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Calculating the effective delayed neutron fraction using Monte Carlo techniques

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We present a true Monte Carlo estimator of the effective delayed neutron fraction β_{eff}. The advantage of this method is that by using the physics at the microscopic level, it obviates the need for adjoint calculations, without making any approximations. We have implemented this estimator into MCNP. In a standard k_{eff} calculation, the code now reports a β_{eff} value. The method does not slow down the code by more than 0.5%. We define an extensive benchmark set for β_{eff}, which we use to test our method, and two known approximate methods. Our method reproduces all experimental values.

KEYWORDS: effective delayed neutron fraction, Monte Carlo, MCNP

1. Introduction

In reactor kinetics, the effective delayed neutron fraction, β_{eff}, plays a key role. It is, in effect, the unit of reactivity, conventionally being referred to as a 'dollar'. Because of the difficulties in measuring β_{eff}, one has traditionally relied heavily on calculations to determine its value in a specific situation. Keepin, in 1965, provided a theoretical framework that has been used ever since for such calculations [1]. These involve an adjoint and spectrum weighting of the delayed neutron production rate, and hence require a calculation of both a flux and an adjoint function, and on top of that a suitable post-processing to calculate the weighted production rate.

The amount of work that this entails is considerable. Not many code packages can calculate β_{eff} in a standard procedure, based on nuclear data without making any major assumptions or approximations along the way. Monte Carlo programs are especially hard pressed to do this, because adjoint calculations are cumbersome in continuous energy Monte Carlo codes [2]. Nevertheless one can argue that there is a need for reliable β_{eff} calculations for systems other than the familiar light water reactor type (LWR), since there is a strong interest in transmutation of plutonium and minor actinides. These isotopes produce fewer delayed neutrons, which reduces the distance to prompt criticality, and hence increases the need for accuracy in the calculation of β_{eff}. Moreover, many proposed systems for transmutation are strongly heterogeneous, which troubles some of the currently used methods for calculating β_{eff}. A Monte Carlo based method would be ideally suited for such a purpose.

Spriggs et al. [3] recently described an approximation that allows the computation of β_{eff} using two eigenvalues. In fact, the approximation was introduced earlier [4], but the theoretical framework was provided in Ref. [3]. This is potentially a considerable improvement, because the adjoint function is not needed anymore, paving the way for continuous energy Monte Carlo codes. However, although the method was shown to work well for a bare, homogeneous uranium sphere (Godiva), it remains unclear how good the approximation is for LWR systems, or for any new reactor type that is contemplated. In fact,

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Spriggs et al. mentioned that for one, heterogeneous, uranium system the approximation did not work well.

At this point, we want to take a step back and think fundamentally about what it is that we want to calculate: the effect of delayed neutrons on reactor transient behavior. As reactors are generally operated on the basis of the power that is generated, the effect that neutrons have on reactor behavior is through their ability to generate fissions (and hence power). Therefore the quantity we are after is the delayed neutron fraction insofar as it is effective in leading to fission.

In this paper, we propose an approach to β_{eff} that is entirely in microscopic terms, and, consequently, easy to implement in a Monte Carlo scheme. This approach involves no approximations. We have implemented our method into MCNP [5], and show that in a standard MCNP eigenvalue calculation, one can get a β_{eff} value by including only some minor bookkeeping in the code. Given the fact that one calculates k anyway, one gets a value for β_{eff} at no extra (CPU) cost. We have computed β_{eff} for a wide variety of benchmark systems, proving that the method is valid for all systems.

This paper is organized as follows. In Section 2 we outline our approach to the effective delayed neutron fraction, and we discuss other commonly used approaches. In Section 3 we report numerical results for many experimental benchmark systems. Section also contains a brief discussion of these results and some conclusions.

