Analysis and optimization of variance reduction techniques for particle transport problems in radiation shielding

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1. CONTEXT

The transport of neutrons and photons in reactors is described by the Boltzmann equation. The solution of this equation by the Monte-Carlo method is based on the simulation of a very large number of random trajectories of particles inside the system. The averages over all the simulated trajectories allow estimating the physical observables of interest [1]. Each trajectory describes a random walk whose mathematical properties are determined in agreement with the underlying physical laws (probability of particle-matter interaction, scattering laws in angle and energy, distribution of the fission multiplicity, etc.). In addition, the Monte-Carlo method is able to deal with arbitrarily complex geometries without introducing any discretization approximation. For all of these reasons, Monte Carlo simulation has always been considered - since its introduction - as the reference method for the calculation of nuclear systems.

However, in some configurations of the nuclear systems of interest, the probability that a path survives from source to detector is very low. A representative example is the presence of a water and steel shields between the reactor core and the ex-core detectors, with attenuations which can sometimes exceed 15 decades relative to the intensity of the source. It was therefore proposed to replace the natural laws of flights and collisions by other “artificial” laws in order to increase the probability of sampling rare events of interest: this takes the name of non-analog Monte-Carlo simulation. These techniques aim to reduce the variance of the response to the detectors, while preserving the average [1]. For this purpose, the unit contribution of each particle is replaced by a statistical weight, whose adjustment makes it possible to ensure that the average obtained using the modified laws be the same as that obtained using the “analog” physical laws. The use of variance reduction methods is an essential tool for the application of Monte Carlo simulation to radiation protection problems.

The Monte-Carlo TRIPOLI-4® code, developed at CEA to cover all the applications of particle transport in the nuclear domains (particularly in radiation shielding and reactor physics), currently has several of these variance reduction methods, each based on distinct mathematical formalisms and algorithmic approaches: the exponential transform method, the “surface restart” method, the adaptive multi-level splitting (AMS) method and the weight window method. Despite their very different formulations, the common point of these methods is the fact that they are all based on the use of an approximate solution of the adjoint Boltzmann equation (the “importance function”): this is the so-called “importance sampling” approach. It is
known that the use of the information contained in the importance function sampling and / or ranking particles makes it possible to design optimized variance reduction schemes (and ideally to obtain schemes with zero-variance in some cases).

2. **PHD TOPIC**

The diversity of methods is both the strong and the weak point of the variance reduction strategies implemented in the codes: the vast existing literature on these subjects has clearly shown that it is not possible to identify a universal winning strategy and that each method is best suited to one or more subclasses of transport problems. The objective of this thesis is to establish a *coherent theoretical framework* that allows guiding the choice of the existing methodologies in relation to the targeted applications.

The approach proposed in this thesis is based on the understanding of the mechanisms by which the information contained in the importance function is exploited by the algorithms which modify the laws of displacement and collision of particles and / or sort the particles which have the highest probability of contributing to the detector.

In particular, we will focus on three aspects:

1 - Importance maps are typically generated by deterministic codes by calculating the adjoint scalar flux on a spatial and energetic mesh. For radiation shielding problems in the presence of strong bypass effects and / or preferential paths ("streaming"), it would be desirable to have importance maps also including the dependence of the *direction* of the particle; this information will then have to be exploited during the transport of the particles (ideally locally, in the vicinity of strong gradients of importance);

2 - In the exponential transform method, the *ideal sampling of non-analog collisions* in practice is not achieved, because it is very complex to implement in transport codes: this generates a loss of performance in terms of reduction of variance. We will study variants of the ideal scheme allowing a compromise between algorithmic complexity and optimum variance reduction to be reached;

3 - In surface restart methods, particles are first propagated from the source to an intermediate surface and then propagated from this surface to the detector. The choice of the importance function used before and after the surface, as well as the choice of the position of the surface are essential for the correct functioning of the method. We will formalize the problem of the *optimal choice of the importance functions* and the surface in order to minimize the variance of the response to the detector.
3. **WORK PLAN**

The planned thesis work will relate partly to the analysis of algorithms already existing in TRIPOLI-4® and partly to the design of new algorithms in a simplified simulation code, such as the Monte-Carlo Patmos mini-app, currently under development at CEA [3].

The thesis work will be structured around the following major steps:

- Bibliographical study of variance reduction methods for Monte-Carlo simulation and importance sampling, particularly in the context of the TRIPOLI-4® code;
- Choice of a selection of benchmarks in order to compare and classify the existing methods according to the problem treated (high attenuation, workaround/bypass configurations, etc.);
- Analysis of the three problems identified above and identification of algorithms that can improve the performance of variance reduction methods;
- Implementation of relevant strategies in TRIPOLI-4® and / or Patmos and performance tests.

4. **REFERENCES**