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Order-of-Convergence Study of a Condensed-History Algorithm Implementation

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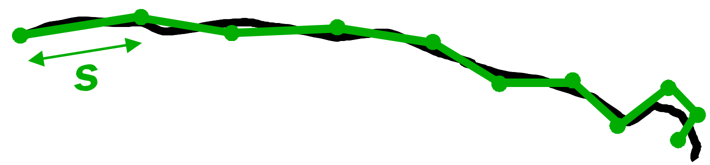
Outline

- **Preliminaries**
  - Condensed History and Pathelngth Convergence
  - Test Problem (albedo)
  - Issues
- **Assessing Order of Convergence**
  - Procedure (using Monte Carlo uncertainties)
  - Results for End-Hinge for Modified ITS
- **Simplified-Physics problem (albedo)**
  - Semi-analytic solution
  - Results for End-Hinge and Random-Hinge
- **Conclusions**

Condensed-History Algorithm and PathLength Convergence



Focus on Angular Scattering and Transport

- **Sample accumulated effects over (*pre-determined*) pathlengths**
- **"Transport-mechanics":**
  - **Hinge at end**
    error O(s)
  - **Random Hinge**
    error O(s^2)
- **Other aspects of ITS remain unchanged**
  - **Steps (for energy loss)**
  - **Secondaries**

- **Accumulated deflections given by Goudsmit-Saunderson:**

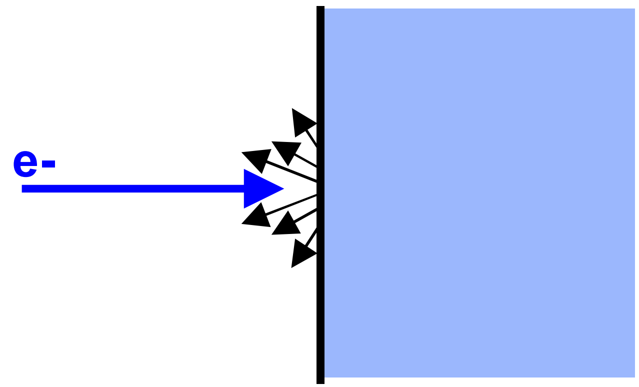
$$\frac{dP_{GS}}{d\Omega}(\mu, s) = \sum_{L=0}^{\infty} \frac{2L+1}{2} e^{-s\,G_L} P_L(\mu)$$

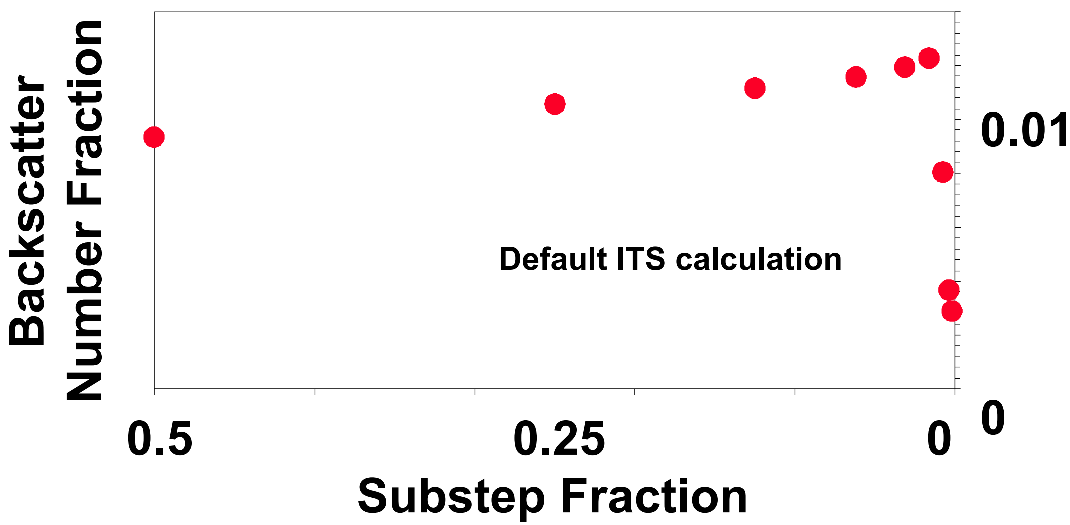
with Transport Moments:

