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LOS ALAMOS SCIENTIFIC LABORATORY
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A CODE FOR REDUCING

MANY-GROUP CROSS SECTIONS TO FEW GROUPS

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A CODE FOR REDUCING

MANY-GROUP CROSS SECTIONS TO FEW GROUPS

by

Ralph S. Cooper

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ABSTRACT

A code (ZOT) has been written which will produce few group neutron cross sections from many group sets based on a given flux spectrum or one computed for an infinite medium. The cross-section format is that of S_n transport theory including the possibility of upscattering in energy. The code is written in the Floco II system for use on the IBM 704.

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Note: In October 1962 this code will be rewritten for production use and compatibility with the IBM 7090. A Fortran version is also planned.

Few Group Cross Sections for Neutron Transport Calculations

While many-group cross sections are necessary for computing a large variety of problems with a single set of cross section parameters, it is often desirable to reduce the number of groups used for particular problems. Multidimensional S_n and diffusion codes are becoming available and are very time-consuming with many energy groups. Where many S_n one-dimensional problems must be run for parameter studies, temperature or perturbation effects, or when coupled to hydrodynamic codes, specially tailored few group cross sections would be advantageous.

George Bell has suggested (memo, July 3, 1958) recipes for collapsing many-group parameters assuming a many-group flux spectrum. This can be obtained from a single many-group calculation for the system or approximated by solving the infinite medium (space independent) equations.

A code (ZOT) has been written which will collapse groups according to a given flux spectrum or using a self-generated infinite medium flux, and the results of several test cases are given.

Equations:

k represents the few-group index, g the many-group index.

Σ will stand for $\displaystyle\sum_{g\ \text{in}\ k}$ unless otherwise noted.

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(1) Fission spectrum

$$x_k = \Sigma \; x_g$$

(2) Fission cross section, absorption cross section

$$\sigma_k^i = \frac{\Sigma \; \sigma_g^i \; \psi_g}{\Sigma \; \psi_g} \qquad \sigma^i = \nu\sigma_f \text{ or } \sigma_a$$

where $\sigma_a^g = \sigma_g^{tr} - \underset{\text{all } g'}{\Sigma} \; \sigma_{g \to g'}$ for SNG cross sections.

(3) Transport cross section

$$\sigma_k = \frac{\Sigma \; \psi_g}{\Sigma \; \psi_g/\sigma_g} \qquad \underline{\text{or}} \qquad \sigma_k = \frac{\Sigma \; \psi_g \; \sigma_g}{\Sigma \; \psi_g} \; ;$$

both options are available.

(4) Transfer cross section from group k' to group k

$$\sigma_{k' \to k} = \frac{\underset{g \text{ in } k}{\Sigma} \; \underset{g' \text{ in } k'}{\Sigma} \; \sigma_{g' \to g} \; \psi_{g'}}{\underset{g' \text{ in } k'}{\Sigma} \; \psi_{g'}}$$

These are sufficient to determine the new set. The elastic scattering (σ_{kk}) can be determined from the others by

$$(5) \quad \sigma_{kk} = \sigma_k - \left(\underset{k' \neq k}{\Sigma} \; \sigma_{k \to k'} \right) - \sigma_a^k \; .$$

Different cross sections may be computed for each region (i.e., core and reflector) separately, but a single velocity spectrum is used for a given problem, and this must be weighted by the total fluxes in each region. The region volumes are used as a measure of the total flux.

$$(6) \quad v_k = \frac{\left(\sum_r V_r \sum \psi_{g,r} \right)}{\left(\sum V_r \sum \psi_{gr}/v_g \right)} \quad .$$

The infinite medium fluxes (ψ^o) can be generated by

$$(7) \quad (\sigma_g - \sigma_{gg})\psi_g^o = x_g + \sum_{g' \neq g} \sigma_{g' \to g} \, \psi_{g'}^o \quad .$$

These are solved successively from the highest energy group until groups with non-zero up-scattering are reached, upon which the remaining equations are solved simultaneously.

General Description of the Code

The code is written for the Floco II assembly system and is intended to be fully compatible with the Floco II assembled SNG routines. The code accepts cross sections and input data on atom densities similar to S_n input and computes collapsed group parameters for the mixtures described for each spacial region. The code will accept flux spectra as input or will compute infinite medium fluxes[*]or can use the flux used in the preceding spacial region (mixture) regardless of its source. The volumes can be given directly or can be computed from the coordinates for planes, infinite cylinders, or spheres. The code assumes there has been sufficient

[*]only without upscattering in the present code.

size allotted to the up and down scattering in the output groups and will stop with an on-line comment if this is not true. The many-group set is divided into a few groups, each containing one or more of the original groups according to the wishes of the user. The input and output are printed off-line (on-line if ss #6 ↓) and the output fission spectrum, velocities, and cross sections are punched on-line, suitable for direct inclusion in the new S_n codes. (They may be used in the old SNG by placing 9 punches in cols. 3 and 21.) The code will normally average $(\sigma_g)^{-1}$ but will average σ_g if sense switch #1 is down. In either case, a comment will be printed describing which was done.

