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TITLE: ZERO-DIMENSIONAL GROUP COLLAPSING

AUTHOR(S): R. B. Kidman and R. E. MacFarlane

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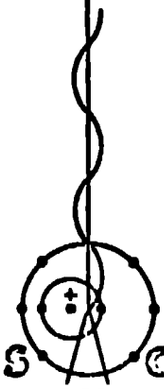

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

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ZERO-DIMENSIONAL GROUP COLLAPSING

by

R. B. Kidman and R. E. MacFarlane

Los Alamos Scientific Laboratory, University of California
Theoretical Division
Los Alamos, New Mexico 87545

The purpose of this work is to develop a zero-dimensional group collapsing capability that will enhance the applicability of ERDA's format[1] and super-group standarization[2] efforts. New physics algorithms are introduced which allow an exact collapsing to a subset group structure.

The link between multigroup processing codes and reactor physics codes is characterized by a multitude of formats and multigroup structures. Standardized formats and a standardized fine-group structure are being introduced in an effort to simplify this area and facilitate the communication of nuclear data between installations and codes involved in the national fast reactor development program.

A computer code, CINX[3], has been developed to accept cross sections in the standardized ISOTXS, BRKOXS, and DLAYXS files,[1] to collapse the cross sections to a subset, fewer-group structure, and to put the results in the original CCCC[1] format. This code allows the user to tailor a multigroup library to his needs without having to re-run an expensive multigroup processing code.

Collapsing can proceed with a built-in weighting function or with one provided by the user. If this weighting function is the same as the one used to generate the original multigroup cross sections, then the resulting collapsed cross sections will be exactly the same as those that would be obtained by generating the course group cross sections directly.

Most infinitely dilute quantities, $\langle\sigma_x\rangle^i$, (quantities which are derived assuming the element is present in low concentration) are collapsed in a straightforward manner by preserving reaction rates

$$\langle\sigma_x\rangle^I = \sum_{i\in I} \langle\sigma_x\rangle^i \phi_0^i \Big/ \sum_{i\in I} \phi_0^i \quad , \tag{1}$$

where

$$\phi_0^i = \int^i \phi_0(E)\,dE \tag{2}$$

is the resonance-smoothed weighting function.

Self-shielding factors, $f_x^i(T,\sigma_0)$, which adjust infinitely dilute cross sections to effective cross sections at temperature T and composition σ_0 are more difficult to collapse. The ability to preserve reaction rates and exactly collapse these f-factors depends on the ability to reproduce the fine group flux used in the original generation of the multigroup constants

$$\phi^i = \int^i \phi_0(E)/[\sigma_t(E,T)+\sigma_0]dE = \phi_0^i/[f_t^i(T,\sigma_0)<\sigma_t>^i+\sigma_0] \quad , \tag{3}$$

where

$$<\sigma_t>^i = <\sigma_f>^i + <\sigma_c>^i + <\sigma_e>^i \quad , \tag{4}$$

and

$$f_t^i(T,\sigma_0) = [f_f^i(T,\sigma_0)<\sigma_f>^i+f_c^i(T,\sigma_0)<\sigma_c>^i+f_s^i<\sigma_e>^i]/<\sigma_t>^i \quad . \tag{5}$$

The resulting exact collapsing algorithm for the capture, elastic, and fission f-factors is

$$f_x^I(T,\sigma_0)<\sigma_x>^I = \sum_{i\epsilon I} f_x^i(T,\sigma_0)<\sigma_x>^i\phi^i \Big/ \sum_{i\epsilon I} \phi^i \quad . \tag{6}$$

One f-factor, f_{tot}^i, is provided so that one can compute an effective diffusion coefficient for use in diffusion theory codes. This requires that the total cross section be weighted by the current ϕ_1 rather than the flux ϕ

$$\phi_1^i(E,\sigma_0,T) = \int^i \phi_0(E)/[\sigma_t(E,T)+\sigma_0]^2 dE$$

$$= \phi_0^i/\left\{[f_t^i(T,\sigma_0)<\sigma_t>^i+\sigma_0][f_{tot}^i(T,\sigma_0)<\sigma_t>^i+\sigma_0]\right\} \quad . \tag{7}$$

The final algorithm for collapsing $f_{tot}^i(T,\sigma_0)$ becomes

$$f_{tot}^I(T,\sigma_0)<\sigma_t>^I = \sum_{i\epsilon I} f_{tot}^i(T,\sigma_0)<\sigma_t>^i\phi_1^i \Big/ \sum_{i\epsilon I} \phi_1^i \quad . \tag{8}$$

Equations (6) and (8) can easily give 1% differences from weighting with just ϕ_0^i. One percent errors in these cross sections can lead to non-negligible effects on reactor parameters which justifies the added complexity of Eqs. (6) and (8).

In order to make MINX[4] (or any CCCC) cross section libraries available to a widely-used set of diffusion theory reactor design codes, CINX has been provided with optional output in the 1DX[5] and PERT-V[6] formats.

CINX running times on a CDC-7600 are relatively short. It takes 29 seconds to collapse a 240 group Pu-239 to 50 groups. (It takes MINX 2410 seconds to generate a 50-group Pu-239 from scratch!) It takes 64 seconds to combine 50-group, 101-isotope ISOTXS and BRKOXS files into the 1DX format.

The CINX code and LIB-IV[7] (an ENDF/B-IV based, 50-group, 101 isotope, MINX-generated, and tested library) are being distributed as a self-contained package by Brookhaven National Laboratory.

The result of this development effort is a convenient, easy-to-use CINX code that can exactly collapse multigroup cross sections in the CCCC format.

REFERENCES:

1. B. M. Carmichael, "Standard Interface Files and Procedures for Reactor Physics Codes, Version III," LA-5486-MS, Los Alamos Scientific Laboratory (1974).

2. C. R. Weisbin and R. J. LaBauve, "Specifications of a Generally Useful Multigroup Structure for Neutron Transport," LA-5277-MS, Los Alamos Scientific Laboratory (1973).

3. R. B. Kidman and R. E. MacFarlane, "CINX: Collapsed Interpretation of Nuclear X-Sections," LA-6287-MS Los Alamos Scientific Laboratory (April, 1976).

4. C. R. Weisbin, P. D. Doran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, J. E. White, and R. B. Kidman, "MINX, A Multigroup Interpretation of Nuclear X-Sections from ENDF/B," Los Alamos Scientific Laboratory, to be published.

5. R. W. Hardie and W. W. Little, Jr., "1DX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections," BNWL-954, Battelle Northwest Laboratory (March 1969).

6. R. W. Hardie and W. W. Little, Jr., "PERT-V, A Two-Dimensional Perturbation Code for Fast Reactor Analysis," BNWL-1162, Battelle Northwest Laboratory (September 1969).

7. R. B. Kidman and R. E. MacFarlane, "LIB-IV, A Library of Group Constants for Nuclear Reactor Calculations," LA-6260-MS, Los Alamos Scientific Laboratory (March 1976).