Application of Adaptive Multilevel Splitting on Coupled Neutron-Photon TRIPOLI-4 Monte Carlo Simulations

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APPLICATION OF ADAPTIVE MULTILEVEL SPLITTING ON COUPLED NEUTRON-PHOTON TRIPOLI-4® MONTE CARLO SIMULATIONS

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In the context of radiation protection simulations, the Adaptive Multilevel Splitting (AMS) algorithm is a challenging variance reduction (VR) technique that has been recently investigated in the field of particle transport simulation. It has been implemented in the forthcoming version 11 of the Monte Carlo code TRIPOLI-4® and successfully tested in neutron-only and photon-only configurations. This paper addresses the application of the AMS algorithm to coupled simulations, and particularly to neutron-photon Monte Carlo calculations. The branching process occurring during the Monte Carlo coupled transport is taken into account in the new coupled-AMS algorithm and is explained in this paper. Two different neutron-photon configurations are then investigated, leading to a comparison of the coupled-AMS algorithm with the analog simulation on the one hand, and with the Exponential Transform (ET) on the other hand, which is the standard VR technique of TRIPOLI-4. Gains up to 30 are obtained in terms of Figure of Merit relatively to the analog simulation, which is about 4 to 6 times more efficient than the ET method for these configurations.

I. INTRODUCTION

Radiation protection simulations performed with Monte Carlo transport codes usually require efficient variance reduction (VR) techniques, so as to provide mean results of the quantities of interest with a satisfactory variance in a reasonable computation time. In this context, the Adaptive Multilevel Splitting (AMS) algorithm is a challenging VR technique that has been recently investigated in the field of particle transport simulation[1-3]. It has been implemented in the forthcoming version 11 of the Monte Carlo code TRIPOLI-4®[†] (Ref. 4) and successfully tested in neutron-only and photon-only configurations[1-3]. This paper addresses the application of the AMS algorithm to coupled simulations, and particularly to neutron-photon Monte Carlo calculations (i.e. simulating a neutron source, neutron transport, photon production induced by neutron reactions and photon transport, and estimating photon tallies). The biasing scheme adjustment required for those coupled simulations is known to be sometimes complicated: primary and secondary particles do not necessarily require

the same biasing scheme, and moreover, it is not always easy for the code user to guess how to define a biasing scheme for primary particles that would be efficient when tallying secondary particles. The branching process occurring during the Monte Carlo coupled transport is taken into account in the new coupled-AMS algorithm[1] and is explained in this paper: Section II is a brief remainder of the main principles of the AMS algorithm, followed by the extension to the new coupled-AMS algorithm. Section III presents the different importance functions used by the coupled-AMS algorithm in the examples of the following section. Two different neutron-photon configurations are then investigated in Section IV, leading to a comparison of the coupled-AMS algorithm with the analog simulation on the one hand, and with the Exponential Transform (ET), which is the standard VR technique of TRIPOLI-4, on the other hand.

II. MAIN PRINCIPLES OF THE AMS ALGORITHM

The AMS method applied to particle transport is a splitting method based on an iterative process[1-3]. The algorithm for coupled simulations[1] works in a similar way to the AMS for single-particle simulations, with a more complex management of importance functions and particles sorting[1]. We first recall the main principles of the AMS algorithm for single-particle simulations (e.g. neutron-only or photon-only simulations) and then explain the extensions needed for the coupled case (e.g. neutron-photon simulations).

II.A. AMS algorithm for single-particle simulations

In this Subsection, we address the case of neutron-only simulations, but similar steps could also be described for photon-only simulations.

