NEW METHODS FOR THE MONTE CARLO SIMULATION OF NEUTRON NOISE EXPERIMENTS IN ADS

Máté Szieberth* and **Jan Leen Kloosterman**
Delft University of Technology, The Netherlands
***On leave from: Budapest University of Technology and Economics, Hungary

Abstract

This paper presents two improvements to speed up the Monte-Carlo simulation of neutron noise experiments. The first one is to separate the actual Monte Carlo transport calculation from the digital signal processing routines, while the second is to introduce non-analogue techniques to improve the efficiency of the Monte Carlo calculation. For the latter method, adaptations to the theory of neutron noise experiments were made to account for the distortion of the higher-moments of the calculated neutron noise. Calculations were performed to test the feasibility of the above outlined scheme and to demonstrate the advantages of the application of the track length estimator. It is shown that the modifications improve the efficiency of these calculations to a high extent, which turns the Monte Carlo method into a powerful tool for the development and design of on-line reactivity measurement systems for ADS.

Introduction

At present accelerator-driven systems (ADS) are being studied, because of their attractive features with regard to safety and transmutation. A crucial point for the practical realisation of ADS is the development of a reliable method to monitor the reactivity of the core. Among others, neutron noise methods such as Feynman-α and Rossi-α measurements are being proposed for this, and experiments like the MUSE project are being conducted to investigate how these techniques can be applied to ADS. Furthermore, new theories are being developed to describe these methods in a more sophisticated way with special attention to spatial, spectral and temporal effects. The development of computer codes that can assist in the design and analysis of reactivity measurement systems has outstanding importance.

Conventional Monte-Carlo codes applying variance reduction techniques are not applicable, because the behaviour of the neutron noise is influenced by the higher-moments of the distribution, which are not preserved by these codes. Therefore, modified versions of existing well-known Monte Carlo codes have appeared like KENO-NR, [1] MCNP-DSP [2] and MVP. [3] In these codes, the real distribution of fission neutrons is sampled as well as the direction of fission neutrons relative to the incident neutron. [4] The MNCP-DSP code contains these modifications even for prompt fission gammas, which makes the code suitable for simulation of measurements applying gamma detectors. Furthermore, the simulation of detection events is done in a fully analogue way: one count is generated for each detector event (capture, fission, scattering, etc.). The counts detected during a predefined period are collected into time bins and processed by the built-in digital signal processing (DSP) routines. The output of this calculation then is the result of the simulated experiment.

As a result of the analogue algorithm, the above-mentioned codes need long CPU times to arrive at acceptable statistics. This causes serious problems if one has to model a large and complicated geometry or if the detector efficiency is very low, which is usually the case in fast reactors. Another problem is that the processing of the simulated detection events is intertwined with the neutron transport calculation itself. This means that, in order to simulate another noise analysis technique, one has to repeat the whole transport calculation.

This paper presents two improvements to speed up the Monte-Carlo simulation of neutron noise experiments. The first one is to decouple the actual Monte Carlo transport calculation from the DSP routines, while the second is to introduce non-analogue techniques to improve the efficiency of the Monte Carlo calculation. For the latter method, adaptations to the theory of neutron noise experiments have to be made to account for the distortion of the higher-moments of the calculated neutron noise.

Structural modifications to the computational flow

The main purpose of the modifications to the calculation scheme is to avoid the repetition of the neutron transport calculation unless the material composition or the geometry changes. This implies that intermediate results (the simulated detector counts) have to be stored to disk after which several neutron noise analysis techniques can be applied to analyse these data. The calculation scheme is divided into three successive steps (see Table 1).

The first one is the neutron transport calculation to collect the travelling time from the source to the detector (t_t) and the history number for each detection event. The latter number uniquely identifies the initiating source event and makes it possible to preserve the correlation between detections. Both external and internal sources (like spontaneous fission and (α, n) reactions) should be considered here.

In a fast reactor, decaying precursor atoms can be considered as a special kind of inherent source as well. It is convenient to perform the transport calculation separately for each source, after which the noise experiments can be simulated for each combination of sources. The result of this step is a data file for each source considered.

The second step is to reconstruct from the data files produced in the first step, the actual experimental data. This means that the individual time (t_{src}) of each source event has to be determined by sampling from the temporal source distribution (uniformly for an internal source, otherwise for pulsed sources). Then the exact time of each detection event (t_d) can be determined as: $t_d = t_{src} + t_t$. The output of this step is a data file containing the actual time of each detection event for a specific linear combination of sources considered.

