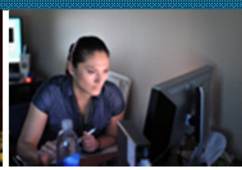
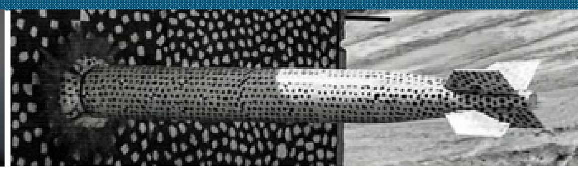
Revisiting the Lockwood Albedo Measurements for Validation of the Integrated Tiger Series Transport Codes





Presented by

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Introduction of Lockwood Albedo

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What is ITS?

ITS = Integrated Tiger Series

A series of coupled electron-photon Monte Carlo radiation transport codes (1, 2)

Used to simulate satellite components for radiation-hardness assessments

Contains a validation suite of seven test problems that vary in geometry, radiation type, material, energy, etc.

Maintained by Sandia National Labs

The Drawbacks of the Validation Suite

Lack of quantitative comparison metrics

Poor quantification of uncertainties

Only qualitative viewgraph norms given to discuss strength of validation suite

Sparse coverage of target materials and source energies

Few overall tests

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The Lockwood Albedo Test Problem

1 of 7 validation problems in the ITS Validation suite

Lockwood took 250 measurements varying in angle, material, and energy

Materials: Be, C, Al, Ti, Ta, Mo, U, UO2

Energies: ~30 keV to 1 MeV (varies for each material)

Angles: ~0 degrees to ~83.5 degrees (varies for each material) (4)

Why Lockwood Albedo?

This is an exemplar measurement set (4)

Contains tabular data for high ease of use in comparison (4-6)

Discussions of measurement errors are there and are sufficient in detail (5)

Robust material selection (comparably)

Wide energy range (comparably)

Simple Geometry, allowing fewer parameters needing to be varied

Challenges with Lockwood Albedo

Legacy measurements make uncertainty quantification difficult

No error information given for Carbon

No reliable measurement errors were given for UO2 (6)

Error publishing was only partial (2 angles, 6 materials, 1 energy)

Needed to estimate proportionality constant, c, based on given information (5, 6)

- C was inversely proportional to the albedo
- C was different for each material, but each C could be used for every angle/energy in material

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Simulations Ran

Lockwood supplies 250 measurements with which to compare to

Over 2000 simulations were performed:

- Three sets of 310 cases were ran (arbitrary number which is a superset of measurements)
- Five sets of 269 cases were ran (also arbitrary; superset of 250)
- Additional sets of cases were ran for other independent comparisons

When comparing simulation to measurement, only the applicable 250 were used

When comparing simulation to simulation, all cases were included.

Chosen Error Metrics and Other Analyses

2 Error Metrics chosen
- Error Relative to measurement
- Error Relative to the combined aleatory (or statistical) uncertainty

Epistemic Uncertainty Study

Cutoff Energy Study

Beryllium Sub-step Study

Change in default thickness

Using and not using ELECTRON-TRAPPING

Error Relative to Measurement

Error relative to measurement simply looks at differences in albedo values

It is an estimate of "how close" the simulation is to Lockwood's data

Standard relative error is calculated for this comparison:

$$\delta = \frac{Actual - Expected}{Expected}$$

No absolute value used to prevent positive limiting of comparison

Error Relative to Combined Aleatory Uncertainty

In terms of number of standard deviation

Y = N independent random variables X_i

X_i is associated with standard deviations $\varepsilon_{Xi}{}^2$

Then error associated with Y can be written as:

$$\epsilon_{TOT} = \sqrt{\Sigma_{i=1}^{N} \epsilon_{X_i}^2 \left(\frac{\partial Y}{\partial X_i}\right)^2} \qquad (13)$$

Epistemic Uncertainty Study

Lockwood estimated zero degrees was good to +/- 0.5 degrees and angles from zero were good for the same range

We examined the effect of +/- 1 degree would have on the albedo, w/ respect to Be

No standard deviation to combine and no error to refer to from Lockwood

Beryllium Sub-step Study

ITS uses a condensed-history approach

Deflections, energy loss, secondary interactions are dealt with over a pre-calculated path length called a substep

Theory: As the substep shrinks, the simulation should converge linearly (10)

Changing Energy Cutoff Values

When an electron falls below a specified energy, the electron is locally deposited and is no longer tracked

Default cutoff is 5% of max source energy

Lowest permitted energy in ITS is 1 keV

Lockwood's bias voltage is +55eV (so 1 keV is appropriate here)

Highest energy used is 1.033 MeV (cutoff is 52 keV)

Change in Default Thicknesses

Albedo problem should be independent of target thickness

Began with 1 cm which was at least twice as large as any actual thickness used in the experiment

Also simulated actual thicknesses from Lockwood's data

Electron Trapping v.s. No Electron Trapping

Electron Trapping is a variance reduction technique used in ITS (also called range rejection)

