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Monte Carlo Method: Theory and Exercises (1)

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Time resolved MCNP neutron transport simulation on multiplying media: GODIVA benchmark

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Abstract

MCNP4C3 feature to sample delayed neutrons by using novel cross section data file for fissile materials was checked through a set of time resolved simulation of the well-known GODIVA fast assembly. Both criticality and source driven simulations were carried out in order to check data and code consistency. The good agreement between results and experimental values permits the application of the methodology to more complex systems.

Introduction

The capability of MCNP [1] to estimates the time resolved behavior of the systems under simulation is a well know feature since the version 4B of the code [2]. The lack of delayed neutrons data in the MCNP cross sections database precluded, up to version 4C, total time resolved transport analysis on multiplying media. Aim of this report is to check the capability of MCNP4C joined with the novel cross section data on delayed neutrons (.61c series) [3,4,5] to simulate the kinetic behavior of a well know and simple critical assembly as GODIVA [6]. The sub-critical, source driven, GODIVA system were also investigated. The good agreement with the experimental values allows us to extend the simulation technique toward more complex systems such as the TRADE and MUSE subcritical configuration.

Methods and plan of calculation

The GODIVA critical assembly is a fast reactor built up realized during the early '50s to extend the basic knowledge in the reactors physics from theoretical and experimental point of view. It consists in a spherical assembly of metallic Uranium enriched at 94% ^{235}U (density 18.8 g cm^{-3}). The critical radius of the assembly is 8.7037 cm. Our MCNP geometry is a sphere of a given radius filled with the proper metallic fuel composition expressed at isotopic level by using new ENDFB-VI cross sections (.61c series). The source driver, where required, was always assumed to be an isotropic, mono-energetic (2 MeV), neutron point source located at the center of the spherical assembly. Three different source time modulations have been considered: an instantaneous neutron burst (All neutron born at t=0), a "short" (100 ns) and a "long" (100 s) square wave period.

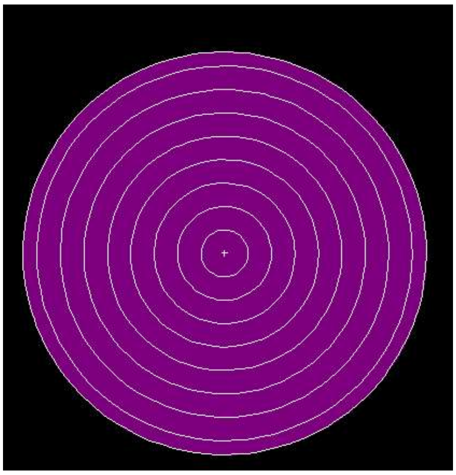

Figure 1. Cross section of the GODIVA model from the MCNP plotter: the system was divided in 9 concentric spherical cells. On each cell flux tallies were estimated.

The flux-time response was estimated by using track length tallies (F4-type) on a set of spherical shells in which the geometry was further subdivided (see fig. 1).

Table I

Item	Problem name	Type of simulation	K_{eff}	Comments
1	TOTAL	KCODE	1.00099 ± 0.00011	Criticality at room temperature.
2	PROMPT	KCODE	0.99461 ± 0.00011	Prompt criticality at room temperature.
3	PC	KCODE	0.98118 ± 0.00034	Sub-critical (r=8.6 cm). Prompt neutrons.
4	P4	SDEF	0.98118 ± 0.00034	2 MeV isotropic source. Neutron burst. Flux tallies. Prompt.
5	PIM	SDEF	0.98118 ± 0.00034	2 MeV isotropic source. 100 ns shoot. Time dependent flux tallies. Prompt.
6	PCR	KCODE	0.98688 ± 0.00034	Sub-critical (r=8.6 cm). Prompt and delayed neutrons.
7	PIR	SDEF	0.98688 ± 0.00034	2 MeV isotropic source. Neutron burst. Flux tallies. Prompt and delayed neutrons.
8	PIR1	SDEF	0.98688 ± 0.00034	2 MeV isotropic source. 100 s shoot. Time dependent flux tallies. Prompt and delayed neutrons.
9	ACD1	ACODE	0.98688 ± 0.00034	Alpha eigenvalue (2.74 ± 0.14) x 10^6 s^{-1}. GODIVA sub critical system.
10	ACD2	ACODE	1.00099 ± 0.00011	Alpha eigenvalue (1.01 ± 0.12) x 10^6 s^{-1}. Godiva critical system.

