Electron Mode in FRENSIE

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Electron Transport in FRENSIE

Forward Mode

- Condensed History
- Secondary Particles
- Atomic Relaxation
- Simulation of hard electron transport events
  - Atomic excitation
  - Hard elastic scattering
  - Electroionization
  - Bremsstrahlung

Adjoint Mode

- Hybrid Multigroup/Continuous-Energy Monte Carlo using Boltzmann-Fokker-Planck Equation (BFP)
- Other Possible Adjoint Methods

Electron Transport in Monte Carlo Codes

MCNP

- Historically has only used a condensed-history approached with Goudsmit-Saunderson multiple scattering techniques.
- MCNP6 implemented a single-event method for energies below 1 keV, were the condensed-history method no longer holds.

Penelope

- Implements a mixed method that simulates soft (condensed-history) events below a cutoff energy/angle and hard (single-events) above.

EGS

- Condensed History Method
- Historically used Molière Multiple Scattering Theory
- EGS5 implemented Goudsmit-Saunderson Multiple Scattering to take into account spin and relativistic effects needed in the MeV range

Electron Mode

FRENSIE

- Hard events implemented using cross-sectional data from MCNP6
- Condensed history method will be chosen in conjunction with an adjoint method
- Ultimately hope to implement a mixed method for forward transport

Current Capabilities

- Single Scattering Events from 100 GeV to 10 eV
- Elastic, Bremsstrahlung, Electroionization, Atomic Excitation
- Secondary particles created, but photons not tracked
- Atomic relaxation implemented

Known Issues

- Absorption at low energies
- Negative energy from Electroionization

Atomic Excitation

Reaction

- There is no angular deflection.
- There are no secondary particles.
- Only energy loss needs to be taken into account

Implementation

- Energy dependent electron energy loss are tabulated in ACE tables.
- No sampling is required for this process.

Hard Elastic Scattering

Reaction

- There is no energy loss.
- There are no secondary particles.
- Only angular deflection needs to be taken into account.

Implementation

- ACE tables provide histogram CDF of the outgoing angle cosine, μ, for 14 – 16 energy groups.
- for $\mu > 0.999999$ an analytical function, $f(\mu)$, derived from Molière's screening factor is used to compute the scattering angle.

$$f(\mu) = \frac{A}{(\eta + 1 - \mu)^2}$$

$$\eta(E, Z) = \frac{1}{4}\left(\frac{\alpha mc}{0.885p}\right)^2 Z^{2/3}[1.13 + 3.76(\alpha Z/\beta)^2]$$

Electroionization

Reaction

- The subshell is directly sampled.
- A knock-on electron is ejected.
- The incident electron energy is reduced by the $E_{knock} + E_{binding}$.
- Conservation of momentum is used to find the scattering and ejection angles.

Implementation

- ACE tables provide CDF of the knock-on energy, E_{knock}, based on the incident electron energy.
- The scattering and ejection angles are sampled independently breaking from a purely analog sampling.
- The shell vacancy is handled using atomic relaxation data.

Electroionization Scattering Angle

Conservation of Momentum

$$(p_{knock}c + p_a c)^2 = (pc)^2 + (p'c)^2 - 2pp'cos(\theta)$$
$$cos(\theta) = \frac{(pc)^2 + (p'c)^2 - (p_{knock}c)^2}{2pp'}$$

Conservation of Energy

$$(E + m_e c^2) + (M_a c^2) = (E' + m_e c^2) + (E_a + M_a c^2) + (E_{knock} + m_e c^2) + E_{Binding}$$

Assume the binding energy is negligible

$$E = E' + E_{knock}$$

Solving independently you obtain:

$$cos(\theta) = \frac{E'}{E}\frac{p}{p'} \quad \text{and} \quad cos(\phi) = \frac{E_{knock}}{E}\frac{p}{p_{knock}}$$

Sampling Electroionization

The original sampling routine implemented in FRENSIE sampled negative electrons energies.

- ACE tables provide CDF of the knock-on energy, E_{knock}, based on the incident electron energy.
- The original implementation randomly selected whether to sample the upper or lower energy bin.
- A correlated sample must be made to avoid non physical values.

Bremsstrahlung

Reaction

- A photon is ejected.
- The incident electron energy is reduced by the E_γ.
- The electron direction is assumed to be essentially unchanged.