If an electron is farther away from a boundary than its range, and below an energy threshold, it is trapped and no longer tracked

The reason for an energy threshold is to allow for bremsstrahlung production which travels much farther than the parent electron

The albedo problem isn't a bremsstrahlung problem, so the threshold is set to the maximum source energy which may implement some sort of bias

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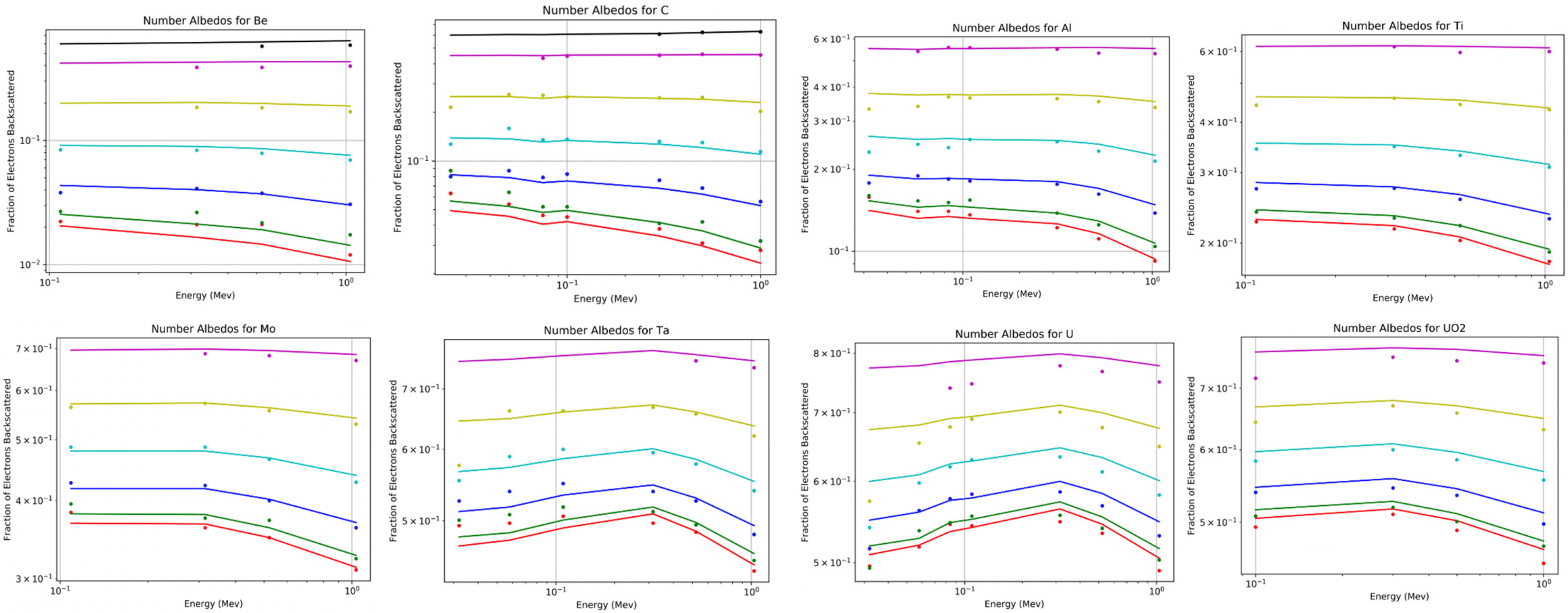
General Albedo Trends



Measured Albedo Values are Dots

ITS Simulations are connected w/ lines, purely to assist in trend illustration

Legend: 0 (1), 15 (16), 30 (31), 45 (46), 60 (61), 75 (76), 82.5 (83.5)

General Albedo Trends

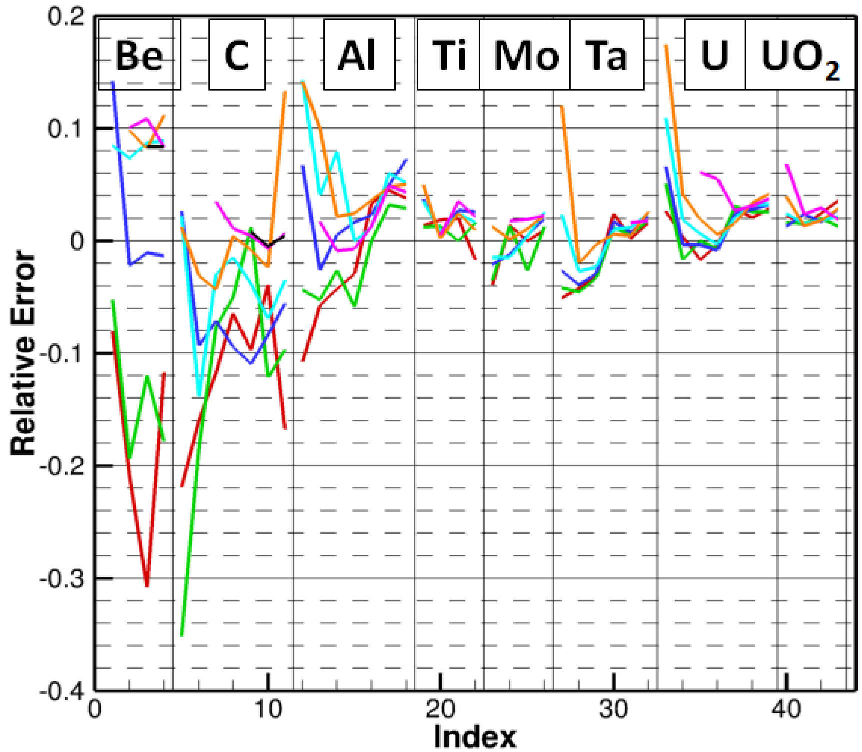
There is a factor of 60 between normal incidence and the largest angle, both at the largest energy for Be

