Hybrid Monte Carlo-Deterministic Methods for Neutral Particle Transport Problems

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Summary

Since the early 1950's, two fundamentally distinct methodologies have been extensively developed to simulate neutron/photon particle transport problems for nuclear systems: *Monte Carlo* and *deterministic* methods [1-3]. In the mid-1990's, researchers began to find ways to combine these two algorithm types, to create new *hybrid transport* methods that significantly enhance the user-friendliness and efficiency of the resulting simulation process. The purpose of these talks is to motivate and describe the work done on this new class of methods [4-21].

To begin, we outline the basic differences between the Monte Carlo and deterministic approaches for simulating neutron/photon transport problems:

1. *Monte Carlo and deterministic methods have independent philosophical foundations.* Monte Carlo methods interpret a particle transport process as a *statistical* one, in which a large number of random histories of individual particles are simulated by the computer and averaged, to obtain estimates of mean fluxes. Deterministic methods interpret a transport process as one governed by the *Boltzmann transport equation*, which is discretized into a (typically large) system of algebraic equations. This system is then solved, typically in an interative manner, to obtain estimates of mean fluxes.
2. *The character of the errors in Monte Carlo and deterministic solutions is different.* If the geometry and cross sections of a physical system are known exactly, then Monte Carlo flux estimates will contain only statistical errors, which tend to zero as $N^{-1/2}$, where N is the number of Monte Carlo particle histories. Deterministic flux estimates contain only truncation errors, which depend on the discretization schemes and the grids chosen for the space, angular, and energy variables.
3. *Monte Carlo solutions are most efficient when a small amount of information is needed and least efficient when global information is needed.* The classic Monte Carlo problem is to determine a single detector response in a "deep" part of the system. *Deterministic methods automatically provide global information across the entire system.*
4. *Monte Carlo and deterministic codes require different kinds of human input to run efficiently.* For geometrically complex source-detector problems, nonanalog Monte Carlo methods must be used to ensure that sufficiently many Monte Carlo source particles will reach the desired "detector" locations in phase space. For this to occur, nonanalog methods must be used, requiring the user to input a large number of problem-dependent biasing parameters. Developing sufficiently optimized values of these parameters can be a costly, intuition-driven, trial-and-error process for the code user. Similarly, deterministic methods require the specification of problem-dependent multigroup cross sections, which also

must be pre-determined by the code user before the deterministic code can be run. This too can be a lengthy and time-consuming process.

5. *The inner workings of Monte Carlo and deterministic transport codes, as well as the skill sets needed to build and develop these codes, are largely distinct.* Historically, Monte Carlo methods development has focused on developing better ways to assess and reduce the statistical errors in Monte Carlo solutions. Deterministic methods development has focused on (i) reducing truncation errors in discretized approximations of the Boltzmann equation, and (ii) devising more efficient and robust iteration strategies for solving the discretized system of equations. Advances in Monte Carlo methods development have had no impact on deterministic methods, and vice versa. The technical teams that have accomplished much of the significant Monte Carlo and deterministic methods and code development are largely disjoint and have worked independently.
6. *Monte Carlo and deterministic methods are not implemented in the same production codes.* Historically, Monte Carlo and deterministic computational approaches have been implemented in different computer codes. Users could not run a Monte Carlo and a deterministic simulation of a specified transport problem using a single code.

In spite of these major differences, Monte Carlo and deterministic methods solve the same particle transport problems. These two algorithm types have coexisted (one has never supplanted the other) because they are complementary – they possess fundamentally different strengths and weaknesses. For certain classes of problems Monte Carlo methods are preferable; for other classes deterministic methods are preferable. For difficult problems, neither methodology offers a "black box" method; both require significant, albeit different, human input (biasing parameters for Monte Carlo; multigroup cross sections for deterministic methods).

For most of the past 60 years, Monte Carlo and deterministic methods have developed independently. Nonetheless, researchers and practitioners have recently begun to devise and implement *hybrid* particle transport methods, in which elements of both methodologies are present. The goal has been to create new numerical particle transport methods that make use of the strengths of the Monte Carlo and deterministic methodologies, and suppress their weaknesses. In the past few years, new hybrid methods have been implemented and successfully run on complex, large-scale problems. Other hybrid methods are still under development. My talks at this 2011 FJOH summer school will discuss the following mix of hybrid methods, which are currently available and under development.

1. *Automated weight window generation for source-detector problems* [4-8]

   In the early 1990's it became understood that for Monte Carlo source-detector problems, one could define efficient weight windows in terms of the

solution of an adjoint transport problem. This led to the idea that an inexpensive deterministic adjoint calculation could be performed to determine an approximate adjoint flux, which could be processed to yield efficient weight windows for a subsequent Monte Carlo simulation. This concept has been implemented in several major codes; by a wide margin, when the phrase *hybrid transport method* is used, this "weight window generation" approach is the one intended.