Implementation

- ACE tables provide CDF of the photon energy, E_γ, based on the incident electron energy.
- An analytical dipole function, $p(\mu)$, is used to sample the direction of the outgoing photon.

$$p(\mu)d\mu = \frac{(1-\beta^2)}{2(1-\beta\mu)^2}d\mu$$

Known Issues

Absorption at low energies

- At energies near the cutoff (10 eV) the reaction cross section is dominated by elastic scattering (by order 10^7 for H barns).
- It is unlikely the electron will scatter below the cutoff energy.
- A temporary fix is to raise the cutoff energy (to 15 eV) to prevent indefinite elastic scattering.
- MCNP notes a similar problem and suggests a minimum cutoff energy of 20 eV.

Testing

Test Problem

- A 10 keV electron delta source was modeled in cold Hydrogen.
- Surface tallies where set on concentric spheres to measure the flux.
- Radii ranged from 0.005 to 0.0025 cm for 5 spheres.
- Electron energy cutoff was set to 15 eV.
- Secondary photons where not tracked.

Verification

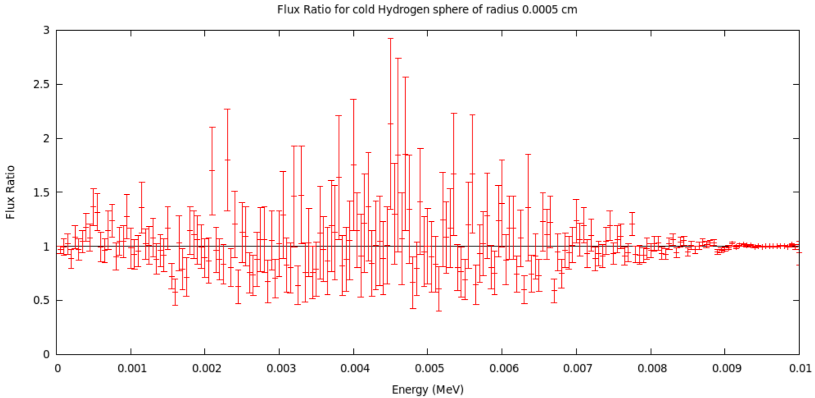
- Test results were verified against MCNP6 using the ratio surface flux
- 10^6 particles history where sampled in MCNP6.
- 10^6 particles history where sampled in FRENSIE.
- The 3σ rule was used to look at the standard deviation of the flux ratio from the expected value of 1
- 68.27%, 95.45% and 99.73% of the ratios should be within $1, 2$ and 3σ respectively for agreement.

3 σ Results

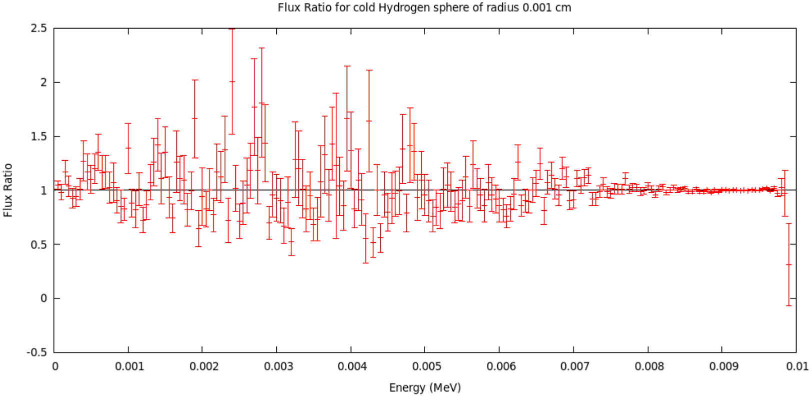
Radius (cm)	0.0005	0.0010	0.0015	0.0020	0.0025
1 σ	72.43%	66.84%	62.18%	57.58%	68.00%
2 σ	96.76%	93.16%	91.71%	93.43%	96.00%
3 σ	99.46%	97.89%	97.93%	98.48%	98.50%

Table: Surface flux ratio and the percentage of energy bins within 1, 2 and 3 σ of the expected value