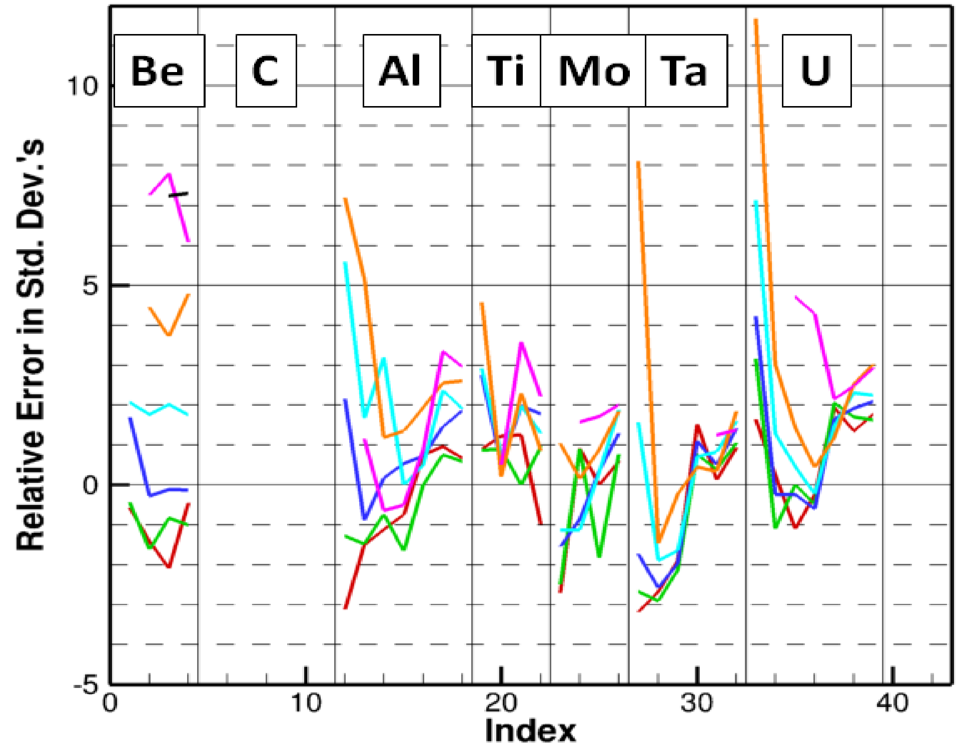
For upper line, ~85% of the simulated albedo values are above or below experimental value

For lower line, ~95% of values are above or below the experimental values

For UO2, 100% are over, illustrating an increased lack of agreement in simulation data for potentially higher Z values

General Albedo Trends – Relative Error





Be and C have large vertical spreads
Associated measurement error for Be was 26% for normal incidence at the highest energy
No error information was given for C or UO2, hence the blank regions on Rel Err. In STDev (combined standard deviations)
Al, Ta, U all have a large orange spike at lowest energy, and appear in both left and right plots, illustrating statistical significance, rather than user error

Error Discussion

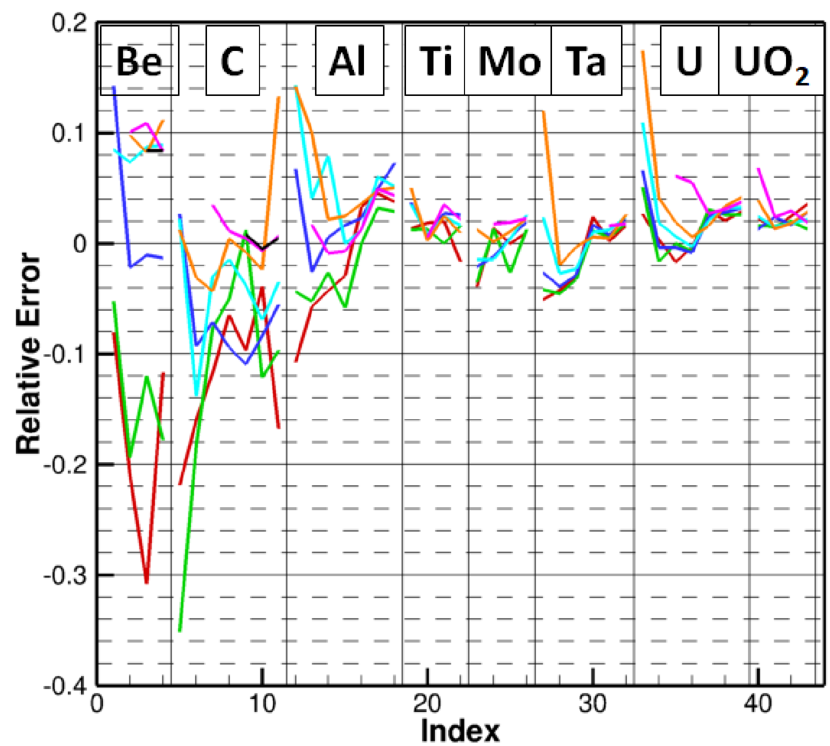
The black and magenta curves near 0.1 Rel Err are a good case for the direction-setting error and substep convergence bias investigation.

