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EVALUATING IMPORTANCE MAPS FOR TRIPOLI-4® USING DETERMINISTIC OR ON-LINE METHODS

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Variance reduction is a key ingredient for solving radiation-protection problems with Monte-Carlo particle-transport codes. Many variance-reduction methods require the definition of an importance map and exhibit optimal performance if the importance map is given by the adjoint flux, the solution of the adjoint Boltzmann equation.

This paper presents the implementation of the Consistent Adjoint-Driven Importance Sampling (CADIS) methodology via a coupling between the TRIPOLI-4® Monte-Carlo particle-transport code and the IDT deterministic solver, Additionally, we describe the implementation of a new TRIPOLI-4® score that makes it possible to estimate the adjoint flux during a direct Monte-Carlo calculation. These new features are expected to simplify the solution of difficult shielding problems.

I. INTRODUCTION

Monte-Carlo particle-transport codes are often the tool of choice for performing quantitative radiation-protection studies. This is mainly motivated by their reference character (i.e. the solution method does not involve any serious approximation) and by their powerful geometrical modelling capabilities. However, the response of a particle detector in a strongly attenuated radiation field, by construction, involves very rare events. The estimation of such a response via Monte-Carlo methods is inevitably computationally intensive. Radiation-protection problems, by definition, fall into this class, and are therefore intractable with Monte-Carlo methods unless suitable *variance-reduction* techniques are applied.

Generally speaking, variance-reduction techniques consist in modifying the estimators and the rules of the Monte-Carlo game in a way that preserves the expected values of the response estimators, while at the same time reducing the expected estimator variance for a given computational effort. The efficiencies of different Monte-Carlo estimates of the same quantity can be compared using the *figure of merit* (FOM), which is formally defined as

$$\mathrm{FOM} = \frac{1}{T \cdot \sigma^2(T)}.$$

Here T is the elapsed calculation time, and $\sigma^2(T)$ is the variance of the considered estimator, which in general is expected to be asymptotically proportional to $1/T$. In practice, the variance of the estimator is usually unknown, but it can be estimated from the sampled events.

Many variance-reduction methods, at some point, need to evaluate how *important* a particle track is, i.e. how promising it looks for the purpose of estimating the desired response. This information may be used to decide if the track is worth following. In some schemes, important tracks are split (duplicated) and unimportant ones are rouletted (possibly killed); in other schemes, the importance of the particle track is used to modify the laws of tracking in order to push the particle towards more important regions. Regardless of the details of the method, it is up to the user to assign an importance to each point of phase space. A function mapping points in phase space to importance values is generally known as an *importance map*.

Of course, the FOM for a Monte-Carlo calculation using variance reduction depends on the chosen importance map. Good importance maps yield a smaller variance (and thus a larger FOM) for a given computational effort. A special role in this context is played by the *adjoint flux*, i.e. the solution $\phi^\dagger$ to the adjoint stationary fixed-source Boltzmann equation[1]:

$$\begin{aligned} -\boldsymbol{\Omega}\cdot\nabla\phi^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega}) + \Sigma_t(\boldsymbol{r},E)\,\phi^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega}) = \\ \int \Sigma_s(\boldsymbol{r},E,\boldsymbol{\Omega}\to\boldsymbol{r},E',\boldsymbol{\Omega}')\,\phi^\dagger(\boldsymbol{r},E',\boldsymbol{\Omega}')\,\mathrm{d}\boldsymbol{\Omega}'\mathrm{d}E' \\ + Q^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega}). \quad (1) \end{aligned}$$

Here $(\boldsymbol{r},E,\boldsymbol{\Omega})$ represent the coordinates in phase space, Σ_t is the total macroscopic cross section, Σ_s is the macroscopic double-differential scattering cross section (for the purpose of this work, fission is considered as included in the scattering kernel) and $Q^\dagger$ is the adjoint source. It is well known that, if $Q^\dagger$ is interpreted as a detector response function, the average expected contribution to the detector from a point $(\boldsymbol{r},E,\boldsymbol{\Omega})$ is a solution of the adjoint equation, Eq. (1)[1]. Thus, in some sense, the adjoint flux can be naturally taken as an indication of the importance of a point in phase space.

It is actually possible to make a stronger statement. For a certain class of variance-reduction algorithms for neutron transport, it has been shown that the adjoint flux results in a *zero-variance* game[2]: this essentially means that every particle history yields exactly the same contribution to the sought response. In order for this to happen, particle histories must not be killed by mechanisms such as Russian roulette and must be allowed to last forever[3]. However, simulation schemes with truncated particle histories still yield excellent FOMs; this is perhaps not obvious, but it has been

empirically verified[3]. As far as it is understood, simulation schemes with truncated histories employing the adjoint flux as an importance map are very nearly optimal.

These remarks trigger two important considerations. First, it is clearly interesting to leverage approximate methods to compute the adjoint flux and use this as an importance map in Monte-Carlo calculations; the use of deterministic solvers for the adjoint Boltzmann equation has indeed given rise to the Consistent Adjoint-Driven Importance Sampling (CADIS) family of methodologies, which has been reviewed by Haghighat and Wagner in Ref. 4. The CADIS methodology has amply proven its worth, as shown in many recent studies; see e.g. Refs. 5–7. Second, the average contribution of particles emitted from a point in phase space is actually accessible during direct Monte-Carlo calculations, at least for the points in phase space that are frequently explored. Therefore, it is conceivable to use the information contained in the particle tracks of the direct Monte Carlo calculation to improve the knowledge of the adjoint flux and thus the efficiency of the importance map *during the direct simulation itself*.

