Computer Code Abstracts

The Integrated TIGER Series (ITS) of Coupled Electron/Photon Monte Carlo Transport Codes

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1. Program Identification: The integrated TIGER series (ITS) of coupled electron/photon Monte Carlo transport codes.[1]

2. Function: The TIGER series of time-independent coupled electron/photon Monte Carlo transport codes is a group of multimaterial, multidimensional codes designed to provide a state-of-the-art description of the production and transport of the electron/photon cascade. The codes follow both electrons and photons from 1.0 GeV down to 1.0 keV, and the user has the option of combining the collisional transport with transport in macroscopic electric and magnetic fields of arbitrary spatial dependence. Source particles can be either electrons or photons. The most important output data are (a) charge and energy deposition profiles, (b) integral and differential escape coefficients for both electrons and photons, (c) differential electron and photon flux, and (d) pulse-height distributions for selected regions of the problem geometry. The base codes of the series differ from one another primarily in their dimensionality and geometric modeling. They include (a) a one-dimensional multilayer code, (b) a code that describes the transport in two-dimensional axisymmetric cylindrical material geometries with a fully three-dimensional description of particle trajectories, and (c) a general three-dimensional transport code that employs a combinatorial geometry scheme. These base codes were primarily designed for describing radiation transport for those situations in which the detailed atomic structure of the transport medium is not important. For some applications, it is desirable to have a more detailed model of the low energy transport. The system includes three additional codes that contain a more elaborate ionization/relaxation model than the base codes. Finally, the system includes two codes that combine the collisional transport of the multidimensional base codes with transport in macroscopic electric and magnetic fields of arbitrary spatial dependence.

3. Method of Solution: ITS is based primarily on the ETRAN system,[2] which combines microscopic photon transport with a macroscopic random walk for electron transport. Electron transport treats energy-loss straggling, elastic scattering, and impact ionization, as well as the production of knock-on electrons, continuous bremsstrahlung radiation, annihilation radiation, Auger electrons, and fluorescence photons. Photon transport treats photoionization, incoherent scattering, and pair production, along with the generation of the corresponding secondary particles. Where macroscopic field transport is involved, a fourth- to fifth-order Runge-Kutta algorithm is used to integrate the Lorentz force equations. Every output quantity is followed by the best estimate of its statistical standard error. The heart of ITS is the Monte Carlo program file. This file was obtained by integrating the eight member codes in such a way as to minimize the repetition of coding that is common to two or more of these codes. Each of the eight member codes will run on the machines of at least four major vendors. The free-format input scheme is based on a set of order-independent descriptive keywords that make maximum use of defaults and internal error checking. Flexibility of construction permits the more sophisticated user to tailor the codes to specific applications and to extend the capabilities of the codes to more complex applications.

4. Related Material: Options are available for plotting the problem geometry in the three-dimensional codes and for plotting electron trajectories in the codes that allow macroscopic field transport. In order to implement this capability, three external plot routines must be modified to call local plot utilities.

5. Restrictions: The machine must have the capability for a word size of at least 60 bits for the real variables. Memory requirements are controlled through the use of Fortran 77 PARAMETER statements to dimension arrays. When running the more complex member codes on machines having limited fast memory, it may be necessary to reduce memory allocations to fit problem requirements by modifying the PARAMETER statements. Similarly, it may be necessary to increase memory allocations for very complex problems.

6. Computers: The system has been tested on the Cray-1, CYBER-76/CDC-7600, VAX-11/780 (double precision), and IBM-3081 (double precision). Use of American National Standards Institute's (ANSI) Fortran 77 should facilitate installation on other machines as well.

7. Running Time: Because run time is a strong function of machine selection, code selection, option selections, and problem details, there is no typical time. As an example, however, the calculation of a one-dimensional energy deposition profile in graphite for normally incident 1.0-MeV electrons required <1.5 s per 100 primary histories on the CYBER-76.

8. Programming Language: Fortran 77 (ANSI X3.9-1978).

9. Operating System: CTSS/COS (CRAY), SCOPE (CDC/CYBER), VMS (VAX), and OS/MVT (IBM).

10. Machine Requirements: no special hardware requirements.
11. Material Available: ITS is disseminated through the Radiation Shielding Information Center at Oak Ridge National Laboratory. In addition to documentation and the input and output from sample problems, the package includes the four basic elements of the system:
    1. XDATA: the electron/photon cross-section data file
    2. XGEN: the cross-section generation program file
    3. ITS: the Monte Carlo program file
    4. UPEML: a machine-independent UPDATE emulator.
12. Acknowledgment: This work was sponsored by the U.S. Department of Energy.
13. *References:*

[1]J. A. HALBLEIB and T. A. MEHLHORN, SAND 84-0573, Sandia National Laboratories (Nov. 1984).

