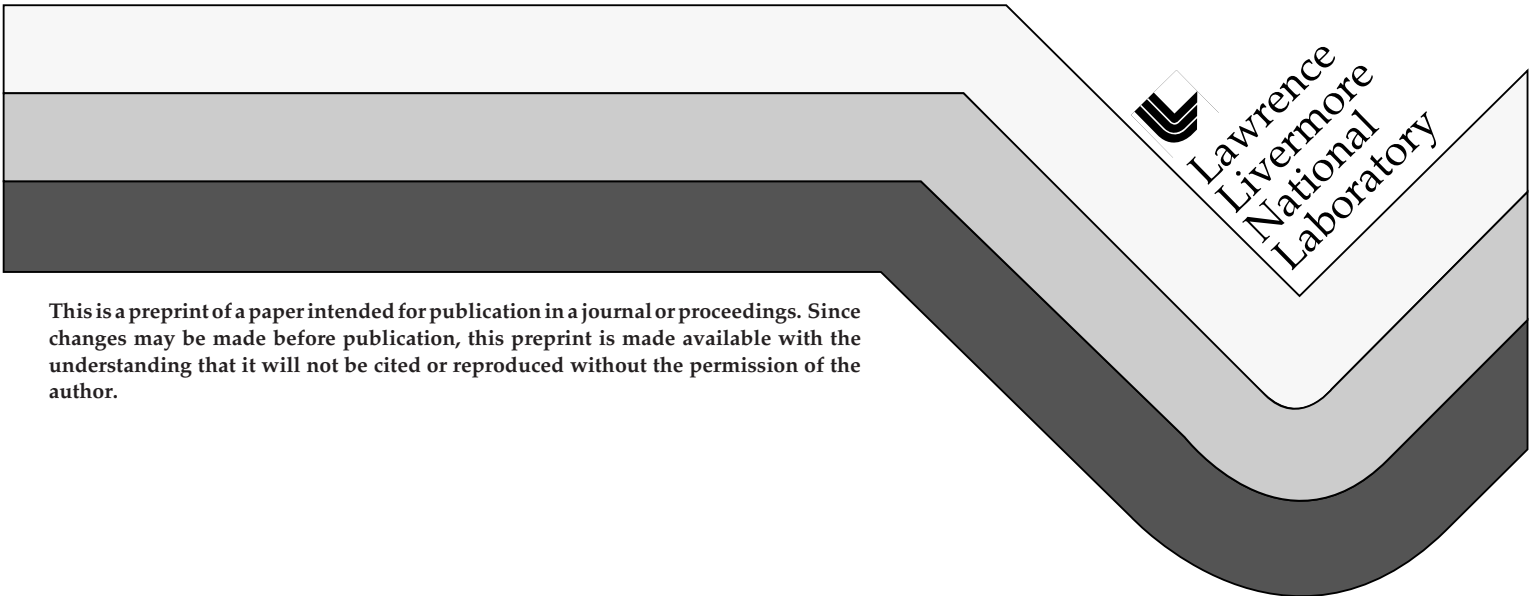


## Efficient Single Scatter Electron Monte Carlo

M. M. Svatos  
J. A. Rathkopf

This paper was prepared for submittal to the  
Joint Russian-American Conference on Computational Mathematics  
Albuquerque, NM  
September 2-5, 1997

November 3, 1997



This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

#### DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

# EFFICIENT SINGLE SCATTER ELECTRON MONTE CARLO

M.M. Svatos and J.A. Rathkopf

Lawrence Livermore National Laboratory  
Livermore, CA 94550

## ABSTRACT

A single scatter electron Monte Carlo code (SSMC), CREEP, has been written which bridges the gap between existing transport methods and modeling real physical processes. CREEP simulates ionization, elastic and bremsstrahlung events individually. Excitation events are usually treated with an excitation-only stopping power, although simulation of individual excitation events is possible. Agreement of these quantities with experimental values is generally quite good.

