

DOORS 3: DISCRETE ORDINATES OAK RIDGE SYSTEM

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ABSTRACT

1. Program Name and Title: DOORS 3: Discrete Ordinates Oak Ridge System, Version 3. DOORS 3 is a code system of the following related programs:

<u>Program</u>	<u>Description</u>
TORT	Three-dimensional neutron/photon transport.
DORT	Two-dimensional neutron/photon transport.
ANISN	One-dimensional neutron/photon transport.
GBANISN	ANISN with "group band" option.
GRTUNC3D	3-D Uncollided flux and first collision source.
GRTUNCL	2-D Uncollided flux and first collision source.
FALSTF	Last collision source projection to point detector.
TORSED	Couple R-Z DORT to X-Y-Z TORT calculation.
TORSET	Couple primary TORT to secondary TORT calculation.
VISA	Prepare a TORSED input file from a DORT output file.
ALC	Material cross-section library maintenance.
GIP	Group cross-section preparation.
ISOPLOT	Display 2-D flux or response contours.
XTORID	Prepare 2-D flux slices from TORT for display in ISPLOT.
BNDRYS	Convert internal boundary flux to internal boundary source.
RTFLUM	Convert flux moment files between various formats.
JDOS	Script for performing calculations.
DRV	DOORS driver module called by JDOS.
CMP	Sandia National Lab. code system maintenance and update.
RSCORS	Sandia National Lab. subroutine library of graphical primitives.

2. Computer for Which Program is Designed and Other Machine Versions Available: DOORS 3 is available for Cray UNICOS, IBM AIX, Sun Solaris, Digital Unix, SGI IRIX, Hewlett Packard HP/UX and Linux computers.

3. Problem Solved: TORT calculates the particle flux or fluence due to particles incident upon the system from extraneous sources or generated internally as a result of interaction within two- or three-dimensional geometry systems, and DORT is used in one- or two-dimensional geometry systems. The principle application is to the deep-penetration transport of neutrons and photons. Reactor eigenvalue problems can also be solved. Numerous printed edits of the results are available, and results can be

transferred to output files for subsequent analysis. Ray-effect anomalies may practically be eliminated using the GRTUNCL or GRTUNCL3D program. Large models may be solved in a bootstrap fashion or smaller volumes may be studied independently for perturbations, through use of the TORSED and TORSET coupling programs.

ANISN solves the one-dimensional Boltzmann transport equation for neutrons or gamma rays in slab, spherical, or cylindrical geometry. GBANISN is based on ANISN but was modified to allow randomizing of multiband fluxes within a group at all interfaces between dissimilar materials and a reduction in the number of outer iterations for problems involving neutron upscatter into higher energy groups. GBANISN requires fewer outer iterations than ANISN by performing "inner iterations" over energy groups within a "band" and converging those groups before moving to the next band. These "inner" iterations slightly resemble outer iterations in ANISN. Thus, a calculation with upscatter and no fission can be solved with one traditional outer iteration.

4. Method of Solution: The Boltzmann transport equation is solved using the method of discrete ordinates to treat the directional variable and weighted finite-difference methods, in addition to Linear Nodal and Linear Characteristic methods in TORT, to treat spatial variables. Energy dependence is treated using a multigroup formulation. Time dependence is not treated in the current release. Starting in one corner of a mesh, at the highest energy, and with starting guesses for implicit sources, boundary conditions and recursion relationships are used to sweep into the mesh for each discrete direction independently. Integral quantities such as scalar flux are obtained from weighted sums of the directional results. The calculation then proceeds to lower energy groups, one at a time.

Iterations are used to resolve implicitness caused by scattering between directions within a single energy group, by scattering from an energy group to another group previously calculated, by fission, and by certain types of boundary conditions. Methods are available to accelerate convergence of both inner and outer iterations. Anisotropic scattering is represented by a Legendre expansion of arbitrary order, and methods are available to mitigate the effect of negative scattering source estimates resulting from finite truncation of the expansion. Direction sets can be biased, concentrating work into directions of particular interest. Fixed sources can be specified at either external or internal mesh boundaries, or distributed within mesh cells.

