Target motion sampling temperature treatment technique with track-length estimators in OpenMC – Preliminary results

TARGET MOTION SAMPLING TEMPERATURE TREATMENT TECHNIQUE WITH TRACK-LENGTH ESTIMATORS IN OPENMC — PRELIMINARY RESULTS

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ABSTRACT

This paper examines the applicability of the Target Motion Sampling (TMS) temperature treatment method together with track-length estimators. Several track-length estimator based quantities are calculated in four test cases using a preliminary implementation of the method in OpenMC. The results are compared to an NJOY-based reference. The study reveals a statistically significant bias in the estimator results, but the errors were found to only affect limited energy regions, and their magnitude is relatively small as long as energy-integrated estimators are considered.

Key Words: **on-the-fly, Doppler-broadening, track-length estimator, TMS, OpenMC**

1. INTRODUCTION

Target Motion Sampling (TMS) temperature treatment technique is a stochastic method for taking the effect of the thermal motion of nuclides on path lengths and reaction rates into account on-the-fly during a Monte Carlo neutron tracking calculation. The method provides for modeling of arbitrary material temperatures with only one set of cross sections stored in the computer memory, significantly decreasing the memory demand of coupled multi-physics calculations involving detailed temperature distributions. Currently, the method is only able to deal with the energy region of resolved resonances and the thermal region of non-bound nuclides, but there are plans to extend the method to $S(\alpha, \beta)$ and the region of unresolved resonances in the future.

Previously, the TMS method has only been studied as a part of the Serpent 2 Monte Carlo code. The implementation of the method in Serpent has been found to be both accurate and well-feasible in terms of performance [1]. Since the calculation of reactor-physical parameters in Serpent relies on collision estimators, the functionality of the TMS method has not previously been studied together with track-length estimators. As there has been discussion whether or not the TMS method can be used together with track-length estimators in the first place, it was decided to scratch the surface of this important topic with a simple hands-on study.

The main application of the TMS method in Serpent is related to the multi-physics interface. Since this interface relies strongly on rejection sampling techniques that can only be applied together with the collision estimators, implementation of the track-length estimators in Serpent only for the purpose of the current study was considered pointless. Hence, the open-source Monte Carlo code OpenMC was chosen as the testing platform [3, 4]. The TMS method was implemented in a currently non-public branch of the OpenMC, primarily, to study the TMS method together with the track-length estimators and, secondarily, to test the performance of the method in a new code. The very first results, including problems that are recognized but not yet solved, are presented in the current article.

2. METHODOLOGY

2.1. OpenMC Monte Carlo Code

OpenMC is an open-source Monte Carlo code originating from the Massachusetts Institute of Technology. The code development has strong emphasis on efficient high-performance computing with current and future parallel computers. The focus on massive parallelization has affected many of the techniques implemented in the code, including for instance the efficiently parallelizable fission bank algorithm and the double-indexing based implementation of the unionized energy grid, which significantly speeds up cross section data retrieval with only a small increase in the memory requirement [3, 5, 6].

OpenMC was the natural choice for the current study for a couple of reasons. First of all, OpenMC, unlike Serpent, uses track-length estimators in the estimation of reaction rates, k_{eff} etc., which makes the study possible in the first place. Second, the source code of OpenMC is freely and easily accessible through the GitHub hosting service. In addition, OpenMC uses the same ACE cross section data format as MCNP and Serpent, significantly facilitating inter-code comparisons.

Since in OpenMC the material-wise macroscopic cross sections are calculated on-the-fly during transport, the code also acts as a very good reference for measuring the performance of the TMS method. This is not the case with the Serpent Monte Carlo code in which the macroscopic cross sections are normally precalculated in the problem initialization phase. As this optimization tweak cannot be utilized together with the TMS method, a normal Serpent calculation does not provide a fair reference for the TMS method, and artificial slowing-down of the Serpent calculations in the hope of a better performance reference, as it has been done for example in Reference [1], has its own issues.

2.2. TMS Temperature Treatment Method

Target Motion Sampling (TMS) temperature treatment technique was introduced for the first time in English-written journals in 2012 [7], but it was recently learned that a similar method has been presented already in 1984 in the Soviet Russia [8] and has been routinely used in Russian Monte Carlo

codes for many years. The efficiency and optimization of the method has been further discussed in References [1] and [9].

