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Evaluating the Efficiency of Estimating Numerous Monte Carlo Tallies

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INTRODUCTION

With the development of faster computers and global variance reduction techniques [1], the Monte Carlo method is being used increasingly often for calculating radiation fields with fine resolution. An important question is being able to quantify the efficiency of a calculation toward estimating a collection of a large number of tallies (e.g., a mesh tally in MCNP [2]).

Considerations on the development of different metrics are explained and three FOMs are defined. Three test problems, one being a simplified splitting model, and the other two involving global variance reduction techniques, generated with an iterative Monte Carlo technique and a deterministic method, are evaluated using these metrics.

EFFICIENCY METRICS

Assessing the efficiency of a calculation for a large number of tallies can be done in several ways. A common approach [3] is to measure the fraction of elements with a relative uncertainty less than some prescribed value, usually ten percent, at a fixed wall-clock time. While this particular metric is useful, it does suffer from a drawback in that the time selected must not be too small such that stochastic noise dominates and may not be too large such that all, or almost all, the elements are less than the particular criteria. This motivates the development of a metric that is time independent for a large number of histories.

For individual tallies, the FOM is typically defined as

$$\text{FOM} = \frac{1}{R^2 T}, \tag{1}$$

where R is the tally relative uncertainty and T is the computation time.

Extending this to a tally collection is not simple because R for the collection is not well defined. Rather, some representative value must be chosen, and there are a virtually unlimited ways to select such a value. This representative value, however, must be selected to preserve the property of the FOM being asymptotically constant so as to provide a time-indpendent basis for comparing variance reduction parameters.

Figures of Merit for a Tally Collection

There are many valid possibilities for an FOM and much depends upon the assumptions about what a practitioner desires. The assumption here is the user desires as many elements having a relative uncertainty $R \leq H$ for the lowest time T possible.

Define a density function of relative variances R^2 of the tally collection. The mean of this density function $\bar{v}$ represents some average relative uncertainty of the collection and is a simple-minded representation of R^2 of the system. It is therefore possible to define a FOM, for convenience called the Type-I FOM,

$$\text{FOM}_1 = \frac{1}{\bar{v} T}. \tag{2}$$

$\bar{v}$ scales as $1/N$ (N is the number of histories) as a consequence of the central limit theorem.

This so-called Type-I FOM is simplistic and intuitive; however, it accounts only for the central tendency of the relative-variance density. Because the tail is always observed to be positively skewed and usually leptokurtic for large N, it is therefore more of a concern given the assumption of desirability. Therefore, it may be instructive to apply a penalty for having a significant fraction of elements greater than the mean and use a larger value as the representation of R^2. There are numerous ways to account for this, but particularly useful are quantities related to higher moments of the relative-variance density: the standard deviation σ_v measuring the dispersion of the density, and the kurtosis κ_v measuring the shape of the tail relative to the peak.

A simplistic approach is to take the representative value of R^2 being one standard deviation greater than the mean $\bar{v}$. This is called the Type-II FOM and has the following form:

$$\text{FOM}_2 = \frac{1}{(\bar{v} + \sigma_v)\, T}. \tag{3}$$

The quantity σ_v scales as $1/N$ so that this satisfies the criteria of being asymptotically constant. This is attractive in that if a set of variance reduction parameters achieves all elements with the same relative uncertainty (ideal because no histories are "wasted" sampling regions already

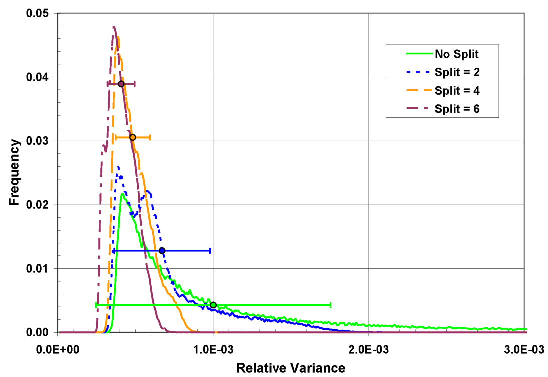


Fig. 1. Relative variance densities for various split parameters.

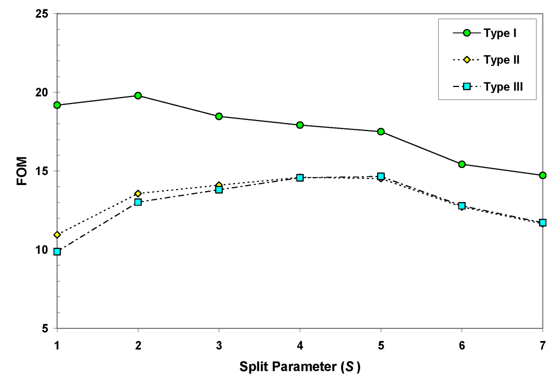


Fig. 2. The three FOMs for the simplified splitting model.

well converged given a fixed-time requirement to do so), then the Type-I and Type-II FOMs are identical.