Direction setting is epistemic, so (albedo + D, albedo, albedo – D) are possible (D is delta)

For the 1 degree offset, there is about 5% error present, which would close the gap between simulation albedo values and experimental albedo values

There was also no convergence in substep size, which introduces bias, which is also about 5%

This illustrates almost little to no change in substep changes with respect to simulated albedo value



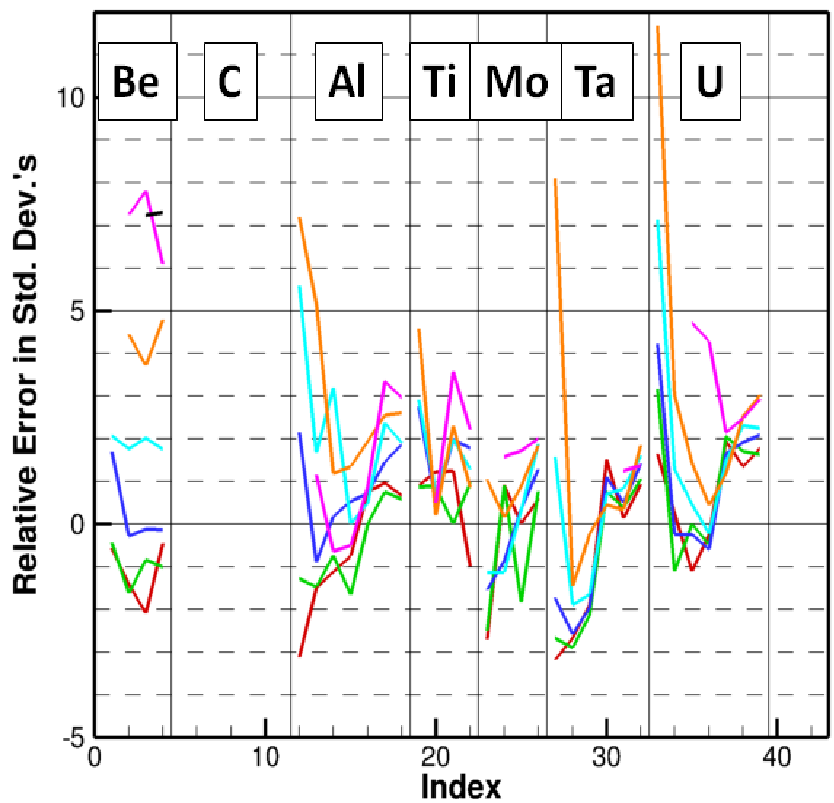
Error Discussion

For the near normal curves (the red and green) of Be, the bias removal is ~30%

Those curves then move to the positive side of the Rel. err. Plot.

Direction setting error then is ~5% so there may be a small negative component.

Adjusted results would be within -2,+2 bounds of the relative err. In terms of the St.Dev plot



