

FIGURES OF MERIT IN MONTE CARLO ISOTOPIC INVENTORY METHODS

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ABSTRACT

In order to determine the efficiency of variance reduction schemes for Monte Carlo isotopic inventory analysis, figures of merit must be developed. Given the specific nature of such calculations, a set of criteria for such figures of merit can be defined: a figure of merit should provide quantitative information about statistical performance, independent of the number of simulated histories, providing guidance on the relationship between computational cost and performance. A number of statistical characteristics of Monte Carlo isotopic inventory calculations are explored for their use in formulating an appropriate figure of merit. While all of them offer interesting information about the performance of the problem under differing modeling schemes, only two offer robust figures of merit: one based on the relative error of a known target isotope ($1/R^2T$) and one based on the overall detection limit corrected by the relative error ($1/D_kR^2T$).

Key Words: variance reduction, isotopic inventories, figure of merit

1 INTRODUCTION

A new Monte Carlo methodology has been developed and implemented for the simulation of changing isotopic inventories in nuclear systems, particularly those with material flowing in arbitrary paths through the system[1]. The current implementation includes the ability to simulate simple, complex and loop flows, and any combination of those. These advanced abilities can then be used to implement features of real systems including sources, sinks, post-irradiation decay and extraction processes.

Monte Carlo inventory analysis is directly analogous in many ways to Monte Carlo neutral particle radiation transport[2-5]; instead of neutral particles traveling through 3-dimensional space and having interactions with the underlying materials that change their energy, inventory analysis simulates atoms moving through (1-D) time and having interactions with the underlying neutron flux that change their isotopic identity. After a description of the fundamental Monte Carlo methodology, including some basic variance reduction methods, and of the motivation and goals for the development of a figure of merit, this paper will explore a number of possible figures of merit and discuss their applicability to different types of simulations.

1.1 Analog Monte Carlo Isotopic Inventory Method

For the development of this methodology, an atom is assumed to experience a sequence of constant irradiation environments, each for a well specified amount of time. For any isotope at any point in time, its total effective reaction rate coefficient, λ_{eff} , can be determined by collapsing the total transmutation cross-section with the neutron flux and adding the decay constant

$$\lambda_{eff} = \lambda_{dcy} + \int \phi(E)\sigma_{tot}(E)dE = \lambda_{dcy} + \sum_{rxn} \int \phi(E)\sigma_{rxn}(E)dE = \lambda_{dcy} + \sum_{rxn} \lambda_{rxn} . \quad (1)$$

The time until the next reaction can be determined from a random variable, $\xi \sim Unif[0,1)$, by

$$t_{rxn} = \frac{-\ln \xi}{\lambda_{eff}} = n_{rxn} \tau_{eff} , \quad (2)$$

where τ_{eff} is the mean reaction time ($1/\lambda_{eff}$) and n_{rxn} is the randomly determined number of mean reaction times until the next reaction.

If the remaining amount of time in this irradiation environment (i.e. remaining amount of time that the atom experiences this neutron flux), expressed as the number of mean reaction times,

$$n_{rem} = t_{rem} \lambda_{eff} , \quad (3)$$

is more than n_{rxn} , then the atom undergoes a transmutation or decay. A new isotope is sampled from the possible reaction pathways, with the relative probabilities based on the individual pathway reaction rates. The amount of time that the atom remains in this irradiation environment is decremented appropriately,

$$t_{rem} = t_{rem} - t_{rxn} , \quad (4)$$

and this new isotope is then followed in the same way, sampling again for the time to the next reaction and so on.

If the remaining amount of time in this irradiation environment is less than n_{rxn} , then the particle moves to another point and λ_{eff} is updated for the flux at this point. The number of mean reaction times until the next reaction is decremented appropriately,

$$n_{rxn} = n_{rxn} - n_{rem} , \quad (5)$$

and the calculation continues. For a calculation at a single point, this second condition indicates the end of the history of an atom and a new atom is sampled.

The basic tally counts the atoms at a particular time of interest, discriminating based on the isotopic identity of the atom, in order to determine the expected value of the isotopic composition.

