A Generalized Boltzmann Fokker-Planck (GBFP) Electron Transport Method

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Overview

GBFP Angular Scattering Approximations

- Discrete
- Hybrid-Discrete
- Hybrid-Exponential

Condensed History (CH) Algorithms

3-Dimensional Simulation (2-Dimensional Results) with a Material Interface

- High-energy electrons in low-Z materials
  - highly anisotropic scattering
- Low-energy electrons in high-Z materials
  - weakly anistropic scattering

Motivation

- **Current electron transport Monte Carlo algorithms are condensed history**
  - This is the scheme implemented in Sandia's electron-photon Monte Carlo code, ITS or the Integrated-TIGER-Series
  - Aggregation of many scattering interactions into an un-transport-like step or linear displacement
  - Known deficiencies, especially at boundary crossings
- **Provide an alternative to condensed-history in our production code, ITS**

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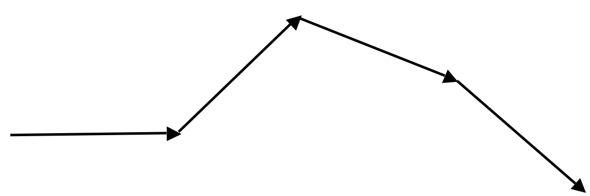
Condensed History and Transport Monte Carlo Algorithms

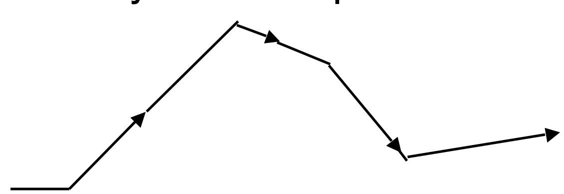
Condensed History Algorithms

Apply an infinite medium angular 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

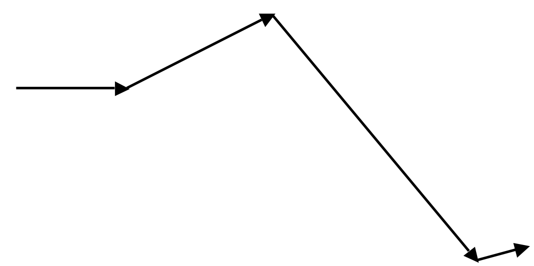


- Angular sampling from a multiple-scattering distribution

Transport Algorithms

Solve Boltzmann transport equation with approximate cross sections.

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

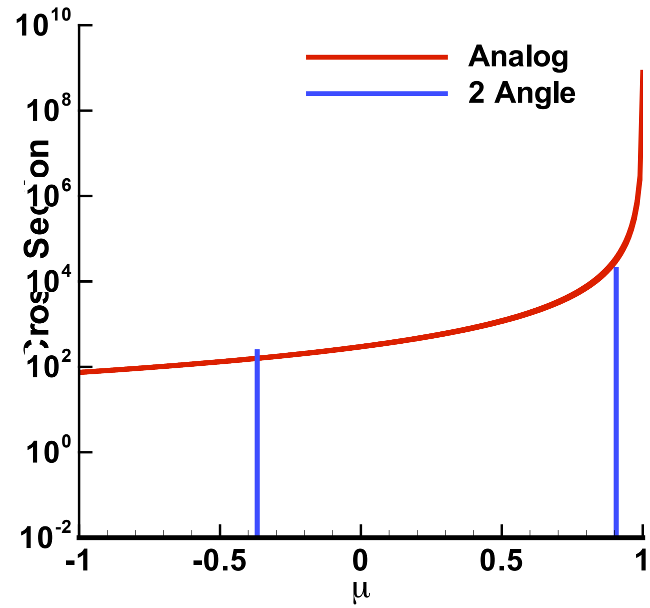


- Angular sampling from analytical, multiple-scattering, discrete, or other distribution

Discrete-Angle Scattering Model for Elastic Electron Scattering

The discrete scattering kernel is:

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



α_n **are amplitudes**

ξ_n **are scattering cosines**

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

Solving by Newton iteration and solving by Sloan's method yield identical results.

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).

