LA-UR -95-2138

CONF-951006--17

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE: STATUS OF ELECTRON TRANSPORT IN MCNP™

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SUBMITTED TO: 1995 ANS Winter Meeting, 10/29 - 11/2/95, San Francisco, CA

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FORM NO 836 R4
ST NO 2629 5/81

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Status of Electron Transport in MCNP™

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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.[1] In this paper I document the continuous-energy electron transport methods currently in use in MCNP, and describe a recent improvement of the energy-loss straggling algorithm. MCNP also supports electron transport calculations in a multigroup mode. This capability is described in another paper in this conference.[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),[5] developed and maintained by Halbleib and his collaborators at Sandia National Lab-

oratories 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, since 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

$$f(s, \Delta)d\Delta = \phi(\lambda)d\lambda \ , \tag{1}$$

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 $\overline{\Delta}$.

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 $\sigma^2 = 10\text{eV}\cdot Z^{4/3}\overline{\Delta}$, 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 $-4 \leq \lambda \leq 100$, 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 $-4 \leq \lambda \leq 100$), 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 correction to the energy-loss algorithm has been successfully implemented and tested.

References

1. Judith F. Briesmeister, Editor, "MCNP™ — A General Monte Carlo N-Particle Transport Code," Los Alamos National Laboratory report LA–12625–M (November, 1993).

   (MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory.)

2. Kenneth J. Adams and Michelle Hart, "Multigroup Boltzmann-Fokker-Planck Electron Transport Capability in MCNP," in these proceedings.

3. M. J. Berger, "Monte Carlo Calculation of the Penetration and Diffusion of Fast Charged Particles," in *Methods in Computational Physics, Vol. 1*, edited by B. Alder, S. Fernbach, and M. Rotenberg, (Academic Press, New York, 1963) 135.

4. Stephen M. Seltzer, "An Overview of ETRAN Monte Carlo Methods," in *Monte Carlo Transport of Electrons and Photons*, edited by Theodore M. Jenkins, Walter R. Nelson, and Alessandro Rindi, (Plenum Press, New York, 1988) 153.

5. J. Halbleib, "Structure and Operation of the ITS Code System," in *Monte Carlo Transport of Electrons and Photons*, edited by Theodore M. Jenkins, Walter R. Nelson, and Alessandro Rindi, (Plenum Press, New York, 1988) 249.

6. H. Bethe, "Zur Theorie des Durchgangs schneller Korpuskularstrahlen durch Materie," *Ann. Phys.* **5**, 325 (1930).

7. C. Møller, "Zur Theorie des Durchgang schneller Elektronen durch Materie," *Ann. Physik.* **14** (1932) 568.

8. S. Goudsmit and J. L. Saunderson, "Multiple Scattering of Electrons,"

Phys. Rev. **57** (1940) 24.

9. N. F. Mott, "The Scattering of Fast Electrons by Atomic Nuclei," *Proc. Roy. Soc. (London)* **A124** (1929) 425.

10. E. Rutherford, "The Scattering of α and β Particles by Matter and the Structure of the Atom," *Philos. Mag.* **21** (1911) 669.

11. G. Molière, "Theorie der Streuung schneller geladener Teilchen II: Mehrfach- und Vielfachstreuung," *Z. Naturforsch.* **3a** (1948) 78.

12. H. A. Bethe and W. Heitler, "On Stopping of Fast Particles and on the Creation of Positive Electrons," *Proc. Roy. Soc. (London)* **A146** (1934) 83.

13. L. Landau, "On the Energy Loss of Fast Particles by Ionization," *J. Phys. USSR* **8** (1944) 201.

14. O. Blunck and S. Leisegang, "Zum Energieverlust schneller Elektronen in dünnen Schichten," *Z. Physik* **128** (1950) 500.

15. O. Blunck and K. Westphal, "Zum Energieverlust energiereicher Elektronen in dünnen Schichten," *Z. Physik* **130** (1951) 641.

