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Benchmarking of nuclear data for TRIPOLI-5, the new Monte Carlo code at CEA

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The PATMOS mini-app is a prototype of a massively parallel Monte Carlo particle transport code, developed at CEA in order to conceive alternative algorithms for novel HPC architectures, in view of the TRIPOLI-5® production code. Recently, the sampling laws for modeling neutron physics as provided in nuclear data libraries have been implemented into PATMOS, first within the so-called « free-gas » model (without treatment of the unresolved resonance range) and then by adding thermal neutron scattering treatment in order to include crystal or molecular bond-effects. As a first step towards the validation and verification of this implementation, code-to-code comparisons have been performed between PATMOS and two other reference Monte Carlo transport codes, TRIPOLI-4® and OpenMC, over around 560 isotopes taken from the JEFF-3.3 nuclear data library. First, the energy or angle distributions have been compared between the three codes for each isotope and reaction, at various incident energies, by resorting to Kolmogorov-Smirnov statistical tests, thanks to dedicated sampling routines. Then, the evaluation of the microscopic cross sections (as well as the multiplicity) by each code has been verified, in order to detect possible discrepancies. Finally, more than 5000 configurations have been tested for a simple benchmark consisting in a sphere filled with a single isotope, irradiated by a single-energy and isotropic source located at the center of the sphere (ten representative incident energies have been considered). The results of the fiducial quantity (flux per unit of lethargy) obtained with PATMOS and with the other reference Monte Carlo codes have then been compared by using the Holm-Bonferroni statistical test. The comparison between PATMOS and TRIPOLI-4® was found to be more involved because of the post-processing of nuclear data; indeed, TRIPOLI-4® relies on ENDF files, while PATMOS relies on ACE files, which leads to discrepancies in underlying nuclear data "seen"by the different codes. Our work has allowed i) validating the implementation of the free-gas model and of the thermal scattering laws in PATMOS, thanks to the perfect statistical agreement between PATMOS and OpenMC; ii) highlighting some inconsistencies in nuclear data; iii) detecting some implementation errors in the sampling routines.

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