1.2 Variance Reduction

Pure analog calculations are limited in the relative inventories they are able to detect. Without implementing variance reduction techniques, large numbers of source atoms must be modeled requiring long runtimes, large parallel clusters, or both, to achieve necessary precision. Variance reduction techniques are applied to improve statistical precision of the analog Monte Carlo modeling by modifying the underlying probability distributions that govern a Monte Carlo particle's processes in order to increase the occurrence of desired effects. The importance or weight of each particle must be appropriately adjusted to obtain unbiased results.

Many variance reduction techniques are being explored and are expected to improve the ability of this method to provide useful results in a broad range of problems. The *forced reactions* technique guarantees that a certain number of reactions happen within a given period of time, increasing the likelihood of contributions from isotopes that occur after many reactions[6]. This method is directly analogous to the forced collision technique common in MC radiation transport methods. *Biased source sampling* increases the number of histories that arise from rare source isotopes, increasing the likelihood of contributions from these isotopes' descendents. *Biased reaction branching* uses a non-physical probability distribution to sample the product isotope at each reaction, and adjusts the weight accordingly, increasing the likelihood of contributions from isotopes that arise from low probability reaction paths. All of these techniques aim at improving statistical results of important isotopes that are consequences of rare reaction channels or atom sources by increasing the number of individual contributions while reducing the value of each contribution closer to the expected value.

1.3 Need for Figure of Merit

Even though these variance reduction techniques have tremendously reduced the statistical error and increased the spectrum of isotopes generated in the Monte Carlo simulation, they also increase the computer time spent calculating each history and thus are not guaranteed to optimize the computing resource for such calculations. That is, in some cases it may be more efficient to simply simulate more histories than use a variance reduction technique. A figure of merit (FOM) is introduced to monitor the efficiency of the Monte Carlo code as different variance reduction techniques are attempted on the same problem[7]. FOMs representing relative efficiencies from biased and unbiased runs of the same physical problem can be calculated and compared quantitatively, assisting a user in determining the optimal variance reduction parameters. This paper will first consider the desired properties of a figure of merit and then introduce a number of possibilities for the figure of merit, discussing situations where each may be a useful measure.

2 PRINCIPLES AND CONSTRAINTS OF FIGURE OF MERIT

Since the underlying distribution that governs the random walk process is rarely known *a priori*, determining the most computationally efficient modeling scheme requires testing a variety of schemes and comparing their performance. In order to be useful, however, a quantitative metric is necessary to permit this comparison. This is the role of a figure of merit (FOM), and as such, defines the characteristics of an ideal figure of merit. In practice, a FOM will be used to determine which set of variance reduction parameters are most efficient for a given problem by comparing the FOMs that result from short problems, each with different variance reduction parameters. The set of parameters with the best FOM would be used to run a simulation with many more histories to achieve the final answer with sufficient precision. Therefore, a FOM should be a quantitative measure that is somehow proportional to the overall efficiency of the problem. This allows a user to compare two alternative modeling schemes. In addition, an ideal FOM is independent of the number of Monte Carlo histories so that a simulation with few histories can be used as an indication of the efficiency of a simulation with many histories. Finally, an ideal FOM should have a clear mathematical relationship to the statistical quantities used to measure the performance and one-to-one functional relationship with the computational cost. This allows a user to estimate the number of histories required to achieve the desired level of precision/performance. If the statistical performance metric, P_t , is measured over a short test time, T_t , and the performance goal is P_g , then an ideal FOM would allow a determination of the time to reach the goal, T_g , as:

$$FOM = f(T_t)g(P_t) = f(T_g)g(P_g) = Const$$

$$T_g = f^{-1} \left[\frac{FOM}{g(P_g)} \right] = f^{-1} \left[\frac{f(T_t)g(P_t)}{g(P_g)} \right] . \quad (6)$$

In summary, an ideal figure of merit has the following characteristics:

- quantitative measure of statistical performance,
- independent of number of Monte Carlo histories, and
- a one-to-one function of the computational cost.

While previous work on determining the efficiency of simulations provides a rigorous decision-theoretic framework evaluating and possibly determining the efficiency of simulations[8], this work takes an approach based more directly in the desired physical outcomes of the simulation. Future work can be carried out to reconcile the efficiency measures developed here with the mathematical development in [8].

The following sections will consider a variety of potential FOMs, both for these characteristics and for other ways that they provide information about the problems performance.