The TMS method is, contrary to other recently-developed on-the-fly temperature treatment techniques [10, 11], in fact a neutron tracking rather than a Doppler-broadening technique. Thus, the Doppler-broadened, effective cross sections are not calculated at any point of the transport calculation, but instead the temperature corrections are based on sampling target velocities at collision sites and using the available cross sections to determine the reaction probabilities in target-at-rest frame. To make this possible, a majorant-based rejection sampling technique must be applied in the sampling of path lengths, as described in Reference [1].

In the current study, "traditional" or DBRC-style truncation of the Maxwellian is used in the generation of the majorant cross section [9]. Thus, the energy range of thermal motion around neutron energy E is defined by limits

$$E_{\min,n}(E) = \left(\sqrt{E} - h\sqrt{\frac{k_{\mathrm{B}}\Delta T_n}{A_n}} \right)^2 \tag{1}$$

$$E_{\max,n}(E) = \left(\sqrt{E} + h\sqrt{\frac{k_{\mathrm{B}}\Delta T_n}{A_n}} \right)^2, \tag{2}$$

where A_n is the atomic weight ratio of nuclide n,

$$\Delta T_n = T_{\max,n} - T_{\mathrm{base}} \tag{3}$$

is the temperature difference between the maximum temperature of the nuclide $T_{\max,n}$ and the cross sections T_{base}, k_{B} is the Boltzmann constant and h specifies the range of thermal motion in terms of dimensionless velocity, similar to the truncation originally used in the Sigma1 kernel broadening method [12]. In other words, h defines the conservativity of the majorant (see Section 2.4).

2.3. Track-length Estimators

The basic idea behind track-lengths is the fact that the integral of neutron flux over a volume is equal to the total track-length of neutrons within the volume in a time interval. Consequently, by keeping track of the neutron track-lengths l during a Monte Carlo transport calculation it is possible to gain information on the spatially integrated neutron flux. When scoring the neutron flux using track-length estimators, the score s_i corresponding to track-length i is defined

$$s_i = w_i l_i, \tag{4}$$

where w_i is the neutron weight, and the estimator for the neutron flux Φ is simply the (normalized) sum of the scores obtained during the transport simulation. Furthermore, the scores can be binned with respect of, for example, energy or spatial domain to gain information on the neutron spectrum or the spatial flux distribution.

The estimators can also be used to calculate reaction rates and other integrals of type

$$\int_t \int_V \int_E f(E, \overline{r}) \Phi(E, \overline{r}) dt d^3 r dE, \tag{5}$$

where the integration is carried over time, some spatial volume and an energy interval, and $f(E, \bar{r})$ is a response function. In this case the scores are multiplied by the value of the response function f_i corresponding to the track-length, i.e.

$$s_i = w_i f_i l_i \,. \tag{6}$$

For example, when calculating the capture reaction rate the value of the response f_i would be the macroscopic capture cross section in the material zone of the neutron track l_i corresponding to neutron energy E, $f_i = \Sigma_\gamma(E, \bar{r}, T)$. When using track-length estimators in the estimation of quantities other than the neutron flux (for which $f_i = 1.0$), the value of the response must represent the whole track-length l_i and, therefore, the material zones in the Monte Carlo transport must be homogeneous with respect to density, nuclide composition and temperature T.

With the TMS temperature treatment method, the effective cross sections at the temperature of the material zone T are not available in general. Hence, the scoring of the estimators must be somehow based on the cross sections at temperature $T_{\mathrm{base}} \leq T$. What comes to *collision* estimators, it was demonstrated in [2] that the effect of thermal motion on cross section responses can be taken into account by first sampling target velocities and then using target-at-rest frame cross sections at T_{base} as responses, similar to the basic idea behind the TMS method. To take also the low-energy effects of thermal motion into account, the responses must be additionally multiplied by the Doppler-integral for constant cross section

$$g_n(E, \Delta T) = \left(1 + \frac{k_{\mathrm{B}} \Delta T}{2 A_n E}\right) \mathrm{erf}\left(\sqrt{\frac{A_n E}{k_{\mathrm{B}} \Delta T}}\right) + \sqrt{\frac{k_{\mathrm{B}} \Delta T}{\pi A_n E}} e^{-A_n E/(k_{\mathrm{B}} \Delta T)} \,. \tag{7}$$

Thus, when scoring the total capture reaction rate within TMS transport, the responses become

$$f_i = \sum_n g_n(E, T - T_{\mathrm{base}}) \Sigma_{\gamma,n}(E'_n, \bar{r}, T_{\mathrm{base}}) \,, \tag{8}$$

where E'_n are the sampled target-at-rest energies for nuclides n.