Table I briefly resumes all the calculation executed in the following flow sheet:

1) Estimation of Total and prompt K_{eff} of the system (Items 1,2 - Table I).

2) The GODIVA system is set to sub-critical state by radius reduction (from 8.7037 to 8.6 cm). Estimation of prompt and total K_{eff} s (Items 3,6 - Table I).

3) A neutron isotropic point source (energy 2 MeV) was placed at the center of the sub-critical GODIVA sphere to simulate the source driver. Two distinct time behavior of the source were investigated: neutron burst and square wave period (Items 4,7 and 5,8 of Table I respectively). Time resolved flux tallies (figs 2a, 2b, 3, 4) were accumulated on nine spherical shells (see fig. 1) in which GODIVA system was ideally subdivided.

4) Estimation of α_p value by:
i) Least square method from the kinetic data obtained in prompt sub-critical runs (item 4 -Table I, figure 2a).

ii) MCNP ACODE routine (item 9,10 - Table I).

iii) Point kinetic theory and thetabular data of the problem summary of the KCODE routine.

The results of those estimations were reported in Table II.

5) Estimation of n_{qs}/n_s ratio from the data of the source jerk like simulation (Item 8 – Table I and figure 4) in the point kinetic approximation (see discussion).

6) Table III reports the comparisons of the estimated α_p and β_{eff} versus the experimental values. The effective delayed neutrons fraction, β_{eff}, was estimated on the basis of the difference between prompt and total K_{eff}s [11].

7) An alternative method to evaluates the system response of a general time shaped source driver was implemented on computer code. The method is based on the convolution of the Monte Carlo results for neutron burst (see Appendix B) to obtain the desired response.

In all cases, the calculation was executed until the KCODE and/or tally results had reached meaningful level of convergence. In the case of KCODE and ACODE calculations convergence was achieved in 10-30 min. of CPU-time of our 677-MHz ALPHA-DEC bi-processor chipset, whereas source driven systems request more than 50 hours on the same computers. The use of 12 CPUs of the Feronia-Beowulf cluster at ENEA-Casaccia center allows us to run the source driven problem in parallel mode and reduces the calculation time of a factor 4. The main purpose of the whole simulation set has to assess the Monte Carlo calculation methodology for kinetic simulation in a regime far from feedback effects. The entire analysis was performed assuming a constant system temperature.

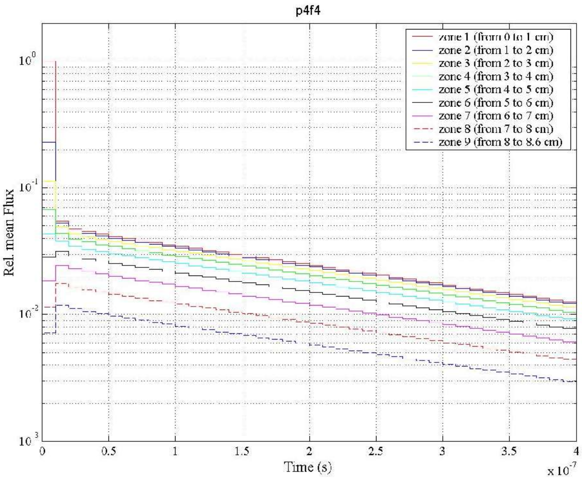

Figure 2a. Prompt neutron flux estimation versus time on the 9 cells of the GODIVA model (Item 4–Table I) when driven by an isotropic neutron point source burst. The fluxes pass through a maximum followed by an exponential decay.

Results and Discussion

The critical GODIVA system behavior was simulated both for prompt and total neutron regimes and the K_{eff}s values were consistent with criticality state (Items 1 and 2-Table I). The radius reduction from 8.7037 to 8.6 cm drives the GODIVA system in a subcritical state with a total K_{eff} value of 0.98688. This level of subcriticality was assumed to be constant during the subsequent source driven calculations.

The prompt flux behaviors versus time were reported on figures 2a and 3 for the neutron burst and square wave. In both cases the prompt flux shown a rise to a maximum, that was slightly time shifted depending of the distance of the tally shell from the source (see fig. 1), then an exponential flux decay, with the same time constant for all shells, take place.