Table 1. **The modified computational scheme**

<table>
<tr><th colspan="2">Step</th><th colspan="3">Operation</th><th>Input</th></tr>
<tr><td rowspan="2">Step 1</td><td rowspan="2">Transport calculation</td><td>spontaneous fission source</td><td>–</td><td>pulsed source</td><td rowspan="2">material composition, source and geometry</td></tr>
<tr><td colspan="3">collecting data about detection events
t_t, nps</td></tr>
<tr><td rowspan="2">Step 2</td><td rowspan="2">Creating measured data</td><td>equally distribute
t_{src}</td><td>–</td><td>special distribution for
t_{src}</td><td rowspan="2">source and measurement data</td></tr>
<tr><td colspan="3">$t_d = t_{src} + t_t$
writing data file</td></tr>
<tr><td>Step 3</td><td>Data processing</td><td>Feynman-α</td><td>–</td><td>auto-correlation</td><td>method of data analysis</td></tr>
</table>

In the third step the data from the previously described file is analysed. If only analogue methods have been applied in the first step (the neutron transport calculation), this step is very similar to the data handling in real experiments (instead of measured counts as a function of time, one has calculated counts). Otherwise, special routines and correction factors are required for each noise analysis technique considered (e.g. Feynman-α and Rossi-α). This is the subject of the next chapter.

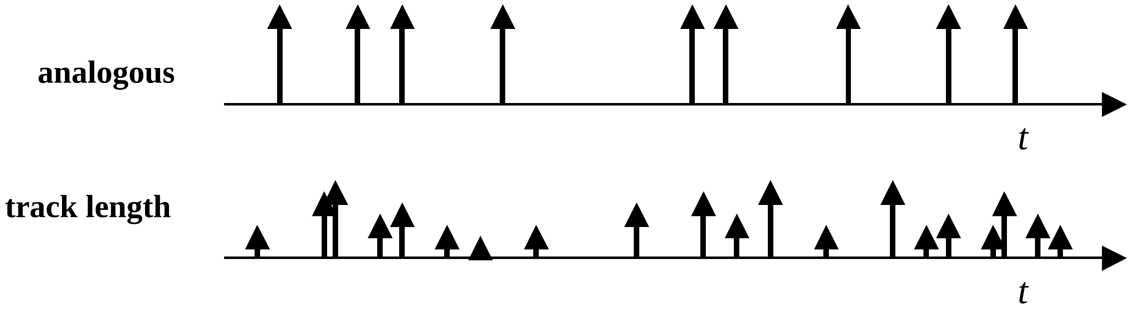
Application of the track length estimator for scoring events

One specific non-analogue technique that can easily be applied in Monte Carlo transport is the track length estimator for scoring. Without this technique, many neutrons simply pass through the detector without detection, which implies a waste of CPU time spent on their transport. The track length method circumvents this problem. Based on the track length one defines an unbiased estimator for the mean value of the number of counts (N) in a time interval T, in a detector with volume V and reaction cross-section $\Sigma(E)$:

$$\langle N\rangle=\int_0^T\int_V\int_0^\infty\Sigma(E)\Phi(E,\mathbf{r},t)\,dE\,dV\,dt=\left\langle\sum_{i=1}^{N_t}\sum_j\Sigma(E_j)d_j\right\rangle=\left\langle\sum_{i=1}^{N_t}w_i\right\rangle \tag{1}$$

where N_t stands for the number of neutrons entering the detector, and the index j sums over all consecutive straight flight paths (d_j) of each neutron with a total contribution to the detector reading of w_i. With this method, instead of having a few counts only, one get many fractional counts (see Figure 1).

Figure 1. **Demonstration of counts in the analogous case and with the track length method**



