

New exclusive CHIPS-TPT algorithms for simulation of neutron-nuclear reactions

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Abstract.

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 Geant4-HP simulation. 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, and of the Doppler broadening of gamma lines in the spectrum, which can be measured by germanium detectors.

1. Introduction

CHIPS-TPT is the successor of CHIPS model formerly included in Geant4 package. Starting from the Geant-4.10 release, CHIPS is no longer supported by the Geant collaboration. The main goals of the CHIPS-TPT project are further maintenance of the universal CHIPS algorithms and the development of exclusive TPT (Toolkit for Particle Transport) algorithms of nuclear reactions at low energies for neutrons and light charged nuclear fragments. The exclusive TPT model can be a replacement for the inclusive NeutronHP model [1] currently used in the Geant4 framework for neutrons below 20 MeV. Exclusive modeling also reproduces kinematic effects such as secondary particle correlations and Doppler broadening of spectral lines and allows to avoid the fluctuations in the simulated response due to energy non-conservation in an inclusive approach. Therefore it is essential for the development of detectors measuring correlation spectra applied to identification of nuclear isotopes.

The main features of CHIPS-TPT are:

- Charge and baryon number conservation.
- Energy and momentum conservation in each nuclear interaction.
- Full isotope coverage.
- All neutron-nuclear reactions below 20 MeV.

2. Reactions

The following reactions have been implemented:

- Elastic neutron scattering.

It is easy to comply conservation laws since elastic scattering is a binary reaction. However, at incident neutron energies near the material temperature scattering is sensitive to the thermal motion of atoms leading to effective cross section

$$\sigma_{eff} = \sigma_0 \cdot \left[\left(1 + \frac{T}{mV^2} \right) \cdot erf \left(\sqrt{\frac{mV^2}{2T}} \right) + \sqrt{\frac{2T}{\pi mV^2}} e^{-\frac{mV^2}{2T}} \right]$$

where V is the incident neutron velocity, m is the mass of the target nucleus, T is the temperature, σ_0 - the cross section at zero temperature. The σ_0 value is a constant at incident energies below the first resonance, so $|\bar{v} + \bar{V}|\sigma_0$ can be averaged over Maxwell distribution to obtain the reaction rate $R = \langle |\bar{v} + \bar{V}|\sigma_0 \rangle = V\sigma_{eff}$. The same result can be found in [2].

- Inelastic neutron scattering.

Inelastic neutron scattering is divided into scattering with excitation of the recoil nucleus and its following step-by-step de-excitation cascade. De-excitation of moving nuclei leads to Doppler broadening.

- Radiative capture.

Radiative capture mainly takes place at thermal energies, so the compound nucleus is at rest, but the first gamma radiation accelerates the compound nucleus and broadens the following gamma-lines of the cascade, whilst the first gamma line remains narrow.

- Production of light nuclear fragments.

In reactions with multiple secondaries the compound nucleus is formed and then fragmented emitting nuclear fragments according to the phase space distribution. The inclusive double-differential spectra available in ENDF-6 databases [3] are not taken into account yet, instead the phase space distributions are used for all nuclear fragments except for the leading fragment (mainly a neutron), which is generated in accordance with the spectrum provided by the database.

- Neutron induced fission.

Fission is implemented by forming the compound nucleus, emitting prompt neutrons and dividing the residual nucleus into two fragments, conserving charge and baryon number in the reaction.

3. Results

We ran a few simulations for testing and verification. Either a simple geometry or scattering on a thin target were used.

Figure 1 shows the energy-momentum conservation up to millielectronvolts for the most complicated CHIPS-TPT process of neutron-induced fission, while an inclusive fission simulation does not conserve neither energy and momentum nor charge and baryon number.

Figure 2 shows the simulated neutron fluence induced by a 14 MeV neutron source located in the center of a water ball of 50 cm radius. The benchmark is similar to the one used for comparison of several other Monte-Carlo neutron codes [4]. Fluence was computed as the sum of the lengths of neutron tracks divided by the integration volume. A good agreement can be seen between CHIPS-TPT and NeutronHP results. The low energy maximum is due to thermal motion of the material atoms.

Figure 3 shows an example of correlated gamma spectra obtained by the scattering of 14 MeV neutrons on nitrogen and oxygen. The peaks correspond to pairs of photons emitted in a single nuclear de-excitation cascade. Similar distribution can be provided by Geant4 in a form of narrow spikes without Doppler broadening if the excited nucleus is stopped in matter and then decayed in gamma and the residual nucleus.