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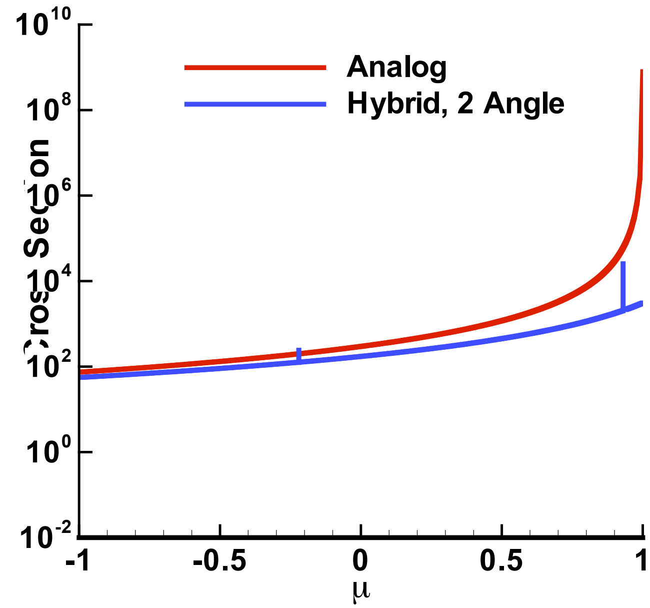
Hybrid/Discrete Angle Scattering Model for Elastic Electron Scattering

The hybrid/discrete scattering kernel is:

$$\tilde{\sigma}_s(\vec{r},\mu_0) = \sum_{n=1}^{N} \frac{\alpha_n(\vec{r})}{2\pi}\delta[\mu_0 - \xi_n(\vec{r})] + \frac{\sigma_{s0}(\vec{r})}{2\pi}\frac{2\eta(\vec{r})\{1+\eta(\vec{r})\}}{\{1+2\eta^*(\vec{r})-\mu_0\}^2}$$



α_n are amplitudes

ξ_n are scattering cosines

η^* is a larger screening parameter than the analog value, η

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

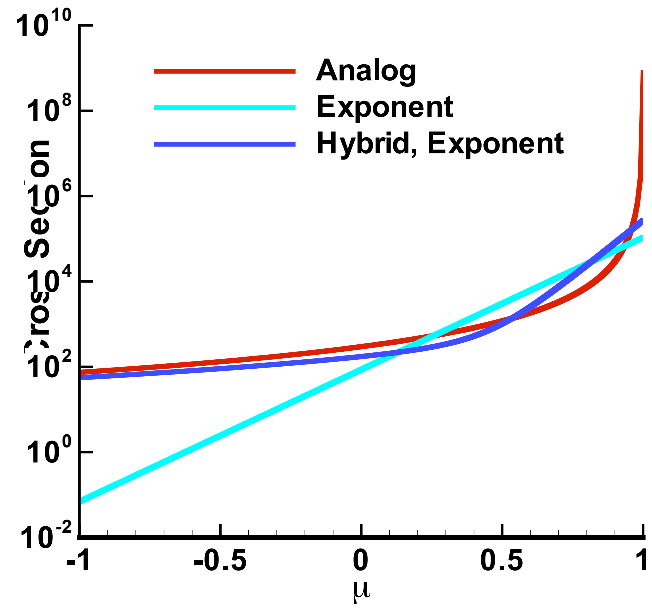
This is solved using Sloan's method.

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).

Hybrid/Exponential Scattering Model for Elastic Electron Scattering

Hybrid/exponential scattering kernel:

$$\tilde{\sigma}_s(\vec{r},\mu_0) = \frac{A(\vec{r})}{2\pi}\exp\left[-B(\vec{r})(1-\mu)\right] + \frac{\sigma_{s0}(\vec{r})}{2\pi}\frac{2\eta(\vec{r})\{1+\eta(\vec{r})\}}{\{1+2\eta^*(\vec{r})-\mu_0\}^2}$$



- η^* is a larger screening parameter than the analog value, η
- *A* and *B* are calculated to preserve two residual momentum transfer moments