The goal of this work is likewise twofold. We present the development of two new functionalities of the TRIPOLI-4® Monte-Carlo particle-transport code[8] that simplify the construction of an efficient importance map. First, a development version of TRIPOLI-4 has been coupled with the deterministic transport solver IDT[9]. The coupling allows users to seamlessly invoke IDT for the construction of the importance map, without having to convert the TRIPOLI-4 simulation geometry to another format. Multigroup cross sections are automatically condensed and homogenized. The TRIPOLI-4/IDT coupling thus allows users to perform Monte-Carlo calculations based on the CADIS methodology. Second, we have implemented a new TRIPOLI-4 response function that makes use of the particle tracks generated by a direct (forward) simulation to produce an online estimate of the adjoint flux for a given detector response. The principle has already been described in the literature[10–13], but we propose a slightly different, collision-based estimator. The final goal of this work is to use the scored adjoint flux as an importance map for the same simulation.

The plan of the paper is the following. Section II presents the codes used for this work, namely TRIPOLI-4 and IDT. Section III describes the coupling between them. Section IV discusses the implementation of the new TRIPOLI-4 feature for scoring the adjoint flux during a direct simulation. Section V illustrates all the developments with some calculation results. Finally, conclusions are drawn in Sec. VI.

II. MATERIALS AND METHODS

We briefly describe here the codes used in this work.

II.A. The TRIPOLI-4® Monte-Carlo code

TRIPOLI-4[8] is a Monte-Carlo particle-transport code developed at SERMA, CEA, Saclay (France). Its main application fields are nuclear reactor physics, instrumentation, criticality safety and radiation protection.

One of the main strengths of TRIPOLI-4 is to offer a wide palette of variance-reduction methods for shielding problems. The traditional approach relies on the *exponential transform* (ET)[14]. In this technique, the physical laws for particle transport are modified in such a way that particles are pushed from regions of phase space with low importance to regions with higher importance. Specifically, given an importance map $I(\boldsymbol{r}, E, \boldsymbol{\Omega})$ one considers the vector field of *directions of interest* $\hat{\boldsymbol{\Omega}}$:

$$\hat{\boldsymbol{\Omega}}(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \frac{\nabla I(\boldsymbol{r}, E, \boldsymbol{\Omega})}{|\nabla I(\boldsymbol{r}, E, \boldsymbol{\Omega})|}.$$

The exponential transform essentially consists in modifying the mean free path for particles as a function of the scalar product $\boldsymbol{\Omega} \cdot \hat{\boldsymbol{\Omega}}$: specifically, the mean free path is extended for particles moving along the direction of interest, and it is contracted for particles moving against it. This way, particles will acquire a general tendency to follow the gradient of the importance map and thus move towards regions with higher importance. The complete formulation of the exponential transform also involves the application of importance sampling at particle emission from the source and after collisions; for historical reasons, TRIPOLI-4 only implements importance sampling at the source.

In recent years, a new major variance-reduction technique called Adaptive Multilevel Splitting (AMS) has been introduced in TRIPOLI-4[15,16]. AMS, in a nutshell, is an iterative algorithm that tracks particles using analogue transport. After each iteration, particle tracks are evaluated with respect to the maximum importance that they have reached so far; the "worst" particles are suppressed, and new particles for the next iteration are generated by splitting the tracks of the remaining ones. The iterations stop when enough particles reach the target detector. It has been proved under very weak conditions that this scheme can yield unbiased estimates of any estimator, including history-based estimators such as energy deposition.

The role played by the importance map in the ET and in AMS is sensibly different. In the former case, the gradient of the importance map is actively used to modify the laws of propagation for particle tracks; in the latter, the importance serves as a criterion to rank particle tracks and decide which ones should be suppressed. The different nature of the two algorithms is also reflected in the fact that the ET admits a zero-variance theorem[3], while AMS does not. This can be understood as a consequence of the fact that transport within each AMS iteration is analogue, and will therefore always result in residual fluctuations.

On the other hand, it has been empirically established that

AMS is more robust than the ET against variations of the importance map[15]. In other words, the ET is more likely than AMS to produce nonsensical results in presence of an inappropriate importance map. This property is crucial for the algorithms of Section IV.

All the work described in this paper was performed on a development version of TRIPOLI-4.

II.B. The IDT deterministic flux solver

IDT[9] is a 3D Cartesian deterministic solver for the multi-group time-independent Boltzmann transport equation for neutral particles. It is also developed at SERMA, CEA, Saclay (France), and it is part of the APOLLO3® suite[17]. We limit the description of the code to the aspects that are relevant for the coupling with TRIPOLI-4.