As the weight w is different for each neutron, and independent of the others, it can be described as a continuous random variable with an unknown probability distribution function (PDF) g(y):

$$P(w<y)=\int_0^y g(\hat{y})d\hat{y} \tag{2}$$

Although the PDF is unknown, the mean value of this distribution can easily be determined. According to (1) the expected value of the sum of all weights equals the expected value of the number of counts. So the estimation of the mean value becomes:

$$\bar{w}=\frac{1}{N_t}\sum_{i=1}^{N_t}w_i=\frac{N}{N_t} \tag{3}$$

In general the detector efficiency (ε) can be written as a product of a geometrical factor (ε_g) and a detection (ε_d) efficiency, which equals the average weight of counts:

$$\varepsilon=\frac{N}{F}=\frac{N_t}{F}\frac{N}{N_t}=\varepsilon_g\varepsilon_d=\varepsilon_g\bar{w} \tag{4}$$

where F is the number of fission events in the core. The probability to have a count in time interval Δt around t with a weight less than y is:

$$P(w<y\,|\,t)\Delta t=\int_0^y g(\hat{y})d\hat{y}\frac{1}{\varepsilon_d}p_c(t)\Delta t$$

where p_c is the probability per unit time of a real count occurring at time t, from which the probability for a neutron entering the detector can be expressed assuming ε_d=1. Thus, the expected value of a weighted count at a given time can be calculated:

$$\langle w\,|\,t\rangle\Delta t=\varepsilon_d\frac{1}{\varepsilon_d}p_c(t)\Delta t=p_c(t)\Delta t$$

which equals the probability to have a count in the case of the analogue method. Although the track length estimator reduces considerably the variance, this formula shows that it preserves the mean value. As noise analysis techniques are usually governed by the higher moments, corrections to the theory are needed. In the following paragraphs the required corrections for the Feynman-α and the auto-correlation method are derived.

The Feynman-α method needs special treatment, because it uses the variance of the measured data, which is radically reduced by the track length estimator. The variance to mean ratio is described by: [5]

$$\frac{\sigma^2(N)}{\langle N\rangle}=1+\frac{\varepsilon D_v}{\rho_p^2}\left(1-\frac{1-e^{-\alpha T}}{\alpha T}\right)=1+Y \qquad (5)$$

where D_v is the Diven-factor, ρ_p is the prompt reactivity and α is the prompt neutron decay constant. Y usually denotes the correlated part, which measures the deviation from the Poisson distribution.

Let λ be the expected value of the number of counts during a time interval T:

$$\lambda=\int_0^T\int_V\int_0^\infty \Sigma(E)\Phi(E,\mathbf{r},t)\,dEdVdt$$

Due to the stochastic nature of neutron transport, λ fluctuates with the flux from time interval to interval, and can be considered as a continuous random variable with an unknown PDF f:

$$P(\lambda<x)=F(x)=\int_0^x f(\hat{x})d\hat{x}$$

The real number of counts can be described as a discrete random variable having a Poisson distribution:

$$P(N=k\,|\,\lambda)=\frac{\lambda^k}{k!}e^{-\lambda}$$

The unconditional probability distribution of N can be written based on the total probability theorem as:

$$P(N=k)=\int_0^\infty\frac{x^k}{k!}e^{-x}f(x)dx$$

From this one can express the first moment of N as:

$$\langle N\rangle=\sum_{k=0}^\infty k\int_0^\infty\frac{x^k}{k!}e^{-x}f(x)dx=\int_0^\infty xf(x)dx=\langle\lambda\rangle \qquad (6)$$

which is trivial from the definition, as well. The second moment can be obtained in a similar way:

$$\langle N^2\rangle=\sum_{k=0}^\infty k^2\int_0^\infty\frac{x^k}{k!}e^{-x}f(x)dx=\int_0^\infty\left(x^2+x\right)f(x)dx=\langle\lambda^2\rangle+\langle\lambda\rangle \qquad (7)$$

From (6) and (7) the variance can be determined:

$$\sigma^2(N)=\langle N^2\rangle-\langle N\rangle^2=\langle\lambda^2\rangle-\langle\lambda\rangle^2+\langle\lambda\rangle=\sigma^2(\lambda)+\langle\lambda\rangle$$

Finally, the variance to mean ratio is:

$$\frac{\sigma^2(n)}{\langle n\rangle}=\frac{\sigma^2(\lambda)}{\langle\lambda\rangle}+1 \qquad (8)$$

This formula demonstrates that the correlated part of the variance to mean ratio comes from the variance of λ, which is related to the variance of the flux in the detector.

