FAST REACTOR CROSS-SECTION PROCESSING CODES - IS THERE A
DOLLARS WORTH OF DIFFERENCE BETWEEN THEM?*

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Since we do not live in an idealized world with infinite computational and monetary resources, the question of dollars worth of difference between ENDF/B cross-section processing codes for fast reactor calculations must be addressed with respect to both the accuracy required in the multigroup constants and the cost of obtaining that accuracy. Unfortunately, no single processing code is an obvious choice since the practical effect of different processing techniques on important reactor parameters is problem dependent. Therefore, it is the purpose of this paper to discuss the range of applicability of several multigroup averaging programs widely used in the United States, as well as the effort that must be expended in using them. The programs selected from the authors' experience include AMPX (1), MINX(2,3)/SPHINX(4), ETOE-2/MC²-2/SDX(5), and ETOX(6)/LDX(7). As is apparent these programs are often systems of linked computer codes and such distinctions will be highlighted in the discussion. Several articles (8-10) have already been published which discuss the different techniques and computer programs employed in cross-section processing. Much of this work, however, is of a survey nature and without numerical detail sufficient to quantitatively contrast the differences between processing codes. Others (11-14) are more quantitative but either do not involve all the programs considered herein, review only a limited number of reaction types, or contain integral results, but limited information on specific group-wise cross sections.

In the next section, a brief summary is given of the status and current capabilities for the programs under discussion. This is followed by a section in which some of the more important processed multigroup constants, obtained with the aforementioned codes (for a particular model of ZPR-6/7) are tabulated to illustrate the magnitude of the differences obtained for individual cross sections and transfer matrix elements. It is essential to note that all of the programs involved have several options and no attempt was made to exploit these options to "fine-tune" or "optimize"

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the resulting data sets to make the agreement appear more satisfactory (as might typically be done in a design effort). The numbers presented are more akin to "most probable values" which would be obtained if each code was run in a straightforward fashion by an interested user. The section also includes a listing of the integral results obtained for k_{eff} and reaction rate ratios using several of these cross-section sets. Significant differences can be observed in even relatively insensitive integral parameters. The last section describes some of the major differences in the physics algorithms employed which lead directly to the differences observed in multigroup constants and integral parameters.

It is expected that with a better understanding of the considerable variation and versatility of these averaging codes, combined with one or more case studies of the type included herein, and the tool of sensitivity analysis presently under development (15,16), the user might better be able to determine how he might best get his "dollars worth."

I. CURRENT CAPABILITIES - GENERAL

Before contrasting specific physical approximations, the prospective user is confronted with more immediate and logistic concerns such as "... is program X operational on my machine and has it ever been successfully used before." Table I illustrates what is thought to be the current capability as of August, 1974. This table will obviously be obsolete shortly after it is written. It does not indicate future plans or the ability to tie to other presently stand-alone modules; nor does it adequately address capabilities in closely related areas such as depletion and sensitivity analysis. However, it should be indicative of the present applicability of these computer programs to specific problem areas.

Three major category headings missing from Table I are timing, prior experience in the generation of multigroup sets, and user convenience. Definitive numbers are not available for the first two since several of these codes are relatively new, operating on different machines, each with a variety of user-control options available to which any timing study would be extremely sensitive. For example, a MINX restart from a Doppler broadened pointwise tape which was preserved from an earlier run might save approximately thirty minutes in the processing of ^{238}U on the IBM 360/91. The third area of user convenience was deemed by the authors to be too

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subjective for inclusion. Other areas of possible interest not tabulated include variable dimensioning, specific reaction types processed, etc. However, incorporation of this level of detail would not allow any room in this paper for anything but Table I.

II. ZPR-6/7 - A CASE STUDY

In order to gain some perspective on the effect that differences in processing methods have on calculated multigroup constants, the ZPR-6/7 critical assembly was selected for joint study. This assembly is a PuO_2/UO_2 fueled, large (3100 liter) core with a soft spectrum and composition typical of the LMFBR Demonstration Plant. Since ENDF/B-IV, as of this writing, was still not released, the assembly was analyzed with ENDF/B-III data in one-dimensional spherical geometry. The transport tool was S_4 , P_1 discrete ordinates with diffusion theory employed only if the former was not available. The atom densities and spatial mesh specified is listed in Table II. The inner and outer boundaries were associated with reflective and vacuum boundary conditions, respectively. The quadrature set, weights and cosines, are listed in Table III, along with the fission spectrum. It is noted here that several of these programs calculate their own mixture-dependent fission spectrum and this can clearly be one source of discrepancy. Perhaps, even more fundamental, is the fact that the fission spectrum is really energy dependent and should thus be represented in matrix rather than vector form. None of the processing codes employed had this feature at the time of comparison. Finally, the calculation was performed at 300°K in 29 groups with the energy boundaries listed in Table IV.

The problem description given above is based on Ref. (17) and differs from the latest CSEWG Fast Reactor Benchmark Description (18) for ZPR-6/7 (19). It was adapted here solely for the convenience of the authors since it was relative differences, rather than correct absolute values, that were being emphasized. In this work, two cores of slightly different composition are defined instead of the single zone core proposed in the newest specifications. The outer core radius and blanket thickness is given here as 92.01 and 33.56 cm instead of 88.16 and 33.81 cm in the more recent definition. Finally, our calculation was done in 29 rather than 27 groups.

As in the earlier work, the homogeneous spherical model was defined by first determining a blanket thickness and then searching for a core radius that gives the spherical reactor the same k_{eff} as the homogeneous two-dimensional cylinder. A heterogeneous-homogeneous correction of 0.0163 has been added to the eigenvalue computed to account for plate heterogeneity. Table V lists the results for k_{eff} along with previously determined values taken from Ref. (14). Differences on the order of one-half percent in k_{eff} are clearly distinguishable. Ratios of reaction rates at the core center are presented in Table VI. The precision between the ratios obtained using different calculational procedures appears to be significantly better than that attained for k_{eff} with the worst discrepancy being on the order of one percent.