2. Theory of Effectiveness

As a first step toward assessing the importance of delayed neutrons in a reactor, one needs to determine how many delayed neutrons are generated. We will restrict ourselves in this paper to a reactor near criticality, and without external source. In general, one writes for the total neutron production rate by fission:

$$P = \int \nu(E)\Sigma_f(\vec{r},E,\Omega)\varphi(\vec{r},E,\Omega)dEd\Omega d\vec{r}\,, \qquad (1)$$

where E, Ω, and $\vec{r}$ are the energy, solid angle, and position of the neutrons, φ is the neutron flux, Σ_f the macroscopic fission cross section of the material at position $\vec{r}$, and ν the average neutron multiplicity per fission. For the production P_d of *delayed* neutrons, one replaces the factor $\nu(E)$ by $\nu_d(E)$, the average delayed neutron multiplicity per fission. For the sake of simplicity, we will not distinguish here between the several delayed neutron time groups, which each have their own energy spectrum. The ratio P_d/P then is the 'fundamental' delayed neutron fraction β_0.

So far, this is fairly straightforward. The problems start when trying to assess how effective this fraction is in terms of reactor kinetics. As stated in the introduction, the effect that neutrons have on reactor behavior is through their ability to generate power, i.e. to induce the 'next' fission. It follows that we should compute the number of fissions that are induced by delayed neutrons, as well as by all neutrons.

2.1 Transport Theory

In transport theory one calculates the effectiveness in generating fission by multiplying by the energy spectrum of the generated neutrons, $\chi(E')$, and by the adjoint function $\psi(\vec{r},E',\Omega')$, (often referred to as 'adjoint flux'). The adjoint function is defined as the fundamental mode eigenfunction of the equation adjoint to the time independent transport equation. Here $\vec{r}$, E', and Ω' are the position, energy, and solid angle of neutrons generated by the fissions that were induced by the incident neutrons characterized by $\vec{r}$, E, Ω. The position $\vec{r}$ is obviously the same for both. The factor $\chi(E')$ is needed because the energy the neutrons start with has an

impact on their effectiveness in inducing fission. The adjoint function $\psi(\vec{r},E',\Omega')$ is used because it is an importance function, which represents the significance of a neutron with properties $\vec{r}$, E', Ω' for producing fission. In the words of Keepin, ψ *is proportional to the asymptotic power level resulting from the introduction of a neutron (…) in a critical system at zero power* [1] (p. 163).

This leads to the so-called spectrum and adjoint weighted neutron production

$$P_{\text{eff}} = \int \psi(\vec{r},E',\Omega')\chi(E')\nu(E)\Sigma_f(\vec{r},E,\Omega)\varphi(\vec{r},E,\Omega)dEd\Omega dE'd\Omega' d\vec{r} \qquad (2)$$

One can calculate the same quantity for delayed neutrons only ($P_{d,\text{eff}}$), by replacing $\chi(E')$ by $\chi_d(E')$ and $\nu(E)$ by $\nu_d(E)$. When one takes the ratio $P_{d,\text{eff}}/P_{\text{eff}}$, one arrives at the Keepin definition of β_{eff}.

It is instructive to interpret P as the neutron source (the number of neutrons produced per unit of time), and P_{eff} as the number of fissions produced by this source per unit of time.

2.2 New Method

Within the context of a Monte Carlo scheme, the transport theory approach is more complicated than need be. In such a scheme, the neutrons are simulated by generating them with a probability that is proportional to P. Assessing the effectiveness of these neutrons in generating the 'next' fission, is then intuitive and straightforward in a Monte Carlo scheme. All neutrons are labeled either 'prompt' or 'delayed' at birth, and subsequently they are tracked through the reactor until they are 'removed' from it by either an interaction such as fission or capture, or by escape to the surroundings. In those cases where the removal is due to a fission, one needs to check whether the incident neutron is a delayed one or not. One can then calculate the average number of fissions generated by delayed neutrons, divided by the average number of fissions generated by all neutrons. This is β_{eff}.

Notice that a calculation of this fraction can be done in a Monte Carlo program by means of some minor bookkeeping in the code, which will give a result for β_{eff} in the same run with which one calculates k. The code will not even be slowed down significantly. We have checked that for a Godiva run the extra amount of CPU time involved was less than 0.5% of the total. For thermal systems, this fraction is even smaller.

In Section 3 we will present calculations based on this method for many different neutron multiplication systems. We will compare it to two often used approximate methods of calculating β_{eff}. In the remainder of this section we will outline these two methods.

