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"Condensed history" algorithms[1] are approximate electron transport Monte Carlo methods in which the cumulative effects of multiple collisions are modeled in a single "step" of (user-specified) path length s_0. This path length is the distance each Monte Carlo electron travels between "collisions." Current condensed history techniques utilize a splitting routine over the range $0 \leq s \leq s_0$.[1] For example, the PENELOPE method[2] splits each step into two substeps; one with length ξs_0 and one with length $(1-\xi)s_0$, where ξ is a random number from $0 < \xi < 1$. Because s_0 is fixed (not sampled from an exponential distribution), conventional condensed history schemes are not transport processes.

Here we describe a new condensed history algorithm that is a transport process. Our method simulates a transport equation that approximates the exact Boltzmann equation. The new transport equation has a larger mean free path than, and preserves two angular moments of, the Boltzmann equation. Thus, the new process is solved more efficiently by Monte Carlo, and it conserves both particles and scattering power.

To derive the approximate transport equation, we begin with the exact Boltzmann equation with continuous slowing down energy dependence. After converting energy loss to path length s, and adding the term ψ/s_0 to both sides, we obtain

$$\frac{\partial}{\partial s}\psi(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},s) + \frac{1}{s_0}\psi(\underline{r},\underline{\Omega},s) = \frac{1}{s_0}\left(1 - s_0 L\right)\psi(\underline{r},\underline{\Omega},s) \quad . \tag{1}$$

Here, assuming $\Sigma_a = 0$, L is the collision-minus-scattering operator:

$$L\psi(\underline{\Omega}) \equiv \sum_{n=0}^{\infty}\left(\frac{2n+1}{4\pi}\right)\left(\Sigma_{s0} - \Sigma_{sn}\right)\int_{4\pi} P_n\left(\underline{\Omega}\cdot\underline{\Omega}'\right)\psi\left(\underline{\Omega}'\right)\, d\Omega' \quad . \tag{2}$$

Now, we make the following approximation to the right side of Eq. (1) (with $s_1 \approx s_0$):

$$(1 - s_0 L)\, \psi(\underline{\Omega}) \approx e^{-s_1 L} \psi(\underline{\Omega}) = \int_{4\pi} G(\underline{\Omega} \cdot \underline{\Omega}', s_1) \psi\left(\underline{\Omega}'\right) \, d\Omega' \ . \tag{3}$$

Here $G(\underline{\Omega} \cdot \underline{\Omega}', s_1)$ is the "Goudsmit-Saunderson" distribution,

$$G(\underline{\Omega} \cdot \underline{\Omega}', s_1) = \sum_{n=0}^{\infty} \left(\frac{2n+1}{4\pi} \right) e^{-(\Sigma_{s0} - \Sigma_{sn}) s_1} P_n \left(\underline{\Omega} \cdot \underline{\Omega}' \right) \ . \tag{4}$$

Eq. (1) then becomes

$$\frac{\partial \psi}{\partial s} + \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{\Omega}) = \frac{-1}{s_0} \left[\psi(\underline{\Omega}) - \int_{4\pi} G(\underline{\Omega} \cdot \underline{\Omega}', s_1) \psi\left(\underline{\Omega}'\right) \, d\Omega' \right] \equiv -M \psi(\underline{\Omega}) \ . \tag{5}$$

Eq. (5) is a legitimate transport equation with mean free path s_0 and scattering kernel $G(\underline{\Omega} \cdot \underline{\Omega}', s_1)$. The parameters s_0 and s_1 are contained in the collision-minus-scattering operator M of Eq. (5). M can be rewritten as

$$M \psi(\underline{\Omega}) = \sum_{n=0}^{\infty} \left(\frac{2n+1}{4\pi} \right) \left(\frac{1 - e^{-(\Sigma_{s0} - \Sigma_{sn}) s_1}}{s_0} \right) \int_{4\pi} P_n \left(\underline{\Omega} \cdot \underline{\Omega}' \right) \psi\left(\underline{\Omega}'\right) \, d\Omega' \ . \tag{6}$$

The $n = 0$ terms of Eq. (2) and Eq. (6) are both zero. Hence, both operators conserve particles. To conserve scattering power, the $n = 1$ term of Eq. (6) must equal that of Eq. (2). This condition dictates that

$$s_0 = \frac{1 - e^{-(\Sigma_{s0} - \Sigma_{s1}) s_1}}{\Sigma_{s0} - \Sigma_{s1}} = \lambda_{tr} \left(1 - e^{-s_1 / \lambda_{tr}} \right) \ . \tag{7}$$

Thus, the user may choose any value for s_0 that is less than one transport mean free path, $\lambda_{tr} = \Sigma_{tr}^{-1}$. Physically, the transport mean free path is the mean penetration depth of particles that have travelled infinite path length. Therefore, this constraint does not forbid any reasonable choice for s_0. In practice, however, we choose s_1 to be any suitable positive path length, and then we use Eq. (7) to determine s_0.