In order to examine, in a more differential sense, the processed multigroup constants, groupwise cross sections for ^{238}U capture and ^{239}Pu fission are presented in Tables VII and VIII. Notable differences occur at the extremes in energy. At high energies, the precise form of the $1/E$ + fission spectrum weight function clearly affects the resulting averages. At lower energies, the structure in the weighting function is of prime concern in the self shielding of the resolved resonances. Although this may have had little impact on the integral parameters examined above (since the total neutron flux in this energy region is small), secondary gamma-ray production and transport would be particularly sensitive to such differences. It is also of interest to note that differences of the same order appear in quantities like α (capture/fission ratio) so that the observed differences are not merely scale factors. Even for a lighter material, such as oxygen, where the cross-section fluctuation is typically less severe, distinction on the order of 6% can be made as given in Table IX. Even larger differences are noted for transfer matrix elements in general and elastic removal in particular.

III. PHYSICS APPROXIMATIONS

Many of the differences observed in the previous section can be attributed to differences in methods and algorithms. Approximations are

required in at least the following broad categories: Doppler broadening, flux estimation and self shielding, groupwise numerical averaging, computation of group-to-group transfer matrices, gamma-ray interaction and production calculations, and space-energy collapse.

A. Doppler Broadening

This discussion will be limited to the resolved energy region since it is here that the observed differences (see Tables VII and VIII) appear to be the largest. Furthermore, most codes presently employ the same type of algorithm in the unresolved energy region. The methods by which various processing codes treat pointwise Doppler broadening tend to differ considerably. At least four different techniques have been employed: these include ψ, χ (20) methods, J* improvements (21), TEMPO (22) procedures, and the σ^1 (23,24) technique. The last approach is, at least potentially, the most accurate and the most time consuming.

If the nuclei in the medium are assumed to be distributed according to a Maxwellian distribution with temperature T, the Doppler broadening equation can be reduced to the form (22)

$$\sigma(E, T) = \frac{1}{E} \sqrt{\alpha/4\pi} \int_0^{\infty} \sqrt{E'} \sigma(E', 0) \left[e^{-\alpha(\sqrt{E'} - \sqrt{E})^2} - e^{-\alpha(\sqrt{E'} + \sqrt{E})^2} \right] dE' \quad (1)$$

where

T = temperature of medium $^{\circ}\text{K}$,

m, M = masses of the neutron and target nucleus respectively,

k = Boltzmann constant,

$\alpha = M/(mkT)$,

$\sigma(E', 0)$ = cross section for incident neutrons of energy E' at temperature $T = 0^{\circ}\text{K}$.

In deriving ψ, χ formulations, the second exponential in Eq. (1) is neglected and the major contribution from the remaining exponential $e^{-\alpha(\sqrt{E'} - \sqrt{E})^2}$ is assumed to come from a narrow region about $E' = E$. This is

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consistent with expanding regions of integration to ∞ and neglecting the energy dependence of the Doppler width. In existing codes using this method, the cross section $\sigma(E',0)$ is assumed to be composed of a series of isolated single-level Breit-Wigner resonances; thus a background file or generalized cross-section formulation is not considered. Often these approximations are adequate for reactor problems but may be unsuitable for shielding applications where appropriate consideration of the background file is important. The background file is really not smooth; it has structure of its own which must be broadened along with the resonance component. This approach may be inadequate for GTR core or military applications where temperatures are much higher.

The J* treatment (21) invokes rational transformations and Gauss-Jacobi quadrature to derive expressions for integrals of the flux-weighted Doppler-broadened cross section directly based on the NR approximation. Several mathematical approximations are introduced with regard to asymptotic properties, parameter selection etc., but these have been demonstrated to be negligible. For a system typical of fast reactor compositions, the newer procedure was shown to be approximately a factor of 100 faster than the corresponding MC² for the same problem and equivalent in accuracy.

The TEMPO approach starts from Eq. (1), neglects the second exponential, and assumes that the reaction rate $[\sqrt{E} \sigma(E,0)]$ is given as a table of values with linear-linear interpolation between entries. The algorithm has the same limitations as the (ψ, χ) technique concerning E large compared to $1/\alpha$, as well as ignoring the energy dependence of the Doppler width. But it has the advantage that it can handle and tabulate reaction rate, not just Breit-Wigner resonances.

The σ^1 method starts from the Eq. (1) and makes only one assumption: the cross section (not the reaction rate) is assumed to be piecewise linear between entries. This technique has all the advantages of the TEMPO method and is applicable to all energies, not just to $E \gg 1/\alpha$.

Comparison between these four techniques illustrates just one of a multitude of tradeoffs between accuracy and cost.

B. Flux Estimation and Self Shielding

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The methods by which the various processing codes treat the resolved resonance energy region tend to differ significantly. These differences can have a significant impact on both the accuracy of the resulting group constants and the execution speed of the processing code. Three basically different techniques have been used quite extensively in cross-section generation codes.

The simplest method assumes that a resonance may be represented by the natural line shape and integrated over group boundaries with an assumed weighting spectrum to obtain group averaged resonance cross sections. Such a method is incorporated in the SUPERTOG (25) and ETOG-I (26) codes. Because self shielding and temperature effects are neglected by this method, its use for fast reactor calculations has been limited. The Nordheim method (27,28) which is in the NYFT (29) and ASDRN (30) codes is also a fast integral method which treats self shielding but assumes isolated resonances. Since resonance overlap effects are particularly important for fissile isotopes this method has also been used sparingly for fast reactor calculations.

