Implementation and Validation of the Pulse-Height Tally in OpenMC

Christopher Fichtlscherer, Friederike Frieß, Malte Göttsche and Moritz Kütt

Abstract

Monte Carlo particle transport tools can simulate gamma spectrometry results using a pulse-height tally. Such a tally calculates how much energy is deposited in a cell by an entire particle history. This makes its implementation a sophisticated task that requires detailed bookkeeping of the particle and its progeny. So far, the open source Monte Carlo code OpenMC lacks the functionality of such a pulse-height tally. This article describes its implementation for photons and presents an extensive validation of its results, which relies on three pillars: analytically-based validation, software-based validation, and experimental-based validation.

Keywords

OpenMC, Gamma spectroscopy, Pulse-height tally, Code validation

Introduction

Gamma spectroscopy is a common measurement approach for a large variety of applications, including, for example, the passive assay of fissile materials or nuclear warhead authentication. Adequate simulation capabilities for gamma spectroscopy support the detailed analysis of future measurements as well as the development of new applications. For simulating gamma spectroscopy applications, a so-called pulse-height tally is needed.

A "tally" in a Monte Carlo particle transport simulation is a function that allows for the estimation of a physical quantity. The pulse-height tally allows users to estimate the energy deposited by gamma radiation in a measurement system. The name is chosen in analogy to actual measurement devices. The height of an electric pulse measured, for example, from the output of a photo-multiplier tube connected to a scintillator crystal is – under ideal conditions – proportional to the energy the photon deposited in the crystal.

This article describes the implementation and validation of a pulse-height tally for the open source Monte Carlo code OpenMC [Romano et al. 2015]. The initial release of OpenMC focused on neutron transport. More recently, developers added the capability to simulate photon transport [Lund and Romano 2018], but OpenMC still lacks the functionality of a pulse-height tally. MCNP, another commonly used Monte Carlo particle transport code, features pulse-height tallies [Sood et al. 2004]. In contrast to OpenMC, however, the software is proprietary, with strict limits on source code access. Implementing a pulse-height tally in OpenMC will allow the software's growing user community to conduct gamma spectroscopy simulations in a transparent and accessible manner.

Implementation

To implement a pulse-height tally (PHT) function, it is necessary to record the total energy deposited in a given volume, both by the incoming photon and by secondary particles. Interactions of the incoming photon with the detector material (e.g. Compton scattering) create such secondary particles. Figure 1 shows four exemplary particle tracks. Particle I does not interact in the detector volume, resulting in a PHT value of zero. The energies lost during the three scattering interactions must be added to obtain the PHT value for particle II. Particle III is absorbed in the cell through the photoelectric effect. In that case, the PHT value corresponds to the full energy of the particle. For particle IV, only the two scattering reactions inside the cell contribute to the PHT value.

Most tallies can be evaluated in parallel to carrying out the particle transport simulation, for example to estimate the total reaction rate in a cell it is sufficient to count each reaction, independent of the reacting particles prior or future interactions. For a pulse-height tally, however, one must calculate the particle's entire history beforehand.

In the object-oriented structure of OpenMC, this is done by adding a method to the "particle class". The new method tracks the energy deposited by the individual particle's interactions in a particular cell. OpenMC considers coherent (Rayleigh) scattering, incoherent (Compton) scattering, photoelectric effect, and pair production. Only the latter three lead to energy deposition. The same method tracks secondary photons from such interactions. If secondary photons leave the cell, their energy is subtracted from the PHT value. The interaction of photons with nuclides can also produce electrons or positrons as secondary particles. OpenMC does not support transport simulations of these particles and uses a simplified model here. Positrons generate two 511 keV photons directly at the location of the positron creation. OpenMC provides two different options for electrons: Either the electron deposits its total energy