IDT solves either the direct or the adjoint transport equation within a multi-group formalism using nodal methods, finite differences or short characteristics for the space part. The S_N formalism is used for the angular part. The calculation geometry is defined on a 3D cartesian mesh; each cell of the mesh is associated with a set of multi-group cross sections (total, scattering, fission) defined on a group structure $[E_{g-1}, E_g]$, with $g \in \{1, 2, \ldots, G\}$. The result of the calculation is the multi-group flux ϕ_g (in the case of the direct equation)

$$\phi_g(\boldsymbol{r}, \boldsymbol{\Omega}) = \int_g \phi(\boldsymbol{r}, E, \boldsymbol{\Omega}) \mathrm{d}u$$

or the adjoint multi-group flux (in the case of the adjoint equation)

$$\phi_g^\dagger(\boldsymbol{r}, \boldsymbol{\Omega}) = \frac{1}{u(E_g) - u(E_{g-1})} \int_g \phi^\dagger(\boldsymbol{r}, E, \boldsymbol{\Omega}) \mathrm{d}u,$$

where $u(E) = -\ln E$ denotes the neutron lethargy. A convenient property of IDT (and of deterministic solvers in general) is that the solution method is essentially the same for the direct and the adjoint equations.

III. CADIS METHODOLOGY IN TRIPOLI-4®

We coupled IDT to TRIPOLI-4 in order to realize a CADIS calculation scheme. The coupling is driven by TRIPOLI-4, which constructs an IDT input file, calls the solver and collects the result in memory. One of the design goals of the coupling was to minimize the user intervention required to set up a calculation. We illustrate here the choices that we have made to this purpose, and the potential pitfalls involved.

III.A. Mesh definition

The importance map is computed on a user-defined Cartesian mesh that can be either regular or variable. The same mesh is also taken as the support for the description of the discretized IDT geometry. TRIPOLI-4 constructs the IDT geometry by querying the TRIPOLI-4 geometry for the material at the center of each cell and assuming that the cell is homogeneous. The same strategy was chosen in Ref. 18. As a comparison, ADVANTG performs ray tracing on the geometry to homogenize the composition of each cell[19]. At any rate, it is the user's responsibility to ensure that the chosen mesh coarseness is suitable for the problem description.

III.B. Cross-section condensation

The multi-group cross sections are part of the input to IDT. It is customary to condense point-wise cross sections $\Sigma(E)$ into multi-group cross sections Σ^g by using the direct flux as a weighting function:

$$\Sigma^g = \frac{\int_g \Sigma(E)\phi(E)\mathrm{d}u}{\int_g \phi(E)\mathrm{d}u}.$$

Similar condensation equations apply to differential cross sections for specific processes, such as (elastic or inelastic) scattering and $(n, 2n)$ reactions. However, the shape of the direct flux $\phi(E)$ is generally not known, so some assumption must be made. For the purpose of the coupling between TRIPOLI-4 and IDT, cross sections are condensed by TRIPOLI-4 using an energy spectrum representative of a pressurized water reactor; this is the same approach used in INIPOND, TRIPOLI-4's native module for the construction of importance maps[14]. Additionally, TRIPOLI-4 only generates isotropic (P_0) cross sections and neglects upscattering. Finally, no attempt is made to account for self-shielding.

Depending on the problem at hand, the current condensation algorithm may or may not be appropriate. The rationale is that the effects currently neglected by TRIPOLI-4 are not expected to be very important as long as the resulting adjoint flux is used for variance reduction. We plan to improve the condensation procedure in the near future.

III.C. IDT solver parameters

The user may also need to fix a few free parameters specific to the deterministic solver:

angular quadrature: using too few angles for the angular (Chebyshev-Legendre) quadrature formulas may result in the appearance of ray effects in the deterministic solution, especially in the case of well-localized (adjoint) sources. For the moment, ray effects can be circumvented by increasing the quadrature order (equal to 8 by default);

mesh refinement: as mentioned above, the user must define a mesh to act as a support for the description of the IDT geometry and for the adjoint flux resulting from the IDT calculation. However, IDT will actually perform its computations on a finer mesh, so as to guarantee appropriate convergence of the solution algorithm. The maximum size of the computation mesh can either be manually set by the user, or it can be automatically

computed by IDT based on the longest optical distance in the existing materials.

Finally, IDT allows the user to compute importance maps for geometries with reflection or leakage boundary conditions, which was not possible with TRIPOLI-4's native module INIPOND.

IV. SCORING THE ADJOINT FLUX DURING THE DIRECT CALCULATION

Many particle tracks are simulated during a Monte-Carlo shielding calculation. Tracks are created at the source and are transported through the geometry; a few of them will actually reach the detector and contribute to the desired response. The result of such a calculation can be described as the expected detector response assuming that particles are created according to the given source. However, the tracks generated by this calculation actually also provide information about the expected detector response from *any point* in phase space that they visited. One can rigorously justify this assertion by invoking the Markov property of the Monte-Carlo process, although the proof needs be carefully phrased for the case of calculations using variance reduction[20]. Since the expected detector response from a point in phase space can also be interpreted as the adjoint flux, it is clearly interesting for the purpose of variance reduction to try to extract the maximum amount of information about it during the direct simulation itself.

IV.A. Definition of the adjoint-flux on-the-fly estimator

For the sake of conciseness, we omit rigorous proofs of most of the results of this section.

