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A Geant4 Implementation of a Novel Single-Event Monte Carlo Method for Electron Dose Calculations

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Outline

1. Introduction
   - Analog Monte Carlo Electron Transport Calculations
   - Practical Solutions to the EBTE
   - Geant4 Physics
2. Results
   - One-Dimension
   - Two-Dimensions
3. Wrap-up
   - Conclusion
   - Questions?

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Boltzmann Transport Equation for Electrons (EBTE)

- Applications: Space Physics, Accelerator Physics, Medical Physics, Shielding, etc.
- Quantities of Interest: Dose, Charge Deposition, Energy and Angular Spectrum, etc.
- Monte Carlo Solutions to the CPBTE
  - Exact Within Statistics
  - Computationally Prohibitive

$$\begin{aligned}\vec{\Omega} \cdot \nabla\psi(\vec{r}, E, \vec{\Omega}) + [\Sigma_{s0}(\vec{r}, E) + \Sigma_{e-0}(\vec{r}, E)]\psi(\vec{r}, E, \vec{\Omega}) \\ = \int_{4\pi} d\Omega' \Sigma_s(\vec{r}, E, \vec{\Omega}' \cdot \vec{\Omega})\psi(\vec{r}, E, \vec{\Omega}') \\ + \int_{Q_{min}}^{Q_{max}} dQ \Sigma_{e^-}(\vec{r}, E', Q)\psi(\vec{r}, E + Q, \vec{\Omega})\end{aligned} \tag{1}$$

$$\psi(\vec{r}_s, E, \vec{\Omega}) = \delta(\vec{\rho} - \vec{\rho}_s)\delta(1 - \vec{\Omega} \cdot \vec{\Omega}_0)\delta(E - E_0) \tag{2}$$

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An analog Monte Carlo algorithm

1. Generate source particle
2. Sample distance to collision
3. Determine collision type
4. Sample collision outcome
5. Repeat (accumulate necessary tallies)

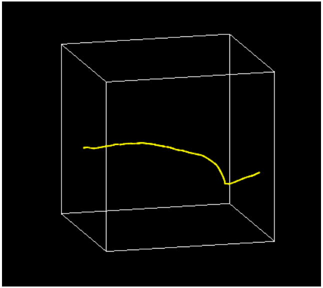

Figure 1 : Trajectory for 1 MeV Electron in Gold

Why is the EBTE Computationally Prohibitive?

- The Screened Rutherford Cross Section

$$\Sigma_s(E,\mu_0) = N\frac{2\pi r_e^2 Z(Z+1)}{\beta^4\gamma^2}\frac{1}{(1-\mu_0+2\eta(E))^2} \tag{3}$$

- The Total Screened Rutherford Angular Deflection Cross Section

$$\Sigma_{s0}(E) \sim \frac{1}{\eta(E)}\ ,\ 10^{-7} < \eta < 10^{-3}$$

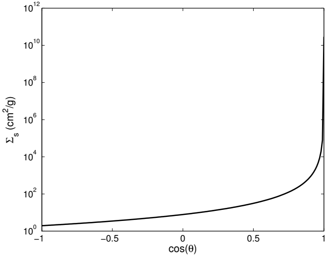

Figure 2 : Screened Rutherford Cross Section for 1 MeV Electrons in Carbon

Why is the EBTE Computationally Prohibitive?

- Rutherford Energy Loss Cross Section

$$\Sigma_{e^-}(E,Q) = N\frac{2\pi r_e^2 Zmc^2}{\beta^2}\frac{1}{Q^2}, \tag{4}$$

- The Mean Energy Loss Per Collision

$$\frac{S(E)}{\Sigma_{e^-0}(E)} \sim ln\left(\frac{Q_{max}}{Q_{min}}\right) Q_{min} << 1 \tag{5}$$

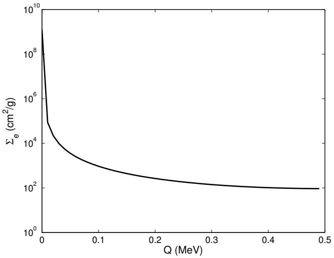

Figure 3 : Moller Cross Section for 1 MeV Electrons in Carbon

Condensed History/Multiple-Scattering Methods (CH/MS)

