

Hybrid Monte Carlo-Deterministic Methods for Simulating Particle Transport

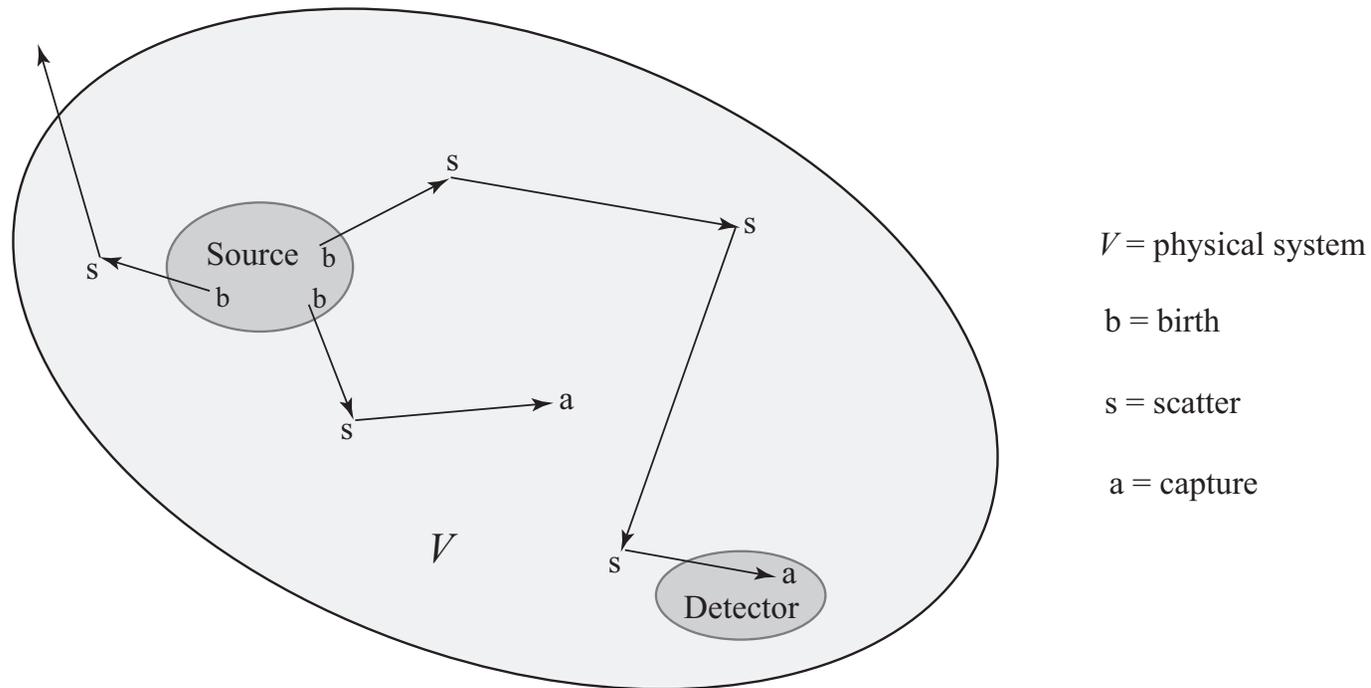
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Abstract:

For the past 50 years, methods for simulating practical neutron and photon transport problems have been developed for two very different classes of algorithms: deterministic (discrete ordinates), and stochastic (Monte Carlo). Almost all production particle transport codes are based on one of these broad approaches, not on both. However, “hybrid” Monte Carlo-Deterministic methods, which advantageously combine Monte Carlo and Deterministic techniques, have recently been developed and shown to be useful. This talk will review, in the context of some well-known hybrid methods, several different hybrid methods that have been developed at the University of Michigan during the past 15 years.

2. Particle Transport (Source Detector Problem)



- Number of physical particles $\approx 10^{15}$.
- Pdf's for: point of birth, initial direction of flight and energy, distance to collision, scattering vs capture, and scattered direction of flight and energy.
- Absorption in the detector can be a rare event.

3. Monte Carlo (Stochastic) Methods

- Simulate the random histories of 10^6 - 10^8 particles and average over all histories.
- Statistical deviations from the mean are much larger than in real life:

$$\text{Error} \approx \frac{\sigma}{\sqrt{N}} \quad , \quad [\sigma = \text{standard deviation is problem-dependent}] \quad . \quad (1)$$

- Estimation of rare events requires nonanalog methods.
- Nonanalog methods (geometric splitting, weight window) require a large number of biasing parameters that historically have been prescribed by the code user. These parameters can be difficult and costly to estimate well. [Monte Carlo is *not* user-friendly.]
- Monte Carlo methods generally work best when estimating limited information (e.g. a single detector response or eigenvalue). It is difficult for Monte Carlo methods to obtain accurate global information.

