EVENT-BY-EVENT
MONTE CARLO TRACKING OF
NEUTRON-NUCLEUS COLLISIONS
IN NEUTRON DETECTORS

MARY CHIN & NICHOLAS SPYROU

Department of Physics, University of Surrey, Guildford GU2 7XH, United Kingdom
A VERY SIMPLE EXPERIMENT

TWO INDEPENDENT MONTE CARLO CODES

THERMAL NEUTRONS IN BORON-10
- ONE ENERGY
- ONE MATERIAL
- ONE CELL

- MCNPX
- FLUKA
WHEN EVERYONE’S BUSY MODELLING
VERY COMPLEX PROBLEMS

THE EXTREME ...
OR AT LEAST ...

TO SEE THINGS
WE WOULDN’T
OTHERWISE SEE

WHY SHOULD WE SIMULATE

SIMPLE SPHERE
SINGLE NUCLIDE
MONOENERGETIC BEAM
SINGLE PARTICLE TYPE
A. The $^{10}\text{B}(n, \alpha)$ Reaction

Probably the most popular reaction for the conversion of slow neutrons into directly detectable particles is the $^{10}\text{B}(n, \alpha)$ reaction. The reaction may be written:

$$^{10}\text{B} + ^{1}\text{n} \rightarrow \begin{cases} \frac{3}{2}\text{Li} + ^{4}\alpha & 2.792 \text{ MeV (ground state)} \\ \frac{3}{2}\text{Li}^* + ^{4}\alpha & 2.310 \text{ MeV (excited state)} \end{cases}$$

From each reaction we expect either NO GAMMA or ONE 0.48 MeV GAMMA.

94% OF THE TIME

6% OF THE TIME
from each reaction we expect either

NO GAMMA

or

ONE 0.48 MeV GAMMA

MCNPX WOULD QUITE HAPPILY GIVE US ONE, TWO, THREE, ...

6% OF THE TIME

94% OF THE TIME
MCNPX WOULD QUITE HAPPILY GIVE US ONE, TWO, THREE, ...

MCNPX SIMULATION
SOURCE: 0.025 eV NEUTRONS
NUMBER OF HISTORIES: 10 MILLION
MEDIUM: $^{10}\text{B}$

OUT OF 10 MILLION NEUTRONS STARTED
632,665 COUNTS OF ZERO GAMMA PER NEUTRON
9,362,277 COUNTS OF 1 GAMMA PER NEUTRON
5,053 COUNTS OF 2 GAMMAS PER NEUTRON
5 COUNTS OF 3 GAMMAS PER NEUTRON
VIOLATES THEORETICAL EXPECTATION
Yet ... can’t be that wrong after all.

Used worldwide to solve a wide range of problems over the years.

Violates theoretical expectation.
FIRST 12 HISTORIES EACH PRODUCED ONE GAMMA

THOUGH YIELD NEVER EVER EXCEEDS ONE

THOUGH YIELD PER HISTORY COULD BE UP TO 3

YIELD = 0.94

EVENTUALLY GETS IT RIGHT... IF WE RUN ENOUGH HISTORIES

A SIMULATION OF 10 MILLION RADIATION HISTORIES

DIP! BECAUSE 13TH HISTORY DIDN'T PRODUCE ANY GAMMA

YIELD NEVER EVER EXCEEDS ONE
<table>
<thead>
<tr>
<th>Level 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>THIS HAS ALWAYS BEEN IN MCNP/MCNPX</td>
</tr>
<tr>
<td>Level 2</td>
</tr>
<tr>
<td>NOT A BUG, BUT A DESIGN FEATURE</td>
</tr>
<tr>
<td>Level 3</td>
</tr>
<tr>
<td>NOT NEW, JUST THAT MOST USERS ARE UNAWARE</td>
</tr>
<tr>
<td>Level 4</td>
</tr>
<tr>
<td>DOESN’T MATTER IN MOST CASES AFFECTS EXCEPTIONS ONLY</td>
</tr>
</tbody>
</table>

VIOLATES THEORETICAL EXPECTATION
MCNP-PoliMi: a Monte-Carlo code for correlation measurements