II.A.1. Algorithm steps

i) For a given iteration, neutron trajectories are sampled in the phase space in an analog Monte Carlo way and are then sorted with respect to the maximum of a given importance function evaluated along the tracks. Each track is composed of the source point, the different flies between collisions and the different collision points of the trajectory. Neutron importance is defined either with a spatial dependency only, or based on space and

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[†] TRIPOLI-4® is a registered trademark of CEA.

energy importance maps pre-calculated by TRIPOLI-4 (as detailed in Section III of this paper). For each iteration of the algorithm, the sorting process allows for the definition of a splitting importance level, which adaptively distinguishes the most interesting simulated particles from the others.

ii) All tracks with an importance below the splitting level are removed from the simulation, and resampled by duplicating some of the better ranking trajectories at their intersection with the current splitting level. In practice, the first point of the track whose importance is above the level is defined as splitting point. The splitting rate is typically 10 percent of the number of source neutrons simulated in a TRIPOLI-4 batch (TRIPOLI-4 sets the default value to 10 percent but this can be changed by the user if needed). This splitting rate can also be seen as the number of neutrons which do not reach the splitting level of the current iteration.

iii) A stopping criterion is tested. It is related to the splitting rate k of the AMS simulation: the iterative process ends when the kth-worst track has reached the target volume defined by the user.

iv) Finally, the following multiplicative correction is applied to the usual Monte Carlo neutron tally:

$$\alpha = \left(1 - \frac{k}{n}\right)^N \qquad (1)$$

where k stands for the splitting rate, n for the number of source neutrons in each simulated batch and N for the number of completed AMS iterations.

II.A.2. Remarks

As an option of Step i), the implicit capture can also be used instead of a full analog simulation mode. However, neutron transport between collisions remains analog when using the AMS algorithm.

The estimation of the requested tally is unbiased[4] after multiplying by the α factor, given by Equation (1), the statistical weight of neutrons reaching the target volume.

II.B. Extension to the coupled-AMS algorithm

II.B.1. Extensions of the previous algorithm steps

In the case of coupled neutron-photon simulations, Step i) of the previous algorithm is replaced by the Monte Carlo analog sampling of both neutron and photon trajectories.

To meet the needs of the AMS algorithm, each track becomes a tree-structure composed of a neutron trajectory and all secondary branches resulting from photon production induced by neutron reactions (and possibly also photo-atomic reactions), as illustrated by Figure 1.
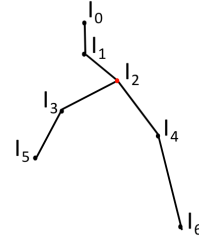

Fig. 1. Example of branching track with a tree-type track structure (the importance in this configuration is assumed to increase from top to bottom of the figure, i.e. with $I_0 < I_1 < I_2 < I_3 < I_4 < I_5 < I_6$, and with importance I_2 at the branching point in red).

In addition, a threshold value is defined for each branch in the following way: the neutron branch has a zero threshold value and, for each photon branch, the threshold is set to the neutron importance value at the collision point prior to the photon production (red point with importance I_2 in Figure 1).

Concerning the sorting process, neutron importance and photon importance functions can be defined separately, with the same possibilities than previously described for neutron importance at Step i) of Subsection II.A.1 (and detailed in Section III of this paper). The importance of the whole track is defined as the maximum importance of all branches within the track.

In Step ii), when a track is removed, all the branches that compose this track are deleted from the simulation. The splitting process for a track selected for duplication (i.e. with an importance greater than the current splitting level) is more delicate in the coupled case. Each branch of this track has to be examined, actually leading to three different possible situations illustrated in Figure 2:

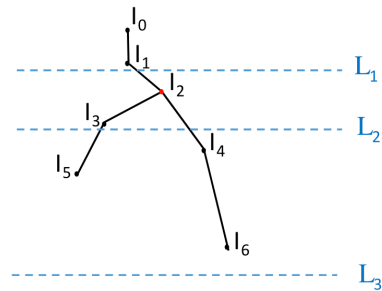**Fig. 2.** Example of splitting levels shown in dashed blue lines (it is assumed that $L_1 < I_2$, $I_2 < L_2 < I_5$ and $I_6 < L_3$).