16. W. Börsch-Supan, "On the Evaluation of the Function

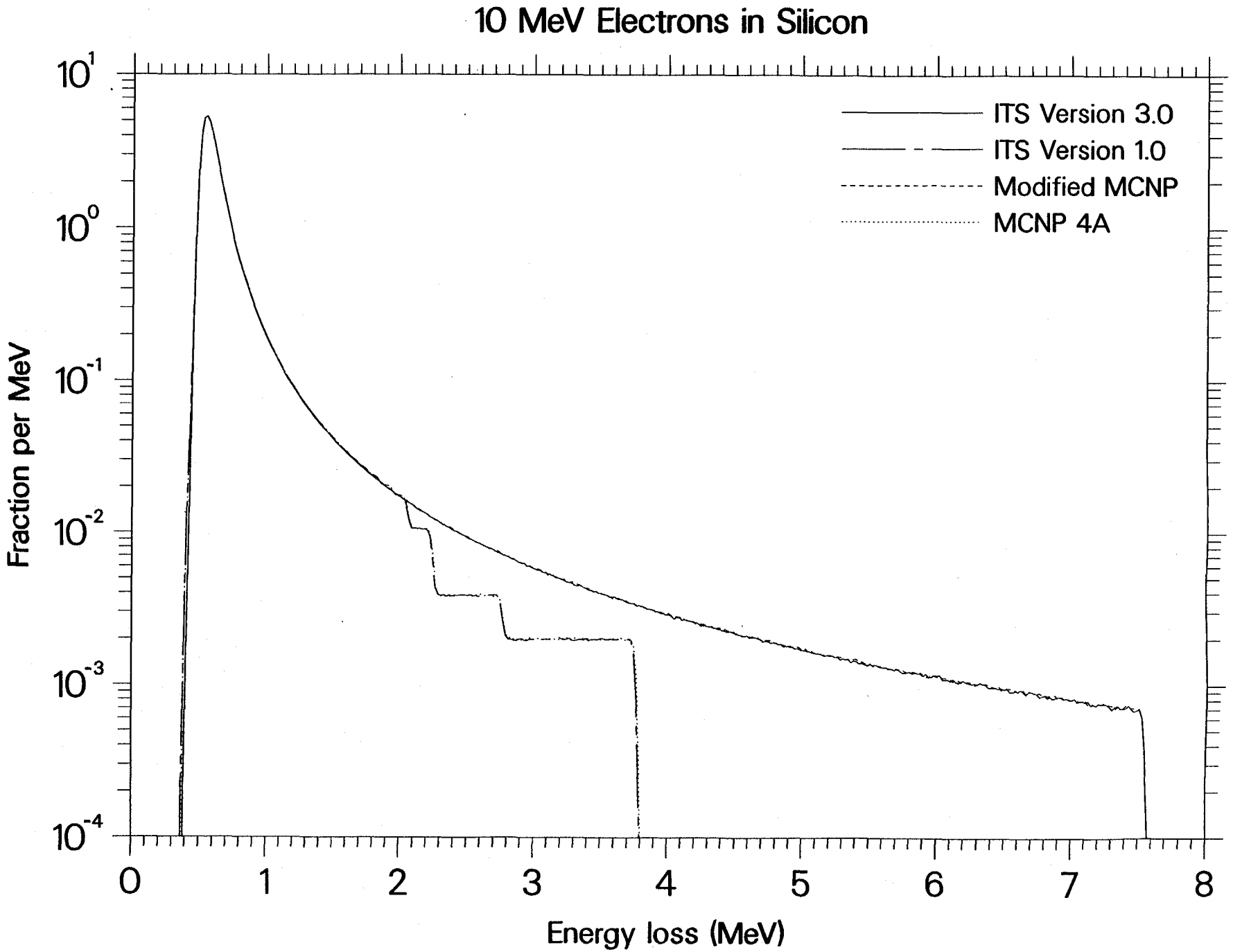
$$\phi(\lambda) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} e^{\mu \ln \mu + \lambda \mu} d\mu$$

for Real Values of λ," *J. Res. National Bureau of Standards* **65B** (1961) 245.

17. Stephen M. Seltzer, "Electron–Photon Monte Carlo Calculations: The ETRAN Code," *Appl. Radiat. Isot.* Vol. 42, No. 10 (1991) pp. 917–941.

Figure Caption

Fig. 1. Collisional energy loss spectrum for 10 MeV electrons in silicon as calculated by ITS 1.0, ITS 3.0, MCNP4A, and the new modified MCNP.


10 MeV Electrons in Silicon
ITS Version 3.0
ITS Version 1.0
Modified MCNP
MCNP 4A
Fraction per MeV
Energy loss (MeV)
10^1
10^0
10^-1
10^-2
10^-3
10^-4
0
1
2
3
4
5
6
7
8