS therefore requests RES assistance to establish independence in the processed nuclear cross-section data used for criticality, source-term, and shielding analyses. Dr. Carlson has worked with Mr. Charles Nilsen of your staff (Division of Regulatory Applications, RES/DRA) to outline the tasks that would provide the requested independent capabilities. Those tasks would have significant synergism with ongoing RES/DRA work at ORNL on using sensitivity methods, in conjunction with ENDF/B cross-section covariance data, to evaluate the applicability ranges of integral criticality data (Job Code W6479). The new work would be accomplished by having ORNL upgrade, test, and document the appropriate modules of AMPX and then use that upgraded code system to process ENDF/B-VI data, as well as selected independent cross-section data from the Russian, European, Japanese, and Chinese evaluated nuclear data files (BROND-2, JEF-2, JENDL-3.2, and CENDL-2), all of which have now adopted the same new formatting standards. The resulting processing capabilities, along with new independent libraries of processed fine-group and continuous-energy cross-section data, would also be available to potential user communities in NRR and the Office for Analysis and Evaluation of Operational Data. Dr. Carlson can be reached at 415-8507 to help address any comments or questions about NMSS needs in this area.

Attachment:
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AMPX Cross Section Processing System Upgrade for ENDF/B-VI and Enhancements

I. Summary of Benefits

Several potentially important benefits should arise from this effort. The most obvious of these are:

- a) **Lower Analytical Uncertainties Give Potential Savings - Safety Criteria** include analytical uncertainties as well as system uncertainties in establishing the margin of safety. While the primary objective is assuring safety, a secondary benefit is an acceptable level of safety at reduced cost. Calculations indicate conditions will still maintain adequate Safety Criteria. With the present situation in the United States, wherein many reactor facilities are running out of spent fuel storage space and legal problems thwart the shipment of this material to centralized reprocessing facilities, the ability to pack more material in the same space is of high desirability. More accurate calculations could demonstrate that the interspersal of new inter-fuel materials would allow more spent fuel to be shipped or stored. Certainly, the methods could prove that closer spacings are possible in fissile material storage.
- b) **Improved Safety Margin Calculations and Performance Predictions** - More accurate analyses of fuel storage loadings, accident consequences, isotopic transmutation studies and pressure vessel aging effects should be possible.
- c) **Enhance Accuracy** - Some of the new procedures will extend the state-of-the-art, especially in the treatment of resonance self-shielding in the unresolved, resolved and thermal energy ranges.
- d) **Range of Applicability** - Extension to all types of reactors (power, research, test) and facilities for entire fuel cycle (enrichment, storage, transportation, reprocessing).
- e) **Window of Opportunity** - AMPX is an established system with a world-wide user community. Leadership and staff capability for this effort are at Oak Ridge National Laboratory. Collaborative interest with other national laboratories and major universities is already in place. Sponsorship on a multi-agency basis (Department of Energy, Nuclear Regulatory Commission, Defense Nuclear Agency) is near-term reality.

II. Background

Prior to the mid-sixties, no comprehensive system of computer codes existed for producing multigroup neutron and gamma cross sections for use in the discrete ordinates, diffusion theory and Monte Carlo programs being developed in that time frame. Rather, a morass of individual codes, were used at most national laboratories and other government facilities to produce these data using very cumbersome and tedious procedures to unite data from a variety of sources. For example, one code might be used to produce elastic scattering data, another to produce inelastic data, another to produce n_2n , another to produce thermal data, etc., etc. Considering the sizes, speeds, and costs of the computers of that era, this was a natural way to approach the problem, because one simply did not have the memory to accommodate all the codes at one time, or the resources to gamble on trying to do everything together.

Cross section data sources were at best, sketchy, with liberal use being made of BNL-325 (the barn book), compiled and produced at Brookhaven National Laboratory.

