LA-UR- 08-5737

Approved for public release; distribution is unlimited.

Title: MCNPX Improvements for Threat Reduction Applications

Author(s): Laurie S. Waters, Joe W. Durkee, Ernst I. Esch, Michael L. Fensin, John S. Hendricks, Shannon T. Holloway, Michael R. James, Andrew Jason, Russell C. Johns, M. William Johnson, Toshihiko Kawano, Gregg W. McKinney, Peter Moller, Denise B. Pelowitz

Intended for: Proceedings of the 20th International Conference on the Application of Accelerators in Research and Industry, CAARI2008
American Institute of Physics Conference Proceedings Series

Los Alamos
NATIONAL LABORATORY
EST. 1943

MCNPX Improvements for Threat Reduction Applications

Laurie S. Waters, Joe W. Durkee, Jay S. Elson, Ernst I. Esch, Michael L. Fensin, John S. Hendricks,
Shannon T. Holloway, Michael R. James, Andrew Jason, Russell C. Johns,
M. William Johnson, Toshihiko Kawano, Gregg W. McKinney, Peter Moller, Denise B. Pelowitz
Los Alamos National Laboratory, Los Alamos, NM 87545

Keywords: Monte Carlo, muons, muon-capture, delayed neutron, delayed photon
PACS codes: 24.10.Lx 25.40Sc

Abstract

The DHS Domestic Nuclear Detection Office (DNDO) is funding a multiyear program of improvements for the MCNPX[TM1] Monte Carlo radiation-transport code. Additional work is also underway for DTRA Active Interrogation programs.

Enhancements contained in the current MCNPX 2.6.0 RSICC release will be presented, including stopped-muon physics, delayed neutron and photon generation, and automatic generation of source photons. Preliminary benchmarking comparisons with data taken with a PSI muon beam will be discussed. We will also describe current improvements now underway, including Nuclear Resonance Fluorescence, pulsed sources, and others. We will also describe very new work begun on a Threat-Reduction user interface, designed to simplify the setup of TR-related calculations, and introduce standards into geometry, sources and backgrounds.

[1] MCNPX is a trademark of Los Alamos National Security, LLC.

Introduction

MCNPX (Monte Carlo N-Particle Extended) [1] is a fully 3-dimensional Monte Carlo radiation transport simulation code. It tracks thirty single particles, and in addition, deuterons, tritons, He-3, alphas, and all heavy ions in the 2.6.0 version. The code uses evaluated nuclear data libraries for interaction probabilities, and in-line physics models when library data are not available. The inclusion of the CINDER'90 [2] transmutation code and data libraries into MCNPX enables burnup calculations as well as the generation of delayed photons and neutrons. The code runs on single or parallel platforms, and on PC, Linux and Macintosh machines.

MCNPX is extensively used in Threat-Reduction applications. Work is now underway on a multi-year code-improvement program sponsored by the Department of Homeland Security (DHS) Domestic Nuclear Detection Office (DNDO). Additional projects are funded by the Defense Threat Reduction Agency (DTRA). This paper reviews new code features related to active and passive interrogation included in MCNPX version 2.6.0, which was released for distribution by the Radiation Safety Information Computational Center (RSICC) in June 2008. The new features include, but are not limited to, muon-capture physics, delayed photon and neutron capabilities, generation of source photons, and tally tagging. Additional features are under development and will be released periodically in the MCNPX beta test program.

Muon-Capture Physics

Negative muons have features that may make them useful for active interrogation. In transport they either lose energy or decay into an electron and two neutrinos. The high-energy electron can cause further interactions, but overall a muon beam induces little beam-clutter background radiation. When a negative muon slows enough to be captured in an atomic orbital, the cascade to ground state first causes the emission of electrons, and finally of muonic x-rays whose energy is greater than an electron x-ray by approximately the ratio of the muon to electron mass, ~207. This results in MeV muonic x-ray energies in the 6 MeV range for uranium. The muon can then either decay or capture on a proton in the nucleus. Spallation or a collective response such as fission can be induced from the nuclear excitation caused by the proton capture or from x-ray absorption. Multiple neutron emission from these processes can occur.