A Direction Parallel (DP) multitasking option, which concurrently sweeps each row in all directions within an octant, is available for solving the Linear Nodal method equations in TORT on UNICOS Cray platforms. A pthreads version of TORT is also available, and work is progressing on a combined MPI-pthreads version.

5. Restrictions on the Complexity of the Problem Solved: External forces and nonlinear physical effects cannot be treated. Penetration through large, non-scattering regions may become inaccurate due to ray effects. Problems with scattering ratios near unity or eigenvalue calculations with closely spaced eigenvalues may be quite time-consuming. Flexible dimensioning is used throughout so that no fixed limits on group, problem size, etc., are applicable.

6. Typical Running Time: Central processor unit (CPU) time used by the flux sweep is roughly proportional to the number of flux calculations: spatial mesh cells * directions * energy groups * iterations/group. Times for running all test cases in the package range from about 1 hour on an IBM RS/6000 Model 590 to several hours on slower machines.

7. Unusual Features of the Program:

Machine resource requirements are determined from the user input of model parameters. Small models may then be analyzed on machines with small memory and small unused disk space availability, while large detailed models run best on fast machines with large memories and multiple gigabytes of free disk space. The programs will also attempt to configure themselves to run within the user-specified amount of memory.

8. Related and Auxiliary Programs: DOORS is a code system of related programs as shown above. The CMP package, developed by Sandia, is used for packaging the DOORS 3 software distribution, allowing for a complete package or an updates-only distribution. CMP, built during the software installation by the user, is then used to build the other programs. ALC is a utility program for preparing an ANISN cross section library. GIP is used to process ANISN cross section libraries and create a group ordered cross section library for use with ANISN/GBANISN, DORT, TORT, and other programs. GRTUNCL and GRTUNCL3D calculate uncollided fluxes and write a first collision source file for use with DORT and TORT, respectively. When large models can be represented as a series of smaller models coupled geometrically, the VISA and TORSED programs may be used to couple an R-Z DORT calculation to an X-Y-Z TORT calculation, while TORSET is used to couple separate X-Y-Z TORT calculations. Coupling occurs through the use of angular boundary sources at the coupling interfaces. ISOPLOT provides flux or other user-defined response contours in a two-dimensional plane. XTORID is used to prepare two-dimensional data for use with ISOPLOT from the TORT three-dimensional data. The ISOPLOT graphics are prepared using the RSCORS subroutine library developed by Sandia. The JDOS script and DRV program provide a useful capability to stack input data for all the programs necessary in a calculation sequence. FALSTF provides a semi-analytic calculation of the last collision source projection to point detectors. The BNDRYS and RTFLUM utilities are included in the DOORS 3 distribution as legacy tools.

9. Status: DOORS has been rigorously tested on Cray and IBM, and has been installed on several other Unix systems. The Cray version runs under UNICOS version 8.0.3 using the CFT77 compiler version 6.0.4.10. Library calls are made to the standard UNICOS library to provide time, date, etc. DOORS was also tested on the following systems:

Cray Unicos 8.0.3, cft77 6.0.4.10 and Cray J90 Unicos 9.2.0.03, f90 3.0.1.3
IBM RS/6000, AIX 4.2, XLF 3.2.2.3 and later
DEC Alpha 3000, Digital UNIX V3.2G - Worksystem Software (Rev. 62),
Digital Fortran Version 4.
SGI IP22, IRIX 5.3, F77 Ver 4.0.2
Sun SparcStation 20, OS5.6, SUN FORTRAN 77 Ver 4.2
HP 9000/715, HP-UX 10.20, HP Fortran 77 Version B.10.20
PC under RedHat 5 Linux with f2c Ver1 19970805 and gcc Ver 2.7.2.3

10. References: (included in Doc/pdf subdirectory as PDF files)

W. A. Rhoades and D. B. Simpson, "The TORT Three-Dimensional Discrete Ordinates Neutron/Photon Transport Code," ORNL/TM-13221 (October 1997).