2.3 'Prompt' Method

Denoting the integral in Eq. (2) as $\langle\chi\nu\rangle$, one can rewrite the expression for β_{eff} as follows, making use of the fact that the integrals are linear.

$$\beta_{\text{eff}} = \frac{\langle\chi_d\nu_d\rangle}{\langle\chi\nu\rangle} = 1-\frac{\langle\chi\nu-\chi_d\nu_d\rangle}{\langle\chi\nu\rangle} = 1-\frac{\langle\chi\nu_p-(\chi_d-\chi)\nu_d\rangle}{\langle\chi\nu\rangle} \approx 1-\frac{\langle\chi_p\nu_p\rangle}{\langle\chi\nu\rangle}, \qquad (3)$$

where we have used $\nu_p=\nu-\nu_d$. The approximation in the last step is based on the following arguments. The term $(\chi_d-\chi)\nu_d$ is two orders of magnitude smaller than the one with $\chi\nu_p$, because ν_d is two orders of magnitude smaller than ν_p. For the same reason, the shape of $\chi(E')$ is almost equal to that of $\chi_p(E')$.

At this point a crucial step is taken. Often it is simply stated that

$$\frac{\langle\chi_p\nu_p\rangle}{\langle\chi\nu\rangle} = \frac{k_p}{k} \qquad \Rightarrow \qquad \beta_{\text{eff}} = 1-\frac{k_p}{k}. \qquad (4)$$

In fact, this is an approximation. It is true that the *k*-eigenvalue is the ratio of production *P* and loss *L*, and that this also holds for the ratio of $P_{d,\mathrm{eff}}$ and $L_{d,\mathrm{eff}}$. But the difficulty lies in the definition of k_p. Since this parameter is supposed to be calculated by means of a transport theory code, it should be defined as the eigenvalue pertaining to a reactor with $\chi=\chi_p$, and $\nu=\nu_p$. The difference is that in such a calculation, the shapes of φ and ψ will not be the same as for the original system with χ and ν, for which the eigenvalue is *k*. This subtlety is generally ignored in papers dealing with the 'prompt' method of calculating β_{eff} based on Eq. (4), see e.g. Ref. [6].

2.4 Spriggs Method

Alternatively, Spriggs et al. [3] rewrite β_{eff} as

$$\beta_{\mathrm{eff}} = \frac{\langle \chi_d \nu_d \rangle}{\langle \chi \nu \rangle} = \frac{\langle \chi_d \nu_d \rangle}{\langle \chi_d \nu \rangle} \cdot \frac{\langle \chi_d \nu \rangle}{\langle \chi \nu \rangle} = \beta_0' \frac{\langle \chi_d \nu \rangle}{\langle \chi \nu \rangle}, \qquad (5)$$

where we have introduced, after Spriggs et al., yet another delayed neutron fraction β_0'. For the present purposes we restrict ourselves to the approximation that $\beta_0' \approx \beta_0$, because we still need to perform adjoint weighting to calculate β_0'. By approximating $\beta_0' \approx \beta_0$ we can simplify the calculation to something that can easily be implemented in a Monte Carlo code. As remarked by Spriggs et al., the approximation $\beta_0' \approx \beta_0$ works well for homogeneous cases.

Also for this method we subsequently introduce a ratio of *k*-values.

$$\frac{\langle \chi_d \nu \rangle}{\langle \chi \nu \rangle} = \frac{k_d}{k} \qquad \Rightarrow \qquad \beta_{\mathrm{eff}} = \beta_0' \frac{k_d}{k}, \qquad (6)$$

As in the case of the 'prompt' method, this is an approximation. Here the problem lies in the definition of k_d. Since this parameter is supposed to be calculated by means of a transport theory code, it should be defined as the eigenvalue pertaining to a reactor with $\chi=\chi_d$ and $\nu=\nu$. Again, the shapes of φ and ψ will not be the same as for the original system with χ and ν, for which the eigenvalue is *k*. This subtlety is explained by Spriggs et al. for their method of calculating β_{eff}.