One application of this code is the generation of probability distribution functions (PDFs) to describe the phase space of a single electron emerging from a sphere of a given material and radius. A library of data sets for such spheres (or “kugels”) is being computed for a variety of incident energies, material types, and sizes. The final goal of this work is to achieve extremely accurate transport results with an efficiency that is similar to that of condensed history methods.

## 1 Introduction

Single scatter Monte Carlo (SSMC) physics is gaining attention for electron transport, despite the fact that it is inherently very time consuming. One reason is that since single scatter calculations conform more closely to the physical processes the electron undergoes, they can serve as a means to explore the validity of assumptions used in other transport techniques. The results of SSMC can also be tallied and fed into a more efficient code.

SSMC allows large angle scatter and backscatter measurements to be calculated with greater accuracy in a reliable manner. Large angle scatter and backscatter, being relatively rare, result in much of the seemingly eccentric energy deposition behavior of electron beams (and photon beams for that matter, since photons deposit their energy to the medium through secondary electrons), including lateral blooming with distance and nonuniformities (“hot” or “cold” spots) found near changes in the medium type or density.

CREEP relies on sampling the Lawrence Livermore Evaluated Electron Data Library (EEDL), which was established at LLNL by 1990 to complement the ENDL (Evaluated Nuclear Data Library) and EPDL (Evaluated Photon Data Library). Complete documents detailing its contents, with derivations, are available [1–3]. Cross sections for ionization (by subshell), elastic scatter, bremsstrahlung, and excitation are tabulated on an energy grid with a variable placement of points between 10 eV and 100 GeV, for atomic numbers 1 to 100. Compounds and mixtures may also be used by combining the appropriate element data via Bragg additivity.

One important application of SSMC is to use it as a foundation for other more efficient methods. This has been called a Local-to-Global approach. It works by breaking the calculation into two stages: a local calculation (SSMC) done over small geometries having the size and shape of the “steps” to be taken through the mesh; and a global calculation which relies on a stepping code that samples the stored results of the local calculation. An example of an SSMC-based Local-to-Global code will be introduced in Section 4.

## 2 Single Scatter Monte Carlo Code

The CREEP code is written in FORTRAN and C, in a very simple style with the intent of being extremely portable. Since this code is intended primarily as a means to explore basic physical properties of the

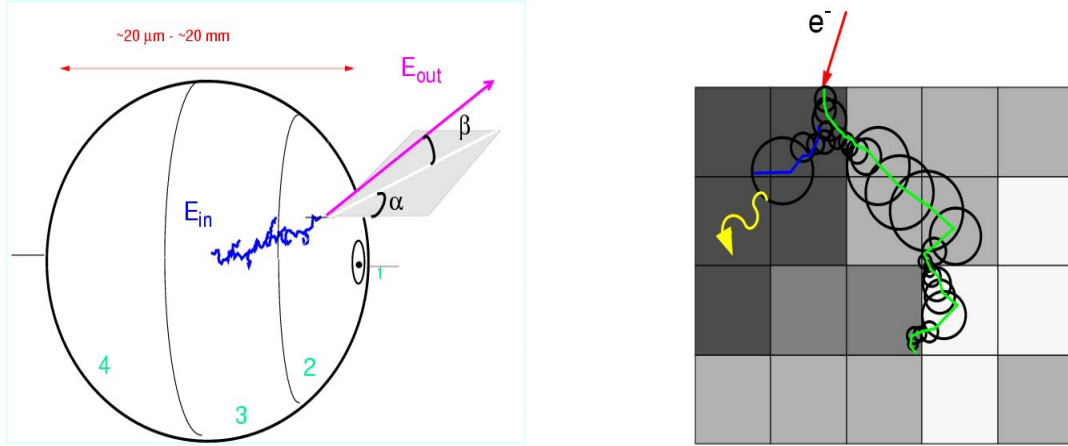


Figure 1: LEFT: The geometry of the local calculation. RIGHT: An example global calculation.

medium, only simple geometries are assumed: either spherical or slab or a slab layered with different materials.

