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## To cite this version:

J.-M. Verbeke, O. Petit. TRIPOLI-4 and FREYA for Stochastic Analog Neutron Transport. Application to Neutron Multiplicity Counting.. 37th ESARDA Annual Meeting (ESARDA Symposium 2015), May 2015, Manchester, United Kingdom. cea-02500827

**HAL Id: cea-02500827**

**https://hal-cea.archives-ouvertes.fr/cea-02500827**

Submitted on 6 Mar 2020

# TRIPOLI-4® and FREYA for Stochastic Analog Neutron Transport. Application to Neutron Multiplicity Counting.

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***Abstract:***

*From nuclear safeguards to homeland security applications, the need for better modeling of nuclear interactions has grown over the past decades. Current Monte Carlo radiation transport codes compute average quantities with great accuracy and performance, but performance and averaging come at the price of limited interaction-by-interaction modeling. These codes often lack the capability of modeling interactions exactly: for a given collision, energy is not conserved, energies of emitted particles are uncorrelated, multiplicities of prompt fission neutrons and photons are uncorrelated. Many modern applications require more exclusive quantities than averages, such as the fluctuations in certain observables (e.g. the neutron multiplicity) and correlations between neutrons and photons. In an effort to meet this need, the radiation transport Monte Carlo code TRIPOLI-4® was modified to provide a specific mode modeling nuclear interactions in a full analog way, replicating as much as possible the underlying physical process. Furthermore, the computational model FREYA (Fission Reaction Event Yield Algorithm) was coupled with TRIPOLI-4® to model complete fission events. FREYA automatically includes fluctuations as well as correlations resulting from conservation of energy and momentum.*

*Neutron Multiplicity Counting (NMC) exploits the correlated nature of fission chains, and thus requires analog neutron transport. With the latest analog neutron transport developments in TRIPOLI-4®, we will show that NMC can now be properly simulated, by reconstructing the mass and multiplication of an object by analyzing the measured signal from $^3$He tubes in a well counter.*

**Keywords:** Monte Carlo radiation transport code; Neutron Multiplicity Counting; TRIPOLI-4®; FREYA; analog transport

## 1. Introduction

Methods based on time-correlated signals have been developed over many years to characterize fissile materials. For NMC, sequences of thermal neutron captures are recorded in $^3$He tubes. To determine features of the measured objects, the sequences are split into time windows, and the numbers of neutrons arriving in each window are recorded to build statistical count distributions. These distributions are in turn analyzed to authenticate or characterize fissile materials. Some materials such as $^{252}$Cf emit several neutrons simultaneously, whereas others such as uranium and plutonium multiply the number of neutrons to form bursts. This translates into unmistakable time-correlated signatures.

General Monte Carlo codes that are used for criticality safety evaluations are typically meant for calculation of an integral reactor parameter such as $k_{eff}$ and for estimation of neutron fluxes and derived quantities of interest. They make use of well established variation reduction techniques leading to more efficient calculations. These techniques are meant to speed up calculations and are sufficient for the calculation of average quantities such as flux, energy deposition and multiplication.

However, they suffer from approximations of the underlying physical interactions, and are thus unsuitable for studying detailed correlations between neutrons and/or photons on an interaction-by-interaction basis, and in particular for NMC which relies on the correlated nature of fission chains.

The first part of this paper will focus on the latest TRIPOLI-4® [1][2] developments that were necessary to simulate NMC experiments: analog neutron transport, coupling with the LLNL Fission Library/FREYA [3]-[5] package for fission interactions, development of a spontaneous fission source, and new options to reduce memory footprint of ROOT [6] track files. The second part will focus on the use of these new capabilities for NMC. We will show that the mass and multiplication of a $PuO_2$ ball in a well counter (see Fig. 1) can be determined from measurements of the neutron captures in the $^3He$ tubes.