2.1 Test Problem

The performance of each FOM was tested by calculating the proposed FOM at shutdown following a 10-year steady-state irradiation of ^{56}Fe with a uniform multi-group neutron flux of 5×10^{12} n/cm²-s. In all cases the FENDL-2/A activation library and FENDL-2/D decay library

were used. The results for the analog case were compared to non-analog cases with forced reaction parameters of 1, 2, 3, 5, and 8. The forced reaction parameter indicates the number of times an isotope will be forced to undergo a reaction within the 10 year irradiation period. The FOM was calculated for each case as a function of time, in increments of 1000 seconds of computer time.

3 DEVELOPMENT OF FIGURES OF MERIT

Based on the above characteristics, developing a Figure of Merit requires first choosing a statistical performance metric and then examining its relationship to the computational cost to arrive at a formulation that is independent of the number of histories. A variety of statistical performance metrics are available and they form the basis for distinguishing among the four FOM formulations proposed in this section. The behavior of the specific statistical performance metric will be considered first and then its usefulness in formulating a FOM will be addressed.

3.1 Statistical Error of Single Result ($1/R^2T$)

The strong analogy between this methodology and Monte Carlo neutral particle transport results in an obvious suggestion for a FOM based on the statistical error of the result. In this case, the statistical performance metric is the square of the relative statistical error, R , which is known to vary inversely with the number of Monte Carlo particles and hence inversely with the computational cost, T . Thus, a FOM based on this metric is

$$FOM = \frac{1}{R^2T}. \quad (7)$$

Implicitly, this metric/FOM is based on the relative error of a single tally result, or single tally bin. Consequently, optimizing this FOM amounts to optimizing the results for only that tally bin and only improves the whole problem to the extent that the tally bin in question represents the rest of the problem. In the current Monte Carlo inventory implementation, the tally bins are based on time (analogous to space in Monte Carlo transport) and/or isotopic identity (analogous to energy in Monte Carlo transport). Using this FOM, therefore, requires the choice of a specific time and isotopic identity.

It is important at this stage to point out a distinct difference between the inventory analysis and the neutral particle transport methods. The energy domain of neutral particle transport is a continuous dimension where two different energies have a clear physically meaningful relationship to each other. This often allows a single energy bin (or the total over all energy bins) to be representative of the results over the entire energy domain. The isotopic identity domain is discrete and two isotopic identities may not have any clear relationship to each other. Hence a single isotopic identity bin is unlikely to be representative of many other isotopic identities, and rarely representative of the whole problem. This FOM is therefore only valuable in optimizing the modeling scheme for a particular isotope, i . For this study, the inventories at the end of a 10-year irradiation period were used to calculate the FOMs, comparing results for a variety of specific isotopes.

Since R^2 is inversely proportional to T and T is directly proportional to the number of histories, FOM should be constant with respect to a number of histories (allowing for statistical

fluctuations at very small numbers of histories). Three isotopes from the test problem, Fe-56, Cr-54 and Co-59, with different relative expected end-of-problem inventories of 9.82×10^{-1} , 3.10×10^{-5} and 4.29×10^{-7} , were chosen to be isotopes in question. The behaviors of the three resulting FOM values are shown in Figure 1(a-c), demonstrating the effects of increasing the forced reaction parameter. The FOM for all three isotopes are constant as expected. For Fe-56, this FOM suggests that the analog scheme is much more efficient than forced reactions technique. This agrees with physical nature of the problem; because Fe-56 is the initial isotope, forcing a reaction will only reduce the variance of the products in the reaction chain, but will make each history have a higher computational cost. On the other hand, both Cr-54 and Co-59 are produced predominantly from the third reaction from Fe-56 and the forced reaction technique with parameter of 3 improves the likelihood of producing these isotopes with the minimum increase in the computational cost of each history. This FOM confirms that this is the optimal choice for these isotopes.