4. Discrete Ordinates or S_N (Deterministic) Methods

- The Boltzmann Equation:

$$\Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x})\psi(\mathbf{x}, \Omega) - \frac{\Sigma_s(\mathbf{x})}{4\pi} \int_{4\pi} \psi(\mathbf{x}, \Omega') d\Omega' = \frac{Q(\mathbf{x})}{4\pi}, \quad \mathbf{x} \in V, \quad \Omega \in 4\pi, \quad (2a)$$

$$\psi(\mathbf{x}, \Omega) = 0, \quad \mathbf{x} \in \partial V, \quad \Omega \cdot \mathbf{n} < 0, \quad (2b)$$

$$R = \int_V \int_{4\pi} \frac{\Sigma(\mathbf{x})}{4\pi} \psi(\mathbf{x}, \Omega) d\Omega dV =? \quad (3)$$

- Discretize all variables (space, direction of flight, energy) in Eqs. (2). Then solve the resulting system of algebraic equations. This yields a global solution, with truncation errors.
- Deterministic methods require the user to select grids for all the independent variables. Typically, this is an easier task than choosing biasing parameters for difficult Monte Carlo problems.

5. Neutron/Photon Transport Code Development

- The technical knowledge and skills needed to develop and implement deterministic methods differ greatly from that needed to develop and implement Monte Carlo codes.
- Advances in deterministic methodology (discretization methods, iterative solvers, etc.) have had almost no impact on Monte Carlo methodology (variance reduction methods, etc.) – and vice versa.
- The particle transport code development community actually consists of two communities: Deterministic and Monte Carlo, which have limited interaction.
- With rare exceptions, “production” particle transport codes written during the past 50 years are based *either* on Monte Carlo methodology *or* on Deterministic methodology.
- Yet, Monte Carlo and Deterministic codes simulate the same physical problem.

6. Hybrid MC/Det Methods

In the past 15 years, a new class of “hybrid” MC/Det methods have been developed, whose purpose is to combine MC and Det concepts in ways that enhance their advantages and suppress their disadvantages.

Typically, these methods operate in the following way:

1. An inexpensive deterministic simulation (usually, adjoint) is first performed.
2. The deterministic results are processed to yield biasing parameters.
3. The biasing parameters are then used in a subsequent nonanalog Monte Carlo calculation.

The overall concept is to use deterministic methods to help make Monte Carlo simulations easier to set up and more efficient to run. The goal is to achieve an unbiased Monte Carlo solution as efficiently as possible.

7. Hybrid MC/Det Methods: Advantages and Disadvantages

Advantages:

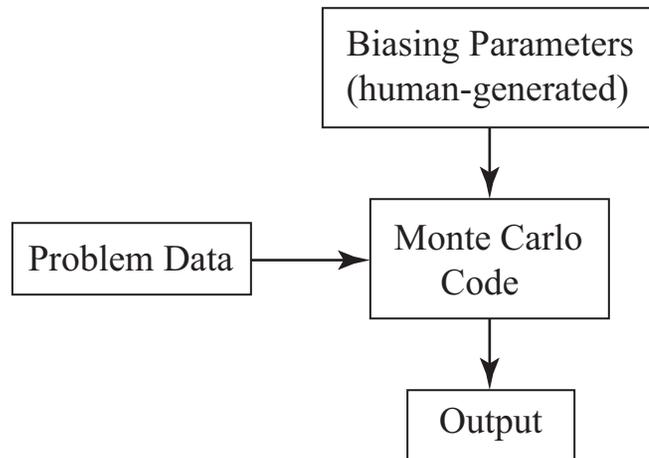
- For difficult problems, setting up, running, and processing a deterministic code to obtain biasing parameters can take much less time than the often-inefficient process of trial-and-error. (The user time is reduced.)
- If the deterministic solution is reasonably accurate, then the resulting biasing parameters are better than ones that would be chosen by a code user. (The Monte Carlo calculation with computer-generated biasing parameters runs more efficiently.)

Disadvantages:

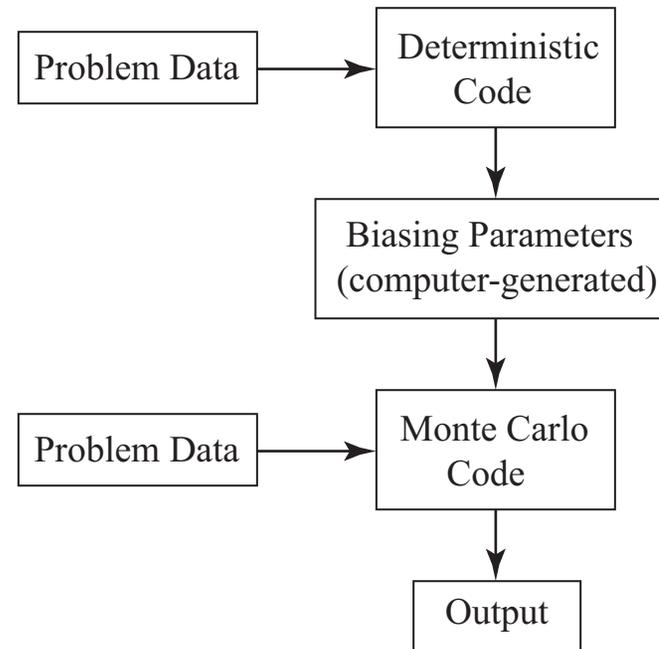
- The code user must (i) set up the problem in two separate codes, and (ii) process and ship results from the Deterministic code to the Monte Carlo code. (The cumbersomeness of this process has been an impediment to the wider use of hybrid methods.)