Eq. (5) may be simulated like a standard analog Monte Carlo code. In this simulation, the distance to "collision" (the distance to where a change of direction occurs) is sampled from an exponential distribution with mean value s_0. After a particle has experienced a collision, the new direction of flight is sampled from the Goudsmit-Saunderson distribution evaluated at path length s_1. We describe this algorithm as a "transport condensed history" method. Like conventional condensed history, this method contains larger distances between collisions than in analog codes. Unlike conventional condensed history, our method is a true transport process.

To test these ideas, let us consider a monoenergetic 12.5 keV electron pencil beam in an infinite medium of aluminum. The continuous slowing down approximation is employed with multigroup cross sections obtained from the EPICSHOW code.[4] Scattering events, which are modeled using the Screened Rutherford kernel, are the only interactions considered. As the electrons slow down to various energies, the mean position and the standard deviation about this mean are calculated. The results are obtained using three different methods: (i) analog Monte Carlo, (ii) transport condensed history, and (iii) PENELOPE condensed history. For the condensed history codes, s_1 is selected as 1/2 the path length required for the electron to lose the energy of one group. One million particle histories are used.

The mean depth $\overline{z}$, the standard deviation about this mean σ_z, and the rms value of the radial deflection σ_r for several energies are shown in Table 1. Because the first two angular moments of the Boltzmann equation are preserved, transport condensed history exactly matches the analog Monte Carlo results for $\overline{z}$. PENELOPE generally overestimates the mean depth by 4%. As neither transport nor PENELOPE preserve higher-order moments, the predictions for σ_z are about 5% too high. Surprisingly, PENELOPE predicts σ_r within 1%, especially at lower energies. For transport condensed history, these results are only within 3%. The time required to generate the analog Monte Carlo results is roughly ten times greater than the run-time for the other two methods.

In summary, we have developed a new condensed history algorithm for electron transport that is a transport process. The new method should be more efficient than current condensed history schemes near material boundaries and interfaces, because the costly expense of shrinking or expanding the step sizes is unnecessary.[5] In future work, we plan to test this idea in heterogeneous media and develop transport condensed history models that preserve additional angular moments of the Boltzmann equation.

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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. S. Goudsmit and J.L. Saunderson, "Multiple Scattering of Electrons," *Phys. Rev.* **57**, 24 (1940).

4. D.E. Cullen, "EPICSHOW," Version 97-1, Lawrence Livermore National Laboratory, (1997).

5. A.F. Bielajew, "PRESTA: The Parameter Reduced Electron-Step Transport Algorithm for Electron Monte Carlo Transport," *Nucl. Instr. Meth. Phys. Research* **B18**, 165 (1987).

TABLE 1: Mean Depth and Standard Deviations for a 12.5 keV Electron Beam (amc = analog Monte Carlo, tch = transport condensed history, pen= PENELOPE condensed history)

Final Energy (keV)	Solution Method	$\overline{z}$ (μm)	σ_z (μm)	σ_r (μm)
10.0	amc	43.56	15.53	29.11
10.0	tch	43.57	17.63	27.88
10.0	pen	45.43	18.55	26.45
8.0	amc	57.82	29.87	51.70
8.0	tch	57.83	32.50	50.07
8.0	pen	59.91	32.60	50.51
6.0	amc	63.01	40.45	66.69
6.0	tch	63.02	42.95	65.09
6.0	pen	65.23	42.98	66.13
3.0	amc	64.47	47.42	75.94
3.0	tch	64.46	49.68	74.45
3.0	pen	66.58	49.81	75.65
1.0	amc	64.51	48.38	77.16
1.0	tch	64.51	50.60	75.70
1.0	pen	66.74	50.76	76.93
0.1	amc	64.51	48.42	77.21
0.1	tch	64.51	50.63	75.76
0.1	pen	66.74	50.81	77.03