[2]M. J. BERGER and S. M. SELTZER, "Computer Code Collection," CCC-107, Radiation Shielding Information Center, Oak Ridge National Laboratory (June 1968).

TEMPS

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1. Program Name and Title: TEMPS, The Evaluation of the One-Group Time-Dependent Neutron Transport Flux in Infinite Media.
2. Description of Problem Solved: The code numerically determines the scalar flux as given by the one-group neutron transport equation with a pulsed source in an infinite medium. Standard plane, point, and line sources are considered as well as a volume source in the negative half-space in plane geometry. The angular distribution of emitted neutrons can either be isotropic or monodirectional (beam) in plane geometry and isotropic in spherical and cylindrical geometry. A general anisotropic scattering kernel represented in terms of Legendre polynomials can be accommodated with a time-dependent number of secondaries given by $c(t) = c_0(t/t_0)^\beta$ where $-1 < \beta < \infty$. The code is designed to provide the flux to a high degree of accuracy (4 to 5 digits) for use as a benchmark to which results from other numerical solutions or approximations can be compared.
3. Method of Solution: A semianalytic method of solution is followed. The main feature of this approach is that no discretization of the transport or scattering operators is employed. The numerical solution involves the evaluation of an analytical representation of the solution by standard numerical techniques. The transport equation is first reformulated in terms of multiple collisions with the flux represented by an infinite series of collisional components. Each component is then represented by an orthogonal Legendre series expansion in the variable x/t where the distance x and time t are measured in terms of mean-free-path and mean-free-time, respectively. The moments in the Legendre reconstruction are found from an algebraic recursion relation obtained from a Legendre expansion in the direction variable μ. The multiple collision series is evaluated first to a prescribed relative error determined by the number of digits desired in the scalar flux. If the Legendre series fails to converge in the plane or point source case, an accelerative transformation, based on removing the singular portion of the flux (near the wave front), is applied. The scattering kernel

$$g(\mu' \to \mu) = \frac{L+1}{2^L}(1 \pm \mathbf{\Omega}\cdot\mathbf{\Omega}')^L$$

is supplied to test the anisotropic scattering option. In addition, fission is accommodated in the isotropic scattering component.
4. Related Material: No additional programs are required other than a plotting routine. A plot file can be generated in a format compatible to standard plotting packages.
5. Restrictions: The number of desired flux calculations, anisotropy of the scattering kernel, and computational accuracy are limited only by the computer storage available through the use of dynamic storage allocation. The largest time t allowed is limited by the greatest floating point number allowed according to

$$c_0(t/t_0)^\beta t/(1+\beta) < \text{largest floating point number}\ .$$

For $x/t \cong 1$ and a beam source, the Legendre series may not converge to the accuracy desired as a result of its poor representation at discontinuities.
6. Special Features of Program: The Legendre flux moments can be stored and read from the stored file to avoid unnecessary recalculation.
7. Computers: The code was developed on a CYBER 175 and is currently being modified for a VAX-11/780.
8. Running Time: The computational time required is problem dependent and therefore cannot be easily specified. As an example, consider a case where the flux is desired to four-place accuracy at 23 time points and 5 space points for an isotropic scattering kernel. The computational time for this case is <2.5 s on a CYBER-175 or ~0.012 s per time and space point.
9. Machine Requirements: None.
10. Programming Language: FORTRAN IV.
11. Operating System: NOS BE CDC/CYBER 175.
12. Additional Programming Information: The code is written in a modular format with 15 subroutines and ~1200 lines of coding.
13. Material Available: The code and documentation may be obtained from the Argonne Software Center, Argonne National Laboratory, or from the author.
14. *Acknowledgment*: This work was partially completed under the AFOSR contract #S-4-77486.
15. *Reference:*

[1]B. D. GANAPOL, *Proc. Int. Mtg. Advances in Nuclear Engineering Computational Methods*, Knoxville, Tennessee, April 9–11, 1985, p. 696, American Nuclear Society (1985).