8. Hybrid MC/Det vs standard MC

Conventional
Monte Carlo:



Hybrid Monte Carlo/
Deterministic:



9. Example: Deterministic Weight Windows (i)

The *forward* source-detector problem:

$$\begin{aligned} \Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x})\psi(\mathbf{x}, \Omega) - \frac{\Sigma_s(\mathbf{x})}{4\pi} \int_{4\pi} \psi(\mathbf{x}, \Omega') d\Omega' \\ = \frac{Q(\mathbf{x})}{4\pi} , \quad \mathbf{x} \in V , \quad \Omega \in 4\pi , \end{aligned} \quad (4a)$$

$$\psi(\mathbf{x}, \Omega) = 0 , \quad \mathbf{x} \in \partial V , \quad \Omega \cdot \mathbf{n} < 0 , \quad (4b)$$

$$R = \int_V \int_{4\pi} \frac{\Sigma(\mathbf{x})}{4\pi} \psi(\mathbf{x}, \Omega) d\Omega dV =? \quad (5)$$

The *adjoint* problem:

$$\begin{aligned} -\Omega \cdot \nabla \psi^*(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x})\psi^*(\mathbf{x}, \Omega) - \frac{\Sigma_s(\mathbf{x})}{4\pi} \int_{4\pi} \psi^*(\mathbf{x}, \Omega') d\Omega' \\ = \frac{\Sigma(\mathbf{x})}{4\pi} , \quad \mathbf{x} \in V , \quad \Omega \in 4\pi , \end{aligned} \quad (6a)$$

$$\psi(\mathbf{x}, \Omega) = 0 , \quad \mathbf{x} \in \partial V , \quad \Omega \cdot \mathbf{n} > 0 . \quad (6b)$$

10. Example: Deterministic Weight Windows (ii)

1. Deterministically solve Eqs. (4) to obtain:

$$\psi^*(\mathbf{x}, \Omega) \quad \text{or} \quad \phi^*(\mathbf{x}) = \int_{4\pi} \psi^*(\mathbf{x}, \Omega) d\Omega .$$

2. Define weight windows:

$$ww^\pm(\mathbf{x}, \Omega) = \lambda^{\pm 1} \frac{C}{\phi^*(\mathbf{x})} \quad [\text{isotropic: MCBEND}]$$

or

$$ww^\pm(\mathbf{x}, \Omega) = \lambda^{\pm 1} \frac{C}{\psi^*(\mathbf{x}, \Omega)} \quad [\text{anisotropic: AVATAR}]$$

3. Run the Monte Carlo code in nonanalog mode using the deterministic weight windows.

Other hybrid methods, such as source-biasing (CADIS), are based on similar ideas.

Next, we discuss some alternate hybrid methods which, for source-detector problems, make use of the same adjoint function as discussed above [see Eqs. (6)].

11. The “LIFT” Method for Source-Detector Problems

The Local Importance Function Transform (LIFT) method for source-detector problems is a hybrid MC/Det method that approximates a zero-variance method. To explain the LIFT method, we first describe the zero-variance method.

We again consider the forward source-detector problem:

$$\begin{aligned} \Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x})\psi(\mathbf{x}, \Omega) - \frac{\Sigma_s(\mathbf{x})}{4\pi} \int_{4\pi} \psi(\mathbf{x}, \Omega') d\Omega' \\ = \frac{Q(\mathbf{x})}{4\pi} \quad , \quad \mathbf{x} \in V \quad , \quad \Omega \in 4\pi \quad , \end{aligned} \quad (7a)$$

$$\psi(\mathbf{x}, \Omega) = 0 \quad , \quad \mathbf{x} \in \partial V \quad , \quad \Omega \cdot \mathbf{n} < 0 \quad , \quad (7b)$$

$$R = \int_V \int_{4\pi} \frac{\Sigma(\mathbf{x})}{4\pi} \psi(\mathbf{x}, \Omega) d\Omega dV =? \quad , \quad (8)$$

and the corresponding adjoint problem:

$$\begin{aligned} -\Omega \cdot \nabla \psi^*(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x})\psi^*(\mathbf{x}, \Omega) - \frac{\Sigma_s(\mathbf{x})}{4\pi} \int_{4\pi} \psi^*(\mathbf{x}, \Omega') d\Omega' \\ = \frac{\Sigma(\mathbf{x})}{4\pi} \quad , \quad \mathbf{x} \in V \quad , \quad \Omega \in 4\pi \quad , \end{aligned} \quad (9a)$$

$$\psi(\mathbf{x}, \Omega) = 0 \quad , \quad \mathbf{x} \in \partial V \quad , \quad \Omega \cdot \mathbf{n} > 0 \quad . \quad (9b)$$