The overall algorithm for a truly single scatter charged particle code is a direct analog of the algorithm that has historically been used in photon and neutron Monte Carlo codes. Briefly, one finds the distance to interaction by finding the total cross section at the present energy and uses the relation  $s = -\lambda \ln(\eta)$ , where  $\eta$  is a random number on the interval  $(0, 1]$ . One then determines which interaction took place, by forming and sampling from a cumulative probability based on the cross sections for each of the four possible interactions (ionization, excitation, elastic scatter, bremsstrahlung). The energy, position and trajectory of the particle are updated to reflect the chosen interaction. Then the same process is begun again, provided the electron has not escaped the medium or fallen below the energy cutoff.

### 3 Results from Single Scatter Monte Carlo

Benchmarking this code with experiment for a variety of elements and select compounds and mixtures, over the energy range of the EEDL database, is a large effort that is still in its infancy.

Historically, backscatter has been difficult for condensed history codes to simulate correctly. Figure 2 shows two examples of backscatter information generated by CREEP compared to experimental values. The agreement is generally quite good.

Comparisons of the CREEP single scatter Monte Carlo (SSMC) code with energy deposition measurements are shown in figure 2. Agreement to experiment is generally quite good for a variety of materials, incident energies, and incident angles. The curves did not require normalization.

In addition to the preceding quantities, CREEP also calculates analog stopping powers (the amount of energy lost per unit distance for both radiative and collisional events), energy deposits due to individual interaction types, and “real” pathlength (cumulative distance between events) which can be used to calculate detour factors (the ratio to the real range compared to the CSDA range).

Obtaining these results is time consuming. Some timings are shown in Table 1. In general, the simulation time increases with the number of histories, the geometry size, and as the energy threshold is lowered.

Table 1: Timings for several CREEP runs on a SunSparc 20 running Solaris OS 2.51. Each medium was a slab of 1 mm thick. Results for the number of interactions, the number of calls to the random number generator (RNG), and the user time are normalized per incident history.

Medium	Density (g/cc)	Interactions	RNG calls	User Time (s)	Ratio
H	$1 \times 10^{-4}$	0.667	8	$2.52 \times 10^{-4}$	1
O	$1.4 \times 10^{-3}$	5.098	39	$1.77 \times 10^{-3}$	7.02
Na	1.0	6714	48001	1.35	5357
$H_2O$	1.0	8057	71714	3.30	13095
Au	19.3	19810	145541	6.98	27698

All of these require more interactions to be simulated. The version of the code which includes compounds and mixtures is also notably slower than the single-element versions. Table 1 gives some feel for how the run time scales with different media.

Clearly if this method is to become practical, there must be a means for a radical speed-up in the execution time. Such a means has been suggested in the Local-to-Global algorithm. [7]

## 4 Using Single Scatter Results in Local-to-Global Transport

In this application, the local calculation is an SSMC (CREEP) run performed in small spheres of various materials. The electron is started in the center and tracked until it crosses the surface of the sphere, at which time the following state variables are tallied: exit energy, exit “position cosine” ( $z/R$ ), elevation angle ( $\beta$ ) and swing angle ( $\alpha$ ) of the trajectory in the exit plane, and the number of secondary particles it set in motion that also escaped the sphere. The sphere, or kugel, is also divided into four surface bands; each band has its tallies kept separately. This geometry is illustrated in figure 1. After many histories, these tallies result in probability distribution functions (PDFs), each having 100 equally-spaced bins, that may be sampled by the global calculation. Knock-on electrons that escape, as well as all photons, are kept in separate distributions.

