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Evaluation of Monte Carlo Electron-Transport Algorithms in the Integrated Tiger Series Codes for Stochastic-Media Simulations

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Overview

- Condensed-history electron transport is based on infinite-medium solutions for angular scattering and energy loss. These methods become less accurate in the presence of material boundaries.
- Stochastic media are material mixtures with random distributions, such as concrete, foam, clouds, pebble-bed reactors, etc. Most stochastic-media problems have numerous material boundaries.
- We have evaluated the ITS condensed history algorithm for use in stochastic media and implemented improvements. We have also evaluated a condensed transport (or Generalized Boltzmann Fokker-Planck - GBFP) algorithm in ITS.
- Most comparisons are performed in a single material, with “material boundaries” artificially included to evaluate their effect. We also compare to analog transport, when possible.

Condensed History and Transport Monte Carlo Algorithms

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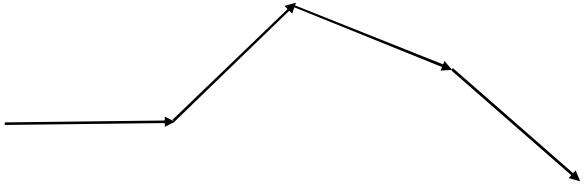
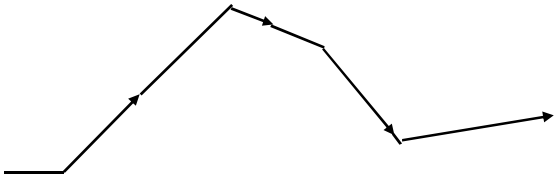
Condensed History Algorithms

Apply an infinite-medium multiple-scattering solution and algorithmically approximate the spatial displacement.

- ETRAN, ITS, MCNP model: particle scatters at the end of the step



- Random Hinge model: particle scatters at a randomly selected point within the step

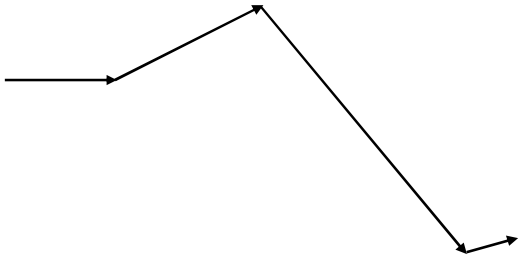


- Angular sampling from a multiple-scattering distribution

Condensed Transport Algorithms

Solve the Boltzmann transport equation with approximate cross sections.

- Random distance-to-collision is sampled from an exponential distribution



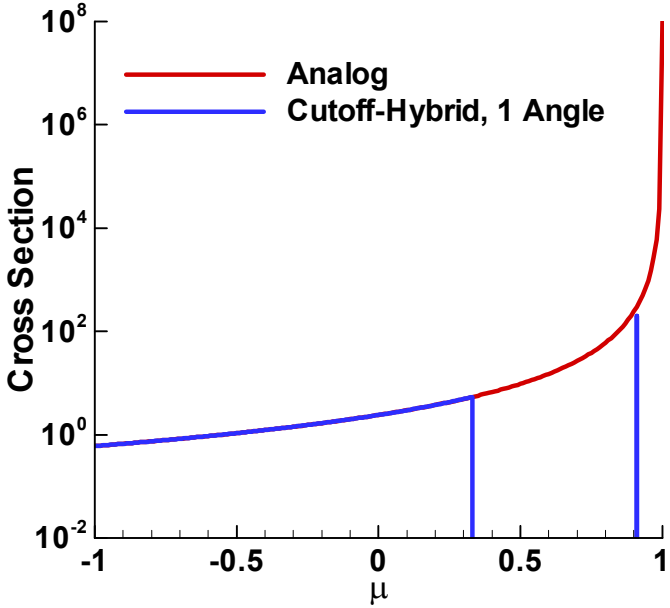
- Angular sampling from analytical, multiple-scattering, discrete, or other distribution

Generalized Boltzmann Fokker-Planck (GBFP) for Elastic Electron Scattering

The "cutoff hybrid" scattering kernel is:

$$\tilde{\sigma}_s(\mu_0) = \sum_{n=1}^{N} \frac{\alpha_n}{2\pi} \delta[\mu_0 - \xi_n]$$

$$+H\left[-\mu_0 + \mu_0^*\right] \frac{\sigma_{s0}}{2\pi} \frac{2\eta\{1+\eta\}}{\{1+2\eta-\mu_0\}^2}$$



α_n are amplitudes

ξ_n are scattering cosines

H is the Heaviside function, one for $\mu_0 < \mu_0$ and zero otherwise

Requiring that α_n and ξ_n preserve $2N$ residual momentum transfer moments (σ_n, $n=1,\ldots,2N$) produces a nonlinear algebraic system.

This is solved using Sloan's method.

Sloan, D.P., "A New Multigroup Monte Carlo Scattering Algorithm for Neutral and Charged-Particle Boltzmann and Fokker-Planck Calculations," Technical Report SAND83-7094, Sandia National Laboratories (1983).

Stochastic-Media Simulations

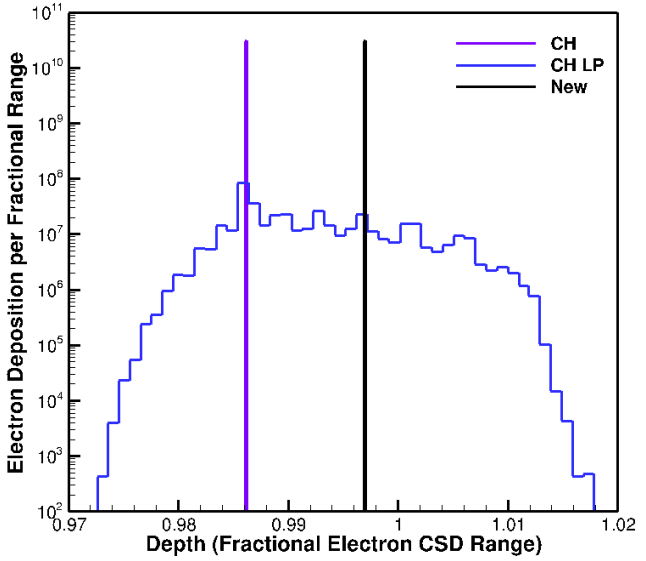
- Simulations are performed using the Levermore-Pomraning (LP) closure or chord-length sampling (CLS) technique. In this approximation, electrons randomly change between materials (i.e., encounter material boundaries) at random locations during transport (i.e., the distance to a material boundary is randomly sampled from an exponential distribution) based on the mean chord length in each material.
- More accurate "limited chord-length sampling" techniques have been demonstrated in Monte Carlo codes, but this work uses only the LP (or CLS) approach.