12. The “Contributon” Flux

Define the contributon flux $\xi(\mathbf{x}, \Omega)$ by:

$$\psi(\mathbf{x}, \Omega) = \frac{\xi(\mathbf{x}, \Omega)}{\psi^*(\mathbf{x}, \Omega)} . \quad (10)$$

Introduce Eq. (10) into Eqs. (7) to obtain the following transport problem for ξ :

$$\begin{aligned} & \Omega \cdot \nabla \xi(\mathbf{x}, \Omega) + \widehat{\Sigma}_t(\mathbf{x}, \Omega) \xi(\mathbf{x}, \Omega) \\ &= \int_{4\pi} \widehat{c}(\mathbf{x}) \widehat{p}(\mathbf{x}, \Omega) [\widehat{\Sigma}_t(\mathbf{x}, \Omega') \xi(\mathbf{x}, \Omega')] d\Omega' + \widehat{P}(\mathbf{x}, \Omega) R , \end{aligned} \quad (11a)$$

$$\xi(\mathbf{x}, \Omega) = 0 , \quad \mathbf{x} \in \partial V , \quad \Omega \cdot \mathbf{n} < 0 , \quad (11b)$$

where:

$$\widehat{\Sigma}_t(\mathbf{x}, \Omega) = \frac{1}{4\pi} \frac{\Sigma_s(\mathbf{x}) \phi^*(\mathbf{x}) + \Sigma(\mathbf{x})}{\psi^*(\mathbf{x}, \Omega)} , \quad (12a)$$

$$\widehat{p}(\mathbf{x}, \Omega) = \frac{\psi^*(\mathbf{x}, \Omega)}{\phi^*(\mathbf{x})} , \quad (12b)$$

$$\widehat{c}(\mathbf{x}) = \frac{\widehat{\Sigma}_s(\mathbf{x}) \phi^*(\mathbf{x})}{\widehat{\Sigma}_s(\mathbf{x}) \phi^*(\mathbf{x}) + \Sigma(\mathbf{x})} , \quad (12c)$$

$$\widehat{P}(\mathbf{x}, \Omega) = \frac{\psi^*(\mathbf{x}, \Omega) Q(\mathbf{x})}{\int_V \int_{4\pi} \psi^*(\mathbf{x}', \Omega') Q(\mathbf{x}') d\Omega' dV'} . \quad (12d)$$

13. A Zero-Variance Problem for Contributons

Note that:

- Contributons are born in the source region with “weight” R .
- $\hat{\Sigma}_t(\mathbf{x}, \boldsymbol{\Omega}) \rightarrow \infty$ as $\mathbf{x} \rightarrow \partial V$ with $\boldsymbol{\Omega} \cdot \mathbf{n} > 0$. [Contributons cannot leak out of V .]
- $\hat{c}(\mathbf{x}) = 1$ outside the detector region and $\hat{c}(\mathbf{x}) < 1$ inside the detector region. [Contributons can be absorbed only in the detector region.]

Therefore: all contributons will die in the detector region with weight R . This implies that an analog Monte Carlo simulation of the contributon problem [Eqs. (11)] will have zero variance.

14. Transport “Mechanics” of the Zero-Variance Problem

Also, note that:

- $$\hat{P}(\mathbf{x}, \Omega) = \frac{\psi^*(\mathbf{x}, \Omega) Q(\mathbf{x})}{\int_V \int_{4\pi} \psi^*(\mathbf{x}', \Omega') Q(\mathbf{x}') d\Omega' dV'}$$

favors the location \mathbf{x} and direction Ω of source particles where $\phi^*(\mathbf{x}, \Omega)$ is largest. [Spatial points \mathbf{x} “nearest” the detector and directions Ω pointing “toward” the detector are favored. (This is the concept underlying source biasing.)]

- $$\hat{\Sigma}_t(\mathbf{x}, \Omega) = \frac{1}{4\pi} \frac{\Sigma_s(\mathbf{x})\phi^*(\mathbf{x}) + \Sigma(\mathbf{x})}{\psi^*(\mathbf{x}, \Omega)}$$

is minimized for directions Ω pointing “toward” the source. [At each \mathbf{x} , contributions traveling in directions Ω toward the detector have the longest mean free paths.]

- $$\hat{p}(\mathbf{x}, \Omega) = \frac{\psi^*(\mathbf{x}, \Omega)}{\phi^*(\mathbf{x})}$$

is maximized for directions pointing “toward” the detector. [When contributions scatter at \mathbf{x} , outgoing directions of flight Ω that point “toward” the detector are favored.]

Therefore: the transport “mechanics” of the zero-variance problem [Eqs. (11)] actively encourage contributions to migrate toward the detector. [Contribution histories are short.]