Applying the track length estimator, the total number of counts *N* is the sum of all weights (1), which means that *N* is now a continuous random variable with the following distribution (assuming that *k* neutrons enter the detector):

$$P\left(N<y\,|\,N_t=k\right)=\int_0^y g_k\left(\hat{y}\right)d\hat{y}$$

Here g_k is unknown again, but considering that the weights of the subsequent counts are independent from each other, and assuming that $\langle w\rangle = m$ and $\sigma^2(w)=\sigma^2$ the followings can be stated based on the rules of summing up independent random variables:

$$\langle N\,|\,k\rangle = km$$

$$\sigma^2\left(N\,|\,k\right)=k\sigma^2$$

$$\left\langle N^2\,|\,k\right\rangle=\sigma^2\left(N\,|\,k\right)+\left\langle N\,|\,k\right\rangle^2=k\sigma^2+k^2m^2$$

From (4), the expected number of neutrons entering the detector is a Poisson variable with mean $\frac{\lambda}{\varepsilon_d}$. So the distribution of *N*, with the condition of λ can be written as:

$$P(N<y\,|\,\lambda)=\int_0^y\sum_{k=0}^{\infty}g_k\left(\hat{y}\right)\frac{\left(\frac{\lambda}{\varepsilon_d}\right)^k}{k!}e^{-\frac{\lambda}{\varepsilon_d}}d\hat{y}$$

The unconditional distribution becomes:

$$P(N<y)=\int_0^y\int_0^{\infty}f\left(x\right)\sum_{k=0}^{\infty}g_k\left(\hat{y}\right)\frac{\left(\frac{x}{\varepsilon_d}\right)^k}{k!}e^{-\frac{x}{\varepsilon_d}}dxd\hat{y}$$

From this, considering that $\varepsilon_d=m$ (see (4)) the first and second moments become:

$$\langle N\rangle=\int_0^{\infty}y\int_0^{\infty}f\left(x\right)\sum_{k=0}^{\infty}g_k\left(\hat{y}\right)\frac{\left(\frac{x}{\varepsilon_d}\right)^k}{k!}e^{-\frac{x}{\varepsilon_d}}dxd\hat{y}=\int_0^{\infty}\frac{x}{\varepsilon_d}mf\left(x\right)dx=\langle\lambda\rangle$$

$$\left\langle N^2\right\rangle=\int_0^{\infty}y^2\int_0^{\infty}f\left(x\right)\sum_{k=0}^{\infty}g_k\left(\hat{y}\right)\frac{\left(\frac{x}{\varepsilon_d}\right)^k}{k!}e^{-\frac{x}{\varepsilon_d}}dxd\hat{y}=\left(\sigma^2+m^2\right)\frac{\langle\lambda\rangle}{m}+\left\langle\lambda^2\right\rangle \qquad (9)$$

From which the variance can be calculated:

$$\sigma^2(N) = \langle N^2 \rangle - \langle N \rangle^2 = \left(\frac{\sigma^2}{m} + m \right) \langle \lambda \rangle + \langle \lambda^2 \rangle - \langle \lambda \rangle^2 = \left(\frac{\sigma^2}{m} + m \right) \langle \lambda \rangle + \sigma^2(\lambda)$$

Finally, the variance to mean ratio in the case of the track length method can be expressed as:

$$\frac{\sigma^2(N)}{\langle N \rangle} = \frac{\sigma^2(\lambda)}{\langle \lambda \rangle} + \frac{\sigma^2}{m} + m, \qquad (10)$$

which means that the required correction can be calculated from the mean and the variance of the count weights. The mean can be estimated like in (3), while the estimation for the variance writes:

$$\bar{\sigma}^2 = \frac{1}{N_t} \sum_{i=1}^{N_t} (w_i - \bar{w})^2 = \frac{1}{N_t} \sum_{i=1}^{N_t} w_i^2 - \left(\frac{1}{N_t} \sum_{i=1}^{N_t} w_i \right)^2$$

Usually, these two parameters can be estimated very accurately, because there are many more fractions of counts than real counts ($N_t >> N$). Assuming real counts with a weight of one, the variance of the weights becomes $\sigma^2=0$, while the mean is $m=1$, and (10) becomes (8) again.

The auto-correlation can be written as:

$$ACF(\tau) = \frac{\langle N_1 N_2 | \tau \rangle}{\langle N_1 N_2 | 0 \rangle} = \frac{\langle N_1 N_2 | \tau \rangle}{\langle N^2 \rangle}$$

where N_1 means the number of counts in a time interval $[t,t+T]$ and N_2 means the number of counts in a time interval $[t+\tau,t+\tau+T]$. The expression in the numerator (the covariance) can be calculated using the track length method, but the denominator equals the second moment, which is not preserved as it was shown above. Therefore, a correction is needed in the case of the auto-correlation as well, which can easily be derived from (9) and (11):

$$\langle N^2 \rangle' = \langle N^2 \rangle + \langle N \rangle - (\sigma^2 + m^2) \frac{\langle N \rangle}{m}$$

The obtained formula can be calculated as simple as (12) and the same is true: in the case of real counts the correction becomes zero.