- CH/MS has error inherent to the method $\sim$ step size
- Boundary crossing issues
- Imposing step limitations improves accuracy but at the cost of efficiency

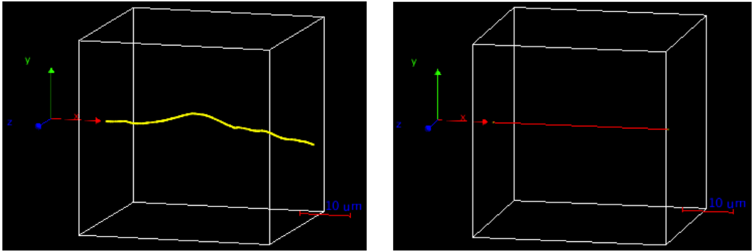

Figure 4 : Comparison of Physics Models over a Step

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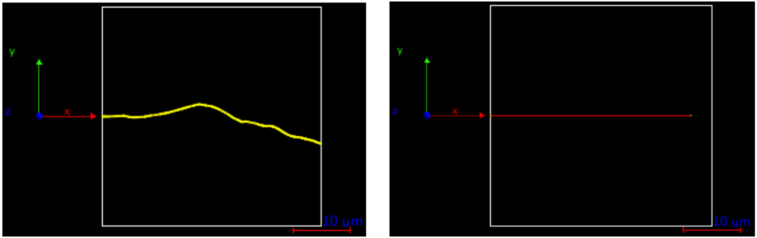

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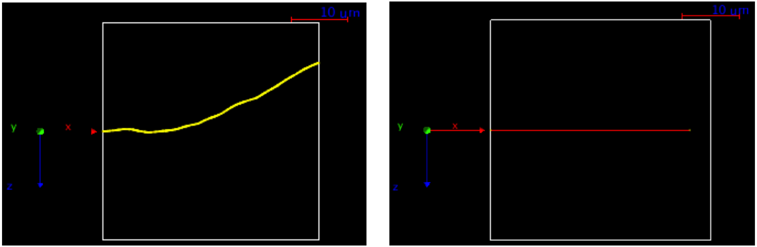


Figure 4 : Comparison of Physics Models over a Step

An Alternative to CH/MS Methods

- The analog EBTE

$$\vec{\Omega}\cdot\nabla\psi(\vec{r},E,\vec{\Omega})+[\Sigma_{s0}(\vec{r},E)+\Sigma_{e-0}(\vec{r},E)]\psi(\vec{r},E,\vec{\Omega}) = \int_{4\pi} d\Omega'\Sigma_s(\vec{r},E,\vec{\Omega}'\cdot\vec{\Omega})\psi(\vec{r},E,\vec{\Omega}') + \int_{Q_{min}}^{Q_{max}} dQ\Sigma_{e^-}(\vec{r},E',Q)\psi(\vec{r},E+Q,\vec{\Omega}) \qquad (6)$$

$$\psi(\vec{r}_s,E,\vec{\Omega}) = \delta(\vec{\rho}-\vec{\rho}_s)\delta(1-\vec{\Omega}\cdot\vec{\Omega}_0)\delta(E-E_0) \qquad (7)$$

An Alternative to CH/MS Methods

- An approximation to analog EBTE

$$\vec{\Omega}\cdot\nabla\psi(\vec{r},E,\vec{\Omega})+[\tilde{\Sigma}_{s0}(\vec{r},E)+\tilde{\Sigma}_{e-0}(\vec{r},E)]\psi(\vec{r},E,\vec{\Omega}) = \int_{4\pi} d\Omega'\tilde{\Sigma}_{s}(\vec{r},E,\vec{\Omega}'\cdot\vec{\Omega})\psi(\vec{r},E,\vec{\Omega}') + \int_{Q_{min}}^{Q_{max}} dQ\tilde{\Sigma}_{e^-}(\vec{r},E',Q)\psi(\vec{r},E+Q,\vec{\Omega}) \quad (6)$$

$$\psi(\vec{r}_s,E,\vec{\Omega}) = \delta(\vec{\rho}-\vec{\rho}_s)\delta(1-\vec{\Omega}\cdot\vec{\Omega}_0)\delta(E-E_0) \quad (7)$$

- We know from Lewis theory that preserving legendre moments of the cross section is equivalent to preserving space-angle moments of the solution
- This provides an excellent starting point for determining $\tilde{\Sigma}$

What is the GBFP approximation?