2.5 Comparison of Monte Carlo Methods

Given the fact that Eqs. (4) and (6) are approximations, one wonders how good these approximations are in a practical situation. In the next section we will investigate the accuracy of these approximations by presenting results for experiments done in the past, but based on the above derivation one can expect that the 'prompt' method is the better approximation. This is because in the derivation, the shape of the flux and of the adjoint function for the k_p eigenvalue calculation are approximated by the respective shapes for the *k* eigenvalue calculation. As the prompt neutrons constitute roughly 99% of the neutron population, this is as good an approximation as one can get. On the other hand, for the Spriggs method, one approximates φ_d and ψ_d by φ and ψ. The delayed neutrons constitute only 1% of the total neutron populations, so in this case the approximation cannot be expected to perform equally well. Still, in section 3 we will show that this method yields good results for most systems considered. Only the results for very heterogeneous systems are unfavorable.

There is also the computational aspect of Eqs. (4) and (6). In the first one, the ratio k_p/k, which is very close to unity, is subtracted from unity, to obtain a value typically below 0.01. This implies that, when one uses a Monte Carlo code to calculate k_p and *k*, one needs very good statistics. Otherwise the statistical uncertainty in β_{eff} will be larger than the result for β_{eff}

itself. The Spriggs method does not have this problem, which gives it a clear advantage over the prompt method, computationally.

In a practical situation, the 'prompt' method is the only method that can be used with, for instance, a standard MCNP executable. The Spriggs method, and the one proposed in this paper, both need a bit of extra programming.

Finally, the 'prompt' method and the Spriggs method both need two eigenvalue calculations, whereas the new method proposed here requires only one.

3. Results and Discussion

We have searched in the literature for measurements of the effective delayed neutron fraction, the result of which is listed below. We will use these experiments as benchmarks for our calculation of β_{eff}. For some systems we have found experimental values for the parameter α, which is linked to β_{eff} through $\alpha=[k(1-\beta_{eff})-1]/l$, where l is the prompt neutron life time. All systems described below are at delayed criticality, so that the parameter we can compare with is the value $\alpha_{dc}=\alpha(k=1)=-\beta_{eff}/l$. For a description of the systems used, including literature references for the experimental values for β_{eff} and α_{dc}, we refer to Ref. [7].

We have calculated β_{eff} for all experiments described in the previous section, based on three different nuclear data evaluations, viz. JEFF-3.0, ENDF-B/VI.8, and JENDL-3.3. The reason why we have listed the results for all three data evaluations in Tables 1–3 is that the differences between these data evaluations are sometimes larger than the differences between the three methods of calculating β_{eff}. We have calculated the results for the prompt method only for a selection of cases, because the run times for the other systems are prohibitively long if we are to get statistically useful results.

The results are presented in Tables 1–3 and in Figure 1. The results are roughly ordered with respect to the average energy at which fission takes place. We conclude the following.

- For most cases, in particular for LWR type applications, all methods yield good results.
- The results for the new method agree with the experimental data, even for the most heterogeneous systems.
- The prompt method also yields good results for all systems. However, this method requires at least 40× more CPU time.
- The Spriggs method performs well in most cases, but for the heterogeneous systems there are clear deviations from the experimental values. The reason for the discrepancy most probably is the additional approximation of β_0' by β_0, so we cannot conclude that the Spriggs method is inadequate for these systems, based on these results alone. On the other hand, Spriggs et al. [3] mention that for Topsy (a high enriched uranium sphere with a natural uranium reflector) the results of their method were 'not very good'. Moreover, if we have to calculate β_0' instead of β_0, we need to apply adjoint weighting, which we cannot easily do in a Monte Carlo program.
- For homogeneous systems, the differences between the results based on the various nuclear data libraries are often at least as large as the differences between the three methods. This allows us to draw conclusions about the nuclear data.
- Judging by the results for TCA, Stacy and Winco, the JENDL-3.3 nuclear data library gives the best α and β_{eff} results for LWR type applications.

In summary, we have introduced a new method to calculate the effective delayed neutron fraction using Monte Carlo techniques. We have implemented this method in a version of MCNP-4C3, and we calculated the effective delayed neutron fraction for a variety of systems.