Calculations

Calculations were performed to test the feasibility of the above outlined calculation scheme and to demonstrate the advantages of the application of the track length method. For this purpose, the required modifications to the physical model of neutrons were transferred from MCNP-DSP to MCNP4C [6] without interfering with the original calculation flow. These modifications are using the actual distribution of fission neutrons and sampling the direction of the fission neutrons relative to the incident neutron. A new source option was created for spontaneous fission where multiple neutrons start at the same source position. However, to sample the actual number of fission neutrons and their direction, the same PDFs were used as in MCNP-DSP. The other two sources considered, the (α,n) and the D-D source (either in pulsed or continuous mode), can be realised by the standard MCNP input options. The collection of the detection events was also realised by the standard options in case of analogue simulation of detection and by a user subroutine in case of the track length estimator. In the first case, the data stored are the time of each count and the history number, while in the second case the length, energy and count weight of each neutron flight path in the detectors are stored.

After the Monte Carlo calculation, the data file was processed with a programme that distributes randomly all the source events in the measuring time, sorts the counts by time, and writes a count file for each detector containing the weight (all unity in the analogue case) and time of each count. This is very similar to real measurement data that contains the arrival time of each count. The count file can be processed with any kind of noise analysis technique. In our case the variance-to-mean ratio and the auto-correlation function were calculated.

The first goal of the calculations was to confirm that the use of the track length estimator influences the result as described above. The examined problem was the Jezebel [7] geometry (a Pu sphere). During the simulation, the sphere was slightly sub-critical (k_{eff}=0.99576±0.00042), because only prompt neutrons were simulated. The system was driven by spontaneous fission neutrons of ^{240}Pu and ^{242}Pu. Two lithium glass (5.08 cm in diameter, 2.54 cm long) detectors are located adjacent to the sphere and are positioned 180° apart. The very simple geometry was chose so that even the analogous method can produce results with good statistics in a reasonable time.

The second goal was to demonstrate the advantages gained by the new methods. For this purpose a complicated geometry, the 1 120 cells configuration of the MUSE-4 benchmark programme (see Figure 4), [8] was used. Now, only the track length method has been applied, because of the complicated geometry, and the small (10 cm long and 2.54 cm in diameter) fission chambers with low-efficiency, which makes it impossible to get accurate results by the analogue method. Three separate calculations were performed for D-D, spontaneous fission and (α,n) source.

Results

The results obtained for the Jezebel benchmark can be seen in Figures 2 and 3. The analogue case required ~40 hours of CPU time to provide as good statistics as the track length method after 2 hours. The fitted α values are summarised in Table 2. In the Feynman results the calculated correction was 0.063, while the fitted one was 0.060±0.025. The discrepancy observed in the asymptotic value of the Feynman curves (Figure 3) can be explained by the small difference in reactivity (<50 pcm) between the two jobs (which is due to the statistical fluctuations), because the absolute value of the reactivity is very small (~425 pcm) and the asymptotic value is inverse proportional to its square. [5]

In the case of the MUSE calculations the k_{eff} was 0.99516. In Figure 5 the auto-correlation function in detector C (located in the reflector) can be seen assuming spontaneous fission, (α,n) and D-D source in continuous mode. The fitted α-value (Table 2) is in the range expected for MASURCA. In Figure 6 the D-D source was considered as a pulsed source and the (α,n) source was omitted to obtain a higher relative source strength of the D-D source. The peaks at every 0.3 ms can be observed due to the source pulsed with a frequency of 3.33 kHz. The presented results show the possibility of the variation of the different source types, and prove that the track length method gives good results, even for a detector far away from the active core zone.