Several things happened in the latter sixties to serve as a catalyst for improving the situation:

- Computers (in particular the IBM 360 family and CDC-6600) became much larger and faster.
- The first version of the Evaluated Nuclear Data Files was distributed on magnetic tape. This effort, championed by Henry Honeck, had evaluations containing all the data concerning a nuclide necessary to make a complete set of cross sections.
- Code developers were beginning to espouse the modular approach, wherein a collection of codes could be coupled together in a single system which employed standard interfaces for communicating between codes. The first of these systems was probably KAPL's NOVA system, but others quickly popped up, including the JOSHUA system at Savannah River, the ARC system at ANL, the COSMOS system at Winfreth, the APOLLO system in France, and the AMPX system at ORNL.

A) Summary of AMPX, AMPX-II, and AMPX-77

The Defense Nuclear Agency (DNA) initiated support for AMPX, a Modular System for Producing Multigroup Neutron and Gamma-Ray Cross Sections, in 1969.

Though it was intended for use primarily in weapons effects studies, the basic modules -- XLACS, LAPHNGAS, SMUG, CHOX, NITAWL, and XSDRNPM -- were based primarily on ORNL codes, which had capabilities tailored for reactor design and shielding analyses. This meant that the system had a wider range of applicability than a system written strictly for

weapons effects because it provided mechanisms for analyzing thermal and resonance self-shielding effects, etc.

The initial release of the system was made in 1973 and consisted of a User's Guide and a system of codes which would only execute on IBM computers.

By 1978, the system had grown to the point where a new release was needed, and a system consisting of 30 modules (albeit with some close functional overlap in 3 or 4 cases) was released.

Some of the new capabilities were provided by BONAMI, a code to perform Bondarenko calculations, ROLAIDS, a general purpose multi-regional integral transport code for resonance self-shielding, RADE, a cross section library checking code, VASELINE, a plotting code, etc.

By this time, support for the system had been reduced to a maintenance level, and, subsequent, further development was on a "by project" basis. Over the ensuing years, several enhancements and new modules were added, and two of three attempts were made to re-issue a new version of the system; however, the lack of a major supporter prevented any of these attempts coming to fruition.

In the latter eighties, a series of events led to the evolution of AMPX into a better and more widely usable product.

1) A new production library was made for the advanced Neutron Source (ANS) reactor which caused several procedures to be automated to make the system more "quality-assured".

2) This led to the decision to produce a new 238 group library for shipping cask analyses using all ENDF/B-V evaluations (a few over 300 nuclides).

3) Financial considerations made it wise to make use of the CRAY-XMP for task 2. This meant that all AMPX modules would have to be converted to FORTRAN-77, a compiler that does not vary significantly between different computers.

When the modules were all converted and used in the production task, it was decided to attempt to make another system release. By combining support from several tasks, we were able to rewrite the User's Guide and to release a new version, AMPX-77, in October 1992. This new version contains around 50 operational modules.

Subsequent to the last release, most modules in the system have been converted for various workstation platforms and are being used in a variety of analysis and production tasks.

B) Summary of NJOY

In the latter sixties and into the seventies, there was a strong fast reactor design effort in the US.

While Milton Shaw was head of the Atomic Energy Commission (AEC), now DOE, it was recognized that each reactor design study group in the US was developing its own computer software to solve the same or similar problems, leading to a large amount of redundancy and duplication, and hence, extra cost. This is understandable, as computers were not that old, and the lack of "off-the-shelf" software made the situation necessary.

At this time of austere budgets, wherein fast reactor research had to receive the lion's share of reactor research monies, it was decided to put cross section processing money into two baskets:

- 1) Two "production" codes called MINX (developed at LANL) and SPHINX (developed at Westinghouse Hanford), and
- 2) Three "benchmarking" state-of-the-art fast reactor codes called ETOE, MC²-2, and SDX (developed at ANL).