Results

18 group cross sections for graphite and water moderated systems were collapsed to 6 and 3 group sets with errors in k_{eff} of the order of 1 or 2%.

For example, a bare graphite moderated system with C/U = 300 was run with the old SNG code, using 18 groups collapsed to 6 and to 3.

# Groups	Flux Source	$\Delta k/k$	Iterations	Relative Time
18	--	(k = .9700)	73	1
6	18g SNG calc.	- .67%	130	.6
6	∞ medium ϕ	+ .80	130	.6
3	18g SNG	-1.15	130	.3
3	∞ medium ϕ	+1.89	130	.3

For new situations, one would want to do a single one-dimensional multigroup calculation to check the accuracy for the cases involved.

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Input

The input is divided into two parts: the parameters which precede the code and data which follow it.

Parameters

The parameters determine the sizes of storage blocks and are used in determining exits and loop lengths. Parameters are put on Floco cards, following a "load parameters" pseudo instruction (*0000S00, see Floco II manual). There are three sets labeled P00, G00, and K00, each requiring a load parameters instruction. All are fixed point numbers.

Position	Symbol	Definition
P01	ID	problem identification number
P02	R	no. of regions
P03	M	no. of mixtures + no. of elements
P04	W	volume specification
P05	N	no. of mixture specifications
G01	G	no. input groups
G02	h_t	position of σ_{tr}, as in SNG input
G03	h_s	position of σ_s
G04	h_ℓ	position of last σ in a group
G05	U	no. of groups with no-zero up-scattering

K01-K04 have similar meaning for the output cross sections. The equivalent of G05 is not needed for the output groups.

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W, Volume Specification

W	Meaning
0	volumes are supplied in WO data block.
1	planar distances of regions are supplied in WO data block; code will compute volumes $V = (r_{i+1} - r_i)$ and place them in WO data block.
2	cylindrical radii supplied in WO, code computes $V = (r_{i+1}^2 - r_i^2)$, etc.
3	spherical radii supplied, $V = (r_{i+1}^3 - r_i^3)$, etc.
4	volumes are not supplied; velocities are computed separately for each region.

Input Data

The data follow the code and are on Floco cards preceded by Floco "load data" pseudo-instructions (*0000S0). The order of the data blocks is immaterial.

Block	Description	Type	Number of Entries
CO	Group separation, a table giving the largest value of g in each output group.	fixed	K
FO	The flux source for each region 0 -- flux supplied 1 -- calculate ∞ medium flux 2 -- use flux from preceding region	fixed	R
F2	The weighting fluxes for each region	floating	GXR
NO	The mixture specifications, similar to the SNG input. For each region there is an identifying number, followed by the labels of the elements in that region.	fixed	N
MO	The atomic densities (x 10^{-24}) of the elements in the order given in NO. Zeros in the positions corresponding to region numbers in NO serve to delimit the regions.	floating	N

WO	Volume or radius input.	floating	R
SO	Input fission neutron spectrum.	floating	G
VO	Input group velocities	floating	G
PO	The input (and mixture) cross section block. The elements are numbered implicitly by the order in which they are placed in the input deck. The regions are labeled by consecutive numbers beginning with E + 1, as in the new (July, 1959) SNG input (DSN code).	floating	h_ℓ x GXR

Output

The output includes off-line (on-line if sense switch #6 is down) listing of all of the input blocks, descriptively labeled and of the mixture cross sections (in the PO block) and the mixture absorption cross sections. This is followed by a print of the output fission spectrum, velocities, absorption cross sections, and mixture cross sections.

The fission spectrum, velocities, and mixture cross sections for each region are punched in that order on separate cards (or blocks of cards), ready for direct insertion into the DSN code. Cards may also be used in the SNG code by putting nine punches in columns 3 and 19. Should trouble arise, one can obtain an input print by transferring to $(1016)_8$ and pressing start twice. One can obtain an on-line output print by putting sense switch no. 6 down and transferring manually to $(1017)_8$ and pushing start twice.

Operation

Deck Arrangement

The present deck (labeled 9-09-59) has all necessary loading and transfer cards in it. The three parameter cards follow ZOT card no. 001 and the data cards follow card no. 077. The ZOT deck should be preceded by an on-line identification card to identify the user on the off-line listing.

Running time -- $\leq$ 1 minute per case + readin time, unless there are greater than 10 upscattering groups.

Problem size -- for the 8K machine about $(4000)_{10}$ words are available for data. The largest block will be the input and mixture cross sections (P0) which will be h_ℓ x G x (E + R) numbers. Almost all problems can thus be done on the 8K (small) 704.