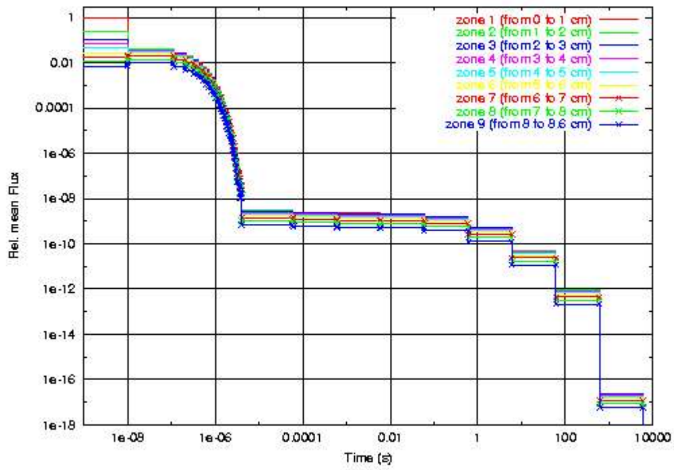

Figure 2b. Total neutron flux estimation versus time on the 9 cells of the GODIVA model (Item 7–Table I) when driven by an isotropic neutron point source burst. The time response shows a net separation between prompt and delayed neutron contribution

The flux became negligible in about 4 µs. Figure 2b reports the total flux time behavior when the subcritical system was driven by a source neutron burst: after a 4 µs (from source shutdown) the flux decays of seven order of magnitude and then due to the delayed neutrons contributions, the flux remains almost constant up to 0.1 s (quasi static state).

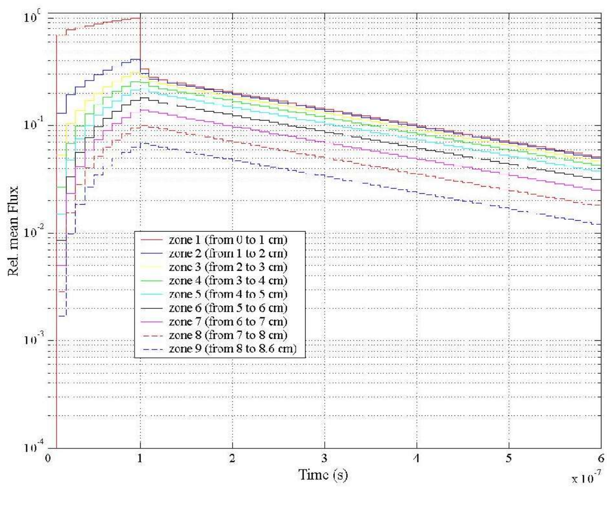

Figure 3. Prompt neutron flux estimation versus time on the 9 cells of the GODIVA model (Item 6–Table I) when driven by an isotropic neutron point source with square time shape (100 ns of shoot).

The total flux becomes practically negligible after 1 s from the source shutdown. The total flux responses in case of the system driven by a square wave source with a period of 100 s (source jerk response) was reported in figure 4a. Before the source shutdown the system was in a stationary state in which all precursor families were near at the equilibrium. After the source shutdown (100 s) the flux starts to decrease and became negligible after 900 s.

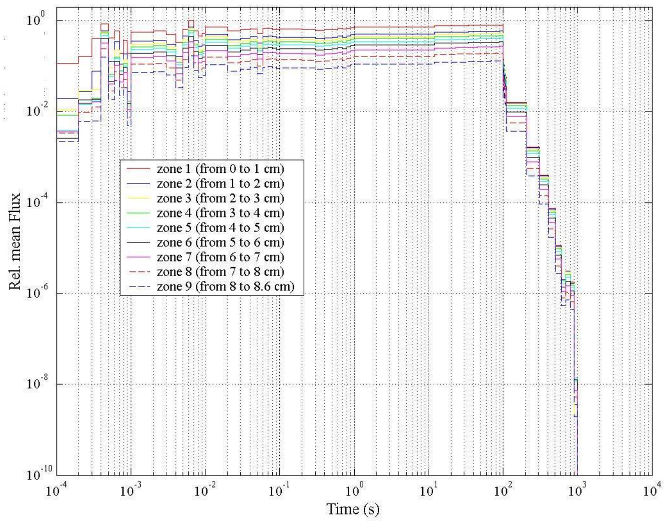

Figure 4a. Total neutron flux estimation versus time on the 9 cells of the GODIVA model (Item 8–Table I) when driven by an isotropic neutron point source with square time shape (100 s of shoot).