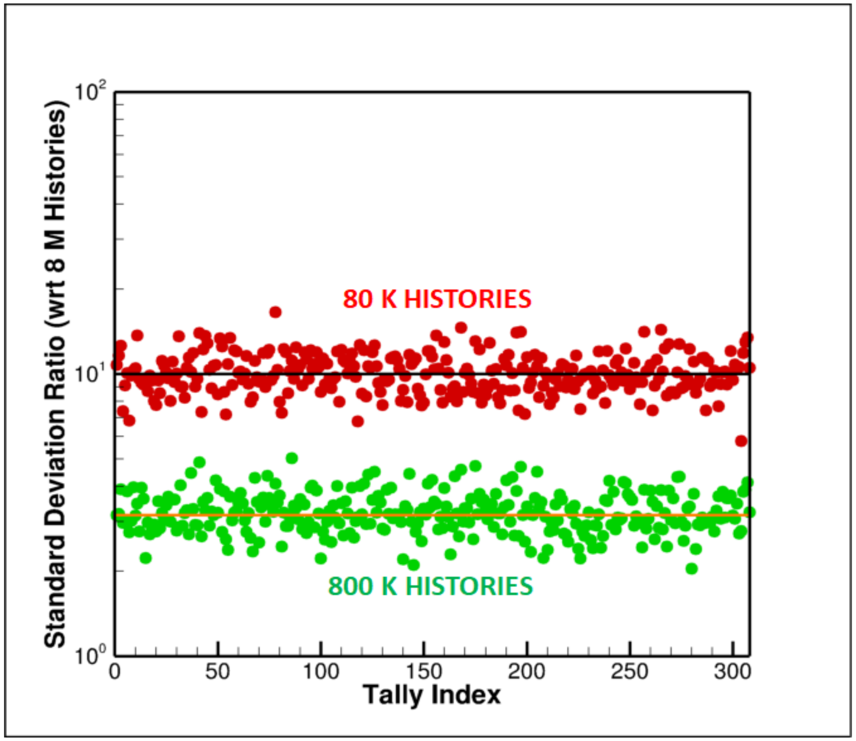
Error due to Combined Uncertainty

80K Histories show an avg. St.Dev of 10.14

800K Histories show an avg. St.Dev of 3.25

Compared to Monte Carlo convergence of 1/sqrt(10) [starting with 100] which is of 10 and 3.16.

Therefore the standard deviations are behaving properly.



Error due to Combined Uncertainty

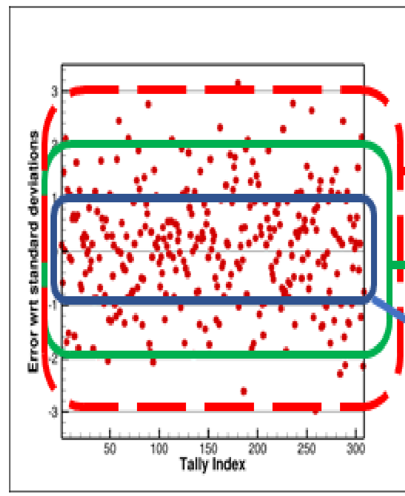
Fraction of values between +/-1 St.Devs is 67.2

Fraction of values between +/-1 St.Devs is 96.4

Fraction of values between +/-1 St.Devs is 99.6

Theoretical Values are 68.3, 95.45, and 99.7 respectively.

This test indicates the computed combined St.Devs yields a normal distribution with unit standard deviation.



800 K vs 8 M	THEORY	80 K vs 8 M
99.6	99.7	99.7
96.4	95.45	93.5
67.2	68.3	64.6

Relative Error in Terms of the Combined St. Devs

Be Sub-step Comparisons

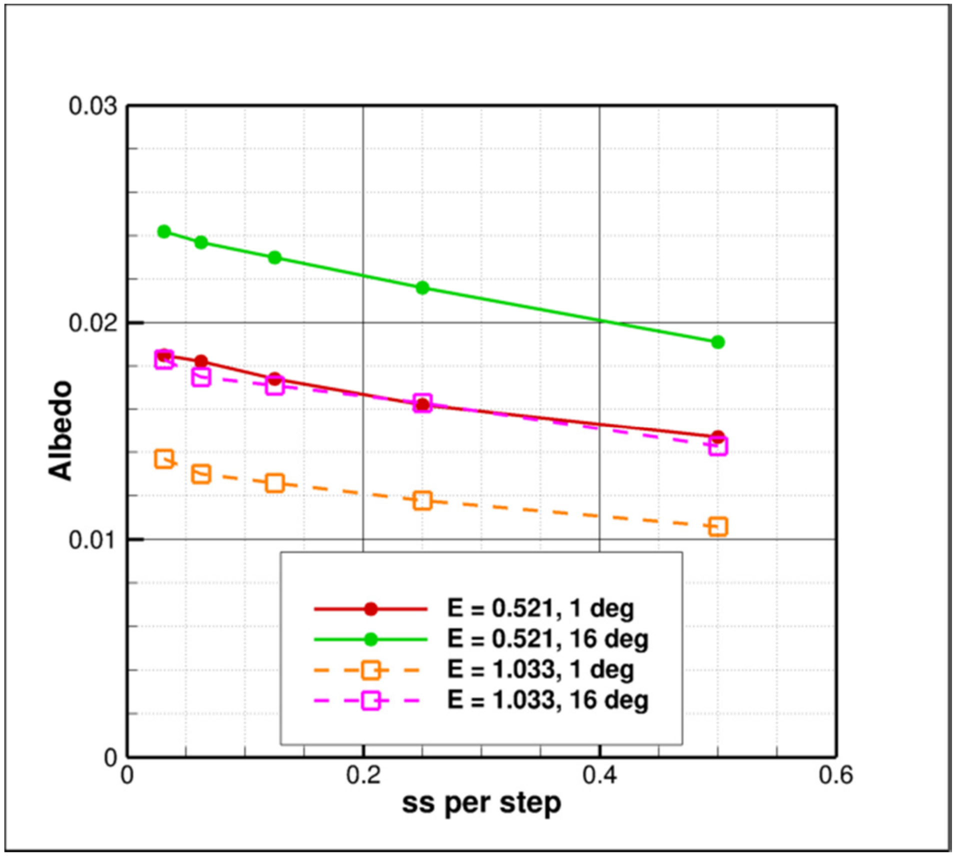
For Albedo:

