2

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Steps Toward Importance Sampling for MCMEG

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Steps toward Importance Sampling for MCMEG

Introduction

A well-known concept in neutron transport theory is that of importance, which may be defined as follows: "The importance, $N^+(\vec{x}, t)$, is defined as the expected or probable contribution of one particle at $\vec{x}$ at time t to the meter reading at time t_f . Thus a particle is "important" to the (future) observable reading". (Reference 1) When the observable is an extensive characteristic of the physical system, a variational principle may be applied to show that importance is in fact the adjoint neutron density. (op. cit.) One such observable, for instance, is the system "alpha".

This has obvious consequences for analog Monte Carlo treatment of neutron transport, which are also well-known. Importance sampling as a means for reducing variance is discussed in reference 2, where it is pointed out that this offers a way to factor prior knowledge into the Monte Carlo process, and that zero-variance sampling is possible in principle (though not in practice!) A similar point is made in reference 3, but with an especially valuable caveat: "The problem of estimating $\overline{Z_j^2}$ or $\overline{Z_j}$ [from which the importance can be obtained] is crucial if importance sampling is to be done. Intuition, approximate calculations, experiments, or previous Monte Carlo calculations can be used to get information about $\overline{Z_j^2}$ or $\overline{Z_j}$. In most problems it is easy for the computer to get some idea of the relative importance of different regions. When it is necessary though, it is worthwhile to go to some effort to get reasonable estimates of $\overline{Z_j^2}$ or $\overline{Z_j}$ for, it can be shown that there are real disasters possible if the assumed importance functions are very badly chosen."

As a first step toward exploiting this powerful method in MCMEG and yet controlling the degree of susceptibility to "real disasters", a straightforward realization of importance has been selected and limited to predetermined (user-input) dependence on independent variables. In particular, the neutron importance is to be identified with the number of Monte Carlo particles allocated to describe unit number of neutrons (say, one mole of neutrons), and this specification of particles per mole is to depend only on spatial location and time. Thus if it is known beforehand, that in a particular problem certain regions of space will have relatively little influence on the neutronic parameters deemed vital for that problem, the computational work and memory space devoted to those regions can be minimized to a definite degree, and the savings pocketed as a less expensive problem or reinvested to improve the quality of results in the more influential regions.

Clearly, once the non-uniform particle allocation algorithm has been derived and established, well chosen prescriptions for estimating relative importances from current and local problem data (rather than predetermined as input) can be explored with care. A distant goal is to estimate relative importances from simple yet well-behaved solutions to the adjoint equation. Another distant goal is to extend the dependence of the importance on independent parameters to include energy and angle in addition to position and time.

Discussion

George Kramer providentially coded MCMEG with a particle tagging system that includes particle weight, even though that weight is the same for every particle. This weight is defined as moles of neutrons per particle. His

coding is also highly segmented according to logical function. Finally, MCMEG's treatment of census requires that at a particular point in time, namely at the beginning of a cycle, splitting or rouletting are done as necessary to effect a determined total number of census particles for following during the cycle as a representation of the previous cycle's Monte Carlo configuration. Therefore the only missing ingredient is the non-uniform particle allocation algorithm, which will supply the needed specification of particles per mole for each individual space zone. (To be explicit about what is obvious from their definitions given here, the importance and the weight ascribed to a given Monte Carlo particle are reciprocals.)

Derivation of the desired algorithm proceeds from the stipulations that (a) neutrons are conserved in each zone separately, and that (b) in a given zone, the weights of freshly generated (source) particles and recycled census particles are the same. Let the number of neutrons in census in zone j be n_C^j and the weight of all particles to be generated in zone j be w_g^j . Then if a subscript r denotes census particles that will be recycled (i.e. original number less those rouletted, with splitting treated as a negative loss), these stipulations may be expressed as

$$(a) \quad n_C^j = n_r^j$$

$$(b) \quad w_g^j = w_r^j$$

It is also necessary to express symbolically two aspects of the particle management procedure in MCMEG. First, particles to recycle are selected randomly from census according to the value of a parameter, say p_ℓ^* , such that

