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Evaluating importance maps for TRIPOLI-4$^{®}$ using deterministic or on-line methods

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ABSTRACT

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.

INTRODUCTION

The goal of this work is to present the development of two new functionalities of the TRIPOLI-4$^{®}$ Monte-Carlo particle-transport code [1] that simplify the construction of an efficient importance map for variance reduction. First, a development version of TRIPOLI-4 has been coupled with the deterministic transport solver IDT [2]. 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. Multi-group cross sections are automatically condensed and homogenized. The TRIPOLI-4/IDT coupling thus allows users to perform Monte-Carlo calculations based on the Consistent Adjoint-Driven Importance Sampling (CADIS) methodology [3]. 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 [4, 5], 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 reader is referred to Ref. 6 for further details about this work.

MATERIALS AND METHODS

We briefly describe here the codes used in this work.

The TRIPOLI-4$^{®}$ Monte-Carlo code

TRIPOLI-4[1] 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) [7]. 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. The exponential transform essentially consists in modifying the mean free path for particles; 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.

In recent years, a new major variance-reduction technique called Adaptive Multilevel Splitting (AMS) has been introduced in TRIPOLI-4 [8, 9]. 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 [10], 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 [8]. 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 that score the adjoint flux, described below.

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

The IDT deterministic flux solver

IDT [2] is a 3D Cartesian deterministic solver for the multigroup 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 [11]. 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 given group structure. The result of the calculation is the multi-group flux or the adjoint multi-group flux (in the case of the adjoint equation). 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.

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.

mesh refinement: the importance map is computed on a user-defined Cartesian mesh that can be either regular or variable. TRIPOLI-4 constructs the IDT geometry on this mesh assuming that cells are homogeneous. It is the user's responsibility to ensure that the chosen mesh coarseness is suitable for the problem description. Note that IDT will actually perform its computations on a finer mesh, so as to guarantee appropriate convergence of the solution algorithm.

angular quadrature: if ray effects are visible in the solution, the user can increase the quadrature order for the angular flux (equal to 8 by default).

cross-section condensation: multi-group cross sections are part of the input to IDT. 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 [7]. Depending on the problem at hand, this condensation algorithm may or may not be appropriate. We plan to improve the condensation procedure in the near future.

boundary conditions: 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.

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. 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.

We developed an on-the-fly estimator for the adjoint flux during the direct simulation. In summary, the recipe for scoring the adjoint flux in a phase-space cell is the following:

1. collect all particles emitted during direct transport by collisions within the cell;
2. associate each collision point with the contribution to the detector response delivered by the particle and its descendants from that point onwards;
3. divide the total contribution from the cell to the detector by the total weight of particles emitted from the cell. This estimates the adjoint flux in the phase space cell.

The reader is referred to Ref. 6 for further details.

RESULTS

We consider the following simple problem: fission neutrons (Watt spectrum) are emitted perpendicularly to the face of a 3 m-thick water slab followed by a 1.2 m-thick concrete slab. The detector is placed at the end of the concrete slab and scores the integral neutron flux. The geometry is infinite in the transverse direction (reflection boundary conditions are applied). 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 [7], 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.

	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.

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 stage using AMS. The result of the score is then injected in a second calculation stage 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 the 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 [8].

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 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.

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-stage calculation:

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

2. During the second stage, 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. 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 stage 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 stage on the length of the first calculation stage. In the ET/SCORED calculation shown in Tab. I, the adjoint flux from the first stage has very small uncertainties on most parts of phase space. It is legitimate to ask whether a shorter calculation would have been sufficient. We plan to investigate this and similar issues in the near future.

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 stage; 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 coupled 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.

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REFERENCES

1. 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).

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

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

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

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

6. D. MANCUSI, M. NOWAK, E. DUMONTEIL, H. LOUVIN, E. MASIELLO, and D. SCIANNANDRONE, "Evaluating importance maps for TRIPOLI-4® using deterministic or on-line methods," in "Proceedings to the 20th Topical Meeting of the Radiation Protection and Shielding Division (RPSD 2018)," Santa Fe, NM, USA (2018).

7. 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).

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

9. 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).

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

11. 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.