GRTUNCL3D: A Three-Dimensional XYZ Geometry First Collision Source and Uncollided Flux Code.

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ABSTRACT

1. **Program Name and Title:** GRTUNCL3D: A Three-Dimensional XYZ Geometry First Collision Source and Uncollided Flux Code.

2. **Computer for Which Program is Designed and Other Machine Versions Available:** GRTUNCL3D was specifically written for an IBM RS/6000 workstation. Versions are available for Cray, Sun, DEC, and Hewlett Packard platforms and for PC's operating under Linux.

3. **Problem Solved:** GRTUNCL3D helps to mitigate anomalous results called "ray effects" that occasionally occur in discrete ordinates radiation transport calculations when isolated point sources exist in weakly scattering media. GRTUNCL3D generates energy and angular (moments) dependent first collision source distributions on three-dimensional XYZ geometric spatial meshes due to one or more energy and/or angular dependent radiation point sources for subsequent input to the three-dimensional discrete ordinates radiation transport code TORT. Both forward and adjoint problems with or without fission may be treated. GRTUNCL3D also generates energy and spatially dependent uncollided fluxes. If required, energy and angular (moments) dependent uncollided fluxes may be generated. No restriction is placed on source location, i.e., the radiation sources may be located anywhere, either inside or outside of the transport geometric model.

4. **Method of Solution:** Since TORT is able to perform calculations on a multilevel discontinuous mesh, i.e., a geometric model in which the number of mesh cells in each row and the number of rows in each plane may vary, GRTUNCL3D was written to generate uncollided flux and first collision source distributions for XYZ discontinuous meshes. GRTUNCL3D employs a semi-analytic technique to estimate the average uncollided flux and first collision source moments within each TORT fine mesh cell. The average uncollided fluxes are estimated by performing a ray trace between each radiation source point and each fine mesh cell center to obtain the number of mean-free-paths along the "source-mesh cell center ray". The average first collision source moments within each cell are then obtained by folding the uncollided fluxes with Legendre scattering coefficients

and modified spherical harmonics evaluated at the directions associated with the "source-mesh cell center ray".

5. **Restrictions on the Complexity of the Problem:** Volumetric radiation sources, e.g., photon decay sources must be approximated using many point sources. In most cases, first collision sources generated from these point sources are concentrated in the original source volume resulting in "ray effects" from the first collision sources. In addition, all point source locations must be common to all reflected and/or periodic spatial boundaries.

6. **Typica1 Running Time:** Typical running times on an IBM RS/6000 MODEL 590 vary between 1 and 5 milliseconds per ray trace, i.e., approximately 1 to 5 milliseconds times the product of the number of fine mesh cells and source points. (In most cases, I/O occupies 10 to 50 % of actual wall clock time).

7. **Unusual Features of the Program:** To simplify the ray tracing procedure employed in GRTUNCL3D, a regular coarse mesh based on material changes is constructed from the discontinuous fine mesh. A simple scheme of cell subdivision coupled to individual cell balance is employed for cells located close to sources or containing sources and for cells that are "optically thick" (in terms of mean-free-paths) to provide improved estimates of the average uncollided flux and first collision source moments within these cells. Because of this scheme, the inverse distance squared problem associated with point sources located inside fine mesh cells is avoided. In addition, GRTUNCL3D performs a system balance to aid the user in determining fine mesh adequacy, it dynamically allocates all memory as needed, and finally, it obtains many of its control parameters and all of the geometry data from the TORT input file thereby eliminating any duplication of input data.

8. **Related and Auxiliary Programs:** GRTUNCL3D is part of the DOORS 3.3 code system package which is available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory.

9. **Status:** GRTUNCL3D was originally developed to be part of the MASH v2.0 code system (see references) released in May 1999. (However, distribution of the MASH code system is restricted). Testing of GRTUNCL3D was completed in December 1998. Testing in a production environment is ongoing.

10. **References:** R. A. Lillie, "GRTUNCL3D: A Discontinuous Mesh Three-Dimensional First Collision Source Code," Proc. of 1998 ANS RP&S Div. Topical Conf.: *Technologies for the New Century*, Nashville, TN (1998).

    "DOORS 3.2, One, Two, and Three Dimensional Discrete Ordinates Neutron/Photon Transport Code System," CCC-650, RSIC Computer Code Collection, Oak Ridge National Laboratory (1998).

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

J. O. Johnson, Ed.,"A User's Manual for MASH v2.0 – A Monte Carlo Adjoint Shielding Code System", ORNL/TM-11778/R2 (May 1999).

11. **Hardware Requirements:** For most problems, 8 megabytes of memory should be more than sufficient. However, since both the uncollided flux and first collision source moment files are generally very large and at least one of these files must exist simultaneously in both sequential and direct access form, many problems may require upwards of 10 or more gigabytes of disk "online" storage.

12. **Programming Language(s):** Although GRTUNCL3D has been successfully compiled with Fortran 77 (extended) and C compilers on Cray, IBM, Sun, DEC, and Hewlett Packard workstations and on PC's running Linux, it is recommended that a Fortran 90 compiler be used.

13. **Operating System:** GRTUNCL3D is operational on Cray (Unicos), IBM (AIX), Sun (Solaris), DEC (Digital Unix), Hewlett Packard (HP-ux), and Intel x86 (Linux).

14. **Other Programming or Operating Information or Restrictions:** Many of the I/O routines, some of the auxiliary routines, and all of the C memory management routines in GRTUNCL3D are contained in the DOORS 3.3 code system. These routines are located in a library called **libtort.a** that is produced when either TORT or the entire DOORS 3.3 code system is built. This library must be available when GRTUNCL3D is compiled.

15. **Name and Affiliation of Author or Contributor:** R. A. Lillie, Oak Ridge National Laboratory, Oak Ridge, TN 37831, arl@ornl.gov, (865) 574-6083.

16. **Material Available:** None. The software package and all documentation must be obtained through the Radiation Safety Information Computational Center (RSIC), (http:/www-rsicc.ornl.gov/) Oak Ridge National Laboratory, Oak Ridge, TN 37831.

17. **Category:** **J.** Gamma Heating and Shield Design

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