In past versions of MCNPX, muons have undergone only slowing down from ionization, and decay in flight with a mean lifetime of 2.19703e-6 seconds. The default lower energy cutoff for muon transport is 0.113 MeV – this value can be changed by the user. In MCNPX version 2.6.0, once the muon reaches the energy cutoff, it enters into the new muon-capture physics routines. The capture nuclide is sampled from all nuclides in the material using F*Z weighting, where F is the atomic fraction of all elements with atomic number Z. Hyperfine-split K- and L-shell x-ray lines are hardwired into MCNPX for ^{10}B, ^{11}B, ^{12}C, ^{13}C, ^{16}O, ^{17}O, ^{18}O, ^{54}Fe, ^{56}Fe, ^{57}Fe, ^{58}Fe, ^{127}I, ^{133}Cs, ^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{235}U, and ^{238}U. Electron emission is currently ignored. One or more L-shell x-rays are sampled and banked for further transport. Next, one or more K-shell x-rays are sampled. A K-shell x-ray may be emitted, in which case it is banked for future transport, or the x-ray may be absorbed by the nucleus, with a probability of absorption that varies by Z for Z~>82. Less than Z~82, the energy of the x-ray is too small to make a significant contribution to absorption and is currently ignored in the code. If the x-ray is absorbed by the nucleus, the CEM physics code [3] is called to calculate the de-excitation by neutron emission, or fission of the excited nucleus. The excited nucleus has no change in Z or A from the original capture nuclide, but it will have the muon attached. In MCNPX, if fission occurs, the muon attaches to the larger of the two fragments. The alternative attachment to the smaller fragment is currently not implement in MCNPX.

The negative muon attached to the nucleus may decay with the free decay mean lifetime, or it may be captured by a proton in the nucleus. A lookup table based on the Primakoff relationship [4] is used to calculate the capture time versus the decay time. If the muon decays, the electron and neutrinos are banked for further transport. If it is captured, the residual is set to (Z-1, A), indicating the preferred channel of capture by a proton. Currently a single excitation distribution is used in MCNPX for all nuclides to assign a nuclear excitation, and CEM is used to determine the subsequent decay or fission of the excited residual. Improvements in the muon-capture routines will be made in the future, especially for the excitation function, and for the fission barriers in CEM that are affected due to the modified charge distribution induced by the presence of the muon in the nucleus.

The improved muon physics involves no change to the MCNPX user interface; this capability is active at all times. Work is also underway to increase the number of hyperfine x-ray lines through direct calculation [5].

In August 2007 muon-beam data was collected at the Paul Scherrer Institute SINQ spallation-neutron source on Depleted uranium and other targets, using a germanium detector to measure gamma emissions. A beam of 140-MeV negative muons was obtained from pion decay, and focused on the target. The experimental setup will be described in more detail in a future paper, and we anticipate increasing the amount of data in this continuing experimental program. Figure 1 shows initial raw gamma data (with background subtraction) between 6.0 to 7.0 MeV from a depleted uranium target compared to an un-normalized MCNPX simulation. Note the correspondence of the muonic x-ray lines, and also the indication of a high-energy continuum in the data and simulation, which is related to the high-energy electrons from muon decay interacting with the experimental setup. The resolution of the germanium detector used for this data was substandard due to damage in shipping, and we expect a substantial improvement in peak resolution in the next measurement.

Delayed Neutrons and Photons

The addition of the CINDER'90 burnup code and data libraries gives MCNPX the ability to generate detailed time and energy distributions of 'delayed' neutrons and gammas emitted by decaying activation products. Two improvements to this capability are now available- the generation of specific neutron emission energies for light nuclides (this feature is still undergoing testing), and the ability to sample individual line data for delayed photons in addition to the current multigroup capability. Figure 2 shows examples of the neutron line data from four light nuclides. This allows MCNPX to accurately model a major competitor to delayed neutrons from fission; the neutron emission of ^{17}N, which has a half-life of 4.17 seconds.

The addition of delayed photon lines is an ongoing process. Data for 979 nuclides is now available, while the remaining nuclides have either no data or multigroup photon-emission spectra. For the code to access the delayed photon data effectively, the entire set of lines needed in the simulation should be loaded into memory. For an actinide problem, about 4 Gbytes of memory is required.

Spontaneous Photon Capability

The ability to generate an appropriate spontaneous-fission neutron distribution and do multiparticle correlations on those particles was added in version 2.5.0 of MCNPX. A similar capability for spontaneous photon emission is now available. The code searches a volume defined in the SDEF source card, and then searches the CINDER gamma-line database for decay gammas and adds these to the source. This capability is activated with the PAR=SF keyword on the SDEF card. Future work will include the ability to assign an age to a material, resulting in a gamma source based on the buildup of decay products at a specific time.

