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cessors are used. However, even with the limited amount of data, it can be seen that efficiency is nearly constant after 200 000 histories. Figure 1 also shows that a considerable efficiency in parallel computing can be obtained even for problems of moderate size.

In conclusion, our experience with ITS and the distributed memory parallel environments suggests that the conversion from a strictly serial implementation to one which uses the full resources of the machine is achievable. Results show that a good degree of speedup can be attained by distributing a single problem across all of the nodes. Our batch partitioning method appear as a very efficient parallel approach to the solution of large Monte Carlo transport problems. Parallel simulations show that one can tackle large problems with a conceptually simple load balancing scheme coupled with nodes that have sufficient computational power as well as memory.

1. J. A. HALBLEIB, R. P. KENZSEK, G. D. VALDEZ, S. M. SELTZER, M. J. BERGER, "The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes – ITS Version 3.0," *IEEE Trans. Nucl. Sci.*, **39**, 1025 (Aug. 1992).

2. "IBM AIX PVMe User's Guide and Subroutine Reference: Release 3.1," IBM, Poughkeepsie, NY (Dec. 1994).

3. V. S. SUNDERAM, "PVM: A Framework for Parallel Distributed Computing," *Concurrency: Prac. Exper.*, **2**, *4*, 315 (1990).

4. Physics of ETRAN and ITS Electron-Photon Monte Carlo Codes, *Stephen M. Seltzer (NIST), invited*

INTRODUCTION

The algorithms and cross sections in the Monte Carlo code ETRAN (Refs. 1, 2, and 3) used for the calculation of coupled electron-photon transport in extended media serve also as the physics engine in the ITS (Integrated Tiger Series) code,[4] which provides a much more elaborate geometrical treatment. In turn, relevant parts of the ITS code have been incorporated into a recent version of the MCNP code[5] to furnish treatment of electron transport. Our improvements to the model tend to proceed from implementation in ETRAN to ITS and then others.

The code was intended to be of general purpose for the calculation of a wide variety of quantities, including all generations in the electron-photon cascade in the energy region from 100 GeV to 1 keV. In an effort to make use of the most accurate cross-section information available, much of the sampling is done from numerical distributions rather than from approximation formulas. This brief overview merely outlines the methods used; further details and references can be found in earlier papers of Berger[6–8] and Seltzer.[2,3]

ELECTRON TRANSPORT

Electrons (and positrons) follow a condensed-history random walk that is comprised of a series of path segments in each of which many elastic and inelastic Coulomb interactions occur. The net energy loss and the net angular deflection for each segment are sampled from multiple-scattering distributions in a scheme classified by Berger[6] as complete-grouping, class 1. The net electronic (collision) energy loss is sampled from the Landau[9] energy-loss straggling distribution, with theoretical and empirical modifications[2,3] of its width for the smaller path lengths. Radiative energy losses are sampled individually from bremsstrahlung production cross sections[10] derived from critically evaluated high-energy theory and exact phase-shift calculations for low electron energies. The energy losses are consistent with the mean energy loss from stopping-power evaluations that have become an industry standard.[11] The net angular deflection is sampled from the exact Goudsmit-Saunderson[12] distribution, based on single elastic-scattering cross sections derived from a combination of high-energy theory and exact phase-shift calculations.

The production of secondary radiation is sampled from relevant cross-section information: the generation of bremsstrahlung photons from the same cross sections; differential in emitted photon energy, as for the radiative energy loss; and the intrinsic bremsstrahlung emission angles from analytical bremsstrahlung theory; the generation of knock-on electrons from the Møller cross section; the generation of characteristic X rays and Auger electrons from cross sections for electron-impact ionization (K shell only for current ETRAN versions, but all shells, including complete atomic relaxation, for ITS); and the generation of annihilation quanta from two-photon positron annihilation at rest (annihilation in flight is not presently implemented). An unbiased weighting scheme allows for the sampling of bremsstrahlung photon and characteristic X-ray histories in excess of their natural production rate to help reduce the statistical fluctuations in the photon results without an increase in the number of more time-consuming electron histories.

The treatment of spatial displacements in the electron history go beyond the assumption of straight-line path segments, and include the sampling from relevant theory for the transverse and longitudinal displacements[3] that result from a wiggly path.

PHOTON TRANSPORT

Successive photon interactions are sampled individually in analogy with the physical process, using cross sections compiled by Berger and Hubbell.[13] At each interaction, the fate of the photon is sampled from among photoelectric absorption, coherent (Rayleigh) scattering, incoherent (Compton) scattering, and pair (and triplet) production processes.

Changes in direction for coherent-scattered photons are sampled from the Thomson cross section combined with atomic form factors. The direction and energy of Compton-scattered photons (and of the Compton electrons) are sampled from the Klein-Nishina cross section combined with incoherent scattering functions. In the case of photoelectric absorption, the emission angle of the photoelectron is sampled from relevant theory, and its energy adjusted to account for the atomic binding; for subsequent atomic emissions, the shells included are the K shell only for ETRAN and all shells for ITS. The kinetic energies and the emission directions of the electron and positron from pair (and triplet) production are sampled according to Bethe-Heitler theory.

DISCUSSION

The transport methods and the underlying cross-section database has been under continued development for more than three decades; with minor exceptions, all the physical processes governing the transport of electrons and photons have been included using rather complete and accurate methods. A large number of comparisons with measured results have accumulated, indicating rather high reliability for the Monte Carlo calculations. Some weaknesses in the model are known, mostly related to low-energy electron transport in high-Z materials where the use of the condensed-history methods are no longer valid.