The MINX code in the first basket, had roughly the same capabilities as the AMPX XLACS module, except that it had no thermal processing capabilities and its resonance processing was based on the Bondarenko approach.

One of the features MINX shares with several codes is to print a banner page at the front of its output which proclaims MINX in large block letters. You should recall the computer named HAL in the movie "2001" (HAL is IBM with the letters decremented by one). It is reputed that Bob MacFarlane of LANL was working on an upgrade to MINX; when his output was returned, the printer chain has slipped causing all letters to be moved forward by one letter; hence, MINX became NJOY (deja vu, I suppose).

NJOY contains significant advances relative to MINX: it is a modular system in itself; it contains thermal processing capabilities; it processes neutron and gamma data; its Bondarenko factors are very much like one has parametrized the Nordheim treatment, an integral transport approach and are considerably more correct than those derived from the Narrow Resonance Approximation; it is only code in the world which comprehensively processes ENDF/B-VI data.

C) Need for Independent, Corroborative Capability

In a recent effort that produced a 199 group library, based on ENDF/B-VI at ORNL and using NJOY, several problems were encountered. Feedback to LANL allowed the problems to be corrected in a timely fashion.

It has been reported that Bob MacFarlane has several times remarked on how uncomfortable he is with a situation where NJOY is the only code which is an ENDF/B-VI processor. (I am sure

that there is also a feeling of satisfaction, as there should be).

For the same reason that Milton Shaw did not put all his eggs in one basket, there should be at least one operational alternative to using NJOY to process ENDF/B-VI. NJOY, of necessity, has picked procedures which may not be adequate for all applications. For example, the shielding factor approach is viewed with suspicion by some, though there is a sizeable number of examples which suggest the treatment can, or could be made to, handle most situations adequately. In any event, while NJOY reportedly processes all formats which are presently used in ENDF/B-VI, there are still other formats which have not been used and have not been addressed. Certainly, future developments could be aided by a "cross-checking" capability.

At present, with NJOY being the only code in the world which processes most or all of ENDF/B-VI data, there is no possibility of these very fruitful code comparison studies.

D) Project Applications Areas for New AMPX

An advantage of a modular system, like AMPX, is that one never has to pick an exclusive option for performing a particular task. While the writing of a code may be quite difficult, its introduction to be used with a suite of existing codes is trivial, requiring only that the new code know how to "talk" to the other codes in the system.

For example, we presently have three separate, and unique methods for resonance self-shielding:

- 1) NITAWL, for using the Nordheim treatment,
- 2) BONAMI, for using the Bondarenko approach,
- 3) ROLAIDS, for a multi-region integral transport theory approach.

We will shortly add a fourth, CENTRM, a multi-region discrete-ordinates or integral transport theory approach.

All of these (and more, if necessary) will remain in the system, giving the user the choice of selecting a treatment adequate and/or efficient enough for his application.

In the sense that we presently provide support necessary to perform weapons effects calculations (the actual analysis calculations are generally made with auxiliary non-AMPX codes which "know" our cross section formats), we will continue to do so. Our codes are used to analyze spent fuel shipping cask studies, critical experiments, reactor designs, shield designs, dosimetry studies, radiation damage analyses, etc.

New capabilities will either be written or imported, as necessary for new applications. For example, a contact has already been made with UC, Berkeley to collaborate on the further development of a two dimensional lattice program, which will greatly enhance our calculational

capabilities. An AMPX module written ten or fifteen years ago called CAMAY which has never been upgraded to production status, has the requisite cross section homogenization capabilities to make use of this new capability.

III. Unique Aspects of ENDF/B-VI Requiring New Processing Methodology

The upgrade to the new ENDF/B-VI formats involves several new and complicated features that were introduced to eliminate deficiencies in earlier versions of ENDF/B.

ENDF/B-VI contains 320 evaluations of which 246 are simple conversions of the ENDF/B-V data to the slightly modified ENDF/B-VI formats. These nuclides are already processable by AMPX, as are many of the 74 new evaluations.

