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Development of a Variance Reduction Scheme in the Serpent 2 Monte Carlo Code

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Abstract - *This paper presents the weight-window based variance reduction scheme recently implemented in the Serpent 2 Monte Carlo particle transport code. Importances used for forming the weight-window boundaries are obtained from a super-imposed mesh, which can be produced using external calculation tools or a built-in light-weight solver based on the response-matrix method. The methodology is introduced and demonstrated by two examples: 1) radiation shielding calculation in a spent fuel transport cask with weight-window mesh produced by SCALE / MAVRIC, and 2) ex-core neutron dosimetry calculation with the internal light-weight solver. In both cases the use of variance reduction results in orders of magnitude increase in computational performance without introducing any biases in the results. The work is part of an on-going effort to expand the use of Serpent from its traditional applications in reactor physics to new fields, such as radiation transport and fusion neutronics.*

I. INTRODUCTION

During the past few years the development of the Serpent Monte Carlo code [1] has been extended from its traditional applications in reactor physics to new fields, including radiation transport and fusion neutronics. The work has been accompanied by the implementation of photon interaction physics routines [2], and the development of a coupled neutron / photon transport mode is currently under way [3]. Broadening the scope of applications is supported by a CAD-based geometry type [4] and a radioactive decay source mode [5, 6], which have been tested in particular for the purpose of fusion applications.

Using the Monte Carlo method for such applications often requires efficient variance reduction techniques. This is especially the case for radiation shielding problems, in which dose rates are calculated in regions where the particles are intentionally kept away from by physical barriers. Since Serpent was originally designed as a reactor physics code, the development has been focused on analog Monte Carlo game. Work on a weight-window based variance reduction scheme was started fairly recently, in order to support expanding the scope of applications to new fields. This paper presents the methodology, together with some of the first results.

II. METHODS

The variance reduction scheme in Serpent 2 relies on the conventional weight-window based approach [7], using an importance mesh overlaid on top of the geometry. The concept of importance can be interpreted as the contribution that a single source particle at given position, energy and direction of motion has to a specified response, such as a physical reaction rate. The population is encouraged to flow in the direction of increasing importance, which makes it more likely that the simulated histories contribute to the desired result. This is accomplished by splitting particle histories that enter a cell of higher importance and terminating histories by Russian roulette in the opposite case. Even though the transport of individual particles is biased in the Monte Carlo game, the simulation preserves the transport of statistical weight. The weight-window boundaries that determine the criteria for splitting and roulette are inversely proportional to the local importance.

Internally the weight-window routines in Serpent 2 support regular Cartesian and cylindrical mesh types in both neutron and photon transport modes, divided into multiple energy groups. The importance mesh used for forming the weight-window boundaries is obtained by solving the adjoint transport problem. Even though it is possible to accomplish this task with continuous-energy Monte Carlo simulation, variance reduction applications typically rely on either multi-group calculation or deterministic transport methods. The work for Serpent 2 is currently focused on two alternative calculation schemes:

i) Support for external tools for importance mesh calculation

ii) Development of an internal light-weight solver based on the response-matrix method

Each approach is briefly described below.

The most significant flaws in the methodology are related to source biasing. The source sampling routine does not account for the weight-window mesh in any way, which may lead to problems when particles are born in locations where the importance differs significantly from unity. These issues are discussed with the examples in Sec. III..

1. Support for external tools

Weight-window based techniques have been used for variance reduction in Monte Carlo simulations for decades, and there exists a wide range of calculation tools, such as ADVANTG [8] and MAVRIC [9], capable of obtaining the adjoint solution. In order to utilize the best available methodology in Serpent calculations, it was decided to include support for standardized and widely-used data formats. The first solution was to implement an input routine capable of reading

weight-window mesh files in the MCNP WWINP format [10]. These mesh files can be produced from other standard formats using existing conversion tools. At the time of this writing the support in Serpent 2 was limited to regular Cartesian mesh with uniform spacing and multiple energy groups.

2. Response-matrix based light-weight solver

The use of external tools requires constructing a separate input model for the importance mesh calculation. This translates into time and effort, and for some cases it might be more convenient to obtain the solution from another Serpent calculation using the same input files. This approach may not work for the most challenging variance reduction problems, but for simple applications a built-in light-weight importance mesh solver can lead to significant improvement in efficiency with minimal user effort. The internal solver obtains the adjoint solution using the response-matrix method, which is briefly described below. At the time of this writing the development was still under way, and the solver was implemented without energy dependence.

