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Efficient Use of Monte Carlo: Uncertainty Propagation

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Abstract—*A new and faster Total Monte Carlo (TMC) method for the propagation of nuclear data uncertainties in Monte Carlo nuclear simulations is presented (the fast TMC method). It addresses the main drawback of the original TMC method, namely, the necessary large time multiplication factor compared to a single calculation. With this new method, Monte Carlo simulations can now be accompanied with an uncertainty propagation (other than statistical), with small additional calculation time. The fast TMC method is presented and compared with the TMC and fast GRS methods for criticality and shielding benchmarks and burnup calculations. Finally, to demonstrate the efficiency of the method, uncertainties due to uncertainties in $^{235,238}U$, ^{239}Pu, and thermal scattering nuclear data, for the local deposited power in 12.7 million cells, are calculated for a full-size reactor core.*

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I. INTRODUCTION

As accredited scientists, one of our obligations is to report reliable uncertainties. They can be seen as a quality flag on measurements, as well as on calculations, and by quoting such numbers (small or large), methodical justifications are expected. Additionally, other actors in today's society will associate these uncertainties with risks, asking detailed explanations in order to manage costs: If trusted, an understanding of them helps in making the correct decisions during different phases of simulation. Therefore, we, scientists, need to be specially careful when dealing with the estimation of uncertainties.

While measurement results are usually reported together with an uncertainty estimate, results of calculations are in fact seldom given with an estimation of uncertainties, questioning the relevance of the above arguments. The origin of such a lack is not in the awareness of the importance of uncertainties as such, but more in the difficulties in reporting reliable uncertainties. Truly, in the ideal case of obtaining pertinent uncertainties and nominal values from the same calculations, scientists would be eager to report both. It is therefore justified to develop practical and ready-to-use methodologies for uncertainty calculations, which can be applied without unnecessary burden. At best, the inclusion of the methodology in simulation codes will integrate uncertainties at the level of standard calculations.

In the specific case of computer simulations, one important source of uncertainty lies in the use of predictive models. Models imply uncertainties (a) from their inherent approximations and (b) from their input parameters. The first origin of uncertainties can be investigated using different theoretical models (if possible). The impact of input parameters on a simulated quantity q, quantified by the uncertainty on q called δq (often presented as $q \pm \delta q$), can be assessed in various ways, and this paper will focus on practical solutions based on Monte Carlo sampling.

In reactor calculations, random sampling has traditionally been used with the GRS code package SUSA (Ref. 1) to assess the influence of uncertainties in technological and thermohydraulic parameters. Stochastic sampling-based uncertainty quantification methods have also successfully been applied outside the nuclear field, e.g., in geochemical simulations,[2] medical applications,[3] and soil acidification.[4] These methods are based on repeating n times the same simulation, each time varying external parameters (such as cross sections) according to given distributions, leading to different calculated quantities $q_1, \ldots, q_n$. δq can then be estimated by the standard deviation of the distribution of q's.

A different attempt using Monte Carlo simulations to provide exhaustive uncertainties in nuclear applications based on the parameters of nuclear reaction models is presented in Ref. 5. This approach, called Total Monte Carlo (or TMC), also relies on the ability to repeat the same calculation enough times—but each time sampling all possible model parameters of a nuclear reaction code (level densities, transmission coefficients, etc.)—and then supplying random external parameters (such as cross sections), thereafter to be used in a reactor simulation code, leading to different calculated quantities $q_1, \ldots, q_n$. In the specific case of nuclear simulations, the novelty of TMC was not to sample (nuclear) input parameters but to do so systematically (for all possible nuclear data) and based on nuclear reaction theories. The TALYS nuclear reaction code[6] was then used to produce "random nuclear data," based on random model parameters.

The main drawback of the stochastic methods (including TMC) is the long time required compared to a single calculation, making them unsuitable for some applications. Recently, a first successful attempt to provide nuclear data uncertainties in a short calculation time was presented in Ref. 7: the fast GRS method, as presented later in this paper. Conscious of the limitation of the TMC method, we are proposing faster solutions, producing uncertainties with approximately no additional calculation time compared to a unique calculation with nominal parameters. If successful, these solutions will provide uncertainties in simulations in a rational manner, allowing for possible automation and integration in simulation codes.

After describing the new methods, examples of three types of Monte Carlo simulation for particle transport are presented, varying different types of nuclear data (such as cross sections for actinides or structural materials): shielding calculations (starting from a given neutron source), criticality calculations (with the so-called k-code for fission chains), and burnup estimation. Finally, the applicability of the method is demonstrated with a computationally intensive case (a full-size reactor core), leading to uncertainties due to the ^{235,238}U and ^{239}Pu transport nuclear data and H in H_2O thermal scattering.

With the possibilities of these new methods, there will be no more pretext for not providing Monte Carlo simulation results without uncertainties due to input parameters (nuclear data or engineering quantities).

II. TMC: A SIMPLE BUT INEFFICIENT SOLUTION

In 2008 a Monte Carlo method to propagate nuclear data uncertainties to parameters of large-scale nuclear systems was presented in Ref. 5, later acquiring the name of "Total Monte Carlo"[a] (or TMC). Other random sampling methods to evaluate reactor calculation uncertainties due to nuclear data uncertainties were later developed by different groups in Refs. 8 through 11; in these references, the sampling is based on information from covariance data contained in the evaluated nuclear

[a]This name was given by M. Herman, National Nuclear Data Center, Brookhaven National Laboratory.

data files or on covariance matrices already processed into a multigroup structure, as contained in the SCALE code package.[12]

Previous cited references[5–11] all rightly point out the advantages of such methods (simplicity, inclusion of nonlinear effects, etc.) together with the main drawback: the large time multiplication factor. In the following, n is the total number of times a given simulation is repeated, and i denotes the i'th simulation. In practice, stochastic sampling methods including TMC are based on repeating similar simulations n times, each time using a random set of input data A_i. For example, for isotope enrichment, A_i is a vector of dimension 1, containing a random value for the enrichment, within some defined boundaries and distributed according to a specific probability density function. For cross sections for a given isotope, A_i is a matrix containing random cross sections (such as fission, elastic, inelastic, etc.). A_i can include nuclear data for one or many isotopes on a simple or a dense energy grid. In the TMC method, A_i is produced by a nuclear reaction code, from random parameters for the level density model, optical model, compound nucleus model, etc. (any inputs of nuclear reaction models). If A_i is used in a simulation i (with a deterministic or Monte Carlo code), a specific value of the quantity q is obtained, called q_i. By repeating the same calculation n times with different A_i, n values for q_i are obtained. The effect of $\vec{A}=[A_1 \ldots A_n]$ can be measured by the standard deviation $\sigma_A(q)$ (square root of the variance) it induces on the calculated quantity $[q_1 \ldots q_n]$ (reaction rate, fluence, heat, etc.):