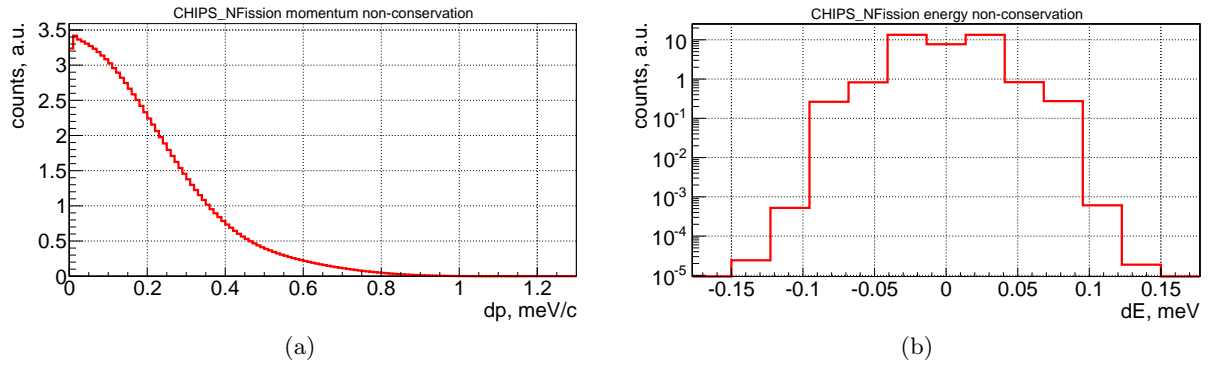


Figure 1: Energy and momentum conservation. Horizontal axis shows the difference of the momentum (left) or energy (right) between initial and final particles in each event.

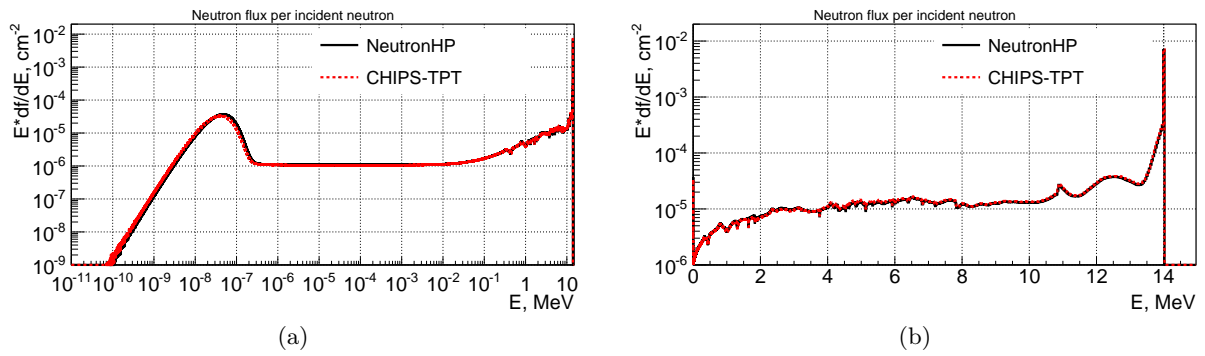


Figure 2: Neutron fluence in water. Horizontal axes show neutron energy, vertical axes show fluence multiplied by the energy. Left panel shows the horizontal axis in the logarithmic scale, while the right panel shows the horizontal axis in the linear scale.

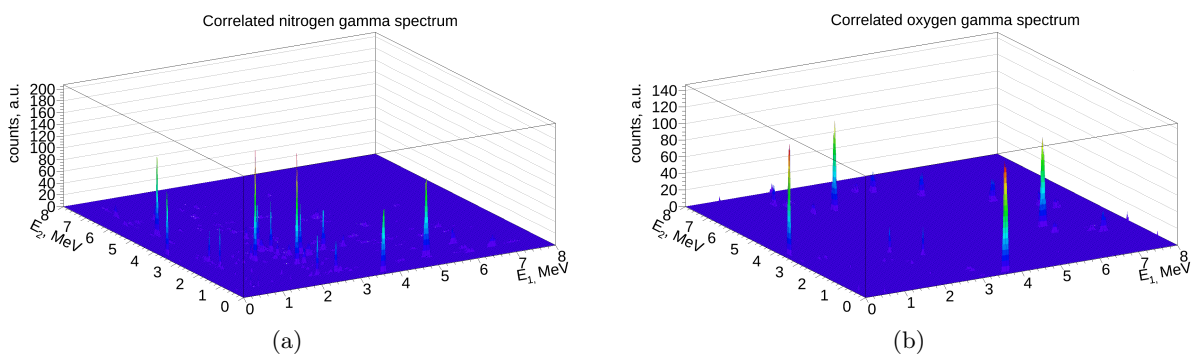


Figure 3: Energy spectra of pairs of photons emitted in a single nuclear de-excitation cascade. Left panel shows spectra for nitrogen, right panel shows spectra for oxygen.

4. Summary and Outlook

The exclusive CHIPS-TPT code reproduces the results of simulations with inclusive Monte-Carlo codes, being capable to simulate quantities obtainable with exclusive codes only. CHIPS-TPT also strictly complies the energy and momentum conservation requirements inherited from

CHIPS. The plans for future development are:

- Improvement of multiple secondary particle production by comparison with experimental data.
- Development of fragmentation models for inelastic interactions of soft charged nuclear fragments.
- Calculation speed-up by caching cross section for each material used in a simulation run.

Updated versions of CHIPS will be publicly available online [5]. For the full CHIPS-TPT library contact the authors via e-mail.

References

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- [5] <http://vniia.ru/cfpi/eng/wptpt.html>