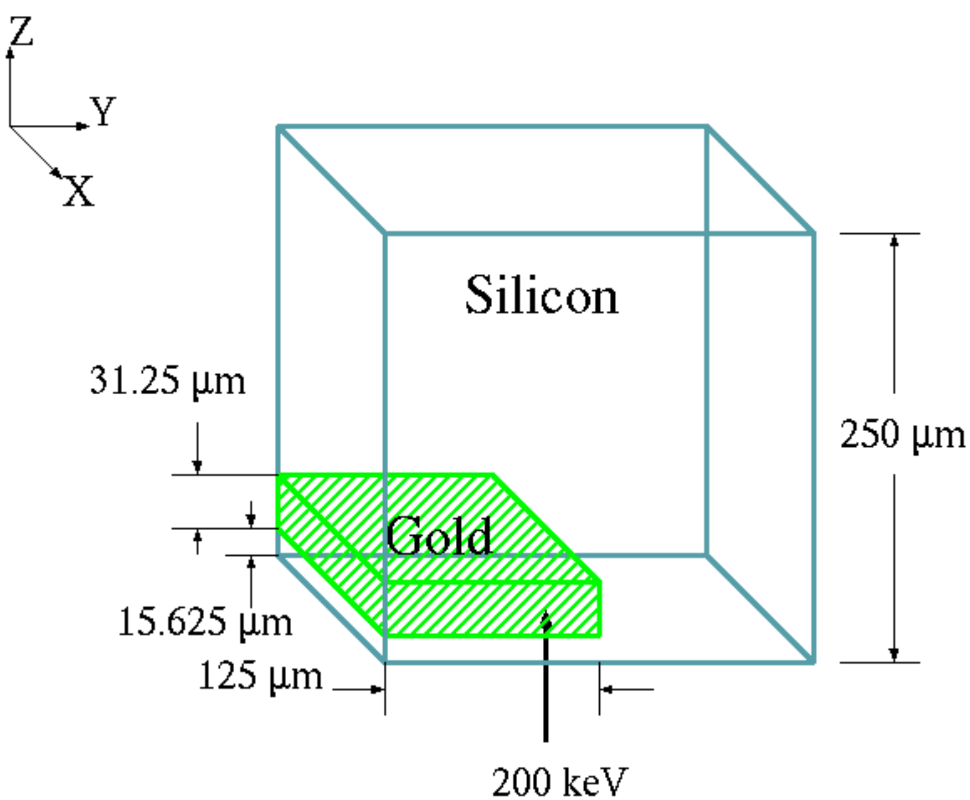
Simplifications for Assessing These Methods

Simplifications for all of our calculations:

- Continuous Slowing-Down (CSD) in energy
- Electron-only simulations without secondary electrons
- Screened Rutherford angular scattering
- These simplifications are not required for the GBFP approach. They are being made to isolate the effects of the approximations.
- We have implemented simple material boundary crossing algorithms for all methods.
  - For GBFP and analog, we preserve distance in mean free paths between interactions. This is the proper transport treatment.
  - For CH, we preserve fractional step-sizes between materials. This is an approximation.

Pencil-Beam Incident on a Block, Gold imbedded in Silicon, 200 keV electrons

The pencil beam is normally incident at the midpoint of the bottom of the block.