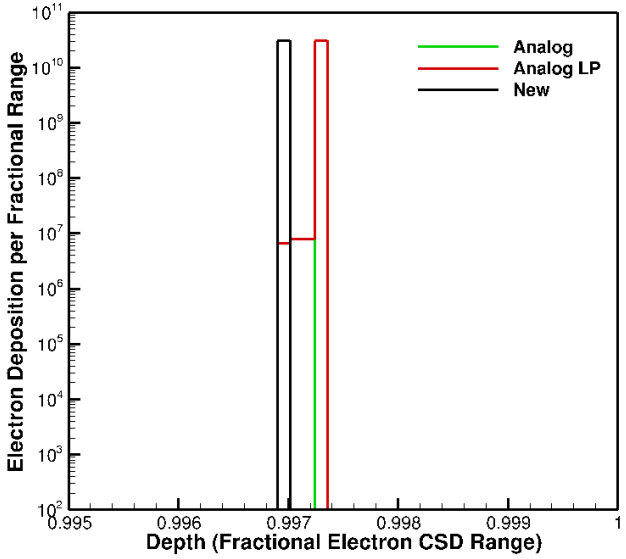
M. Adams, E. Larsen, and G. Pomraning, "Benchmark Results for Particle Transport in a Binary Markov Statistical Medium," *J. Quant. Spectrosc. Radiat. Transfer*, **42**, 253-266 (1989).
R. Sanchez, "Linear Kinetic Theory in Stochastic Media," *J. Math. Physics*, **30**, 2948-2511 (1989).
G. Zimmerman and M. Adams, "Algorithms for Monte-Carlo Particle Transport in Binary Statistical Mixtures," *Trans. Am. Nucl. Soc.*, **64**, 287-288 (1991).

Boundary Effects with Continuous Slowing Down

- Even in pure CSD calculations (with no angular scattering and no energy-loss straggling), the algorithms showed effects from material boundaries.
- The CH algorithm did a new nearest-neighbor lookup to find the energy-dependent stopping-power data being used when a material boundary was encountered.
- All algorithms were not stopping electrons at the cutoff energy, but would allow them to slow down to some lower-energy checkpoint.
- In the revised algorithms, all are consistent on the CSD range of the electrons to the cutoff energy. (Electron deposition is not at a CSD range of 1.0 because the cutoff is not at zero energy.)

30 keV electrons on Si with a 1 keV cutoff

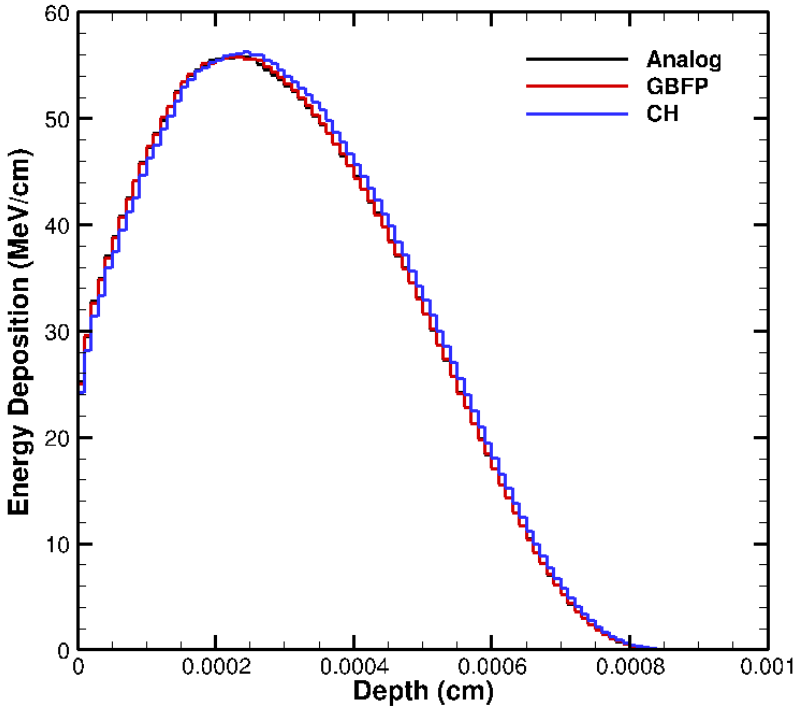




Energy Deposition Test Problem

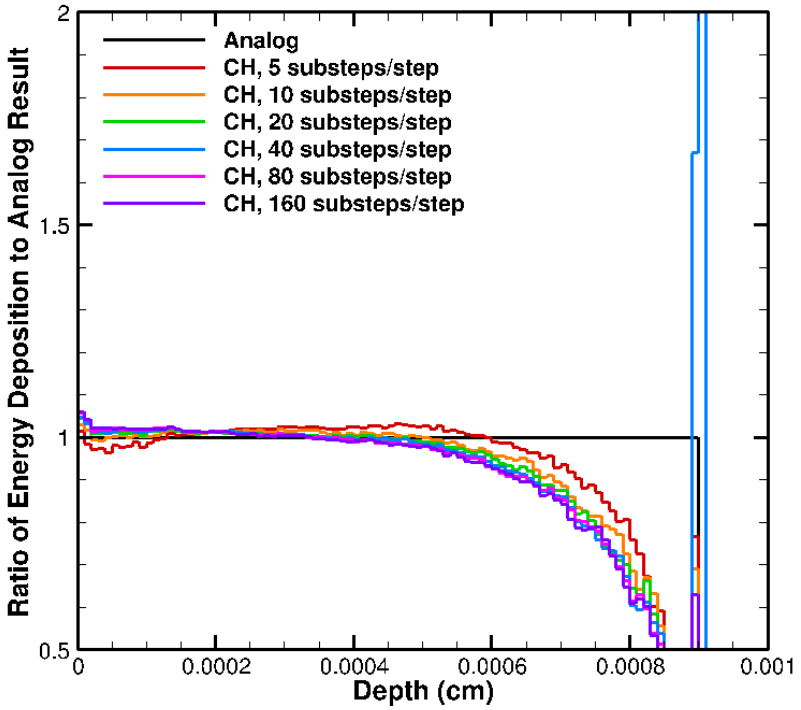
First test problem:

- Energy deposition from 30 keV electrons normally incident on Silicon.
- Angular scattering is modeled using only the screened Rutherford kernel.
- Continuous-slowing down (CSD) in energy for ionization and excitation.
- Bremsstrahlung production permits energy-loss straggling in the transport of the electrons.
- All photon transport is neglected. (Photons are deposited where created.)
- Knock-on electrons are produced and transported.