Table 2. **Fitted α-values in different cases**

Prompt decay constant (1/s)	Jezebel		MUSE
	Analogue	Track length	Track length
Auto-correlation	$1.98 \cdot 10^6$	$2.01 \cdot 10^6$	10 059
Feynman	$2.11 \cdot 10^6$	$2.00 \cdot 10^6$	–

Figure 2. **Auto-correlation in Jezebel**

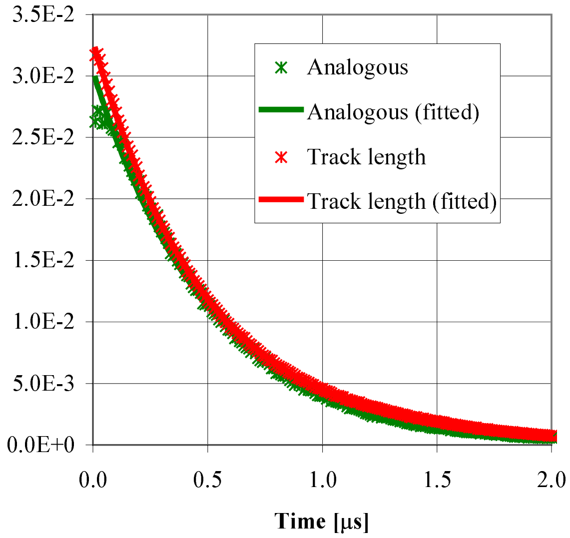


Figure 3. **Variance to mean ratio in Jezebel**

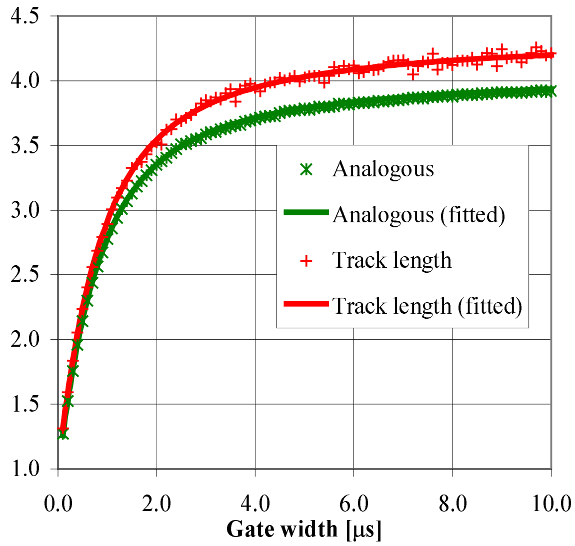


Figure 4. **The MUSE 1112 cells geometry with detector positions (capital letters)**

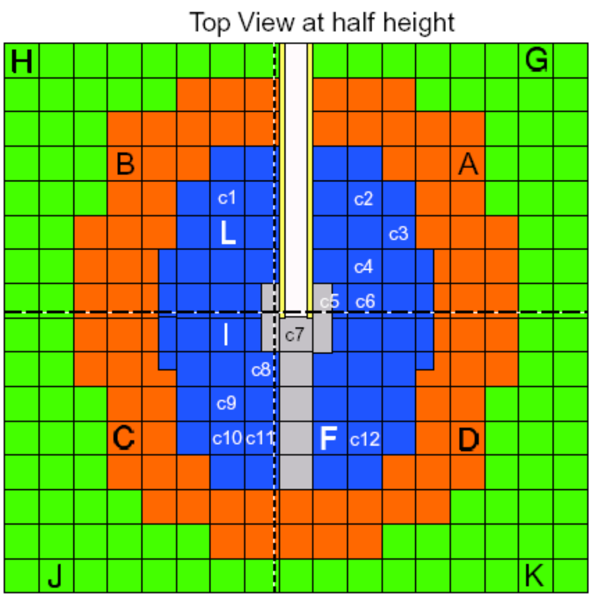
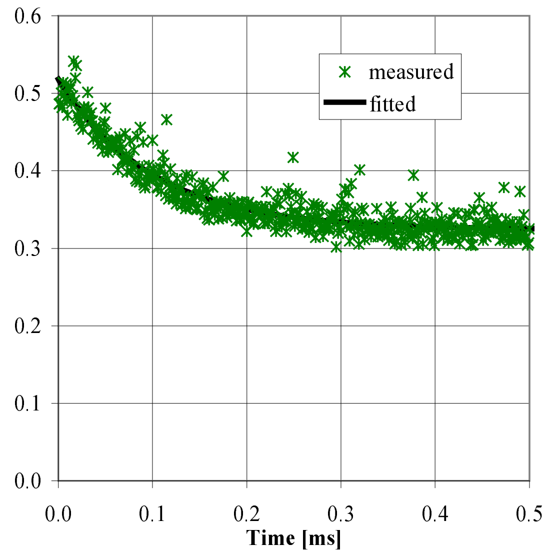


