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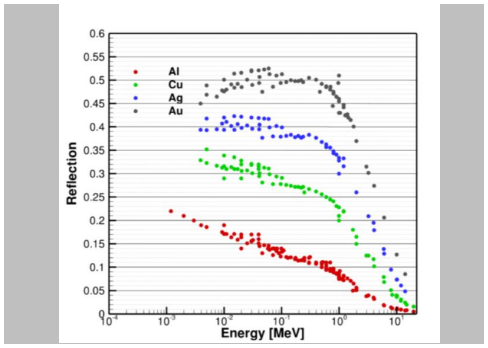

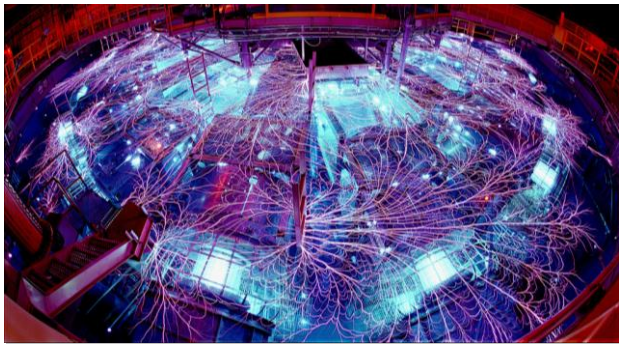

Data Needs and Desires for ITS and SCEPTRE

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(telecon)

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Who are we? (Mainly Electron/Photon Transport)

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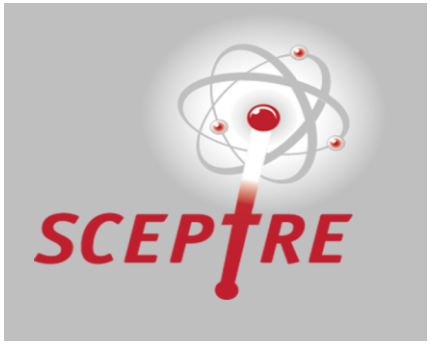
- ITS (Integrated TIGER Series)
  - Monte Carlo
  - Electron Transport:
    - Condensed History (process cross sections)
    - Single Scatter (Based on LLNL Evaluated Data Library)
  - Hybrid Continuous-Energy/Multigroup (process cross sections)
    - Sloan's algorithm (angular moments w/ integrals)

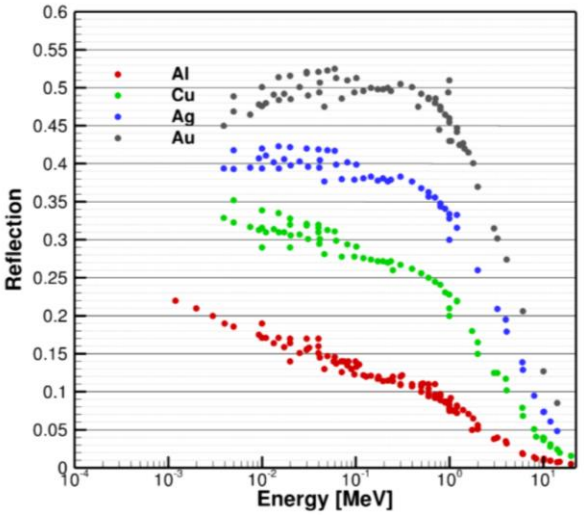
- SCEPTRE (Sandia's Computational Engine for Particle Transport for Radiation Effects)
  - Deterministic Boltzmann Equation Solve
    - Option to use a variety of Solvers for different parts of phase space
  - Multigroup/Finite-elements (process cross sections w/ integrals)
    - Interest with proton 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
  - EPIXS – (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 ~eV energies (plasmon decay, polarons)