The response-matrix method is based on the preservation of particle balance and the continuity of particle current over the boundaries of the modeled system. When the geometry is divided into smaller sub-zones, the continuity of current implies that these zones are coupled to their neighbors by the interface currents. The implementation in Serpent 2 relies on spatial division based on a regular Cartesian or a cylindrical mesh, and the currents are integrated over the boundary surface, time, energy and direction of motion.

The preservation of particle balance inside each mesh cell is expressed using a number of pre-calculated coupling coefficients between the cell and its nearest neighbors. These constants are easily calculated using the Monte Carlo method and standard cell flux and surface current tallies. The coupling coefficients for cell m are formed by tallying the partial currents, with a flag indicating the interface through which the particle entered the cell:

$$\alpha_{m,i,j} = \frac{J^+_{m,i,j}}{J^-_{m,j}}, \tag{1}$$

where $J^+_{m,i,j}$ is the outward particle current that passes through the cell from neighbor j to neighbor i, and $J^-_{m,j}$ is the net inward current that is passed into the cell from neighbor j. In a three-dimensional Cartesian mesh these coefficients form a 6×6 matrix for each mesh cell m:

$$\mathbf{A}_m = \begin{pmatrix} \alpha_{m,1,1} & \alpha_{m,1,2} & \dots & \alpha_{m,1,6} \\ \alpha_{m,2,1} & \alpha_{m,2,2} & \dots & \alpha_{m,2,6} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{m,6,1} & \alpha_{m,6,2} & \dots & \alpha_{m,6,6} \end{pmatrix} \tag{2}$$

Also required for the calculation are the source terms which determine the fraction of source particles that escape the cell to neighbor i, and response terms that determine the contribution of particles entering the cell from neighbor j to the user-defined result. The source vector for cell m can be written as:

$$\mathbf{S}_m = \begin{pmatrix} S_{m,1} \\ S_{m,2} \\ \vdots \\ S_{m,6} \end{pmatrix}, \tag{3}$$

where $S_{m,i}$ is the fraction of source particles that are emitted inside the cell and escape through the boundary to neighbor i. The contribution of inward currents to user-defined responses is given by the response vector:

$$\mathbf{F}_m = (F_{m,1} F_{m,2} \dots F_{m,6}) \tag{4}$$

formed by coefficients:

$$F_{m,j} = \frac{f_{m,j}}{J^-_{m,j}}, \tag{5}$$

where $f_{m,j}$ is the contribution of particles that entered the cell from neighbor j to the given response.

The forward solution proceeds in iterations. The outward currents are mapped into the inward currents of the adjacent cells. If cell (b) is located east of cell (a), the outward current component from (a) through its east face becomes the west inward component of (b), and so on (see Fig. 1). The inward current vector for each cell is then multiplied by the coupling matrix, which yields the outward currents for the next iteration:

$$\mathbf{J}^+ [k+1] = \mathbf{A}\mathbf{J}^- [k], \tag{6}$$

where k is the iteration index and the cell index m is omitted for convenience. The procedure starts with the source distribution, which forms the outward current vectors for the first iteration:

$$\mathbf{J}^+ [0] = \mathbf{S}. \tag{7}$$

The iteration is terminated when the current vectors become negligible. Reaching a converged solution requires that the system is sub-critical or non-multiplying, in which case the currents are diminished from iteration to iteration. The algorithm cannot be applied as such to critical or super-critical configurations.

Each inward current component makes a contribution to the results. The contribution is obtained by vector multiplication:

$$R [k] = \mathbf{F}\mathbf{J}^- [k], \tag{8}$$

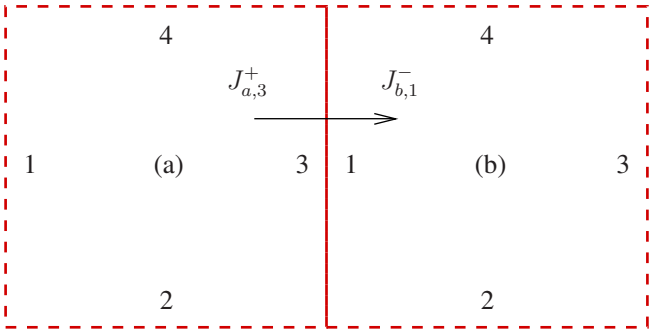

Fig. 1. Mapping of outward to inward currents. The outward current from cell (a) through face 3 becomes the inward current 1 of cell (b).

where **F** is the response vector. The final results are given by:

$$R = R_s + \sum_k R\,[k]\,, \tag{9}$$

where R_s is the direct contribution from source particles, obtained from the Monte Carlo simulation similar to the coupling coefficients and source and response vectors.