The global geometry for cases of interest is divided into voxels of varying density and material type. An example is shown in figure 1. For each history, a kugel of appropriate size and incident energy is chosen from the library and centered on the electron’s location. The exit conditions are then sampled from that kugel’s PDFs, starting with the exit band  $b$ , on which the other variables depend. The exit energy is then sampled, which sets the (target) energy loss,  $E_{loss} = E_{in} - E_{out}$ . The exit trajectory is determined by sampling two correlated angles,  $\alpha$  and  $\beta$ , from which three correlated direction cosines can be obtained. The target exit position on the sphere is found by sampling the  $z$  coordinate, and then randomizing  $x$  and  $y$  on the  $z$ -ring. This exit point is used to define the endpoint of a vector which starts at the center of the kugel. It is along this projected pathlength vector that  $E_{loss}$  is deposited. Since a kugel can be larger than a transport zone, the energy deposited in each zone is scaled by two factors: the fraction of the projected pathlength vector through the zone, and the density of the zone. If the density of a zone is greater than the nominal density that was used in the global calculation, the energy will be deposited before the edge of the kugel was reached; thus a new exit position is found along the same trajectory, but closer to the center (or vice versa for a less dense region). If a new material is encountered during the energy deposition scheme, the step is stopped at the boundary, and only the energy deposited up to that point is subtracted from  $E_{in}$ . The next step is taken in the new material.

After each kugel step, the average number of secondary electrons escaping from (anywhere on) the kugel is sampled,  $n_e$ , given that the primary escaped from band  $b$  with exit energy  $E_{out}$ . The state variables for  $n_e$  secondary electrons are then sampled in a manner exactly like that above, but the results are taken from

the secondary electron distributions. The same is done for photons, which are not tracked, but passed off to another code for transport.

## 5 Summary

Single scatter Monte Carlo provides the most accurate way to simulate electrons, however it is too slow to be practical for general use. It is possible to have a code with both speed and accuracy by using the Local-to-Global method of precalculating distributions. A current implementation of this algorithm uses approximately  $5 \times 10^4$  bytes per kugel PDF set. If the application can be defined by a limited number of materials and step sizes, the total amount of storage is quite feasible.

The speed-up in the global calculation comes from needing a fewer number of steps per history and also a fewer number of operations per step. The accuracy converges to that of the local SSMC calculation as many histories are run, provided the PDF sampling routine is faithful. Further investigation as to the degrees of speed-up and accuracy in various geometries is an ongoing effort.

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

## References

- [1] D.E. Cullen and S.T. Perkins. *The Livermore Bremsstrahlung Database*. UCID-21627, 1989. Lawrence Livermore National Laboratory.
- [2] S.T. Perkins and D.E. Cullen. *The Livermore Electron Impact Ionization Database*. UCID-21628, 1989. Lawrence Livermore National Laboratory.
- [3] S.T. Perkins and D.E. Cullen. *The Livermore Electron Elastic Scattering Database*. UCRL-ID-103170, 1990. Lawrence Livermore National Laboratory.
- [4] G.J. Lockwood, L.E. Ruggles, G.H. Miller, and J.A. Halbleib. *Calorimetric Measurement of Electron Energy Deposition in Extended Media – Theory vs Experiment*. Sandia Report SAND79-0414, 1980.
- [5] E.H. Darlington. *Backscattering of 10-100 keV electrons from thick targets*. *J. Phys. D Appl. Phys.*, **8**:85–93, 1975.
- [6] G. Neubert and S. Rogaschewski. *Backscattering Coefficient Measurements of 15 to 60 keV electrons for Solids at various angles of incidence*. *Phys. Stat. Sol.*, **59**:35–41, 1980.
- [7] M.M. Svatos, C.T. Ballinger, H. Neuenschwander, T.R. Mackie, W.P. Chandler, C.L. Hartmann Siantar, J.A. Rathkopf, and P.J. Reckwerdt. *Electron Transport in Radiotherapy using Local-to-Global Monte Carlo*. In *Proceedings of the International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses*, pages 866–875, La Grange Park, IL, 1995. American Nuclear Society, Inc.