15. Contributons and Physical Particles

The contributon flux $\xi(\boldsymbol{x}, \Omega)$ and the particle flux $\psi(\boldsymbol{x}, \Omega)$ are related by:

$$\psi(\boldsymbol{x}, \Omega) = \frac{\xi(\boldsymbol{x}, \Omega)}{\psi^*(\boldsymbol{x}, \Omega)} . \quad (13)$$

A contributon has constant weight R outside the detector region. A contributon with weight R at (\boldsymbol{x}, Ω) corresponds to a physical particle at (\boldsymbol{x}, Ω) with weight:

$$w(\boldsymbol{x}, \Omega) = \frac{R}{\psi^*(\boldsymbol{x}, \Omega)} . \quad (14)$$

Thus, the physical particles at (\boldsymbol{x}, Ω) that correspond to contributons have a deterministic (non-random) weight, $w(\boldsymbol{x}, \Omega)$.

16. The Impracticality of the Zero Variance Method

To implement the zero variance method for correctons, it is necessary to exactly know the adjoint angular flux $\psi^*(x, \Omega)$ for all $x \in V$ and $\Omega \in 4\pi$.

Generally, this is impossible; the zero-variance method requires infinitely more knowledge than the originally-desired response R (a single number)!

Hence, the zero-variance method is impractical.

But – this does not mean that it cannot be approximated in a way that *is* practical.

17. The LIFT Method – An Approximate Zero-Variance Method

The Local Importance Function Transform (LIFT) method is a practical approximation to the zero-variance method for contributors. Suppose that one has an approximate adjoint flux $\tilde{\psi}^*(\mathbf{x}, \Omega)$, which is obtained by a deterministic code; and suppose that one defines an approximate contributor flux $\tilde{\xi}(\mathbf{x}, \Omega)$ by:

$$\psi(\mathbf{x}, \Omega) = \frac{\tilde{\xi}(\mathbf{x}, \Omega)}{\tilde{\psi}^*(\mathbf{x}, \Omega)} . \quad (15)$$

Introducing Eq. (15) into Eqs. (7), we obtain the following transport equation for $\hat{\xi}$:

$$\begin{aligned} & \Omega \cdot \nabla \hat{\xi}(\mathbf{x}, \Omega) + [\Sigma_t(\mathbf{x}) + \Omega \cdot \nabla \ln \hat{\psi}^*(\mathbf{x}, \Omega)] \hat{\xi}(\mathbf{x}, \Omega) \\ &= \frac{\Sigma_s(\mathbf{x})}{4\pi} \int_{4\pi} \frac{\hat{\psi}^*(\mathbf{x}, \Omega)}{\hat{\psi}^*(\mathbf{x}, \Omega')} \hat{\xi}(\mathbf{x}, \Omega') d\Omega' + \frac{Q(\mathbf{x})}{4\pi} \hat{\psi}^*(\mathbf{x}, \Omega) , \quad \mathbf{x} \in V , \end{aligned} \quad (16a)$$

with the boundary condition:

$$\hat{\xi}(\mathbf{x}, \Omega) = 0 , \quad \mathbf{x} \in \partial V , \quad \Omega \cdot \mathbf{n} < 0 . \quad (16b)$$

18. Some Properties of the Transport Problem for $\hat{\xi}(x, \Omega)$

The transport problem for $\hat{\xi}(x, \Omega)$ has the following properties:

- Source points x “nearest” the detector and initial directions of flight Ω pointing “toward” the detector are still favored.
- The longest mean free paths still occur for particles traveling “toward” the detector.
- Scattered directions of flight pointing toward the detector are still favored.
- Particles are generally not forbidden to leak out of the system.
- Outside the detector region, the effective scattering ratio is not = 1, but it is ≈ 1 . Thus, in collisions, MC particles will experience *small* changes in weight.
- The computer arithmetic necessary to process Monte Carlo streaming and scattering for Eqs. (16) is greater than that for Eqs. (1).

Thus, an analog Monte Carlo simulation of Eqs. (16) for $\hat{\xi}$ will not be zero-variance, but it will generally be *low-variance*. Like the zero-variance method, it will actively encourage MC particles to migrate toward the detector, helping to ensure that histories are short.

If $\hat{\psi}^*(x, \Omega)$ is “simple,” the time to process Monte Carlo simulations of Eq. (16) is minimized.

19. The LIFT Form of $\hat{\psi}(\mathbf{x}, \Omega)$

The LIFT method approximates $\hat{\psi}^*(\mathbf{x}, \Omega)$ and carries out the steps described in the previous slides. The algebraic form of $\hat{\psi}^*$ is as follows. We divide the system V into J disjoint spatial cells V_j , and within each j^{th} cell we take:

$$\hat{\psi}^*(\mathbf{x}, \Omega) = \hat{\psi}_j^*(\mathbf{x}, \Omega) \equiv A_j \frac{e^{\rho_j \cdot (\mathbf{x} - \mathbf{x}_j)}}{1 - \rho_j \cdot \Omega} , \quad \mathbf{x} \in V_j , \quad 1 \leq j \leq J , \quad (17)$$

where \mathbf{x}_j is a chosen point in V_j , and A_j and ρ_j are constants defined in each cell, obtained by processing the deterministic adjoint flux in and around V_j .

This form of $\hat{\psi}^*$ leads to an exponential transform with angular biasing, with transform parameters (A_j and ρ_j) that are computer-generated and defined locally within each spatial cell V_j . (Care must be taken at cell edges, where the transform parameters can be discontinuous.)

