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Title: A New MCNP6 Electron-Photon Transport Validation Test: The Lockwood Energy Deposition Experiment: version 1.

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Memorandum

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Subject: A New MCNP6 Electron-Photon Transport Validation Test: The Lockwood Energy Deposition Experiment: version 1.

Summary

This memo announces the availability of a new validation test for quantifying the accuracy of the MCNP6 electron-photon transport algorithm for use in energy-deposition calculations. Specifically, energy-deposition results are compared with the Lockwood energy-deposition experiment [1, 2]. The comparison includes energy-deposition profiles in a variety of different single-element materials including beryllium, aluminum, carbon, copper, iron, molybdenum, tantalum, and uranium for pencil beam electron sources with energies including 0.05-, 0.1-, 0.3-, 0.5, and 1-MeV and angles of incidence including normal, 30°, and 60° off-normal.

The purpose of this memo is to discuss the contents of the Lockwood validation directory and to outline the procedure for generating the input files, running the tests, processing the results, and comparing results to the experimental and numerical benchmark. Each step is mostly automated by a makefile that executes the necessary perl script.

Lockwood validation directory structure

The Lockwood directory is located in the MCNP6 Testing/ELECTRON directory and contains the following files and sub-directories:

Files

./compare_results.pl

./Makefile

./mcnp_ep_lockwood_utils.pm

./process_lockwood.pl

./run_lockwood.pl

./setup_lockwood.pl

./plotResults.py

./plot_all.sh

Sub-directories

./input_files

./experimental_benchmark

./numerical_benchmark

./results

Generating the input files

Input file generation is straightforward. From the lockwood directory where "Makefile" is located, one simply enters the following command highlighted in blue:

~/lockwood: make setup_all

This command will make two directories, "condensed_history" and "single_event," in the input_files directory. In both "condensed_history" and "single_event," a directory for each material is created where each of the corresponding input files are placed after they are generated. The input files follow a specific naming convention, or <material>_<energy>_<angle>_cell_<cell number>_. For example, for 1-MeV electrons normally incident on molybdenum, the input filename for the 4th cell is "mo_1mev_0deg_cell_4_." The number of input files is problem dependent and can range from a single cell up ~20 cells.

Alternatively, one can generate a test for a single material for a given mode "condensed_history" or "single_event" by entering the following command (for aluminum in single-event mode):

~/lockwood: make MAT="al" MODE="single_event" setup_one.

Running the test

Once the input files are generated, one can elect to run the test for a single material or all materials, using both condensed history and/or the single-event physics modes for electrons. To run all of the tests for each enters the following command:

~/lockwood: make run_all

Alternatively, one can run the test for one mode by entering the following commands

~/lockwood: make run_all_ch

or,

~/lockwood: make run_all_se

While this is a simple command for running all of the tests, it is recommended that the tests be run for each material individually because runtime can be significant. To do so for aluminum using condensed history, one enters the following command:

~/lockwood: make MAT="al" MODE="condensed_history" run_one.

To run the same test using single event one enters:

~/lockwood: make MAT="al" MODE="single_event" run_one.

The validation test is currently fixed to check if one is running on the yellow HPC machine called "Mapache." If so, the test will be submitted with parallel processing using the Moab command "msub." If not, the script assumes that the mcnp6 executable can be found by searching the PATH variable, and will run the jobs in serial (the assumption is that job is being run on a local machine).

Processing the results

Similar to the previous section, one can process all of the results simultaneously for a given mode, or individually by material. Keep in mind that the processing scripts relies on an MCNP6 perl module, so the results must be processed from the corresponding MCNP6 Lockwood validation directory. To process all of the condensed history results one enters:

~/lockwood: make MODE="condensed_history" process_all.

Alternatively, one can process a results single material by entering:

~/lockwood: make MAT="al" MODE="condensed_history" process_one.

After the results are processed, they are placed in "./results/condensed_history/"or "./results/single_event". The results files, including an energy deposition profile and a relative difference profile, are generated for each source energy and angle.

Comparing the results

Finally, one can compare the results to the numerical benchmark included with the test to verify if any changes in results have occurred perhaps as a result of modifying the source code. The numerical benchmark was generated using MCNP6 version 1.0 in condensed history mode. To compare all of the results one enters:

~/lockwood: make MODE="condensed_history" compare_all.

Alternatively, one can process a result for a single material by entering:

~/lockwood: make MAT="al" MODE="condensed_history" compare_one.

For those interested in studying the accuracy of MCNP6 with respect to the experimental results, one can simply view the results in the results directory. In addition, a python script for

plotting results is available. To generate plots for all of the materials, run the bash script "plot_all.sh" by entering:

~/lockwood: ./plot_all.sh.

This will generate plots of the results in pdf format similar to those found in reference [2]. See the "plot_all.sh" for examples of the proper usage of "plotResults.py."

References

[1] G.J. Lockwood, G.H. Miller, and J.A. Halbleib, Calorimetric Measurement of Electron Energy Deposition in Extended Media – Theory vs. Experiment, Sandia National Laboratory report, SAND79-0414, 1987.

[2] D. Dixon and H.G. Hughes, Validation of MCNP6® Electron Energy Deposition in Extended Media for Source Energies ≤ 1-MeV, Los Alamos National Laboratory report, LA-UR-16-22749, April 12th, 2016.

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