- the splitting level is less than the threshold of the branch: in this case, the (photon) branch is not duplicated because the duplication only concerns the inducing neutron (which already had an importance greater than the splitting level when the photon was produced). For

example, the splitting level L_1 is less than the threshold I_2 in Figure 2.

- the splitting level is greater than the branch threshold but less than the branch importance, either for a source neutron or for a photon: the first point of the branch whose importance is above the level is then defined as splitting point. For example, the splitting level L_2 is greater than the threshold I_2 but less than the branches importance I_5 and I_6 in Figure 2.

- the splitting level is greater than the branch importance (splitting level L_3 in Figure 2 for example): then, the (neutron or photon) branch is not duplicated, by definition of the duplication, as introduced in Step ii) of Subsection II.A.1.

Finally, the same multiplicative correction (1), as introduced in Step iv) of Subsection II.A.1, is applied to the usual Monte Carlo photon tally, the splitting rate k being global for the whole tracks and n standing for the number of source neutrons.

II.B.2. Remarks

As an option of Step i), the photon production induced by neutron reactions can also be biased, by artificially increasing the photon multiplicity by a reasonable factor (2 to 10 for example) and correcting the photon statistical weights accordingly.

We also mention that the photon production, sampled by accessing only to the averaged probability density data available in the evaluated data files, is generally not analog but can be handled as it is by the coupled-AMS algorithm. Coupled neutron-photon TRIPOLI-4 simulations are currently working this way (photon production is for the moment not analog, even if the analog neutron transport mode is activated).

III. IMPLORTANCE FUNCTIONS USED BY THE AMS AND COUPLED-AMS ALGORITHMS

As mentioned in Subsections II.A.1 and II.B.1, different importance functions (needed by the sorting process of the AMS and coupled-AMS algorithms) can be chosen for neutrons and for photons. This choice is even independent for each type of particle and has to be made in accordance with the type of configuration and transport problem to simulate.

III.A. Spatial importance function

The simplest importance function to be tried with the AMS and coupled-AMS is defined by the inverse of the distance between the current particle and the target volume. When used in the same simulation for neutrons and photons, no importance normalization concern comes up during the sorting process. Even if this importance function does not include any energy dependency, it can be handled successfully by the AMS and coupled-AMS algorithms.

Several simple spatial functions are actually available: the inverse of the distance to a point, a line, a plane, a sphere, a cylinder or a ring. The distance instead of the inverse of the distance can also be chosen, for repulsive effects instead of attractive ones. In this paper, only the cases of attraction towards a point and towards a plane have been used.

III.B. Space and energy importance map pre-calculated by TRIPOLI-4

The INIPOND module of TRIPOLI-4 pre-calculates an importance map for the needs of its standard VR technique, based on the ET method. A brief description of the INIPOND module follows, for further details the reader is referred to Refs. 5 and 6. The importance function is factorized in space, energy, angle and time, with a coupling between space and energy variables. The user has to define a space and energy grid and to specify the areas of interest or "attractors". A strength parameter β must also be set, typically between 0 and 1, which makes the attraction of particles towards the areas of interest more or less strong.

This pre-calculation step can be performed for each type of particle of the simulation, or only for some of them, as requested by the user (for example, only for neutrons or only for photons in a coupled neutron-photon simulation). Even if the ET is not used afterwards during the simulation, these pre-calculated maps can be used by the sorting process of the AMS or coupled-AMS algorithms. The advantage of this kind of importance function relies in better taking into account the energy variable of the transport problem, at least if the pre-calculated map was able to catch an energy dependency, in addition to the space dependency.

III.C. Other available importance functions

Other importance functions have been implemented in the frame of the AMS algorithm, such as those useful in streaming configurations[3] for example, but we have listed in this section only importance function types that were used in the following section of this paper.