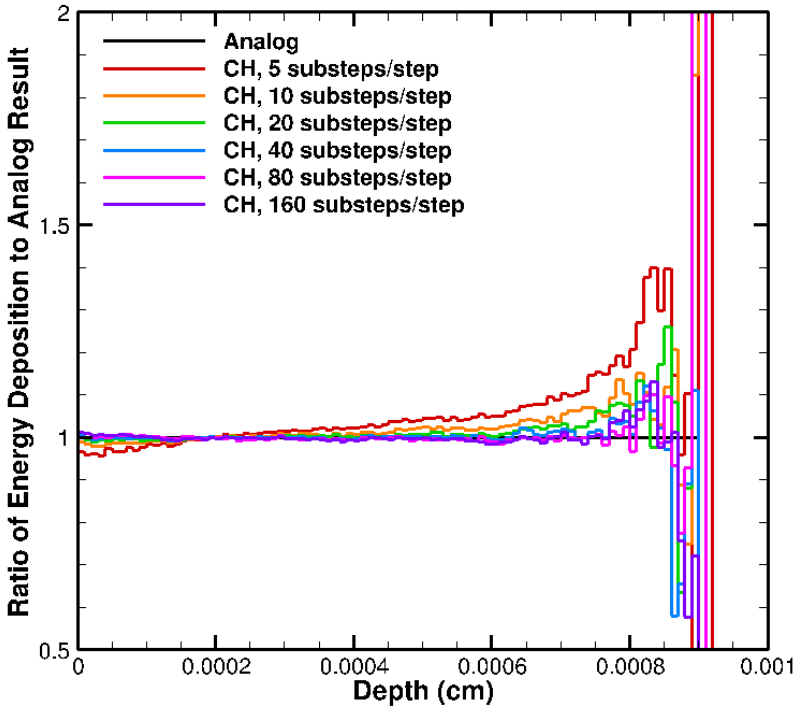
Condensed History Energy Deposition with No Material Boundaries (Old Algorithm)

- The condensed history results for this problem are compared with analog results.
- The default condensed history algorithm uses 5 substeps/step. The substep size is decreased by factors of 2.
- The condensed history results are incorrect and converge to an incorrect result due to the algorithm always continuing the "step" using the initial nearest-neighbor data despite energy loss during the step.
- In this case, the 30 keV energy does not coincide with a point on the energy grid on which data was precomputed.



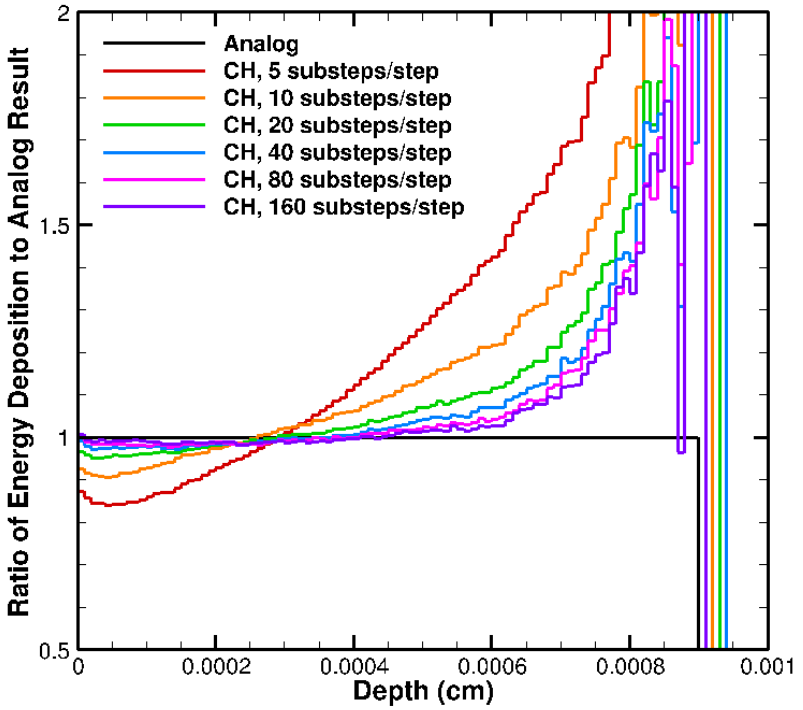
Condensed History Energy Deposition with No Material Boundaries (Old Algorithm with Improvement)

- Better results are achieved when the energy boundary is enforced. That is:
  - If the nearest-neighbor energy point changes during the substep, the substep is truncated.
  - The nearest-neighbor look-up is performed at the start of each substep. The nearest grid-point may change due to energy loss from a bremsstrahlung event.
- Decreasing substep size now converges to the analog result.



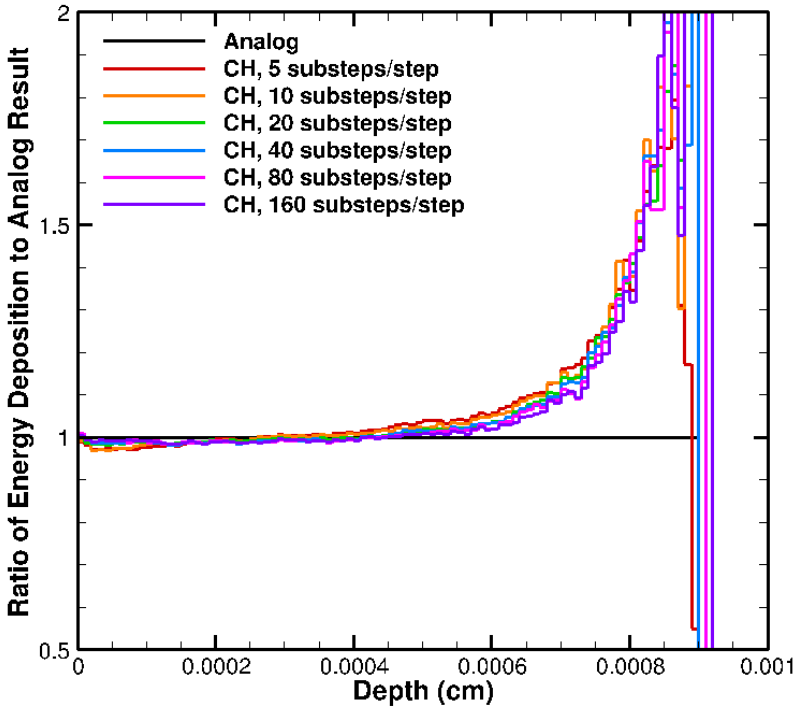
Condensed History Energy Deposition with Material Boundaries (Old Algorithm)

- Including artificial material boundaries introduced significant error. The CH is not converging to the correct result with decreasing substep size.
- This is due to two effects:
  - When a substep is truncated at a material boundary, the ETRAN model samples the angular deflection at the boundary. The algorithm uses rejection sampling to prohibit electrons from backscattering at this point.
  - To avoid geometry confusion, electrons are "pushed" off of a material boundary.



