Preprint
UCRL-JC-139318

A Moment-Based Condensed History Algorithm

D. R. Tolar, Jr. and E. W. Larsen

This article was submitted to
American Nuclear Society 2000 Winter Meeting,
Washington, DC, November 12-16, 2000

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

June 15, 2000

A Moment-Based Condensed History Algorithm

Danny R. Tolar, Jr.
Defense and Nuclear Technologies
Lawrence Livermore National Laboratory
Livermore, California 94551 USA

Edward W. Larsen
Department of Nuclear Engineering and Radiological Sciences
University of Michigan
Ann Arbor, Michigan 48109 USA

"Condensed History" algorithms[1] are Monte Carlo models for electron transport problems. They describe the aggregate effect of multiple collisions that occur when an electron travels a path length s_0. This path length is the distance each Monte Carlo electron travels between Condensed History steps. Conventional Condensed History schemes employ a splitting routine over the range $0 \leq s \leq s_0$.[1] For example, the Random Hinge[2] method splits each path length step into two substeps; one with length ξs_0 and one with length $(1-\xi)s_0$, where ξ is a random number from $0 < \xi < 1$.

Here we develop a new Condensed History algorithm to improve the accuracy of electron transport simulations by preserving the mean position and the variance in the mean of electrons that have traveled a path length s *and* are traveling with the direction cosine μ. These means and variances are obtained from the zeroth-, first-, and second-order spatial moments of the Boltzmann transport equation. Hence, our method is a Monte Carlo application of the "Method of Moments".

For deriving these spatial moments, we consider the one speed transport equation in planar geometry with continuous slowing down energy dependence. Neglecting absorption, this equation is given by

$$\frac{\partial}{\partial s}\psi\left(z,\mu,s\right) \;+\; \mu\frac{\partial}{\partial z}\psi\left(z,\mu,s\right) \;+\; \Sigma_s\,\psi\left(z,\mu,s\right) = \int_{-1}^{1} \Sigma_s(\mu,\mu')\,\psi(z,\mu',s)\,d\mu' \;\;, \qquad (1)$$

with the initial condition of one particle at $z = 0$ traveling down the z-axis in the direction $\mu = 1$,

$$\psi(z,\mu,0) = \delta(z)\,\delta(\mu-1) \;\;. \qquad (2)$$

To obtain the zeroth-order spatial moment, we integrate Eqs. (1) and (2) over all space. That is, we operate by $\int_{-\infty}^{\infty}(\cdot)\,dz$, and we define the function:

$$\psi_0(\mu,s) \equiv \int_{-\infty}^{\infty} \psi\,(z,\mu,s)\;dz \quad . \tag{3}$$

The resulting differential equation for $\psi_0(\mu,s)$ is given by

$$\frac{\partial}{\partial s}\psi_0(\mu,s) + \Sigma_{s0}\psi_0(\mu,s) = \sum_{n=0}^{\infty} \frac{2n+1}{2}\,\Sigma_{sn}\,P_n(\mu) \int_{-1}^{1} P_n(\mu')\psi_0(\mu',s)\,d\mu' \quad , \tag{4}$$

where $\Sigma_{s0} = \Sigma_s =$ macroscopic scattering cross section, and $\psi_0(\mu,0) = \delta(\mu-1)$. The solution to Eq. (4) is the following:

$$\psi_0(\mu,s) = \sum_{n=0}^{\infty} \frac{2n+1}{2}\,P_n(\mu)\,\exp(-\Sigma_{an}s) \quad , \tag{5}$$

where $\Sigma_{an} = \Sigma_{s0} - \Sigma_{sn}$. $\psi_0(\mu,s)$ is known as the Goudsmit-Saunderson distribution. Physically, it is the probability distribution function for the direction cosine μ for particles that have traveled a path length s.