Let us consider a given Monte Carlo scheme for the calculation of some detector response, possibly including variance reduction. Let c be the contribution to the detector response generated by a particle of weight w created at the phase-space point $(\boldsymbol{r}, E, \boldsymbol{\Omega})$. For given values of $(\boldsymbol{r}, E, \boldsymbol{\Omega}, w)$, c is a random variable described by a conditional probability distribution $k(c|\boldsymbol{r}, E, \boldsymbol{\Omega}, w)$. The quantity we wish to estimate with Monte Carlo is $I(\boldsymbol{r}, E, \boldsymbol{\Omega})$, the expected detector response from point $(\boldsymbol{r}, E, \boldsymbol{\Omega})$ in phase space. If the Monte Carlo game between $(\boldsymbol{r}, E, \boldsymbol{\Omega})$ and the detector is fair, then the expected value of c over k must be proportional to w, and I can thus be expressed as

$$I(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \frac{1}{w} \int c \cdot k(c|\boldsymbol{r}, E, \boldsymbol{\Omega}, w)\, \mathrm{d}c. \tag{2}$$

Now let us fix the particle source for the direct calculation and let $f(\boldsymbol{r}, E, \boldsymbol{\Omega}, w)$ represent the probability density for a particle being produced at $(\boldsymbol{r}, E, \boldsymbol{\Omega})$ (by the source or by a collision) with weight w during one Monte-Carlo history. Then, by the law of conditional probability, the joint probability distribution for all the variables is given by

$$d(c, \boldsymbol{r}, E, \boldsymbol{\Omega}, w) = k(c|\boldsymbol{r}, E, \boldsymbol{\Omega}, w) \cdot f(\boldsymbol{r}, E, \boldsymbol{\Omega}, w)$$

and it is crucial to observe that d is the distribution of the events generated by the direct Monte Carlo calculation. Therefore, Eq. (2) can be rewritten as

$$I(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \frac{\displaystyle\int c \cdot d(c, \boldsymbol{r}, E, \boldsymbol{\Omega}, w)\, \mathrm{d}c}{w \cdot f(\boldsymbol{r}, E, \boldsymbol{\Omega}, w)}. \tag{3}$$

Eq. (3) allows us to construct an approximate estimator for the integral of $I(\boldsymbol{r}, E, \boldsymbol{\Omega})$ over a certain neighbourhood X of $(\boldsymbol{r}, E, \boldsymbol{\Omega})$. We consider a Monte-Carlo history, represented by a sample of n events

$$\mathcal{S} = \{(c_1, \boldsymbol{r}_1, E_1, \boldsymbol{\Omega}_1, w_1), \ldots, (c_n, \boldsymbol{r}_n, E_n, \boldsymbol{\Omega}_n, w_n)\},$$

which are intermediate states of the Monte-Carlo Markov process. The $\boldsymbol{r}_i$ should be taken to be collision or source sites of particles with outgoing weight w_i, outgoing energy E_i and outgoing direction $\boldsymbol{\Omega}_i$; c_i represents the contribution to the target score (which may vanish) delivered by the particle and its descendants *after* the given point. The sample $\mathcal{S}$ is constructed by recording collision sites during the direct simulation and associating each collision site with the eventual score contribution.

Armed with the event sample $\mathcal{S}$, we define

$$\hat{F} = \sum_{i=1}^{n} w_i\, \mathbb{I}_X(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i). \tag{4}$$

Here $\mathbb{I}_X(\boldsymbol{r}, E, \boldsymbol{\Omega})$ is the characteristic function of the phase-space subset X (equal to 1 inside X and to 0 outside). Clearly the expectation value of $\hat{F}$ is the integral

$$\mathbb{E}(\hat{F}) = \int \mathrm{d}w \int_X \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}E\, \mathrm{d}^2\boldsymbol{\Omega}\, [w \cdot f(\boldsymbol{r}, E, \boldsymbol{\Omega}, w)]\,.$$

Likewise, we define

$$\hat{D} = \sum_{i=1}^{n} c_i\, \mathbb{I}_X(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i); \tag{5}$$

its expectation value is

$$\mathbb{E}(\hat{D}) = \int \mathrm{d}w\, \mathrm{d}c \int_X \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}E\, \mathrm{d}^2\boldsymbol{\Omega}\, [c \cdot d(c, \boldsymbol{r}, E, \boldsymbol{\Omega}, w)]\,.$$

We can then define our approximate estimator of $I(\boldsymbol{r}, E, \boldsymbol{\Omega})$:

$$\hat{I} = \frac{\hat{D}}{\hat{F}}. \tag{6}$$

In practice, the estimators $\hat{D}$ and $\hat{F}$ are actually separately cumulated over batches of several Monte-Carlo histories. Eq. (6) then yields one estimate per batch. We have omitted this detail from the presentation for the sake of simplicity.

There are several reasons why $\hat{I}$ is approximate. First, $\hat{D}$ and $\hat{F}$ estimate *weighted* averages of their integrands over a

certain neighbourhood X of $(\boldsymbol{r}, E, \boldsymbol{\Omega})$. Second, clearly $\hat{I}$ is biased because of Jensen's inequality, i.e.

$$\mathbb{E}(\hat{I}) \neq \frac{\mathbb{E}(\hat{D})}{\mathbb{E}(\hat{F})}.$$

However, $\hat{I}$ is consistent (asymptotically unbiased) as the sample size n tends to infinity and the size of the neighbourhood X tends to zero, in this order:

$$\mathbb{E}(\lim_{X\to 0}\lim_{n\to\infty}\hat{I}) = I(\boldsymbol{r}, E, \boldsymbol{\Omega}).$$

In summary, we propose the following recipe for scoring the adjoint flux in a phase-space cell:

1. collect all particles emitted by collisions within the cell;
2. associate each point with the contribution to the detector response delivered by the particle and its descendants from that point onwards;
3. calculate $\hat{D}$ (Eq. (4)) by summing the particle contributions;
4. calculate $\hat{F}$ (Eq. (5)) by summing the particle weights;
5. divide $\hat{D}$ by $\hat{F}$ to estimate the adjoint flux in the phase space cell.