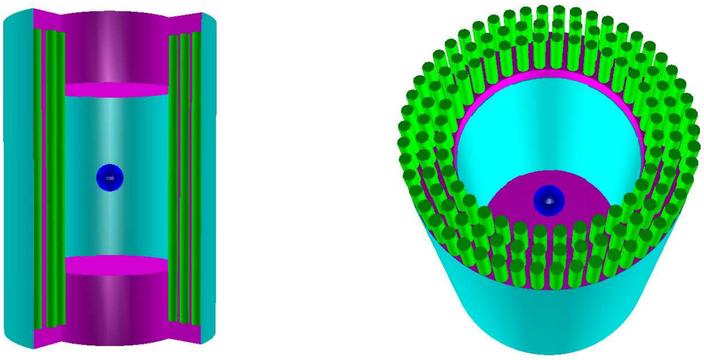

**Figure 1:** (color online) Cutouts to show the inside of a well counter. Polyethylene (magenta), Cadmium (cyan), $^3He$ tubes (green), representation of a generic neutron source to be characterized (blue). Left: multiple $^3He$ tubes removed for clarity. Right: upper polyethylene plug removed.

## 2. Developments in TRIPOLI-4® for NMC

TRIPOLI-4® solves the linear Boltzmann equation for neutrons, photons, electrons and positrons with the Monte Carlo method, in any 3-D geometry. The code uses ENDF format continuous-energy cross sections from various international evaluations. It has advanced variance reduction methods to address deep penetration issues and can be run in parallel. TRIPOLI-4® is used as a reference code for industrial purposes (fission/fusion) for CEA[1], EDF[2] and branches of AREVA, as well as an R&D and teaching tool, for radiation protection and shielding, core physics, nuclear criticality safety and nuclear instrumentation.

This section presents the list of the most important TRIPOLI-4® developments that were required for the NMC application, starting from version 9 of the code. These developments were made using a recent version of TRIPOLI-4® with analog mode capabilities [7]. While simulating the well counter was the objective of this study, these developments would also apply to multiplicity counting with liquid scintillators for fast neutrons and photons.

### 2.1. Coupling of FREYA and TRIPOLI-4® for fission modeling

To model fission, general-purpose Monte Carlo codes TRIPOLI-4®, MCNP6/X [8], TART [9], COG [10], Geant [11], etc.) employ the “average fission model” which is characterized by outgoing projectiles (fission neutrons and photons) that are uncorrelated, and sampled from the same probability density functions.

During the past decade several code extensions have been developed that allow the modeling of correlations in fission. MCNP-DSP [12] and MCNPX-PoliMi [13] added limited angular correlations of

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fission neutrons. The LLNL Fission Library [14], introduced in MCNPX2.7.0 [15], Geant 4.9 [11] and MCNP6 featured time-correlated sampling of photons from neutron-induced fission, photofission and spontaneous fission. The capabilities for correlations are, however, limited, as they sample outgoing particles from average fission distributions instead of sampling them from individual realizations of a fission process.

In recent years, various simulation treatments addressed fluctuations of and correlations between fission observables. In particular, a Monte Carlo approach was developed [16] for the sequential emission of neutrons and photons from individual fission fragments in binary fission. The more recent event-by-event fission model, FREYA, has been specifically designed for producing large numbers of fission events in a fast simulation [17]. Employing nuclear data for fragment mass and kinetic energy distributions, using statistical evaporation models for neutron and photon emission, and conserving energy, momentum, and angular momentum throughout, FREYA is able to predict a host of correlation observables, including correlations in neutron multiplicity, energy, and angles, and the energy sharing between neutrons and photons. For modeling of fission on an interaction-by-interaction basis, the new LLNL Fission Library/FREYA package was coupled with TRIPOLI-4®.

### 2.2. Development of a spontaneous fission source

A spontaneous fission source was developed to sample time-correlated neutrons and photons from fission. This source emits bursts of time-correlated prompt neutrons and photons from individual fission events, whose multiplicities and energies are sampled from the LLNL Fission Library/FREYA package. TRIPOLI-4® accesses this source as an *external source* (see User Manual [1]). The times of spontaneous fissions are sampled randomly and uniformly within a given time interval $\Delta T$[3]. The rate of spontaneous fissions has to match the rate $F_s$ of spontaneous fissions of the object to be measured experimentally. It is therefore essential to set the correct number of particles accordingly.

