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THE CNCSN-2: ONE, TWO- AND THREE-DIMENSIONAL COUPLED NEUTRAL AND CHARGED PARTICLE DISCRETE ORDINATES CODE SYSTEM

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ABSTRACT

1. NAME AND TITLE

CNCSN-2: One, Two- and Three-Dimensional Coupled Neutral and Charged Particle SN Code System.

AUXILIARY CODES

KATRIN-2.5: Parallel three-dimensional neutral and charged particle transport code.

KASKAD-S-2.5: Two-dimensional neutral and charged particle transport code.

ROZ-6.6: One-dimensional neutral and charged particle transport code.

ARVES-2.5: Preprocessor for the working macroscopic cross-section FMAC-M format for transport calculations.

MIXERM: utility for preparing mixtures on the base of multigroup cross-section libraries in ANISN format.

CEPXS-BFP: A version of Sandia National Lab. multigroup coupled electron-photon cross-section generating code CEPXS, adapted for solving the charged particle transport in the Boltzmann-Fokker-Planck formulation with the use of discrete ordinate method.

SADCO-2.4: Institute for High-Energy Physics modular system for generating coupled nuclear data libraries to provide high-energy particle transport calculations by multigroup method.

KATRIF: Postprocessor for KATRIN code.

KASF: Postprocessor for KASKAD-S code.

ROZ6F: Postprocessor for ROZ-6 code.

ConDat 1.0: code for converting by the tracing algorithm the combinatorial geometry presentation to the bit-mapped one.

MCU Viewer: code for combinatorial geometry visualization.

Maplook: Script for SURFER to automate geometry visualization on the base of material maps given as atlas boundary (*.bna) files.

SYNTH: utility for construction of an approximate solution of the 3D transport equation in a vicinity of reactor pressure vessel by the synthesis method.

2. CONTRIBUTOR

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3. CODING LANGUAGE AND COMPUTER

Fortran 90, multicore PC/workstation under Windows XP/XP 64 Edition/Vista 64-bit.

4. PROBLEM SOLVED

KATRIN [1], KASKAD-S [2] and ROZ-6 [3] codes solve the multigroup transport equation for neutrons, photons and charged particles in 3D (x, y, z and r, ϑ, z), 2D (x, z, r, z and r, ϑ) and 1D (plane, spherical and cylindrical) geometries, respectively. The transport equation for charged particles can be solved with direct treatment of the continuous slowing-down (CSD) term; for 1D plane and spherical geometries the Bolzmann-Fokker-Plank equation can be solved with direct treatment both CSD and continuous scattering terms. The scattering anisotropy can be treated in the P_L approximation. The adjoint solution of the problem can be also obtained (for neutral particles only). The principal application is the solving of the deep-penetration transport problems, typical for radiation protection and shielding calculations. The fission problems (subcritical boundary value problem and k_{eff} problem), problems with upscattering (the thermalization problem, etc), electron-photon and hadron cascade problems can be also solved.

A few standard types of reflecting boundary conditions can be used. Several types of boundary and volumetric sources, including point anisotropic source (for x, y, z, r, ϑ, z and r, z geometries), point and line isotropic sources for 1D spherical and cylindrical geometries, respectively (for neutral particles only); boundary monodirectional source (with given spatial distribution in the perpendicular section of the beam) that is normally incident on the bottom of x, y, z, r, ϑ, z and r, z geometry regions, plane monodirectional source, volumetric distributed isotropic source with factorized energy dependence and boundary both isotropic and anisotropic sources with factorized spatial dependence, have been implemented. In solving problems with fission the volumetric fission source file can be generated or used as input volumetric fission source file. In solving hadron cascade transport problems the anisotropic spallation source file can be generated (or used as input anisotropic source file). It is important to note that the meshes used for presentation of the sources are independent from the mesh used for approximation of transport equation.