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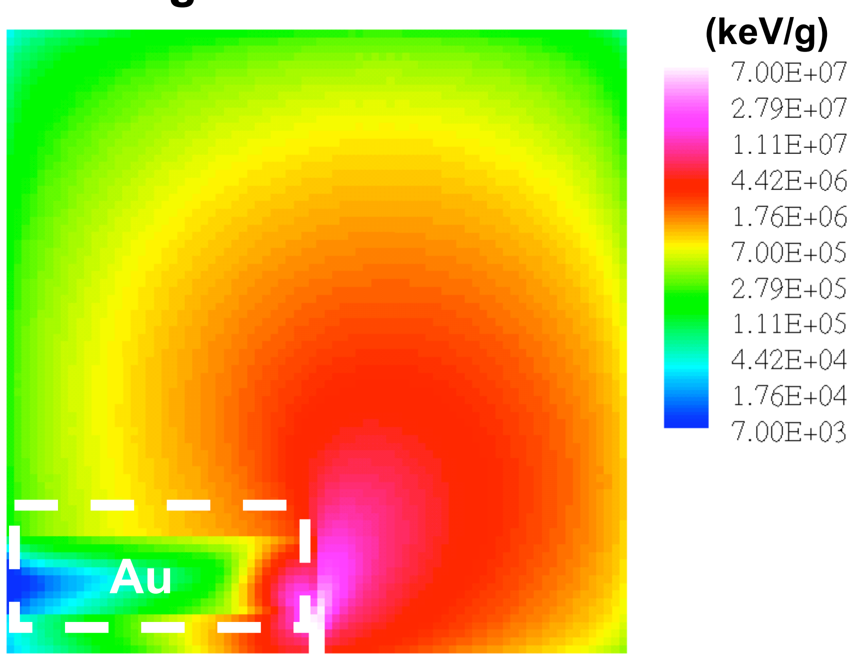
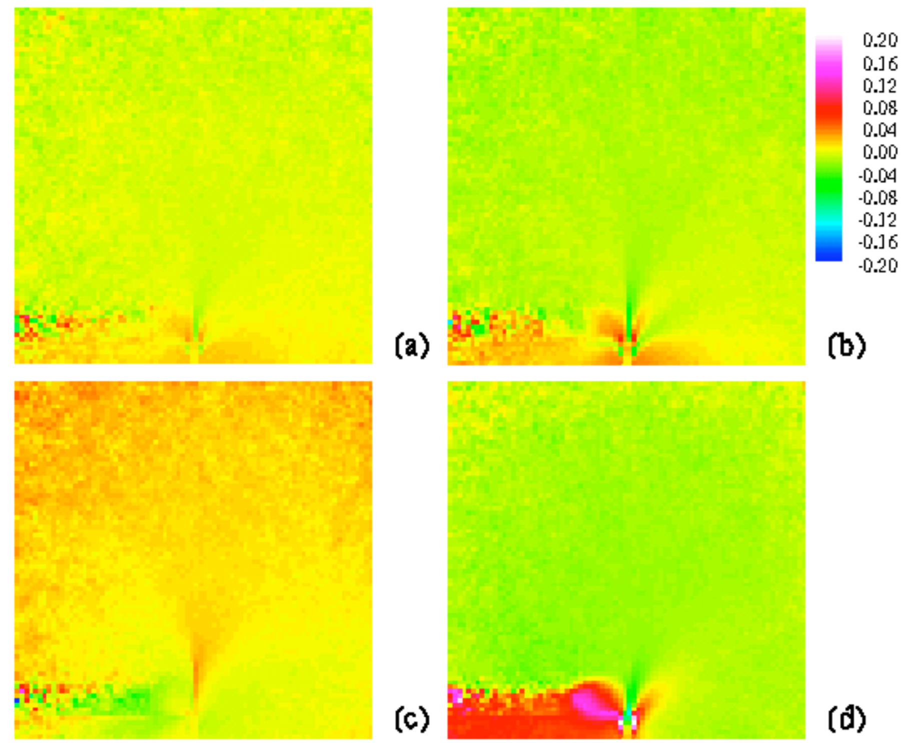
200 keV Electrons Incident on Silicon and Gold

Analog Benchmark Dose



Relative Difference with Benchmark

Hybrid-Discrete **Hybrid-Exponential**



Random Hinge **ITS-like Algorithm**

The relative differences in the approximate methods are shown for 4 calculations requiring approximately the same runtime and using the same number of particles.