Largest effect is for Be – 30% increase seen for normal incidence near 1 MeV

For largest angle of 83.5 degrees, the increase is only 5%

As substep size tends toward zero, the simulations converge to a point where a straight-line extrapolation would intersect the y-axis

This allows for numerical bias to be removed from the substep size analysis



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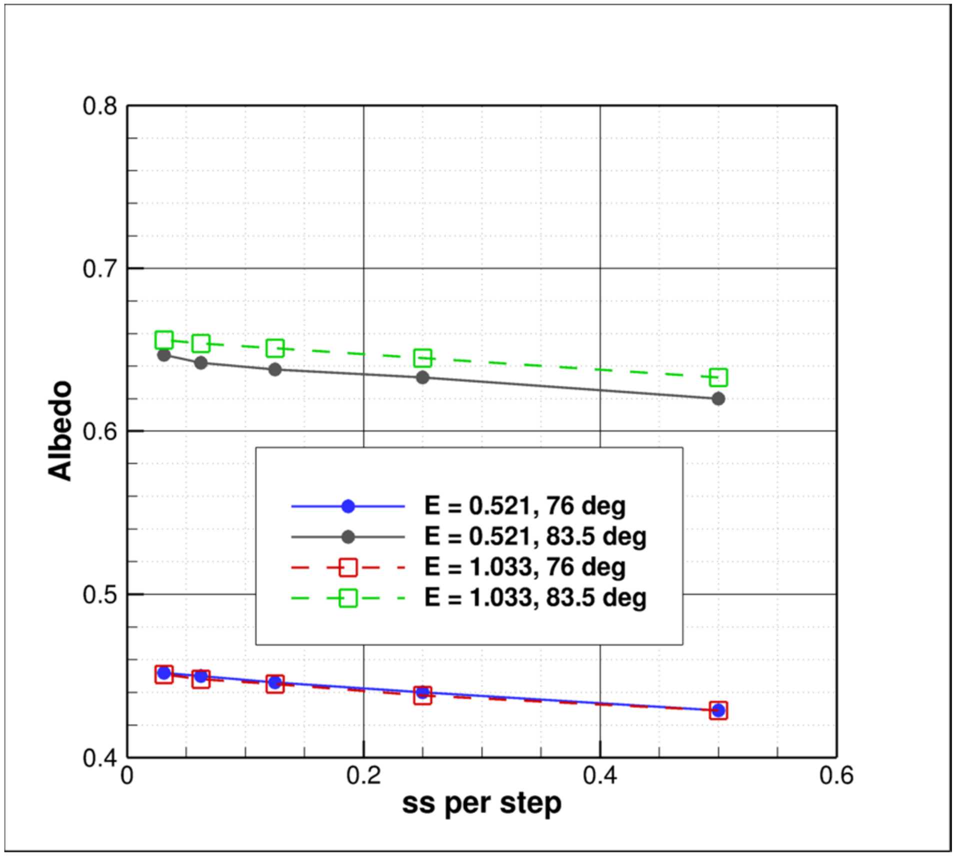
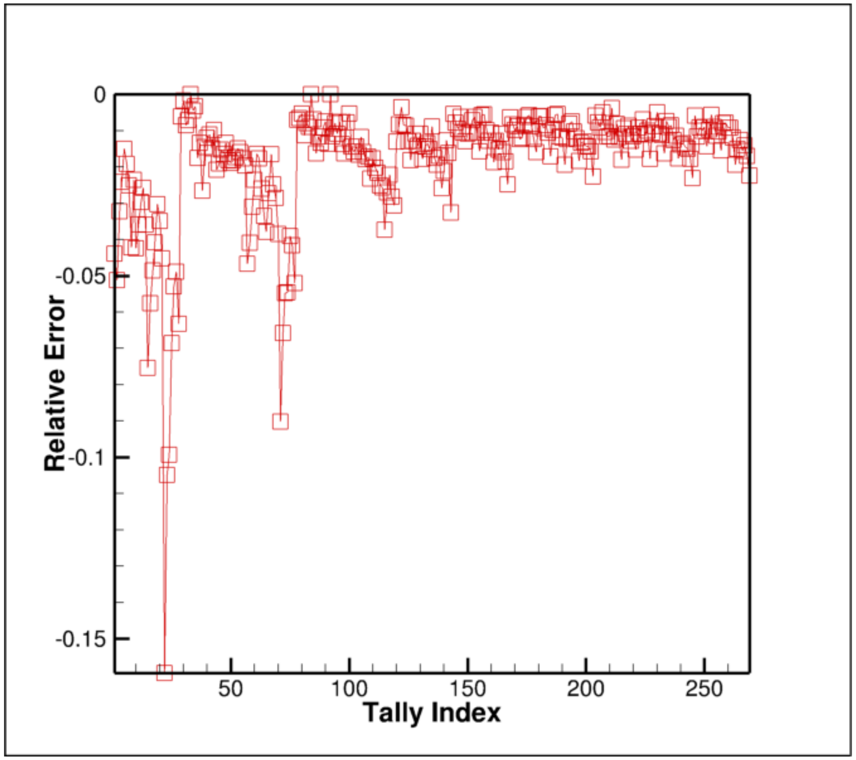


Cutoff Comparisons

Largest error for cutoffs are at lower Z (less scattering) materials at about 16% for normal incidences.