Tally Tagging

Neutron, photon and electron interactions in MCNPX can now be scored by production mechanism and physical origin. This feature can aid in determining whether a signal is actually coming from a threat object. A user may specify tallies based on nuclide or residual nuclide from which the particle is emitted, the reaction type as determined by ENDF reaction numbers, and the geometry cell from which particles are produced. The capability is controlled by an FT card with the keyword 'TAG', and an additional parameter that determine various treatments for collided particles. The user enters the desired cells and reaction channels on an FU card. Figure 3 shows an example consisting of photons tallied within a sphere of lead, that has a 14-MeV neutron point source at its center. Separate tallies are obtained for neutron-capture gammas, bremsstrahlung and fluorescence photons, K shell x-rays, 511-keV annihilation photons and the Compton continuum.

Conclusion

In addition to the features described here, the MCNPX team is working on other code capabilities of interest to Threat Reduction applications. Nuclear Resonance Fluorescence cross sections and emitted photons are being included into the ENDF format, and processed into ACE files for use by MCNPX. Two beam-related capabilities of interest to active interrogation are now being tested. These include a simplified way to designate accelerator beams from micropulse to macropulse, and a new source definition that allows the user to input beam emittance parameters to enable focusing of charged particle beams.

A major project under development is the formulation of a special-purpose wrapper for MCNPX, which will enable the simple specification of Threat Reduction problems. Standardization of input and output options is achieved through the use of templates for venues, geometries, primary and background sources, detectors, and analysis methodologies. This code is meant to greatly simplify the input and analysis process, and we anticipate release in mid FY'09.

References:

1. D. B. Pelowitz, ed., "MCNPX™ User's Manual, Version 2.6.0", Los Alamos National Laboratory, LA-CP 07-1473 (April 2008).

2. M. L. Fensin, J. S. Hendricks, S. Anghaie, "The Enhancements and Testing of the MCNPX Depletion Capability," Los Alamos National Laboratory Report, 2008 International Congress on Advances in Nuclear Power Plants Embedded International Topical Meeting at the 2008 ANS Annual Meeting, ICAPP '08, Anaheim, CA (June 8-12, 2008).

3. S. G. Mashnik, K. K. Gudima, M. I. Baznat, A. J. Sierk, R. E. Prael, and N. V. Mokhov, "CEM03.S1, CEM03.G1, LAQGSM03.S1, and LAQGSM03.G1 Versions of CEM03.01 and LAQGSM03.01 Event-Generators," Los Alamos National Laboratory report LA-UR-06-1764 (March 6, 2006).

4. H. Primakoff, *Muon Physics*, eds. Highes and Wu, vol. II (Academic Press, 1975) p 3.

5. G. A. Rinker, "Static and Dynamic Muonic-Atom Codes – MUON and RURP", Computer Physics Communications 16 (1979) 221-242.