Results

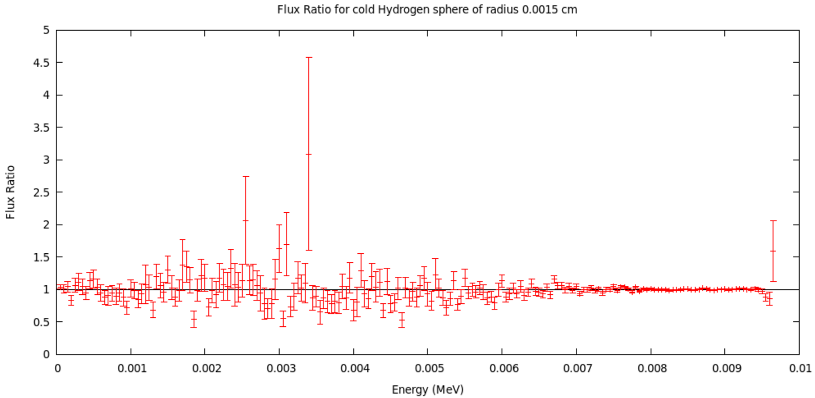

Flux Ratio for cold Hydrogen sphere of radius 0.0005 cm
Flux Ratio
Energy (MeV)
0
0.5
1
1.5
2
2.5
3
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
0.01

Results



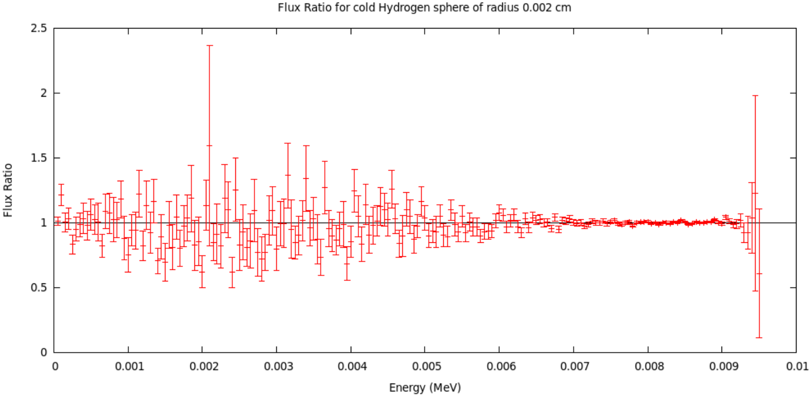
Flux Ratio for cold Hydrogen sphere of radius 0.001 cm
Flux Ratio
Energy (MeV)
2.5
2
1.5
1
0.5
0
-0.5
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
0.01

Results



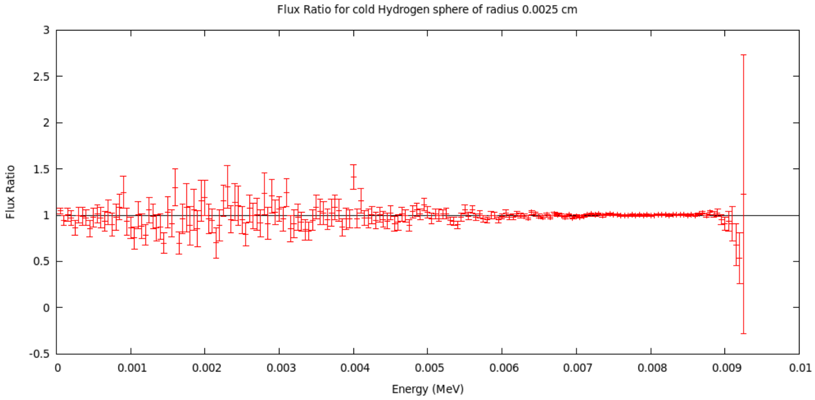
Flux Ratio for cold Hydrogen sphere of radius 0.0015 cm
Flux Ratio
Energy (MeV)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
0.01

Results



Flux Ratio for cold Hydrogen sphere of radius 0.002 cm
Flux Ratio
Energy (MeV)
2.5
2
1.5
1
0.5
0
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
0.01

Results



Flux Ratio for cold Hydrogen sphere of radius 0.0025 cm
Flux Ratio
Energy (MeV)
3
2.5
2
1.5
1
0.5
0
-0.5
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
0.01

Conclusions

- The agreement is slightly below the 3 σ rule.
- There appears to be a tail off in the upper energy bins.
- Further testing is planned to evaluate the the single scattered spectrum.
- FRENSIE code currently runs 100x slower than MCNP6 for a simple geometry.
- Modifications need to be made to speed up transport in DAG geometry by reducing the number of ray firings.
- Implementation of Root's combinational geometry would also speed up geometry transport.

Possible Adjoint Methods

Hybrid Multigroup/Continuous-Energy BFP

- The same basic multigroup cross-section data can be used for forward and adjoint calculations.
- The adjoint transport model is nearly identical to the forward making implementation easy.

Generalized Particle for Adjoint Transport

- The CSDA is used with Molière's multiple scattering theory.
- No secondary particles are produced. One particle enters an event and one leaves.