$$G_L = \int_{-1}^{1} \frac{d\sigma}{d\mu} \left[1 - P_L(\mu)\right] d\mu$$

Test Problem: Albedo Number Fraction

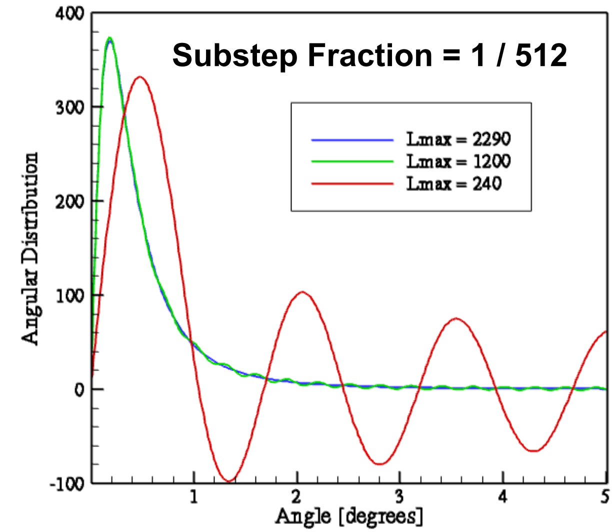
- **Normally incident electrons on thick slab (1D)**
- **Calculate total number of reflected electrons (albedo)** ***(minimal use of boundary-crossing logic)***
- **Particulars for this talk: 1-MeV electrons on Be**

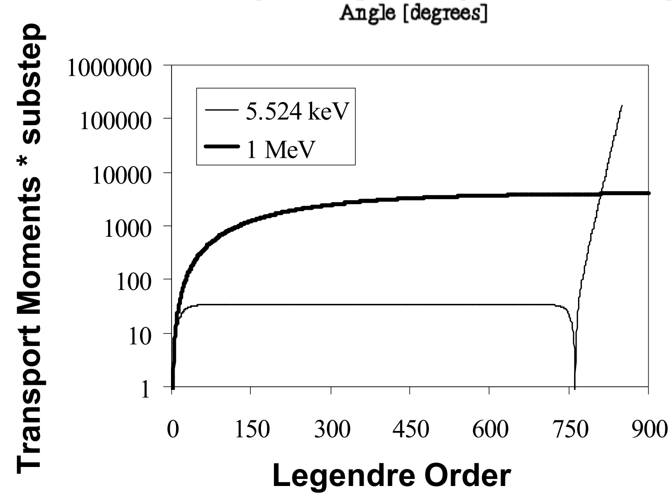




Failure of substep convergence
Culprit: Angular Representation

- **Too few terms in Legendre expansion**
  - Historical prescription is used to determine number of terms (also use of forward or reverse forms)
    - » Never exceeds 240
  - Unstable transport-moment recurrence relations used
- **Histogram representation**
  - Need greater resolution at small angles for small substeps (*addressed through input*)
- **Modified code:**
  - Increased Lmax
  - Screened-Mott xs only
  - Forward recurrence only
  - Used energy at start of substep





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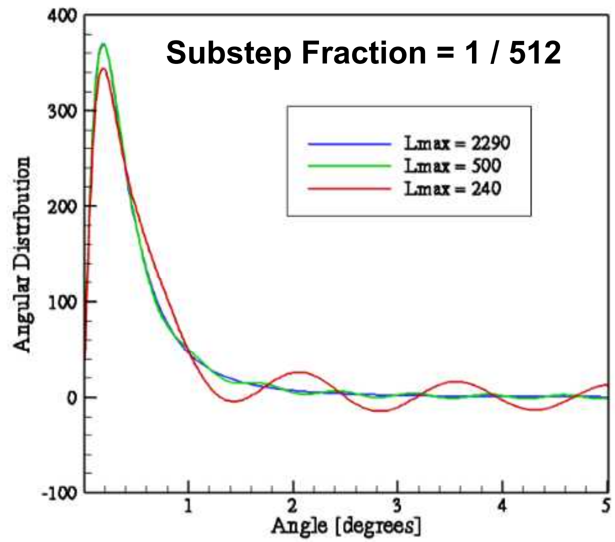
Potential Convergence Acceleration

- **Berger&Wang (1988) indicated improved convergence for small substep sizes may be obtained by first separately evaluating:**
  - **Uncollided**
  - **First collided**
- **For this study, the "convergence" criteria is actually on the transport moments themselves**
  - **Will be moved to attribute of angular representation - i.e., integration of histogram bin**



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Procedure: Minimizing Chi-squared

