

## Data Needs and Desires for ITS and SCEPTRE

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# Who are we? (Mainly Electron/Photon Transport)

- ITS (Integrated TIGER Series)

- Monte Carlo
- Electron Transport:
  - Condensed History (process cross sections)
  - Single Scatter (Based on LLNL Evaluated Data Library)
- Hybrid Continuous-Energy/Multigroup (process cross sections)
  - Sloan's algorithm (angular moments w/ integrals)



- SCEPTRE (Sandia's Computational Engine for Particle Transport for Radiation Effects)

- Deterministic Boltzmann Equation Solve
  - Option to use a variety of Solvers for different parts of phase space
- Multigroup/Finite-elements (process cross sections w/ integrals)
  - Interest with proton and alpha data for satellite applications
- Legendre moments (angular integrals)



- Cross-Section Generators (each use variety of data/models)

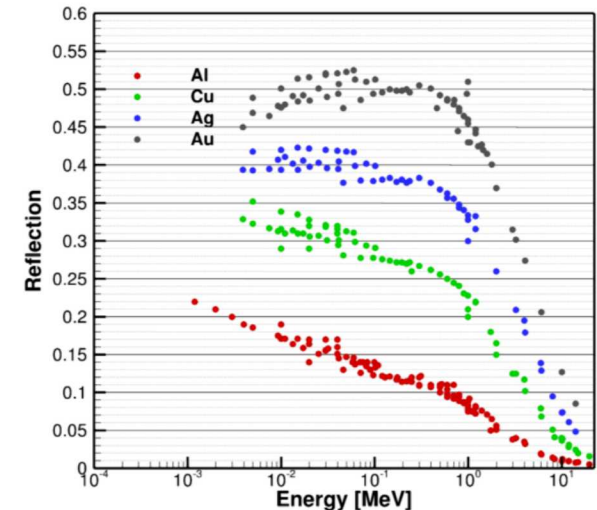
- XGEN (ITS only) – continuous-energy cross sections
- CEPXS (both ITS and SCEPTRE) - multigroup
- EPIX – (new project) – eventual replacement

- Mainly use content of LLNL EDL (more complete and robust) plus:

- Electron stopping power, electron straggling
- **Line-width data** (for time sampling of relaxation), atomic parameters for Seltzer's impact ioniz.

# Other Considerations

- Quantify uncertainties and covariances
  - Validation data from e.g., Geant consortium
    - Could lead to better quantified uncertainties
    - Might be mined for variability vs uncertainty
    - Hopefully includes metadata (reasons for rejecting some data)
  - Covariances may need modeling support
    - Example: ELSEPA code for electron elastic scattering
- Models should be archived
  - Our cross-section data are generally generated
    - Model is ultimate interpolation
    - Possible NGP impact (memory vs run-time tradeoffs)
- Ability to Mix and Match Models and/or Data (probably not your scope)
  - E.g., EADL has a detailed set of relaxation parameters. Binding energies are somewhat outliers.
  - Eventually we would like to consistently use EADL with different set of Binding energies
- Better Form Factors/ Scattering Factors
  - Measured Form Factors for compounds of interest
    - Can be calculated with atom-coordinate model
  - Doppler broadening for Incoherent Scattering Factor
    - Perhaps just the Compton profiles



# More Considerations

- Reconsider using cosine for very-forward-peaked distributions
  - Use 1-cosine [or (1-cosine)/2] instead of just the cosine

As an example (and to point out an anomaly in ENDF data from the website):

9.999851-1	4.450490+3	9.999871-1	5.936520+3	9.999891-1	8.313490+3820026526	279
9.999901-1	1.007690+4	9.999917-1	1.433410+4	9.999930-1	2.014980+4820026526	280
9.999941-1	2.836000+4	9.999950-1	3.948400+4	0.999996+0	5.595180+4820026526	281
0.999996+0	8.056210+4	0.999997+0	1.096450+5	0.999997+0	1.578740+5820026526	282
0.999998+0	2.237270+5	0.999998+0	3.044980+5	0.999999+0	4.384470+5820026526	283
0.999999+0	5.837020+5	0.999999+0	8.152080+5	0.999999+0	9.863740+5820026526	284
0.000000+0	0.000000+0	0	0	0	0820026	099999

- Above can be found in BNL and IAEA websites (VII.1 and VIII.0)
  - Note format change, losing a significant digit just where it causes problems!
  - EEDL(1991) does **not** have this problem (all colored numbers are distinct)
- Polarization models and data?
- Weird physics at  $\sim$ eV energies (plasmon decay, polarons)