- Based on concept of moment preservation
  - Moments capture physical properties
  - Systematically controllable accuracy (more moments→more accurate)
- Maintains true form of Boltzmann collision operator
  - Restores transport mechanics
  - Eliminates boundary crossing issues
- Single-scatter monte carlo
  - Easily plugs into existing single-scatter algorithms
  - Code overhaul/refactorization unnecessary
- Cross Section Models Currently Implemented
  - Discrete
  - Hybrid

GBFP Cross Section Generation

- Define Moment Operator M_l

$$M_l f(\mu_0) = 2\pi \int_{-1}^{1} P_l(\mu_0) f(\mu_0) d\mu_0 \tag{8}$$

- We do not require $\Sigma_s(E,\mu_0) = \tilde{\Sigma}_s(E,\mu_0)$ but rather

$$M_l \Sigma_s(E,\mu_0) = M_l \tilde{\Sigma}_s(E,\mu_0), \;\; l = 1, 2, ...2N \tag{9}$$

- The hybrid cross section has a smooth portion and discrete portion
    - Smooth defined from [-1,μ_{cut}]
    - Discrete defined from [μ_{cut},1]

$$M_l f(\mu_0) = 2\pi \int_{\mu_{cut}}^{1} P_l(\mu_0) f(\mu_0) d\mu_0 \tag{10}$$

The GBFP Cross Section

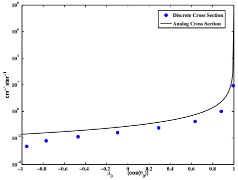
- What is a discrete cross section?

$$\tilde{\Sigma}_s(E,\mu_0) = \sum_{n=1}^{N} \frac{\alpha_n(E)}{2\pi} \delta[\mu - \xi_n] \qquad (11)$$

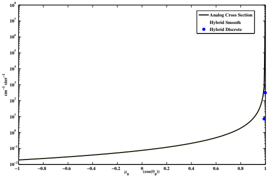
- What is a hybrid cross section?

$$\tilde{\Sigma}_s(E,\mu_0) = \begin{cases} \sum_{n=1}^{N} \frac{\alpha_n(E)}{2\pi} \delta[\mu_0 - \xi_n], & \mu_0 \in [\mu_{cut}, 1] \\ \Sigma_s(E,\mu_0), & \mu_0 \in [-1, \mu_{cut}) \end{cases}$$

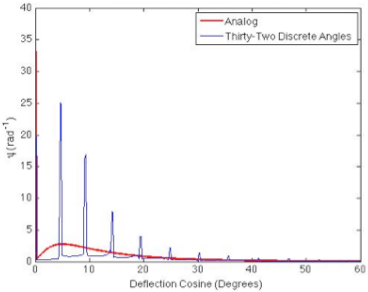
Discrete Cross Section



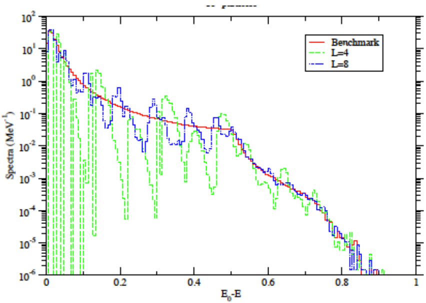
Hybrid Cross Section



Why Use Hybrid?



(a) Angular Distributions for 100 *keV* Electrons on Gold.



(b) Energy Spectrum Using Discrete.