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5. Status of Electron Transport in MCNP, *H. Grady Hughes (LANL)*

INTRODUCTION

In recent years, an ongoing project within the radiation transport group (XTM) at Los Alamos National Laboratory has been the implementation and validation of an electron transport capability in the Monte Carlo code MCNP (Ref. 1). This paper documents the continuous-energy electron transport methods currently in use in MCNP and describes a recent improvement of the energy-loss straggling algorithm. MCNP also supports electron transport calculations in a multigroup mode. This capability is described elsewhere.[2]

ELECTRON TRANSPORT METHODS IN MCNP

The principal original reference for the condensed history Monte Carlo method is the 1963 paper by Berger.[3] Based on the techniques described in that work, Berger and Seltzer developed the ETRAN series of electron/photon transport codes.[4] These codes have been maintained and enhanced for many years at the National Institute of Standards and Technology. The ETRAN codes are also the basis for the Integrated TIGER Series (ITS) (Ref. 5), developed and maintained by Halbleib and his collaborators at Sandia National Laboratories in Albuquerque, New Mexico. The electron physics in MCNP is largely derived from that of the ITS.

The electron random walk in MCNP is based on a precalculated set of condensed-history steps selected so that, on the average, the kinetic energy of the electron decreases by a fixed ratio (specifically $2^{-1/8}$) during each step. After the selection of step lengths, the radiative stopping power is modeled explicitly by the sampling of bremsstrahlung photons. The average collisional stopping power is obtained analytically from Bethe's[6] theory for small energy transfers combined with an integral of the Møller[7] cross section to account for larger energy transfers. Collisional energy straggling is also modeled, as discussed in the next section.

For the actual representation of the electron's path, the electron step is divided into smaller substeps. Substep angular deflections are sampled from the Goudsmit-Saunderson[8] theory applied to a combination of the Mott[9] and Rutherford[10] cross sections, with a screening correction due to Molière.[11] For partial substeps to a boundary, MCNP approximates the Goudsmit-Saunderson distribution by a linear interpolation in the cosine of the deflection angle.

Bremsstrahlung photons are sampled from tabulated data based on Bethe-Heitler[12] Born-approximation results. The sampling of a bremsstrahlung photon causes a correlated decrease in the electron energy. By contrast, the sampling of a secondary electron is not correlated with the electron energy, because the collisional stopping power has already been included in the substep energetics. Secondary "knock-on" electrons are sampled from an appropriately normalized cumulative integral of the Møller cross section.[7]

IMPROVED ENERGY STRAGGLING

Because an energy step represents the cumulative effect of many individual random collisions, fluctuations in the energy loss rate will occur, leading to a probability distribution $f(s,\Delta)\,d\Delta$ from which the energy loss Δ for the step of length s can be sampled. Landau[13] studied this situation under several simplifying assumptions, including the assumption that the formal upper limit of energy loss can be extended to infinity. With these simplifications, Landau found that the energy loss distribution can be expressed as

$$f(s,\Delta)\,d\Delta = \phi(\lambda)\,d\lambda\ , \qquad (1)$$

in terms of $\phi(\lambda)$, a universal function of a single dimensionless variable λ related to Δ; s, the energy of the electron; and various properties of the medium. The asymptotic form of $\phi(\lambda)$ is such that an unrestricted sampling of λ leads to an unbounded mean energy loss. Therefore, a cutoff value λ_c is imposed to ensure a finite mean energy loss $\bar{\Delta}$.

Blunck and Leisegang[14] extended Landau's result to include the second moment of the expansion of the cross section. Their result can be expressed as a convolution of Landau's distribution with a Gaussian distribution:

$$f^*(s,\Delta) = \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{+\infty} f(s,\Delta')\exp\left[\frac{(\Delta-\Delta')^2}{2\sigma^2}\right]d\Delta'\ , \qquad (2)$$

with the variance of the Gaussian $\sigma^2 = 10\ \text{eV}\cdot Z^{4/3}\bar{\Delta}$, as given by Blunck and Westphal.[15]

Earlier versions of MCNP, following Version 1.0 of the ITS, sampled Δ from Eqs. (1) and (2) using a 501-point tabulation of $\phi(\lambda)$ in the range $-4 \le \lambda \le 100$, based on the work of Börsch-Supan.[16] This approach suffered from two major shortcomings. First, the resolution of the table was insufficient to provide a smooth sampled function for large values of λ. Second, the arbitrary fixing of $\lambda_c = 100$ caused the mean energy loss to be incorrect except in a limited electron energy range. As is done in the current version of ITS, MCNP now employs a tabulation with greater resolution (5001 points in $-4 \le \lambda \le 100$), an analytic approximation to the asymptotic form given by Börsch-Supan for $\lambda > 100$, and a variable energy- and material-dependent cutoff λ_c, to ensure correct mean energy loss. In addition, an empirical modification of σ^2 described and recommended by Seltzer[17] is made. Figure 1 shows the effect of these improvements on the energy-loss spectrum for 10-MeV electrons in silicon, and also shows the excellent agreement between the current version of ITS and the new version of MCNP for this case.

CONCLUSIONS

The current methods used in MCNP for condensed history electron transport have been briefly presented. An important