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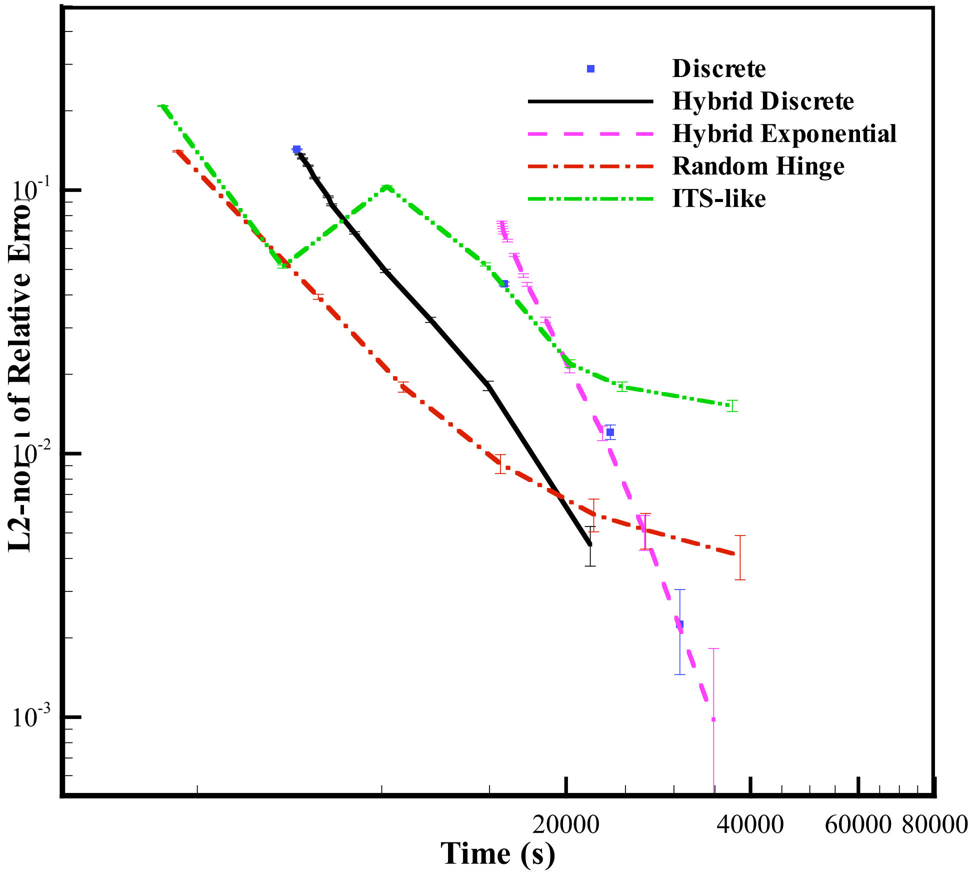
200 keV Electrons Incident on Silicon and Gold

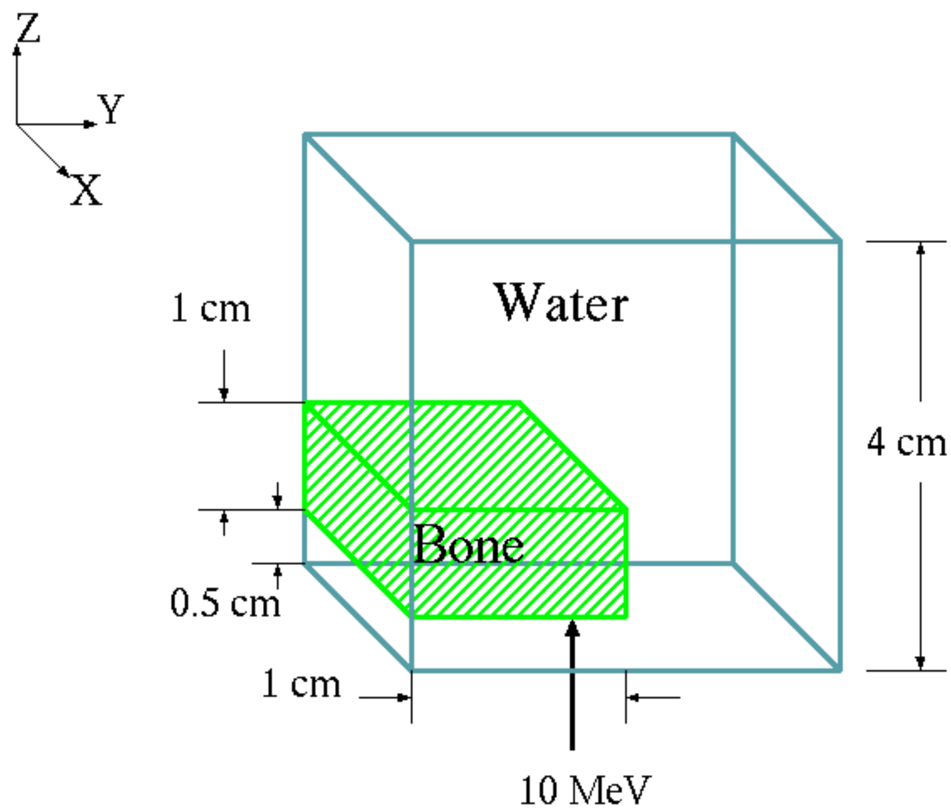
Relative Error vs. Runtime



A parameter was varied in each of the approximate methods to increase accuracy and increase runtime (e.g., substep size, discrete angles, smooth mean free path).