We can also find the first-order spatial moment by operating on Eqs. (1) and (2) by $\int_{-\infty}^{\infty} z(\cdot)\,dz$ and by defining the function:

$$\psi_z(\mu,s) \equiv \int_{-\infty}^{\infty} z\psi\,(z,\mu,s)\;dz \quad . \tag{6}$$

The differential equation governing $\psi_z(\mu,s)$ is given by

$$\frac{\partial}{\partial s}\psi_z(\mu,s) + \Sigma_{s0}\,\psi_z(\mu,s) = \mu\,\psi_0(\mu,s) + \sum_{n=0}^{\infty} \frac{2n+1}{2}\,\Sigma_{sn}\,P_n(\mu) \int_{-1}^{1} P_n(\mu')\psi_z(\mu',s)\,d\mu' \quad , \tag{7}$$

with the initial condition $\psi_z(\mu,0) = 0$. The solution for this first-order moment is shown below:

$$\begin{aligned} \psi_z(\mu,s) \;=\; & \sum_{n=0}^{\infty} P_n(\mu) \left\{ \frac{n}{2} \left[\frac{\exp(-\Sigma_{an}s) - \exp(-\Sigma_{a,n-1}s)}{\Sigma_{sn} - \Sigma_{s,n-1}} \right] \right. \\ & + \left. \frac{n+1}{2} \left[\frac{\exp(-\Sigma_{an}s) - \exp(-\Sigma_{a,n+1}s)}{\Sigma_{sn} - \Sigma_{s,n+1}} \right] \right\} \quad . \end{aligned} \tag{8}$$

Similarly, we can obtain the second-order spatial moment by operating on Eqs. (1) and (2) by $\int_{-\infty}^{\infty} z^2(\cdot)\,dz$ and by defining the function

$$\psi_{zz}(\mu,s) \equiv \int_{-\infty}^{\infty} z^2\psi\,(z,\mu,s)\;dz \quad . \tag{9}$$

After performing this operation, we solve the resulting equation for $\psi_{zz}(\mu, s)$.[3]

As the zeroth-order moment provides the Goudsmit-Saunderson distribution, the first-order moment provides the mean position $\langle z \rangle(\mu, s)$ for electrons that have generated a path length s *and* are traveling in the direction μ. The mean position is defined as

$$\langle z \rangle(\mu, s) \equiv \frac{\int_{-\infty}^{\infty} z\,\psi\,(z, \mu, s)\; dz}{\int_{-\infty}^{\infty} \psi\,(z, \mu, s)\; dz} = \frac{\psi_z(\mu, s)}{\psi_0(\mu, s)} \quad . \tag{10}$$

The second-order moment allows the variance in the mean position to be determined. The variance is given by

$$\sigma_z^2(\mu, s) \equiv \langle z^2 \rangle(\mu, s) - \langle z \rangle^2(\mu, s) = \frac{\psi_{zz}(\mu, s)}{\psi_0(\mu, s)} - \left[\frac{\psi_z(\mu, s)}{\psi_0(\mu, s)}\right]^2 \quad . \tag{11}$$

Our new Monte Carlo algorithm is designed such that the mean and variance are preserved in each Condensed History step. Similar to existing methods, the user specifies the path length s (step size) at the beginning of each step. Next, the direction of flight μ is sampled from the Goudsmit-Saunderson distribution given by Eq. (5). However, unlike existing methods, we use μ and s to evaluate $\langle z \rangle(\mu, s)$ and $\sigma_z^2(\mu, s)$. Then, at the end of the step, we move the electron history to a position that is sampled from a Gaussian distribution with mean $\langle z \rangle(\mu, s)$ and variance $\sigma_z^2(\mu, s)$.

To test the Moment Condensed History method, we simulate a monoenergetic 12.5 keV electron pencil beam at $z = 0$ cm in an infinite medium of aluminum. The continuous slowing down approximation is employed with multigroup cross sections from EEDL database.[4] As the electrons slow down to 0.06 keV, the dose (energy deposited per unit mass) is calculated as a function of depth (z coordinate). Three different simulations are used to obtain these results: (i) Moment Condensed History (MCH), (ii) Random Hinge Condensed History (RH), and (iii) Analog Monte Carlo (AMC). For the Condensed History models, s is chosen to be the path length required for the electron to lose the energy of one group. The MCH and RH methods use 36 steps, while AMC, on the average, needs 355 collisions to model this problem. We simulate one million electron histories.

The depth-dose curve for the 12.5 keV beam is shown in Figure 1. The dose predicted by MCH resembles the AMC distribution more closely than the results determined by RH. The differences are as much as 7% at the depths $0 < z < 5\text{x}10^{-5}$ cm. Figure 1 indicates that MCH's capability of preserving higher-order moments enhances the accuracy of dose calculations as compared to RH which does not preserve these moments. This improvement in accuracy, however, is slightly offset by a loss in efficiency. While the RH simulation is about ten times more efficient than AMC, the MCH algorithm is only about eight times faster.

In summary, we have developed a new Condensed History algorithm for electron transport that preserves the zeroth-, first-, and second-order spatial moments of the transport equation.