### 2.3. Reduction in tracks memory footprint

To model NMC for the well counter shown in Fig. 1, it is necessary to store the time tags of all the neutron capture reactions in the $^3$He tubes. It was quickly realized that the ROOT tracks stored by TRIPOLI-4® became bloated for large simulations, leading to files that were close to terabytes in size for seconds of experimental data. Most of the tracks did not result in $^3$He(n,p) reactions and were thus cluttering the disk. When filtering out tracks failing to traverse detector cells, we were able to substantially decrease the memory footprint, but not enough. Two new options were therefore introduced to further reduce the size of the track files. The first option enables us to store full tracks containing one or several events of interest, whereas the second option enables storage of only specific events with those tracks. With these two additional filters, we could keep the footprint of the ROOT track files in check.

## 3. $PuO_2$ ball

Let's consider a $PuO_2$ object spherical in shape, of weight equal to 5.5366 kg, density 3 g/cc, and of outer radius 7.62 cm [4]. Knowing the neutron yields of the different isotopes composing the object, we calculated the rate of spontaneous fissions to be 140170 spontaneous fissions/s. The spontaneous fission source is uniformly distributed across the sphere. A simulation of the $PuO_2$ source in the well counter shown in Fig. 1 was performed. While the intensity of the $(\alpha,n)$ source could be calculated, we will neglect this contribution for the purpose of this study.

### 3.1. Fitting count distributions to determine system parameters

The arrival times of the neutrons in each of the $^3$He tubes were recorded in the simulation. Randomly splitting the sequence of time tags into $N$ segments of width $T$ (where $T$ is of the order of microseconds to hundreds of microseconds) one can count how many neutrons arrive in the first

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[3] The time tags of the $^3$He(n,p) reactions in the $^3$He tubes are re-ordered chronologically in post-processing.

[4] The isotopics of the plutonium are 0.014% $^{238}$Pu, 93.5% $^{239}$Pu, 6% $^{240}$Pu, 0.5% $^{241}$Pu, 0.03% $^{242}$Pu, and traces of other isotopes.

segment, how many in the second segment, in the third one, etc. to build a distribution $B_n(T)$ of the number *n* of neutrons arriving in the segments of width *T*. The blue dots labelled "simulated data" in the left-hand graph of Fig. 4 show a typical count distribution.

The probability distributions $b_n(T)$ (where $b_n(T)$ is the probability of recording *n* counts in a time gate *T*, which is equivalent to $B_n(T)$ normalized by the number of segments of width *T*) can be reconstructed theoretically [18] using different sets of the three free parameters ($M$, $\varepsilon$, $\overline{\nu}_{sp} F_s$), where *M* is the multiplication of the object, ε the efficiency of the detector array, $\overline{\nu}_{sp}$ the average number of neutrons emitted per spontaneous fission and $F_s$ the intensity in units of spontaneous fissions per second of the spontaneous fission sources in the object. Using a likelihood function, one can determine which parameters ($M$, $\varepsilon$, $\overline{\nu}_{sp} F_s$) generate the theoretical count distribution $b_n^{theory}(T)$ closest to the measured data points $b_n(T)$. This method is best described in Ref. [19].

Each set of parameters ($M$, $\varepsilon$, $\overline{\nu}_{sp} F_s$) has an associated likelihood that the reconstructed $b_n^{theory}(T)$ will be a good match to the measured $b_n(T)$. Using Bayes' theorem, we calculate the posterior probability of each such set. To determine the region of the ($M$, $\varepsilon$, $\overline{\nu}_{sp} F_s$) space that contains the solution with a credibility of 68.27%, we have to accumulate high posterior probability sets until the cumulative probability reaches 68.27%. Fig. 2 shows the credible regions in the ($M$, $\varepsilon$) and ($M$, $\overline{\nu}_{sp} F_s$) parameter spaces for credibilities of 68.27% (red), 95.45% (yellow) and 99.73% (blue). The top two graphs are computed with FREYA. The bottom two graphs are computed without FREYA. Without FREYA, $\overline{\nu}$ is statistically rounded up or down at each fission site to get a number of neutrons. Fig. 3 shows the same credible regions for 2530 seconds.