The adjoint problem is solved in a similar way, starting from the responses and iterating backwards. The solution provides the contribution of each inward current component and source term to the response. The sum of these components is interpreted as the cell importance.

The main advantage of the response-matrix method is its simplicity. The coupling coefficients, source and response vectors are easily obtained from a forward Monte Carlo simulation using standard cell flux and surface current tallies. The forward solution preserves the results of the Monte Carlo simulation, not only to within statistics, but to within the numerical precision of floating point artithmetics. This means that the calculation of the various coefficients needed for obtaining the adjoint solution is easily verified.

The built-in response-matrix solver was implemented in Serpent version 2.1.27. It works for both neutrons and photons, and takes full advantage of OpenMP parallelization. Responses are provided using standard detectors (tallies) and the importance mesh is written in a file that can be read directly into a second Serpent calculation. As mentioned above, the methodology is currently implemented without energy dependence.

III. FIRST RESULTS

Development of the variance reduction scheme is still under way, and the methodology is not yet in routine use. Two test cases are presented below to demonstrate the methodology. The purpose of these tests is to: 1) verify that the results remain unbiased, and 2) show that the variance reduction scheme leads to a significant improvement in computational efficiency. The metric used for evaluating the efficiency is the figure-of-merit (FOM):

$$FOM = \frac{1}{T\sigma^2}\,, \tag{10}$$

where T is the wall-clock running time and σ is the relative statistical error associated with the result estimator.

1. Transport cask calculation with MAVRIC-Serpent

The use of external solvers for the production of importance maps was studied in a special assignment at Aalto University during the Summer of 2016 [11]. Two test cases were covered: the Kobayashi variance reduction benchmark [12] and a shielding calculation involving a spent fuel transport cask with photon and neutron sources from radioactive decay [13]. In both cases the adjoint solution was obtained using SCALE / MAVRIC. Selected results of the second test case are presented below. Since the purpose was to evaluate the variance reduction capabilities in Serpent 2, the results are not compared to any reference data.

The computational model consists of a simplified description of the TN-24P transport cask developed by Transnuclear, Inc. The cask holds 24 fuel assemblies inside a 27 cm thick steel canister and external radial neutron shield. The Serpent input was constructed based on the SCALE model in Ref. [13]. Fuel assemblies were modeled as homogenized material zones and source spectra and flux-to-dose conversion factors were provided in point-wise tabular form. The geometry is illustrated in Figure 2.

Neutron and photon transport calculations were run using MAVRIC to provide the importance meshes for variance reduction. The calculation was optimized for dose rates outside the cask. In both cases the geometry was covered by a 66×66×90 Cartesian mesh. The number of energy groups was set to 27 for neutrons and 19 for photons. The conversion to WWINP format was carried out using the *mim2wwinp* utility included in the SCALE code package.

Reference results were obtained by running Serpent simulations without any variance reduction scheme. A total of 17 billion ((1.7×10^{10}) neutron histories and 215 billion photon histories were run in a single 20-core 2.2 GHz Intel Xeon cluster node with OpenMP parallelization. The calculations took 108 and 178 hours, respectively. Good statistics were obtained for neutrons, but because of the more effective shielding, the largest statistical errors for the photon transport simulation remained at few percent. The calculations were repeated with variance reduction, using one billion neutron and 10 billion photon histories. The corresponding running times were 3 and 18.5 hours, respectively.

Neutron and photon dose rates were evaluated using a cylindrical mesh tally, divided into a single axial and 200 equally-spaced radial bins. The results are presented in Figure 3. Dose rates obtained using variance reduction agree with the results of the reference analog simulations to withing statistics, which suggests that the weight-window based variance reduction scheme works as expected without introducing any biases in the results.