IV.B. Variance reduction

The explicit treatment of the particle weights in the estimator outlined in the previous section hints at the fact that the estimator remains applicable in presence of variance reduction. In particular, the estimator works in presence of AMS, although care must be exercised in the definition of the weights.

Being able to use AMS for the estimation of the adjoint flux is crucial. Indeed, as mentioned above, AMS is more robust than the ET against variations of the importance map. An overly eager variance-reduction technique such as ET will intentionally suppress exploration of supposedly uninteresting regions of phase space. Therefore, there is some tension between the need to improve the importance map of the present calculation and the wish to maximise the figure of merit for the sought response. If the initial importance map is inadequate, it is entirely possible that the variance-reduction technique may make it impossible to improve it. For this reason, we mostly centre our discussion of the adjoint-flux score around the use of AMS, which guarantees a better balance between exploration and exploitation.

On the other hand, the ET can yield much larger figures of merit with a suitable importance map. This suggests calculation schemes where AMS is used to score the importance map, and the ET is used to accelerate the convergence of the calculation. One possible scheme consists in starting the calculation as an AMS calculation with a rough importance map; the adjoint flux is scored until sufficient statistics is cumulated, at which point the ET takes over and uses the scored adjoint flux as an importance map. More sophisticated schemes are possible, in which AMS keeps updating the importance map until the ET becomes efficient.

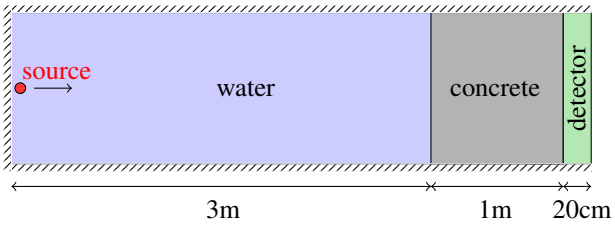

Figure 1. Geometry for the strong-attenuation problem. A mono-directional neutron source with a Watt spectrum is placed in a 3 m-long tank of water. The detector is a 20 cm-wide part of a 120 cm-long concrete wall. Reflection boundary conditions are applied to all surfaces except for the outer surface of the detector, from which neutrons can leak out.

IV.C. Similar work

Similar approaches for scoring the importance map have already been proposed in the literature[10–12], sometimes in conjunction with non-parametric interpolation techniques[13]. Since our estimator is collision-based, it can be straightforwardly incorporated in an interpolation framework. A smoothed importance map may make variance-reduction methods more efficient, but the cost of the interpolation framework needs to be accounted for in the estimation of the figure of merit. We leave exploration of this subject for future work.

V. RESULTS

We now illustrate the TRIPOLI-4 developments described in the previous sections with some calculation results.

V.A. Strong-attenuation problem

We start with the simple problem depicted in Fig. 1, which concerns the transport of neutrons in a geometry made of a 3 m-thick water slab followed by a 1.2 m-thick concrete slab. The detector is placed at the bottom of the concrete slab and scores the integral neutron flux. The geometry is infinite in the transverse direction (reflection boundary conditions are applied). A Watt neutron source is placed at the top of the water slab and emits mono-directional neutrons towards the detector.

The problem can be essentially characterized by the strong attenuation factor incurred by neutrons. The attenuation is so strong that it is not possible to produce a reference result by means of analogue calculations in any reasonable

time. We have no choice but to resort to variance reduction.

In order to evaluate the sensitivity of variance reduction to the importance map, we present results obtained with the following maps, roughly sorted from least to most sophisticated:

INIPOND: this 6-group importance map was produced by INIPOND, TRIPOLI-4's native deterministic module[14], with manually adjusted Placzek coefficients. The default Placzek coefficients produced by INIPOND (in "automatic mode") are unable to push any particle towards the detector within a reasonable time. Note that the number of groups was limited to 6 because manual parameter adjustment rapidly becomes unwieldy as the number of groups increases.

IDT: this 57-group importance map was produced by IDT, as invoked by TRIPOLI-4 within the framework of the coupling described above. As explained above, cross sections were condensed by TRIPOLI-4 and assumed to be isotropic.

IDT+AP3: this importance map uses the same group structure as the previous one, but the multi-group cross sections were produced by an external condensation calculation performed with the APOLLO3® code. The resulting cross sections used an anisotropy order of 5.

SCORED: this importance map is the adjoint flux scored by TRIPOLI-4 during a first, direct calculation pass using AMS. The result of the score is then injected in a second calculation pass using the ET method. The map also uses IDT's 57-group structure.

All importance maps used the same one-dimensional mesh for space discretization (42 10 cm-wide cells) except for the IDT+AP3, which consists in 100 4.2 cm-wide cells.

Table I shows the results of calculations performed with both variance-reduction methods, namely AMS and the ET, for each of the importance maps. For each combination we present the average detector response, its standard error, the calculation time and the figure of merit. Calculations were stopped when the standard error dropped below 10 %. Computing times do not include the time needed for the generation of the importance map.

The first remark is that all AMS calculations yield similar results. The average detector responses are mutually compatible within their errors, and the figures of merit are within a factor of 2 of each other. More refined importance maps do yield larger figures of merit, but overall AMS is seen to be relatively robust. This property of AMS is probably exacerbated in this example problem, which uses a very simple, one-dimensional geometry, but it holds in a rather general setting[15].