As will mentioned again below, the two major changes in data representation that require new programming are the use of the Reich-Moore formalism to represent resolved resonances and the activation of "FILE 6" to present energy-angle correlated data for scattering processes.

Of the 74 new evaluations, 27 use FILE 6, 21 have Reich-Moore and FILE 6, which means we can probably process 292 of the 320 evaluations, though there are some other format conversions, which may be used, that the AMPX modules will not recognize.

Incidentally, the 28 "non-processable" nuclides include many very important nuclides. They are shown in Table 1.

The known areas requiring changes are listed below:

A) Reich-Moore Resonance Data

In point of fact, the Reich-Moore treatment has been implemented in AMPX, using a procedure suggested by Nancy Larson of ORNL, which allows one to calculate accurate cross section values using single precision arithmetic, whereas alternate approaches require at least double precision arithmetic. This does not solve all of the precision problem, however.

The structural nuclides all have resolved resonance ranges which extend into the hundreds of KeV range. On an IBM machine with 32 byte words, one gets around 6 and a half digits of precision. This means that one cannot even accurately represent the energy mesh of such high energy resonances since so many digits are "eaten up" just getting the resonance energy.

All our resonance processing codes use single precision arithmetic, except NITAWL, which was recently converted to double precision.

If we converted to the multi-pole approach, this would allow these SLBW resonances to be passed to NITAWL which could then process these data.

The new CENTRM program is already in double precision. However, the codes which make point data for CENTRM are not and will need to be converted. This should be a relative minor task.

B) New Energy-Angle Correlated Data (FILE 6)

Physically any scattering interaction involves a correlation between the initial and final energies and the angle of scatter. For example, in elastic and discrete level neutron scattering, a particle with a specified energy that scatters through a particular angle can only lead to a neutron that has a particular energy. For processes such as n_2n , n_3n , etc., the solution of the equations describing the processes is impossible without many assumptions of questionable validity. At higher neutron energies, the inelastic levels become so closely spaced that one cannot "see" the levels, and, hence, the measurement of the scattered particles looks like a cloud of multiple energies at varying angles.

For these reasons, scattering data are often reported as a probability function which varies with initial and final energies and angle. The representation can take several forms, including tabular and any of several analytic forms.

In previous versions of ENDF/B, this most general form of data representation was not used. Rather, for elastic and discrete-level inelastic scattering, one had the cross section as a function of energy, and the differential scattering distribution as a function of energy and angle. Using these data, along with the δ -function arising when one writes the equations for conserving energy and momentum, a procedure can be written to generate scattering matrices.

For other process, in most cases the cross section is specified as a function of energy and the secondary energies are specified as a function of initial energy, with most processes assumed to scatter isotopically in the LAB system.

For a few processes wherein it was known that the process scatters anisotropically in the LAB system, the differential scattering distribution is specified as a function of energy and angle. This form of presentation is called "uncorrelated energy-angle data," and is a misnomer. Furthermore, this misnomer which implies that the energy distribution can be treated independently of the angular scattering distribution is misleading and has, at least in AMPX, led to it being treated improperly.

In actuality, this situation is just as complicated as the "correlated energy-angle" case and should be treated in exactly the same fashion. What we are recognizing is that if an energy distribution varies in between two energies, and the angular distribution varies between two energies, then the file has defined an inherent correlation between energy and angle which should be treated as such. In short, the two distributions should be folded together to form a function of the three variables initial energy, final energy, and scattering angle.

In AMPX, scattering matrices are calculated for neutron-neutron interactions, gamma-gamma

interactions, and neutron-gamma interactions. Each of the separate codes which perform these operations use significantly different treatments, because the codes were written at different times by different personnel with different philosophies: To make matters even more confusing, in the neutron-neutron code, there are separate processes for calculating elastic, inelastic, n2n, thermal, etc., matrices, many of which are quite different.