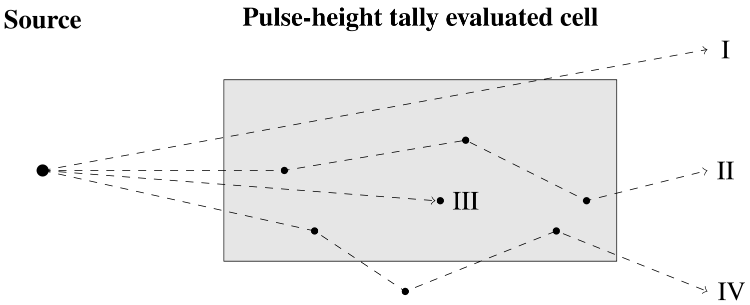

Figure 1. *Four exemplary particle histories (points: location of interactions, dashed lines: particle tracks).*

at the location of creation, or photons are created in the form of bremsstrahlung (OpenMC is using the so-called thick-target bremsstrahlung approximation [Lund and Romano 2018].). The simulations presented here use the second option. OpenMC stops transporting ("kills") photons that fall under a user-specified energy limit, to improve computing efficiency. The default cut-off value is one keV. The PHT function also takes into account the energy of photons killed in the cell of concern.

Currently, the implementation only allows for the software execution with an active pulse-height tally as a single-core process because of limitations with particle ID handling in OpenMC. To execute a pulse-height tally simulation on multiple cores, several such simulations must be started using different random number seeds. Afterward, results can be combined to reduce statistical uncertainties. We have worked with this procedure using an additional Python script for data aggregation.

In an actual measurement of a gamma spectrum, different physical effects such as charge collection statistics, electronic noise, and variations in the detector response over its active volume contribute to the intrinsic resolution of a detector [Knoll 2010]. Instead of narrow lines, peaks appear broadened. The energy resolution of a detector describes how well it can distinguish nearby peaks. If the energies of incoming photons are too close to each other, the detector will measure them as a single peak. The resolution of a detector depends on the energy of the incoming particle and is proportional to $1/\sqrt{E}$ [Heath 1964]. Typically, the resolution is given as the quotient of the full width at half maximum (FWHM) of the full energy peak divided by its energy. The broadening can be approximated by a Gaussian distribution [Heath 1964]. The standard deviation $\sigma(E)$ of the approximating distribution for a given energy E, is by

$$\sigma(E) = \frac{\mathrm{FWHM}(E)}{2\sqrt{2\ln 2}} \tag{1}$$

related to the FWHM of a peak of a certain energy. To replicate experimental results, we have added a functionality to the OpenMC pulse-height tally to automatically broaden spectral results, using a user-provided energy-dependent detector resolution function.

Validation

To ensure that our implementation delivers correct results, we carried out extensive validation with an analytical method, through comparison with other simulation software and experimental data.

Analytical validation

The analytical validation of the new pulse-height tally follows an approach described by [Shuttleworth 1994] and [Sood et al. 2004]. Here, we consider a simplified setup: A cylinder with a length and diameter of $\ln(2)$ cm (shown in Figure 2) contains three theoretical elements Kneeon, Moron, and Odium. Interactions with these elements are simplified versions of pair production, photoelectric absorption, and Compton scattering. The material in this cylinder has a total macroscopic cross section of $1/\mathrm{cm}$. Half of the interactions are simplified pair productions, 30 percent simplified Compton scattering events, and 20 percent simplified photoelectric absorption. Photons start with an energy of 3.2 MeV towards the cylinder. The simplified pair production creates two photons, each with a quarter of the incoming photon's energy. If the incoming photon energy was above 1.0 MeV, one of these photons is scattered through ninety degrees. The simplified photoelectric effect leads to the absorption of the incoming particle. Simplified Compton scattering reduces the energy of the incoming photon by half without changing its direction. Photons below a threshold energy of 0.15 MeV are killed.

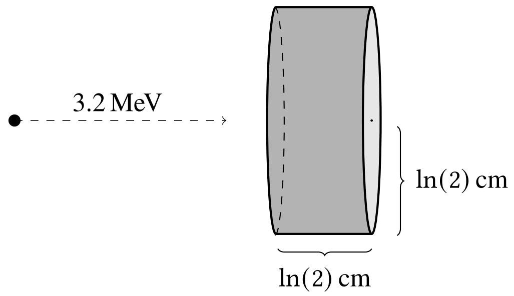

Figure 2. *A schematic representation of the setup for the analytical validation of the pulse-height tally.*