Figure 5. **Auto-correlation function in detector C with spontaneous fission, (α,n) and D-D source**

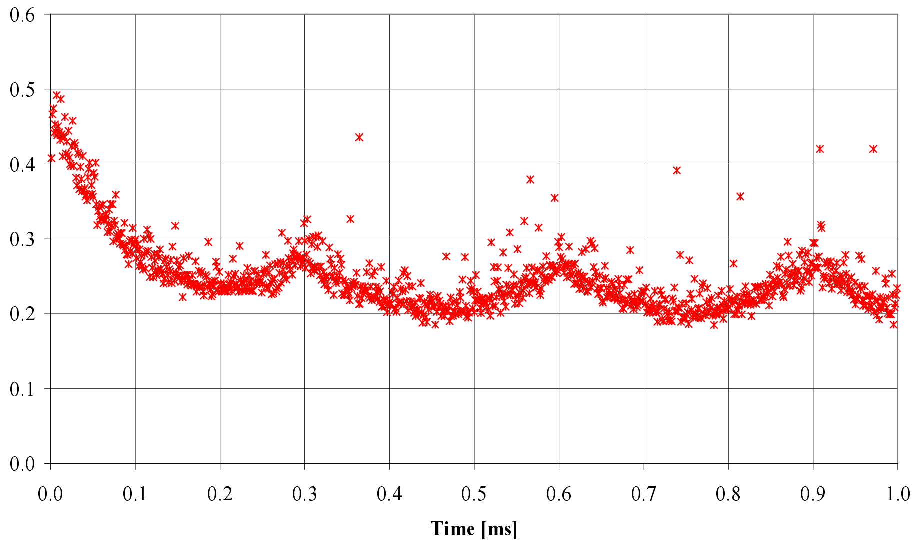


Conclusions

To speed up the simulation of neutron noise experiments, improvements were made to the computational flow applied by the standard analogue codes. The Monte Carlo simulation and the noise analysis techniques have been separated, which enables us to simulate multiple measurement techniques using the results of only one Monte Carlo calculation. Furthermore, using the track length estimator, the Monte Carlo calculations could be made much more efficient, which makes it possible to apply these techniques to complicated geometry and to detectors with low efficiency (like in

MUSE). Because the application of the track length estimator gives a distortion of the distribution of the detected neutron population, adaptations to the theory of Feynman-α and the auto-correlation were made. The test calculations show that the new computation scheme gives unbiased results in much shorter CPU time.

Figure 6. **Auto-correlation function in detector C with spontaneous fission and pulsed D-D source**
(f=3.33 kHz)



Acknowledgements

The authors acknowledge the European Commission for co-funding this work under project number FIKW-CT2000-00063 and for the travel grants provided, and the other members of the MUSE project for their co-operation.

REFERENCES

[1] E.P. Ficaro (1991), *KENO-NR: A Monte Carlo Code Simulating the ^{252}Cf-Source-driven Noise Analysis Experimental Method for Determining Subcriticality*, Ph.D. Dissertation, University of Michigan.

[2] T.E. Valentine (1997), *MCNP-DSP Users Manual*, ORNL/TM-13334, Oak Ridge Nat. Lab, January.

[3] T. Mori, K. Okumura, Y. Nagaya (2001), *Development of the MVP Monte Carlo Code at JAERI*, Transactions of the ANS, 84, pp. 45-46.

[4] T.E. Valentine (1999), *Review of Subcritical Source-driven Noise Analysis Measurements,* ORNL/TM-1999/288, Oak Ridge Nat. Lab., November.

[5] Robert E. Uhrig (1970), *Random Noise Techniques in Nuclear Reactor Systems*, The Roland Press Company, New York.

[6] J.F. Briesmeister (ed.) (2000), *MCNP-A General Monte Carlo N-Particle Transport Code, Version 4C*, LA-13709-M, UC700 (March).

[7] R. Douglas O'Dell (evaluator) (2001), *^{240}Pu Jezebel: Bare Sphere of Plutonium-239 Metal*, in: International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA Nuclear Science Committee, NEA/NSC/DOC(95)/03/I, Volume I, Plutonium Systems.

[8] D. Villamarin, R. Soule, E. Gonzalez (2001), *Benchmark on Computer Simulation of MASURCA Critical and Subcritical Experiments (MUSE-4 Benchmark)*, OECD/NEA, NEA/SEN/NSC/WPPT(2001)5, JT001117874.