R. L. Childs, W. A. Rhoades, "Theoretical Basis of the Linear Nodal and Linear Characteristic Methods in the TORT Computer Code," ORNL/TM-12246 (January 1993).

J. O. Johnson, the DORT section of "A User's Manual for MASH 2.0 - A Monte Carlo Adjoint Shielding Code System," ORNL/TM-11778/R2 (March 1999).

W. W. Engle, Jr., "ANISN, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering," K-1693 (March 1967).

W. W. Engle, Jr., M. A. Boling, and B. W. Colston, "DTF-III, A One-Dimensional, Multigroup Neutron Transport Program," NAA-SR-10951 (March 1966).

R. L. Childs and D. E. Cullen, "GROUPBAND-ANISN: A Code to Perform Multiband Calculations," Informal Notes (June 1994).

RSICC, "Input Modifications Required for ANISN and GBANISN" (July 1998).

W. A. Rhoades and M. B. Emmett, "DOS: The Discrete Ordinates System," ORNL/TM-8362 (September 1982).

R. A. Lillie, the GRTUNCL3D section of "A User's Manual for MASH 2.0 - A Monte Carlo Adjoint Shielding Code System," ORNL/TM-11778/R2 (March 1999).

R. L. Childs, "GRTUNCL: First Collision Source Program," ORNL Informal Notes (1982).

R. L. Childs, "The FALSTF Last-Flight Computer Program," ORNL/TM-12675 (January 1996).

W. A. Rhoades and D. B. Simpson, "Splicing and Bootstrapping Methods for DORT/TORT-to-TORT Coupling," ORNL/TM-13350 (to be published).

C. O. Slater, "The XTORID and ISPL3D Codes for Plotting TORT Activities," ORNL Internal Memo (March 25, 1996).

W. A. Rhoades, "The ALC1 Program for Cross-Section Library Management," ORNL/TM-4015 (December 1972).

11. Hardware Requirements: The software will install and run on most Unix workstations presently in use. Small problems may be calculated with just a few megabytes of memory available to the user, while larger or more detailed models may require 32 or greater megabytes of memory. If sufficient memory is not available to store all model data in memory at once, the programs will attempt to calculate one group in memory at a time, followed by modes in which several blocks in memory at a time are analyzed with or without the I/O of data used for acceleration.

12. Programming Languages: Over 99 percent of the software is written in Fortran, with the remainder being C language utilities. The software has recently been modified to use the `date_and_time` subroutine available in the Fortran 90 standard, but Fortran 77 substitutes are provided by the C utilities provided.

13. Operating System: The operating systems used for testing the software are listed in section 9 above. More recent versions of each operating system are expected to be satisfactory for installing and running the programs.

14. Other Programming or Operating Information or Restrictions: As distributed, full optimization of the programs is not provided. Successful optimization is very compiler version dependent. Since the developers do not have access to each of the combinations of vendor hardware, operating system, and compiler version, successful full optimization is left to the user.

15. Names and Affiliations of Author or Contributor: There have been many authors and contributors to the development of this software over many years, and they are too numerous to list here. Many of the names are provided in the references above and with the software documentation provided with the distribution. Current developers include Yousry Azmy, Ed Blakeman, and Dave Simpson, all members of the Nuclear Analysis and Shielding section of the Computational Physics and Engineering Division at Oak Ridge National Laboratory.

16. Material Available: A compact disk containing the program software, documentation, and test problem output is available from the Radiation Safety Informational and Computational Center at Oak Ridge National Laboratory.

17. Keywords: DISCRETE ORDINATES; NEUTRON; GAMMA-RAY; MULTIGROUP; ADJOINT; SPHERICAL GEOMETRY; SLAB; CYLINDRICAL GEOMETRY; ONE-DIMENSION; TWO-DIMENSIONS; THREE DIMENSIONS; COMPLEX GEOMETRY; WORKSTATION.

18. Sponsor: There have been different sponsors in the past for development of the software, and these are noted in the documentation. The current sponsor of continued development of the software is from in-house funding, while some development is provided by support to another DOE laboratory.