We are working toward unifying all these procedures to make use of a single scattering matrix calculation procedure. This will serve all needs and, therefore, will be more consistent and easier to maintain as a quality-controlled product. Furthermore, the new product should be slightly more accurate, though the present procedures seem adequate for most situations. In any event, we have to change, because the existing procedures will not handle the correlated energy-angle scattering data.

C) New Thermal Data Representations

The formats for thermal data have remained unchanged for all early versions of ENDF/B, at least from ENDF/B-II to ENDF/B-V. Indeed, the data remained unchanged for all these versions.

Thermal elastic scattering data were given as energy-angle pairs, augmented by data which specified the differential scattering distributions as a function of energy. The inelastic data were presented in a special file of what is called scattering law (or $S(\alpha, \beta)$) data which is a compact way of presenting scattering data in dimensionless energy and momentum transfer variables. A complicated, though straightforward, expression relates $S(\alpha, \beta)$ to the differential scattering cross section, $\sigma(E \rightarrow E', \mu)$.

An assumption called "detailed balance" reduces the size of the large thermal files by a factor of two. What this assumption, in essence, says is that to have scattering equilibrium, the net flow down must be balanced by the flow up. Detailed balance requires an assumption about the thermal flux shape (typically taken to be a Maxwellian). The $S(\alpha, \beta)$ data allows one to calculate the downscatter cross sections, while detailed balance can be used to calculate upscatters.

In ENDF/B-VI, a completely different procedure is used to calculate thermal elastic scattering with different parameters added to the special thermal data file. A code, called HEXSCAT, can be procured which will process the new data. The inelastic $S(\alpha, \beta)$ data can now be presented for downscatter and upscatter, which eliminates the need for the approximate detailed balance assumption.

AMPX needs changing to accommodate these modifications. The introduction of HEXSCAT is thought not to be too difficult, while the treatment without detailed balance should be very straightforward.

D) Relocation of Some Data Types

In version V and earlier, neutron interaction data were all carried in separate files, as were gamma production data and gamma interaction data.

Version VI allows the mixing of these data. For example, a neutron interaction which produces a secondary particle, be it a gamma or whatever, can have the secondary particles scattering distribution data given in the "neutron files." Likewise for gammas, which can produce neutrons through the(γ ,n) reaction.

Our present codes, would either ignore these data or designate them incorrectly, and, therefore, must be modified. The magnitude of this work has not been scoped, though the availability of the generalized scattering data procedure mentioned above should greatly facilitate the task.

E) New Designation for Some Data

Another modification in ENDF/B-VI which will cause coding changes is the use of new identifiers for some interactions, and, in particular, gamma interactions. These changes will be minor and easy to make and will involve a code or two in the system.

IV. Methods Enhancements

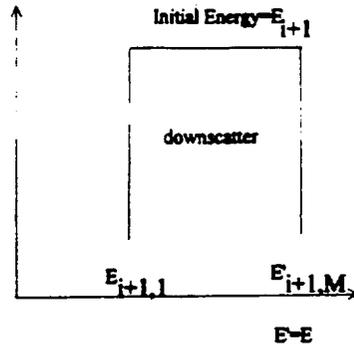
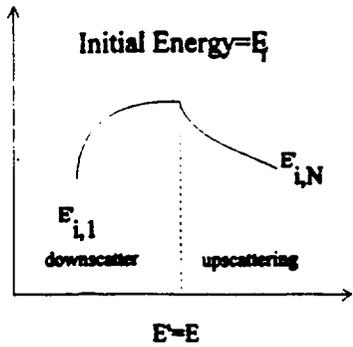
Several aspects of the planned developments should produce a system which could become the state-of-the-art for cross section processing.