$p_\ell^* < 1$ requires rouletting and $p_\ell^* > 1$ requires splitting, while $p_\ell^* = 1$ demands that the ℓ^{th} census particle is certain to be recycled without splitting. Now the ℓ^{th} census particle represents w_ℓ neutrons, while the number of MC particles assigned to represent those neutrons in the forthcoming cycle is $(1/w_r^j) \times w_\ell$. The ratio of the new to the old number of particles assigned to represent these same neutrons is the parameter p_ℓ^* . That is,

$$p_\ell^* = \{(1/w_r^j) \times w_\ell\} / \{1\} = w_\ell / w_r^j \quad (1)$$

Since w_ℓ is just the value of the tag found on the ℓ^{th} census particle, all that is now needed to evaluate p_ℓ^* for use in MCMEG with importance sampling, is the value of w_r^j that satisfies the stipulations (a) and (b) above. This value can be determined uniquely in terms of MCMEG variables by noting the second required aspect of the particle management procedure in MCMEG, namely that a fixed total number of particles, say N_a^T , are specified a priori (as input) to be tracked each cycle. Thus

$$N_a^T = N_g^T + N_r^T \quad (2)$$

Finally, let the given importance profile be V_j , and note that

$$w_r^j = n_r^j / N_r^j \quad (3)$$

Then the appropriate algebraic manipulation of equations (a), (b) and (1) - (3) yields the needed expression for w_r^j :

$$w_r^j = (\bar{n}_g + \bar{n}_c) / N_a^T V_j, \text{ where } \bar{n} \equiv \sum_j V_j n_j^j \quad (4)$$

Summarizing, the desired non-uniform particle allocation algorithm is as follows. The total number of Monte Carlo particles to be tracked each cycle, N_a^T , the relative importance of each space zone, V_j , and the number of neutrons in each zone, n_j^j , are combined according to equation (4). The resulting values of the weights for new MC particles to be tracked in the upcoming time cycle, w_r^j , are used with a census particle's weight, w_ℓ , to obtain p_ℓ^* , the selection parameter used in MCMEG for determining the fate of the ℓ^{th} census particle (p_ℓ^* is called, in MCMEG, the "particle utilization determinant"). The w_r^j are also used with the expression given below as equation (5) to obtain N_g^j , the number of particles assigned to carry neutrons freshly generated in zone j .

$$N_g^j = n_g^j / w_r^j \quad (5)$$

Results

All MEG versions after F85 permit importance sampling as described above. Time dependent specification of the spatial profile of the importance function is accomplished with MEG input card type 54 according to the standard MEG format for sources, boundary temperatures, etc.

The most common problem for which the present importance sampling capability is suitable is one in which neutrons exit almost completely from latently dominant regions during settle and/or early times. Of those problems in this class, a particularly interesting one presented an exacerbated condition due to the addition of a huge quantity of air to the exterior of the problem. In that problem, nearly all the MC particles available were required to represent neutrons that had departed from the neutronicly significant regions and were trapped in the innermost air region. Therefore,

inadequate numbers of particles were devoted to the significant neutronics in the problem, and incorrect calculations of yield resulted. In fact, the air-less problem itself was marginally calculated.

Specifically, taking the accepted yield based on the air-less problem run with uniform importances and 5000 particles per cycle as 1.00, the addition of the surrounding air, raised the yield in this problem as high as 1.15. But when the air-less problem was run on an experimental code that permitted 20,000 particles per cycle, yields of .84 and .89 were obtained in two independent runs.

This problem, with air, was then run using 7000 particles per cycle and importance profiles that trebled particle allocations to certain interior neutronically significant regions and diminished allocations to the air by a factor of 10^3 , until a problem time was reached where no regions were neutronically important but subsequent transport into and through the air was of interest (at that time uniform importances were restored). The yield was .87.

Conclusion

MCMEG now admits the use of prior knowledge to improve Monte Carlo efficiency via importance sampling. When used with care, even the simple realization described here is sufficiently powerful that factors of two or three in running time or even the ability to run at all have been achieved in real problems of current interest. Future steps toward providing the full power of importance sampling in MCMEG include extension to dependence on energy and angle in addition to space and time, and various degrees of automation, as discussed in the Introduction.

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