Sara A. Pozzi, Enrico Padovani*, Marzio Marseguerra

Department of Nuclear Engineering, Polytechnic of Milan, Via Ponzio 34/3, Milan 20133, Italy

deviation from physical reality: the emission of secondary gamma rays from neutron collisions. In fact, in MCNP secondary photons are sampled independently from the type of neutron collision. For example, it is possible for a neutron in a collision with uranium to generate fission photons in the course of an elastic scattering. This technique provides correct answers when we consider the average outcome of a large number of histories, and it is well suited for biased calculations, but it fails when considering the single history [2]. This is a severe drawback in the simulation of correlation measurements in which the experimental quantity of interest is the delay between particles emitted by a single event [1,3].

In this paper we describe the MCNP-PoliMi of the standard MCNP cod. A major deviation to the introduced by inverting the photon production and neutron particle tracking. This means equal to one to each of the source and to each of the born at a collision. With particles have weight equal escape or are absorbed, a process simpler to model.

The modifications to the transport can be grouped in first concerns secondary whereas the second concern
A. The $^{10}\text{B}(n,\alpha)$ Reaction

Probably the most popular reaction for the conversion of slow neutrons into high-energy charged particles is the $^{10}\text{B}(n,\alpha)$ reaction. In this reaction, a neutron collides with a boron-10 nucleus, and the reaction proceeds through a series of nuclear reactions to produce an alpha particle and a helium nucleus. 

The energy released in this reaction is given by the reaction energy, which is the difference between the incident neutron energy and the kinetic energy of the alpha particle. The reaction energy is typically on the order of several MeV.

The reaction proceeds via several intermediate steps, including the formation of a compound nucleus and the emission of a 0.48 MeV gamma ray. We will assume that this photon always escapes and does not contribute to the response of the detector.

**LOOKS NICE & CLEAN IN THE TEXTBOOKS**

**BUT IF WE REALLY START THERMAL NEUTRONS IN $^{10}\text{B}$ WE'LL GET CAPTURE GAMMAS AS WELL**
What do we get from a FLUKA‡ simulation?

‡ developed by INFN & CERN
OBSERVATION #1

NO BACKGROUND/CONTINUUM

COZ THESE ARE GAMMAS CREATED, NOT GAMMAS ‘DETECTED’ BY A PHYSICAL DETECTOR

MONTE CARLO CAN BE USED AS A PERFECT DETECTOR

AFTER REMOVING 0.48 MeV PEAK
**OBSERVATION #2**

BANDS INSTEAD OF LINES DUE TO MULTIGROUP TREATMENT, WHERE THE CONTINUOUS ENERGY RANGE IS APPROXIMATED AS DISCRETE INTERVALS

AFTER REMOVING 0.48 MeV PEAK
OBSERVATION #2
BANDS INSTEAD OF LINES
MATCH WITH NUCLEAR DATA

Thermal Neutron Capture Gammas — Target Nucleus $^{10}B$

<table>
<thead>
<tr>
<th>$E_Y$ (keV)</th>
<th>$\Delta E_Y$ (keV)</th>
<th>$I_Y/I_Y(\text{max})$ (%)</th>
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<tbody>
<tr>
<td>2120.00</td>
<td>0.00</td>
<td>4.6</td>
<td>0.21</td>
</tr>
<tr>
<td>2295.00</td>
<td>2.00</td>
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<td>4.67</td>
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<td>2534.00</td>
<td>2.00</td>
<td>23.0</td>
<td>3.26</td>
</tr>
<tr>
<td>4444.00</td>
<td>2.00</td>
<td>100.0</td>
<td>6.53</td>
</tr>
<tr>
<td>4711.00</td>
<td>2.00</td>
<td>38.4</td>
<td>2.35</td>
</tr>
<tr>
<td>5019.00</td>
<td>0.00</td>
<td>3.0</td>
<td>0.14</td>
</tr>
<tr>
<td>6739.00</td>
<td>2.00</td>
<td>26.2</td>
<td>2.05</td>
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<tr>
<td>7006.00</td>
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</tr>
<tr>
<td>8916.00</td>
<td>2.00</td>
<td>25.0</td>
<td>3.26</td>
</tr>
<tr>
<td>11447.00</td>
<td>2.00</td>
<td>9.0</td>
<td>1.60</td>
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</table>
**OBSERVATION #2**