In the current work a similar approach is applied for the track-length estimators. However, some problems are expected due to the usage of non-representative cross section responses in the scoring. To demonstrate the problem, let us consider N monoenergetic neutron tracks with energy E_{m} that are used to estimate the reaction rate of reaction r. In conventional neutron transport the expected value (EV) of the estimator is

$$
\begin{aligned}
EV[R_{\mathrm{eff}}] \quad &= EV\Big[\sum_i^N s_i\Big] = EV\big[w_1 \Sigma_{\mathrm{eff},r}(E_{\mathrm{m}}, \bar{r}, T) l_1 + w_2 \Sigma_{\mathrm{eff},r}(E_{\mathrm{m}}, \bar{r}, T) l_2 + \dots\big] \\
&= \Sigma_{\mathrm{eff},r}(E_{\mathrm{m}}, \bar{r}, T) EV\Big[\sum_i^N w_i l_i\Big]
\end{aligned} \tag{9}
$$

where $\Sigma_{\mathrm{eff},r}(E_{\mathrm{m}}, T)$ is the effective cross section of reaction r at material temperature T. With TMS transport the effective cross sections must be approximated with sampled cross section responses and the corresponding EV becomes

$$
\begin{aligned}
EV[R_{\mathrm{TMS}}] \quad &= EV\big[w_1 g_n(E_{\mathrm{m}}, \Delta T) \Sigma_r(E'_1, \bar{r}, T_{\mathrm{base}}) l_1 + w_2 g_n(E_{\mathrm{m}}, \Delta T) \Sigma_r(E'_2, \bar{r}, T_{\mathrm{base}}) l_2 + \dots\big] \\
&= EV\Big[\sum_i^N w_i g_n(E_{\mathrm{m}}, \Delta T) \Sigma_r(E'_i, \bar{r}, T_{\mathrm{base}}) l_i\Big] \,,
\end{aligned} \tag{10}
$$

where n is the target nuclide of reaction r. If the track-lengths were independent of the sampled responses, the expected value in (10) would correspond to [13]

$$EV[\sum_i^N w_i g_n(E_{\mathrm{m}}, \Delta T)\Sigma_r(E_i', \overline{r}, T_{\mathrm{base}})l_i] \quad = EV[g_n(E_{\mathrm{m}}, \Delta T)\Sigma_r(E_i', \overline{r}, T_{\mathrm{base}})]EV[\sum_i^N w_i l_i]$$

$$= \Sigma_{\mathrm{eff},r}(E_{\mathrm{m}}, \overline{r}, T)EV[\sum_i^N w_i l_i], \qquad (11)$$

i.e. the correct expected value. However, the sampled cross section responses are also used in the neutron tracking process while determining whether a collision point candidate is accepted, terminating the neutron track and ultimately defining the track-length, or rejected, in which case the tracking proceeds by sampling of a new collision point candidate. Consequently, the track-lengths and responses are at least somewhat correlated, meaning that Equation (11) does not hold. This may introduce bias in the estimator results. The correlation effects are emphasized if the response reaction r has significant impact on the neutron transport process and involves a strongly energy-dependent cross section. The basic cause for the problem persists also when calculating energy-integrated estimators.

To reduce the correlations, all of the information on sampled cross sections obtained along each track-length is utilized instead of using only one cross section sample per nuclide per score. In practice, every time the velocity of a target nuclide is sampled during the TMS tracking process, the corresponding target-at-rest cross sections are used to accumulate nuclide-wise cross section sums and the average of the cross sections (multiplied by g_n) is used as the response when finally scoring the track-length estimator. In case the cross sections for some nuclides have not been sampled even once before the track ends, cross sections for these nuclides are sampled prior to scoring the estimator.

2.4. Implementation of TMS in OpenMC

The Target Motion Sampling (TMS) temperature treatment method was implemented in the OpenMC Monte Carlo code using the Elevated Basis Temperature approach, meaning that the basis cross sections can be at any temperature between zero Kelvin and the minimum temperature of the nuclei in the system. In the original TMS method the basis cross sections were forced to zero Kelvin, but it was later realized that the performance of the method can be significantly increased by elevating the basis cross section temperature [1]. The method was implemented such that the TMS method is only used for user-specified materials and the remaining materials are treated normally using pre-broadened cross sections.

