Exclusive CHIPS-TPT algorithms for simulation of neutron-nuclear reactions

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Published 1 September 2016

The CHIPS-TPT physics library for simulation of neutron-nuclear reactions on the new exclusive level is being developed in CFAR VNIIA. The exclusive modeling conserves energy, momentum and quantum numbers in each neutron-nuclear interaction. The CHIPS-TPT algorithms are based on the exclusive CHIPS library, which is compatible with Geant4. Special CHIPS-TPT physics lists in the Geant4 format are provided. The calculation time for an exclusive CHIPS-TPT simulation is comparable to the time of the corresponding inclusive Geant4-HP simulation and much faster for mono-isotopic simulations. In addition to the reduction of the deposited energy fluctuations, which is a consequence of the energy conservation, the CHIPS-TPT libraries provide a possibility of simulation of the secondary particles correlation, e.g. secondary gammas or n - γ correlations, and of the Doppler broadening of the γ -lines in the simulated spectra, which can be measured by germanium detectors.

Keywords: Geant4; neutron inelastic scattering; Monte Carlo simulation.

PACS numbers: 24.10.Lx, 25.40.Fq, 28.20.Cz.

1. Introduction

The CHIPS-TPT^{1,2} physics package is a successor of the CHIPS physics package, a package used for simulation of nuclear reactions at energies of several tens of MeV, formerly included in Geant4.^{3,4} Starting from the Geant-4.10 release, CHIPS is no longer supported by the Geant4 Collaboration. The main goal of the CHIPS-TPT project is further maintenance of the universal CHIPS algorithms and development of the exclusive Toolkit for Particle Transport (TPT) algorithms of nuclear reactions at low energies for neutrons and light charged nuclear fragments. The exclusive TPT model can be used as a replacement for the inclusive NeutronHP models⁵ currently used in the Geant4 framework for neutrons with energy below 20 MeV. Unlike inclusive modeling which

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reproduces values averaged over large statistics, exclusive modeling reproduces each interaction exactly including kinematic effects, such as kinematic correlations of secondary particles and Doppler broadening of spectral lines, and avoids fluctuations in the simulated detector responses, which are typical for inclusive approaches of Geant4-NeutronHP and MCNP.

The main features of CHIPS-TPT algorithms are:

- charge and baryon number conservation,
- energy and momentum conservation in each nuclear interaction,
- full isotope coverage, and
- full neutron-nuclear reaction coverage below 20 MeV.

2. Continuum Neutron Inelastic Scattering

This paper is focused on the exclusive modeling of the so-called continuum neutron inelastic scattering. Earlier we implemented inelastic scattering with excitation of discrete nuclear levels including the angular distributions of scattered neutrons along with other nuclear reactions with production of multiple nuclear fragments.² Inelastic neutron scattering cross sections include channels where particular excited levels are unknown, cannot be separated from other levels, or cannot be represented in the ENDF-6 format.⁶ In the ENDF-6 files, the events are assigned to a separate “continuum” section and are given with the energy-angle distribution for secondary neutrons. The neutron spectra assume azimuthally symmetric distributions and depend on the initial and final energies, and the polar scattering angle. The neutron spectrum can be described in several different formats, in either laboratory (LAB) or center of mass (CM) reference frames. The approximated spectra are given for each particle independently, so the exclusive TPT algorithm should take care of the kinematic limits and the energy and momentum conservation.

The continuum excitation has an energy threshold similar to the discrete level excitations, so in the CM system, the energy distribution of secondary neutrons should not have an overlap between discrete levels and the continuum. That is right for exclusive TPT simulation, but not right for the inclusive simulation. It should be noted that sometimes in data bases, the continuum threshold lies below some high discrete levels. The TPT algorithms consider the overlap as true complementary information.

One more problem is the correspondence between the continuum spectrum and the real known levels of excitation within the continuum energy range. Most frequently there are a lot of known narrow discrete levels within the continuum excitation. If the discrete levels are more or less homogeneous within the continuum excitation energy range, then the continuum distribution can be considered as an appropriate average spectrum, but if there are big gaps in the discrete level distribution, then one should expect corresponding dips in the continuum spectrum. To assess the systematic errors, the TPT algorithms provide a possibility to attract the continuous excitation to the known excitation levels. So far the levels' strengths are not taken into account, and the continuous events are

attracted to the closest known level. The simulation version can be selected by a special TPT flag.