The approach's simplicity leads to 161 potential interaction histories for an incoming photon, resulting in nine different energies for the PHT value. We have implemented the artificial elements and the simplified reactions in OpenMC as described above. For the OpenMC simulation, 10^{10} particles were started. To provide estimates for the statistical uncertainty of resulting values, we calculated the standard deviation of the results of 1,000 sub-samples (with 10^7 particles each) to the average result of all sub-samples. Furthermore, we calculated the probabilities for the 161 interaction histories through a separate numerical calculation. Table 1 summarizes the results. The OpenMC calculations and the numerical calculations agree within the range of the statistical errors. The table also shows analytical solutions for the different possible energies from two sources. Comparing the OpenMC simulations to the results from [Sood et al. 2004], one finds larger discrepancies. In fact, the authors themselves found similar inconsistencies between their MCNP simulation results and the analytical values. Likely, this points to an error in the analytical solution. Analytical values published earlier in [Sood, Reed, and Forster 2003] are much closer to OpenMC and numerical results. Overall, the validation using this simplified physics model shows that the implemented PHT produces valid results.

Energy [MeV]	OpenMC result	Standard deviation	Numerical result	Analytical result [Sood, Reed, and Forster 2003]	Analytical result [Sood et al. 2004]
0.0	0.500005	$1.609 \cdot 10^{-4}$	0.499988	0.5	0.5
1.6	0.190617	$1.242 \cdot 10^{-4}$	0.190609	0.190616	0.190615
2.0	0.060757	$7.594 \cdot 10^{-5}$	0.060754	0.060758	0.059594
2.2	0.025117	$5.108 \cdot 10^{-4}$	0.025127	0.025118	0.027446
2.4	0.068594	$8.065 \cdot 10^{-5}$	0.068595	0.068597	0.067084
2.6	0.010005	$3.171 \cdot 10^{-5}$	0.010008	0.010006	0.010565
2.8	0.024178	$4.820 \cdot 10^{-5}$	0.024178	0.024176	0.023878
3.0	0.005745	$2.400 \cdot 10^{-5}$	0.005745	0.005745	0.006057
3.2	0.114981	$1.301 \cdot 10^{-5}$	0.114995	0.114986	0.114760

Table 1. *Results for pulse-height tally estimates with a simple photon interaction model in simple geometry. OpenMC results were derived from an implementation of that model and simulations using* 10^{10} *particles. The standard deviation is calculated from 1,000 sub-samples of the entire simulation. The third column shows numerical results from separate calculations for the potential particle interaction histories. The two right columns show values of analytical solutions as presented in two different publications.*

Software-based validation

For the software-based validation, a simplified scintillation detector was modeled in MCNP6 [Werner et al. 2018] and OpenMC (cf. Figure 4). The model is based on the NaI-based "802 Scintillation Detector" by Mirion Technology [Mirion Technology Inc 2017]. OpenMC used the photon interaction cross section library ENDF/B-VII.1, MCNP6 the ENDF/B-VII.0 library. The photon source was modeled as a disk of the same radius as the detector (with casing), 10 cm in front of the detector. The photons are produced at random positions on this disk and emitted parallel to the source surface normal towards the detector. We used the pulse-height functionality to simulate the measurement of this detector for different gamma sources and compared the results.

Cs-137 spectrum Figure 3 shows simulation results for a scintillation detector with 100 detector channels and a mono-energetic source with an energy of 0.6617 MeV (Cs-137). The plot shows the various characteristics, such as the full energy peak, the Compton edge, and the backscatter peak. Overall, results are nearly identical, indicating good agreement between the newly implemented pulse-height tally and the tally functionality of MCNP6. The smaller peak near 0.63 MeV is a simulation artifact, which needs further investigation. As it is present in both simulations, we still conclude that our PHT implementation provides valid results.