A) Improved Method for Processing Scattering Matrix Data

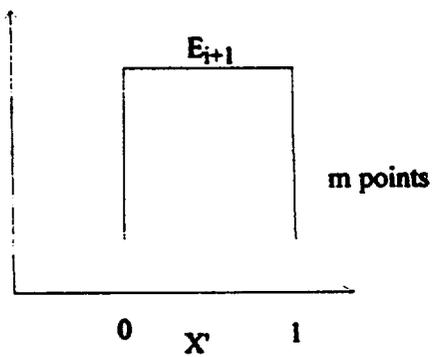
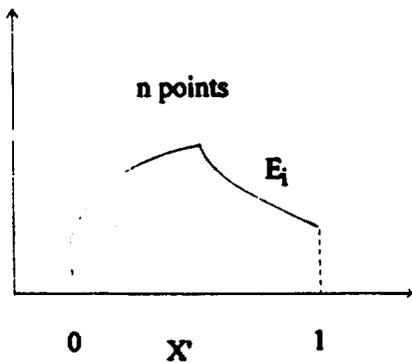
The method mentioned in II(b) above involves the integration over a three dimensional surface, $\hat{\mu}(E \rightarrow E', \mu)$, multiplied by cross sections, fluxes and Legendre Polynomials.

ENDF/B-VI proposes two approaches for this processing:

1) The NJOY method of corresponding energies, wherein scattering distributions are examined and integrated in a cumulative manner that assumes the distributions "match" at energy points corresponding to where a particular fraction of the function lays below the energy point. For example, if a 5 % tolerance is specified, one would find the point in both functions wherein 5 % of the distributions lay below the points, and where 10 % lay below the next two points, etc., etc., and where 95 % of the functions The distributions are assumed to match along these lines in a linear fashion. While this is "exact" for elastic scattering, it becomes non-physical, if one, for example, wanted to interpolate between a thermal distribution and a free atom distribution, because what we desire is that the $E=E'$ point be a match point.



2) The LLL developed a method called unit base transform, which transforms all distributions to a space wherein the secondary variable ranges from 0 to 1 and interpolates linearly between the corresponding points in this new space.



Clearly if applied without thought, this approach would not match along $E=E'$. However, if one tacks on a zero tail to the second function, which extends from $E_{i+1,m}$ to $E_{i+1,m+1}$ where this latter point is determined from

$$\frac{E_i}{E'_{i,m} - E'_{i,1}} = \frac{E_{i+1}}{E'_{i+1,m+1} - E'_{i+1,1}}$$

then we get the match we desire.

This, however, requires one use the same kind of judgement with every situation, something which may be difficult, or impossible to automate.

An easier approach to obtain the above match is to use an energy scaling, wherein each distribution is transformed to a space where

$$\frac{z'}{E} = \frac{E'_{i,k}}{E_i} = \frac{E'_{i+1,l}}{E_{i+1}}$$

In other words, if E is the interval (E_i, E_{i+1}) , where tabulations of E'_i and E'_{i+1} , specify the secondary distribution, the z' distribution at E picks a point in the surrounding distributions where the ratio of the final to initial energies is equal. This would inherently force the match line $E=E'$ to be taken as desired. This has the very desirable characteristics of not requiring the integration of the panels as method one above does, nor does it require the care of representation that the unit base transform does.