The calculation of the nuclide-wise majorant cross sections is done in the problem initialization phase and the cross sections are kept in the computer memory. The majorant boundaries are chosen according to the "traditional" method (Equations (1)–(2)), which is based on the truncation of the Maxwell-Boltzmann distribution. The studies performed in [9] showed that the conservativity of the majorant can be decreased by changing the value of the h parameter in Equations (1)–(2) from original value of $h = 4.0$ to $h = 3.0$. This increases the performance of the TMS method without affecting the neutron transport in practice.

The usage of TMS slightly increases the memory consumption of OpenMC, because nuclide-wise majorant cross sections and the sums of sampled cross sections used in the scoring of the estimators are stored, in addition to the normal data. The memory consumption of the sampled cross sections is very small, so in practice the increase in memory consumption comes from one additional cross section to be scored per nuclide. As the number of nuclides in problems involving burned fuel is around 300 and the number of points in the nuclide-wise energy grid is usually below 200 000, the increase in memory consumption should be less than 100 MB, multiplied by the number of parallel MPI processes.

3. TEST CASES

The first "PWR-Gd" case involves a 17x17 PWR fuel assembly with 16 Gadolinium-doped fuel rods in an infinite two dimensional lattice. The geometry and material definitions of the fuel assembly are from an NEA benchmark [14]. The only differences to the benchmark specifications are related to temperatures: the moderator temperature is risen to 600 K for simplicity and the originally flat temperature profiles of the fuel rods are replaced with 3-step distributions such that the pellets are divided into three equi-thick annular regions with temperatures 600 K, 900 K and 1200 K from outside in.

The second case is abbreviated "PWR-BU" and features the previously introduced "PWR-Gd" bundle irradiated to 40 MWd/kgU burnup. The irradiated material compositions were obtained by running a burnup calculation using Serpent 2.1.14. The resulting compositions contain 241 actinide and fission product nuclides with cross sections available in the data libraries.

The "HTGR" test case consists of TRISO particles within graphite matrix in an infinite three dimensional lattice. The specifications of the TRISO particles and the composition of the graphite matrix are based on a NEA benchmark for HTGR fuel depletion [15], and the lattice pitch is 0.16341 cm. The fuel kernel in the spherical TRISO particles is divided in two equally thick parts such that the innermost 0.0125 cm is at 1800 K temperature and the outer layer is at 1200 K. The temperature of all other materials is 1200 K.

The last of the test cases, "SFR", involves a fuel assembly from the sodium cooled fast reactor JOYO in an infinite two dimensional lattice. The specifications of the assembly can be found in [16]. The geometry and material definitions correspond to the benchmark definition for the $250°C$ core. Again, the fuel temperature is modified such that the inner half (radius) of the fuel pellets is at 1200 K and the outer half at 900 K temperature. All other materials are at 600 K temperature in the model.

4. RESULTS

The calculations were made using the development branch version of OpenMC 0.5.2 with extended xml support and the TMS temperature treatment method preliminarily implemented. It is empha-

sized that the implementation is not yet working correctly. Hence all results, particularly those considering the performance of the method, are very preliminary. Fixing the present problems in the implementation is expected to slightly decrease the performance.

The TMS method is used only for the fuel materials, while other materials are treated conventionally using NJOY-broadened cross sections. The basis temperature of the cross sections for the TMS treatment T_{base} equals the minimum temperature of the fuel material in each system. In the reference calculations all materials are modeled using NJOY cross sections as-is. The only difference between the TMS calculation and the reference is in the modelling technique of the thermal motion, i.e. the materials, the geometry definitions and the temperature profiles are identical. Probability table treatment for unresolved resonances is turned off in all of the calculations.

OpenMC was run using MPI parallelization on 12 Intel Xeon CPUs running at 3.47 GHz with the exception that the HTGR-case was run using only one processor due to an unidentified problem that caused random termination of the calculations for this test case. The cross section library is based on JEFF-3.1.1 and has been processed with NJOY using 0.001 reconstruction tolerance for high accuracy.
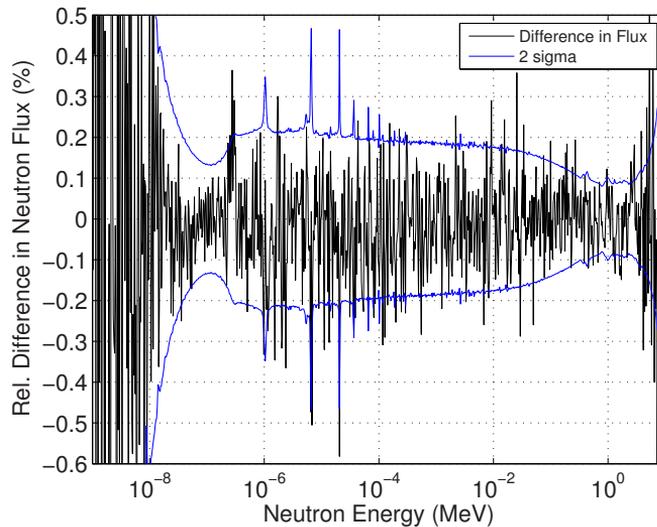

Figure 1. Comparison of the neutron spectra of the PWR-BU case between the TMS calculation and the reference.