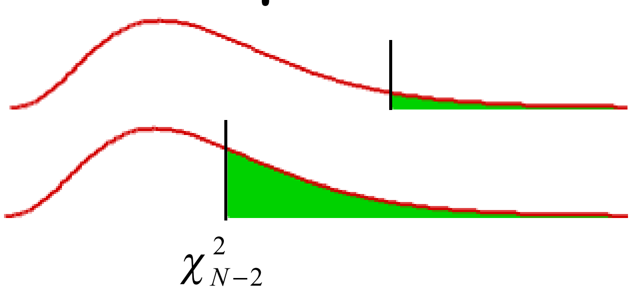
- **Need parameterized expression for fit in asymptotic region (based on theory)**

$$y = b + a\,s^{M}$$

- **Determine parameters from minimizing a χ^2_{N-2} statistic using the Monte Carlo results $\{(y_i, \sigma_i)\}$**

$$\chi^2_{N-2} = \sum_{i=1}^{N} \left(\frac{y - y_i}{\sigma_i} \right)^2$$

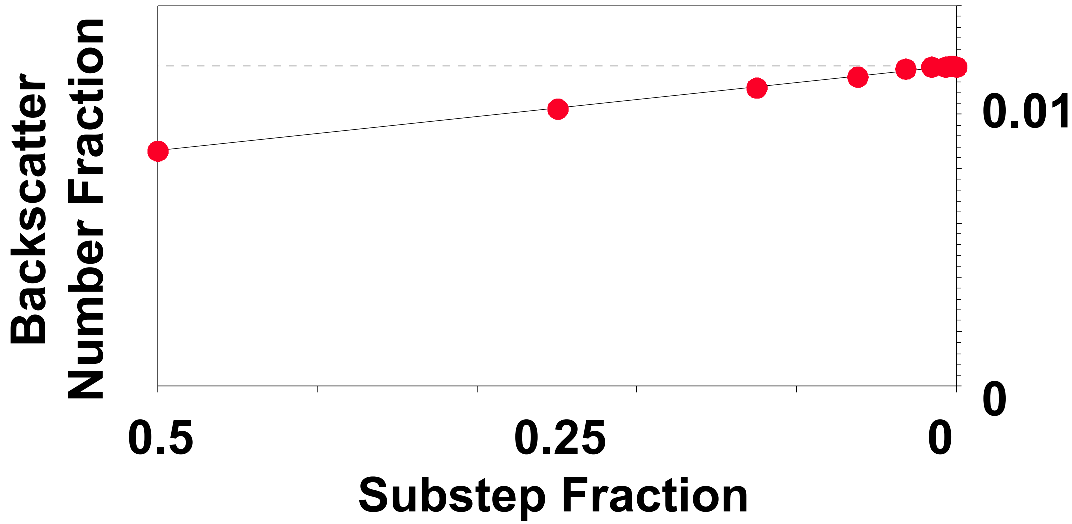
- **Evaluate q-value of χ^2_{N-2} to determine goodness of the fit.**



$$q.value(\chi^2_{N-2}) < 0.05 \Rightarrow$$ 👎

$$q.value(\chi^2_{N-2}) > 0.05 \Rightarrow$$ 👍

Results modified ITS



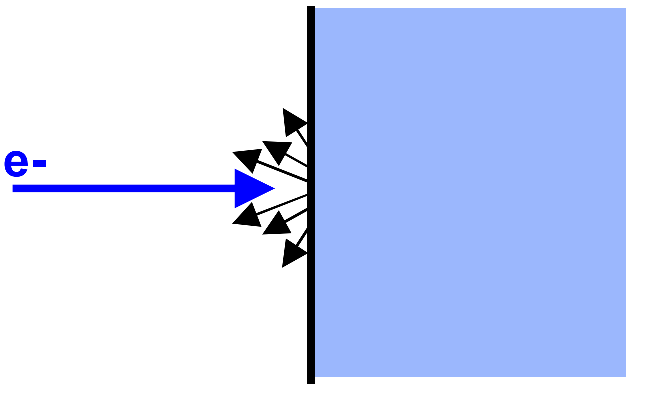
	Results	Uncertainty
Intercept	$1.179\ 10^{-2}$	$1.216\ 10^{-5}$
Slope	$-6.274\ 10^{-3}$	$6.442\ 10^{-5}$

$$\chi^2_{N-2} = 8.816$$

$$q.value(\chi^2_{N-2}) = 0.358$$

Modified Test Problem: Classical Albedo Number Fraction

- To simplify implementation of random hinge within ITS, a simpler problem was used
- Reduced physics:
  - Isotropic elastic scattering
  - Absorption added
  - Nothing else (no energy loss, no secondaries)
- Calculate total number of reflected electrons (albedo) *(minimal use of boundary-crossing logic)*
- *Semi-analytic* solution is available



- Particulars for this talk:
  - Default substep length has about 15 collisions on average
  - Ratio of absorption to total cross section ~ 10^{-5}