This enables Moment Condensed History to more accurately predict the locations of electrons after Condensed History steps. In the future, we plan to improve the efficiency of our scheme by alleviating the costly expense of evaluating the infinite summations involved with the moments. Perhaps Molière theory[5], which has been used to approximate the Goudsmit-Saunderson distribution by replacing it with a simpler function, could be extended to the first- and second-order solutions.

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

References

1. E.W. Larsen, "A Theoretical Derivation of the Condensed History Algorithm," *Ann. Nucl. Energy* **19**, 701 (1992).

2. J. Baro, J. Sempau, J.M. Fernandez-Varea, and F. Salvat, "PENELOPE: An Algorithm for Monte Carlo Simulation of the Penetration and Energy Loss of Electrons and Positrons in Matter," *Nucl. Instr. Meth. Phys. Research* **B100**, 31 (1995).

3. D.R. Tolar, Jr., "Advanced Multiple Scattering Algorithms for Electron Transport", PhD Dissertation, University of Michigan (1999).

4. S.T. Perkins, et al, "Tables and Graphs of Electron-Interaction Cross Sections Derived from the LLNL Evaluated Electron Data Library (EEDL)", LLNL UCRL-50400, **31**, (1991).

5. H.A. Bethe, "Molière's Theory of Multiple Scattering", *Phys. Rev.* **89**, 1256 (1953).

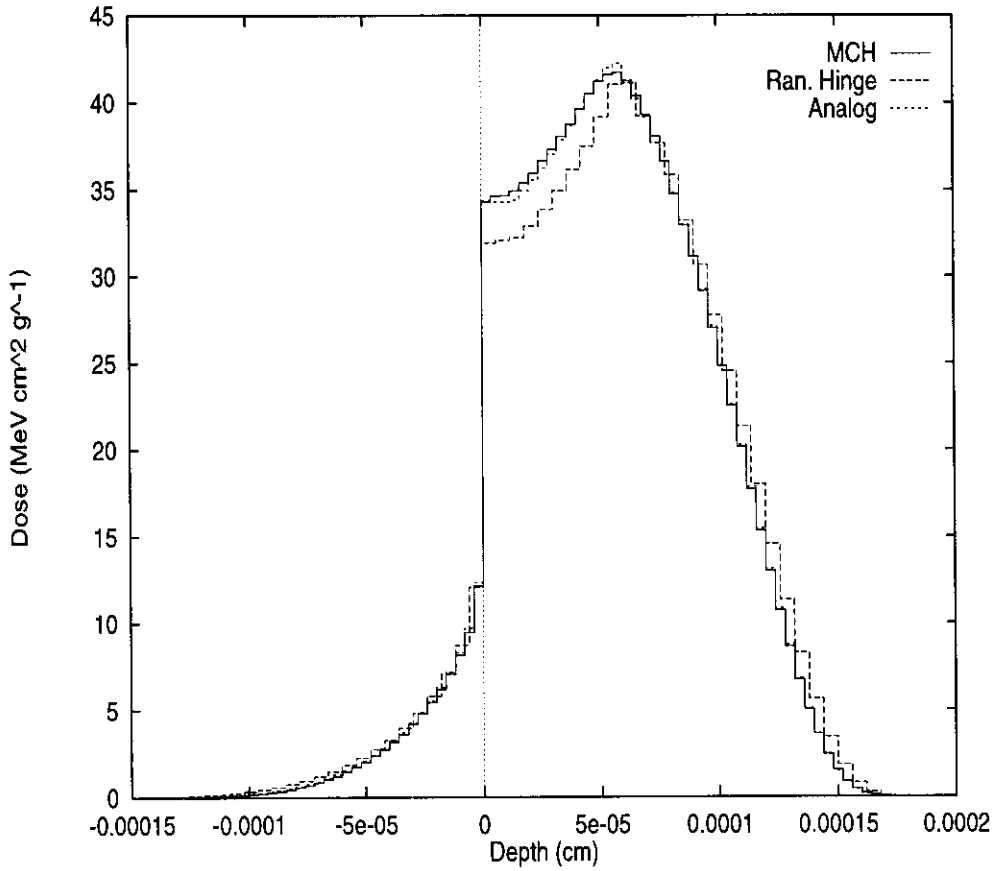

Figure 1: Dose Deposited as a Function of Depth into Aluminum ($E_0 = 12.5$ keV)