Monte Carlo simulation of multiple particle spectra with energy and momentum conservation

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A Monte Carlo toolkit for the simulation of the passage of particles through matter.

Originally used for High Energy Physics experiments

Increased precision stimulates to simulate lower energy secondary particles

New applications: medical, microelectronics, neutron physics
Background
ParticleHP in Geant4

- Data-based model for neutrons and light charged particles
- Originally NeutronHP for neutrons below 20 MeV
- Aims to reproduce MCNP results
- Has a flag to correct energy by emitting additional gammas
Background

CHIPS-TPT physics list

- Built on top of CHIPS model formerly included in Geant4
- Light charged particles and neutrons up to 20 MeV
- Quantum numbers conservation in each interaction
- Energy and momentum conservation in each interaction
Motivation

- Avoids artificial fluctuations
- Allows to simulate correlated measurements
- Reproduces kinematic effects
- Imposes physical constrains on the data
Problem

- Secondary particle spectra are given uncorrelated
- Uncorrelated sampling of secondary particles leads to energy non-conservation
- Rejection of events with non-conserved energy disturbs the spectra
- Many ways to construct correlated particle spectra exist
Formal Problem Statement

Set the order in which the particles are simulated. Assume the energy distributions of the first and the second particles are given:

\[ f(e) \ni h(e), \ e \in (0, e_{\text{max}}) \]

\[
\int_{0}^{e_{\text{max}}} f(e) \, de = \int_{0}^{e_{\text{max}}} h(e) \, de = 1
\]

In the non-relativistic approximation the maximum energies \((e_{\text{max}})\) are the same.

The energy distribution of the second particle \(g(e|e_1), \ e \in (0, e_{\text{max}})\) when the energy of the first particle is \(e_1\) must satisfy the conditions:

\[
\int_{0}^{e_{\text{max}}} g(e|e_1) \, de = 1
\]

\[
\int_{0}^{e_{\text{max}}} g(e|e_1) f(e_1) \, de_1 = h(e)
\]
Solution

We find the solution in the form:

\[ g(e|e_1) = \frac{\theta(e_{\text{max}} - e_1 - e)}{\int_0^{e_{\text{max}}-e_1} g(e'|e_1) \, de'} g(e), \]

where the integral in the denominator

\[ \int_0^{e_{\text{max}}-e_1} g(e'|e_1) \, de' \]

is the normalization factor, and Riemann \( \theta \) function

\[ \theta(x) = \begin{cases} 
0 & x \leq 0 \\
1 & x > 0 
\end{cases} \]

represents the kinematic boundary ignoring relativistic effects and the recoil nucleus energy.
Solution

Substituting the anzats into the condition we obtain

\[
\int_0^{e_{\text{max}}} \frac{g(e) \cdot \theta(e_{\text{max}} - e_1 - e)}{1 - \int_{e_{\text{max}} - e_1}^{e_{\text{max}}} g(e')de'} f(e_1)de_1 = h(e),
\]

which easily transforms into

\[
g(e) = \frac{h(e)}{\int_{e_{\text{max}}}^{e} \frac{f(e_{\text{max}} - e_f)}{1 - \int_{e_f}^{e_{\text{max}}} g(e')de'} de_f},
\]

where \( e_f = e_{\text{max}} - e_1 \).
To calculate the cumulative distribution $G = \int g(e)de$ which is needed for the Monte Carlo simulation we transform the formula using finite bins

$$\Delta G_i = \frac{\Delta H_i}{\sum_{j>i} \frac{\Delta F_j}{1-\sum_{k>j} \Delta G_k}} ,$$

where $\Delta G_i = g_i \Delta e_i$, $\Delta H_i = h_i \Delta e_i$, $\Delta F_i = f(e_{max} - e_i) \Delta e_i$. Because $i < j < k$ it can be iteratively calculated starting from the upper bin where $G$ approaches 1.
Solution
Comparison with a standard solver

The integral equation is transformed to a differential equation of the second order:

\[
\frac{d}{de} \frac{h(e)}{G'(e)} + \frac{f(e_{\text{max}} - e)}{G(e)} = 0,
\]

which has no solution with the boundary conditions \( G(0) = 0, \ G(e_{\text{max}}) = 1 \), but has a solution with boundary conditions

\[
G(\delta) = \epsilon, \ G(e_{\text{max}} - \delta) = 1 - \epsilon,
\]

where \( \delta \text{ и } \epsilon \) - small quantities to avoid singularities on the edges of the interval.
Solution
Comparison with a standard solver

Green - example function $f = h = x \times (1 - x) \times e^{-5x}$
Blue - solution using a standard solver
Orange - recursive solution

The solution using finite sums automatically avoids singularities.
Solution
The third and subsequent particles

Using the obtained distribution $G$, one can evaluate the distribution of the sum of the energies of the first two particles:

$$\phi(e) = \int_{0}^{e_{\text{max}}-e} \frac{G'(e' - e)}{G(e_{\text{max}} - e')} f(e') \, de'$$

It can be regarded as the energy distribution of a quasi-particle to be used to obtain the spectrum of the second particle with the same formulae. This substitution allows to simulate an arbitrary number of kinematically correlated particles.
Results: The Good (Perfect)
Smooth data, heavy nucleus - $^{109}\text{Ag}(n, 2n)^{108}\text{Ag}$

Red line - initial distribution, blue dots - simulation result, black dash line - ratio.
Results: The Bad (Still Pretty Good)
Reinterpolated data, medium nucleus $^{56}\text{Fe}(n, 2n)^{55}\text{Fe}$

Red line - initial distribution, blue dots - simulation result, black dash line - ratio.
Results: The Ugly (Better Than Expected)
Irregular data, light nucleus $^9\text{Be}(n, 2n)2\alpha$, CENDL

Red line - initial distribution, blue dots - simulation result, black dash line - ratio.
Results: Correlated Spectrum

\( ^9\text{Be}(n, 2n)2\alpha \) at 19 MeV, CENDL

![Graph showing neutron energy-energy distribution](image-url)
TALYS is the main program for nuclear data evaluation which includes complex physical models. The recoil excitation is not included in the evaluated data library and was simulated with TALYS and reconstructed from TPT simulation.
Comparison With TALYS

The distributions are in agreement.
Conclusion

- Method to sample correlated secondary neutrons
- Energy and momentum conservation in each scattering
- Reasonable reconstruction of the inclusive spectra
- Very simple model, little overhead
- Extensible to other boundary conditions