The exponential transform, on the other hand, is much more sensitive to the importance map. We draw the attention of the reader to the fact that the ET/IDT result for the

	INIPOND	IDT	IDT+AP3	SCORED
Adaptive Multilevel Splitting				
average (a.u.)	2.58	2.61	2.78	2.66
error (%)	9.90	9.83	7.11	9.88
time (ks)	167	120	159	108
FOM (10^{-5})	9	12	16	14
Exponential transform				
average (a.u.)	2.55	2.04	2.81	2.77
error (%)	6.51	6.60	0.82	0.52
time (ks)	94.1	239	3.27	4.33
FOM (10^{-5})	38	22	57 561	109 602

Table I. Results for the strong attenuation problem. We present the integrated average response in the detectors and the standard error after a certain simulation time. Values are given for both AMS and the ET method with four importance maps: INIPOND, IDT (cross sections from TRIPOLI-4), IDT+AP3 (external cross sections from APOLLO3®, with anisotropy order 5) and SCORED (adjoint score); see text for further details.

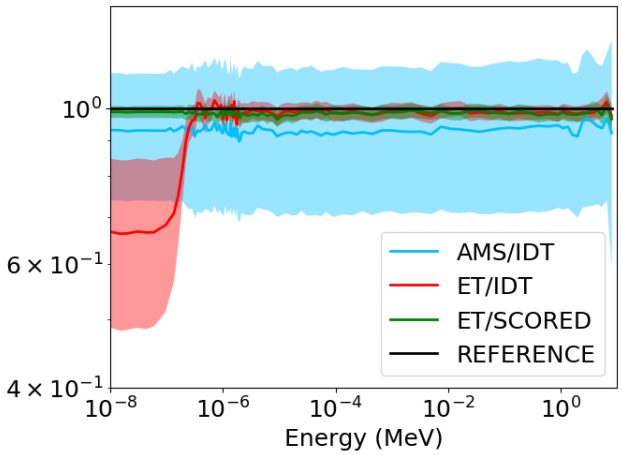

Figure 2. Comparison of the energy dependence of the neutron flux in the detector for the strong-attenuation problem. The plot shows the results for AMS/IDT (blue), ET/IDT (red) and ET/SCORED (green) calculations, relative to the reference ET/IDT-AP3 calculation, as a function of the neutron energy. The shaded regions represent the combined 3σ confidence interval.

average is significantly smaller than the others: the second smallest result, ET/INIPOND, is more than two combined standard deviations away. The statistical evidence is not very strong, but it should be sufficient to raise some suspicion about the ET/IDT calculation. The figure of merit of the ET/IDT-AP3 calculation, on the other hand, is more than *three orders of magnitude* larger than any other. This suggests that ET/IDT-AP3 is probably very close to the actual adjoint flux.

The suspicion about ET/IDT is reinforced by inspection of the energy spectrum of the neutron flux in the detector. We take ET/IDT-AP3 as a reference, which seems warranted given its small standard error, and we plot the ratio between ET/IDT and ET/IDT-AP3 in Figure 2. For comparison, we also plot the ratio of AMS/IDT and ET/IDT-AP3, which does not exhibit any bias. Combined 3σ error bars are shown as shaded regions. It is clear that the ET/IDT calculation underestimates the reference below 0.1 eV, suggesting that this importance map hinders neutron thermalization.

V.A.1. Using the scored adjoint flux as an importance map

Finally, we wish to illustrate TRIPOLI-4's new capability to score the adjoint flux. We performed a two-pass calculation:

1. The first pass is an AMS calculation using the IDT+AP3 importance map. During this pass, TRIPOLI-4 scores the adjoint flux using the estimator described in Sec. IV.

2. During the second pass, the adjoint flux is used as an importance map for an ET calculation. The results of this calculation are referred to as ET/SCORED.

Table I shows that the integrated neutron flux calculated by ET/SCORED is in statistical agreement with the ET/IDT+AP3 result. Fig. 2 shows that the energy spectrum of the neutron flux is also coherent with ET/IDT+AP3. The figure of merit, on the other hand, is slightly larger, about a factor of 2.

This encouraging result suggests that the new score for the adjoint flux is a promising tool to accelerate the convergence of difficult shielding calculations. Of course the computational cost for the production of the importance map should be accounted for in the estimation of the figure of merit, which is not the case for the values shown in Tab. I. As a general indication, the CPU time required for the production of the IDT+AP3 importance map is of the order of one hour, while the time required for the first calculation pass of ET/SCORED is of the order of a few hundred hours.

Still, we have not investigated the dependence of the figure of merit of the second pass on the length of the first calculation pass. In the ET/SCORED calculation shown in Tab. I and Fig. 2, the adjoint flux from the first pass has very small uncertainties on most parts of phase space. It is legitimate to ask whether a shorter calculation would have sufficed. We plan to investigate this and similar issues in the near future.

V.B. Neutron-photon coupled calculation

As an additional illustration of TRIPOLI-4's new capability to score the adjoint flux, we present the result of a coupled neutron-photon calculation. A neutron source is placed at the left end of the geometry depicted in Figure 3; a photon detector is placed on the other side of a stack of plastic material and iron slabs. The goal is to estimate the response of the photon detector. The reference calculation is an analog one.