Evaluation of Semi-analytic Solution

- The semi-analytic solution for the albedo (current) is

$$y = \frac{c}{2}\mu_0 H(\mu_0)\int_0^1 \frac{\mu H(\mu)}{\mu + \mu_0} d\mu$$

where $\mu_0 = 1$

$$c = \sigma_{SCATT} / \sigma_{TOTAL}$$

- $H(\mu)$ is the "Chandrasekhar ***H*** function" (defined through an integral equation)

  Used Ganapol's procedure with
  - Quad precision
  - Quadrature order 40, 64 or 100
  - Iteration convergence 1.E-08
- To evaluate the albedo integral, we used quadrature of the same order, or a 15000-point trapezoid rule, also in quad precision

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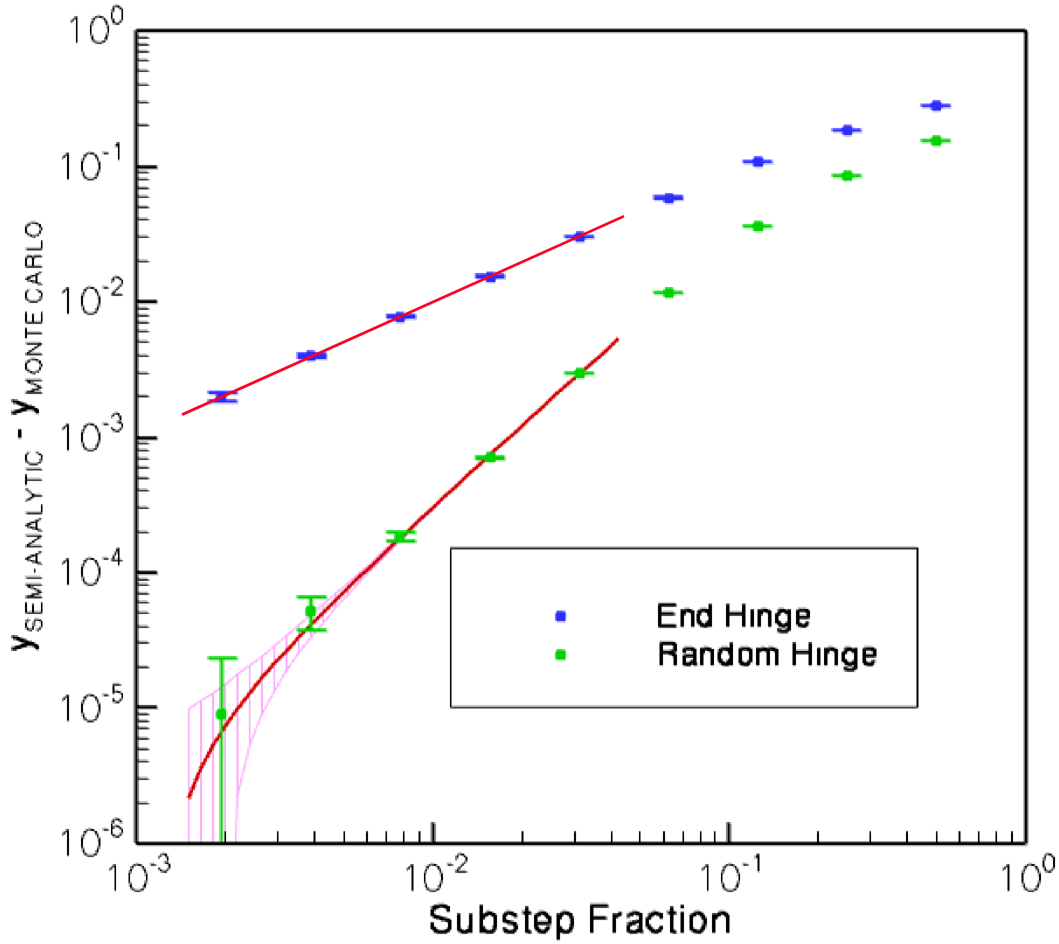
Results



- **End Hinge**:

N=5

$$\chi^2_{N-2} = 3.00$$

$$q.value(\chi^2_{N-2}) = 0.391$$

👍

- **Random Hinge**:

N=5

$$\chi^2_{N-2} = 3.10$$

$$q.value(\chi^2_{N-2}) = 0.376$$

👍

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Conclusions

- Demonstrated procedure for verifying order-of-convergence testing for condensed-history Monte Carlo
- Revealed that the number of terms in multiple-scattering angular distribution is inadequate in ITS for very small substep sizes
- Gained a better appreciation for “semi-analytic” solutions
- Can only conclude whether results are statistically consistent with model

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