For all these systems, the new method reproduces the experimental values for β_{eff} with satisfactory accuracy. The 'prompt' method gives similarly good results, although one needs at least 40× longer run times. The method described by Spriggs et al. [3] also yields good results, except for heterogeneous systems.

Therefore we consider the new method to be the preferred one in all cases, because it involves no approximations, it reproduces all experimental values considered, it needs no extra Monte Carlo runs, and it has a low standard deviation.

Table 1 C/E results for the new method of calculating β_{eff}

Benchmark Experiment		**JEFF-3.0**	**ENDF/B-VI.8**	**JENDL-3.3**
Proteus	3.60±0.02 s^{-1}	1.061±0.020	1.050±0.020	1.025±0.020
SHE-8	6.53±0.34 s^{-1}	0.974±0.052	0.953±0.051	0.930±0.050
Stacy-029	122.7±4.1 s^{-1}	0.996±0.039	1.014±0.040	0.985±0.039
Stacy-033	116.7±3.9 s^{-1}	1.024±0.040	1.015±0.040	0.966±0.038
Stacy-046	106.2±3.7 s^{-1}	1.029±0.041	1.012±0.041	0.976±0.040
Stacy-030	126.8±2.9 s^{-1}	1.024±0.032	1.055±0.032	0.989±0.031
Stacy-125	152.8±2.6 s^{-1}	1.062±0.029	1.044±0.028	1.010±0.028
Stacy-215	109.2±1.8 s^{-1}	1.049±0.027	1.059±0.027	0.998±0.027
Winco	1109.3±0.3 s^{-1}	1.054±0.012	1.051±0.012	0.988±0.012
TCA	771±17 pcm	1.060±0.026	1.053±0.026	0.987±0.025
Masurca R2	721±11 pcm	1.019±0.018	1.035±0.019	1.018±0.018
Masurca Z2	349±6 pcm	1.026±0.023	0.983±0.022	0.994±0.022
FCA XIX-1	742±24 pcm	1.034±0.035	1.005±0.034	0.985±0.034
FCA XIX-2	364±9 pcm	1.063±0.030	1.003±0.028	1.022±0.029
FCA XIX-3	251±4 pcm	1.016±0.023	1.016±0.023	0.996±0.022
Sneak-7A	395±12 pcm	0.965±0.032	0.932±0.031	0.937±0.031
Sneak-7B	429±13 pcm	1.042±0.034	0.981±0.032	0.993±0.032
Sneak-9C2	426±19 pcm	0.927±0.043	0.911±0.042	0.897±0.042
Sneak-9C1	758±24 pcm	0.999±0.033	0.978±0.032	0.978±0.032
Zpr-Pu	222±5 pcm	1.095±0.033	1.005±0.032	0.991±0.032
Zpr-Mox	381±9 pcm	0.979±0.028	0.953±0.027	0.945±0.027
Zpr-Heu	667±15 pcm	1.061±0.027	1.010±0.026	1.030±0.027
Zpr-U9	725±17 pcm	1.043±0.027	1.037±0.027	0.999±0.026
BigTen	720±7 pcm	1.062±0.014	1.017±0.013	1.010±0.013
Godiva	659±10 pcm	1.027±0.020	1.017±0.020	1.006±0.020
Topsy	665±13 pcm	1.002±0.023	0.962±0.022	0.952±0.022
Jezebel	194±10 pcm	1.031±0.059	0.964±0.056	1.010±0.061
Popsy	276±7 pcm	1.025±0.032	1.007±0.031	1.036±0.032
Skidoo	290±10 pcm	0.979±0.038	1.079±0.043	1.076±0.042
23-Flattop	360±9 pcm	0.953±0.029	0.997±0.030	1.017±0.030