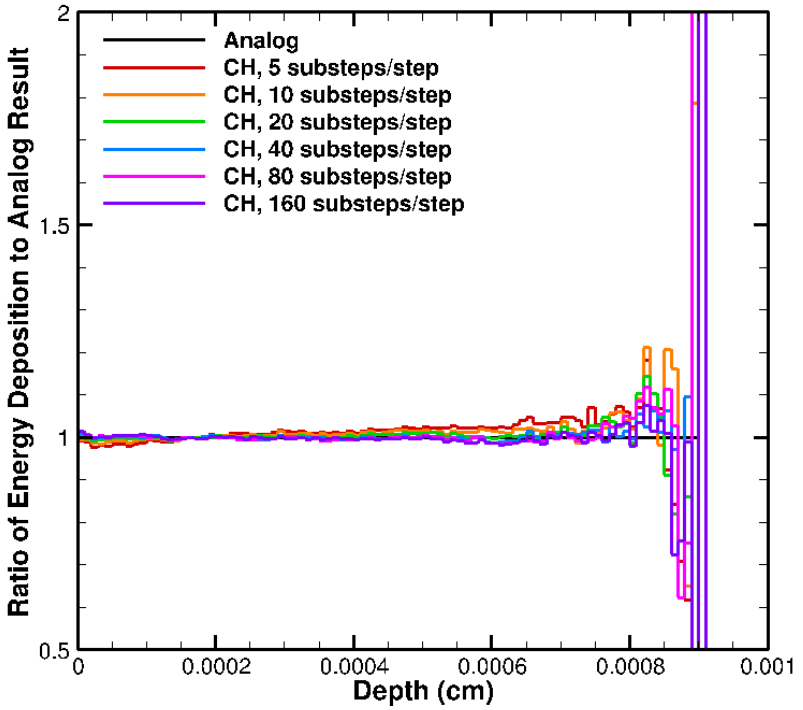
Condensed History Energy Deposition with Material Boundaries (Old Algorithm with Improvements)

- Removing the prohibition on backscatter at material boundaries improves agreement between results with large and small substep sizes, but the CH results are still converging to the same incorrect result.



Condensed History Energy Deposition with Material Boundaries (New Algorithm)

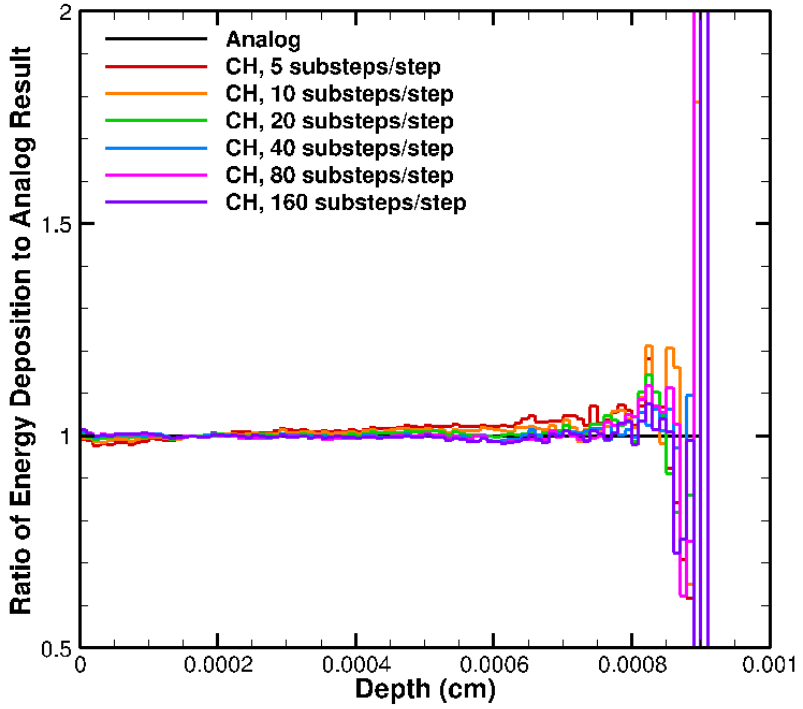
- The boundary "push" feature was the source of remaining error. Electrons are moved 1 nm off of the boundary in their direction of travel. With 100 boundaries over 10 μm, this had a discernible effect on the range of the electrons.
- The "push" feature is unnecessary in the 1D code.
- This feature is also unnecessary for algorithmic "boundary crossings", such as in the LP algorithm.
- The feature may not be necessary in the 3D code, but requires careful revision of the geometry-interrogation logic.



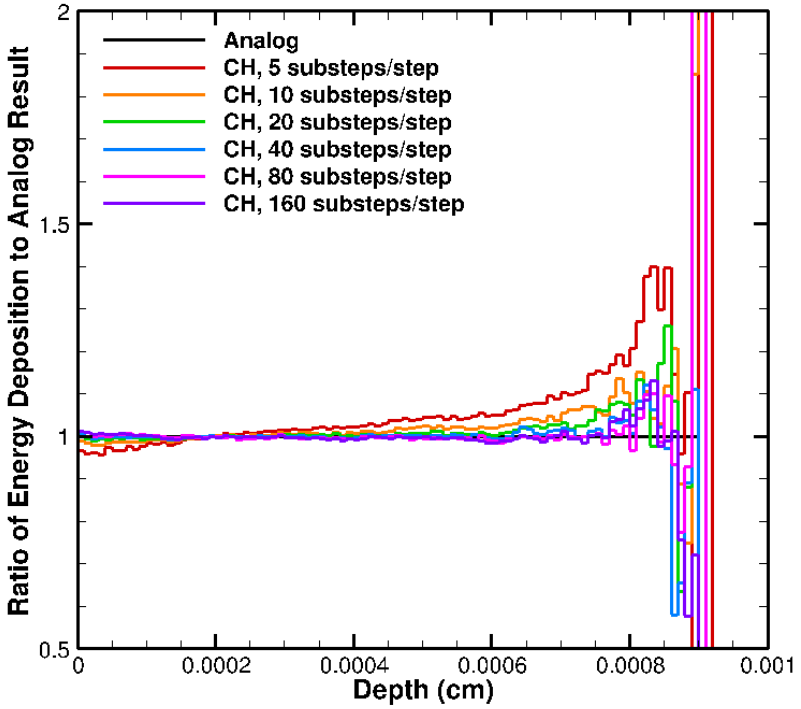
Condensed History Energy Deposition with and without Material Boundaries

The inclusion of material boundaries is now making the condensed history ***more accurate***! This is because in the revised algorithm the boundaries are reducing some of the substep sizes.

