LA-UR-10-00213

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Intended for: RPSD-2011 conference proceedings

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MCNP/X Form Factor Upgrade for Improved Photon Transport

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INTRODUCTION

Executive Summary

The angular distribution of scattered photons is incorrect in MCNPX [1] and MCNP5 [2] because the incoherent and coherent form factors are obsolete. We have upgraded MCNP/X and NJOY [3] to utilize newer ENDF/B-VII [4] form factor data and provided a new photoatomic data library to more accurately model photon transport.

Background

The inadequacies of the MCNP/X form factors were identified by Brian Quiter, Bernhard Ludewigt, and Vladimir Mozin in their study [5] of nuclear resonance fluorescence (NRF). Simulation of a 2 MeV endpoint energy bremsstrahlung photon beam striking uranium significantly underestimated the backwards scattered photon background This error was because the elastic scatter coherent form factors were incorrect. Quiter pointed out that the MCNP/MCNPX form factor data has remained nearly unchanged since the predecessor code, MCP [6], in 1973. These data are specified on a fixed grid of 21 points for incoherent form factors applied to Compton scattering and 55 points for coherent form factors applied to Thomson scattering. The grid is in units of inverse angstroms and for coherent scatter the maximum value allowed in MCNP/X is 6 A^{-1} even though the evaluated photon data library (EDPL97) [7], which is the basis of ENDF/B-VII photoatomic data, allows values up to $1x10^{11}$ A^{-1}. Consequently, Quiter observed that the truncated form factors make all the 1.7 MeV photons undergoing coherent Thomson scattering on uranium to go within 5^o of the forward direction, completely eliminating coherent backscatter. Indeed, all coherent scatter is affected for energies > 74 keV, and there is no coherent backscatter > 105 keV.

Fortunately, these large errors in photon scattering angular distributions generally have a negligible effect on most transport problems. The effect is greatest at high energies where Thomson scattering is small relative to the competing channels of incoherent scatter and pair production. Also the effect is greatest for high-Z materials where incoherent scatter and pair production are even more significant. But when looking at the photon backscatter background, Compton scatter, photoelectric fluorescence, and pair production all emit photons of lower energy and the elastic Thomson scatter photons stand out with their unchanged energy. For these coherent scatters the truncation of the form factors is most pronounced.

DESCRIPTION OF THE ACTUAL WORK

We have upgraded MCNP/X and are upgrading NJOY to utilize the newer ENDF/B-VII form factor data. A new photoatomic data library of 100 elements, unofficially named MCPLIB05, has been prepared using the latest ENDF/B-VII form factors. Coherent backscatter is now possible to 10^7 keV.

In previous MCNP/X, NJOY, and MCPLIB versions the incoherent Compton and coherent Thomson form factors were restricted to a 21-point and 55-point fixed momentum grid with any data points from the library evaluated at only those points. In Quiter's groundbreaking work coherent form factors were evaluated on a 77-point fixed momentum grid. In our work, form factor data can be represented on any arbitrary grid size which can be different for each element. All the ENDF data for both coherent and incoherent scatter are provided without interpolation to fit on a common grid.

As with ACE-format neutron cross section data, linear-linear interpolation is used for form factors even though the ENDF/B-VII source may use log-log interpolation. But NJOY can always add more linear points if required to minimize the error of not using log-log interpolation. Note that the photoatomic cross section data are interpolated on a log-log grid.

Although we have significantly improved the photon scattering treatment in MCNP/X by the upgraded form factor data, the MCNP/X treatment still omits Delbruck scatter, nuclear Thomson scatter, and anomalous scattering factors.

There are no user interface changes required for MCNP/X. The new form factors are used when available in the ACE libraries. Backwards compatibility is maintained in that use of the old (MCPLIB04 [8] and earlier) photoatomic data causes no changes to MCNP/X tracking.

RESULTS

Figure 1 illustrates the MCNPX sampled coherent Thomson scattering of monodirectional, monoenergetic, 1.7 MeV photons on uranium using both the old MCPLIB04 data and the new MCPLIB05 data.

MCPLIB04 coherent scatter is extremely forward peaked, truncated below $\mu > .996$ (blue line – nearly a delta function.) MCPLIB05 coherent scatter is also forward peaked, but backscatter is now present, and the forward peak is only 77% as high in the 1^{o} angle bin (black line).