**BANDS INSTEAD OF LINES MATCH WITH NUCLEAR DATA**

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**Thermal Neutron Capture Gammas — Target Nucleus $^{10}\text{B}$**

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</table>

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**OK**
OBSERVATION #3
DIFFERENT BAND WIDTHS

counts

energy (MeV)

WIDER?
### Table 10.2: Gamma energy group structure of the ENEA library

<table>
<thead>
<tr>
<th>Gamma group n.</th>
<th>Lower limit (GeV)</th>
<th>Upper limit (GeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.4 \cdot 10^{-2}$</td>
<td>$2.0 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>2</td>
<td>$1.2 \cdot 10^{-2}$</td>
<td>$1.4 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>3</td>
<td>$1.0 \cdot 10^{-2}$</td>
<td>$1.2 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>4</td>
<td>$8.0 \cdot 10^{-3}$</td>
<td>$8.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>10</td>
<td>$5.0 \cdot 10^{-3}$</td>
<td>$5.5 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>11</td>
<td>$4.5 \cdot 10^{-3}$</td>
<td>$5.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>12</td>
<td>$4.0 \cdot 10^{-3}$</td>
<td>$4.5 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>13</td>
<td>$3.5 \cdot 10^{-3}$</td>
<td>$4.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>14</td>
<td>$3.0 \cdot 10^{-3}$</td>
<td>$3.5 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>15</td>
<td>$2.5 \cdot 10^{-3}$</td>
<td>$3.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>16</td>
<td>$2.0 \cdot 10^{-3}$</td>
<td>$2.5 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>17</td>
<td>$1.5 \cdot 10^{-3}$</td>
<td>$2.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>18</td>
<td>$1.0 \cdot 10^{-3}$</td>
<td>$1.5 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>19</td>
<td>$4.0 \cdot 10^{-4}$</td>
<td>$1.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>20</td>
<td>$2.0 \cdot 10^{-4}$</td>
<td>$4.0 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>21</td>
<td>$1.0 \cdot 10^{-4}$</td>
<td>$2.0 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>22</td>
<td>$1.0 \cdot 10^{-5}$</td>
<td>$1.0 \cdot 10^{-4}$</td>
</tr>
</tbody>
</table>

**Observation #3**

**Different Band Widths**

Indeed wider
Hi Mary,

there are two neutron cut-offs in FLUKA. 1.960E-02 GeV is the cut-off for high-energy neutrons, below which the special multigroup treatment starts. With the present version it cannot be changed: it could be changed only when using a different library for low-energy neutrons (one with a different maximum energy). This cut-off is changed with PART-THR, but only when allowed by the low-energy neutron library.

The second cut-off, which is changed with LOW-BIAS, is the real cut-off. It is not expressed in energy, but as a neutron group number. Look carefully in the output:

The first cut-off is reported as follows:
Cut-off kinetic energy for NEUTRON transport: 1.960E-02 GeV

And the second cut-off as follows: (here the group cut-off has been set as 73 for regions 1 and 2 - which means no cut-off at all - and group 65 in regions 3 and 4)

<table>
<thead>
<tr>
<th>Region</th>
<th>Particle number</th>
<th>Particle importances</th>
<th>RR factor</th>
<th>Cut off group</th>
<th>N.A. abs. group</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>73</td>
<td>72</td>
</tr>
<tr>
<td>2</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>73</td>
<td>72</td>
</tr>
<tr>
<td>3</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>65</td>
<td>72</td>
</tr>
<tr>
<td>4</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>65</td>
<td>72</td>
</tr>
</tbody>
</table>

Here the group cut-off has been set as 73 for regions 1 and 2 - which means no cut-off at all - and group 65 in regions 3 and 4, which means 7.3375E-09 GeV (see energy group structure in the Manual).