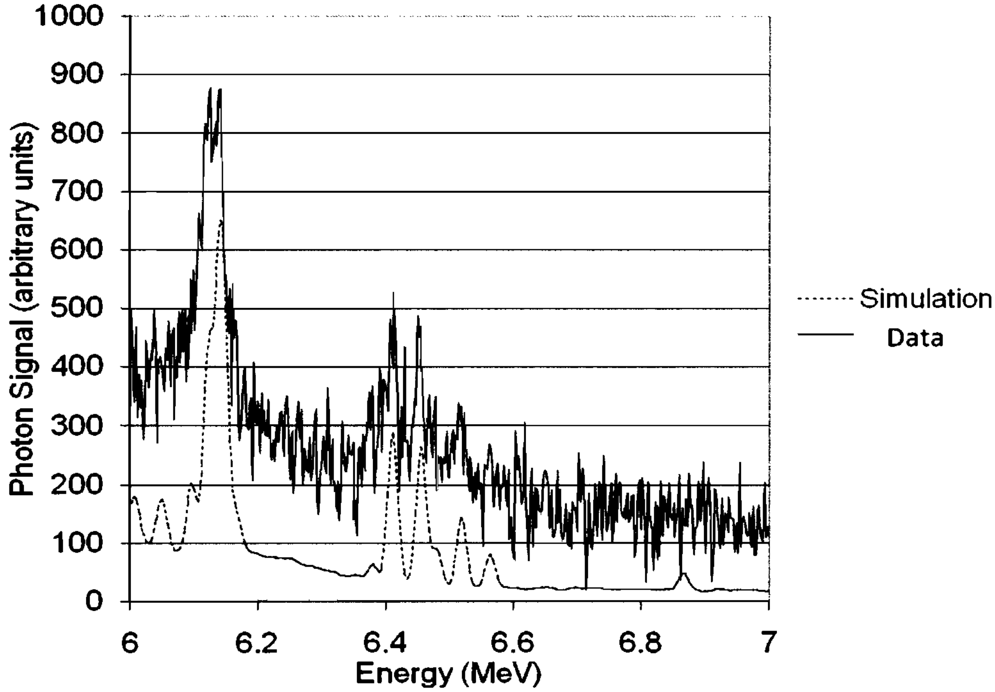

Figure 1: Comparison of MCNPX muon x-ray simulations with PSI raw experimental data

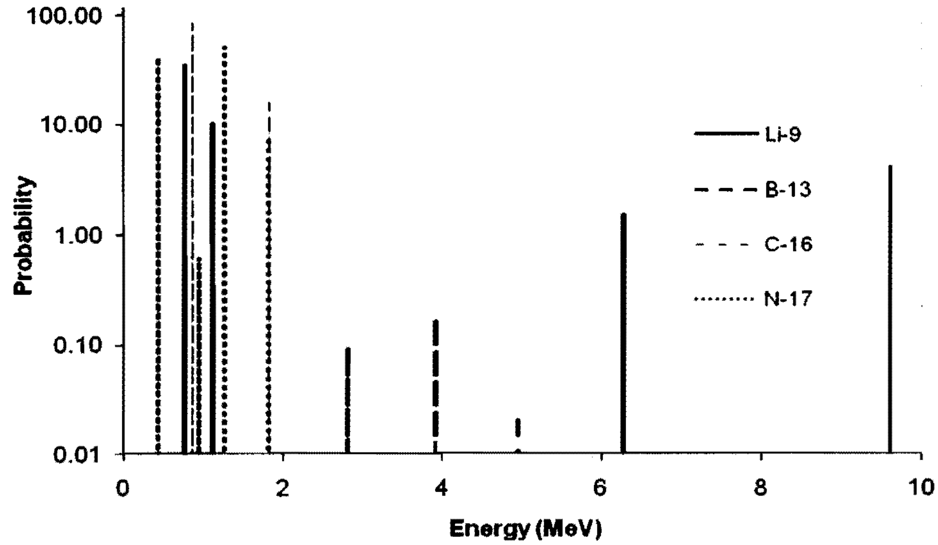

Figure 2: Neutron emission lines from light-ion decay.

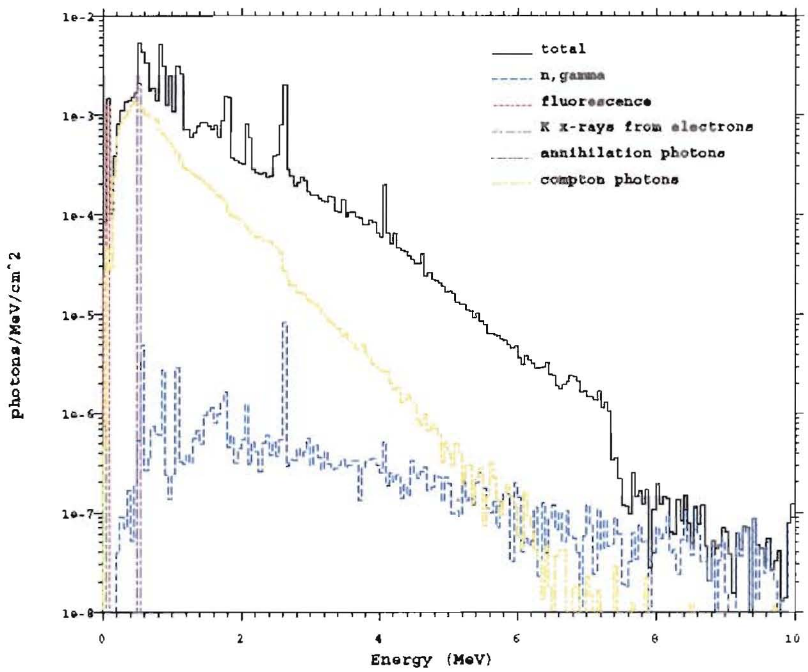

Figure 3: Photons generated from a 14-MeV neutron source at the center of a 5.0 cm radius lead sphere, from different production mechanisms.