With Material Boundaries

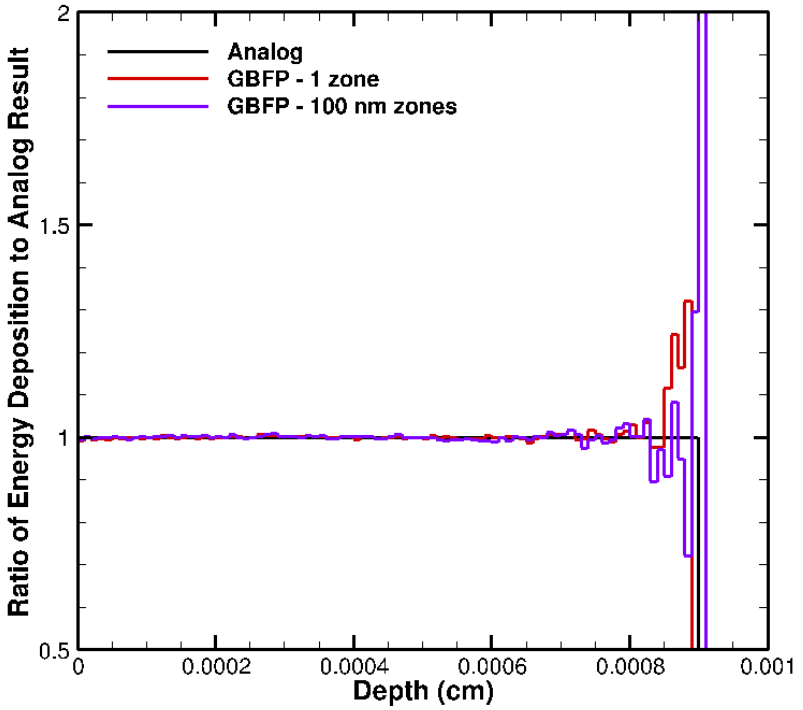


Without Material Boundaries



GBFP Energy Deposition

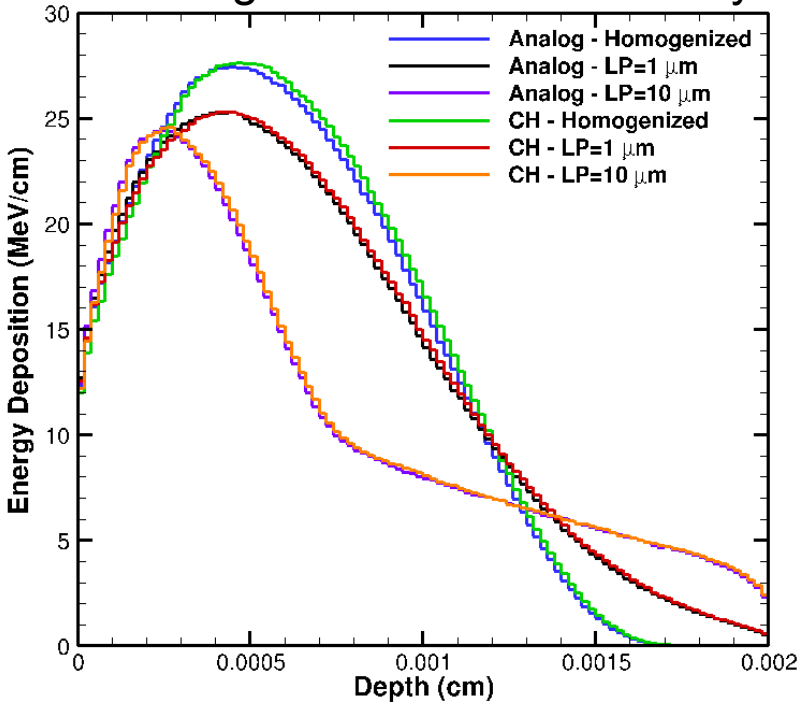
- The GBFP algorithm performs well on this test problem using the default scattering kernel parameters. Results appear to be within statistical agreement with and without material boundaries.



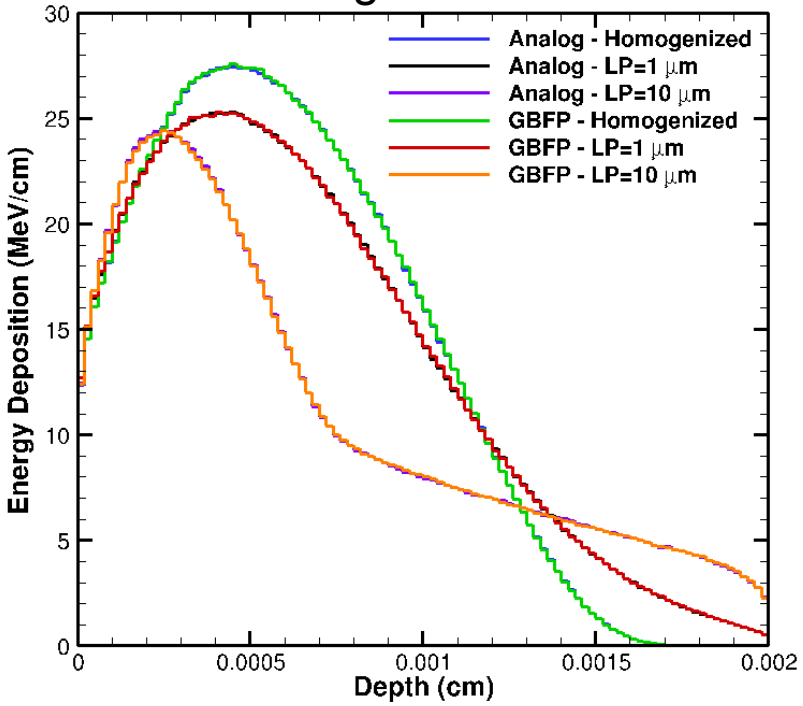
Energy Deposition Test Problem in a Stochastic Mixture

In a 50/50 stochastic mixture of silicon and nitrogen and varying mean chord lengths, both condensed history and GBFP using default parameters now provide reasonable agreement with analog results.