20. Performance of the LIFT Method

The LIFT method is described in detail in two papers [S.A. Turner & E.W. Larsen, *Nucl. Sci. Eng.* **127**, pp. 22-35 and 36-53 (1997)].

- Problems run were 3-D, relatively simple geometries (but with heterogeneous geometries with ducts), few-groups, linearly anisotropic scattering.
- Adjoint calculations were performed by diffusion, simplified P_N , and S_N .
- Comparisons were made against the AVATAR (automatic weight window) method.
- LIFT can be run with or without a weight window. Generally, running LIFT with a weight window was found to be *disadvantageous*.
- LIFT is most advantageous for problems with strong absorption. As the scattering ratio decreases, the benefit of LIFT increases. LIFT is not advantageous for highly scattering problems.
- Basic conclusion: For the problems tested, LIFT usually (but not always) outperforms AVATAR. For deep penetration problems, when ψ^* is fairly accurate, LIFT often outperforms AVATAR by about a factor of 5 (ratio of figures-of-merit).

21. The LIFT and VVR Methods – Overview

The LIFT method is an approximation to a zero-variance method. The principal action of the LIFT method is to alter the transport mechanics in ways that (i) encourage Monte Carlo particles to migrate toward the detector and (ii) minimize the random weight change of particles in collisions.

There is another zero-variance method (for both source-detector and eigenvalue problems), which is based on a variational principle using – as before – the forward and adjoint fluxes. As in the LIFT method, if we approximate this impractical “variational” zero-variance method, we obtain a practical low-variance “Variational Variance Reduction” (VVR) method. The action of the VVR method is to alter the manner in which information from the Monte Carlo particle histories is processed and stored.

The VVR method has been developed mainly for k -eigenvalue problems, so we will describe the method in that context. First, we discuss the zero-variance method on which VVR is based.

22. k -Eigenvalue Problems

We now consider the forward k -eigenvalue problem:

$$\begin{aligned} \Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x})\psi(\mathbf{x}, \Omega) - \frac{\Sigma_s(\mathbf{x})}{4\pi} \int_{4\pi} \psi(\mathbf{x}, \Omega') d\Omega' \\ = \frac{\nu \Sigma_f(\mathbf{x})}{4\pi k} \int_{4\pi} \psi(\mathbf{x}, \Omega') d\Omega' , \quad \mathbf{x} \in V , \quad \Omega \in 4\pi , \end{aligned} \quad (18a)$$

$$\psi(\mathbf{x}, \Omega) = 0 , \quad \mathbf{x} \in \partial V , \quad \Omega \cdot \mathbf{n} < 0 , \quad (18b)$$

or:

$$T\psi = \frac{1}{k}F\psi . \quad (19)$$

The corresponding adjoint k -eigenvalue problem is:

$$T^*\psi^* = \frac{1}{k}F^*\psi^* . \quad (20)$$

Multiplying Eq. (19) by $\psi^*(\mathbf{x}, \Omega)$ and integrating over $\Omega \in 4\pi$ and $\mathbf{x} \in V$, we obtain

$$\frac{1}{k} = \frac{\int_V \int_{4\pi} \psi^*(\mathbf{x}, \Omega) T\psi(\mathbf{x}, \Omega) d\Omega dV}{\int_V \int_{4\pi} \psi^*(\mathbf{x}, \Omega) F\psi(\mathbf{x}, \Omega) d\Omega dV} . \quad (21)$$

23. The Variational Functional $F[\Psi^*, \Psi]$

Eq. (21) suggests that for any functions $\Psi(\mathbf{x}, \Omega)$ and $\Psi^*(\mathbf{x}, \Omega)$, we define the functional:

$$F[\Psi^*, \Psi] = \frac{\int_V \int_{4\pi} \Psi^*(\mathbf{x}, \Omega) T \Psi(\mathbf{x}, \Omega) d\Omega dV}{\int_V \int_{4\pi} \Psi^*(\mathbf{x}, \Omega) F \Psi(\mathbf{x}, \Omega) d\Omega dV} . \quad (22)$$

F has the following property: if

$$\Psi^*(\mathbf{x}, \Omega) = \psi^*(\mathbf{x}, \Omega) + \delta\psi^*(\mathbf{x}, \Omega) , \quad (23a)$$

$$\Psi(\mathbf{x}, \Omega) = \psi(\mathbf{x}, \Omega) + \delta\psi(\mathbf{x}, \Omega) , \quad (23b)$$

then:

$$\begin{aligned} F[\Psi^*, \Psi] &= \frac{\frac{1}{k} \iint [\psi^* F \psi + \delta\psi^* F \psi + \delta\psi F^* \psi^*] d\Omega dV + \iint \delta\psi^* T \delta\psi d\Omega dV}{\iint [\psi^* F \psi + \delta\psi^* F \psi + \delta\psi F^* \psi^*] d\Omega dV + \iint \delta\psi^* F \delta\psi d\Omega dV} \\ &= \frac{1}{k} + O(\delta\psi^* \delta\psi) . \end{aligned} \quad (23c)$$

Therefore:

1. If $\Psi = \psi$, then for any Ψ^* , $F[\Psi^*, \psi] = \frac{1}{k}$.
2. If $\Psi^* = \psi^*$, then for any Ψ , $F[\psi^*, \Psi] = \frac{1}{k}$.
3. If Ψ is a first-order approximation to ψ and Ψ^* is first-order approximation to ψ^* , then $F[\Psi^*, \Psi]$ is a second-order approximation to $\frac{1}{k}$.