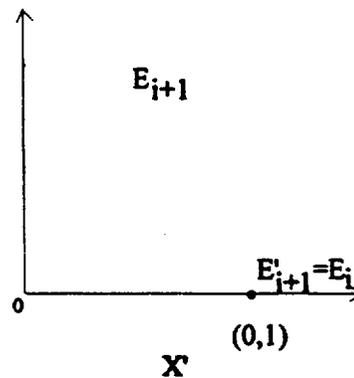
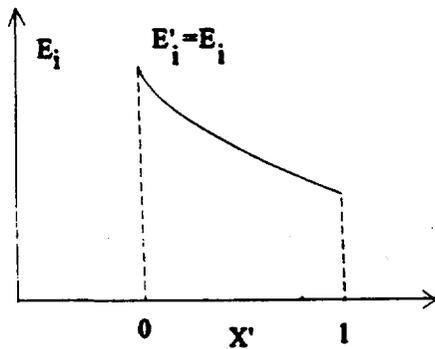
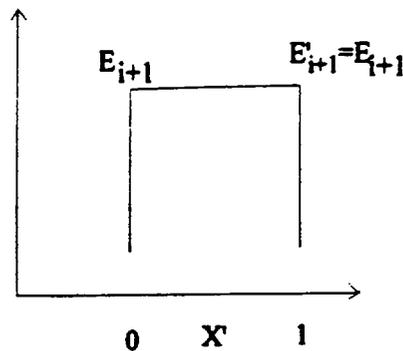
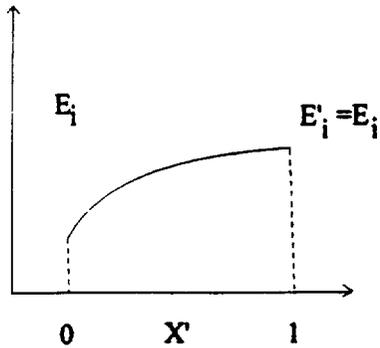
Unfortunately, this is not "physical" either because any intermediate energy, E , will have a distribution formed from a combination of the two distributions at E_i and E_{i+1} as

$$F(E) = hF_i(E'_i) + (1-h)F_{i+1}(E'_{i+1})$$

which says that, for example, if the distribution at E_i upscatters to an E' that is two times E_i , then every E in the interval will see an upscattering component at two times E .

In a interesting paper written by some researchers from the Peoples Republic of China, a method based on the unit base transform approach was discussed, which recognized that what really makes more sense is to look at corresponding features in the distributions (in their case, they considered the maxima points in the distributions) and then used unit base transform interpolation between the regions in between corresponding areas on the surrounding distributions.

In our simple example, one would interpolate in two regions:



This approach allows one to smoothly move from a case with an upscatter of two times E_i to no upscattering at E_{i+1} .

In AMPX, we plan to use hybrid of the unit base transform approach with the energy scaling mentioned earlier.

B) Improved Resonance Data Re-construction to Produce Point Data, Multipolar Representation, Temperature Dependence, Probability Tables for the Unresolved Range

As mentioned earlier, the fact that structural nuclides have important resonances in the hundreds of KeV range requires a double precision energy mesh. This is a problem on short-word machines, such as IBMs and workstation, but not on long word machines such as CRAYs.

The multipolar re-fitting of Reich-Moore data will be examined as an alternative to the straightforward approach, since this allows the use of simpler techniques for Doppler

broadening. At very low energies, a technique developed by Hwang and Leal may be implemented which allows one to accurately Doppler broaden these data.

The use of the probability table approach will be explored to more accurately treat self-shielding in the unresolved energy region. The URR computer code, developed by Leal for cross section calculations based on the probability table method, may be adopted. This may be especially important for the analysis of configurations whose primary neutron spectra is at intermediate energies, such as some shipping cask and shielding problems.

C) New One-Dimensional, Fine-group Technique for Resonance Self-Shielding.

The CENTRM code, developed at LSU for our use at ORNL, has extended state-of-the-art in several respects:

- it allows for at least a P_3 expansion of the anisotropic cross sections for all nuclides in the LAB system,
- it allows S_n theory on a many energy point mesh (other codes have done this, but used crude transport approximations for treating scattering),
- it can couple multigroup calculation above the resolved region to the point calculation in a manner which allows inelastic, n_2n , fission neutrons, etc., all to be treated as sources in the point range,
- it will couple the point calculation to a multigroup thermal calculation, which will allow thermal self-shielding effects to be properly treated.