An alternative to the simple integration methods which retains their simplicity and computational efficiency is the Shielding Factor Method (SFM) most commonly associated with the text introduced in 1969 by Prof. Bondarenko (31). In this scheme a flux weighting spectrum is assumed on the basis of physical arguments and all other cross sections in the mixture are assumed to be constant over the energy interval of the group. In this case the mixture dependence of the microscopic cross sections may be characterized by a single parameter and the cross sections may be precomputed for a range of values of this parameter. Composition and temperature dependent cross sections may then be obtained by interpolation methods; thus the treatment of detailed physics mechanisms is clearly separated from problem-dependent considerations. The main limitation is the deficiency of not properly accounting for the localized fluctuations in the background cross section due to resonances of other nuclei present.

The elastic removal cross section may be considerably in error for compositions which include strong resonance scattering isotopes. The absorption in heavy element resonances, and thus the Doppler effect, are incorrectly predicted if mutual resonance interference effects are not treated. Approximate treatments of these latter effects have been incorporated into more recent extensions of the Shielding Factor Method (32) in the present generation. An alternative parametric representation has been developed by Stacey (33) to account for the relative flux shape in a group and the location of a resonance in the group in the Bondarenko calculation of elastic removal cross sections. Because of its relative simplicity, accuracy, and economy, the Bondarenko scheme has been widely used in the USA and Europe as well as the USSR.

The third method which has been used extensively is based on a detailed calculation of the flux weighting spectrum by means of an ultra-fine-group fundamental mode calculation. This method has the advantage of rigor but the disadvantage that a costly spectrum calculation must be performed for each different composition. In the MC² code (20), the detailed numerical integration of the resonance line shape may account for as much as 60% of the total execution time of the code.

Few studies have been performed to test the sensitivity of group cross sections to the generation methods. In a comparison of codes using the SFM scheme and ultra-fine-group methods, Little found (13) that the methods agreed about as well as codes using the same method agreed with each other. Kidman made a detailed comparison of the ETOX/1DX and MC² (11) codes for a characteristic fast reactor composition and concluded that the agreement was quite good in the calculation of a multiplication factor and sodium void, but the Doppler calculations were in poor agreement. Several improvements were identified for each code which, if implemented, would reduce the original Doppler 18% discrepancy to ~9%. However, because of coding inconsistencies, it was not possible to clearly delineate differences caused by the methods alone.

New methods are being developed which seek to speed up and extend the existing codes that incorporate the SFM and the detailed spectrum

calculation. The new methods are incorporated in the codes MINX/SPHINX (2-4) and MC²-2/SDX (5) which are currently under development. The MINX/SPHINX code system is designed to include anisotropic scattering matrices and a transport theory option. It also provides a detailed treatment of the resolved energy domain using the Bondarenko scheme through the incorporation of a temperature-dependent, pointwise library. The MC²-2/SDX resolved resonance calculation makes use of accurate and economical numerical algorithms developed by Hwang. Because of the relative economy of the resonance calculation and the intermediate-group energy structure, it is possible for these methods to take account of spatial dependence in considerably more detail than the direct-ultrafine-group methods. Thus SDX treats cell heterogeneity explicitly through use of integral transport-theory methods and accounts for multiregion spatial effects by use of fine-group one-dimensional diffusion-theory calculations. Similarly, LDX provides space-energy collapsing using one-dimensional diffusion theory.

Detailed methods sensitivity studies are required to determine how the different algorithms affect the calculation of fast reactor parameters. Some work has been done comparing the SDX resonance calculation with that of MC² and it was found that the agreement between the two methods was quite good in most cases. In many cases differences between the results could be attributed to the more rigorous algorithms within SDX. Pennington found (34), however, that for certain benchmark assemblies, the fine-group method in the SDX code was not accurate for the treatment of the resolved resonances of intermediate mass materials because of the composition dependence of the flux spectrum used to obtain the fine group cross sections. The MINX/SPHINX code system will permit the use of the self-shielding factor method at the fine-group detail; however, one must consider the huge amounts of data that will be generated.

C. Groupwise Numerical Averaging

There is indeed more than a "Dollars Worth" of difference in the way various processing codes use and/or process the ENDF/B File 3 data.

For instance, not only do the techniques of obtaining weighted averages from this File vary, but the previous sections has already demonstrated the diversity in the forms used for the resonance smooth weighting function. Weighting functions vary from arbitrary input functions, to standard forms (e.g., $1/E$, constant, E , fission spectrum), to calculated spectra, to combinations of these.

Techniques for performing the weighted averages can roughly be classed as either numerical or analytical. Numerical evaluations usually proceed by dividing the original broad group into a number of equal lethargy fine groups so that the cross section and weighting function can each be assumed to vary little across any fine group. The broad group integration is then reduced to a summation of the products of mid-lethargy fine group values of cross section and weighting function. This technique can ultimately handle any weighting function shape. Also, a single energy mesh can be used which can be very convenient. However, the technique must solve the problem of putting too many points in some regions and not enough in other regions.

Adaptive procedures (35) differ from this in that the mesh solution for integration is obtained by combining original data points selected by an adaptive Simpson's scheme.

The analytic technique usually operates with a weighting function that, when combined with any of the five possible ENDF interpolation schemes, will yield a function that is analytically integrable. Thus a broad group average is obtained by summing the analytical contributions from the panels defined by the File 3 points contained within the broad group interval. Of course this method has the advantage of being exact and following precisely the given File 3 data points. The principal disadvantage of this approach is that the product function (flux times cross section) representation can become very long.

Almost any step in the above general procedures can be a source of difference in processed results. A specific example can be cited: ENDRUN (36) joins a $1/E$ shape with a fission spectrum to form its weighting function, the two shapes are normalized so that they will be

continuous at the point, E_c , where they join. In order to avoid the normalization procedure, ETOX (7) arbitrarily uses the fission spectrum throughout the group in which E_c falls.

MINX is the only code that follows the prescribed ENDF/B recipe of Doppler broadening the File 3 data. This is accomplished by using a point Doppler broadening kernel on files of energy cross section pairs.