IV. INVESTIGATION OF TWO COUPLED NEUTRON-PHOTON CONFIGURATIONS

In order to investigate the efficiency of the coupled-AMS algorithm, we simulated two different neutron-photon configurations with TRIPOLI-4 and, for each of them, we compared the FOM results with the analog simulation and with simulations using the standard ET method of TRIPOLI-4.

IV.A. Photon dose calculation in a slab configuration

IV.A.1. Configuration

This neutron-photon configuration has already been studied with TRIPOLI-4 in a previous work[6] using the

standard ET method of TRIPOLI-4. It consists of a neutron source (with a Watt spectrum) placed in a paraffin collimator, a cylindrical detector of photon dose rate placed in the air and, in between, a slab configuration alternating five stainless steel and five polyethylene slabs, with a thickness of 5 cm each and separated by a 0.5 cm layer of air. Photon production takes place in the different slabs, along the neutron trajectories. Figure 3 shows a two-dimensional view of this configuration.
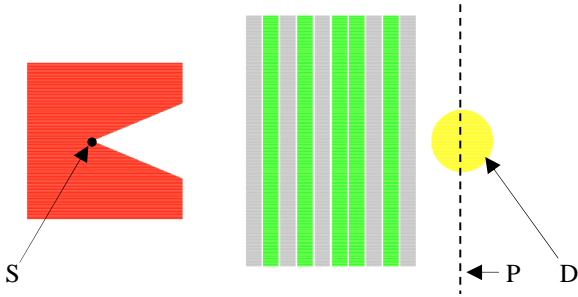

Fig. 3. 2D-view of the configuration (the neutron source S is placed at the cone apex of the red left part, the photon detector D on the yellow cylinder at the right part, the stainless-steel slabs are shown in gray and the polyethylene slabs in green. Plane P is used in the following Subsection).

IV.A.2. Results

An analog neutron-photon TRIPOLI-4 simulation of this configuration was first performed. Then, simulations using variance reduction techniques, either the standard ET method or the coupled-AMS method were compared.

The parameters of the ET method were calculated automatically by the code[5,6] on a space and energy grid with 5 energy groups. A discrete attractor was placed in the middle of the detector volume and the strength parameter β was set to 1 (if needed by the reader, Subsection III.B recalls the parameters to be set by the user for the pre-calculation of the importance map by the code). Only photon transport was simulated with this VR technique, since it turned out to produce the best results in terms of FOM for this configuration, according to Ref. 6. Photon production was also biased by multiplying the photon yield by a factor of 10 in the stainless-steel slabs, as recommended by Ref. 6 as well.

For the AMS needs, the photon detector volume was defined as target and different importance functions for neutrons and photons were successively tried. AMS for only one of the particles was also tried. In the following, plane P (shown in Figure 3) is the plane placed in the middle of the detector and point C is placed at the center of the detector. In Table I:

- "coupled-AMS1" refers to a coupled-AMS algorithm with a spatial neutron importance function attracting neutrons towards plane P and a spatial photon importance function attracting photons towards point C

- "coupled-AMS2" refers to a coupled-AMS algorithm with spatial neutron and photon importance functions attracting both neutrons and photons towards point C

- "coupled-AMS3" refers to a coupled-AMS algorithm with space and energy importance maps for neutrons on the one hand and for photons on the other hand, chosen for neutron and photon importance functions (as presented in Subsection III.B, with a choice of parameters detailed at the beginning of the current Subsection)

- "coupled-AMS4" refers to a coupled-AMS algorithm with a spatial neutron importance function attracting neutrons towards plane P and a space and energy importance map chosen for the photon importance function (as presented in Subsection III.B, with a choice of parameters detailed at the beginning of the current Subsection)

- "AMSn1" refers to an AMS algorithm for neutrons only, with a spatial importance function attracting neutrons towards plane P

- "AMSg1" refers to an AMS algorithm for photons only, with a spatial importance function attracting photons towards point C.