The comparison of figure-of-merits shows that the use of weight-windows leads to a considerable improvement in computational performance in the region of interest (outside the cask). For the neutron transport simulation the gain in efficiency is about a factor of 20. The difference is even more significant for photons, in the order 10,000. This is explained by the fact that very few particles are able to penetrate the thick wall of the steel canister, and obtaining reasonable statistics outside the cask requires running a very large number of particle histories. The effect of variance reduction is also demonstrated in the mesh plots in Figure 2, in which the simulations were run using a low number of particle histories. Most tracks in the analog simulation are terminated inside the cask, and the few individual particles that escape draw visible tracks in the mesh.

Even though the transport cask test case can be considered a successful demonstration of the implemented variance reduction scheme, the calculations also revealed a significant flaw in the methodology. The current source sampling routine in Serpent does not account for the weight-window mesh in any way. All particles are born with unit weight, which means that they may be immediately subjected to splitting or Rus-

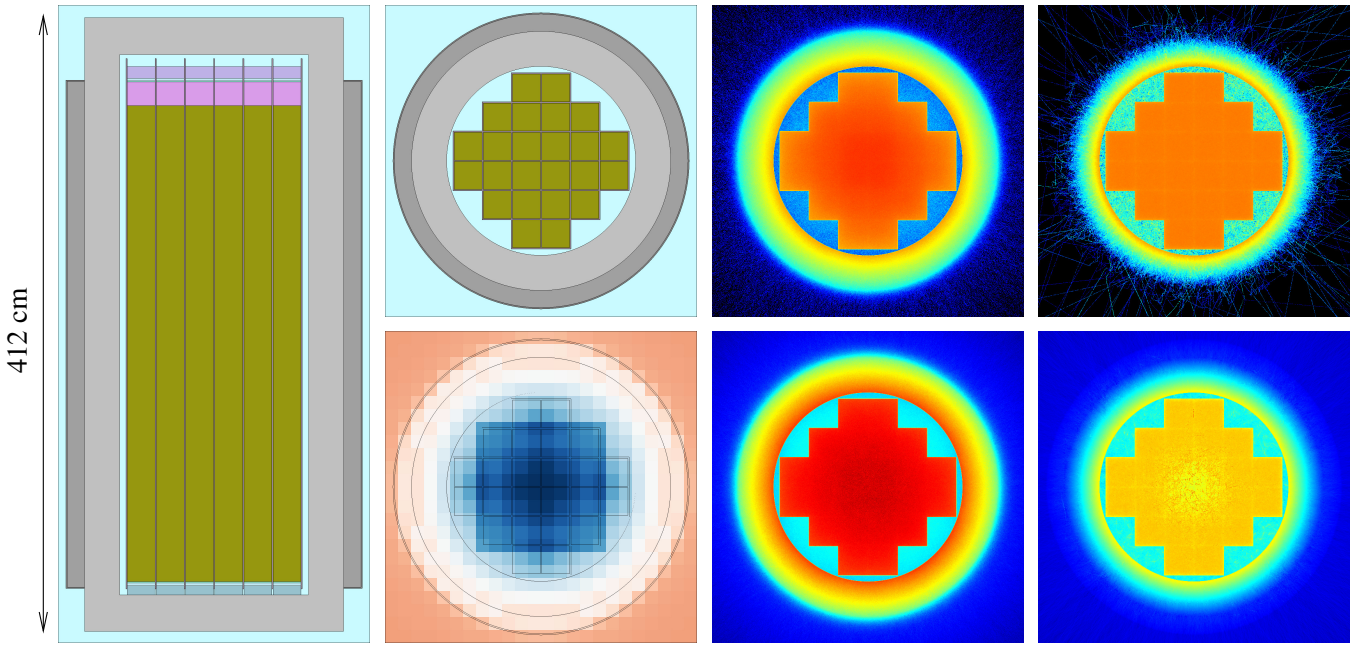

Fig. 2. Transport cask calculation case. 1st column: axial geometry plot of the TN-24P transport cask. 2nd column: radial geometry plot (top) and example importance mesh (bottom). 3rd column: Serpent mesh plot of radial neutron dose rate distribution from analog simulation (top) and using variance reduction (bottom). 4th column: Serpent mesh plot of radial photon dose rate distribution from analog simulation (top) and using variance reduction (bottom). The mesh plots were produced by running a relatively low number of particle histories to emphasize the difference between analog and implicit simulations.

sian roulette if the local importance differs from unity.[1] High importance can lead to over-splitting of the source particles, which may cause the calculation to hang completely.