Run Number	Random Input		Simulated Quantity	With a Monte Carlo Simulation Code
$i=1$	A_1	$\Rightarrow$	q_1	$\pm\sigma_{\text{statistics},1}$
$i=2$	A_2	$\Rightarrow$	q_2	$\pm\sigma_{\text{statistics},2}$
·	·		·	·
·	·		·	·
·	·		·	·
$i=n$	A_n	$\Rightarrow$	q_n	$\pm\sigma_{\text{statistics},n}$
$(1 \ldots n)$	$\vec{A}=[A_1 \ldots A_n]$	$\Rightarrow$	$[q_1 \ldots q_n]$	

If a deterministic simulation code is used, only the $[q_1 \ldots q_n]$ values are obtained, whereas with a Monte Carlo simulation, each q_i comes with its own uncertainty $\sigma_{\text{statistics},i}$. A few applications of this method can be found in the literature (see, for instance, Refs. 13 through 17). This original TMC method has the merit of being an alternative way of propagating uncertainties for a nuclear system, compared to the well-established and accepted perturbation methods. It also allows the propagation of uncertainties for quantities where the perturbation methods were not applied for different practical reasons (no covariances available or no realistic methods).

The originality of the TMC approach is that $\vec{A}$ comes from parameters used in a nuclear reaction code (such as TALYS), randomly varied within some boundaries and according to given probability density functions. The probability distribution of the nuclear reaction code outputs arose from a *physical* theoretical background and not directly from arbitrary assumptions. In general, $\vec{A}$ can also be engineering quantities (such as dimensions, densities, etc.), and different types of parameters can be varied at once. Virtually any quantity in the simulation code could be varied.

In the original description, n should be large enough to obtain a converged standard deviation (the variations of the standard deviation of the distribution of q_i, $\sigma_A(q)$ as a function of n should become smaller than an arbitrary value, such as 2%). In practice, it was found that n was larger than 500 (but often less than 1000). Regarding the simulation codes, the TMC method can indifferently be applied using Monte Carlo or deterministic codes [transport, depletion, or transient codes such as CASMO (Ref. 18) or MCNP (Ref. 19)]. There is no fundamental difference in the application of TMC to either of these, apart from the introduction of the statistical uncertainty σ_{stat} in the Monte Carlo code. For Monte Carlo codes, the original TMC method can be summarized as follows:

Original TMC

Given that a unique Monte Carlo simulation $C(m)$ provides a calculated quantity q with a statistical uncertainty σ_{stat} within T s and m histories (σ_{stat} satisfactorily small),

1. Repeating n times $C(m)$ with each time a random realization of the input data A_i ($i=1 \ldots n$) provides a distribution of q_i in $n \times T$ s.
2. The standard deviation σ_{observed} of the q_i distribution is directly related to the variations of $\vec{A}=[A_1 \ldots A_n]$.

For each new calculation, the same seed s for the random number generator of the m source particles was used. In principle, the spread (or standard deviation) σ_{observed} in the calculated quantities q_i reflects the variations in $\vec{A}$, and a standard approach can provide different moments of the distribution:

$$\begin{cases} \bar{q} & = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} q_i & (1) \\ \sigma^2_{\text{observed}} & = \dfrac{1}{n-1}\displaystyle\sum_{i=1}^{n} (q_i-\bar{q})^2 . & (2) \end{cases}$$

If one is using a deterministic description of a system, the observed σ_{observed} is only due to the variations of the input data A_i:

For a deterministic simulation code:

$$\sigma_{\text{observed}} = \sigma_A(q) \; . \tag{3}$$

In this case, the impact of $\vec{A}$ on the calculated quantity is simply given by σ_{observed}. In the specific case of a Monte Carlo simulation code, an additional difficulty emerges due to the statistical uncertainties. Each simulated quantity q_i has a standard deviation $\sigma_{\text{statistics},i}$ due to the considered random samples. Still, in this case, the observed standard deviation can be related to $\sigma_A^2(q)$ by the following simple equations:

For a Monte Carlo simulation code:

$$\begin{cases} \sigma^2_{\text{observed}} & \approx \overline{\sigma^2}_{\text{statistics}} + \sigma_A^2(q) \qquad (4) \\ \overline{\sigma^2}_{\text{statistics}} & = \dfrac{1}{n}\sum_{i=1}^{n} \sigma^2_{\text{statistics},i} \; . \qquad (5) \end{cases}$$

Equation (4) assumes that the statistical uncertainties do not depend on A_i (no correlation between $\sigma_{\text{statistics},i}$ and A_i). This assumption is not demonstrated here, but it is believed that the correlation term is very small. If the $\sigma^2_{\text{statistics},i}$ are assumed to be unbiased estimates of the statistical variance in each simulation, $\overline{\sigma^2}_{\text{statistics}}$ used in Eq. (5) is an efficient unbiased estimate of the statistical variance of the final distribution.

Monte Carlo simulation codes usually provide an estimation of $\sigma_{\text{statistics},i}$, for various calculated quantities, such as the multiplication factor or reaction rates, which can then be used to extract $\sigma_A^2(q)$ from Eq. (4) (see Ref. 5 for the original description).

In Refs. 5, 7, and 11, each individual simulation i was performed with a large number of histories, necessary to obtain small statistical uncertainties $\sigma_{\text{statistics},i}$ (with the following rule of thumb: $\overline{\sigma}_{\text{statistics}} \simeq 0.05 \times \sigma_{\text{observed}}$) and therefore leading to a precise value of $\sigma_A(q)$.

It can nevertheless be recognized that the stochastic sampling methods including TMC are an inefficient way of propagating uncertainties with Monte Carlo simulation codes, due to the minimization of the statistical uncertainty appearing in Eq. (4). The long calculation time is often considered as the main drawback of TMC and TMC-like methods, compared to faster perturbation/sensitivity methods, which are in general more appropriate for a large number of applications, even if they only provide an approximate answer. In the case of extremely long calculation time for a single simulation (such as weeks on hundreds of processors), it is not realistic to apply the TMC method, and other solutions should be used as presented in Sec. III.

