Computer Code Abstracts

PARTI

1. Name or Designation of Program: PARTI (Pronounced "party").
2. Computer for Which Program is Designed and Others Upon Which it is Operable: Direct Couple IBM 7040-7094, CDC-6500.
3. Programming Language Used: Fortran IV.
4. Nature of Physical Problem Solved: PARTI is a group collapsing code which determines the optimum discrete representation of a variable for subsequent repetitive calculations.
5. Method of Solution: PARTI uses the results from an initial detailed calculation (such as a slowing down calculation for an energy-dependent flux application) and reduces the corresponding space and/or energy structure to an optimal few-interval and/or few-group representation in accordance with the minimization of an objective response function. This minimization is attained employing a method of steepest descent in piece-wise constant, non-convex, multidimensional phase space.
6. Restrictions on the Complexity of the Problem: PARTI will optimize the discrete representation of an arbitrary function of one or two independent variables. The present program storage allocation permits up to eighty nodes for each coordinate of a detailed representation and allows collapsing up to forty nodes for each coordinate of the reduced representation.
7. Related and Auxiliary Programs: None. However, PARTI may be considered to be an auxiliary program to almost any neutron diffusion theory or neutron transport program.
8. Typical Running Time: The running time is strongly dependent upon the number of groups treated and regularity of the function of interest. Running times of typical cases have seldom exceeded 10 sec.
9. Unusual Features of the Program: This is the only computer program known to the authors which performs group or mesh collapsing in an optimal sense.
10. Machine Requirements: 32K Core storage and a random number generator.
11. Operating System or Monitor Under Which Program is Executed: IBSYS (IBM-7904), SCOPE (CDC-6500).
12. Any Other Programming or Operating Information or Restrictions: A random number generator with the function name RANF (X) is used.
13. *References*:

[1]A. A. HARMS and N. J. McCORMICK, *Trans. Am. Nucl. Soc.*, **11**, 527 (1968).

[2]A. A. HARMS and A. L. BABB, *Trans. Am. Nucl. Soc.*, **12**, 143 (1969).

[3]A. A. HARMS, "Variable Phase-Space Neutron Transport Analysis," PhD dissertation, University of Washington (1969).

A. A. Harms

Dept. of Engineering Physics
McMaster University
Hamilton, Ontario, Canada

J. A. Stoddard

TRW Systems Group
One Space Park
Redondo Beach, California 90278

Received November 3, 1969

XSDRN

A Discrete Ordinates Spectral Averaging Code

1. Name of Code: XSDRN.
2. Computer for Which Code is Designed: XSDRN is designed to use computers in the IBM-360 series with a 512K byte directly addressable storage. A special version of the code is available which makes effective use of the bulk storage on the ORNL 360/75. (Present 123 group cross-section library tapes need the 512K byte storage for efficient execution, but could be made to operate on a smaller machine through various out-of-core storage capabilities.) No machine language programming is required.
3. Programming Language Used: The version of XSDRN for the IBM-360-65 uses IBM H-level Fortran and will execute directly on the 360/75. A version which makes use of the ~500K word bulk storage on the ORNL 360/75 needs one machine language routine.
4. Problems Solved: XSDRN uses the Nordheim integral treatment, narrow resonance, or infinite mass approximation to process resonance data on a master cross-section library and thus obtain microscopic fine-group cross sections for a nuclide. The code will then use these cross sections in an independent one dimensional calculation (slab, spherical, or cylindrical geometry) to solve for fluxes, eigenvalues, critical dimensions, etc., using discrete ordinates, diffusion, or an infinite

medium theory calculation. The fine-group fluxes thus obtained can then be used to collapse the fine-group cross-section data to a more tenable broad-group structure for use in several independent computer codes.

5. Method of Solution: The principal calculations performed by XSDRN (resonance calculation and flux calculation) both employ numerical finite-difference techniques. For the resonance calculation, this involves a Simpson's integration to solve for the collision density in the resonance range. The flux calculations employ a multigroup energy structure, an arbitrary spatial mesh and a discrete angular quadrature, all of which are used in the various integration and differencing schemes in the code.

6. Restrictions on the Complexity of the Problem: The principal restriction is the availability of adequate core storage to build required arrays. The code is flexibly dimensioned which means that array sizes are set for the *particular* problem *at* execution time. (Provisions are also available for storing certain large data arrays out-of-core, if need be.) No restrictions are placed on the number of fine energy groups, the number of broad energy groups, the number of upscatters, the number of downscatters, the number of space points, etc., except as they affect the total space needed for the problem.

7. Related and Auxiliary Programs: The master library tape for XSDRN is produced by XLACS. Cross-section tapes can be generated for ANISN, DOT, CITATION, ROD, or the EXTERMINATOR-II codes.

8. Typical Machine Time: (Times quoted are for the IBM 360/75). Resonance calculations: Typical running times have been on the order of one half to one minute per nuclide. Flux calculation: It is extremely difficult, if not impossible, to assign accurate times for the flux calculation, since it depends on number of energy groups, number of space points, geometry, calculational option, cross section order, angular quadrature, convergence criteria, and even on out-of-core storage allocation. A "typical" problem ($S_4 P_3$, 25 space points, 123 energy groups, cylinder, k-calculation, reduce cross sections, 4 resonance nuclides) generally runs ~10 to 12 min (total time). A fixed source calculation for the same system would take approximately the same time.

9. Unusual Features of the Program: The flexible dimensioning scheme employed by the code allows one to make optimal use of his core storage. A unique method of storing cross sections is employed which eliminates impossible and/or zero-transfer cross sections. Two extensive cross-section libraries are available—a 123-group and a 100-group library. The first library (123 groups) contains around 200 sets of data; the second library ~100 sets. The data on the first library was constructed by combining various sets of P_3 GAM-II data with 30-group P_0 THERMOS data. The second library has the GAM-II energy structure with one thermal group. Its data was primarily derived from ENDF/B values.

10. Status: This code is in production use at ORNL. Several options are planned for addition to the present package.

11. Machine Requirements: IBM-360/65 with ~90K words of directly-addressable core storage available for the program. The various calculational options require from four to thirteen input-output devices, depending on the problem. At least one device must be directly-accessible.

12. Operating System: IBM OS/360 with Fortran H compiler.

13. Programming Information: The program consists of ~80 subroutines on 6000 source cards. The program is presently used in a four-level overlay structure consisting of fourteen separate links. With this structure ~90K words are required on the IBM-360/65.

14. User Information: The code and report can be obtained through the Argonne Code Center at ANL and the Radiation Shielding Information Center (RSIC) at ORNL.

15. *Acknowledgment*: This work is based on work performed under U.S. Atomic Energy Commission Contract W-7405-eng-26.

16. *References*:

[1]N. M. GREENE and C. W. CRAVEN, Jr., "XSDRN: A Discrete Ordinates Spectral Averaging Code," USAEC Report ORNL-TM-2500, Oak Ridge National Laboratory.

[2]N. M. GREENE and R. Q. WRIGHT, "XLACS: Cross Section Production Package for XSDRN," Computing Technology Center (to be published).

N. M. Greene

Union Carbide Corporation, Nuclear Division
Computing Technology Center
Oak Ridge, Tennessee 37830

C. W. Craven, Jr.

Union Carbide Corporation, Nuclear Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

Received November 6, 1969
Revised December 5, 1969