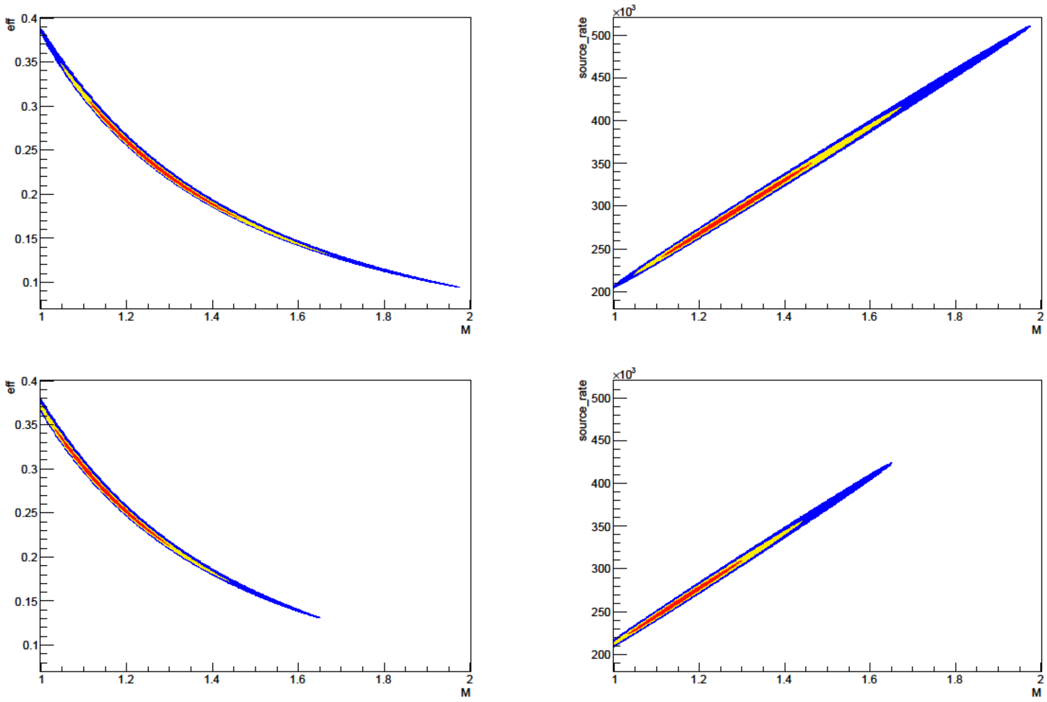

**Figure 2:** (color online) Credible regions for theoretical reconstructions of PuO$_2$ ball:
68.27% (red), 95.45% (yellow), 99.73% (blue).
Nuclear data for induced fission of $^{239}$Pu at 1 MeV. The measurement time is equivalent to 350 seconds.
Top left: ($M$, $\varepsilon$) with FREYA. Top right: ($M$, $\overline{\nu}_{sp} F_s$) with FREYA.
Bottom left: ($M$, $\varepsilon$) without FREYA. Bottom right: ($M$, $\overline{\nu}_{sp} F_s$) without FREYA.

