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Title: Validation of the MCNP6 electron-photon transport algorithm: multiple-scattering of 13- and 20-MeV electrons in thin foils

Author(s): Dixon, David A.
Hughes, Henry Grady III

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Validation of the MCNP6 electron-photon transport algorithm: multiple-scattering of 13- and 20-MeV electrons in thin foils

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David Dixon[1]
H. Grady Hughes[1]

[1]Monte Carlo Methods and Applications Group
Los Alamos National Laboratory
ddixon@lanl.gov

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MCNP6 electron-photon transport V & V

- Motivated by:
  - Information gap in electron-photon V & V
  - New physics/transport algorithm – i.e. the EPRDATA
- Current status:
  - Completed comparison to Lockwood energy deposition experiment
  - Wrapping up the work presented today
  - Will revisit Gierga and Adams (Bremms, electron e-spec, so on)
  - Early stages of collaboration with ANL for GeV range validation
  - Might study the Tabata charge deposition experiments

The multiple-scattering experiment (Ross *et al.*)

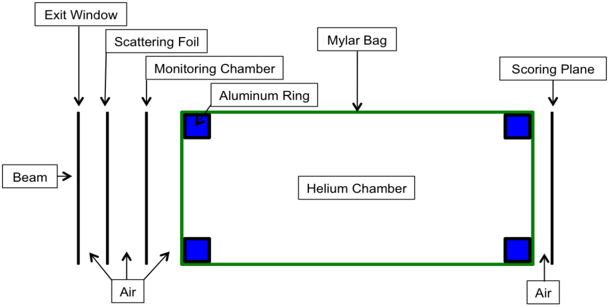
- Purpose: obtain data used to test models of electron scattering
- Measurement of electron fluence at angles from from 0 to 9 degrees
- Materials tested include atomic numbers from 4 to 79
- Key References:

C. K. Ross *et al.*, *Measurement of Multiple Scattering of 13 and 20 MeV electrons by thin foils*, Med. Phys., 35, 4121–4131(2008).

B. A. Faddegon *et al.*, *Accuracy of EGSnrc, Geant4, and PENELOPE Monte Carlo Systems for Simulation of Electron Scattering in External Beam Radiotherapy*, Phys. Med. Biol., 54, 6151–6163 (2009).

Experimental setup

- Experimental features:
  - Beam
  - Scattering foil
  - Monitor Chamber
  - Mylar bag



Simulation setup

- **Geometry**:
  - Each component approximated by a cylinder or cylindrical shell
  - Several very thin regions
- **Source**:
  - Mono-directional, mono-energetic beam with Gaussian spread in plane orthogonal to beam
  - nps=1e9
- **Physics**:
  - Tranport algorithm and data:
    - Electrons: condensed history (EL03)
    - photons: single event (EPRDATA)
  - Parameterized step-size via *ESTEP* and *EFAC*
  - Cut-offs: 1-keV for electrons and photons (probably insignificant)
- **Tallies**:
  - F2: surface flux tallies + surface divisor

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13-MeV beam on various targets

Table 1: Comparison of measured and calculated characteristic angles for 13-MeV electrons on Be, Al, Cu, Ta, and Au. Three different physics configurations are studied: default, *ESTEP*, and *EFAC*=0.99.

				Default		*ESTEP*		*EFAC*	
Material	Thickness (mg/cm2)	Ross *et al.* (deg.)	Dixon & Hughes (deg.)	Calc. (deg.)	Rel. Diff. (%)	Calc. (deg.)	Rel. Diff. (%)	Calc. (deg.)	Rel. Diff. (%)
Be	926	8.143	8.089	8.363	3.382	8.846	9.353	9.081	12.26
Al	70.1	4.003	3.981	4.308	8.223	4.558	14.48	4.289	7.745
	140	5.268	5.226	5.602	7.196	5.798	10.93	5.652	8.150
Cu	43.0	4.219	4.167	4.541	8.968	4.745	13.86	4.450	6.786
	86.4	5.630	5.562	5.970	7.310	6.161	10.74	5.956	7.056
	129.6	6.861	6.803	7.115	4.593	7.323	7.645	7.210	5.989
	174.5	7.956	7.911	8.521	7.704	8.681	9.722	8.619	8.938
Ta	44.3	5.558	5.503	5.812	5.608	5.787	5.158	5.799	5.385
Au	31.2	4.878	4.798	5.061	5.473	5.346	11.43	5.164	7.626
	54.8	6.329	6.260	6.568	4.911	6.769	8.124	6.650	6.216
	93.7	8.243	8.231	8.812	7.052	9.013	9.495	8.986	9.163

20-MeV beam on various targets

Table 2: Comparison of measured and calculated characteristic angles for 20-MeV electrons on Be, C, Al, Cu, Ta, and Au. Three different electron physics configurations are studied: default, *ESTEP*, and *EFAC*=0.99.