Pencil-Beam Incident on a Block, Bone Imbedded in Water, 10 MeV electrons

The pencil beam is normally incident
at the midpoint of the bottom of the block.



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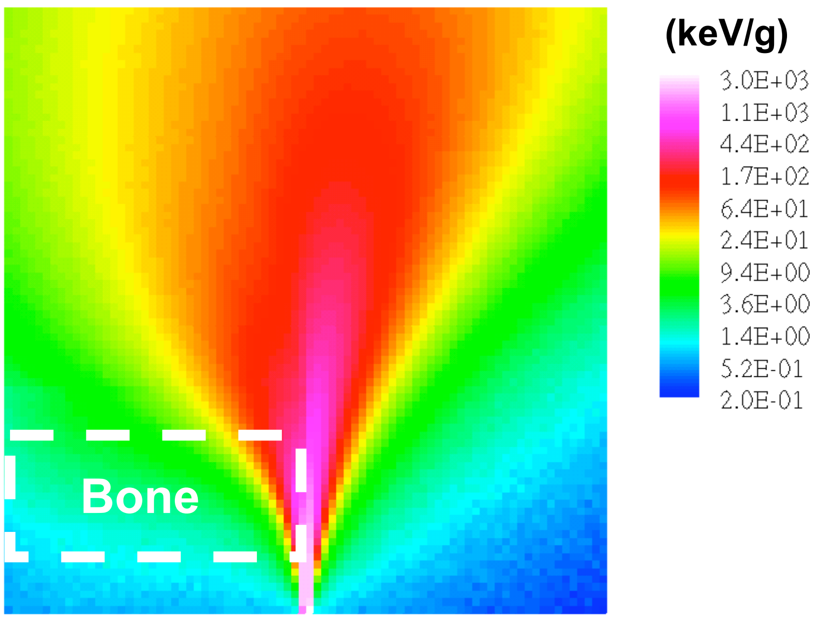
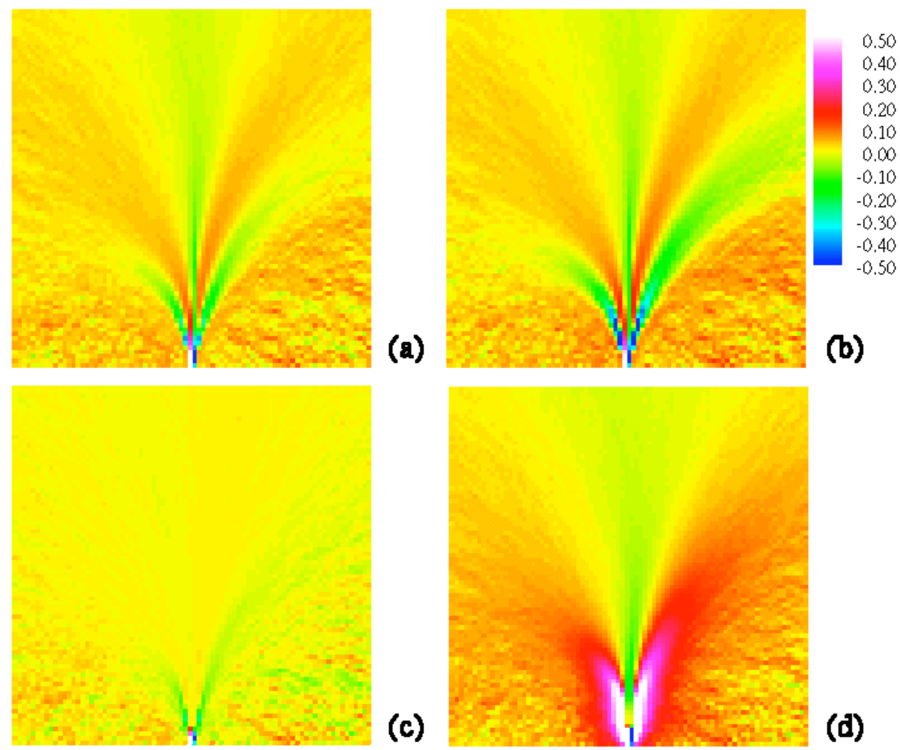
10 MeV Electrons Incident on Water and Bone