Alberto
10.2 Pointwise transport

For a few isotopes only, neutron transport can be done also using continuous (pointwise) cross-sections. For $^1\text{H}$, $^6\text{Li}$ and $^{10}\text{B}$, it is applied as a user option (above 10 keV in $^1\text{H}$, for all reactions in $^6\text{Li}$, and only for the reaction $^{10}\text{B}(n,t\gamma)^4\text{He}$ in $^{10}\text{B}$). For the reaction $^{14}\text{N}(n,p)^{14}\text{C}$, pointwise neutron transport is always applied.

10.3 Secondary particle production

10.3.1 Gamma generation

In general, gamma generation by low-energy neutrons (but not gamma transport) is treated in the frame of a multigroup scheme too. A downscattering matrix provides the probability, for a neutron in a given energy group, to generate a photon in each of 22 gamma energy groups, covering the range 10 keV to 20 MeV. With the exception of a few important gamma lines, such as the 2.2 MeV transition of Deuterium and the 478 keV photon from $^{10}\text{B}(n,\gamma)$ reaction, the actual energy of the generated photon is sampled randomly in the energy interval corresponding to its gamma group. Note that the gamma generation matrix does not include only capture gammas, but also gammas produced in other inelastic reactions such as $(n,n')$. 

EXCERPT FROM FLUKA MANUAL
NOT COVERED IN THIS TALK
BUT DETAILED IN SUMMARY (ANS TRANS)

B. The $^6\text{Li}(n, \alpha)$ Reaction
The next most popular reaction for the detection of slow neutrons is the $(n, \alpha)$ reaction in $^6\text{Li}$. Here the reaction proceeds only to the ground state of the product and is written simply as:

\[
^6\text{Li} + ^1\text{n} \rightarrow ^3\text{H} + ^4\alpha
\]

\[Q \quad 4.78 \text{ MeV}\]

Calculation of the reaction product energies for negligible incoming neutron energy yields the following:

\[E_{^3\text{H}} = 2.73 \text{ MeV} \quad E_{\alpha} = 2.05 \text{ MeV}\]

The alpha particle and triton produced in the reaction must be oppositely directed when the incoming neutron energy is low.

The thermal neutron cross section for this reaction is 940 barns. Figure 14-1 shows that the cross section remains below that for the $^{10}\text{B}$ reaction until the
BEHIND THE SCENES

How we use FLUKA as a perfect detector
ENTRY USDRAW ( ICODE, MREG, XSCO, YSCO, ZSCO )
   IF ( .NOT. LFCOPE ) THEN
      LFCOPE = .TRUE.
   IF ( KOMPUT .EQ. 2 ) THEN
      FILNAM = '/'//CFDRAW(1:8)//' DUMP A'
   ELSE
      FILNAM = CFDRAW
   END IF
   OPEN ( UNIT = IODRAW, FILE = FILNAM, STATUS = 'NEW', FORM =
   & 'UNFORMATTED' )
   END IF

IF ( JTRACK .EQ. 8 .AND. Np.GT.0) THEN
   IF ( Np .EQ. 1 .AND. Kpart(1) . EQ. 8) THEN
   ELSE
      DO I = 1, Np
         WRITE (IODRAW) NCASE, Np, SNGL (ETRACK), Kpart(I),
         & SNGL (Tki(I))
      END DO
   END IF
END IF
RETURN
*=== End of subroutine Mgdraw ==================================*
<table>
<thead>
<tr>
<th>ANALOG TRANSPORT</th>
<th>FLUKA</th>
<th>INFN + CERN</th>
</tr>
</thead>
<tbody>
<tr>
<td>CROSS SECTION</td>
<td></td>
<td>LOS ALAMOS</td>
</tr>
</tbody>
</table>
Chin & Spyrou. Monte Carlo simulation of ($\gamma$, n) and (n, $\gamma$) activations: a multi-code comparison with theory. 12th Int Conf Modern Trends in Activation Analysis. Tokyo, 2007.


“GEOMETRY CODING IS THE EASIEST WITH GATE, SO WE USE GATE.”

“OUR GROUP HAS ALWAYS USED MCNP, SO WE USE MCNP FOR EVERYTHING.”
Different codes combine to give the full picture

We need to understand each code

Scratching the surface is not enough
We need different codes (with independent history and different philosophy) so that Monte Carlo results may be used to validate each other.