4.1. Checking the Implementation

The very first thing to do is to check that the neutron transport with TMS is working properly. Almost all of the output parameters of OpenMC are calculated using track-length estimators, scored with sampled and, thus, potentially non-representative responses as described in Section 2.3. Since this kind of results may be biased, the validity of the implementation can only be checked via

neutron flux estimators for which the values of the responses are known to properly represent the track-lengths ($f_i = 1.0$).

The neutron flux spectra between a TMS calculation and the reference were compared in all of the four test cases and the comparison for the PWR-BU case is shown in Figure 1. Neutron flux spectra were in agreement in all of the four test cases, which indicates that the neutron transport is working properly.

4.2. Integral and Performance Results

The results of energy-integrated parameters and performance measures are provided in Table I. To emphasize the potential biases related to TMS and track-length estimators the reaction rates estimators were scored in fuel materials only. The combined k_{eff}, provided in Table I, is a combination of different track-length estimator based multiplication factors that OpenMC calculates by default.

Table I. Performance measures and integral results. The statistical deviations correspond to one sigma.

	PWR-Gd	PWR-BU	HTGR	SFR
Number of Neutrons	5×10^8	2×10^8	1×10^7	2.5×10^8
Reference Calculation				
Combined k_{eff}	1.15612 ± 4 pcm	0.93621 ± 6 pcm	1.21053 ± 29 pcm	1.78781 ± 4 pcm
Transport time (h)	2.4	13.5	9.5	4.7
XS Memory size (MB)	68	382	31	78
Tot. reaction rate (1/s)	$5.7107 \pm 1\text{E-}4$	$5.8728 \pm 1\text{E-}4$	$3.1481 \pm 6\text{E-}4$	$20.1789 \pm 9\text{E-}4$
Figure-of-Merit	4.64E+5	5.50E+4	9.48E+2	3.27E+4
Tot. absorption rate (1/s)	$0.92494 \pm 3\text{E-}5$	$0.92023 \pm 4\text{E-}5$	$0.98426 \pm 3\text{E-}4$	$0.98248 \pm 5\text{E-}5$
Figure-of-Merit	9.75E+4	1.20E+4	3.31E+2	2.30E+4
TMS Calculation				
Δk_{eff} (pcm)	5 ± 6	**-32 ± 8**	-34 ± 41	3 ± 6
Transport time, abs/rel (h/-)	2.6 / 1.09	14.0 / 1.04	9.6 / 1.02	4.8 / 1.01
XS Memory size, abs/rel (MB/-)	32 / 0.47	136 / 0.36	16 / 0.51	50 / 0.64
Tot. reaction rate (1/s)	$5.7088 \pm 1\text{E-}4$	$5.8707 \pm 1\text{E-}4$	$3.1455 \pm 6\text{E-}4$	$20.1811 \pm 9\text{E-}4$
Figure-of-Merit, abs/rel	4.15E+5 / 0.90	5.28E+4 / 0.96	9.38E+2 / 0.99	3.24E+4 / 0.99
Tot. absorption rate (1/s)	$0.92431 \pm 3\text{E-}5$	$0.91938 \pm 4\text{E-}5$	$0.9830 \pm 3\text{E-}4$	$0.98252 \pm 5\text{E-}5$
Figure-of-Merit, abs/rel	9.02E+4 / 0.92	1.15E+4 / 0.96	3.40E+2 / 1.03	2.27E+4 / 0.99