BOT3P-5.1 mesh generator [4] can be used as preprocessor. KASKAD-S and KATRIN codes can enter problem geometry from a file both in the 'matmap' and 'mixmap' formats, defined in the BOT3P-5.1 code manual [4]. In the 'matmap' format spatial zone dimensions, material map, spatial mesh and density factor are stored. In this case the original material mass conservation is supported globally for problem bodies. The 'mixmap' format stores the fine mesh boundary arrays, the material map distribution and the sequence of original material numbers, contained in meshes, where a few original materials are available, together with the related volume fractions for these meshes, so, the 'mixmap' format enables the material mass conservation locally with the use of the volume fraction method. If geometry data are entered from a file in the 'mixmap' format then KASKAD-S and KATRIN codes generate additional mixtures, if required, to maintain the mass of original materials conservation for every spatial cell.

ConDat converter [5] can be also used as preprocessor. ConDat code includes geometrical module NCG [6] of Monte Carlo MCU transport code [8] and is able to enter combinatorial geometry definition of problem geometry in terms of NCGSIM language [8], used by NCG. MCU Viewer [7] can be used to visualize and to test combinatorial geometry defined in terms of NCGSIM language that simplifies essentially preparing combinatorial geometry definition in solving real complicated geometry problems. To convert a combinatorial problem geometry form to a "bit-mapped" one and generate the problem geometry file in the 'mixmap' format, ConDat code uses the tracing algorithm [9] that is natural for geometrical module NCG of MCU code.

The possibility to calculate spectra/doses in a void outside KATRIN x, y, z and r, ϑ, z, and KASKAD-S r, z geometries is also implemented (for neutral particles only). Numerous printed edits of the results are available and output solution/source files can be written for subsequent analysis by postprocessors. Both KASKAD-S and KATRIN codes, and postprocessors KASF [2] and KATRIF [1] can generate the Atlas boundary files with the problem and material maps for given region section that can be used by SURFER™ to visualize the geometry entered before and (or) after transport calculation. A specially designed script Maplook [5] is available to automate geometry visualization.

ARVES-2.5: cross-section preprocessor (the package of utilities for operating with the cross-section file in FMAC-M format) [10] is included. It consists of utilities those are able:

a) perform interface: ANISN format (given in a binary or ASCII form) or GIP format (in a binary form) → binary FMAC-M format;
b) make listing and perform consistency tests of cross-sections in the FMAC-M format;
c) cut unused groups;
d) generate the adjoint cross-section file in the FMAC-M format;
e) transform the by particle type organized group sequence in the coupled cross-section file to by energy organized group sequence;
f) transform the cross-section file with direct treatment of the CSD term to the file with indirect treatment of this term;
g) collapse the cross-sections prepared in the FMAC-M format by given spectra to a file with less number of groups;
h) transform the binary form of the FMAC-M format to the ASCII one and vice verse.

MIXERM: utility for preparing mixtures with the use of binary cross-section libraries in ANISN format (with user-friendly input interface, similar to used in CONSYST) is also included. The current version of MIXERM is applicable for BUGLE96, BGL1000, BGL440 and CASK coupled neutron and photon problem-dependent cross-section libraries.

CEPXS-BFP [11, 12]: adapted version of Sandia National Lab. multigroup coupled electron-photon cross-section generating code CEPXS is available in the CNCSN. The following additional options, based on the "Monte-Carlo" option of CEPXS, have been implemented in CEPXS-BFP:
a) "Sn-CSD" option. In this case the stopping power at group boundaries is available in the cross-section file generated. So, it is expected that in S_n code used the CSD operator is treated directly, but the continuous-scattering operator is treated indirectly in the P_L approximation.
b) "Sn-BFP" option. In this case both the stopping power at group boundaries and restricted momentum transfer are available in the cross-section file. So, it is expected that in S_n code used both the CSD operator and continuous-scattering operator are treated directly.

Last implemented additional option is:
c) "Sn-indirect" option. It is nearly identical with standard option, used by ONEDANT-LD, but the header cards have been changed to make one's more convenient for the use by the cross-section preprocessor ARVES-2.5 that transforms cross-section matrices prepared in ANISN format to FMAC-M format.