Some programs weight derive quantities simply with the input weighting spectrum while others use information from other cross sections. For example, the average cosine from elastic scattering is weighted with the input flux in some programs and with the elastic scattering collision density in others.

All differences have by no means been enumerated. For example, there are differences in the way programs treat discontinuities in data, in the way background and resonance files are combined, in the characterization of redundant reactions (such as absorption), and even in definitions such as that for the transport cross sections. Some programs use the scattering cross section as derived from matrix element column sums, others from direct averaging of the scattering cross section. And on, and on, and on.....

D. Computation of Group-to-Group Transfer Matrices

Some of the greatest differences among existing multigroup processing codes are in the manner that secondary angular and energy distributions are treated. Data are available in Files 4 and 5 of ENDF/B to describe the angular and energy distributions of secondary neutrons respectively. Processing codes use these data along with cross-section data derived from File 3 and the resonance data to generate multigroup transfer matrices which are defined in terms of double integrals over the source and sink groups.

The most important reactions for which secondary angular distributions are provided are elastic and discrete inelastic scattering. The kinematics of these reactions may be used to derive the energy of the scattered

neutron as a function of the initial energy and the scattering angle. The various processing codes, however, treat the energy-angle correlation with different degrees of rigor. Elastic scattering distributions are treated in detail by codes such as MC² (20), MC²-2 (5), MINX (28,3), ETOG (26), SUPERTOG (25), and XLACS (37). The first three codes perform the integration over the sink group analytically and treat the source group numerically. MC²-2 treats the source group in a semi-analytic manner for heavy isotopes. The other codes treat the double integration numerically. There are two basic problems involved in performing the integrations: (1) at high energies the distributions are highly anisotropic causing significant oscillations in the integrand; (2) at resonance energies the scattering is essentially isotropic but the cross section is a rapidly changing function of energy. These problems are particularly pronounced when calculating high order Legendre moments and the codes MINX and MC²-2 appear particularly reliable for such calculations. Both the ETOX and MC² (fine-group option) codes treat elastic scattering in an approximate manner.

Discrete inelastic and (n,2n) scattering tends to be treated in a far more approximate manner by the various programs, ETOG, SUPERTOG, XLACS, and MC², for example, assume isotropic scattering in the center of mass and consider only the average energy loss per collision thus, effectively, neglecting the energy-angle correlation. In addition MC² neglects the center of mass-lab corrections. All of these codes treat the scattering on a relatively coarse energy mesh. The MINX procedure treats discrete inelastic scattering in the same manner as elastic scattering and thus takes full account of the energy-angle correlation (38). The only approximation made by MINX is the neglect of the double valued region near threshold. The MC²-2 code also treats discrete inelastic scattering rigorously on an ultra-fine-group mesh but is limited to linearly anisotropic distributions in the center of mass. The various approximations of the processing codes have been found to have a significant impact on the calculation of reactor parameters. Segev found (39) that MC² eigenvalues were in error by as much as .6% for some systems compared to calculations which properly accounted for energy-angle correlations. The neglect of the sink energy bank width in discrete inelastic scattering

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has been found to cause errors on the order of .1% in k_{eff} for typical fast reactor configurations. Thus, the approximations made by most processing codes in the treatment of discrete inelastic scattering can have a significant impact on the accuracy of calculations.

The energy distribution of secondary neutrons is given in File 5 of ENDF/B in the form of tabulations or analytical expressions. Versions of all the codes mentioned above exist which handle all or most forms of the File 5 data. The principal differences among the codes is the manner in which the integrations are performed but this tends to have a greater impact on the efficiency of the coding than on the results. The neglect of incident energy dependence in the calculation of fission spectra or the failure to account for the ENDF/B specified integration limits in certain processing codes has not been investigated completely enough to provide quantitative estimates of the effects on calculated parameters.

D. Processing for Gamma Ray Interaction and Production Data from ENDF/B

Multigroup gamma-ray calculations require the use of two types of computer codes in most applications: (1) there is a code which produces "transfer coefficients" for the production of gamma rays from neutron interactions. These "cross sections" are the weighted product of neutron interaction cross sections and gamma-ray yields. (2) The second type of computer code produces matrix elements which correspond to the neutron multigroup cross section and scattering transfer matrices. These represent the gamma-ray interactions.

So-called coupled neutron-gamma cross-section sets are produced by cleverly arranging neutron interaction, gamma production and gamma interaction cross sections into a single set such that one can obtain neutron and gamma transport results in a single calculation. This technique is today receiving wide use by installations concerned with neutron and gamma transport. Only the AMPX (1) system can, today, generate coupled sets in a single computer run.

It is safe to assert that gamma processing, as presently done, cannot affect the reactivity of a conventional reactor, since there is no treatment of $\gamma \rightarrow n$ reactions. However, these data will soon be part of new ENDF gamma libraries, and procedures can be modified to treat them.

The LAPJ (40) code developed by Don Dudziak et al. at Los Alamos fostered a whole family of computer codes which are specifically written to make gamma production cross sections from ENDF data. These include:

1. The LAPHANO (41) and OAPHAN (42) codes developed at Los Alamos, and
2. the LAPHNGAS (42) module of the Oak Ridge AMPX system.

LAPH was written to process the initial version of ENDF photon production files. Significant format revisions led to the writing of the LAPHANP program. LAPHANO produces isotropic gamma production matrices and allows a wide variety of weighting options. An interesting feature of this code is that it can use input neutron fluxes and a description of

a one-dimensional system to collapse from fine neutron groups to broad group neutron-gamma production matrices. It will also output a gamma source to use in a separate gamma transport calculation.

LAPHAN was written to give an anisotropic gamma production capability. It is variably dimensioned.

LAPHNGAS was written using an early version of LAPHANO as its basic framework. It is variably dimensioned and makes anisotropic gamma production matrices as does LAPHAN. It was written for an IBM 360, though an early version is available in a CDC 6600 version of AMPX.