The results show that in three cases out of four the k_{eff} estimate of the TMS calculation agrees with the reference within statistics. For the PWR-BU case the difference is 32 pcm, which is a relatively small error, but still statistically significant. Small biases can also be seen in the reaction rate estimators of the three thermal systems: the TMS results are consistently slightly smaller than the reference, but the errors are again small, less than 0.1 %. In the SFR case the estimators agree within statistics. The overhead from the TMS method varies between 1.01–1.09 for this preliminary implementation.
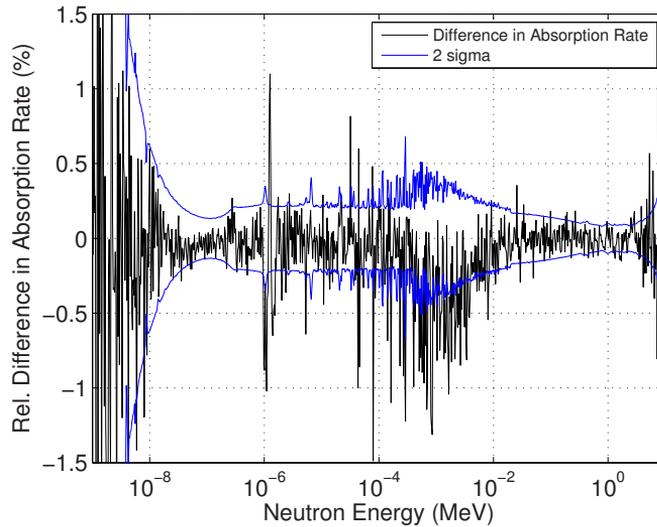
Figure 2. Comparison of the absorption spectra of the PWR-BU case between the TMS calculation and the reference.

4.3. Comparison of Reaction Rate Spectra

As the usage of track-length estimators together with the TMS method clearly introduces a small bias in some of the energy-integrated results, it is beneficial to take a look at the reaction rate spectra to get more information on the origin of the error. The absorption spectra for the PWR-BU case are compared in Figure 2. In this plot a region of negative bias can be seen in the surroundings of 1 keV and, additionally, several narrow error peaks can be recognized. The biases were otherwise similar in all of the thermal systems, but the lowest 1 eV bias peak was only present in the PWR-BU system.

The bias around 1 keV was studied further by calculating reaction rate spectra for the partial absorption reactions. It was noticed that the main contribution to the bias comes from ^{238}U. On the other hand, the absorption rate of ^{234}U did not have any contribution to the bias even though it has a strongly energy-dependent cross section. These observations indicate that the bias originates from correlations between the track-lengths and the sampled cross sections and is specific to "important" nuclides, as anticipated. It also seems that there are no coarse errors in the implementation of the track-length estimators.

The 1 eV bias peak of the PWR-BU was traced back to nuclides ^{103}Rh, ^{239}Pu and isotopes of Sm, which are only present in the PWR-BU case. Excluding ^{103}Rh from the fuel compositions (both TMS and reference) made the positive part of the error peak disappear, and the negative part disappeared after removing ^{239}Pu and Sm.

5. CONCLUSIONS AND FUTURE PROSPECTS

In the current study, the applicability of the TMS method together with track-length estimators was studied in four systems with different neutron spectra and characteristics. The calculations were performed using a preliminary implementation of the TMS method in the OpenMC Monte Carlo code.

Comparison of neutron fluxes in Section 4.1 showed that the implementation of the TMS is working correctly what comes to the neutron transport. Instead, a small but clear bias can be seen in the reaction rates and their derivatives that are calculated in OpenMC using track-length estimators. By comparing the reaction rate spectra it was noticed that the bias concerns a rather narrow energy region around 1 keV and, additionally, some individual resonances. The bias seems to originate from correlations between the track-lengths and the sampled cross sections that are used as responses. Since a negative correlation exists between the sampled cross section responses and corresponding track-lengths, a negative bias emerges in the estimator results at certain energies. However, also positive bias peaks were observed at a few narrow energy intervals. The exact origin of the positive peaks was not identified within the current study.

In general, using TMS-originated, sampled cross sections as responses in the scoring of the track-length estimators had surprisingly small effect on the accuracy of the reaction rates, at least when energy-integrated values are considered. Nevertheless, some unacceptable bias exists in the results and this bias must be removed before the implementation can be considered complete and the TMS method can be included in the official version of OpenMC.

It should be possible to fix the problems by, first, finding a way to recognize the problematic energy regions and cross sections and, then, increasing the number of cross section samples per response within these energy regions by artificially increasing the majorant cross sections. Since the bias exists only at a relatively narrow energy spectrum and sampling cross sections is computationally cheap, this brute-force approach should have only minor effect on the overall performance of the method. However, before proceeding on this path, the topic will be discussed together with the developers of the PRIZMA Monte Carlo code, who have previous experience on the application of track-length estimators together with a tracking method similar to TMS.

ACKNOWLEDGMENTS

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