It is pointed out in Ref. 7 that for a sampling-based sensitivity and uncertainty analysis with Monte Carlo transport codes, it is not necessary to perform each Monte Carlo run with the same high number of neutron histories as in the reference calculation to obtain sufficiently accurate uncertainties and sensitivities. The corresponding method, henceforth called the fast GRS method, will be described in Sec. IV.

III. FAST TMC: SIMPLE AND FASTER SOLUTIONS

It should be mentioned that the following descriptions and tests can be applied indifferently to the original TMC (with the use of a nuclear reaction code to generate random data) or to any stochastic sampling method (without the use of a nuclear reaction code, but with existing covariance matrices to generate random data), as long as a Monte Carlo simulation code is used.

III.A. Using Shorter Monte Carlo Runs

It can be argued that using the original TMC method with a Monte Carlo simulation code applies a Monte Carlo method twice, internally and externally. The first time, or the internal Monte Carlo, uses the random characteristics of simulated particles (such as neutrons or gammas), and the second time uses external random input parameters ($\vec{A} = [A_1 \ldots A_n]$). As presented in Ref. 5, the original TMC method is highly time-consuming because of the necessity to obtain a small $\sigma_{\text{statistics},i}$ value for each of the n random runs used in Eq. (4).

The value $\overline{\sigma}_{\text{statistics}}$ is derived from relatively small $\sigma_{\text{statistics},i}$ values from Eq. (5). If $\overline{\sigma}_{\text{statistics}}$ is too large compared to $\sigma_A(q)$, $\sigma_A(q)$ will be known with a poor precision.

To bypass this difficulty, a new (and faster) solution called fast TMC is presented in the following, with the preceding two observations:

1. Repeating the same $C(m)$ calculations n times, each time with different $A_{i=1\ldots n}$ provides n different values in $n \times T$ s (original TMC).

2. Alternatively, repeating the same $C(\frac{m}{n})$ calculations n times with $A_{i=1\ldots n}$ provides n values in $\approx T$ s.

Therefore,

> **Fast TMC**
>
> Given that a unique calculation $C(m)$ provides σ_{stat} within T s and m histories,
> 1. Repeating n times $C(\frac{m}{n})$ each time with different $A_{i=1\ldots n}$ and different seed s_i provides σ_{observed} in $\approx T$ s.
> 2. Equations (4) and (5) still hold, with a calculation time of $1 \times T$ instead of $n \times T$.

Uncertainties can now be provided for a Monte Carlo simulation within the same calculation time as a single run.

In this description, the fast TMC and TMC methods differ by (a) the number of histories for each run and (b) the use of different seeds in each run.

Examples of fast TMC calculations are presented in Figs. 1 and 2 for the curves "fast TMC," as a function of particle history per individual run. For the original TMC (indicated with a vertical arrow in Figs. 1 and 2), the same seed for the random number generator was used and each of the n repeated simulations had a small statistical uncertainty compared to the observed spread ($\overline{\sigma}_{\text{statistics}} \simeq 0.05 \times \sigma_{\text{observed}}$; see the top x-axis in Fig. 1). Each point in Figs. 1 and 2 represents $n = 700$ calculations, varying the neutron history per run. The gray bands in Figs. 1 and 2 represent the results obtained with the original TMC method $\pm 15\%$.

Again, these simple examples test the validity of Eq. (4) for different neutron histories. They are well representative of the results obtained with the fast TMC method. As seen in Figs. 1 and 2 (and tested by the authors on many other systems), the fast TMC method performs relatively well (within 15% of the correct answer) as long as $\overline{\sigma}_{\text{statistics}} \lesssim 0.50 \times \sigma_{\text{observed}}$. As is often the case in statistical methods, this limit of 0.5 can be changed from one case to another and represents more an indication rather than a firm limit. This represents an important improvement compared to the 0.05-or-less ratio of the original TMC method.

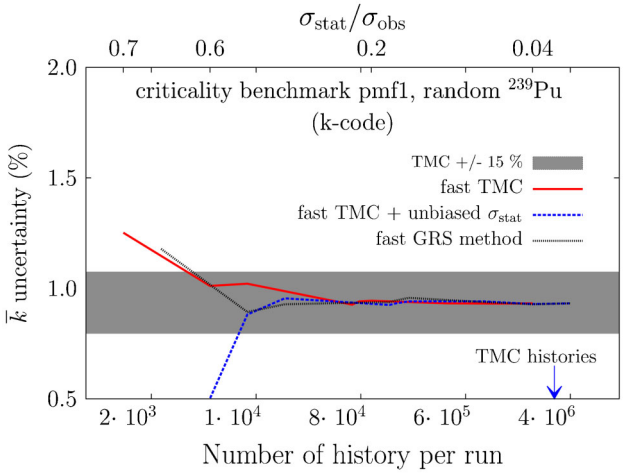


Fig. 1. Different fast TMC versions applied to the pmf1 criticality benchmark,[20] changing ^{239}Pu nuclear data. The calculated quantity is the effective multiplication factor $\bar{k}$. The dimension of $\vec{A}$ is >5000. In each case, the number of histories was varied. The top x-axis indicates the ratios of the statistical uncertainty over the observed uncertainty (a quantity that can be checked while running TMC). The original TMC uses a large number of histories, as presented by the arrow. The curves labeled "fast TMC + unbiased σ_{stat}" and "fast GRS method" are presented in Secs. III.C and IV.

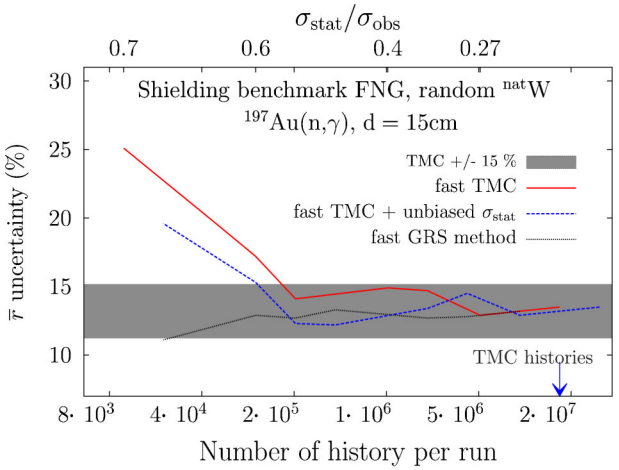


Fig. 2. Different TMC versions applied to the ^{nat}W FNG shielding benchmark with the ^{197}Au(n,γ) reaction rate $\bar{r}$, changing 700 ^{nat}W data libraries. The dimension of $\vec{A}$ is >1000. In each case, the number of histories was varied. The original TMC uses a large number of histories, as presented by the arrow.