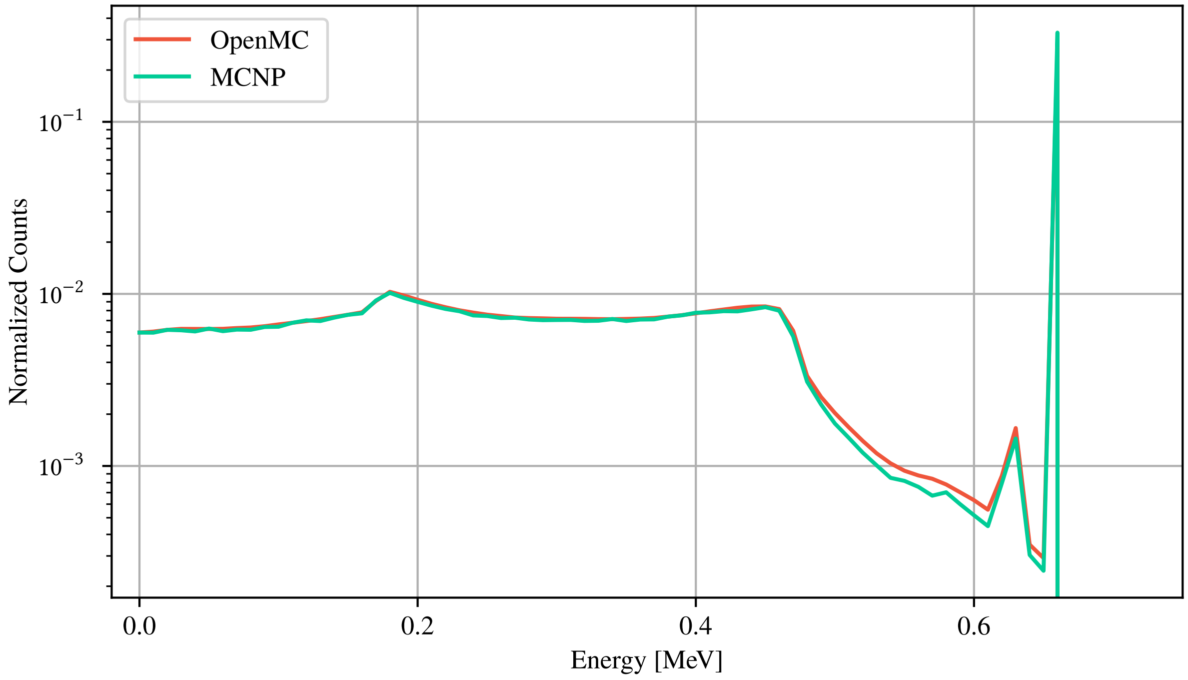

Figure 3. *The simulation result of the measurement of a Cs-137 gamma spectrum with a pulse-height tally in MCNP6 and OpenMC.*

Comparing various energies We ran 300 simulations for incoming photons with energies between 0 MeV and 3 MeV in steps of 10 keV. Each simulation result is an individual spectrum with 2048 energy bins. The full-energy peak is placed in the last energy bin. The simulations included 10^8 starting particles each.

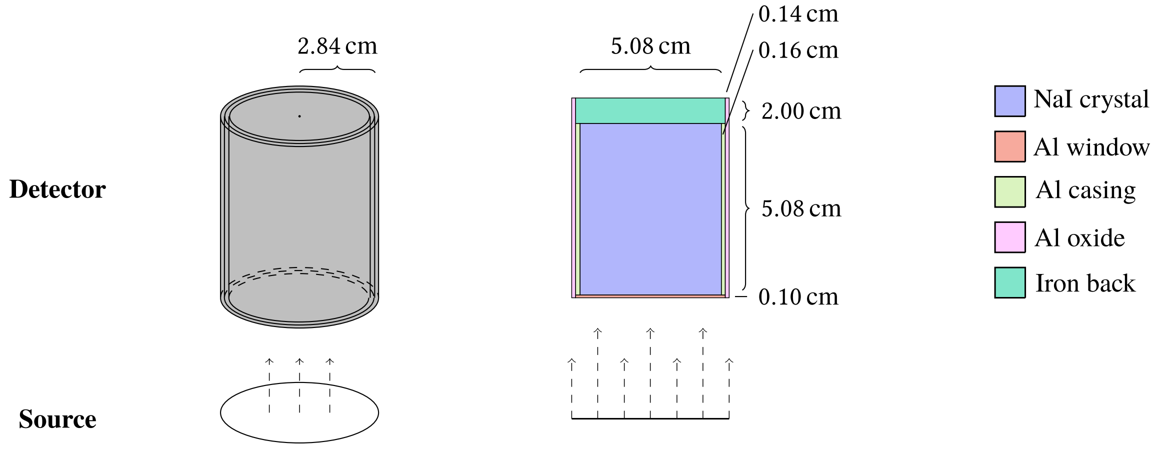

Figure 4. *Detector model used for simulations with OpenMC and MCNP, based on "802 Scintilation Detector" by Mirion Technology [Mirion Technology Inc 2017].*