Table I shows different results obtained: photon dose rates (actually dose equivalent rates H*(10)), with their relative standard deviations σ, are presented in order to check the absence of any bias in the results and FOM (defined as the inverse of the product of the variance of the tally and the calculation time) are presented and also compared after normalization by the FOM of the analog simulation.

TABLE I. Photon dose rate and FOM results: comparison of analog, ET, coupled-AMS and AMS simulations

VR technique	dose rate (μSv/h) $\pm\ \sigma$ (%)	FOM (and normalized)
Analog	$1.063e^3 \pm 3.650$	$4.255e^{-3}$ (1)
E.T	$1.029e^3 \pm 1.387$	$1.940e^{-2}$ (4.56)
coupled-AMS1	$1.036e^3 \pm 0.804$	$1.088e^{-1}$ (25.57)
coupled-AMS2	$1.034e^3 \pm 0.820$	$1.048e^{-1}$ (24.63)
coupled-AMS3	$9.914e^2 \pm 2.247$	$8.321e^{-3}$ (1.96)
coupled-AMS4	$1.040e^3 \pm 1.879$	$2.848e^{-2}$ (6.69)
AMSn1	$1.009e^3 \pm 1.449$	$1.335e^{-2}$ (3.14)
AMSg1	$1.059e^3 \pm 2.823$	$1.817e^{-2}$ (4.27)

The comparison of photon dose rate results from Table I shows that all mean results obtained using the coupled-AMS algorithm are compatible with those of the analog and ET simulations (the 3 sigma confidence intervals overlap).

Moreover, simulations with the coupled-AMS VR technique are more efficient than the analog simulation, and most of them are also more efficient than the ET simulation. Relatively to the analog simulation, FOM gains up to 25.57 are obtained, which is about 5 times better than the FOM gains obtained with the ET method. Best results are obtained with the choices coupled-AMS1 and coupled-AMS2 which consist in coupled-AMS with spatial importance functions for both neutrons and photons. For this configuration, the use of space and energy importance maps for both neutrons and photons (i.e. coupled-AMS3 choice), or for photons instead of a spatial importance function (i.e. coupled-AMS4 choice) does not improve the efficiency of the simulation, when compared to the coupled-AMS1 and coupled-AMS2 cases. Finallly, when the AMS algorithm is used for photons only or neutrons only (i.e. AMSg1 and AMSn1 choices), the FOM gains are lower, which shows that, for this neutron-photon configuration, a coupled-AMS algorithm is more efficient than a simple AMS for only one of the particle types.

IV.B. Photon fluxes and kerma calculation in the NESDIP neutron-photon benchmark

IV.B.1. Configuration

The neutron-photon NESDIP benchmark we are referring to in this paper consists in one of the experiments performed in the ASPIS facility of the NESTOR reactor at Winfrith AEA, in UK. This experiment took place in 1987 and aimed at validating coupled neutron-photon transport calculations in a shield of iron and water[7]. The neutron source was generated in a ^{235}U fission plate (placed in a volume between 26.61 cm to 26.81 cm along Z axis). Neutron activation detectors and gamma ray TLD were positioned on the horizontal center line of the configuration, at different depths along Z axis. Figure 4 shows a two-dimensional view of this configuration, where the deeper photon detector positions are marked with black points. In this paper, only the tally results for photon fluxes and photon kerma responses at the deeper detectors (ranging from 58.6 cm to 93.69 cm) are investigated (neutron results are not examined). In this Section, results are presented only for the deepest detector at 93.69 cm (i.e. at around 67 cm from the fission source) and are not collected at point D position but on the width of Figure 4: the flux tally is integrated on plane Q. The benchmark measurements are not compared with the calculation results here, only TRIPOLI-4 calculations results using different VR techniques are compared with one another.
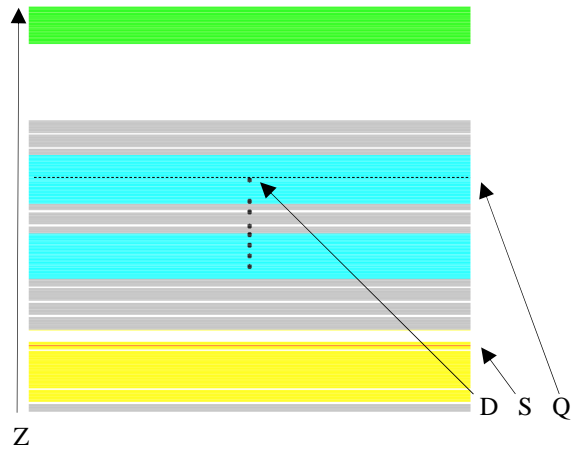