Table 2 C/E results for the Spriggs method of calculating β_{eff}

Benchmark Experiment		JEFF-3.0	ENDF/B-VI.8	JENDL-3.3
Proteus	3.60±0.02 s^{-1}	1.081±0.015	1.069±0.015	1.011±0.015
SHE-8	6.53±0.34 s^{-1}	0.969±0.051	0.968±0.051	0.926±0.049
Stacy-029	122.7±4.1 s^{-1}	1.019±0.036	1.033±0.037	0.988±0.035
Stacy-033	116.7±3.9 s^{-1}	1.033±0.037	1.040±0.037	0.968±0.035
Stacy-046	106.2±3.7 s^{-1}	1.037±0.038	1.042±0.039	0.990±0.037
Stacy-030	126.8±2.9 s^{-1}	1.035±0.027	1.061±0.028	0.997±0.026
Stacy-125	152.8±2.6 s^{-1}	1.066±0.023	1.046±0.022	1.011±0.022
Stacy-215	109.2±1.8 s^{-1}	1.051±0.022	1.036±0.022	1.006±0.021
Winco	1109.3±0.3 s^{-1}	1.058±0.007	1.056±0.007	0.996±0.007
TCA	771±17 pcm	1.049±0.024	1.051±0.024	1.016±0.023
Masurca R2	721±11 pcm	1.067±0.018	1.062±0.018	1.042±0.017
Masurca Z2	349±6 pcm	1.166±0.022	1.103±0.021	1.112±0.021
FCA XIX-1	742±24 pcm	1.005±0.033	0.978±0.032	0.960±0.032
FCA XIX-2	364±9 pcm	1.294±0.034	1.253±0.033	1.245±0.033
FCA XIX-3	251±4 pcm	1.239±0.023	1.203±0.023	1.195±0.022
Zpr-Pu	222±5 pcm	1.077±0.028	1.032±0.027	1.009±0.026
Zpr-Mox	381±9 pcm	0.937±0.024	0.929±0.024	0.916±0.024
Zpr-Heu	667±15 pcm	1.043±0.025	1.057±0.025	1.015±0.024
Zpr-U9	725±17 pcm	1.041±0.025	1.006±0.025	0.999±0.024
Sneak-7A	395±12 pcm	1.218±0.038	1.165±0.036	1.170±0.037
Sneak-7B	429±13 pcm	1.124±0.035	1.068±0.033	1.084±0.034
Sneak-9C2	426±19 pcm	1.146±0.052	1.106±0.050	1.099±0.050
Sneak-9C1	758±24 pcm	1.073±0.035	1.044±0.034	1.050±0.034
BigTen	720±7 pcm	1.074±0.012	1.026±0.011	1.028±0.011
Godiva	659±10 pcm	0.983±0.017	0.989±0.017	0.945±0.016
Topsy	665±13 pcm	1.248±0.027	1.223±0.026	1.197±0.025
Jezebel	194±10 pcm	0.964±0.052	0.928±0.050	0.938±0.051
Popsy	276±7 pcm	1.913±0.052	1.880±0.051	1.855±0.050
Skidoo	290±10 pcm	0.921±0.035	1.010±0.037	1.007±0.037
23-Flattop	360±9 pcm	1.661±0.044	1.733±0.046	1.722±0.045

Table 3 C/E results for the 'prompt' method of calculating β_{eff}

Benchmark Experiment		JEFF-3.0	ENDF/B-VI.8	JENDL-3.3
Stacy-029	122.7±4.1 s^{-1}	1.068±0.043	1.043±0.043	0.970±0.041
Stacy-033	116.7±3.9 s^{-1}	1.020±0.043	1.003±0.042	1.011±0.048
Stacy-046	106.2±3.7 s^{-1}	0.998±0.045	1.073±0.047	0.942±0.050
Stacy-030	126.8±2.9 s^{-1}	1.033±0.039	1.065±0.040	1.080±0.047
Stacy-125	152.8±2.6 s^{-1}	1.106±0.038	1.080±0.038	0.936±0.042
Stacy-215	109.2±1.8 s^{-1}	1.062±0.033	1.007±0.040	0.989±0.040
Winco	1109.3±0.3 s^{-1}	1.055±0.027	1.064±0.036	0.974±0.036
TCA	771±17 pcm	1.054±0.027	1.042±0.026	1.003±0.026
BigTen	720±7 pcm	1.046±0.018	1.018±0.019	0.972±0.018
Godiva	659±10 pcm	0.991±0.020	0.970±0.020	0.998±0.020
Topsy	665±13 pcm	1.041±0.024	1.053±0.025	1.041±0.024
Jezebel	194±10 pcm	0.995±0.069	0.928±0.067	0.907±0.066
Popsy	276±7 pcm	1.047±0.045	1.000±0.044	1.036±0.045
Skidoo	290±10 pcm	0.997±0.044	1.062±0.048	0.990±0.046
23-Flattop	360±9 pcm	1.056±0.038	1.042±0.038	1.097±0.039