Analog vs. Condensed History



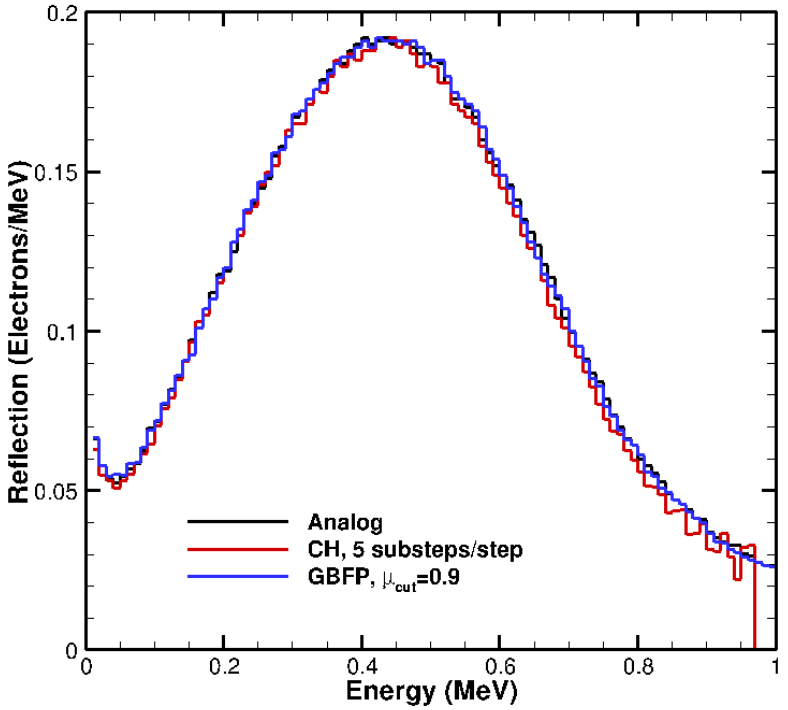
Analog vs. GBFP



Electron Reflection Test Problem

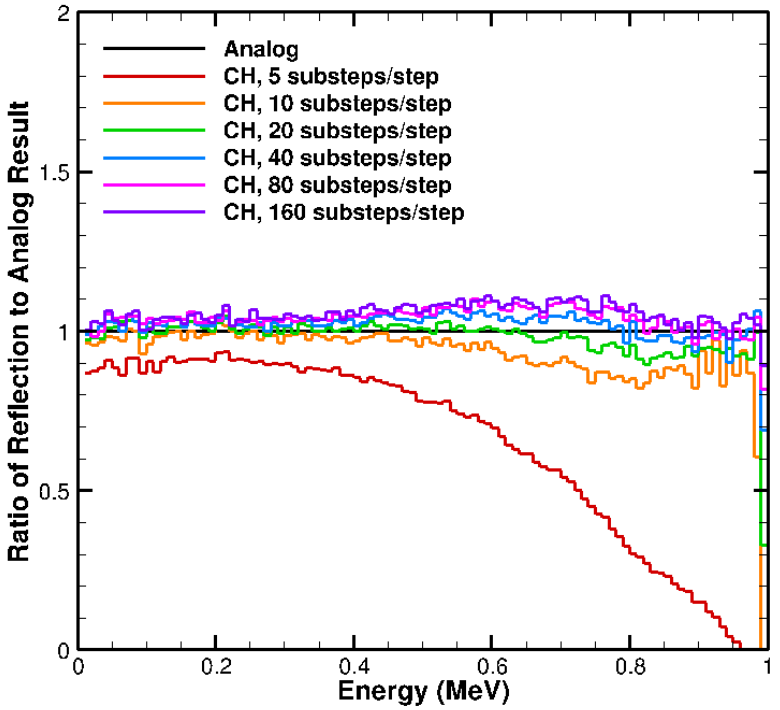
Second test problem:

- Reflected electron spectrum from a 1 MeV electron source normally incident on a thick silicon slab.
- Angular scattering is modeled using the screened Rutherford kernel.
- Continuous-slowing down (CSD) in energy for ionization and excitation.
- Bremsstrahlung production permits energy-loss straggling in the transport of the electrons.
- All photon transport is neglected. (Photons are deposited where created.)
- Knock-on electrons are produced and transported.



Condensed History Reflection with Material Boundaries (Old Algorithm)

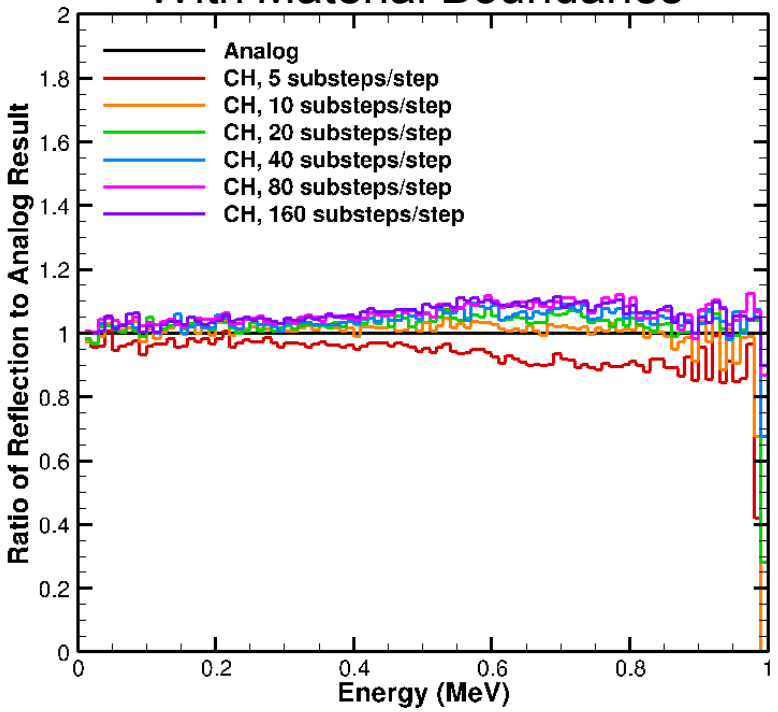
- Material boundaries were placed every 25 μm (compared to the electron range of 2.3 mm and default substep size of 232 μm at 1 MeV). Without improvements to the condensed history algorithm, the default substep size significantly underestimates electron reflection, especially at high energies.
- The condensed history algorithm is not converging to the analog results with decreasing substep size. The reason for this is not yet known. We suspect it is due to deficiencies in the convergence of the Goudsmit-Saunderson multiple-scattering distribution.



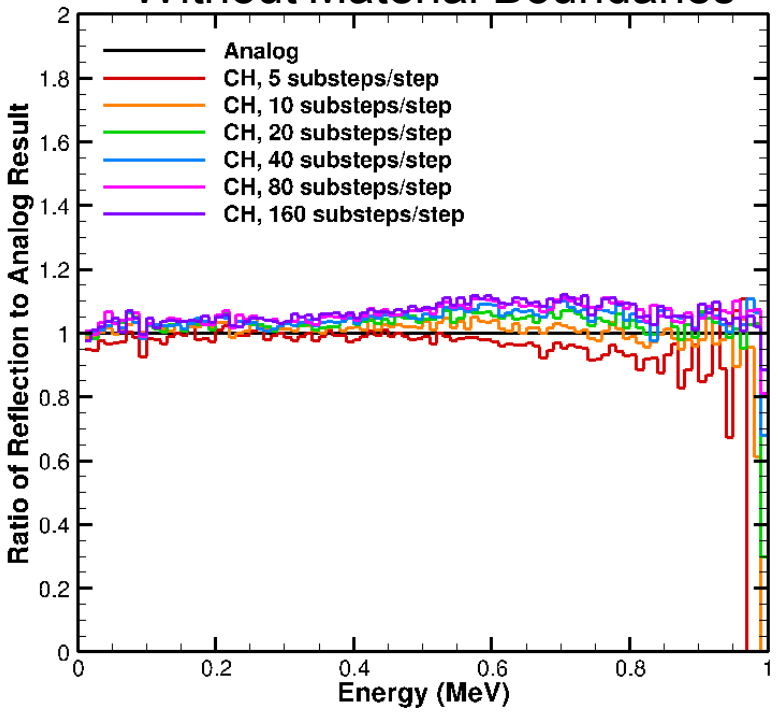
Condensed History Reflection with and without Material Boundaries (New Algorithm)

The previously described improvements in the condensed history algorithm improve performance with the default substep size, to nearly in agreement with simulations performed without boundaries.