To overcome this problem Serpent allows re-normalizing the importance mesh. Setting the highest importances in the source region close to unity removes the issue with over-splitting, but may cause a large fraction of particle histories started in regions of low importance to be terminated by Russian roulette without making any contribution in the results. The normalization had to be adjusted manually, by method of trial and error. Even though it was easy to find values that produced good results, there are no guarantees that the normalization was set up in the optimal way.

2. Ex-core dosimetry calculation with the internal solver

The second example involves neutron dosimeter activation calculation for the surveillance chains in a VVER-440 reactor. The study is related to the monitoring of structural integrity of the Loviisa-1 and -2 reactor pressure vessels, and the purpose was to evaluate the viability of using Serpent for this task in the future [14]. The results are for the most part proprietary, but for the purpose this paper it is sufficient to compare the relative differences between the analog and implicit simulations, together with the associated performance indicators.

[1] An exception to this is the radioactive decay source mode [6], in which the spatial variation in photon emission rate can be accounted for by adjusting the weight.

The geometry in the test case was a simplified 3D model of the Loviisa VVER-440 reactor (the various simplifications are discussed in Ref. [14]). The simulations were run in external source mode with fissions switched off. The neutron source was obtained by combining the full-core power distribution from the HEXBU nodal diffusion code [15] with assembly-wise power distributions calculated using Serpent. The surveillance chains are positioned in the space between core barrel and pressure vessel wall. The flux is determined using activation measurements consisting of 8 dosimeters listed in Table I. The main challenge in the modeling of these experiments was getting sufficient statistics for the high-energy reactions. The detector was positioned outside the barrel 5.7 cm below core mid-plane, and modeled by calculating track-length estimates inside a 2 cm diameter sphere. The same detector was used as the response for the importance mesh solver.

The core geometry was covered by a 50×50×70 regular Cartesian mesh, and the importances were calculated using the built-in response-matrix based solver. The resulting importance mesh is illustrated in Fig 4. It is seen that neutrons that contribute to the results are mostly born in the outer region of the core. The results are presented in Table I. Similar to the transport cask shielding calculation, the differences between the analog and implicit simulation are within the range of statistical accuracy, although the relative statistical errors in the reference results are relatively large.

The reference results were obtained by running an analog Monte Carlo simulation with 500 billion (5×10^{11}) neutron histories. The same calculation was then repeated with 200

