Monte Carlo Analysis

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These notes were written to accompany NE582, which is a graduate level course in Monte Carlo Analysis. This course is aimed primarily at nuclear engineering graduate students and follows a course (NE583) in deterministic neutral particle transport calculation methods.

Since the present course comes second (for most students) the actual derivation of the Boltzmann transport equation occurs in the first course and is not repeated here.

But a stronger effect of this being a follow-up course is the actual approach taken. Toward the Monte Carlo method itself. In the first decades of my career (at the Savannah River Plant and Laboratory) I worked more with deterministic methods of neutral particle transport (diffusion theory, discrete ordinates, integral transport methods) than I did with Monte Carlo. So, when I arrived at the university and it fell to me to teach a Monte Carlo course, I was never quite satisfied with how the method is presented (or even understood by most practitioners). I was more used to studying and coding numerical methods that began with a clear statement of the functional approximation that is occurring (e.g., expanding a desired function in a truncated Legendre polynomial series or values at distributed points on the domain) and then solving for the coefficients. It bothered me that Monte Carlo methods do not do this, even though they are obviously approximating a continuous function, the particle flux, with a finite representation, just like the "deterministic" methods. In my zeal to correct this shortcoming I began teaching my (somewhat bewildered) students the function substitution approach, which is now relegated (in its full treatment) to the end of the semester (Chapters 6-8 of this text), and wrote a paper explaining the approach. The paper was rejected and the students remained bewildered, so I eventually bowed to the reality that most developers and students regard Monte Carlo as a statistical simulation and not a method of solving an equation, and I returned to the more conventional order of presenting the material that you see here.

Although my heart is still with the function-substitution approach, I have relegated it to the later chapters and focused this course on the more immediately usable material in Chapters 1-5. Even when I tentatively introduce the Dirac substitution in Chapter 6, I lay low on the fuller development until the advanced chapters beginning with Chapter 7.

So, the structure of the material is such that:

- Chapters 1 & 2 cover the basic mathematical tools needed for Monte Carlo sampling and scoring.
- Chapter 3 applies these tools to an event-based neutral particle transport approach
- Chapter 4 explores the mathematical approach to sampling of integrals
- Chapter 5 applies the Chapter 4 ideas to the traditional variance reduction techniques.
- Chapter 6 introduces the function substitution approximation.
- Chapter 7 applies the function substitution approach to the random walk utilizing the Dirac delta approximation with Neumann decomposition.
- Chapter 8 applies the function substitution approach to flux-based tallies, producing the traditional collision, track-length and point-flux estimators. It also explores some particle-path extension possibilities, mainly scoring along the path ray of the particle, but beyond the next collision site

Beyond Chapter 8, the chapters explores particular possible improved algorithms—some suggested by the function-substitution approach and some from other experiences. At the present time, the candidates for these addition chapters are (in no particular order):

- Markov chain source problems. The second approach for recursive equations, an iterative Markov chain approach, is described and applied to source problems. The result is a series of samples that only asymptotically approach a sample of the solution, like the traditional eigenvalue approach.
- Vector applications. Extension of the function substitution to vectors (discrete functions), utilizing linear algebra notation. Examples of use of vector substitution, primarily to explore other ways of formulating multigroup energy algorithms.
- Forward random-walk source problems: Analog
- Generalized Woodcock method. An extension to another somewhat useful random walk approach, which avoids the need for ray tracing (at the expense of more particle events to keep up with).
- Variance reduction 1: Applying the PDF-changing approach to every decision in the random walk. The main gap from the traditional approach finding better PDFs for distance to next collision. The others are straight-forward application of emission adjoints and collision adjoints.
- Variance reduction 2: Applying the variance-control method to every decision in the random walk, to compare to the results of the previous one.
- Adjoint random-walk source problems.The adjoint transport equation is laid out and possible general approaches are discussed. The basis of this is that "analog"—i.e., natural—approaches to the adjoint flux calculation would involve forward-flux weighting. So, the successful adjoint calculational methods involve some sort of approximation of the forward flux—perhaps implicit.
- Other eigenvalue approaches. As seen in Chapter 5, the current Markov chain approaches to fission source distributions rely on a "batch" method for the subset of fission source locations used. Other possible solutions will be explored. Maybe, if this was shown useful for source problems, a complete Markov chain approach (including emerging particles) might be explored.
- Lattice k-effective calculations. Possible gains from having particles only move within a single cell within a regular lattice—with particle weights used in other lattice cells.
- Adjoint k-effective problems. Although the forward flux spectrum varies by large orders of magnitude, the adjoint flux is very flat, especially for thermal problems. The usefulness of doing k-effective calculations this way is explored.
- Adjoint lattice k-effective problems. If it looks promising in forward problems.
- Monte Carlo solutions of discrete ordinates equations. Quite a stretch here. Since discrete ordinates equations are just big matrices, can the vector Monte Carlo approach be used to get solutions—especially "bad" solutions that might be useful for importance weighting

of forward Monte Carlo calculations? (The idea being to use the inverse square law to our advantage!) Not sure if this will work.

- Perturbation calculations. The most useful of possible advantage to take of the separation of the PDF from the physics. Possible applications—beyond some that have already reached the literature—for using simultaneous calculation of multiple problems to hone in on differences. The idea is to identify maximum and minimum parameter values, possibly without needed accuracy in the tally values themselves. Maybe even do a mixed calculation—more histories for the base case and/or adapting the base case—to get both to similar uncertainty.
- Multigroup with continuous energy correction. This involves the use of multigroup for the random walk, with weight corrections for continuous energy. This might be particularly useful for continuous-energy adjoint (if it is needed).
- Isotopic decay. Application of Monte Carlo to decay problems. Analog is straight-forward, but are there any suggestions for improvement?
- Space/time decay. Putting space and time calculations together (on decay time scales).
- Diffusion calculations. Examination of the walk on spheres approach—its basis in adjoint and possible improvements. Could be useful way to incorporate heat transfer into the Monte Carlo calculation itself. (Follow up if promising.)
- 1D shield optimization, tournament style. Use of maximization search using a tournament style approach. By "tournament style" I mean start with all possible solutions, dropping off the 3-5 sigma "losers" as the calculation proceeds.
- Importance weighting with uncertainty. Extension of the Markov chain examination for source problems, this involves adaptive importance weight using true variances that occur—rather than the assumption the variance equals importance (a Poisson distribution).
- Spherical 1D calculation. Current 1D spherical geometry, just uses 3D and forgets angular information. Is there a Green's function that could solve the curvilinear equations directly?
- Schrodinger equation applications. This is a big area of Monte Carlo practice that I am completely unfamiliar with. Can any of these ideas help those kinds of applications? (Similar to the diffusion application.)