				Default		*ESTEP*		*EFAC*	
Material	Thickness (mg/cm2)	Ross *et al.* (deg.)	Dixon & Hughes (deg.)	Calc. (deg.)	Rel. Diff. (%)	Calc. (deg.)	Rel. Diff. (%)	Calc. (deg.)	Rel. Diff. (%)
Be	926	5.238	5.214	5.434	4.234	5.694	9.208	5.839	11.99
C	546	5.132	5.108	5.198	1.764	5.456	6.825	5.561	8.873
Al	70.1	2.653	2.634	2.873	9.094	3.148	19.51	2.877	9.221
	140	3.484	3.463	3.657	5.611	4.018	16.02	3.823	10.39
	274	4.777	4.750	4.978	4.798	5.269	10.94	5.268	10.91
Cu	43.0	2.790	2.768	3.025	9.284	3.279	18.49	2.999	8.375
	86.4	3.714	3.685	3.891	5.605	4.245	15.21	4.041	9.666
	129.6	4.493	4.454	4.758	6.843	4.979	11.81	4.900	10.02
	174.5	5.198	5.147	5.429	5.496	5.724	11.22	5.688	10.51
Ta	206.3	7.913	7.809	8.207	5.099	8.306	6.364	8.793	12.60
Au	54.8	4.127	4.111	4.382	6.590	4.652	13.17	4.563	10.99
	164.2	7.278	7.258	7.593	4.605	7.775	7.113	8.025	10.57

Combined results

Table 3: Average of the relative differences between measured and calculated characteristic angles for 13-MeV and 20-MeV electrons for three different physics configurations including: default, *ESTEP*, and *EFAC*, along with results from Faddegon *et al.*

	Average Relative Difference	
Physics Setting	13-MeV	20-MeV
Default	6.4%	5.8%
ESTEP	10.1%	12.2%
EFAC	7.3%	9.5%
EGS	-1.3%	1.0%
Geant4	0.7%	0.9%
Penelope	1.1%	1.1%

Sources of disagreement

- Truncation error in the computation of the scattering distributions
- Tally type
- The underlying differential cross-section
- Simulation geometry and boundary crossings

Truncation Error

- The angular deflection distribution is computed from:

$$F_{gs}(s,\theta) = \sum_{\ell=0}^{L} \frac{2\ell+1}{2} \exp(-sG_\ell) P_\ell(\cos(\theta))$$

- Currently, MCNP truncates at L=240
- 240 terms is not appropriate for a wide range of parameters
- Particularly, for increasing energies and decreasing substeps
- New feature added to allow for arbitrary L

Truncation Error cont.

- Impact of new feature on results:

Table 4: Comparison of measured and calculated characteristic angles for 13-MeV electrons on Be, Al, Cu, Ta, and Au before and **after adding new feature**. Three different physics configurations are studied: default, *ESTEP*, and *EFAC*=0.99.

		Default		*ESTEP*		*EFAC*	
Material	Thickness (mg/cm2)	Calc. (deg.)	Rel. Diff. (%)	Calc. (deg.)	Rel. Diff. (%)	Calc. (deg.)	Rel. Diff. (%)
Al	70.1	4.308	8.223	4.558	14.48	4.289	7.745
Au	31.2	5.061	5.473	5.346	11.43	5.164	7.626
Al	**70.1**	**4.265**	**7.124**	**4.543**	**14.119**	**4.256**	**6.923**
Au	**31.2**	**5.016**	**4.537**	**5.338**	**11.254**	**5.130**	**6.921**

Tally type

- Used an F2 surface flux tally
    - Other codes used a cell volume tally...
    - Surface flux tallies make an approximation for grazing angles
    - Unlikely that grazing angles are the problem
- Will attempt a *F8 tally

Differential cross-section model

- Screened Mott:

$$\sigma_{el}^{M}(E,\mu) = \frac{(\tau+1)^2}{\tau^2(\tau+2)^2}\frac{2\pi r_0^2 Z^2}{[1+2\eta-\mu]^2}\left[\frac{\Sigma_{el}^{M}(\mu)}{\Sigma_{el}^{R}(\mu)}\right] \quad (1)$$

- Doubtful that the underlying DCS is the cause
- Will use EPRDATA14 to make determination
  - Single-event electron-photon DCS library
  - Well be included in MCNP6.2 release
  - See Grady Hughes presentation for details

Simulation geometry

- Small regions + boundary crossing approximation could be a source of error
  - Boundary crossing approximation

$$\tilde{\mu} = 1 - [1 - \mu(s)] \left(\frac{s_\delta}{s} \right) \quad (2)$$

  - Thin regions: scattering foil, monitoring chamber, and Mylar bag
- Sensitivity study
  - Method of last resort
  - Could help identify errors in model

Conclusions

- Overall performance not great (relative to class II codes)
- Uncertain about expectations
- Number of sources of disagreement

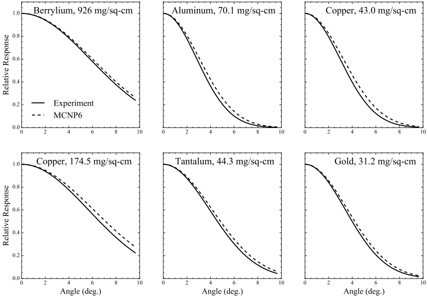

Figure 1: Comparison of Gaussian fits to experiment (solid curve) and calculated (dashed curve) angular distributions for 13-MeV electrons on various foils.

Conclusions cont.

- Overall performance not great (relative to class II codes)
- Uncertain about expectations
- Number of sources of disagreement

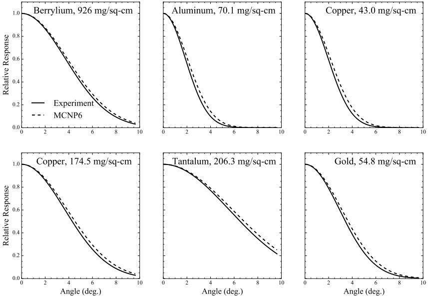

Figure 2: Comparison of Gaussian fits to experiment (solid curve) and calculated (dashed curve) angular distributions for 20-MeV electrons on various foils.

Questions?