This particular example is interesting because, in general, neutron-photon problems are difficult to solve using INIPOND, TRIPOLI-4's native module for the generation of importance maps. Using our new adjoint-flux score, we can compute the importance map during a first calculation with AMS; the resulting adjoint flux can then be injected as an importance map into a new calculation with the ET and hopefully yield large figures of merit.

The first AMS calculation used simple, energy-independent, purely geometric importance maps (the importance for any particle is taken to be equal to the inverse of the distance from the photon detector). During the direct simulation, we scored the adjoint flux for both neutrons and photons. Figure 3 shows the score result after a few hundred CPU hours.

A clear feature of the resulting importance maps is that very little information could be collected in the low-density regions of the geometry: since the material for the world

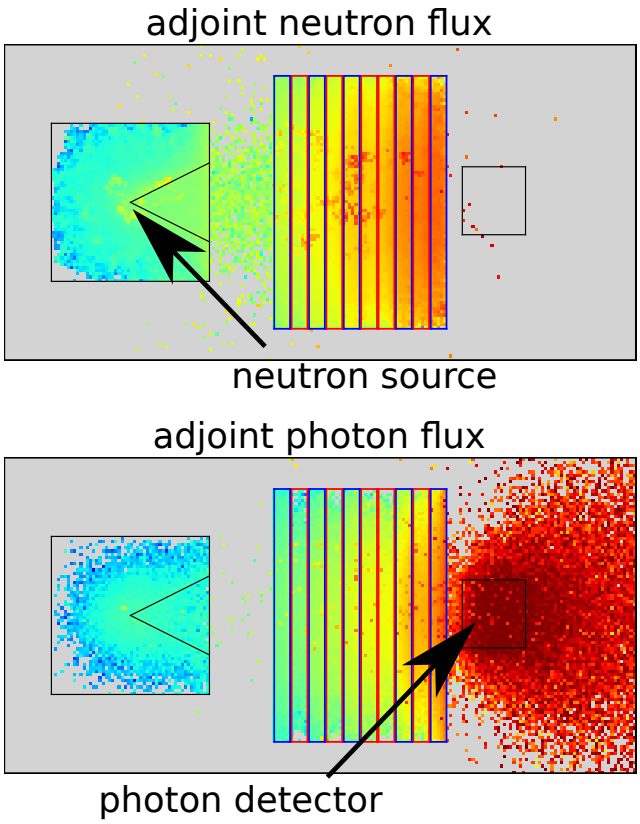

Figure 3. Neutron and photon adjoint flux scored by TRIPOLI-4 for a coupled neutron-photon shielding problem. The plots highlight the lack of information in low-density regions (air, grey).

volume is air, only few collisions can contribute to the estimation of the adjoint flux.

If the scored adjoint flux is to be reused as an importance map for variance reduction, this may or may not be an issue. On the one hand, sparsely filled importance map are problematic for many variance-reduction methods; for instance, the ET uses the gradient of the importance map, which vanishes between empty cells. A precise estimate of the adjoint flux in these regions is possible but requires very long runs, which are detrimental to the overall figure of merit; one should keep in mind that the estimation of the adjoint flux is only an intermediate step towards the solution of the shielding problem. Ideally, the adjoint-flux calculation should be as long as necessary for the second step to converge, but no longer.

On the other hand, some regions of the scored adjoint flux are sparsely populated *exactly because* the variance-reduction method did not consider necessity to push particles towards those regions and force collisions there. Therefore, one may argue that the presence of sparsely-populated regions of the adjoint score should not necessarily hamper variance reduction. It clearly appears that quantitative tests are indispensable to assess this.

VI. CONCLUSIONS

We have presented two recent developments of the TRIPOLI-4® code aiming to provide an implementation of the CADIS methodology, and generally to help users solve complicated radiation-protection problems. To this end, TRIPOLI-4 was coupled with IDT, a deterministic solver for the adjoint Boltzmann equation, to generate efficient importance maps with minimal user intervention. Moreover, we implemented an estimator for the adjoint flux during direct calculations. The rationale behind these choices is that using the adjoint flux as an importance map in a wide range of variance-reduction methods is expected to yield large speed-ups.

We have shown that importance maps calculated with IDT can yield very large speed-up factors in a simple one-dimensional strong-attenuation problem, provided that the solver is fed with accurate multi-group cross sections. We have also proved that the scored adjoint flux, when used as an importance map, can yield even larger figures of merit. The computational cost for the direct determination of the adjoint flux is of course larger than for a deterministic calculation, and this must be taken into account in the evaluation of the calculation efficiency. Nevertheless, the adjoint flux probably need not be calculated very precisely in the first calculation pass; a short calculation may be sufficient to bootstrap the importance map. We believe that this method may represent a promising complement to the CADIS methodology.

Finally, we have shown that the new adjoint-flux score may help with the calculation of importance maps for cou-

pled neutron-photon problems, which are usually among the hardest ones for TRIPOLI-4 users.

The developments described in the present work should be considered as a stepping stone towards the implementation of an intelligent, semi-automatic and dynamic method for the generation of the importance map for variance reduction. The general idea of the scheme is to use the result of a deterministic calculation, a scored adjoint flux, or both, to update the importance map at the beginning and during the calculation, possibly alternating between different variance-reduction methods. To this end, a few questions must be addressed. For instance, how long should we keep scoring the adjoint flux before recycling it as an importance map? Should the code update the importance map only once, or several times? At which point should we switch from AMS (which is robust against poor importance maps) to the ET (which yields very large figures of merit if the importance map is very good)? Finally, is it possible to combine a deterministic importance map produced by IDT with a scored adjoint flux calculated by TRIPOLI-4? If so, how? Answering these questions is left as the subject of future work.