With Material Boundaries



Without Material Boundaries

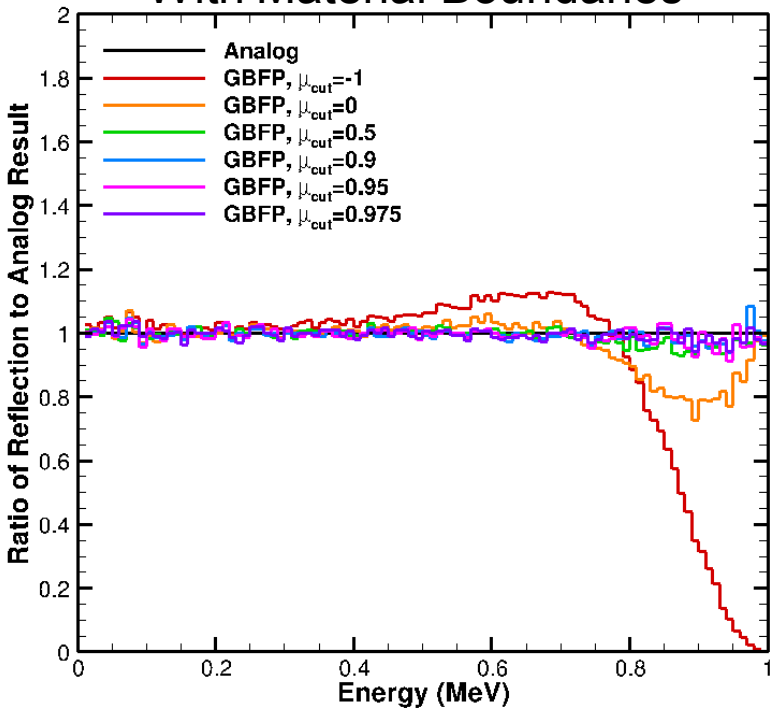


Persistent error at high energies is a result of the ETRAN hinge-at-the-end model.

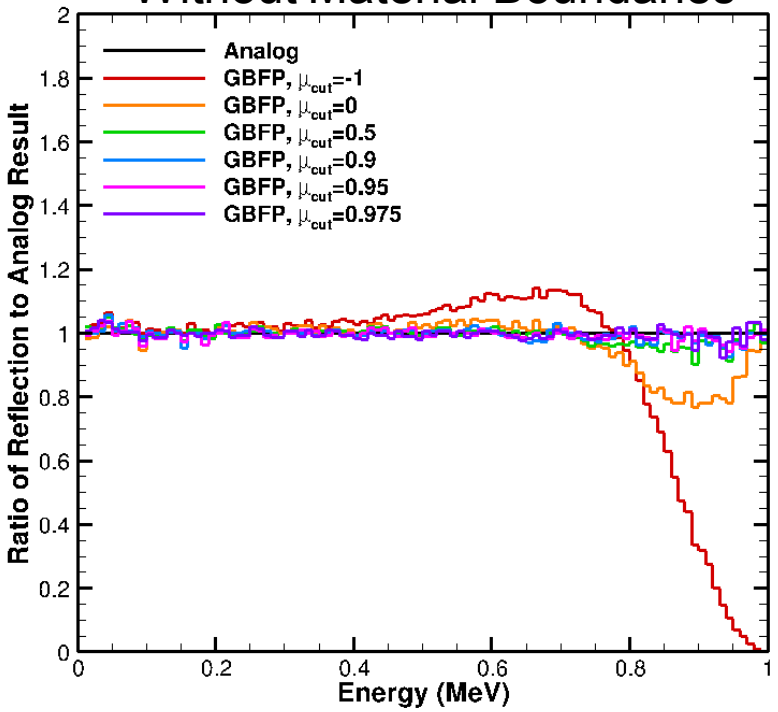
GBFP Reflection with and without Material Boundaries

The GBFP method with default parameters yields good agreement with analog results on this problem. Backing off to a higher cutoff angle or a scattering kernel with one discrete deflection angle does degrade the results.

With Material Boundaries



Without Material Boundaries



Runtime Comparisons

Runtime in Seconds/History

Problem:	30 keV Silicon		1 MeV Silicon	
Method	No Boundaries	100 Boundaries	No Boundaries	100 Boundaries
Analog	6.27E-4	9.58E-4	5.34E-3	1.15E-2
CH	9.33E-4	1.24E-3	9.70E-5	7.23E-4
GBFP	2.98E-4	3.84E-4	1.53E-4	8.64E-4

Speedup (Ratio of Analog Runtime to Method Runtime)

Problem:	30 keV Silicon		1 MeV Silicon	
Method	No Boundaries	100 Boundaries	No Boundaries	100 Boundaries
CH	0.67	0.77	55	16
GBFP	2.1	2.5	35	13

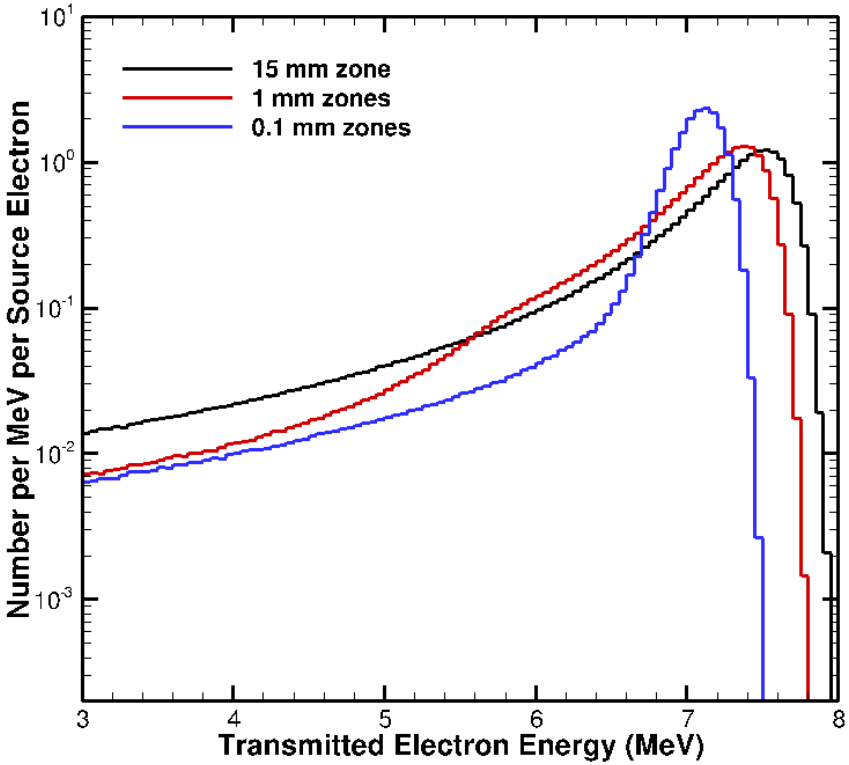
Caveats: Runtimes are given for default method parameters. A more rigorous comparison should vary parameters and evaluate error versus runtime. CH was showing greater error for default parameters. CH is a true production capability that may be burdened by greater overhead expenses.