D) New Multi-dimensional, Fine-group Technique for Fuel Assembly Averaging

A capability based on 2- or 3-dimensional collision probability methods will be used to account for geometrical coupling effects in reactor or fuel storage lattices, or in other situations which need a generalized geometric representation. The fluxes from this module can be use in the existing ORNL code, CAMAY, to further homogenize cross sections for use in diverse analyses.

E) Compatibility of AMPX Libraries with Neutronics Analysis Software

The collision probability code mentioned in the last paragraph must be able to read AMPX working cross sections which will produce fluxes that can be used to collapse cross section data on either an AMPX master of working library.

An AMPX master library contains data in its most elemental form; for example, it contains separate matrices for all scattering processes, is not problem dependent, has not been resonance self-shielded, etc. Subsequent processing by several modules may be required to produce an AMPX working library, which is situation-dependent, and which is ready to be used to calculate fluxes, or whatever.

V. Enhanced Capabilities and Applications Areas

Since several of the modifications noted earlier can be argued to be more theoretically correct than any available counterpart method, we would certainly hope for improvement in the accuracy of calculations using the new data with the associated comfort of knowing the treatments should be more reliable. From our experiences of having to maintain several, quite different procedures for calculating scattering matrices, we have encountered many "special situations" with most of them at some time requiring modifications to the procedures. Just having one scattering matrix calculator should go a long way towards eliminating these nuisance situations.

Additional enhancements accrue from the 74 new evaluations in ENDF/B-VI. Also available in ENDF/B-VI format are the European JEF-II, Japanese JENDL, and Russian Cross section libraries.

Areas that come to mind which may benefit from the new capabilities are given below:

- a) INEL Storage of Spent Naval Fuel - The improvements in resolved and unresolved treatments should allow a better assessment of the situation which would develop if some or all of the water moderator was lost.
- b) Weapon's Parts Storage - The quantity of this material has apparently already inundated available space. An accurate analysis might lead to the possibility of using alternate, or much closer parts spacing arrangements, thereby optimizing the use of storage facilities.
- c) Waste Storage in Fuel Drums - The new methods should allow for a closer qualification on the fissile limits that can be accommodated.
- d) Depletion and Resonance Overlap Studies - The new multiregion resonance self-shielding code should allow more accurate assessment of these effects of particular importance in fissile material processing.
- e) Thermal Self-Shielding - The ability to extend self-shielding in a proper fashion into the thermal range will allow a better assessment of the potential positive reactivities which might be encountered in Plutonium systems, if the flux peaked in the half eV region.
- f) The new multidimension collision probability code will allow for a more accurate analysis of LWR or HTGR fuel assembly performance for actinide burning or burnup credit.

g) Pressure Vessel Surveillance Studies - more accurate resonance and thermal treatments will yield more accurate fluence levels in these energy ranges and a better spatial distribution for secondary gamma rays.

h) Alternate Cross Section Weighting Techniques - For deep penetration calculations or high leakage situations, the ordinary zone and cell weighting techniques, based on simple reaction rate preservation, do not work well in many cases because of the exponential nature of the flux or because leakage effects may be more important than reaction-rate preservation. A technique could be designed that weighted in such a manner as to preserve exponential flux shapes and leakages from small systems.

² H	⁵⁴ Cr	⁶⁰ Ni	²⁰⁶ Pb
⁹ Be	⁵⁰ Mn	⁶¹ Ni	²⁰⁷ Pb
¹¹ B	⁵⁴ Fe	⁶² Ni	²⁰⁸ Pb
¹⁹ F	⁵⁶ Fe	⁶³ Ni	²³⁵ U
⁵⁰ Cr	⁵⁷ Fe	⁶⁴ Ni	²³⁸ U
⁵² Cr	⁵⁸ Fe	⁶⁵ Ni	²³⁹ Pu
⁵³ Cr	⁵⁸ Ni	⁶¹ Co	²⁴¹ Pu

Table 1. Listing of Isotopes not Processed by AMPX