Stops -- the only programmed stops are for the cases where insufficient down or upscattering has been allowed in the output groups. The code will print an on-line comment and stop. One can then transfer to $(1016)_8$ to obtain an input print.

Sense switches -- Sense switch #1 down gives a linear (rather than an inverse) average of σ_g (transport).

Sense switch #6 down causes on-line printing of both input and output. An on-line print of the results can be obtained by transferring manually to $(1017)_8$ and pushing start twice (with SS #6 down).

Example

Consider an H_2O reflected, H_2O moderated sphere, where it is desired to reduce the Hansen-Mills 18 group cross sections to 3 groups. There are thus two regions with the following composition:

Atom density x 10^{-24}	Core	Reflector
H	.0663	.0668
O	.0332	.0334
U^{235}	1.288×10^{-4}	

Assume one wishes to compute the infinite median fluxes for the core and reflector compositions to use in weighting the 18 group cross sections and that the core and reflector radii will be supplied for weighting the velocities. The three output groups will contain 6, 9, and 3 input groups, respectively, starting from the high energy end. Parameter and data for the above problem follow on Floco coding forms and are included in the ZOT decks.

FLOCO 704

77	78	79	80	PROBLEM Example		
				PROGRAMMER	DATE	PAGE

Left block

C	P (2)	R (3)	S (4)	S (5)	X (6)	R (7)	S (8)	S (9)	REMARKS
9	*					P	0	0	load instruction
(10)								1	ID #
(19)								2	# regions
(28)								5	# elements and mixtures
(37)								3	volume spec.
(46)								7	
(55)									.
(64)						P	0	0	
9	*					G	0	0	load instruction
(10)						1	8		G
(19)								2	pos. of σ_g
(28)								3	pos. of σ_{gg}
(37)								8	pos. of last $\sigma_{g'g}$
(46)								0	# upscattering
(55)									
(64)						G	0	0	
9	*					K	0	0	
(10)								3	K
(19)								2	pos. of σ_k
(28)								3	pos. of σ_{kk}
(37)								5	last $\sigma_{k'k}$
(46)									
(55)									
(64)						K	0	0	
9	*					C	0		"load data"
(10)								6	
(19)							1	5	
(28)							1	8	
(37)									
(46)									
(55)									
(64)						0	C	0	

Right block

C	P (2)	R (3)	S (4)	S (5)	X (6)	R (7)	S (8)	S (9)	REMARKS
9	*					N	0		
(10)								4	1st region (core)
(19)								1	H
(28)								2	0
(37)								3	U^{235}
(46)								5	2nd region (re-flec.)
(55)								1	H
(64)								2	0 N 0 0
9	*					M	0		
(10)								0	mixture
(19)			.0	6	6	3			N_H
(28)			.0	3	3	2			N_O
(37)	.	00	0	1	2	8	8		N_U
(46)								0	mixture
(55)				.	0	6	6	8	
(64)				.	0	3	3	4	0 M 0
9	*					F	0		
(10)								1	⎰ fixed pt. flux-
(19)								1	⎱ source
(28)									
(37)									
(46)									
(55)									
(64)									0 F 0
9	*					W	0		
(10)						1	6	.	*radii
(19)		3	1	.	2	7			
(28)									
(37)				(no decimal point allowed in					
(46)				last column of a field)					
(55)									
(64)									

FLOCO 704

	C	OPERATION P R S	ADDRESS X R S	REMARKS		C	OPERATION P R S	ADDRESS X R S	REMARKS
0	9	*	S 0		0				
1	(10)				1	(10)			
2	(19)	This card followed by 18 group			2	(19)			
3	(28)	fission spectrum			3	(28)			
4	(37)				4	(37)			
5	(46)				5	(46)			
6	(55)				6	(55)			
7	(64)			0 S 0	7	(64)			
0	9	*	V 0		0				
1	(10)				1	(10)			
2	(19)				2	(19)			
3	(28)	This card followed by 18 group			3	(28)			
4	(37)	velocity set			4	(37)			
5	(46)				5	(46)			
6	(55)				6	(55)			
7	(64)			0 V 0	7	(64)			
0	9	*	P 0		0				
1	(10)				1	(10)			
2	(19)	This card followed by 18 group			2	(19)			
3	(28)	cross sections in the order, H,			3	(28)			
		0, U235							
4	(37)				4	(37)			
5	(46)				5	(46)			
6	(55)				6	(55)			
7	(64)				7	(64)			
0					0				
1	(10)				1	(10)			
2	(19)				2	(19)			
3	(28)				3	(28)			
4	(37)				4	(37)			
5	(46)				5	(46)			
6	(55)				6	(55)			
7	(64)				7	(64)			