Condensed History Energy-Loss Straggling (Old Algorithm)

We have reproduced results previously obtained by Grady Hughes in MCNP.

The transmitted electron spectrum is shown for 10 MeV electrons through 15 mm of water without angular scattering and without production of secondary particles.

A structured grid of material boundaries causes the old algorithm to produce poor results. Energy-loss straggling in this algorithm was sampled based on a step distance. When the step was truncated due to a material boundary, the algorithm obtained the correct mean energy loss, but underestimated the straggling.

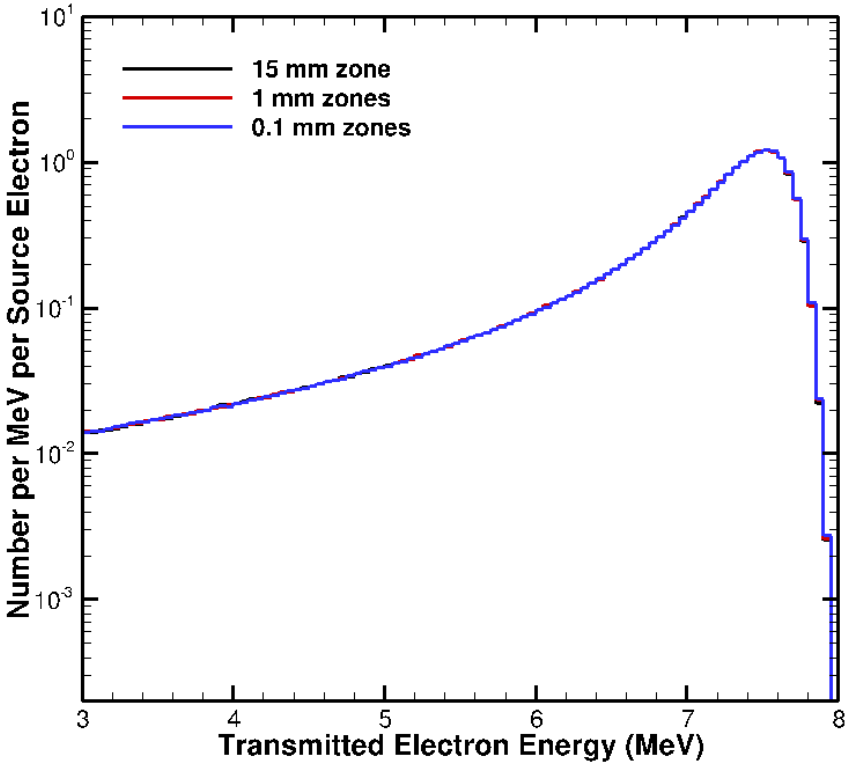


H. Hughes, "Improved Logic for Sampling Landau Straggling in MCNP5," *Proc. Mathematics and Computation, Supercomputing, Reactor Physics, and Nuclear and Biological Applications (M&C 2005)*, Palais des Papes, Avignon, France, September 12–15, 2005.

Condensed History Energy-Loss Straggling (New Algorithm)

The revised algorithm samples the energy-loss straggling based on a predetermined distance to be travelled, either a substep distance or the distance to a material boundary.

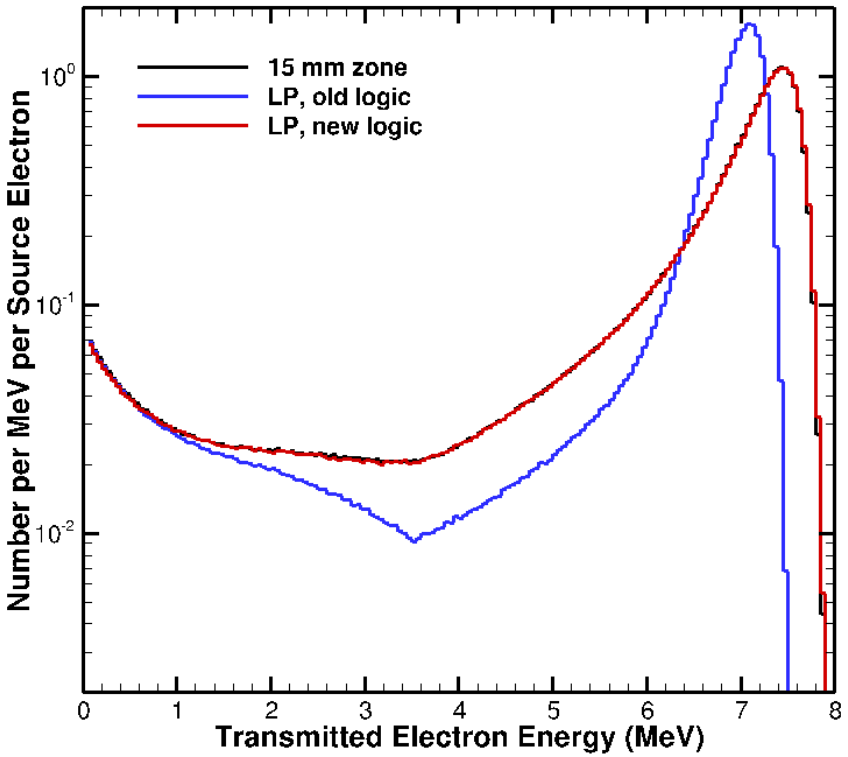
This uses Seltzer's correction to the Landau-Blunck-Leisgang energy-loss straggling. Seltzer provided an approach to scale the energy-loss sampling as a function of distance travelled. That logic has been used for escaping electrons in ITS, but is now applied for each substep. In addition, almost all data is now calculated on-the-fly based on the electron energy, rather than precalculated on an energy grid.



Condensed History Energy-Loss Straggling in a Stochastic Mixture

Hughes' test problem was adapted to include the Levermore-Pomraning closure (exponentially distributed material boundaries) and mean chord lengths of 0.1 mm. This version of the test also includes the production of knock-on electrons.

Consistent with the test using structured material boundaries, the old algorithm introduced significant error but the new algorithm provides excellent agreement with results obtained without material boundaries.



Summary and Future Work

- Improvements in the boundary crossing logic in the ITS condensed history algorithm have been made. It appears that reasonable results can now be obtained in many stochastic-media problems.
  - These assessments were performed in the 1D code. Assessment in the 2D or 3D codes has not been performed.
  - Elimination of the boundary "push" feature requires improvements in the 3D geometry logic, though that may not be required for the Levermore-Pomraning (or chord-length sampling) approach to stochastic media.
- Efforts are underway to implement production capabilities for analog and GBFP electron transport in ITS.

Acknowledgement

- Thanks to John Jones for performing much of the work in implementing the existing analog electron transport capability in ITS.