KATRIN 1.0: THREE-DIMENSIONAL MULTIGROUP DISCRETE-ORDINATES TRANSPORT CODE

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<u>1. Program Name and Title:</u> KATRIN-1.0: Three-Dimensional Multigroup Discrete-Ordinates Transport Code.

<u>2. Computers and Operating Systems for Which Program is Available:</u> Intel-based PCs, Windows XP.

<u>3. Problem Solved:</u> The code KATRIN-1.0 solves the multigroup transport equation for neutrons and photons in 3D x, y, z and r, ϑ, z geometries. The scattering anisotropy can be treated in the P_L approximation. The adjoint solution of the problem can be also obtained. The principal application of the code is the solving of the deep-penetration transport problems, typical for radiation protection and shielding calculations. The fission problems (subcritical boundary value and k_{eff} problems) and problems with upscattering (the thermalization, photo-neutron problems, etc.) can be also solved.

A few standard types of boundary albedoes (vacuum, reflective, white, Lambert's low, periodic) can be used. The boundary spatially distributed isotropical and anisotropical sources, and volumetric internal isotropical source with given spectrum have been implemented. It is important to note that the spatial meshes used for presentation of the sources are independent from the meshes used for approximation of transport equation.

<u>4. Method of Solution:</u> Two variants of the second-order of accuracy adaptive weighted diamond difference (AWDD) scheme: a) standard and b) with iterative refinement of the weighting coefficients of the AWDD scheme in a cell (the IAWDD scheme) have been implemented in the code. The IAWDD scheme gives more accurate choice of the weighting coefficients of the WDD scheme in problems with large flux gradients, especially, in vacuum regions.

The P_1 synthetic acceleration (P_1SA) scheme for acceleration of inner iterations convergence, consistent with the WDD scheme has been implemented in the code. For solving the P_1SA system for acceleration corrections the cyclic symmetric ADI (SADI) method with adaptive refinements of eigenvalue bounds in solving heterogeneous problems is used.

The code works with symmetrical and asymmetrical angular meshes. A module that generates suitable quadrature meshes (ES_n type, Gauss-Chebychev product type, composite S_n type (the last quadrature can be used in the case when it is necessary to give more nodes in the desirable angular directions)) is included in KATRIN-1.0 code. The number of discrete-ordinates directions and the order of the P_L approximation can vary in energy groups. The code can produce output files those can be used as input data for solution treatment utilities (for example, by the post-processor KATRIF).

<u>5. Restrictions on the Complexity of the Problem:</u> The number of discrete ordinate directions, space intervals, energy groups and the order of the scattering anisotropy approximation are limited only by the computer storage available through the use of dynamic storage allocation. All calculations in PC-version of KATRIN-1.0 are performed with the double-precision arithmetic. The number of words needed for working arrays of the problem solved if no acceleration algorithm is used can be estimated by the following formula:

$$IJK\left[3J_L+4\right]+M\left(4IJ+2JK+2IK+J\right),$$

where I, J and K = number of spatial intervals in radial, circular and axial spatial variables, respectively; $J_L=(1+L)^2$ = number of angular flux moments; L = order of P_L approximation used; M = number of angular directions.

6. Typica1 Running Time: CPU time used is roughly proportional to the number of flux calculations: spatial mesh cells × directions × energy groups × iterations/group. It also depends on the order of the P_L approximation used. The possibility to continue calculation after an interruption (needed in calculation of large variants) is also implemented in the code.

7. Unusual Features of the Program: No.

8. Related and Auxiliary Programs: ARVES-2: the cross-section preprocessor (the package of utilities for operating with the cross-section files in the FMAC-M format). It includes utilities those are able:

a) to perform interface: ANISN format → FMAC-M format;

b) to make listing and perform consistency tests of cross-sections in the FMAC-M format;

c) to cut unused groups;

d) to generate the adjoint cross-section file in the FMAC-M format;

e) to collapse the cross-sections prepared in the FMAC-M format by given spectra to a file with less number of groups.

Input macroscopic cross-sections can be given both in the ANISN (or GIP) format for materials used or in the more economical FMAC-M format. Typical cross-sections libraries used are CONSYST/ABBN-93-2.A (coupled neutron and photon cross-sections), CASK, BUGLE-96, BGL1000, etc.

KATRIF: the postprocessor for KATRIN-1.0. This utility edits flux/source files and prepares input data for graphical software codes: GRAPHER-3.0 and SURFER-7.0 to display spectra for given spatial points (or material zones), and 1D and 2D both flux and response distributions for given spatial sections.

ROZ-6.5: the 1D predecessor of KATRIN-1.0.

KASKAD-S-2.0: the 2D predecessor of KATRIN-1.0.

9. Hardware Requirements: Code runs on Pentium PC equipped typically with 0.5-1.5 Gbytes of fast memory and 60-180 Gbytes of hard disk memory.

10. Programming Language(s): The Fortran 77 language standard is followed closely. The PC executables were created using the Compaq Visual Fortran 6.6A compiler.

11. Other Programming or Operating Information or Restrictions: In the code real, double-precision, integer and character arrays are stored separately. No EQUIVALENCE statement is used between variables of different types. So, the code can be easily compiled with the use of other modern Fortran compilers, Operating Systems and computers those support sufficiently large fast memory and data files.

12. References:

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A. M. Voloschenko and A. V. Shwetsov, "KASKAD-S-2.0 – two-dimensional discrete-ordinates neutron, photon and charged particles transport code," User's guide, Report No. 7-2-2000, *Keldysh Inst. of Appl. Math.,* Moscow, 2000 (in Russian).

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A. M. Voloschenko, S. V. Gukov and A. V. Shwetsov, "ARVES-2 - a package of utilities for operating with the FMAC-M format: a multigroup macroscopic cross-section format for discrete-ordinates transport codes," User's guide, Report No. 7-3-2000, *Keldysh Inst. of Appl. Math.,* Moscow, 2000 (in Russian).

13. Appendix: Code package includes the referenced manuals (both in Russian and in English), Fortran source, batch files for compile/link/run, executables, and sample problems input/output.