LAPHANO, LAPHAN, and LAPHNGAS are very similar codes as one would expect if their genealogy is examined. All have benefited from the collaboration of Los Alamos and Oak Ridge personnel. They are unique in their capability to process ENDF gamma production data, and the choice of the best one is a matter of what codes one plans to use with the gamma production data, one's computer and whether one needs anisotropic gamma production arrays.

Until recently two codes (or their variants) have almost exclusively been used to make multigroup gamma interaction matrices. These are the GAMLEG (44) and the MUG (45) programs. These codes are very similar. Their transfer matrices are formed by integrating the Klein-Nishina equation. This, of course, limits their use to applications well above X-ray energies. Pair production is included in the transfer matrices isotropically. Versions are available which access some ENDF data. As with the gamma production codes, the proper choice of which of these codes to use is a matter of installation and the auxiliary codes to be employed.

E. Space-Energy Collapse

The reactor designer would prefer to run his calculations with one energy group, if at all possible. The object of the space-energy collapse is to approach this desirable state. Typically fast reactor calculations are run in 8 or 9 groups, and 21 groups are used for reactivity and void calculations. These calculations use cross-section sets derived from a more detailed library of 30 or more groups.

The current trend is to go to a large number of groups for a basic standard cross-section library (46) and collapse from that for different applications. The existence of such standardized data sets would focus even more attention on the process of space-energy collapse.

The ideal space-energy collapse tries to preserve reaction rates and leakages although the former has been given until recently the most attention. The actual mechanics of performing the collapse are fairly trivial and do not differ widely between codes. However, the whole crux of the problem is to get the right spectrum over which to collapse. This is where the processing codes differ most. The range is from zero dimensions and a large number of energy points to few group with great spatial detail. Table X presents a summary of some of the currently available codes.

The relative emphasis which must be placed on the energy and space variables is an important question which deserves further attention.

REFERENCES

1. N. M. Greene and F. R. Mynatt, "The AMPX Modular Code System for Generating Coupled Neutron-Gamma Multigroup Cross-Section Sets," Trans. Am. Nucl. Soc. 15, 568 (1972); see also N. M. Greene et al., "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," ORNL-TM-3706 (to be published).
2. C. R. Weisbin, P. D. Soran, D. R. Harris, R. J. LaBauve, and J. S. Hendricks, "MINX - A Multigroup Interpretation of Nuclear X-Sections," Trans. Am. Nucl. Soc. 16, 127 (June 1973); see also C. R. Weisbin, P. D. Soran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, and J. E. White, "MINX, A Multigroup Interpretation of Nuclear Cross Sections from ENDF/B," Los Alamos Scientific Laboratory report to be published.
3. D. R. Harris, R. J. LaBauve, R. E. MacFarlane, and P. D. Soran, Los Alamos Scientific Laboratory, and C. R. Weisbin and J. E. White, Oak Ridge National Laboratory, "MINX, A Modular Code System for Processing Multigroup Cross Sections from Nuclear Data in ENDF/B Format," LA-UR-1766, presented at the Seminar on Codes for Nuclear Data Processing held at NEA-CPL, CONF-731207-1, Ispra, December 5-7, 1973.
4. N. C. Paik, C. Durston, W. Davis, and M. B. Yarbrough, "Physics Evaluations and Applications - Quarterly Progress Report for Period Ending January 31, 1974," WARD-XS-3045-5 (March 1974).
5. H. Henryson, II, B. J. Toppel, and C. G. Stenberg, "ETOE-2/MC²-2/SDX Multigroup Neutron Cross-Section Processing," presented at the Seminar on Codes for Nuclear Data Processing held at NEA-CPL, CONF-731207-1, Ispra, December 5-7, 1973; see also B. J. Toppel and H. Henryson, II, "Methodology and Application of the MC²-2/SDX Cross Section Capability," Trans. Am. Nucl. Soc., 16, 126 (1973).
6. R. E. Schenter, J. L. Baker, and R. B. Kidman, "ETOX - A Code to Calculate Group Constants for Nuclear Reactor Calculations," BNWL-1002 (1969).
7. R. W. Hardie and W. W. Little, Jr., "IDX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections," BNWL-954 (March 1969).
8. N. E. A. Computer Program Library, "Seminar on Nuclear Data Processing Codes," Ispra, December 5-7, 1973, Newsletter #16.
9. D. K. Truhey and Jane Gurney, Compilers, "A Review of Multigroup Nuclear Cross Section Preparation Theory, Techniques, and Computer Codes," ORNL-RSIC-27 (January 1970).
10. W. M. Stacey, Jr., et al., "The U. S. Theoretical and Computational Program," International Symposium on the Physics of Fast Reactors, Oct. 16-23, 1973, Tokyo, JAPAN, paper #7.