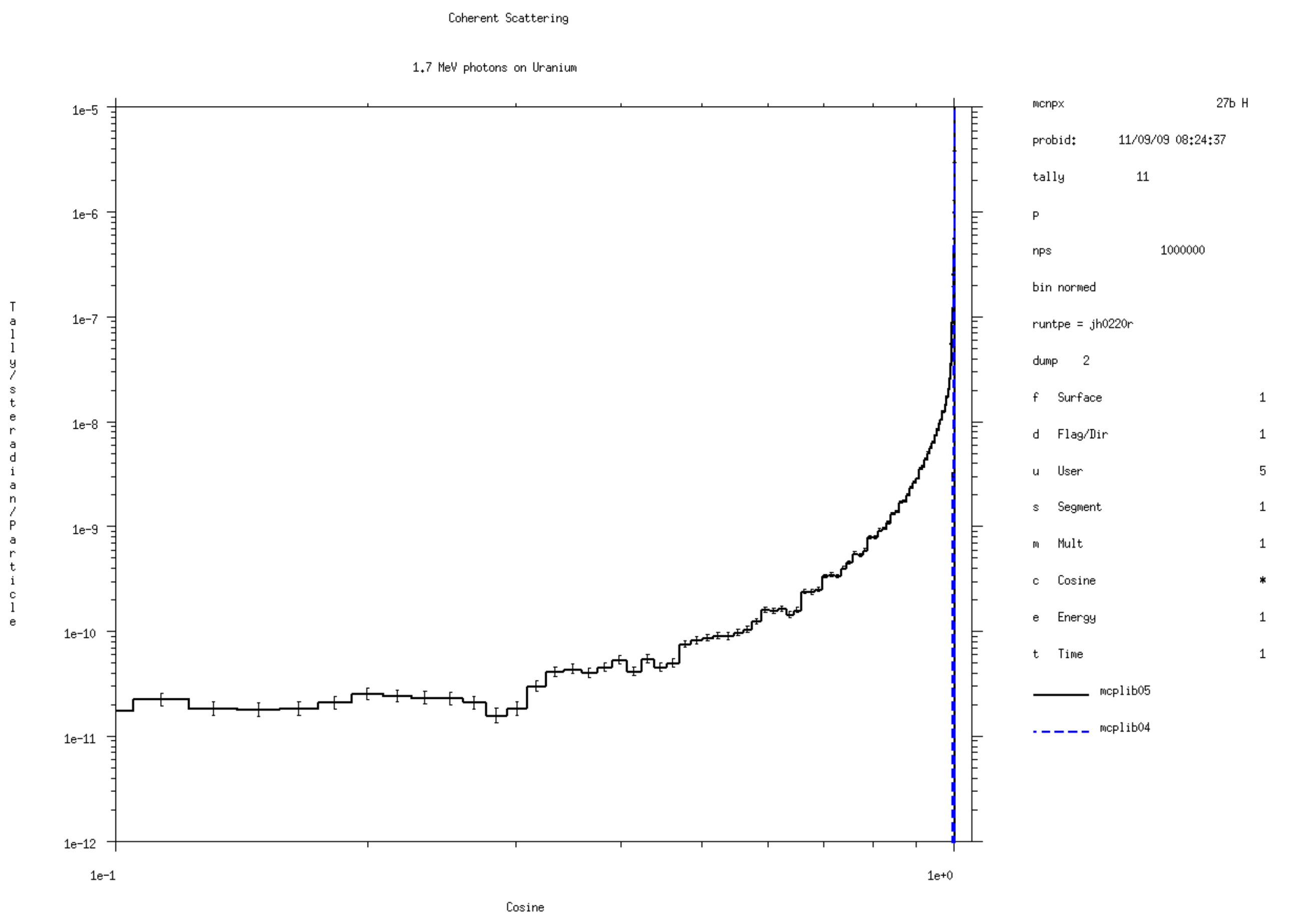

Figure 1. Coherent Thomson scattering of 1.7 MeV photons on uranium. The old MCPLIB04 data are the blue dashed forward-peaked line, and the new MCPLIB05 data are the black solid line extending from $-1 < \mu < 1$.

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