As a metric to compare OpenMC to MCNP, we computed the result of the Kolmogorov-Smirnov test [Massey Jr. 1951] for each pair of simulations of all 300 energy levels. The Kolmogorov-Smirnov test is a versatile statistical test to compare probability distributions. To calculate the test, we first determined the cumulated function of the spectra. Then, we searched for the maximum difference between the two functions. We reject a null hypothesis at a significance level α if the maximum value between the two cumulative functions is larger than a particular critical value

$$d_\alpha = c(\alpha) \cdot \sqrt{\frac{n_1 + n_2}{n_1 \cdot n_2}}, \tag{2}$$

where $c(\alpha)$ is the Kolmogorov distribution. The null hypothesis assumes that both results come from the same distribution. In our case, $n_1 = n_2 = 2048$. Assuming a significance level of $\alpha = 0.01$, the critical value is $d_\alpha = 0.072$.

The comparison results for all the simulations can be seen in Figure 5. We do not find energies for which the Kolmogorov-Smirnov test is higher than the critical value. We can conclude that the simulations give very similar results, again providing evidence that the new PHT in OpenMC provides valid results.

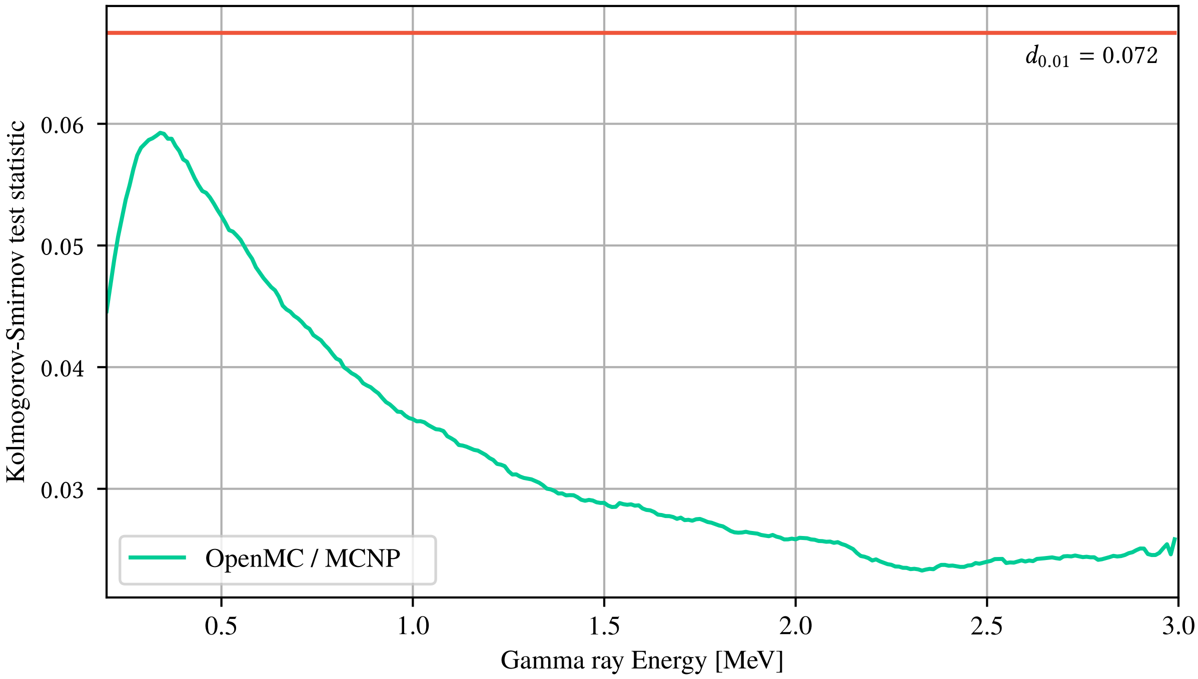

Figure 5. *Comparison of 300 spectra in the energy range from 0 MeV to 3 MeV, generated with MCNP6 and OpenMC. For the comparison, we use the Kolmogorov-Smirnov test. Simulation results are considered equal if the test result is below the critical value.*

Experimental validation

A comprehensive set of experimental results is provided by [Heath 1964]. The authors used a 3 × 3 inch cylindrical NaI detector to measure the gamma spectra of many isotopes. We modeled this detector in OpenMC. Figure 6 shows a concept drawing of the model. To simulate experimental results, both the PHT function and the spectrum-broadening functionality were used. Since no specific information was given about the source, we approximated it as a point source. Also, [Heath 1964] does not provide details about the background, which we ignore in our simulation. Hence, the following results are mostly a qualitative comparison.