III.B. Using Fewer Random Variations of Inputs

A second gain can then be realized by taking just enough variations of the input parameter A_i. As there is a relatively small difference (or bias) with the fast TMC method compared to TMC, a lower limit in the number of random A_i may be achievable, without impacting the precision of the result. This is illustrated in Fig. 3 for four criticality benchmarks, where the convergence of the final uncertainty is plotted as a function of the number of random realizations n. Four benchmarks are considered, varying for each of them different types of nuclear data: ^{56}Fe for hmi1, ^{239}Pu for pmf1, ^{238}U for imf1-3i, and ^{241}Pu for pmf1. The total number of histories is fixed for all the benchmarks at $m = 10^4$. It is then possible to study the rate of convergence for systems where the impact of nuclear data is high to systems where the impact is low. Different ratios $\overline{\sigma}_{\text{statistics}}/\sigma_{\text{observed}}$ are obtained from Fig. 3 from low values (high impact for nuclear data compared to the statistical uncertainty) to high values (low impact for nuclear data). These four examples are representative of the different cases studied. It can be seen that when $\overline{\sigma}_{\text{statistics}}/\sigma_{\text{observed}} \lesssim 0.50$ or 0.60, an acceptable value of $\sigma_A(q)$ (within 15% of the value given by the original TMC method) is obtained around 300 random A_i. In favorable cases, 200 random A_i are enough. This number is naturally dependent on the considered system, but after testing many cases, we have noticed that for the TMC constant, $n_{\text{TMC}} = 300$ can be used. It is interesting to realize that as the ratio m/n is fixed by σ_{stat} (see the "Fast TMC" box in Sec. III.A), an increased number of A_i (higher n) will generally not lead to a more precise answer, contrary to an increase in the number of

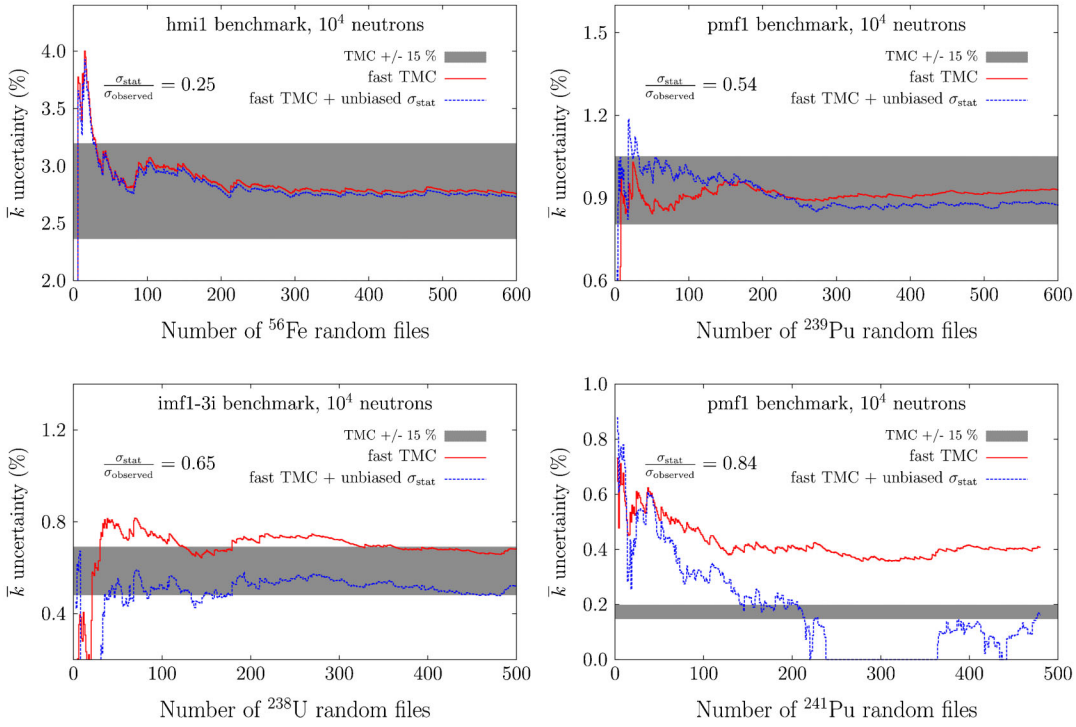


Fig. 3. Examples of convergence of the k_{eff} uncertainties for different criticality benchmarks as a function of the number of random input files, with different values of $\frac{\sigma_{stat}}{\sigma_{observed}}$. The band represents the uncertainties from the original TMC method $\pm 15\%$. For the cases of $\frac{\sigma_{stat}}{\sigma_{observed}} \gtrsim 0.5$, the fast TMC method cannot be applied.

source particles (m). In the unfavorable cases presented in Fig. 3 ($\overline{\sigma}_{statistics}/\sigma_{observed} \gtrsim 0.50$), the statistical uncertainties are too large to obtain a precise estimation of $\overline{\sigma}_{statistics}$ with Eq. (5). A simple solution to lower the $\overline{\sigma}_{statistics}/\sigma_{observed}$ ratio is to increase m. Table I summarizes the characteristics of the original TMC and fast TMC methods.

Two limitations should be mentioned in the application of fast TMC. The first is related to the effective calculation time. If the number of source particles (histories) is similar to a unique calculation with the desired statistical uncertainty, each of the n subcalculations uses new random input data A_i, loaded in computer memory. This leads to an additional loading time, increasing the total time needed to perform the n calculations. For relatively long subcalculations, this loading time becomes negligible. The second limitation lies in the use of the statistical uncertainty provided by the Monte Carlo simulation code. For nuclear transport Monte Carlo codes such as MCNP or SERPENT (Ref. 21), as well as others, it is known that for the k-code mode, the correlation of fission cycles can introduce significant

TABLE I

Summary and Comparison of the Original TMC and Fast TMC Methods

	Single Calculation	Original TMC	Fast TMC
Histories per calculation	m	m	m/n
Number of random $\vec{A}$	$n = 0$	$n \geq 500$	$n \simeq 300$
Random seed	—	No	Yes
Condition on $\overline{\sigma}_{statistics}/\sigma_{observed}$	—	$\simeq 0.05$	$\lesssim 0.50$
Running time	T	$n \times T$	$\simeq T$
Uncertainty due to $\vec{A}$	—	$\sigma_A(q)$	$(0.85 \text{ to } 1.15) \times \sigma_A(q)$

negative bias into the estimation of the k_{eff} statistical uncertainty.[22–25] Additionally, in unfavorable conditions, it may happen that the true uncertainty is substantially underestimated, as has been observed, e.g., when calculating the power distributions in large reactor cores.[26] For the original TMC, a bias in $\sigma_{\text{statistics}}$ exists, and according to the previous references,[7,10] this can be as high as 50%. As $\sigma_{\text{statistics}}$ is relatively small compared to $\sigma_A(q)$, this effect is not noticeable. For the fast TMC method, as $\sigma_{\text{statistics}}$ is not negligible compared to $\sigma_A(q)$, there is a perceivable bias on $\sigma_{\text{statistics}}$ and $\sigma_A(q)$. A solution is presented in Sec. III.C, but in cases other than eigenvalue calculations, this bias does not exist.