Analog Benchmark Dose



Relative Difference with Benchmark

Hybrid-Discrete | Hybrid-Exponential

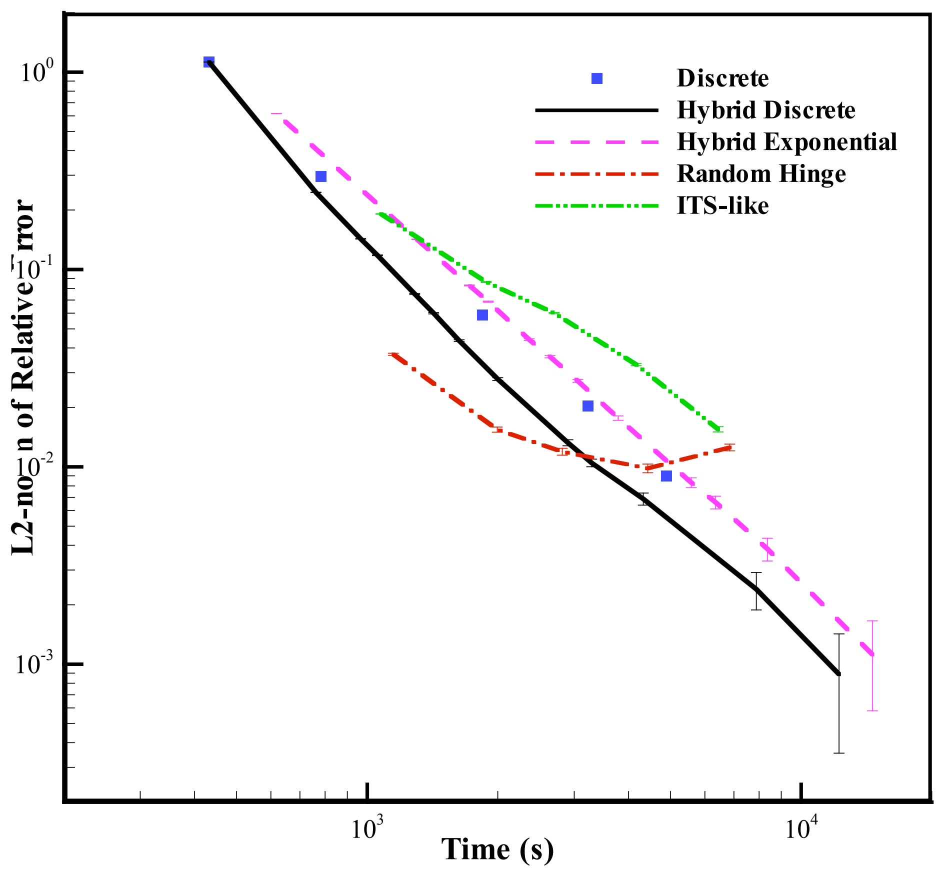


Random Hinge | ITS-like Algorithm

The relative differences in the approximate methods are shown for 4 calculations requiring approximately the same runtime and using the same number of particles.

10 MeV Electrons Incident on Water and Bone

Relative Error vs. Runtime



A parameter was varied in each of the approximate methods to increase accuracy and increase runtime (e.g., substep size, discrete angles, smooth mean free path).

Summary / Future Efforts

- **GBFP is a viable alternative to CH**
- **Implement GBFP in ITS for general use**
  - **Users will have an option of selecting GBFP or CH**
  - **Energy-loss Treatment**
    - » **Similar Approaches Can Be Applied**
    - » **Lee Harding and Anil Prinja are developing this.**
  - **Implement more realistic physics**
    - » **We Are Developing Mott Angular Scattering for Hybrid Methods**
    - » **Secondary particle production issues (e.g. bremsstrahlung) need to be integrated into GBFP for general purpose.**