3. Results

We ran a few simulations for testing and verification of our code. Only simple geometry simulation or just a neutron scattering on a thin target were used for the testing. ^{56}Fe was chosen as a target because iron is an important construction material, but due to a rich level structure has a high continuum neutron inelastic cross section. ^{55}Mn was chosen as a similar nucleus where the agreement between different simulations is not that good. Figures 1 and 2 show the energy and momentum conservations for the CHIPS-TPT (red) and the NeutronHP (black) processes of neutron inelastic scattering, calculated in the LAB system, where δE is the difference between the sum of the energies of the initial (the incident neutron and the target nucleus) and the final (scattered neutron, recoil nucleus, gammas and other products) particles, and δp is the absolute value of the difference between the sum of the momentums of the initial and the final particles.

Fig. 1. Energy conservation. Horizontal axis shows the absolute value of the energy difference for the initial and the final particles in each event.

Fig. 2. Momentum conservation. Horizontal axis shows the absolute value of the momentum difference of the initial and the final particles in each event.

One can see that CHIPS-TPT conserves the reaction momentum and the reaction energy up to 0.1 meV in the LAB system, so in the CM system the discrepancy is as also very small. The NeutronHP package does not conserve either energy or momentum, and consequently the measure of non-conservation depends on the reference system. The discreteness of the energy difference distribution is due to the machine rounding errors.

Figure 3 shows a comparison of the continuum neutron distribution data given in ENDF/B-VII.1 with the results of TPT randomization based on the same distribution. The spectra are presented in the database ENDF/B-VII.1 as a step histogram for iron and as a linear-linear interpolation for titanium. The TPT algorithm always transforms the histogram to the linear-linear interpolation to avoid discontinuity and for the accurate modeling of the distribution near the threshold and the kinematic limits. The NeutronHP algorithms do not perform such corrections.

Fig. 3. Energy distribution for the neutron inelastic scattering at a fixed angle with emission of photons. Horizontal axis shows the neutron energy; vertical axis shows the relative distribution.

Figures 4 and 5 show the energy distribution of all secondary neutrons after non-elastic scattering in the CM system. The initial neutron energy was set to 11 MeV for iron and 10 MeV for manganese to suppress the contribution of reactions other than (n,n γ). The red line shows the TPT attempt to excite the known levels in the continuum energy

region. The levels were taken from the TALYS database,⁷ but one needs to take into account the real widths of the levels, which are not always known. The thin peaks at higher than continuum energies correspond to the excitation of discrete levels. For Mg, the NeutronHP peaks seem to be shifted to higher energies by a value, which looks like a difference between the incident neutron energy in the LAB and the CM systems. For both elements, the TPT continuum (green lines) lies strictly below the discrete levels, because the continuous nucleus spectrum normally starts higher than any discrete level, while for the NeutronHP simulation (black), the continuous and discrete contributions overlap.

Fig. 4. The energy distribution of inelastically scattered neutrons on ^{56}Fe . Horizontal axis shows the neutron energy; vertical axis shows the normalized distribution.

Fig. 5. The energy distribution of inelastically scattered neutrons on ^{55}Mn . Horizontal axis shows the neutron energy; vertical axis shows the normalized distribution.

Figure 6 shows the simulated neutron fluence induced by a 14 MeV neutron source located in the center of iron and manganese balls of 50 cm radius. The fluence was

Fig. 6. Neutron fluence inside the iron and manganese balls induced by 14 MeV neutrons.

computed as a sum of steps of neutron tracks divided by the integration volume. For iron, the agreement is satisfactory at energies above 10 MeV. Near 9 MeV, there is excess in the NeutronHP result due to the continuum overlapping with discrete levels. One can see that because of the usage of step histograms between 4 MeV and 9 MeV, the NeutronHP graph is stepped and the TPT graph is smooth due to the different interpolation schemes. For manganese, the energy shift in NeutronHP leads to simulated neutrons with energies higher than the initial one, and there are discrepancies all over the energy range. The difference below 4 MeV is due to the current isotropic secondary neutron distribution for the TPT simulation of the (n, α) reaction.

4. Conclusion

We implemented continuum neutron inelastic scattering based on ENDF-6 data. We conducted a comparison of simulations made with the NeutronHP model from Geant4 and our implementation. We showed that the TPT simulation conserves energy and momentum in each interaction and reproduces the flux calculated with NeutronHP. Our comparison proves the importance of the energy and momentum conservation not only for higher quality of simulation, but also as a tool for error indicator for the simulation processes. One can acquire a free version of the open part of the TPT physics libraries on the TPT page¹ or contact the authors to get TPT processes in the Geant4 applicable form.

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