Figure 6 : Demonstration of discrete artifacts resulting from the discrete cross section

GEANT4 Physics Models Modifications

- Some modifications were made to ensure all models are based on consistent cross sections
- G4UrbanMscModel95
  - Modified screening parameter and material constant
  - Turned-off transport cross section corrections
- G4MollerBhabhaModel
  - Modified definition of stopping power (default is Berger-Seltzer formula)

$$S(E) = \int_{Q_{min}}^{Q_{max}} Q\Sigma_{e^-}(E, Q)dQ \tag{12}$$

  - Turned off energy-loss fluctuations
- Step limitation parameter

$$s = F_r \cdot \max(R(E), \lambda_1), \tag{13}$$

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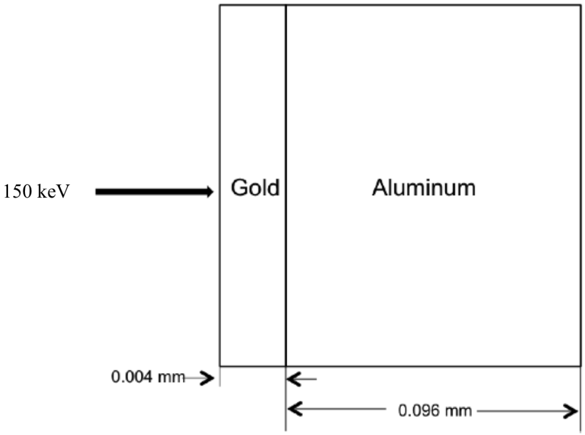
Low Energy Problem Setup



Low Energy Problem Results

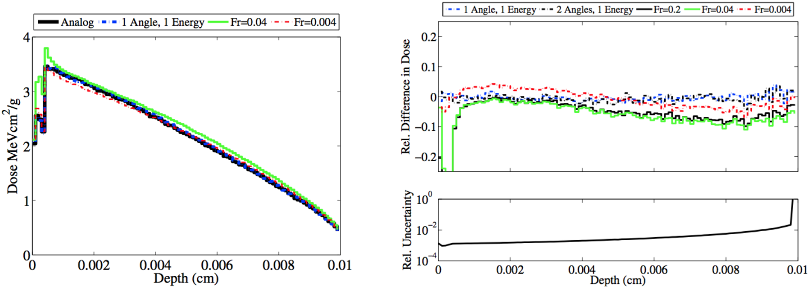
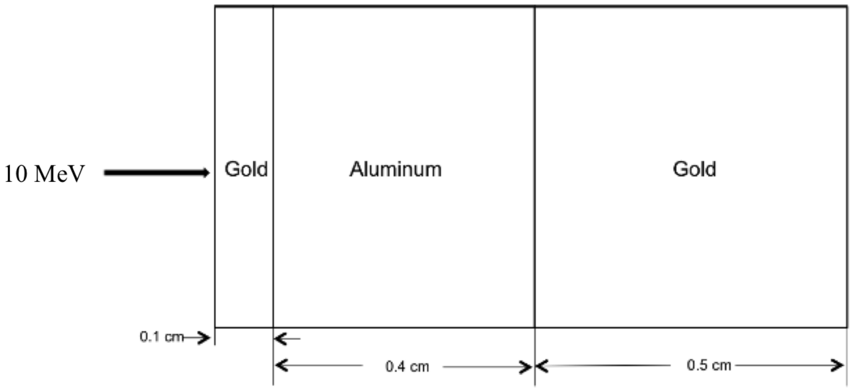


Figure 7 : Results for 150-keV electrons incident on Gold/Aluminum slab

High Energy Problem Setup



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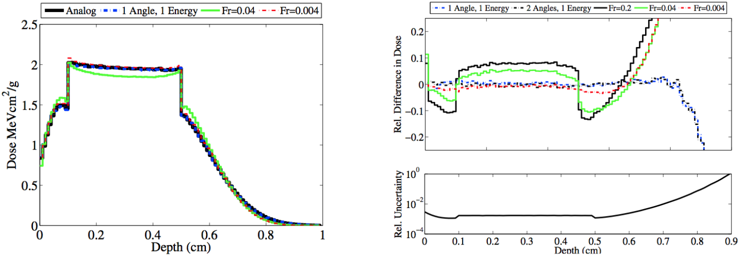