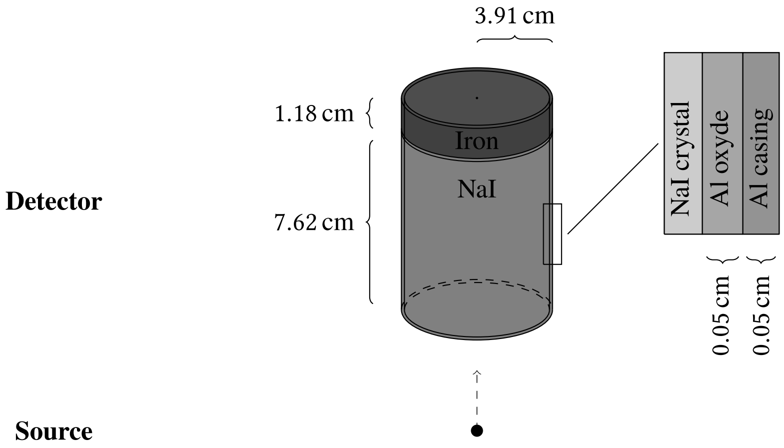

Figure 6. *The setup modeled in OpenMC for comparison of the results of the pulse-height tally with experimental data.*

To determine the energy-dependent resolution of the detector, we fit the function

$$f(E) = a \cdot \frac{1}{\sqrt{E}} + b \tag{3}$$

to data points read manually from Figure 6 in [Heath 1964, p. 9]. Figure 7 shows the individual values and the fit, using parameters $a = 3.756$ and $b = 3.991$ with a mean squared fitting error of 0.507. The figure also shows detector resolutions calculated from the nine experiments presented below.

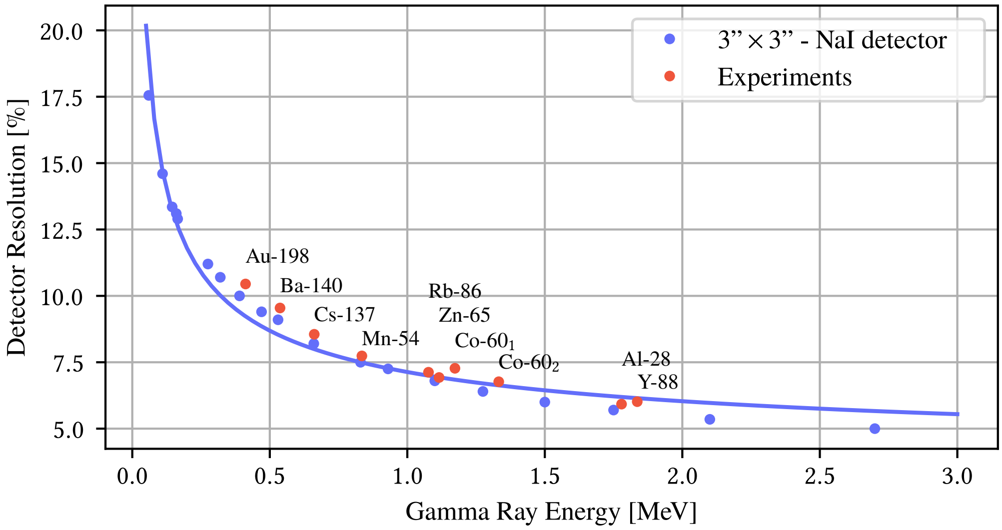

Figure 7. *Detector resolution. Blue dots show the values given in [Heath 1964]. The blue line uses the fit parameters described in the text. Red dots show the resolution for the experimental spectra considered here.*