Because of the poor resolution of the time logarithmic scale the quasi-static state due to delayed neutron contribution is not clearly visible in the figure. In the figure 4b a magnification of the first 5 s after to source shutdown was reported. As expected the quasi-static flux was about the 26% of the flux of the stationary state.

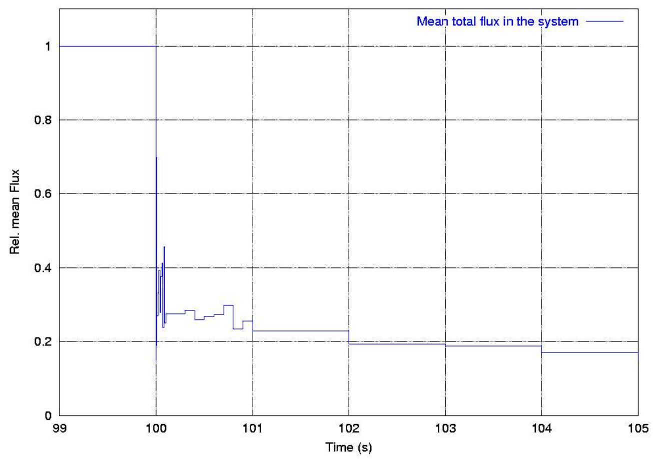

Figure 4b. Magnification of the total neutron flux estimation of the GODIVA model (Item 8–Table I) for the first 5 s after the source jerk

The great difference between the flux in the quasi-static state for the source burst and the one induced by the source jerk was due to the small amount of delayed neutron precursors created in the former. From the quantitative point a view the code was checked for internal consistency by using different estimator for the main kinetic parameter of the system under simulation.

Table II

α_p from Linear Regression*	α_p from ACODE	α_p from Point Kinetic **
3.517 x 10^6 s^{-1}; StD=4.564 x10^3	2.740 x 10^6 s^{-1}; StD=1.400 x10^5	3.45E x10^6 s^{-1}; StD=6.00 x10^4

α_p estimation based on different techniques with MCNP simulation data.

***Based on the prompt flux kinetic evolution after a source neutron burst (Item 5 – Table I and fig. 2a)**

****Based on the point kinetic relationship $\alpha_p=\rho_p/\Lambda$ (see discussion).**

The α_p values reported in Table II, calculated with three different methods, were in sufficiently good agreement. The ACODE estimator tends to underestimate α_p respect to the other two estimators. It is worth of noticing that the point kinetic estimator (third column, Table II) is based on the well-known formula:

$$\alpha_p = \rho_p/\Lambda \qquad \textbf{(1)}$$

Where

ρ_p = prompt reactivity;

Λ= neutron generation time;

If

$$\rho_p = (K_{pc} - K_{ps})/(K_c * K_{ps});$$

where

K_c = prompt K_{eff} of the GODIVA critical system (Item 1 –Table I)

K_{ps} = prompt K_{eff} of the GODIVA sub-critical system (Item 3- Table I)

And approximating Λ to the neutron generation lifespan [10] from the tabular data of MCNP KCODE calculation (Item 3 –Table I) the α_p value reported in Table II is readily obtained.

Table III

Theoretical		MCNP	
n_{qs}/n_s	Standard Deviation	n_{qs}/n_s	Standard Deviation
0.332	0.007	0.26	0.05

Quasi-static to static neutron ratio comparison between the value obtained from the theoretical formulation and the MCNP estimation based on the Kinetic data of the square wave source response (Item 10 – Table I).

Table III reports a comparison between the quasi-static to static neutron ratio as obtained from theoretical relation [7]:

$$\frac{n_{qs}}{n_s} = \frac{1}{1 + \frac{1-k_s}{k_s * \beta_{eff}}}$$

and the MCNP tally flux data averaged on the first 7 ms after the source jerk shutdown (Item 8-Table I).

Table IV

	Experimental		MCNP		
	Mean	Standard Dev.	Mean	Standard Dev.	Method
β_{eff} (pcm)	659	10	637	16	k-eigenvalues
$\alpha_p (s^{-1})$	1.01 x 10^6	--	1.0078 x 10^6	1.1 x 10^5	ACODE

Comparison between calculated and experimental values of β_{eff} and α_p from reference [8] and [9] respectively

The fraction of delayed neutrons was calculated as difference between the two K_{eff} 's values [11]. The so obtained β_{eff} value appears to be 2.8% lower than the experimental value quoted by Hansen [8] (first row of Table IV). The second row of Table IV reports a comparison between the experimental [8] and calculated α_p values that are in good agreement. The calculated α_p value was obtained from ACODE routine in the case of critical configuration (Item 10 Table I) differs substantially from the previous value, relative to ACODE estimation on the sub-critical GODIVA system (Item 9 – Table I).