All results with the lower cutoff showed higher albedo values than the default cutoff.

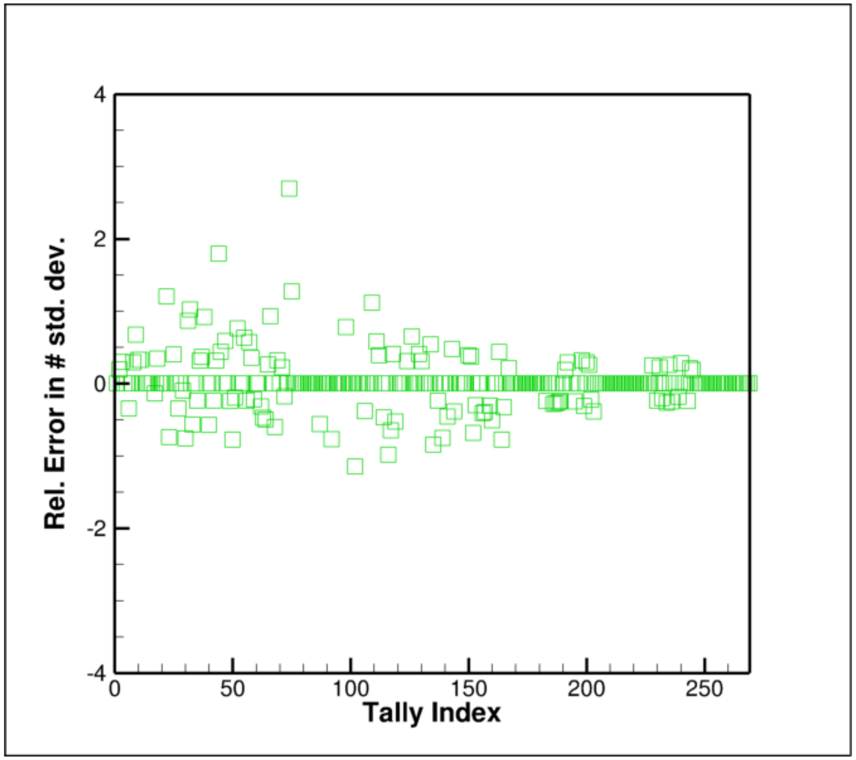
This is in line with theory as there were fewer electrons stopped prematurely.



Thickness Comparisons

Spread here is significantly less than in the MC statistics discussed previously.

There is no clear difference in using a 1-cm thick target (very thick) or not for this problem.