24. The “Variational” Zero-Variance Method

Let us consider a Monte Carlo scheme in which:

$$\begin{aligned}\Psi^*(\boldsymbol{x}, \Omega) &= \psi^*(\boldsymbol{x}, \Omega) \\ &= \text{the exact adjoint angular flux}\end{aligned}\tag{24}$$

and

$$\begin{aligned}\Psi(\boldsymbol{x}, \Omega) &= \text{any estimate of } \psi(\boldsymbol{x}, \Omega) \text{ obtained} \\ &\text{by a forward Monte Carlo simulation .}\end{aligned}\tag{25}$$

Then from results on the previous slide,

$$F[\psi^*, \Psi] = \frac{1}{k} ,\tag{26}$$

so the exact eigenvalue is always obtained. Hence, this Monte Carlo method – which is distinguished by how it processes the information obtained from particle histories – has zero variance.

As before, this zero-variance method is impractical because it requires perfect knowledge of $\psi^*(\boldsymbol{x}, \Omega)$.

25. The VVR Method

The Variational Variance Reduction method uses an approximate deterministic estimate of the adjoint function:

$$\Psi^*(\mathbf{x}, \Omega) = \Psi_j^*(\mathbf{x}, \Omega) \quad , \quad \mathbf{x} \in \partial V_j \quad , \quad \Omega \in 4\pi \quad , \quad (27)$$

where Ψ_j^* is a specified continuous function with parameters determined by the deterministic adjoint solution. Eq. (22) becomes:

$$\begin{aligned} F[\Psi^*, \Psi] &= \frac{\sum_{j=1}^J \int_{V_j} \int_{4\pi} \Psi_j^*(\mathbf{x}, \Omega) T \Psi(\mathbf{x}, \Omega) d\Omega dV}{\sum_{j=1}^J \int_V \int_{4\pi} \Psi_j^*(\mathbf{x}, \Omega) F \Psi(\mathbf{x}, \Omega) d\Omega dV} \\ &= \frac{\sum_{j=1}^J \left[\int_{\partial V_j} \int_{4\pi} [\Omega \cdot \mathbf{n}_j \Psi^*] \Psi(\mathbf{x}, \Omega) d\Omega dS + \int_{V_j} \int_{4\pi} [T^* \Psi_j^*] \Psi(\mathbf{x}, \Omega) d\Omega dV \right]}{\sum_{j=1}^J \int_{V_j} \int_{4\pi} [F^* \Psi_j^*] \Psi(\mathbf{x}, \Omega) d\Omega dV} \\ &\approx \frac{1}{k} \quad . \end{aligned} \quad (28)$$

Estimates of each of the above integrals involving Ψ can be obtained by processing the histories of forward Monte Carlo particles as they migrate through V . If $\Psi^*(\mathbf{x}, \Omega)$ is accurate, the variance in the resulting estimate of k is low, and if $\Psi^*(\mathbf{x}, \Omega)$ is simple, the Monte Carlo estimation of these integrals is not expensive.

26. Performance of the VVR Method

The VVR method for eigenvalue calculations is described in detail in [J.D. Densmore and E.W. Larsen, *Nucl. Sci. Eng.* **146**, pp. 121-140 (2004)].

- Problems run were 3-D, diffusive, relatively simple heterogeneous geometries, few groups.
- Adjoint calculations were performed by diffusion.
- The adjoint flux is represented in each spatial cell as a low-order polynomial in x and Ω .
- Comparisons were made against standard Monte Carlo.
- It is more efficient to run VVR without implicit capture.
- Basic conclusion: for the problems tested, VVR outperformed standard Monte Carlo by $O(10)$.

27. Generalizations of LIFT and VVR

- The VVR method can also be applied to deep penetration source-detector problems. The relevant functional is:

$$F[\Psi^*, \Psi] = \int_V \int_{4\pi} \Sigma \Psi \, d\Omega dV - \int_V \int_{4\pi} \Psi^* \left(T\Psi - \frac{Q}{4\pi} \right) d\Omega dV \approx R . \quad (29)$$

A logical choice of Ψ^* is given by Eq. (17):

$$\Psi^*(\mathbf{x}, \Omega) = \Psi_j^*(\mathbf{x}, \Omega) \equiv A_j \frac{e^{\rho_j \cdot (\mathbf{x} - \mathbf{x}_j)}}{1 - \rho_j \cdot \Omega} , \quad \mathbf{x} \in V_j , \quad 1 \leq j \leq J . \quad (30)$$

We plan to investigate this approach.