III.C. Other Improvements

One should notice that these two methods (TMC and fast TMC) use the estimator for the statistical uncertainties of each run given by the Monte Carlo simulation code. Because of the possible bias in $\sigma_{\text{statistics}}$, it can be helpful to have a separate estimation of $\sigma_{\text{statistics}}$, by repeating the same simulation p times (p can be different from n), each time with a different random seed $s_{i=1\ldots p}$ and a unique input parameter A_0. Other solutions have been investigated in different papers. In Ref. 22, a different batching method is proposed, leading to a reduction in the correlation between the different variance estimates. An expression of the bias in the variance estimation is presented in Ref. 27, which uses an iterative method to estimate the variance better. In Ref. 28, autoregressive and moving-average models were used to account for correlations between batches. Finally, Ref. 29 presents the fission source distribution intercycle correlation method, using the cycle-by-cycle stochastic error propagation model, which is more accurate than the previous methods in specific cases. Some Monte Carlo simulation codes such as McCARD (Ref. 30) include different estimations of the real variance, leading to a convenient comparison of the performance of the estimators. The accuracy of the real variance estimations with these methods is demonstrated in Ref. 29. Depending on the experience of the user and on the simulation code, different solutions are then available.

In the case of repetition of the same simulations with different seeds (the first proposed solution), the independent estimation of $\sigma_{\text{statistics}}$ can in general be performed more quickly than with random nuclear data ($p < n$). The advantage is that the variance of the calculated quantities provides an unbiased estimator of $\overline{\sigma^2}_{\text{statistics}}$. The drawback of such estimation is that a new set of simulations is needed, increasing the total calculation time (n for random A_i and random s_i, and p for the random s_i only). The obtained unbiased $\overline{\sigma^2}_{\text{statistics},i}$ would then be used in Eq. (4). As the standard deviation estimator from the Monte Carlo code is underestimated, the unbiased one would be systematically larger, leading to a lower $\sigma_A(q)$ from Eq. (4). Examples of this method, where a second set of runs is used to estimate $\sigma_{\text{statistics}}$, are presented in Figs. 1, 2, and 3 with the curves labeled "fast TMC + unbiased σ_{stat}."

As seen in Figs. 1 and 3, neither of these two methods converges faster than the others (fast TMC and fast TMC with an unbiased estimation of $\sigma_{\text{statistics}}$), which was relatively surprising to the authors.

If a user is willing to accept a 15% difference in the uncertainty with the original TMC method (considered as the method of reference in this work), then either of the following two solutions is acceptable: (a) fast TMC and (b) fast TMC with an unbiased σ_{stat}, as long as $\overline{\sigma}_{\text{statistics}}/\sigma_{\text{observed}} \lesssim 0.5$ and the system is realistic (it is possible to create a weakly coupled fissile array problem to simulate anomalous fission source convergence for which the mentioned criteria do not apply, as presented in Ref. 31).

IV. FAST GRS METHOD

A different approach to give faster uncertainty propagation was taken by Zwermann et al. as presented in Ref. 7, where the advantages of the properties of identically distributed and conditionally independent output variables are exploited. Detailed descriptions can be found in Ref. 7 with several examples. One advantage of this method is that it avoids the use of Eq. (4) and the inherent approximation from the estimation of $\overline{\sigma}_{\text{statistics}}$. It can be performed as follows:

(1) n calculations with m/n histories each, using different $A_{i=1\ldots n}$ and a unique seed s_1. A given distribution for the calculated quantity is obtained: $\overset{(1)}{q}_{i=1\ldots n}$.

(2) n other calculations with m/n histories each, using different $A_{i=1\ldots n}$ [similar to case (1)] and a unique seed s_2. A given distribution for the calculated quantity is obtained: $\overset{(2)}{q}_{i=1\ldots n}$.

(3) The covariance between calculations (1) and (2) is equal to the variance due to $\vec{A}$: $\text{cov}(q^{(1)}, q^{(2)}) = \sigma_A^2(q)$.

An example of application of the fast GRS method is presented in Fig. 4, for the criticality benchmark imf1-1 with random ^{235}U nuclear data files. It was applied with $n = 500$ runs and individual statistical uncertainties of 600 pcm. The correlation between runs (1) and (2) was $\rho = 0.48$ (as presented by the straight line in Fig. 4), and the standard deviations for each distribution were 1100 and 1120 pcm, leading to $\sigma_A(q) = 770$ pcm (the TMC method gives 800 pcm).

Additional results are also presented in Figs. 1, 2, and 3 with the curves labeled "fast GRS method."

With this method, nuclear data uncertainty can be propagated by performing, instead of n long runs, $2 \times n$ individual short runs with two different seeds of the random number generator of the Monte Carlo transport code.

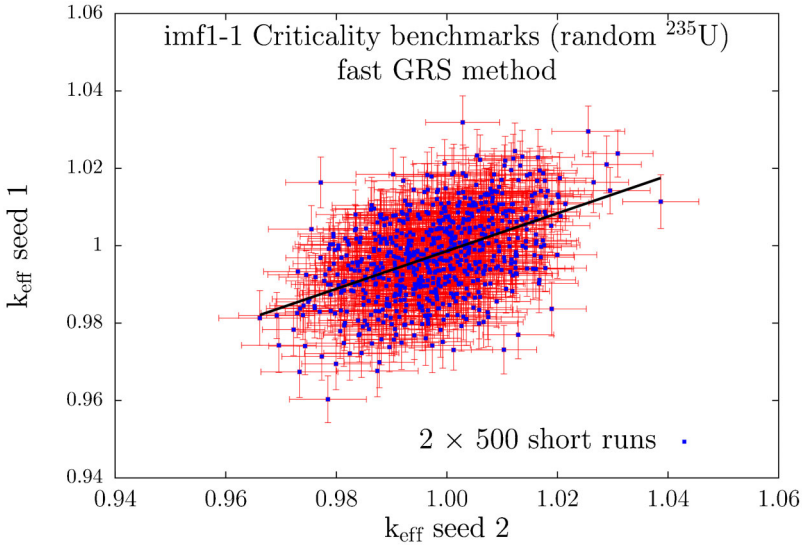


Fig. 4. Example of the fast GRS method applied to the criticality benchmark imf1-1 with random ^{235}U nuclear data. The uncertainties on each point are statistical.