11. R. B. Kidman, "A Comparison of Two Fast Reactor Cross Section Processing Codes," HEDL-TME 72-57 (February 1972).
12. R. Q. Wright, R. E. Schenter, and J. D. Jenkins, "A Comparison of the Group Constants Generated by the ENDF/B Processing Codes ETOX and SUPERTOG," ORNL-TM-4041 (April 1973).
13. W. W. Little et al., "Numerical Comparison of Data Processing Codes for Fast Reactors," Trans. Am. Nucl. Soc., Vol. 12, No. 1, 144 (1969).
14. H. Alter, "Report on the Cross Section Evaluation Working Group - Status of Fast Neutron Cross Section Data Testing Using ENDF/B Version 3 File," contained in the minutes of the CSEWG Meeting, November 1972.
15. E. G. Silver, E. M. Oblow, J. M. Kallfelz, C. R. Weisbin, D. E. Bartine, G. F. Flanagan, and F. R. Mynatt, "Generalized Reactor Sensitivity Program at ORNL," Trans. Am. Nucl. Soc., 18 (June 1974).
16. H. Henryson, II, H. Hummel, R. Hwang, W. M. Stacey, Jr., and B. J. Toppel, "Sensitivity of Integral Neutronics Properties of LMFBR Assemblies to Cross Section Preparation Methods and Data Uncertainties Using the ETOE-2/MC²-2/SDX Code System," proceedings of this conference.
17. L. G. LeSage, E. M. Bohn, J. E. Marshall, and M. Salvatores, "ZPR-6/7 - The Single-Zone Demonstration Reactor Benchmark Assembly," Initial Experimental Results," ZPR-TM-45 (January 1971).
18. S. Pearlstein, Editor, "CSEWG Benchmark Specifications," ENDF-202 (August 1974).
19. E. M. Bohn, L. G. LeSage, J. E. Marshall, W. R. Robinson, G. S. Stanford, and T. J. Yole, "ZPR-6 Assembly 7 Experimental Results Part IP Critical Mass, Neutron Spectrum and Reaction Rates," ZPR-TM-76 (September 1971).
20. B. J. Toppel, A. L. Rago, and D. M. O'Shea, "MC², A Code to Calculate Multigroup Cross Sections," ANL-7318 (1967).
21. R. N. Hwang, "Efficient Methods for the Treatment of Resonance Cross Sections," Nucl. Sci. Eng. 52, 157 (1973).
22. K. Gregson and M. F. James, "TEMPO - A General Doppler Broadening Programme for Neutron Cross Sections," Atomic Energy Establishment, Winfrith, AEEW-M518 (1965).
23. D. E. Cullen, O. Ozer, and C. R. Weisbin, "Exact Doppler Broadening of Evaluated Neutron Cross Sections," Trans. Am. Nucl. Soc. 16, 320 (1973).
24. D. E. Cullen, Program SIGMA1 (Version 74-1), UCID-16426 (January 1974).
25. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, Jr., "SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B," ORNL-TM-2679 (1969).

26. D. E. Kusner, R. A. Dannels, and S. Kellman, "ETOG-I, A Fortran IV Program to Process Data from the ENDF/B File to the MUFT, GAM, and ANISN Formats," WCAP-3845-1 (1969).
27. L. W. Nordheim, "A Program of Research and Calculations of Resonance Absorption," GA-2527, General Atomic (August 1961).
28. L. W. Nordheim, "The Theory of Resonance Absorption, in Symposium on Applied Mathematics, Vol. XI (1961).
29. H. Bohl, Jr., and A. P. Hemphill, "MUFT-5, A Fast Neutron Spectrum Program for the Philco-2000," WAPD-TM-218 (February 1961).
30. N. M. Greene and C. W. Craven, Jr., "XSDRN: A Discrete Ordinates Spectral Averaging Code," ORNL-TM-2500 (July 1969).
31. I. I. Bondarenko, ed., Group Constants for Nuclear Reactor Calculations, Consultants Bureau, New York (1964).
32. R. B. Kidman, R. E. Schenter, R. W. Hardie, and W. W. Little, "The Shielding Factor Method of Generating Multigroup Cross Sections for Fast Reactor Analysis," Nucl. Sci. Eng. 48, 189-201 (1972).
33. W. M. Stacey, Jr., "The Effect of Wide Scattering Resonances on Neutron Multigroup Cross Sections," Nucl. Sci. Eng. 47, 19 (1972).
34. E. M. Pennington, "ENDF/B Version-III Fast Reactor Data Testing Using Cross Sections Produced by Both MC² and SDX."
35. W. M. McKeeman, "Algorithm 145 - Adaptive Numerical Integration by Simpson's Rule," Comm. of the Association for Computing Machinery 5, (12) (December 1962); see also, D. Kahaner, "Comparison of Numerical Quadrature Formulas," Los Alamos Scientific Laboratory Report LA-4137 (June 1969).
36. B. A. Hutchins, C. L. Cowan, M. D. Kelley, and J. E. Turner, "ENDRUN-II, A Computer Code to Generate a Generalized Multigroup Data File from ENDF/B," GEAP-13704 (1971).
37. N. M. Greene, R. Q. Wright, J. L. Lucius, C. W. Craven, Jr., J. E. White, and M. L. Tobias, "XLACS: A Program to Produce Weighted Multigroup Neutron Cross Sections from ENDF/B," ORNL-TM-3646 (April 1972).
38. C. R. Weishin, P. D. Soran, and J. S. Hendricks, "A New Procedure for the Determination of Neutron Multigroup Transfer Matrices," accepted for publication in Nuclear Science and Engineering, July 1974.
39. M. Segev, "Group Transfer Matrices and Their Relation to Basic Cross Section Data," Nucl. Sci. Eng. 45, 3, 269 (September 1971).
40. D. J. Dudziak, A. H. Marshall, and R. E. Seamon, "LAPH, A Multigroup Photon Production Matrix and Source Vector Code for ENDF/B," LA-4337 (1969).

41. D. J. Dudziak, R. E. Seamon, and D. V. Susco, "LAPHANO: A P₀ Multigroup Photon-Production Matrix and Source Code for ENDF," LA-4750-MS (1972).
42. D. J. Dudziak, "LAPHAN: A Code to Compute the P₀ to P₄ Multigroup Photon Production Matrices," LA-4963 (ENDF-182 (January 1973)).
43. W. E. Ford, III, and J. L. Lucius, "LAPHNGAS: AMDX Module for Generating Multigroup Secondary Gamma-Ray Production Cross Sections," ORNL-TM-3706 (to be published).
44. K. D. Lathrop, "GAMLEG, A Fortran Code to Produce Multigroup Cross Sections for Photon Transport Calculations," LA-3267, Los Alamos Scientific Laboratory (1965).
45. J. R. Knight and F. R. Mynatt, "MUG: A Program for Generating Multigroup Photon Cross Sections," CTC-17 (January 1970).
46. C. R. Weisbin and R. J. LaBauve, "Specification of a Generally Useful Multigroup Structure for Neutron Transport," LA-5277-MS (May 1973).