The implementation of this concept is nontrivial. Because Monte Carlo and deterministic methods have not been implemented in the same computer codes, and because of the expense of writing an entirely new code, the most practical way to implement this approach is to use two already-existing codes, one deterministic, and one Monte Carlo. But then the user must (i) write two separate input decks for the system geometry and materials, (ii) ship the necessary information to the deterministic code and run it, (iii) process the output from the deterministic code into weight windows and ship these (in the proper format) and the geometry/material information to the Monte Carlo code, and finally, (iv) run the Monte Carlo code with the computer-generated weight windows. Clearly, this process is unwieldy. However, it is a process that can be – and has been – automated. In the automated process, the user writes a single input deck, specifying the geometry and materials of the system and the grid for the deterministic calculation. The computer then does everything else: the necessary information is sent to the deterministic code, this code runs, the output is processed into weight windows, these and the original system parameters are sent to the Monte Carlo code, and finally, the Monte Carlo code runs with the deterministically-calculated weight windows.

This methodology has been implemented at Oak Ridge National Laboratory, in the *Consistent Adjoint-Driven Importance Sampling*, or CADIS technique. In this implementation, the deterministic adjoint transport calculations are performed by TORT or the new DONOVO code, and the Monte Carlo calculations are performed by the MONACO code. These codes are linked in the MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) code sequence, which has been publicly released in SCALE 6. The resulting automated procedure has been demonstrated to be advantageous in two ways: (i) the code user no longer has to determine weight windows by a tedious trial-and-error, intuition-driven process, and (ii) the deterministically-obtained weight windows are usually more optimized than the weight windows that a human would obtain; consequently, the Monte Carlo simulation runs more efficiently.

2. *Automated biasing of neutron physics* [9-11]

   The same deterministic adjoint solution has also been used in nonanalog Monte Carlo codes to "actively but fairly" modify the neutral particle physics (distance-to-collision, probability of absorption, angle-of-scatter, etc.). The biased physics "steers" particles to more quickly migrate in phase space from the source to the detector. The implementation of this method is more costly than the implementation of a weight window. However, because the method actively biases particles to travel from the source to the detector, the length of particle histories can be greatly decreased, particularly for deep penetration problems. In these situations, the physics-biasing approach is significantly more efficient.

3. *Automated weight window generation for global problems* [12-17]

   The successful use of automated weight windows for Monte Carlo source-detector problems raised the question of whether a successful automated weight window could be developed for "global" Monte Carlo problems, in which the neutron flux is desired at all spatial points in the system. (This problem occurs routinely in the design and optimization of nuclear reactor cores.) The answer to this question is *yes*. The *Forward-Weighted CADIS* (FW-CADIS) method, which accomplishes this, is publicly available in the SCALE 6 code package, and implemented in the same MAVRIC sequence as described above for the CADIS method.

4. *Functional Monte Carlo methods* [18-21]

   For large, diffusive, optically thick systems (such as commercial reactor cores), standard Monte Carlo methods can be extremely inefficient in the estimation of eigenfunctions. Also, because of the correlations between the fission sources for successive neutron generations, the estimated variance can be significantly smaller than the true variance. To deal with this, new *functional Monte Carlo* (FMC) methods have been developed in which Monte Carlo is not used to directly generate estimates of the neutron flux. Instead, Monte Carlo is used to generate estimates of *nonlinear functionals*, which have the character of multigroup cross sections and have smaller statistical errors than the neutron flux estimates. After these functionals are estimated, a *low-order* algebraic system of equations containing the functionals is solved to obtain (more accurate) estimates of the eigenvalue and eigenfunction. Several different FMC methods have been developed and undergone preliminary testing. This evaluation process is still under way.

In general, the goal of hybrid transport methods is to overcome the deficiencies inherent in "pure" Monte Carlo or deterministic transport methods. Thus, deterministic methods are used to automatically (i) determine useful biasing parameters for

geometrically complex Monte Carlo simulations and (ii) suppress the effect of correlations in estimates of the fission source from one fission generation to the next. Also, continuous-energy Monte Carlo methods can be used to automatically generate accurate multigroup cross sections and other necessary parameters for deterministic methods.

Hybrid transport methods also attempt to make the simulation process for complex particle transport problems much more of a "black box" approach than it has been historically. In other words, the intent is to make the simulation process one in which (i) the code user specifies the system geometry and materials and the grids on which information is desired, and (ii) the computer does everything else – without the need for a human to provide approximate biasing parameters for a Monte Carlo simulation or approximate multigroup cross sections for a deterministic simulation. By removing the guesswork involved in the specification of biasing parameters or multigroup cross sections, the burden on the code user is greatly reduced, and the resulting simulations should become more accurate and reliable.

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