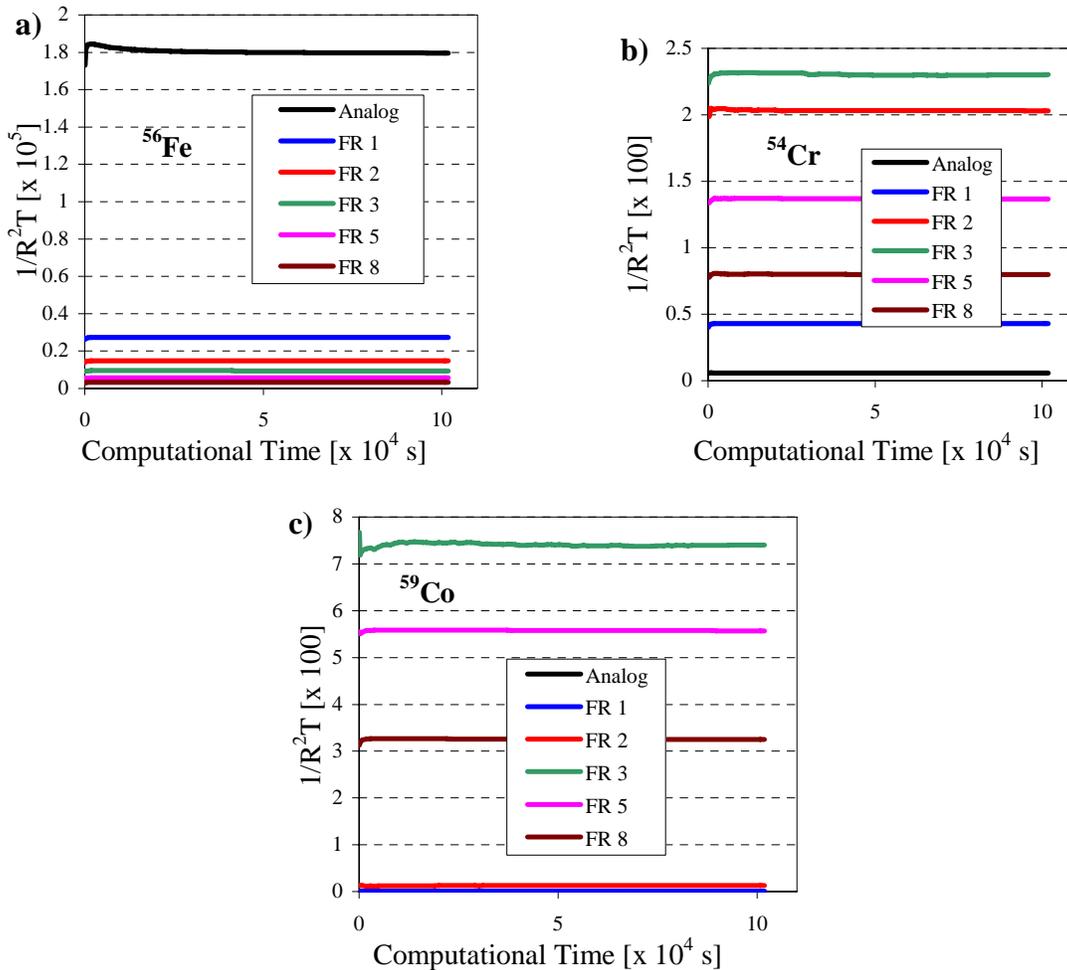


Figure 1. Traditional figure of merit based on relative error, shown for three different isotopes as a function of time and for different forced reaction (FR) parameters: a) ^{56}Fe b) ^{54}Cr c) ^{59}Co .

Finally, this FOM can be used to estimate a computing time to achieve a target error for the isotope in question:

$$T_g = \frac{1}{R_g^2 \cdot FOM} = \frac{R_t^2 T_t}{R_g^2}, \quad (8)$$

as described in equation (6). This FOM has all of the characteristics of an ideal FOM defined above, but the performance metric itself is only useful in special circumstances. Since the important isotopes are not always known *a priori* and one isotope's results are rarely indicative of another's, other potential performance metrics and FOMs will be explored.

3.2 Number of Qualified Isotopes (N_k)

Another performance metric for the Monte Carlo inventory method is a number of isotopes produced by a given set of modeling parameters. If the statistical error for a particular isotope is too high, however, it should be disregarded. The number of qualified isotopes, N_k , is defined as the number of isotopes that have relative error less than k percent. This quantity is the simplest measurement of the performance for a given modeling technique.