SADCO-2.4 [13, 14]: Institute for High-Energy Physics modular system for generating the coupled multigroup cross-sections for protons, pions and neutrons in high-energy region (20 MeV< E <10 GeV), coupled with standard coupled neutron/photon multigroup cross-sections below 20 MeV, is also included in the CNCSN.

CNCSN-2 is the new release of the CNCSN system [15, 16].

5. METHOD OF SOLUTION

The second-order of accuracy adaptive weighted diamond difference scheme (AWDD scheme) [17, 18, 19, 20, 21] for spatial and angular variables is implemented. The AWDD scheme is also used for approximation the continuous slowing-down term in solving the charged particle transport problems [12].

The fourth-order of accuracy linear moments/quadratic continuous (LM/QC) [22] and third-order of accuracy linear discontinuous (LD) schemes in spatial variables are implemented for 1D and 2D *x-z* and *r-z* geometry case. A variant of the adaptive weighted LM/QC-weighted LD (AWLM/QC-WLD) scheme is available for 1D geometries case.
The P_1 Synthetic Acceleration (P_1SA) scheme [23, 24, 25, 26] for acceleration of inner iterations convergence, consistent with the WDD scheme, is implemented. For 1D geometries case the P_1SA scheme for acceleration of inner iterations convergence, consistent with the WLM-WLD scheme, is available. The consistent P_1SA scheme for acceleration of fission up-scattering iterations convergence in solving subcritical problems and thermal up-scattering iterations convergence with the use of the estimated by Fourier analysis spectrum shape function for homogenized problem is also implemented. For solving the P_1 system for acceleration corrections the direct through-computations, iterative cyclic ADI [23, 24] and splitting-up [25, 26] methods are used in 1D, 2D and 3D geometries, respectively.

Parallelization of KATRIN code is performed via a 2-D spatial decomposition in $x, y / r, \vartheta$ transverse section of the problem geometry, which retains the ability to invert the source iteration equation in a single sweep (the KBA algorithm). The solving of the P_1 system for acceleration corrections is also parallelized by performing the array of through-computation runs in parallel.

For point, linear and monodirectional sources the unscattered component of the flux is selected and treated by analytical formulas. The codes work both with symmetrical and asymmetrical angular meshes, modules those generates suitable quadrature meshes (ES_n type [17], Gauss-Chebychev and 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 direction)) is included in KATRIN. The number of discrete ordinates directions and the order of the P_L approximation can vary in energy groups.

To calculate spectra/doses in a void outside KATRIN or KASKAD-S geometry the last-flight algorithm is implemented (for neutral particles only).

To receive a fast estimation of the 3D transport equation solution in a vicinity of reactor pressure vessel, the synthesis method is implemented in the SYNTH utility [27].

6. RESTRICTIONS OR LIMITATIONS

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 codes are performed

with the double-precision arithmetic. The number of words needed for working arrays of the problem solved is available in the code abstracts.

7. TYPICAL RUNNING TIME

Central processor unit (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 transport codes included.

8. COMPUTER HARDWARE REQUIREMENTS

All codes of the package run on Intel Core 2 Duo or Core i7 PC equipped with 2.0-12.0 Gb RAM and 40-200 Gb HD memory under Windows XP/XP 64 Edition/Vista Ultimate 64-bit. The use of RAID 0 HD arrays to decrease total time of problem calculation is recommended.

9. COMPUTER SOFTWARE REQUIREMENTS

The Fortran 90 language standard is followed closely. The Intel Visual Fortran 11.0 compiler is recommended to make the PC executables. Parallelization of KATRIN code is performed using OpenMP 3.0. The Compaq Visual Fortran 6.6C compiler can be also used to make the PC executables for solving problems, which require the RAM memory volume < 2 Gb. No parallelization is available in this case. Some routines from IMSL library are used for estimation of spectral shape of acceleration corrections in outer iterations acceleration algorithm. Commercially available graphical software codes GRAPHER™ and SURFER™ are used to visualize geometry/results of calculations.

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11. CONTENTS OF CODE PACKAGE

Included are the referenced manuals, Fortran source, makefiles to compile/link, executables, and sample problems input/output.

12. DATE OF ABSTRACT

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