These parameters are used in the custom broadening function for the pulse-height tally. Figure 8 shows the results of nine experimental measurements and the simulated spectra. The individual plots also show the initial sources of photon energies as vertical lines. In our simulations, we use the Python package PyNE 0.7.1 Scopatz et al. 2012 to determine energy and intensity of source photons. Some experimental spectra were only given in a normalized form, marked by the letter "n" in Figure 8. For comparison, the simulation results were normalized using the number of total counts. We used the detector efficiency given in [Heath 1964] for the other experiments to determine the total number of simulated particles. Per isotope, we used the efficiency of the full energy peak. Certain experimental spectra did not match the expected source energies by two or three energy bins. For the plots shown in the figure, the data was shifted by the respective bin count. We also notice some unexpected behavior in the low-energy regions of the experimental results. Very likely, the high count rates are the result of electronic noise. Mostly, the simulations match the experimental results well. For Zn-65, we see an additional peak at 511 keV in the experimental data that our simulation results do not include. The peak results from photons produced by the annihilation of positrons produced in the β^+ decay of Zn-65. OpenMC does not transport the non-gamma decay products, hence the effect is not yet simulated. The source function should be modified to include isotropically emitted photons for source isotopes with β^+ decay to include this in the future. A difference is also visible for the Co-60 spectrum. After the β^- decay, two photons with energies 1.17 MeV and 1.33 MeV are emitted in succession at intervals of only 23 ps on average. Experimental gamma spectra include a summation peak, which occurs if the detector absorbs both photons. In the figure, we have inserted the sum of the two energies as a purple dashed line. Modeling such effects with OpenMC would require the software to start correlated particles, which is currently impossible.

Overall, the experimental comparisons show the validity of the newly implemented pulse-height tally. While some challenges remain, we consider the functionality ready to use for other applications. An example use case is presented at this conference [Fichtlscherer, Göttsche, and Kütt 2021].