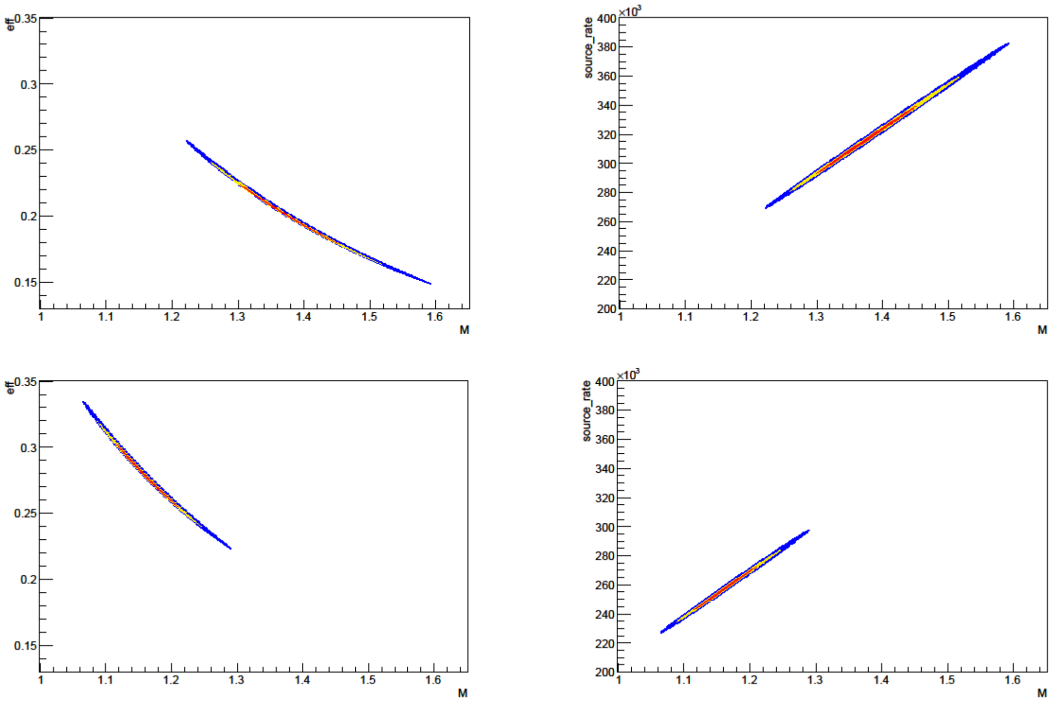

**Figure 3:** (color online) Credible regions for theoretical reconstructions of $PuO_2$ ball: 68.27% (red), 95.45% (yellow), 99.73% (blue).
Nuclear data for induced fission of $^{239}$Pu at 1 MeV. The measurement time equivalent to 2530 seconds.
Top left: ($M$, $\varepsilon$) with FREYA. Top right: ($M$, $\bar{\nu}_{sp} F_s$) with FREYA.
Bottom left: ($M$, $\varepsilon$) without FREYA. Bottom right: ($M$, $\bar{\nu}_{sp} F_s$) without FREYA.

## 3.2. Discussions

Table 1 shows the multiplication calculated by TRIPOLI-4® in different modes: either a criticality calculation including a convergence process of the fission source, or a fixed source criticality calculation where the same neutron source is kept during the whole simulation and fission neutrons are sampled but not used for the source convergence (see TRIPOLI-4® User Manual [1]).

| TRIPOLI-4® simulation mode | LLNL Fission Library/FREYA | $M \pm \sigma$ |
|---|---|---|
| CRITICALITY | no | 1.3312 ± 0.0012 [5] |
| FIXED_SOURCES_CRITICALITY | no | 1.3140 ± 0.0007 |
| FIXED_SOURCES_CRITICALITY | yes | 1.3124 ± 0.0008 |

**Table 1:** Neutron multiplication for $PuO_2$ ball in the well counter calculated with TRIPOLI-4®.

With TRIPOLI-4® running in analog mode, the multiplication of the $PuO_2$ ball within the well counter was calculated to be 1.3124 ± 0.0008 with FREYA, and 1.3140 ± 0.0007 without FREYA. These multiplications are very close and show that average quantities are not affected by the choice of the fission model, whether it statistically samples $\bar{\nu}$ rounded up or down, or a full neutron multiplicity distribution.

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[5] This multiplication was calculated using $M = 1/(1-k_{eff})$ and the k-eigenvalue method of TRIPOLI-4® for $k_{eff}$. Since this method does not solve the same problem as the FIXED_SOURCES_CRITICALITY method [20], it is not expected to produce the same multiplication. It is only shown for the sake of completeness.

For the reconstruction with FREYA, the best solution is $(M, \varepsilon, \bar{\nu}_{sp} F_s)$ = (1.35, 20.9%, 308368 n/s).

One may wonder whether the credible regions shown in the top two graphs of Fig. 3 contain the true solution, which is the one with the source intensity used for the simulation and the multiplication computed by TRIPOLI-4®. The solution (1.33, 21.5%, 303041 n/s) in these two graphs is within the 68.27% credible region and gives the correct source intensity of 302799 n/s. The small discrepancies are likely to be attributed to systematic errors, and to inadequacies in the theory to model the experiment. This is discussed at length in Ref. [19].