Figure 2 shows the results for this performance metric for a k of 1% and for a variety of modeling schemes represented by the forced reaction parameter. For very short run times, all cases produce approximately the same number of qualified isotopes. As the computing time progresses, Figure 2 clearly shows that forced reaction problems with higher parameters (3, 5 and 8) perform similarly, but better than problems with lower forced reaction parameters. Increasing a number of Monte Carlo particles and thus computing time would decrease relative errors of all isotopes. Consequently, more isotopes would be counted as qualified isotopes. This performance measure is expected to have this step behavior until the maximum number of isotopes is qualified, with the more efficient variance reduction schemes approaching this maximum more quickly. (In theory, the maximum number of qualified isotopes is equal to the full scope of the data library since any isotope has a finite probability of being produced, even if minute. In a different study using a forced reaction parameter of 8 and a computing time of 3×10^6 s, 94 isotopes were included for this ^{56}Fe problem, of which 30 had relative errors below 1%.) While this measure does provide quantitative information about the performance of the modeling scheme, its functional relationship to the number of simulated histories is unclear making it difficult to form a FOM that meets the other criteria: independent of number of histories and a one-to-one functional relationship with computational cost. This measure could be retained for comparing the efficiency of two schemes, but does not provide all the necessary information expected of a figure of merit.

3.3 Detection Limit ($1/D_k T$)

Often, an isotope with a relatively small inventory may have a disproportionate importance to the analysis in question due to some property of the isotope (e.g. its contribution to an engineering response such as the overall activity, the radiotoxicity or the waste disposal rating). The ability of a simulation to detect such a small existence of a particular isotope should also be taken into consideration when creating a FOM for an inventory problem. Moreover, since the specific isotope in question might not be known, it is important to use metric that provides information about the overall precision of the simulation. The detection limit can serve that purpose.