- Also, LIFT and VVR can be combined. The resulting method would alter both the transport mechanics (LIFT) and the calculation of tallys (VVR). We plan to investigate this as well.

28. “Global” Transport Problems

In source-detector problems, an estimate of a single number – the response R – is desired. In global problems, estimates of the flux ψ are desired at all points (x, Ω) of phase space. [Global problems are the “opposite” of source-detector problems.]

No zero-variance methods exist for obtaining global estimates of ψ .

For deep-penetration problems, estimates of ψ are difficult at points distant from the source, where few analog Monte Carlo particles go. To achieve comparably good estimates of ψ everywhere, it is necessary to populate the system more uniformly with Monte Carlo particles.

29. Cooper's (Weight Window) Method

Consider a forward transport problem with forward angular flux $\psi(\mathbf{x}, \Omega)$ and scalar flux $\phi(\mathbf{x})$. Suppose that a weight window is used:

$$ww^\pm(\mathbf{x}) = \lambda^{\pm 1} f(\mathbf{x}) \quad , \quad (31)$$

where $\lambda \approx 3$ and $f(\mathbf{x})$ is the prescribed "center" of the weight window at \mathbf{x} . Also, let:

$$D(\mathbf{x}) = \text{density of Monte Carlo particles at } \mathbf{x} \quad , \quad (32a)$$

$$N(\mathbf{x}) = \frac{1}{v} \phi(\mathbf{x}) = \text{density of Monte Carlo particles at } \mathbf{x} \quad . \quad (32b)$$

Then:

$$\boxed{N(\mathbf{x}) \approx D(\mathbf{x}) f(\mathbf{x}) \quad .} \quad (33)$$

If we estimate $N(\mathbf{x})$ deterministically and choose $f(\mathbf{x}) = CN(\mathbf{x})$, then

$$D(\mathbf{x}) \approx \frac{1}{C} \quad , \quad (34)$$

and the density of Monte Carlo particles will be approximately uniform in phase space. This will uniformly populate the "deep" parts of problems with Monte Carlo particles, and will help ensure that the relative statistical errors in estimates of ψ are relatively constant throughout V .

30. Cooper's Method - Discussion

- This method is described in detail in [M.A. Cooper and E.W. Larsen, *Nucl. Sci. Eng.* **137**, 1 (2001)].
- Problems run were 3-D, heterogeneous, with and without voids, with few energy groups.
- The method worked very well.
- If large numbers of groups are used, the method can work *too* well. Since all groups are treated equally, Cooper's method can spend too much time populating groups that are not "important," and this slows down the simulation.
- A remedy: If some groups (or other regions in phase space) are deemed to be less "important" than others, then increase the center of the weight window there. This will decrease the number of Monte Carlo particles that go there. (Peplow)
- Is there an "optimal" way to do this?

31. The “Correcton” Method

Consider a deep-penetration problem with a forward angular flux $\psi(\boldsymbol{x}, \boldsymbol{\Omega})$ and a deterministically-estimated forward angular flux $\Psi(\boldsymbol{x}, \boldsymbol{\Omega})$. Define the *correcton* flux $f(\boldsymbol{x}, \boldsymbol{\Omega})$ by:

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) f(\boldsymbol{x}, \boldsymbol{\Omega}) . \quad (35)$$

Then if $\Psi \approx \psi$, $f \approx 1$.

Hence, if we:

- Insert Eq. (35) into Eqs. (2) to obtain the transport problem for f , and
- Use Monte Carlo to simulate the transport problem for f ,

then the transport mechanics of the Monte Carlo simulation will automatically ensure that the density of f -particles (correctons) will be roughly uniform in phase space. Also, the same transport mechanics will make correcton histories short, with relatively small random changes in weight.

32. Correcton Method - Discussion

- The implementation of this method is similar to that of the LIFT method.
- The correcton method is more complicated to implement than Cooper's method, but it seems to be more efficient – because particle histories are shorter, and because it is not necessary to use a weight window.
- The correcton approach will suffer from the same problem as Cooper's method: for multigroup problems with many groups, some not-so-important, correctons will try to populate all groups equally. To adjust for this, Eq. (35) should be modified so that the correcton flux is smaller in the less-important groups.
- The correcton approach is still a work-in-progress. For details and 1-D results, see: [T.L. Becker, A.B. Wollaber, and E.W. Larsen, *Nucl. Sci. Eng.* **155**, 155 (2007).]

33. Conclusions

- Hybrid MC/Det methods are known and, to a limited extent, used in practical source-detector problems.
- Practical hybrid methods use deterministic adjoint functions to obtain deterministic weight windows (MCBEND, AVATAR) or to perform source biasing (CADIS).
- Deterministic adjoint solutions can also be used to advantageously bias the transport mechanics (LIFT) and the estimation of tallys (VVR).
- It is also possible to use deterministic forward solutions to obtain global Monte Carlo estimates. (Cooper, Correcton, Peplow)
- The ideas that underlie these “new” approaches are straightforward and have a solid theoretical basis.
- A greater acceptance and use of hybrid methods is not likely until software improvements are made to make these methods easier to apply.