Table I. Current Capabilities of Four ENDF/B Cross Section Processing Codes

	ETOX/1DX	ETOE-2/MC ² -2/SDX	AMPX	MINX/SPHINX
Applicability				
a) Fast reactors	X	X	X	X
b) Thermal reactors			X	
c) Shielding				
1. Neutron			X	*
2. Gamma			X	
d) Weapons				X
Output format				
a) CCCC	**	X	**	X
b) Discrete ordinates	X		X	
c) CITATION			X	
d) Local		X	X	X
Documentation				
a) Distributed	BNWL-1102 BNWL-954			
b) In preparation		X	ORNL-TM-3706	X
Availability	ANL Code Center	ANL Code Center - Jan. 1975	RSIC	ANL Code Center - Jan. 1975
Machine Compatibility	UNIVAC-1108 CDC-6600 IBM-360/***	IBM-360/***	IBM-360/*** CDC-6600 UNIVAC-1108	CDC/*** IBM-360/91
Basic library	ENDF/B	ENDF/B	ENDF/B	ENDF/B
Coupled sets			X	
Flux Model				
1. Energy	Self-Shielding Factor Tables	Composition Dependent Calculation	Fixed Spectrum	Self-Shielding Factor Tables
2. Space	Diffusion Theory	Diffusion Theory	Transport Theory	Diffusion Theory

*Diffusion theory limitation to P₀ matrices.

** ISOTXS only.

***Operable on several machines of this type.

Table II. Atom Densities and Geometrical Configuration
Employed in Modelling ZPR-6/7

Material	Inner Core	Outer Core	Blanket
<u>Regional Densities</u>			
(Density 10^{24} at/cc)			
^{235}U	0.00001249	0.00001254	0.00008522
^{238}U	0.005775	0.005798	0.04005
^{238}Pu	0.00000031	0.00000045	
^{239}Pu	0.0008874	0.0008886	
^{240}Pu	0.0001178	0.000118	
^{241}Pu	0.00001341	0.00001483	
^{242}Pu	0.00000141	0.00000179	
Mo	0.0002251	0.0002273	
Na	0.009278	0.009146	
O	0.01378	0.01466	
Fe	0.01306	0.01360	0.004221
Ni	0.001173	0.001168	0.0005087
Cr	0.002713	0.002700	0.001175
Mn	0.0002074	0.0002066	0.00009

Spatial Description

20 intervals - inner core
40 intervals - outer core
20 intervals - blanket

Inner core radius: 24.34 cm
Outer core radius: 92.01 cm
Blanket thickness: 33.56 cm

Note: These do not conform to the latest CSEWG benchmark specifications for ZPR-6/7 (which may be weighted averages of the inner and outer core specified above).

Table III. Quadrature Constants and Fission Spectrum
Used in the Analysis of ZPR-6/7

Quadrature Constants

<u>Angle</u>	<u>ω_m</u>	<u>μ_m</u>
1	0	-1.00000-00
2	1.73927-01	-8.61136-01
3	3.26073-01	-3.39981-01
4	3.26073-01	3.39981-01
5	1.73927-01	8.61136-01

Fission Fractions

<u>Group</u>	<u>Fission Fraction</u>	<u>Group</u>	<u>Fission Fraction</u>
1	0.32480-01	16	0.43500-03
2	0.12177+00	17	0.20600-03
3	0.21094-00	18	0.98000-04
4	0.22296-00	19	0.19000-04
5	0.17278-00	20	0.15000-04
6	0.11047+00	21	0.12000-04
7	0.36131-01	22	0.22000-04
8	0.26621-01	23	0.10000-04
9	0.33162-01	24	0.50000-05
10	0.16770-01	25	0.20000-05
11	0.82560-02	26	0.10000-05
12	0.40000-02	27	0.00000
13	0.18390-02	28	0.00000
14	0.56600-03	29	0.00000
15	0.42800-03		

Table IV. Twenty-Nine Group Structure Used in the
Analysis of ZPR-6/7

<u>Group</u>	<u>Energy Boundaries (eV)</u>	<u>Lethargy Interval</u>
1	6.065+06 to 1.000+07	0.500
2	3.679+06 to 6.065+06	0.500
3	2.231+06 to 3.679+06	0.500
4	1.353+06 to 2.231+06	0.500
5	8.209+05 to 1.353+06	0.500
6	4.979+05 to 8.209+05	0.500
7	3.877+05 to 4.979+05	0.250
8	3.020+05 to 3.877+05	0.250
9	1.832+05 to 3.020+05	0.500
10	1.111+05 to 1.832+05	0.500
11	6.738+04 to 1.111+05	0.500
12	4.087+04 to 6.738+04	0.500
13	2.554+04 to 4.087+04	0.470
14	1.989+04 to 2.554+04	0.250
15	1.503+04 to 1.989+04	0.280
16	9.119+03 to 1.503+04	0.500
17	5.531+03 to 9.119+03	0.500
18	3.355+03 to 5.531+03	0.500
19	2.840+03 to 3.355+03	0.167
20	2.404+03 to 2.840+03	0.167
21	2.035+03 to 2.404+03	0.167
22	1.234+03 to 2.035+03	0.500
23	7.485+02 to 1.234+03	0.500
24	4.540+02 to 7.485+02	0.500
25	2.754+02 to 4.540+02	0.500
26	1.301+02 to 2.754+02	0.750
27	6.144+01 to 1.301+02	0.750
28	1.371+01 to 6.144+01	1.500
29	6.826-01 to 1.371+01	3.000

Table V. Effective Multiplication Constant for ZPR-6/7

Calculated in this work (Model taken from Ref. 17)

<u>Processing Code</u>	<u>k_{eff}</u>	<u>Organization</u>
AMPX	1.0075	ORNL
ETOX-1DX	1.0089	HEDL
ETOE-2/MC ² -II	1.0009	ANS