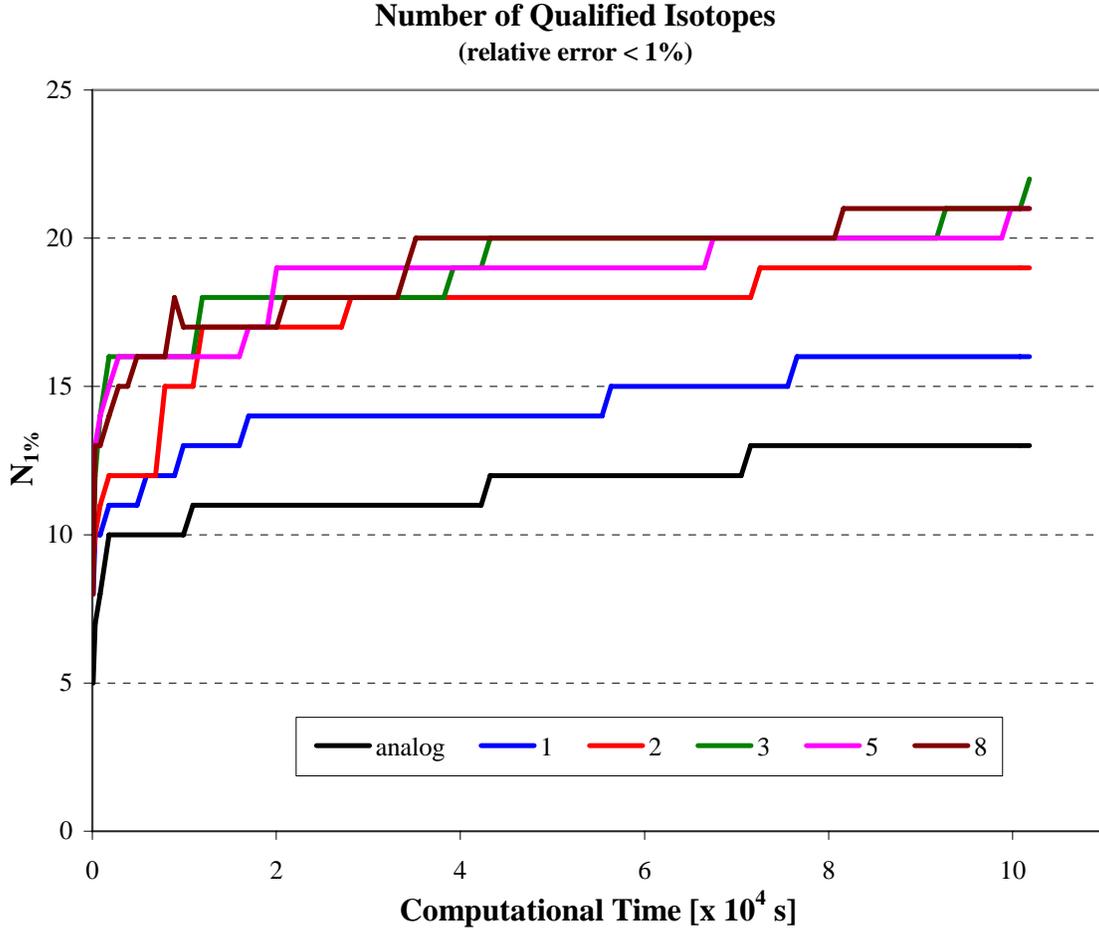


Figure 2. The performance of the test problem is compared using the number of qualified isotope metric.

3.3.1 Detection limit in Monte Carlo isotopic inventory

A k -percent detection limit (D_k) is defined as the lowest relative production (yield) of all isotopes with relative error less than k percent. For analog problems it can be derived analytically from the definition of the relative error:

$$R_j = \sqrt{\frac{\sum_{i=1}^N x_{ij}^2}{\left(\sum_{i=1}^N x_{ij}\right)^2} - \frac{1}{N}}. \tag{9}$$

By the definition of analog Monte Carlo, the contribution x_{ij} from history i to the tally for isotope j is 1 if the atom is isotope j and 0 otherwise. By defining the yield, Y_j , as the probability of producing isotope j from a source atom, this can be reduced to

$$R_j = \sqrt{\frac{Y_j \cdot N}{(Y_j \cdot N)^2} - \frac{1}{N}} = \sqrt{\frac{1}{N} \left(\frac{1}{Y_j} - 1 \right)}$$

$$R_j^2 = \frac{1}{N} \left(\frac{1}{Y_j} - 1 \right)$$
(10)

Since the goal is to determine the detection limit for rare product isotopes, $Y_j \ll 1$, and the detection limit is defined as the yield at which the relative error is exactly equal to k percent,

$$Y_j \approx \frac{1}{N \cdot R_j^2}, \text{ and } D_k \equiv \frac{100^2}{N \cdot k^2}.$$
(11)

For a given a value of k the detection limit for analog Monte Carlo simulations is inversely proportional to N . However, this continuous $1/N$ behavior implicitly assumes that the isotopic yields are continuous, that is, an uncountably infinite number of isotopes exist. This is certainly not the case for the Monte Carlo inventory method where the isotopic yields are distributed discretely.

For any results from a Monte Carlo isotopic inventory simulation, there can be only a finite number of isotopic products. The results will form a set of yields, $\{Y_j\}$, which can be sorted in descending order. At any point, the detection limit, D_k , will be defined by one of those isotopes, i , that has the smallest yield of all the isotopes with relative error less than k percent. The isotope, $i+1$, has a smaller yield and a relative error larger than k percent. As N is increased, the relative error of both isotopes i and $i+1$ will decrease ($R^2 \propto 1/N$), but the detection limit will remain unchanged until the relative error of isotope $i+1$ drops below k percent, at which point D_k will drop suddenly to the value Y_{i+1} . The overall shape of the detection limit in a discrete problem should therefore be a series of steps where the leading edge follows the $1/N$ ($\propto 1/T$) dependence.

3.3.2 Analyzing the detection limit in a real problem

Figure 3 shows the 1% detection limits for an analog case and three different forced reaction parameters for the test problem. As expected, the detection limits for the analog case exhibits a $1/T$ dependence. In addition to the step behavior caused by the discrete nature of the isotopic yields, the detection limits for the non-analog cases are all lower than that of the analog case and appear to depend similarly on $1/T$. Power law curves were fit to the leading edge of each of these results to examine the relationship with T . The parameters of each fit are shown in the figure, where the multiplicative constant represents the relative improvement of the variance reduction method and the exponents are reasonably close to -1. Once again, the discrete nature of the detection limit combined with the discrete time sampling of this test problem can contribute to an apparent departure from the $1/T$ behavior.