Fig. 4. 2D-view of the configuration (the neutron source S is shown in red, iron in gray, water in cyan, concrete in green, air in white, other materials such as lead, aluminum, bore and graphite in yellow, TLD positions are marked in black and D is the deepest photon detector. Z axis is oriented from the bottom to the top of the figure. Plane Q is used in the following Subsection).

IV.B.2. Results

An analog neutron-photon TRIPOLI-4 simulation of this configuration was first performed. Then, simulations using variance reduction techniques, either the standard ET method or the coupled-AMS method were compared.

The parameters of the ET method were calculated automatically by the code[5,6] on a space and energy grid with 4 neutron groups and 2 photon groups. A discrete neutron attractor was placed behind detector D of Figure 4 and the associated strength parameter β was set to 1.5 for neutron biasing. Additionally, neutrons of energy higher than 1 MeV were favored, with the use of the exponential form of the energy biasing (available in the INIPOND module[5,6]) for neutrons in those groups. A discrete photon attractor was placed at the same position as for the neutron attractor and the associated strength parameter was set to 0.5 for photon biasing.

For the AMS needs, the volume just behind detector D (along Z axis) was defined as target and different importance functions for neutrons and photons were successively tried. AMS for only one of the particles was also tried. In the following, plane Q (shown in Figure 4) refers to the plane placed at 93.69 cm, orthogonal to Z axis. In Tables II and III:

- "coupled-AMS5" refers to a coupled-AMS algorithm with spatial neutron and photon importance functions attracting both neutrons and photons towards plane Q

- "coupled-AMS6" refers to a coupled-AMS algorithm with a spatial neutron importance function attracting neutrons towards plane Q and a space and energy

importance map chosen for the photon importance function (as presented in Subsection III.B, with a choice of parameters detailed at the beginning of the current Subsection)

- "coupled-AMS7" refers to a coupled-AMS algorithm with space and energy importance maps for neutrons on the one hand and for photons on the other hand, chosen for neutron and photon importance functions (as presented in Subsection III.B, with a choice of parameters detailed at the beginning of the current Subsection)

- "AMSg2" refers to an AMS algorithm for photons only, with a space and energy importance map chosen for the photon importance function (as presented in Subsection III.B, with a choice of parameters detailed at the beginning of the current Subsection).

For the ET simulation and for all coupled-AMS and AMS simulations of this subsection, photon production was also biased by multiplying the photon yield by a global factor of 2.

Table II and Table III show different results obtained: photon fluxes (integrated in energy and on plane Q) in Table II, and photon kermas (integrated on plane Q) in Table III, are presented with their relative standard deviations σ. FOM are also presented, followed by their normalization by the FOM of the analog simulation.