In Sec. V, we will present some comparisons for the three methods: original TMC, fast TMC, and fast GRS, for a few systems, showing the different performances of the fast methods compared to the slower one.

V. COMPARISON OF RESULTS

To test the performance of the fast uncertainty propagation methods, their results were compared to those from the original TMC, the latter being considered as the reference solution. Comparisons of calculated uncertainties can easily be done, since the same transport and depletion codes are used, as well as the same random nuclear data $\vec{A}$. Four different cases were considered: criticality safety benchmarks (k_{eff} calculations) from the International Criticality Safety Benchmark Evaluation Project collection,[20] shielding benchmarks, a simple model of a pin-cell burnup,[13] and finally a full-size pressurized water reactor (PWR) core as defined in Ref. 32. The MCNP transport code was chosen for the full core, and the criticality and shielding benchmarks were used, whereas the SERPENT code was used for the burnup calculation. The SERPENT code has the advantage that it includes a depletion module that uses the same nuclear data as the transport module, which allows easy uncertainty propagation to inventories due to nuclear data (cross sections or fission yields).

V.A. Shielding and Criticality Safety Benchmarks

For the criticality and shielding benchmarks, reaction rates, neutron/gamma fluxes, or k_{eff} were calculated, together with the uncertainties due to statistics and the random data. The random nuclear data for a few isotopes were used, depending on the type of benchmark: ^{239,240,241}Pu, ^{235,238}U, ^{56}Fe, and tungsten isotopes, taken from the TENDL-2011 library.[33] This gives the flexibility to investigate small uncertainties (<100 pcm) to large ones (>1000 pcm and a few tens of percent for shielding benchmarks) by selecting a given benchmark in combination with random nuclear data for selected isotopes. Because of the availability of codes and licenses, MCNP version 4C3 was used. Results are presented in Fig. 5.

In Fig. 5, the calculated uncertainties for either k_{eff}, reaction rates, and neutron and gamma spectra from the fast methods (fast TMC and the GRS method) are plotted as a function of the original TMC method. The criticality benchmarks considered are all fast and intermediate systems, allowing a reasonable calculation time (<1 h for a single calculation, with 30 to 60 pcm statistical uncertainties for 10^6 neutrons). Three shielding benchmarks are considered: the FNS, FNG, and OKTAVIAN benchmarks.[34]

If the fast methods yield the same results as the original TMC, all uncertainty values can be represented on a single $y=x$ line. From Fig. 5 it can be seen that the results are scattered along the $y=x$ line for both the fast TMC and fast GRS methods. Significant deviations start to be noticeable for small uncertainty values (<300 pcm, corresponding to $\sim 0.3\%$), but the results still show good agreement, considering the statistical uncertainties for criticality benchmarks (presented as x and y error bars in Fig. 5). These results confirm the good agreement for the fast GRS method presented in Ref. 7, where the studied systems provided uncertainties from 500 to 1400 pcm.

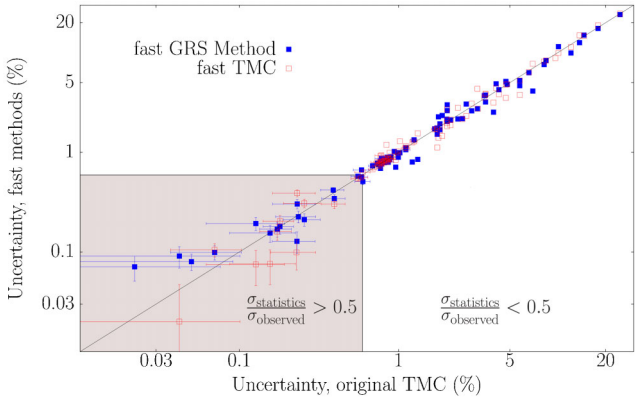


Fig. 5. Results for many criticality benchmarks and shielding benchmarks (FNS, FNG, and OKTAVIAN). If the fast methods agree with the original TMC, the results are on the diagonal. The uncertainty bars are statistical. For $\sigma_{statistics}/\sigma_{observed} \lesssim 0.5$, differences are noticeable.

One should, nevertheless, notice that for small nuclear data uncertainties and k_{eff} calculations $\left(\frac{\sigma_{statistics}}{\sigma_{observed}} \gtrsim 0.5\right)$, a difference up to a factor of 2 can be observed in some cases.

Similar calculations were realized for spectral indexes, presenting good agreement between methods, given the higher level of uncertainties for these quantities (at the percent level). For all the benchmark cases tested (about 100), the average ratio of fast TMC over TMC was 0.998 with a standard deviation of 0.02. For the fast GRS method, similar results were obtained (average of 0.99 and a standard deviation of 0.01).

V.B. Burnup Calculation

For the burnup calculations, the chosen system was a typical fuel rod from the Three Mile Island Unit 1 PWR, with a 15×15 assembly design, and an average power density of 33.58 W/g U (4.85% enriched, see Ref. 13 for more details). Different quantities were considered with a burnup from 0 to 120 GWd/tonne U (to obtain large nuclear data impacts): k_{eff}, macroscopic cross sections, and number densities (inventory of fission products during burnup). The SERPENT code (version 1.1.16) was used for the Monte Carlo transport and for the depletion of the fuel. Figures 6 and 7 present the uncertainties for a few quantities as a function of burnup level, varying the ^{235,238}U transport data (cross sections and single/double differential data) or the ^{239}Pu fission yields (k_{eff}, macroscopic cross sections, and number densities).

Burnup calculations were performed using a combination of Monte Carlo transport and deterministic depletion. With SERPENT, as for many other Monte Carlo transport codes, there was no information on the statistical uncertainties for number densities after the burnup steps. For the uncertainty propagation with the TMC method (original or new), one has to evaluate the statistical uncertainties to be used in Eq. (5). As in the case of the steady-state calculation, the statistical uncertainties can be calculated by repeating the same calculation many times with different random seeds for the random number generator. If in the case of steady-state calculations the independent calculation of statistical uncertainties is optional (to eliminate possible bias), it is mandatory for burnup calculations. For the fast GRS method, the statistical uncertainties are not needed.