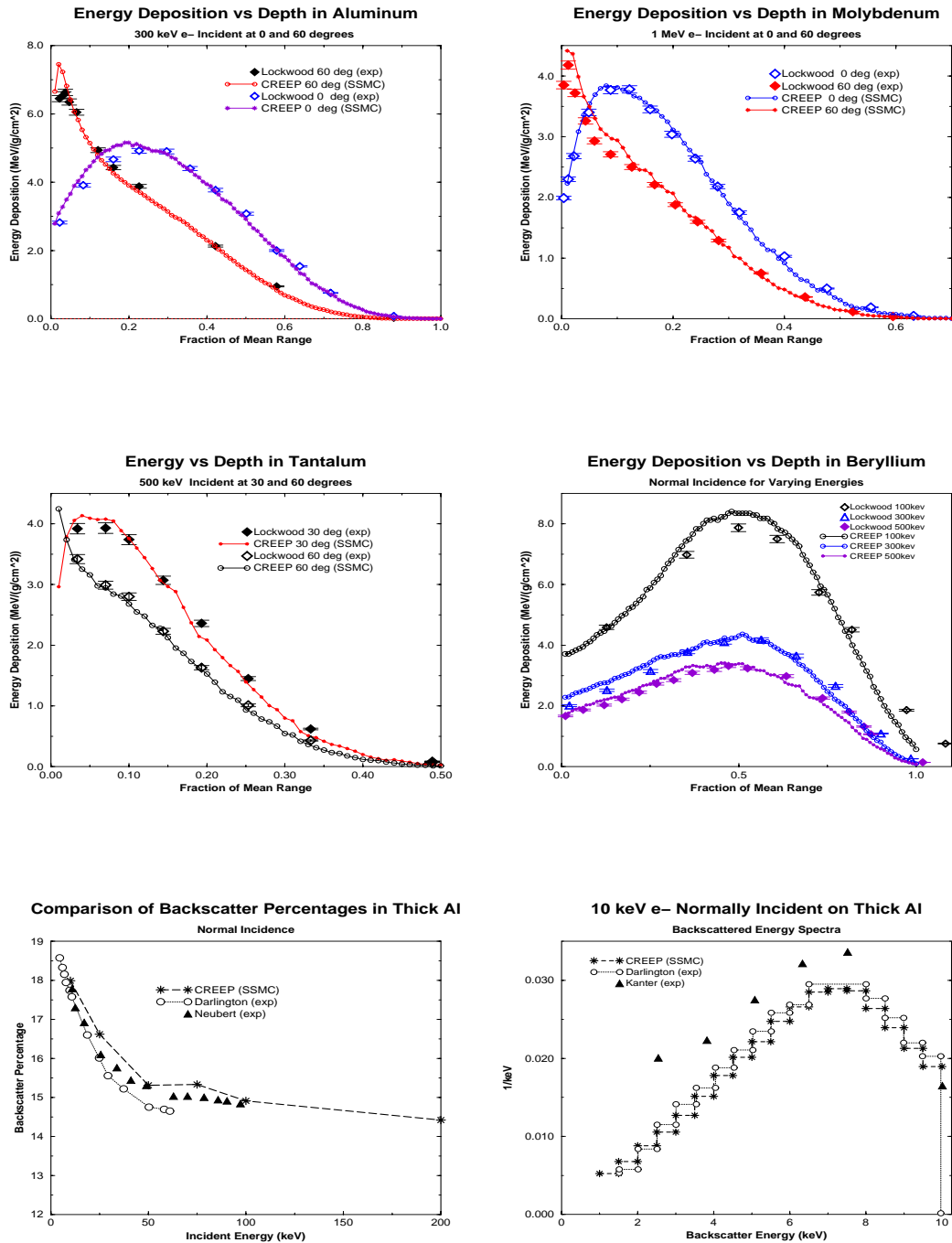


Figure 2: TOP and MIDDLE: Energy deposition is shown as a function of depth into the medium, where the depth has been normalized to the CSDA range of the electron in each case. The points attributed to Lockwood *et al* are from calorimetric measurements [4]; the comparisons are absolute. BOTTOM LEFT: CREEP backscatter percentage (including backscattered secondary electrons) compared to the experiments of Darlington *et al* [5] and Neubert *et al* [6]. BOTTOM RIGHT: The backscattered energy spectrum resulting from a 10 keV electron impinging on an aluminum slab that is large in x, y, and z compared to the mean free path of the incident electron.

*Technical Information Department • Lawrence Livermore National Laboratory*  
*University of California • Livermore, California 94551*