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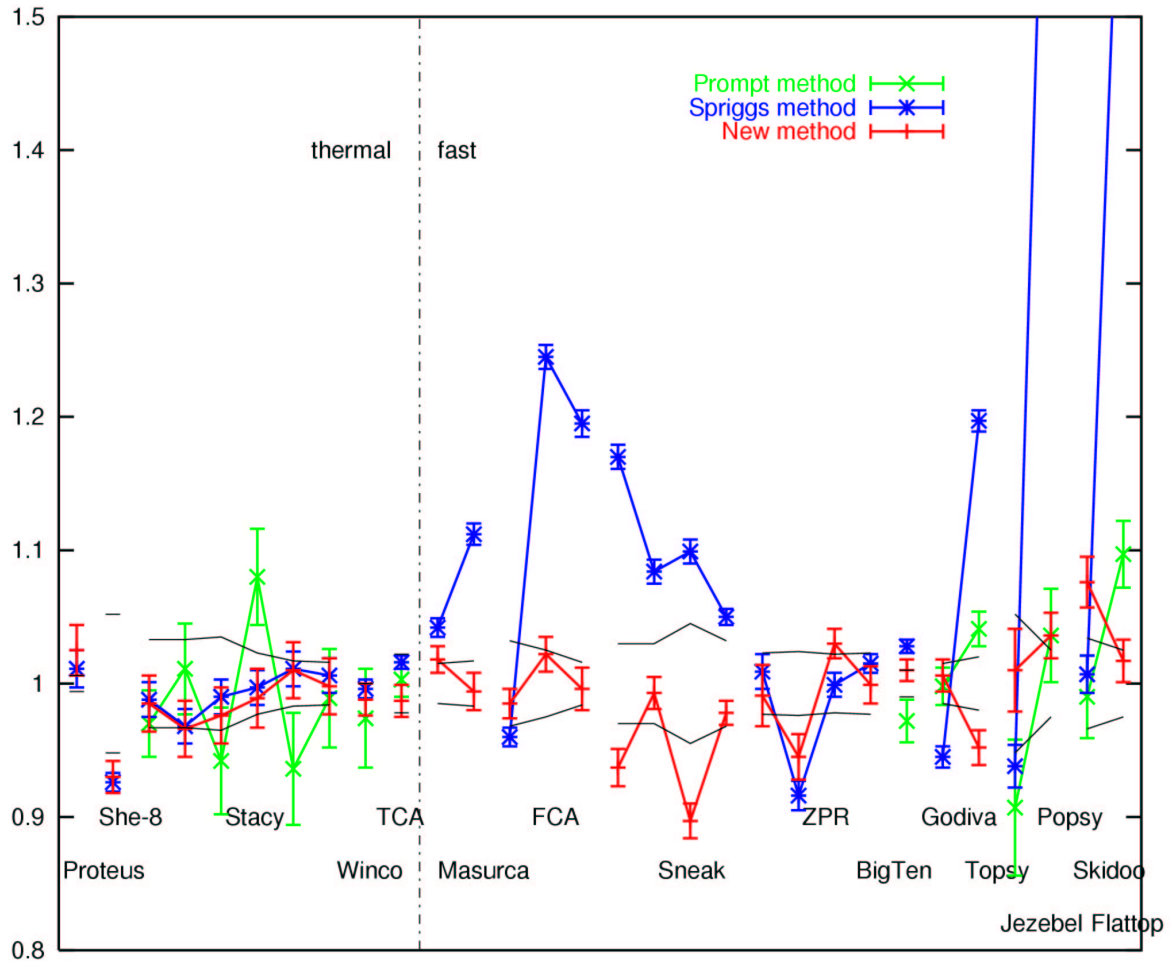

Figuur 1 C/E results for β_{eff} for the various methods, based on JENDL-3.3