One can see in Fig. 7 that small and large uncertainties for the number densities are well represented by the fast methods. This effect is rather different than for k_{eff}, where small uncertainty values were less well reproduced by the fast TMC method. For all the burnup results tested (about 1530), the average ratio of the fast TMC over TMC was 0.997 with a standard deviation of 0.003. For the fast GRS method, the ratio was 1.00 with a standard deviation of 0.001 (for 320 studied cases).

V.C. Full-Sized Reactor Core Benchmark

We used the Hoogenboom benchmark description[32] to present nuclear data uncertainty propagation for a full-size PWR core. This full-core description presents a challenging test for Monte Carlo transport methods, even without uncertainty propagation. It is required to calculate the generated local power in $241 \times 264 \times 100$ cells of 5.8 cm^3 with a statistical uncertainty $< 1\%$. In the following, we will calculate the effect of nuclear data in 12.7 million cells with the fast TMC method, showing that the statistical uncertainty is not the largest uncertainty for this type of quantity.

This benchmark consists of a reactor core with 241 identical fuel assemblies, each consisting of 17×17 regions, 264 of which are filled with pins and the remainder are for guide tubes. In the MCNP model, a tally grid was defined with $357 \times 357 \times 100$ identical regions, so that the active core and some space around it are covered. The size of each region was $1.26 \times 1.26 \times 3.66$ cm^3. The tally used was f7. The model was run for some time to obtain a reasonably converged fission source, which was the starting point for all subsequent simulations. All these subsequent simulations were done with 10 inactive cycles and 90 active cycles of 4×10^6 histories. In total 508 runs were performed with random nuclear data sets for ^{235}U, ^{238}U, and ^{239}Pu, and for H in H_2O thermal scattering data. For each of these 508 runs, a different random number seed was used in MCNP. Also, 389 runs were performed with constant nuclear data, but with identical seeds as the first 389 of the 508 runs, to have unbiased estimates of the standard deviations. These calculations were performed with $\simeq 200$ processors during 2 months of calculations.

The results of the 508 runs with random nuclear data can be combined into a single set of tally results, using the

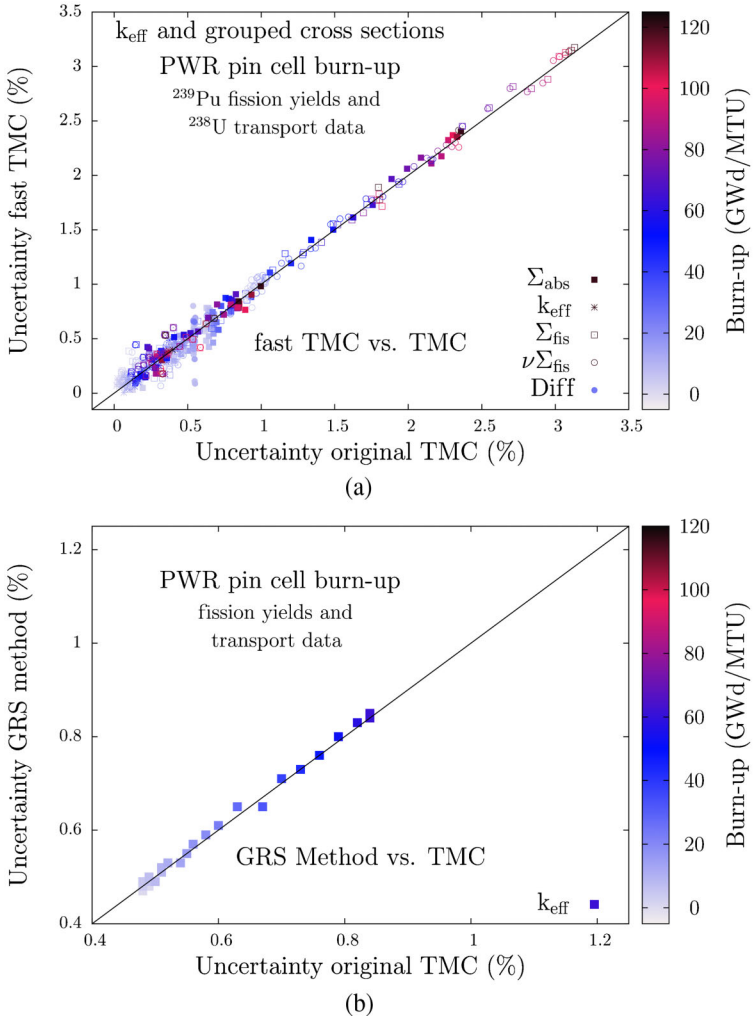


Fig. 6. (a) Uncertainties in k_{eff} and macroscopic group cross sections (Σ_{abs}, Σ_{fis}, $\nu\Sigma_{fis}$, and D_1) for burnup calculation (0 to 120 GWd/tonne U) due to random ^{238}U transport data and random ^{239}Pu fission yields. The results from the fast TMC are plotted as a function of the results of the original TMC method. (b) The results for the fast GRS method are plotted.

method outlined in Ref. 35. The results for the uncertainties for the generated fission power at mid-height in the core are shown in Fig. 8.

The cut at $z=0$ shows the distributions of the uncertainties at the center of the reactor. The local generation of power happens in the fuel elements and not in the guide tubes, represented by white spots in Fig. 8. The presented results were obtained with the fast TMC method without independent estimation of σ_{stat}. The cut at $z=0$ and $y=0$ (Fig. 8b) shows two results with and without independent estimation of σ_{stat}, both fitted with a parabolic function. One can see that as in the previous examples, there is not a large difference between the results for both methods ($<0.1\%$), leading to a preference for the fast TMC method because of its simplicity and faster realization.

In the middle of the core, the impact of the nuclear data is minimal, leading to $0.75\pm0.13\%$ uncertainty (from the fast TMC method). Toward the outer edges of the core, their impact increases up to $\sim3\%$.

For simple models such as a pin cell or an assembly, the uncertainties for generated power can be easily calculated with the fast TMC method, and the different nuclear data component can be disentangled by varying only one type of nuclear data. For a PWR mixed-oxide assembly as defined in Ref. 36, the uncertainty of the power is 0.7%, including 0.45% from ^{239}Pu, 0.28% from ^{235}U, 0.35% from ^{238}U, and 0.28% from the H in H_2O thermal scattering. This is in agreement with the 0.75% found at the center of the full-size core, which can be well approximated by a simple pin cell or assembly model with reflective boundaries.