The choice of one standard deviation is completely arbitrary. The number of standard deviations taken should be a function of the shape of the relative-variance density. This can be measured via its kurtosis, which is constant for large N.

A distribution can have the same mean and standard deviation, but have a tail that is either fat and concentrated near the peak (low kurtosis) or a thin tail with a small number of elements having a large relative uncertainty (high kurtosis). For example, suppose the mean and standard deviation of two different variance reduction schemes are identical at time T, but the maximum uncertainty for the first is aH ($a > 1$) while the maximum uncertainty of the other (despite being for a smaller fraction) is $2aH$. Assuming N is already large, the total time required to get all elements with $R \leq H$ is a^2T and $4a^2T$ respectively. Therefore, the latter has significantly more "wasted" histories than its counterpart.

A possible form that takes this into account, the Type-III FOM, is

$$\text{FOM}_3 = \frac{1}{\left[\bar{v} + (\kappa_v/3)^{1/4}\,\sigma_v\right] T}. \tag{4}$$

The semi-empirical factor $(\kappa_v/3)^{1/4}$ denotes the number of standard deviations to take the penalty. The division by three is to make the penalty for a normal distribution be one standard deviation such that the Type-III and Type-II FOMs are identical under this condition. If the distribution becomes less kurtic than a normal distribution, there is a "reward" present over the Type-II FOM. The exponent of 1/4 is present because the kurtosis is a function of scores to the fourth power and this scales the magnitude to be on the order of one, although this factor has been observed to be above ten for highly kurtic distributions. One drawback is that this representative value of R^2 can take on non-realizable values for relative variance ($R^2 > 1$) distributions that are far from normal; however, this usually only occurs when the distribution has been poorly sampled.

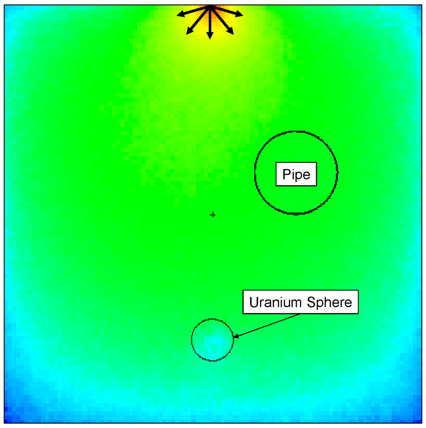
An issue inherent is the treatment of elements that are not sampled. In this case, nothing can be said about them and their relative uncertainties are undefined; therefore, they are not included in the relative-variance density moment calculation. This subject is not addressed here.

TEST PROBLEMS

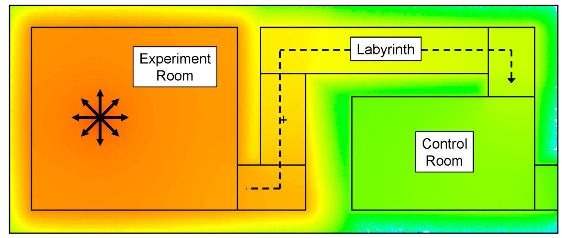
Simplified Non-Transport Splitting Model

Simplified Monte Carlo models without transport physics are often useful to test metrics. The model used contains 100,000 elements. Each history, every element is sampled with a probability that is distributed uniformly (chosen prior to simulation) between 0.01 and 0.10. If the element is sampled, a corresponding tally accumulator is appended with an exponentially distributed variable with a unit parameter.

A common technique for improving the efficiency of a calculation is splitting. In a transport sense, this involves taking a particle and splitting it into S (the split parameter) copies, simulating each copy individually, and modifying each score by $1/S$ to preserve the expected value of the tally. In this simplified model, all elements with $p \leq 0.05$ will have S chances of scoring each history to simulate the splitting seen in transport. Doing so gives low probability elements a higher chance of success, reducing the variance in the score; however, each additional simulation takes ad-



(a)



(b)

Fig. 3. (a) Photon flux distribution of the neutron on ground problem. (b) Neutron flux distribution of a criticality accident.

ditional time, potentially decreasing the overall efficiency.

Fig. 1 displays the relative-variance density function for different splitting parameters: The dot with error bars on each curve denote the mean and standard deviation of the distribution. Increasing the splitting parameter reduces the mean of the distribution, the standard deviation, and appears to shorten the tail. This gives evidence that higher moments are useful in determining a "quality". The three types of FOMs as a function of S are shown in Fig. 2. As expected, all experience some gain in efficiency until some point where the increase in computational time overtakes the diminishing gains from additional splitting. The Type-I FOM suggests an optimal split parameter $S = 2$, whereas the others suggest $S = 4$ or 5. Analyzing Fig. 1, the dispersion and tail are significantly smaller from the $S = 2$ and $S = 4$ cases.