Figure 8 : Results for 10-MeV electrons incident on Gold/Aluminum/Gold slab

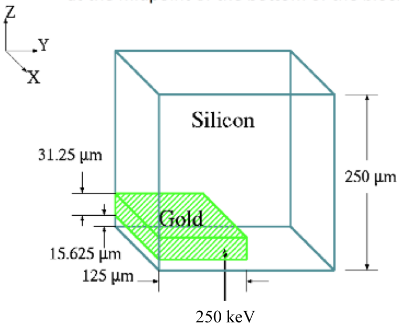
Speed-ups

Table 1: Efficiency of Tested Models

Model	Speedup Factor: 10-MeV on Au/Al/Au	Speedup Factor: 150-keV on Au/Al
1 angle, 1 energy	179.7	23.7
2 angles, 1 energy	84.9	15.8
Geant4, $F_r = 0.2$	178.2	10.3
Geant4, $F_r = 0.04$	163.5	10.2
Geant4, $F_r = 0.004$	76.9	7.3

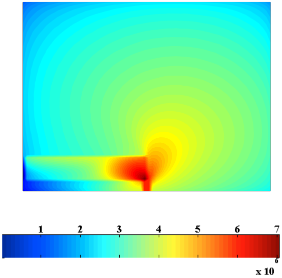
Low Energy Problem Setup

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



Low Energy Problem Results: GBFP and Geant4 Default EM Physics

Analog Benchmark



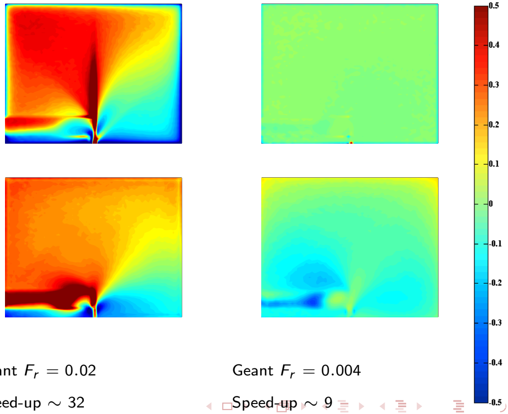
$\frac{keV}{g}$

Discrete 1 angle

Speed-up ∼35

Discrete 8 angles

Speed-up ∼9



Geant $F_r = 0.02$

Speed-up ∼ 32

Geant $F_r = 0.004$

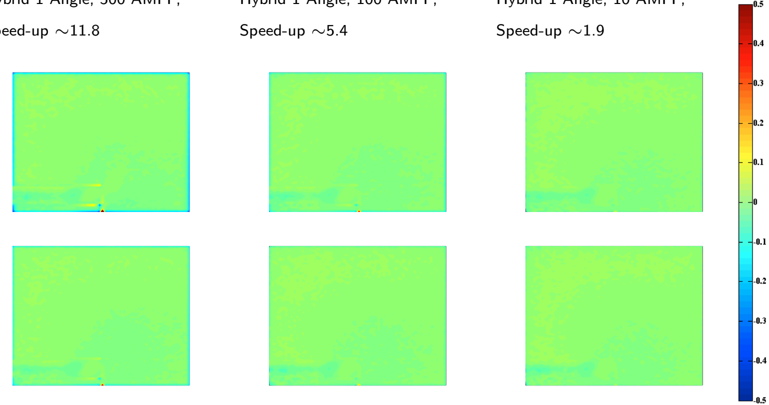
Speed-up ∼ 9

Low Energy Problem Results: The Hybrid Cross Section

Hybrid 1 Angle, 500 AMFP, Speed-up ∼11.8

Hybrid 1 Angle, 100 AMFP, Speed-up ∼5.4

Hybrid 1 Angle, 10 AMFP, Speed-up ∼1.9



Hybrid 2 Angles, 500 AMFP, Speed-up ∼5.8

Hybrid 2 Angle, 100 AMFP, Speed-up ∼2.9

Hybrid 2 Angle, 10 AMFP, Speed-up ∼1.5

Figure 10 : Two-d dose comparison for 250-keV electrons in Si/Au cube

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Conclusion

- GBFP provides a single-scatter alternative
- Transport mechanics are restored through use of GBFP
- Accuracy is controllable systematically and adaptively with the GBFP
- GBFP exceeded the speed and accuracy of Geant4 default EM physics
- A direct comparison with the Geant4 default EM physics is desirable
- Implementation of GBFP physics was straightforward
  - Pre-existing algorithms for transporting particles can be used
  - If single scatter model is available, most of the work is done
  - Cross section generation tools are needed

Questions?