TABLE II. Photon flux and FOM results: comparison of analog, ET, coupled-AMS and AMS simulations

VR technique	flux (photon/s) $\pm \sigma$ (%)	FOM (and normalized)
Analog	$2.373e^1 \pm 3.238$	$1.423e^{-2}$ (1)
E.T	$2.389e^1 \pm 1.495$	$1.330e^{-1}$ (9.35)
coupled-AMS5	$2.389e^1 \pm 1.790$	$2.946e^{-1}$ (20.70)
coupled-AMS6	$2.426e^1 \pm 1.712$	$4.478e^{-1}$ (31.47)
coupled-AMS7	$2.402e^1 \pm 1.785$	$1.348e^{-1}$ (9.47)
AMSg2	$2.340e^1 \pm 1.727$	$3.775e^{-1}$ (26.53)

TABLE III. Photon kerma and FOM results: comparison of analog, ET, coupled-AMS and AMS simulations

VR technique	kerma (MeV/(cm.s)) $\pm \sigma$ (%)	FOM (and normalized)
Analog	$3.187e^{-1} \pm 2.929$	$1.740e^{-2}$ (1)
E.T	$3.173e^{-1} \pm 2.833$	$3.704e^{-2}$ (2.13)
coupled-AMS5	$3.247e^{-1} \pm 2.817$	$1.189e^{-1}$ (6.83)
coupled-AMS6	$3.413e^{-1} \pm 2.856$	$1.599e^{-1}$ (9.20)
coupled-AMS7	$3.235e^{-1} \pm 3.234$	$4.107e^{-2}$ (2.36)
AMSg2	$2.954e^{-1} \pm 2.989$	$1.260e^{-1}$ (7.24)

The comparison of the tally results, respectively from Table II, then from Table III, shows that all mean results of flux and kerma obtained using the coupled-AMS algorithm are compatible with those of the analog and ET simulations (the 3 sigma confidence intervals overlap).

In terms of FOM, whatever the choice of neutron and photon importance functions (among those presented here), the coupled-AMS method is always more efficient than the analog simulation, and also than the ET simulation. Satisfactory FOM gains seem more difficult to achieve for the photon kerma response than for the photon flux response, most probably because of the shape of the response function, which increases with photon energy. Best FOM results are obtained with the choice coupled-AMS6: relatively to the analog simulation, FOM gains up to 31.47 for photon fluxes and 9.20 for photon kermas are obtained, which is about 3 to 4 times better than the FOM gains obtained with the ET method. The energy dependency taken into account by the photon importance map seems to have a positive impact on the behavior of the simulation with the coupled-AMS method for this configuration. However, when space and energy neutron maps are used for both particle types (i.e. coupled-AMS7 choice), the global FOM efficiency drops. As a remark, when using more energy groups for the photon importance map of case coupled-AMS6 (e.g., 4 groups instead of 2), the results (not shown in Tables II and III) are not better in terms of FOM gains. And last, in the same way as for the previous neutron-photon configuration, when the AMS algorithm is used for photons only (i.e. AMSg2 choice), the FOM gains are a bit lower, which shows that, for this neutron-photon configuration, a coupled-AMS algorithm turns out to be more efficient than a simple AMS for only one of the particle types (results with AMS for neutrons only are not shown here but are not better).

V. CONCLUSIONS

This paper is in line with ongoing work on the AMS algorithm recently implemented in the Monte Carlo code TRIPOLI-4 and successfully tested as VR technique in neutron-only and photon-only simulations[1-3]. The new coupled-AMS algorithm has been addressed here: its specificities, on the basis of the AMS algorithm, have been detailed in this paper. Two application examples have then been investigated in the context of coupled neutron-photon transport calculations. The efficiency of the method was examined in terms of FOM results. Interesting efficiency results were obtained when using the coupled-AMS VR technique, which behaved better than the analog simulation, but also better than an ET simulation, and at last better than simulations using the AMS algorithm for only one of the particle types. Similarly to the AMS algorithm for single-particle simulations, the coupled-AMS algorithm turned out to be an interesting alternative to the standard VR technique of TRIPOLI-4 based on the ET method. The coupled-AMS method could also be used in the frame of photon-electron-positron spectrometry simulations, enabling the

use of a VR technique in TRIPOLI-4 spectrometry simulations with multiple particle types.

ACKNOWLEDGMENTS

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