Transport Problems with Global Weight-Window Maps

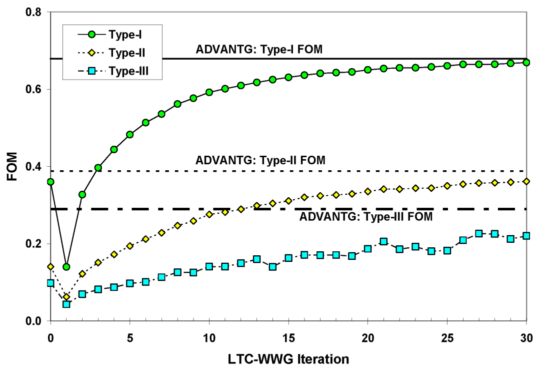
Two radiation transport problems are employed to test the efficiency metrics. For illustration, flux plots of the two problems are given in Fig. 3. Global weight-window maps are generated with an iterative linear-tally-combination with the MCNP weight-window generator (LTC-WWG) in a patched MCNP version [4] and with a deterministic method employed by ADVANTG [5].

The first has a neutron source on ground with a 5 cm radius sphere of uranium-238 buried 80 cm directly below the source. To complicate the geometry, a cylindrical pipe of radius 10 cm is located in the ground. The problem is a coupled neutron-photon problem (global mesh tally is uniform 100 x 100 x 100), where the weight windows (map is 40 x 40 x 40) are optimized to both fields.

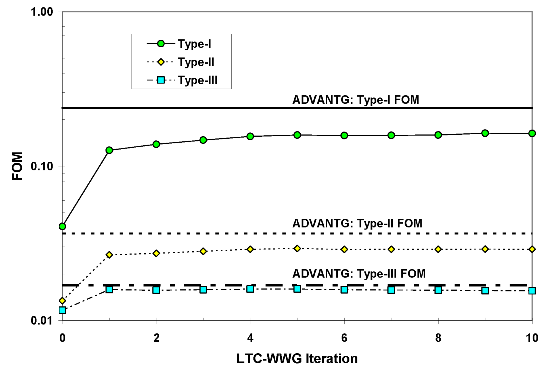
The second problem simulates a criticality accident with the neutron flux being desired throughout the entire facility. A point source of neutrons is located in an experiment room. A labyrinth hallway (walls are concrete) connects the experiment room and the control room. The neutron flux is desired throughout the entire facility; the tally map is 1200 x 500 x 1, spanning the problem neglecting the floor and ceiling, and the weight-window map is 10 x 10 x 10, including the entire problem.

The FOMs of the photon mesh tally of the sphere detection problem are displayed in Fig. 4a, and the FOMs of the neutron flux tally for the criticality accident problem are displayed in Fig. 4b. General observation is, as desired, a global weight-window map (whether generated iteratively via Monte Carlo or via a deterministic method) improves the efficiency of the calculations as defined by the new FOMs. This is confirmed by the traditional approach of evaluating the fraction of elements with a relative uncertainty less than some threshold as a function of time. The advantage of the FOMs, however, is that they provide a time-independent basis (for large N) for comparing the efficiency of different variance reduction parameters.

One drawback is that importance maps contain numerous degrees of freedom, i.e., each mesh element, and there may be temporary decreases in the FOMs as parameters are adjusted iteratively despite getting closer to an optimal value – a challenge for automated approaches. The fraction of elements with scores or less than a certain threshold seems less sensitive to this, and therefore is still use-



(a)



(b)

Fig. 4. FOMs for LTC-WWG iterations and ADVANTG for (a) the photon field from a neutron source, and (b) neutron field from a criticality accident.

ful in trying to evaluate which set of parameters is better. The higher moments give more information, and additional gains beyond the Type-I FOM can often be observed as the penalty for dispersion and kurtosis decreases. Unfortunately, because there even more degrees of freedom with the higher moments, these are even more prone to decreases in the FOM while iterating and more susceptible to noise.

CONCLUSIONS

Three versions of FOMs for collections containing a large number of tallies are defined based upon moments of the relative-variance density function. These parameters are time independent for large N, which is an attractive feature for an efficiency metric. Unfortunately, any metric involves some arbitrariness and inherently has shortcomings of not being able to anticipate the exact needs of every user. Despite this, some metric is better than none, and offers insight into the issue of optimizing variance reduction parameters. These metrics could be used to assess the efficiency of differing weight-window mesh resolutions as well as the employment of different variance reduction techniques in conjunction with global weight-window maps.

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