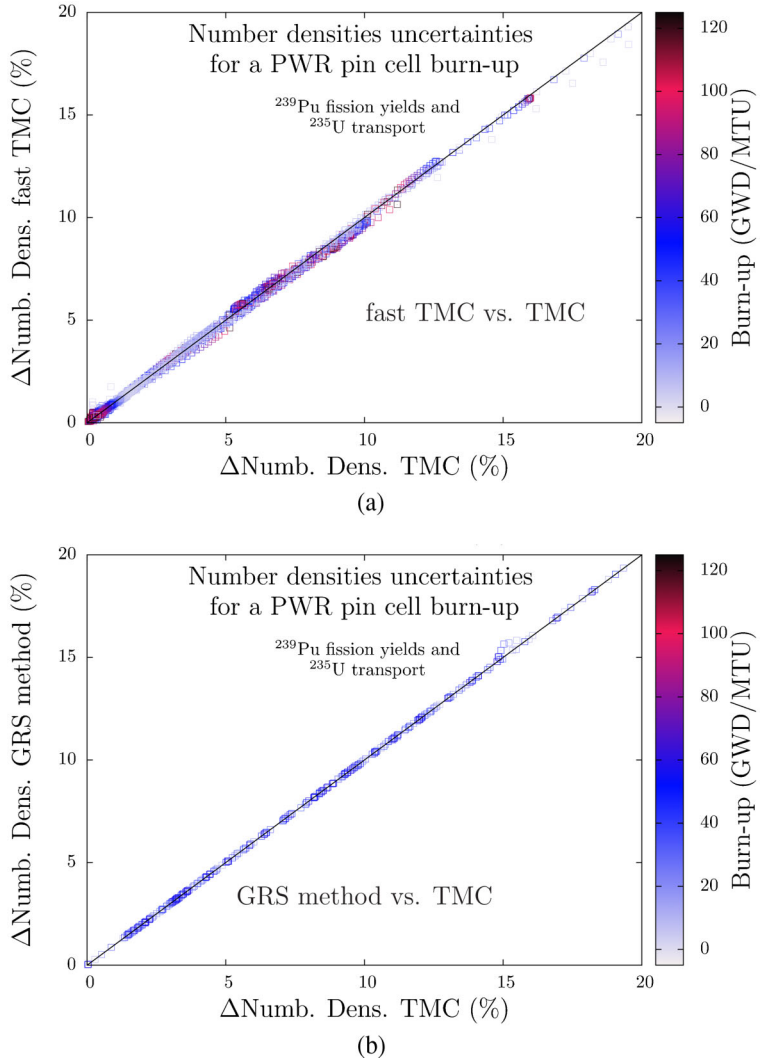


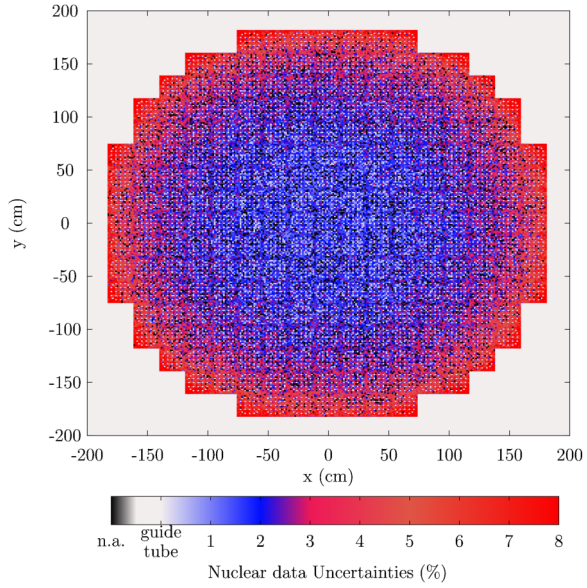
Fig. 7. (a) Uncertainties for the inventory of nuclei from 0 to 120 GWd/tonne U burnup due to random ^{235}U transport data and random ^{239}Pu fission yields. The results from fast TMC are plotted as a function of the results of the original TMC method. Each square represents a given isotope burnup value, and the color of the squares indicates the value of the burnup (color online). (b) The results for the fast GRS method are plotted.

With the fast TMC method, we were thus able to calculate the local generated fission power for the 12.7 million cells, demonstrating the capability of this uncertainty propagation method for a full-size system.

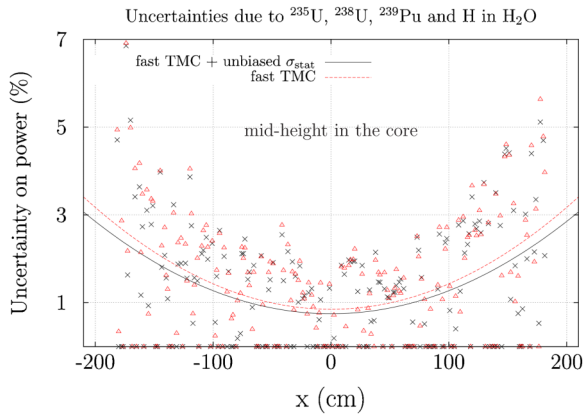
VI. CONCLUSION

In 2008, the TMC method was presented for propagating nuclear data uncertainties, with the handicap of multiplying the required calculation time by $n > 500$ (n being the number of random cases considered). Five years later, we now present a faster solution for Monte Carlo simulations: the fast TMC method. This new method was tested with criticality and shielding benchmarks, as well as with a simple burnup benchmark, together with the fast GRS method. The comparisons show the good performance of both fast methods. As a demonstration of its capabilities, the fast TMC method was applied to a full-size reactor core with 12.7 million cells. The uncertainties for local generated power due to ^{235,238}U, ^{239}Pu, and H in H_2O thermal scattering data were calculated in each cell, showing the power of the fast TMC method.

It is now possible to provide uncertainties due to nuclear data for any type of Monte Carlo simulation with a time multiplication factor between 1 and 2, making any justification for not providing uncertainties on calculations obsolete.



(a)



(b)

Fig. 8. (a) Local generated fission power for the coordinates $z=0$ for the full-size PWR core. ^{235,238}U, ^{239}Pu, and thermal scattering for H in H_2O were randomly varied over 508 runs. The colors indicate the level of uncertainties (color online). The white spots point out the position of the guide tubes. (b) Cut at $z=0$ and $y=0$ with parabolic fits as an eye-guide (both with and without independent estimation of σ_{stat}).

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