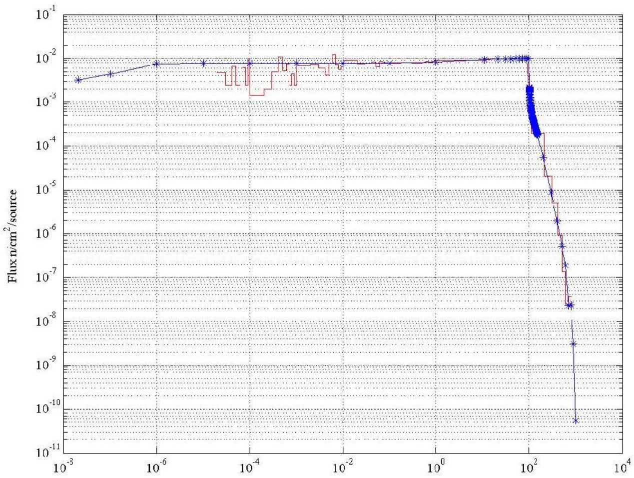

Figure 5. Comparison of the total neutron flux obtained in the inner GODIVA shell in a MCNP run (Item 8, Table I, red solid line) with the one obtained by convolution of burst response with a square shaped source (100 s of shoot, blue asterisk)

In order to avoid complicated time consuming simulation a computer program able to executes the convolution of a neutron burst source response with a general source time shape was implemented by using OCTAVE [10] prototyping system scripts. The main advantage of this technique is in the speed up of the calculation for more complicated source time shape. The relative simple GODIVA problems permit us to check the consistency of the results and the robustness of the algorithm (see Appendix A for the technical details). Figures 5 reports a comparison between the direct and the convolute GODIVA response: the agreement was excellent.

Conclusions

The inner consistency of the results from the MCNP routines KCODE, ACODE and SDEF were optimal: the .61c microscopic cross section series from ENDF-B VI were adequate to represents the behavior of the GODIVA system. The ACODE routine shows discrepancy respect to kinetic methods when the system was driven into a subcritical condition. The agreement with the experimental values was adequate. The kinetic simulations, even in the relative simple GODIVA case, require very long calculation time and the use of parallel computers became mandatory. Works are in progress to extend this analysis toward more complex systems in which heterogeneous effects, such the ones induced by reflector and/or moderator, could complicate the response. The convolution code developed in our lab could help the analysis of the transient response of the accelerator "beam trip" in the simulation of Accelerator Driven System.

Appendix A (Convolution technique)

Definitions:

G: transfer function operator, time independent and linear;

f(t): input function;

δ(t): Dirac delta function;

$g(t) \equiv G[f(t)]$; $h(t) \equiv G[\delta(t)]$.

From the delta-dirac definition we know that:

$$f(t) = \int_{-\infty}^{+\infty} f(\tau)\delta(t-\tau)d\tau$$

$$G[f(t)] = \int_{-\infty}^{+\infty} f(\tau)G[\delta(t-\tau)]d\tau = \int_{-\infty}^{+\infty} f(\tau)h(t-\tau)d\tau = g(t)$$

from MCNP output we have:

$$h(t) = \sum_{i=1}^{N} h_i[\Theta(t-t_{i-1}) - \Theta(t-t_i)]$$

where:

- h_i i=1,2,…,N are the results of the system defined from the G operator to the delta function that, in the MCNP output, are in the tally histogram form;
- $t_0<t_1<\ldots<t_{i-1}<t_i<\ldots<t_N$ is the sequence of the boundaries of the time-bins of the MCNP tallies;
- $\Theta(t)$ is the heaviside step function,

than:

$$G[f(t)] = \sum_{i=1}^{N} h_i \int_{-\infty}^{+\infty} f(\tau)[\Theta(t-\tau-t_{i-1}) - \Theta(t-\tau-t_i)]d\tau = \sum_{i=1}^{N} h_i \int_{t-t_i}^{t-t_{i-1}} f(\tau)d\tau$$

This technique is valid for the MCNP model in the hypothesis that the correlation introduced by the convolution from the G [δ(t)] and G [δ(t+τ)] results is negligible.

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