REFERENCES

1. G. I. BELL and S. GLASSTONE, *Nuclear reactor theory*, Van Nostrand Reinhold Company, New York (1970).

2. S. R. DWIVEDI, "Zero variance biasing schemes for Monte-Carlo calculations of neutron and radiation transport problems," *Nucl. Sci. Eng.*, **80**, *1*, 172–178 (1982).

3. J. E. HOOGENBOOM, "Zero-variance Monte Carlo schemes revisited," *Nucl. Sci. Eng.*, **160**, *1*, 1–22 (2008).

4. A. HAGHIGHAT and J. C. WAGNER, "Monte Carlo variance reduction with deterministic importance functions," *Prog. Nucl. Energy*, **42**, 25–53 (2003).

5. E. D. BIONDO, A. DAVIS, and P. P. H. WILSON, "Shutdown dose rate analysis with CAD geometry, cartesian/tetrahedral mesh, and advanced variance reduction," *Fusion Eng. Des.*, **106**, 77–84 (2016).

6. J. M. RISNER and E. D. BLAKEMAN, "Analysis of dpa Rates in the HFIR Reactor Vessel using a Hybrid Monte Carlo/Deterministic Method," *EPJ Web of Conferences*, **106**, *03003* (2016).

7. A. ČUFAR, B. KOS, I. A. KODELI, I. LENGAR, Ž. ŠTANCAR, and L. SNOJ, "The analysis of the external neutron monitor responses in a simplified JET-Like tokamak using ADVANTG," *Fusion Sci. Technol.*, **71**, *2*, 162–176 (2017).

8. E. BRUN, F. DAMIAN, C. M. DIOP, E. DUMONTEIL, F.-X. HUGOT, C. JOUANNE, Y. K. LEE, F. MALVAGI, A. MAZZOLO, O. PETIT, J. TRAMA, T. VISONNEAU, and A. ZOIA, "TRIPOLI-4®, CEA, EDF and AREVA reference Monte Carlo code," *Ann. Nucl. Energy*, **82**, 151–160 (August 2015).

9. I. ZMIJAREVIC and R. SANCHEZ, "Deterministic solutions for 3D Kobayashi benchmarks," *Prog. Nucl. Energy*, **39**, *2*, 207–221 (2001).

10. T. E. BOOTH, "Automatic importance estimation in forward Monte-Carlo calculations," *Trans. Am. Nucl. Soc.*, **41**, 308–309 (1982).

11. T. E. BOOTH and J. S. HENDRICKS, "Importance estimation in forward Monte-Carlo calculations," *Fusion Sci. Technol.*, **5**, *1*, 90–100 (1984).

12. I. MURATA, D. FILGES, and F. GOLDENBAUM, "A new approach to estimate importance for weight window in forward Monte Carlo calculations," *Nucl. Sci. Eng.*, **159**, *3*, 273–283 (2008).

13. E. DUMONTEIL, "On a new variance reduction technique: neural network biasing - a study of two test cases with the Monte Carlo code Tripoli4," *Nucl. Technol.*, **168**, *3*, 793–798 (2009).

14. J. P. BOTH, J. C. NIMAL, and T. VERGNAUD, "Automated importance generation and biasing techniques for Monte-Carlo shielding techniques by the TRIPOLI-3 code," *Prog. Nucl. Energy*, **24**, *1–3*, 273–281 (1990).

15. H. LOUVIN, *Development of an adaptive variance reduction technique for Monte Carlo particle transport*, Ph.D. thesis, Université Paris-Saclay (2017).

16. H. LOUVIN, E. DUMONTEIL, and T. LELIEVRE, "Three-Dimensional Neutron Streaming Calculation Using Adaptive Multilevel Splitting," in "M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering," (2017).

17. D. SCHNEIDER, F. DOLCI, F. GABRIEL, ET AL., "Apollo3®: Cea/Den Deterministic Multi-Purpose Code for Reactor Physics Analysis," in "Proceedings to PHYSOR 2016: Unifying theory and experiments in the 21st century," Sun Valley, ID, USA (May 2016), pp. 2274–2285.

18. J. SWEEZY, F. BROWN, T. BOOTH, J. CHIARAMONTE, and B. PREEG, "Automated variance reduction for MCNP using deterministic methods," *Radiat. Prot. Dosim.*, **116**, *1–4*, 508–512 (2005).

19. S. W. MOSHER, A. M. BEVILL, S. R. JOHNSON, A. M. IBRAHIM, C. R. DAILY, T. M. EVANS, J. C. WAGNER, J. O. JOHNSON, and R. E. GROVE, "ADVANTG — An Automated Variance Reduction Parameter Generator," Tech. Rep. ORNL/TM-2013/416, Oak Ridge National Laboratory (2013).

20. T. E. BOOTH, "Common misconceptions in Monte Carlo particle transport," *Appl Ṙadiat. Isot˙*, **70**, *7*, 1042–1051 (2012), proceedings of the 8th International Topical Meeting on Industrial Radiation and Radioisotope Measurement Applications (IRRMA-8).