CSEWG November 1972 (Model taken from Ref. 18)

ETOE-MC ²	0.9987	AI
ETOX/1DX	0.9944	BNL
ENDRUN-TDOWN	0.9902	GE
ETOX/1DX	0.9932	WARD

Experimental Value (19): 1.0000 ± 0.001

Table VI. Unit Cell Reaction Rate Ratios in ZPR-6/7

	<u>"Equivalent"^a Homogeneous Measurement</u>	<u>Reference (18) (1-D Homogeneous)</u>	<u>ETOE-2/ MC²-2</u>	<u>ETOX/ 1DX</u>	<u>AMPX</u>
$\sigma_c^{28}/\sigma_f^{49}$	0.1432	0.1570	0.1581	0.1566	0.1553
$\sigma_f^{28}/\sigma_f^{49}$	0.02406	0.02304	0.02234	0.02227	0.02204
$\sigma_f^{25}/\sigma_f^{49}$	1.049	1.096	1.0975	1.0994	1.0928

^aMeasurement results multiplied by heterogeneity factor (homogeneous result/heterogeneous) taken from Ref. (19).

Table VII. Inner Core Weighted Multigroup Capture Cross
Sections for ^{238}U in ZPR-6/7

Group	Lower Energy Boundary (eV)	AMPX	ETGX/LDX	ETOE-2/ MC ² -2	MC ² -2 (Integral Transport) Option
1	6.065+6	6.414-3	5.96-3	6.431-3	
2	3.679+6	1.182-2	1.19-2	1.179-2	
3	2.231+6	2.850-2	2.68-2	2.853-2	
4	1.356+6	6.561-2	6.24-2	6.564-2	
5	8.209+5	1.216-;	1.21-1	1.214-1	
<u>Better than 2% Agreement in Groups 6-11</u>					
13	4.087+4	4.436-1	4.36-1	4.291-1	
14	2.554+4	5.211-1	5.01-1	4.969-1	
15	1.989+4	5.849-1	5.69-1	5.631-1	
16	1.503+4	6.598-1	6.45-1	6.454-1	
17	9.119+3	7.691-1	7.70-1	7.688-1	
<u>Agreement for Groups 18-23 No Better than 3% and Gets Worse as Energy Decreases</u>					
24	4.54+2	1.277+0	1.313+0	1.308+0	
25	2.754+2	1.128+0	1.265+0	1.323+0	1.343+0
26	1.301+2	1.415+0	1.415+0	1.636+0	1.795+0
27	6.144+1	2.858+0	2.897+0	2.583+0	3.128+0
28	1.371+1	1.826+0	3.531+0	1.951+0	1.899+0
29	6.826-1	3.069+0	3.173+0	1.319+0	1.247+0

Table VIII. Inner Core Weighted Multigroup Fission
Cross Section for ^{239}Pu in ZPR-6/7

Group	Lower Energy Boundary (eV)	AMPX	ETOX/1DX	ETOE-2/ MC ² -2	MC ² -2 (Integral Transport)
					Option
1	6.065+6	2.081	2.084	2.078	
.... Similar Excellent Agreement - Groups 2-14					
15	1.503+4	1.831	1.831	1.807	
16	9.119+3	1.964	1.978	1.947	
17	5.531+3	2.240	2.244	2.206	
~3-5% Agreement - Groups 18-23					
24	4.540+2	8.583	9.462	8.344	
25	2.754+2	9.390	9.864	9.672	9.997
26	1.301+2	15.150	15.35	16.201	15.50
27	6.144+1	32.31	30.09	22.10	23.98
28	1.371+1	35.41	28.87	73.02	38.27
29	6.826-1	65.12	27.61	45.23	44.28

Table IX. Inner Core Weighted Multigroup Total
Cross Section for Oxygen in ZPR-6/7

<u>Group</u>	<u>Lower Energy Boundary (eV)</u>	<u>AMPX</u>	<u>ETOX/1DA</u>	<u>ETOE-2/MC²-2</u>
1	6.065+6	1.101	1.094	1.094
2	3.679+6	1.822	1.734	1.799
3	2.231+6	1.423	1.423	1.409
4	1.356+6	2.032	1.922	2.028
5	8.209+5	4.053	3.883	3.984
6	4.979+5	3.259	3.158	3.268
7	3.877+5	8.600	8.565	9.154
8	3.020+5	3.886	4.053	4.028
9	1.832+5	3.544	3.544	3.545
10	1.111+5	3.562	3.562	3.562

Cross Section Essentially Constant Here

**Table X. Typical Computer Programs Performing Space-Energy
Collapse of Neutron Cross Sections**

Code	Geometry	Type of Solution	No. of Groups	Origin
MC ² (Version I) ELMØE, FRESCØ	Simple Buckling	Fundamental Mode	1,800	ANL-7318 (MC ²)
1DX, SPHINX, TDØWN	1D Sphere, Cylinder Slab (Finite Difference)	One-Dimensional Diffusion Theory	Variable with Problem Size	BNWL-954 (1DX)
XSDRN, AMPX	1D Sphere, Cylinder Slab (Finite Difference)	One-Dimensional Transport Theory (Discrete Ordinates)	Variable with Problem Size	ORNL-TM-2500 (XSDRN)
RABBLE, RABID	1D Slab, Cylinder (Multiregion)	Exact Slowing Down in Lethargy Interface Currents Integral Transport using Collision Probabilities	Variable with Problem Size	ANL-7326 (RABBLE)
GARØL	1D Slab, Cylinder, Sphere (Two Region)	Exact Slowing Down in Energy, Collision Prob- abilities-Reciprocity	Pointwise	GA-6637
RØLAIDS	1D Slab, Cylinder, Sphere (Multiregion)	Exact Slowing Down in Energy, Interface Cur- rents Integral Transport	Pointwise	ORNL (Unpublished)