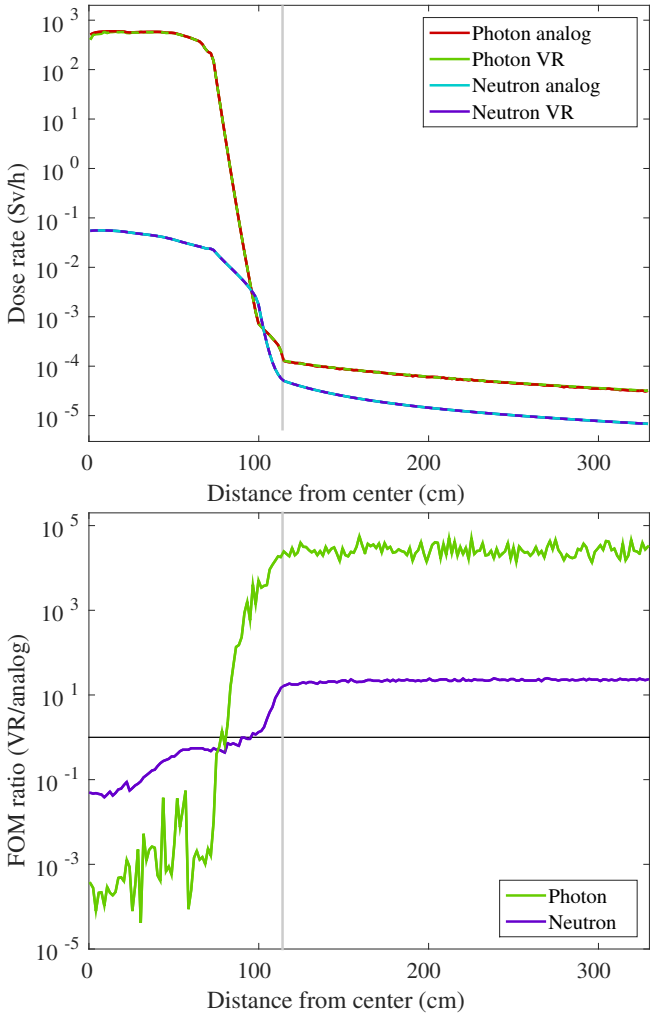

Fig. 3. Neutron and photon radiation dose rates calculated for the TN-24P transport cask using Serpent 2 with and without variance reduction. Top: dose rates as function of radial distance. Bottom: FOM ratios showing the efficiency gain from the use of variance reduction. The vertical line marks the outer radius of the transport cask.

billion histories applying the variance reduction scheme based on the built-in light-weight importance mesh solver. Both calculations were run with OpenMP parallelization in a 20-core 2.2 GHz Intel Xeon cluster node. The analog simulation run for 1478 hours. The use of variance reduction reduced the running time to only 68 hours, as only a small fraction of the simulated histories were started in a region in which the importance was high enough to survive the Russian roulette. Transport simulation for producing the importance mesh took 3 hours, and the response matrix solution converged in less than 30 seconds.

The comparison shows that the weight-window based variance reduction scheme leads to a factor of 500-2700 improvement in computational efficiency. As mentioned above, the built-in importance solver does not yet support energy discretization. In this test case particles of all energies contributed in the results, as the detector responses included both threshold and non-threshold reactions. This is not always the case, and the use of a multi-group weight-window mesh will generally lead to higher performance. Energy dependence becomes important in particular in dose rate calculations, in which the radiation damage depends on particle energy.

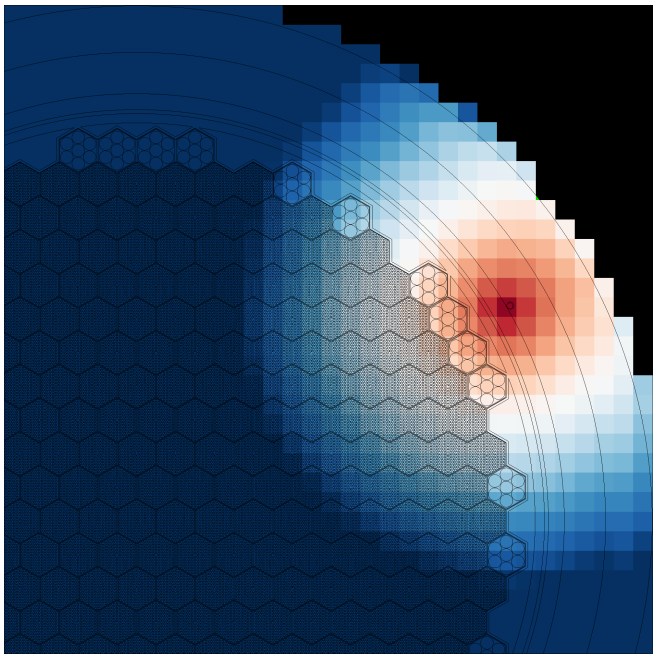

Fig. 4. Serpent geometry plot showing a quadrant of the VVER-440 reactor core, together with the importance mesh produced by the built-in response-matrix based solver. The color scheme is logarithmic, and extends from blue (low importance) to red (high importance). The importance peaks at the position where the detector is located.

IV. SUMMARY, DISCUSSION AND FUTURE PLANS

A weight-window based variance reduction scheme was implemented in the Serpent 2 Monte Carlo code version 2.1.27, released in September 2016. The importance mesh can be provided by an external calculation tool or obtained from a previous Serpent calculation using a built-in light-weight solver based on the response-matrix method. The methodology was put to test in two calculation cases. An importance mesh produced by SCALE / MAVRIC was used in a shielding calculation involving a spent fuel transport cask and photon and neutron sources from radioactive decay. The use of the light-weight solver was demonstrated in a reactor calculation, in which the ex-core flux was determined using neutron dosimeters.