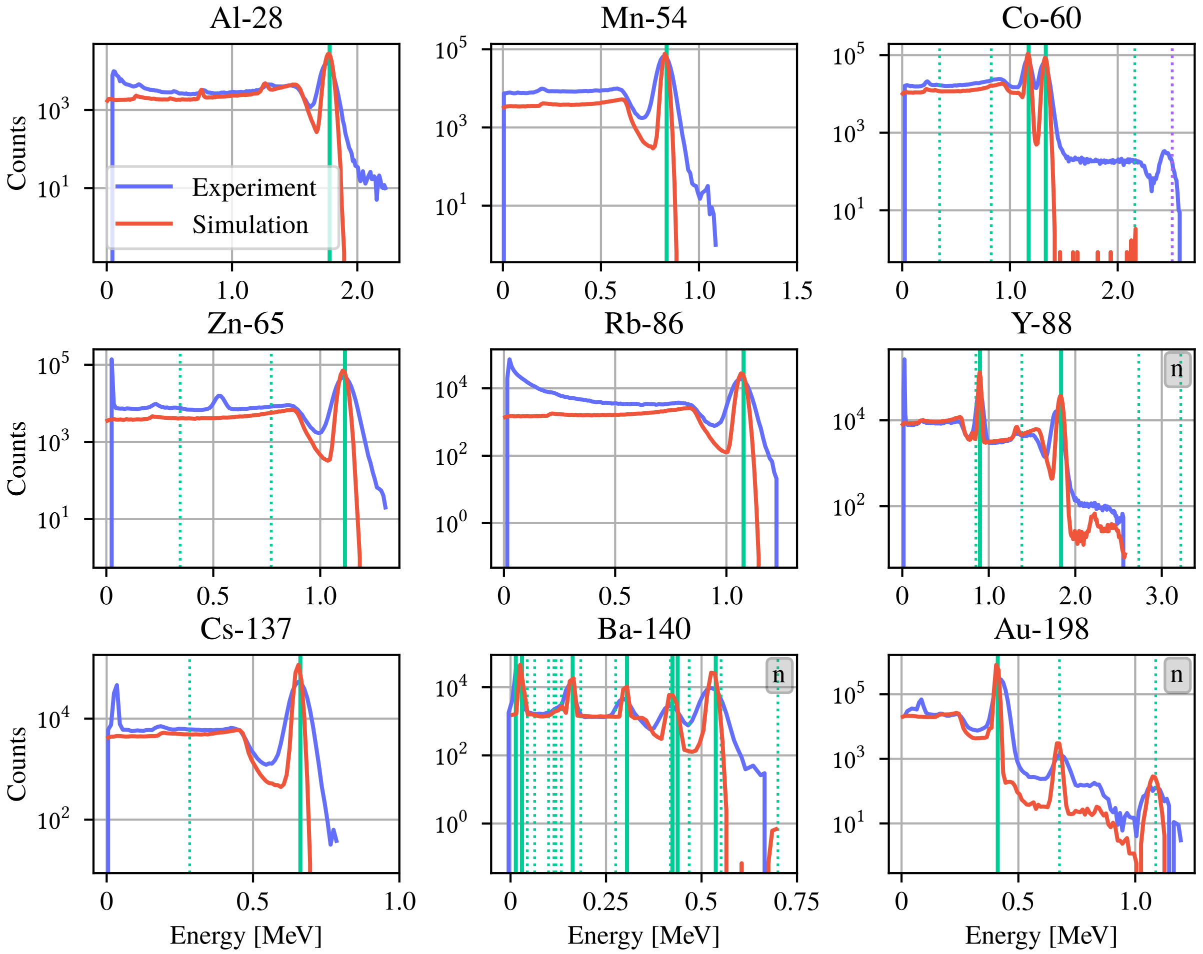

Figure 8. *Comparison of nine experimental spectra and pulse-height tally results. Simulations include energy broadening according to the detector resolution. The energies of initial source photons are marked with green vertical lines, dotted for energy levels contributing less than one percent to the total intensity.*

Conclusion and Outlook

This publication described the implementation of a new pulse-height tally function for photons in the open source Monte Carlo particle transport software OpenMC. Extensive comparisons and validation calculations demonstrate that the function can provide valid results. With the new functionality, simulations of new applications are made possible, including the simulation of gamma spectroscopy with various detector systems.

In the near future, we plan to contribute the functionality to the main OpenMC source code repository. Ideally, such a contribution would allow direct simulations on multiple processor cores or for distributed calculations. Further improvements could consider correlated particles from individual decay events (e.g. Co-60), and better treatment of source materials, for example, to simulate annihilation of photons from the positrons of β^+ decays. In the longer term, the tally could be extended to be applicable to neutron transport simulations.

References

Fichtlscherer, C., M. Göttsche, and M. Kütt. 2021. Can We Fake Gamma Emissions of Nuclear Warheads? An Exploratory Study. In INMM & ESARDA Joint Virtual Annual Meeting.

Heath, R.L. 1964. Scintilation Spectrometry. Gamma-ray Spectrum Catalogue, Volume 2 of 2. Phillips Petroleum Co. Atomic Energy Div., Idaho Falls, Idaho.

Knoll, G.F. 2010. *Radiation detection and measurement.* John Wiley & Sons.

Lund, A.L., and P.K. Romano. 2018. Implementation and Validation of Photon Transport in OpenMC. Technical report. Argonne National Lab.(ANL), Argonne, IL (United States).

Massey Jr., F.J. 1951. The Kolmogorov-Smirnov Test for Goodness of Fit. *Journal of the American Statistical Association.*

Mirion Technology Inc. 2017. 802 Scintillation Detectors. Accessed: 2021-07-24, https://www.mirion.com/products/802-scintillation-detectors.

Romano, P.K., N.E. Horelik, B.R. Herman, A.G. Nelson, B. Forget, and K. Smith. 2015. OpenMC: A state-of-the-art Monte Carlo code for research and development. *Annals of Nuclear Energy* 82:90–97.

Scopatz, A., P.K. Romano, P.P.H. Wilson, and K.D. Huff. 2012. PyNE: Python for Nuclear Engineering. In Am. Nuc. Soc. Winter Meeting 2012, vol. 107. San Diego, CA, USA.

Shuttleworth, T. 1994. The Verification of Monte Carlo Codes in Middle Earth. In Eighth International Conference on Radiation Shielding, Arlington, Texas, USA.

Sood, A., R.A. Forster, B.J. Adams, and M.C. White. 2004. Verification of the pulse height tally in MCNP 5. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 213:167–171.

Sood, A., M.S. Reed, and R.A. Forster. 2003. New Results for Pulse Height Tally Verification in MCNP5. LA-UR-03-4271. Los Alamos National Laboratory.

Werner, C.J., J.S. Bull, C.J. Solomon, F.B. Brown, G.W. McKinney, M.E. Rising, D.A. Dixon, R.L. Martz, H.G. Hughes, L.J. Cox, et al. 2018. MCNP version 6.2 release notes. LA-UR-18-20808. Los Alamos National Laboratory.

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