It is interesting to compare the count distributions reconstructed from the different solutions within the 68.27% credible region. A set of three such distributions is shown in the left-hand graph of Fig. 4. All the solutions within the credible region are essentially indistinguishable, which explains the size of the uncertainty in that region, and illustrates the highly degenerate nature of the model.

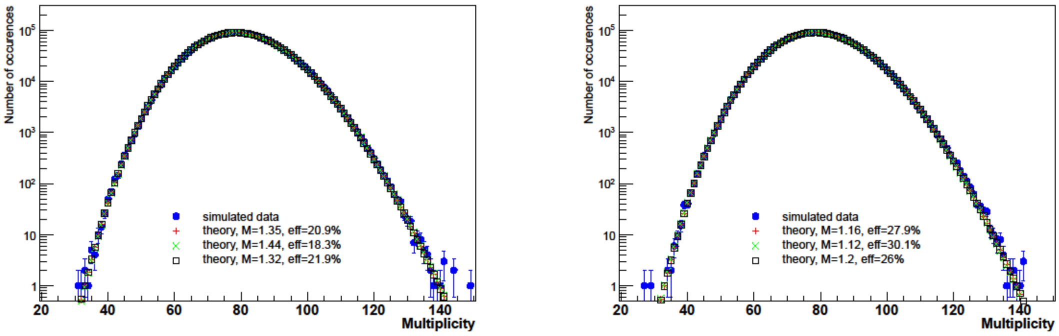

**Figure 4:** (color online) Comparison between theoretically reconstructed count distributions within the 68.27% credible region in Fig. 3. Random time gate count distribution. Time gate width = 1 ms. Simulation result in blue. Nuclear data for induced fission of $^{239}$Pu at 1 MeV. The measurement time is equivalent to 2530 seconds. Left: with FREYA. Right: without FREYA.

Without FREYA, the best solution for the reconstruction is $(M, \varepsilon, \bar{\nu}_{sp} F_s)$ = (1.16, 27.9%, 257174 n/s). Within the 68.27% credible region, the solution that gives the closest source intensity is $(M, \varepsilon, \bar{\nu}_{sp} F_s)$ = (1.2, 26.0%, 269471 n/s). The model still gives very good count distribution reconstructions, as the right-hand graph of Fig. 4 illustrates, but unfortunately, these reconstructions are for the incorrect parameters. For correlated quantities and low multiplication, sampling the full distribution for the fission neutron multiplicity is important. The correct solution could be found with FREYA, whereas without FREYA the default neutron multiplicity sampling gave incorrect solutions.

## 4. Conclusion

FREYA was coupled to TRIPOLI-4® for the purpose of using the latter for NMC. With the addition of a few modifications such as analog transport, spontaneous fission sources and improved tracking capabilities, we demonstrated by way of a $PuO_2$ ball simulation that TRIPOLI-4® when coupled with FREYA can simulate physical correlations sufficiently well to reproduce predicted count distributions measured by a well counter.

Average quantities like neutron flux, reaction rate, multiplication are not affected by the choice of the fission model. Whether the fission model statistically samples $\bar{\nu}$ rounded up or down, or a full fission neutron multiplicity distribution, to emit a number of secondary neutrons, has little to no impact on the result.

For methods using correlated quantities, sampling the full distribution for the fission neutron multiplicity is paramount. The correct solution to the $PuO_2$ ball problem could be found with the fission model

FREYA, whereas the default neutron multiplicity sampling gave incorrect solutions[6]. Thus, including such capabilities in Monte Carlo transport codes is important.

## 5. Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

TRIPOLI-4® is a registered trademark of CEA. We gratefully acknowledge EDF for their long term partnership and AREVA for their support.

J.M. Verbeke wishes to acknowledge the Office of Defense Nuclear Nonproliferation Research and Development in DOE/NNSA for their support, and to thank the stochastic team (LTSD) of the Service d'Etudes de Réacteurs et de Mathématiques Appliquées (SERMA) in the CEA at Saclay, France for hosting him while this paper was being written and while FREYA was being coupled with TRIPOLI-4®.

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