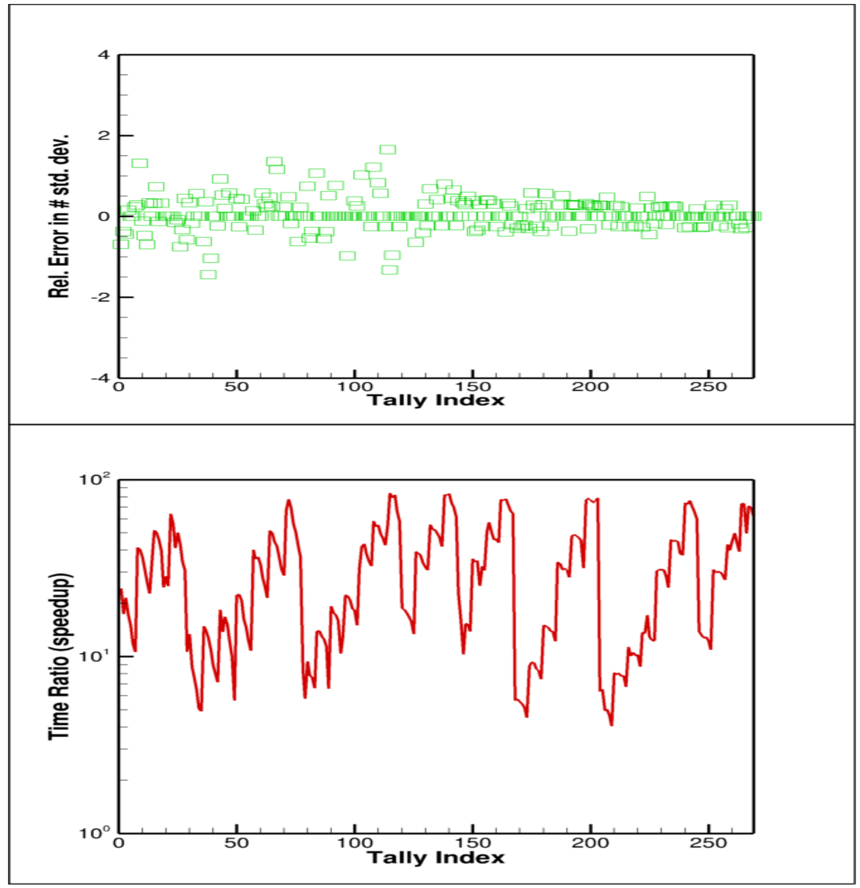


Electron Trapping Comparisons

Top figure shows ratios of run times plotted for a set not using trapping to a set using trapping.

Lowest speed up is about a factor of 4 while the highest is about 80.

The lower figure illustrates that there is no discernable statistical difference in the results of using TRAP-ELECTRONS or not for this problem set.



Final Thoughts on Results

90% of the relative error comparisons of five materials (Al, Ti, Mo, Ta, U) fall between +/- 5%

Only 78% compared to the desired 95.45% of the same comparisons are between +/- 2 St. Devs.

This suggests there may be systematic bias in either the albedo values or assessed uncertainties in either the measurements or simulations.

There are considerably more comparisons with simulations higher than the measurements, suggesting the bias may be in the albedo values.

Be was left out due to large measurement error.

C was left out due to no statement of measurement error (5)

UO2 had no reliable statement of error (6)

The tests have been scripted in bash shell and will soon be incorporated into the weekly test suite to ensure any future versions of ITS may routinely be assessed with this suite.

Overview

Future Work

Investigate discrepancy at lowest energies.

Investigate more robust moment calculation.

Complete a numerical bias calculation for other elements (only have done Be).

Error Analysis in direction-setting needs to be done for all cases.

Continue expanding tests and quantification of further uncertainties.

ITS is not yet set up to handle uncertainty information on cross sectional data.

References

B. C. FRANKE, R. P. KENSEK, "Electron Transport Algorithms in the Integrated Tiger Series (ITS) Codes," American Nuclear Society RPSD (2018).

B. C. FRANKE, et al., "ITS Version 6: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport codes, Revision 5," SAND2008-3331, Sandia National Laboratories, PO Box 5800, Albuquerque, NM. 87185, September 2013.

R. DAVIS, R. P. KENSEK, A. OLSON, C. PERFETTI, B. FRANKE, "Expansion of the ITS Validation Suite," SAND-2021-2344 C, Sandia National Laboratories, PO Box 5800, Albuquerque, NM. 87185, March 2021.

G. J. LOCKWOOD, L. E. RUGGLES, G. H. MILLER, and J. A. HALBLEIB, "Electron energy and charge albedos calorimetric measurement vs Monte Carlo theory," Tech. Rep. SAND80-1968, Sandia National Laboratories (1981).

G. J. LOCKWOOD, G. H. MILLER, and J. A. HALBLEIB, "Simultaneous Integral Measurement of Electron Energy and Charge Albedos," IEEE Transactions on Nuclear Science, **NS-22**, 6 (1975).

G. J. LOCKWOOD, J. A. HALBLEIB, and G. H. MILLER, "Electron Transport in Reactor Materials," IEEE Transactions on Nuclear Science, **NS-25**, 6 (1978).

B. C. FRANKE, A. J. OLSON, and S. D. PAUTZ, "Differential-Operator and Correlated-Sampling Methods with Electron-Photon Transport in the Integrated TIGER Series" in "M&C 2017," Jeju, Korea (April 16-20, 2017).

S. PERKINS, D. CULLEN, and S. SELTZER, "Tables and Graphs of Electron-Interaction Cross Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Electron Data Library (EEDL), Z=1,100," Tech. Rep. UCRL-50400 Vol 31, LLNL (1991).

X. LLOVET, C. J. POWELL, F. SALVAT and A. JABLONSKI, "Cross Sections for Inner-Shell Ionization by Electron Impact," Journal of Physical and Chemical Reference Data, 43, 013102 (2014).

H. SEO, M. G. PIA, P. SARACCO and C. H. KIM, "Ionization Cross Sections for Low Energy Electron Transport," IEEE Transactions on Nuclear Science, 58, pp. 3219-3245 (2011).

E. LARSEN, "A Theoretical derivation of the condensed history algorithm," Ann. Nucl. Energy, 19 pp. 701-714 (1992).

W. BEEZHOLD, D. E. BEUTLER, J. C. GARTH and P. J. GRIFFIN, "A Review of the 40-Year History of the NSREC's Dosimetry and Facilities Session (1963-2003)," IEEE Transactions on Nuclear Science, 50, pp. 635-652 (2003).

G. DAHLQUIST and A. BJORK, "Numerical Methods," (Prentice-Hall, 1974).

R. G. MCCLARREN, "Uncertainty Quantification and Predictive Computational Science," (Springer, 2018).