The use of variance reduction showed a considerable gain in computational efficiency in both test cases. In the shielding calculation the figure-of-merit for photon dose rate outside the transport cask was increased by a factor of 10,000 compared to an analog reference calculation. In the ex-core dosimetry calculation the use of the built-in importance solver enabled obtaining acceptable statistics within a reasonable calculation

TABLE I. Results of the VVER-440 ex-core dosimetry calculation. The first three columns provide the detector materials, reactions and threshold energies, followed by the relative difference between the results (the actual results are proprietary) given by analog and implicit simulations, relative statistical errors and figure-of-merits. The last column shows the gain in computational efficiency (ratio of FOM's). Differences and statistical errors are in percent. The reference analog simulation was run for two wall-clock months (1478 hours) and the implicit simulation with variance reduction for 68 hours. Transport simulation for producing the importance mesh took 3 hours. The response matrix solution converged in less than 30 seconds.

Detector	Reaction	E_{min}	Diff.	$\mathrm{Err}_{\mathrm{ana}}$	$\mathrm{Err}_{\mathrm{vr}}$	$\mathrm{FOM}_{\mathrm{ana}}$	$\mathrm{FOM}_{\mathrm{vr}}$	Gain
Iron-54	^{54}Fe (n,p)^{54}Mn	2.2 MeV	3.0	3.2	0.6	1.07E-02	7.16E+00	× 671
Nickel-58	^{58}Ni (n,p)^{58}Co	1.8 MeV	3.3	2.9	0.5	1.38E-02	9.32E+00	× 673
Copper-63	^{63}Cu (n,α)^{60}Co	4.7 MeV	0.6	8.9	1.9	1.41E-03	7.08E-01	× 503
Titanium-46	^{46}Ti (n,p)^{46}Sc	3.7 MeV	2.8	5.7	1.1	3.47E-03	1.90E+00	× 549
Niobium-93	^{93}Nb (n,n') $^{93\mathrm{m}}$Nb	0.8 MeV	2.2	1.2	0.2	7.41E-02	5.28E+01	× 713
Cobalt-59	^{59}Co (n,γ)^{60}Co	-	0.0	1.3	0.1	7.15E-02	1.64E+02	× 2297
Niobium-93	^{93}Nb (n,γ)^{94}Nb	-	-1.0	2.4	0.2	1.91E-02	5.19E+01	× 2711
Iron-58	^{58}Fe (n,γ)^{59}Fe	-	0.3	1.0	0.1	1.20E-01	2.39E+02	× 1995

time. Reaching a similar level of statistical accuracy would have required running an analog simulation for several CPU-years. Both test cases also showed that the results obtained using the weight-window based variance reduction scheme reproduced the reference results to within statistics, which suggests that the methodology works as expected, without introducing any computational biases in the simulation.

The methodology used for variance reduction in Serpent 2 is still very much under development. There are currently several limitations that need to be addressed:

i) The MCNP format weight-window mesh structure currently supports only regular Cartesian mesh with uniform spacing. In order to provide full support for the state-of-art importance calculation tools, also cylindrical and multi-dimensional formats need to be included.

ii) Source biasing is currently limited to killing particles with Russian roulette if the importance at the source point is low. More efficient means for sampling from a biased source distribution will be studied in the near future.

iii) The built-in light-weight response-matrix based solver currently lacks energy dependence in the solution. This is a major deficiency that clearly affects the performance of the variance reduction scheme, especially in radiation dose rate calculations where the particle energy plays a major role.

It is not likely that the built-in light-weight solver could replace external tools in the production of importance meshes, at least in the most challenging calculation cases. Even so, the method offers certain interesting possibilities for future studies. One of the advantages of the response-matrix method is that even though the solution is currently obtained in a regular Cartesian or cylindrical mesh, the method is not bound to any spatial discretization, and the actual algorithm is completely dimensionless. This means that the solution could be relatively easily extended to adaptive Cartesian or even completely unstructured meshes, which are already used in some of the advanced geometry types supported by the Serpent 2 code [16, 17].

The implementation of variance reduction methods in Serpent 2 is part of an on-going effort to broaden the scope of applications beyond reactor physics. The focus is particularly on radiation transport and fusion neutronics [5, 6].

V. ACKNOWLEDGMENTS

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