The detection limit, D_k , can be used to evaluate the overall performance of the modeling scheme since a lower value D_k indicates a greater precision in the answer. In Figure 3, orders of magnitude improvement are seen in the precision of the problem by invoking forced reaction variance reduction. Because of the $1/T$ dependence of the detection limit, the most appropriate choice for a FOM is

$$FOM = \frac{1}{D_k T}. \tag{12}$$

This FOM for the various cases of the test problem are shown in Figure 4. As expected, the overall shape of detection-limit-based FOM still exhibits the step behavior from $1/D_k$. However, the $1/T$ factor helps to lessen a strong step-function behavior and causes the FOM to oscillate about a constant value.

3.4 Error Corrected Detection Limit ($1/D_k R^2 T$)

The fluctuations in the detection limit based FOM are due to the $1/T$ factor while the detection limit, D_k , is constant. Similarly, the relative error, R_i , of the isotope, i , that is defining the detection limit is declining continuously with time while that the detection limit is constant at that isotope's yield, Y_i . It should therefore be possible to mitigate the oscillatory behavior of the detection limit based FOM by using the relative error as a correction.

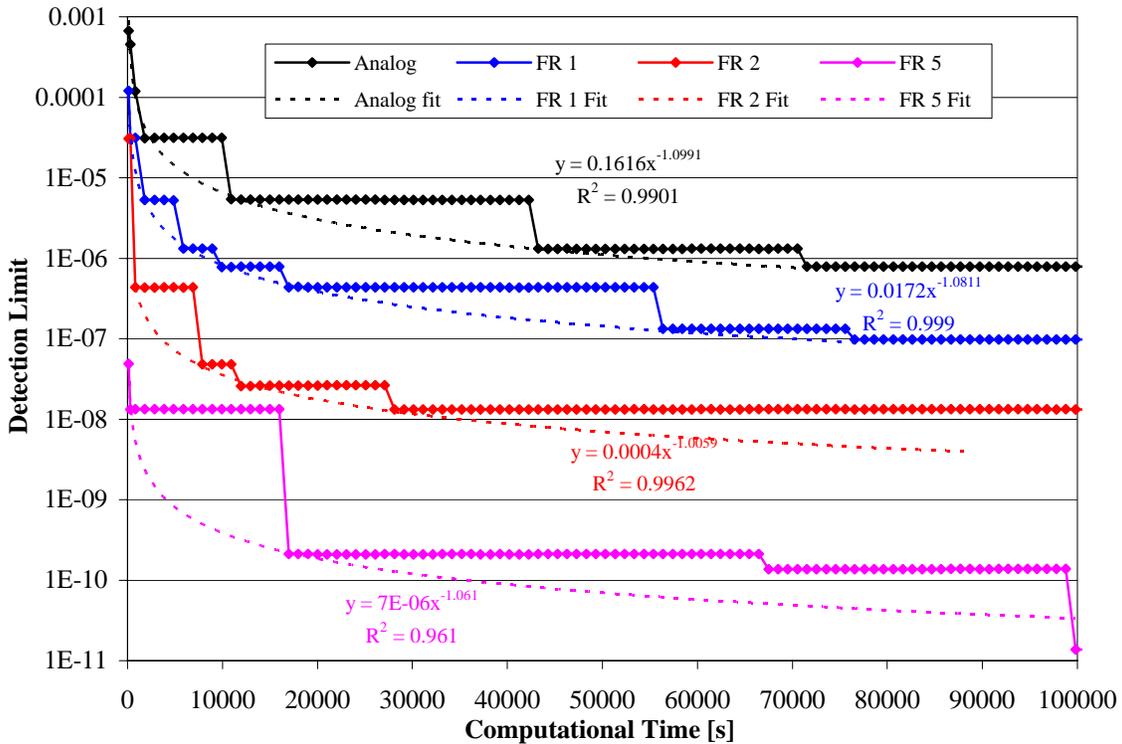


Figure 3. Detection limit as a function of computing time for an analog problem and three different forced reaction (FR) parameters. For each case, the points at the leading edge have been used to generate a power law fit whose parameters are also shown.

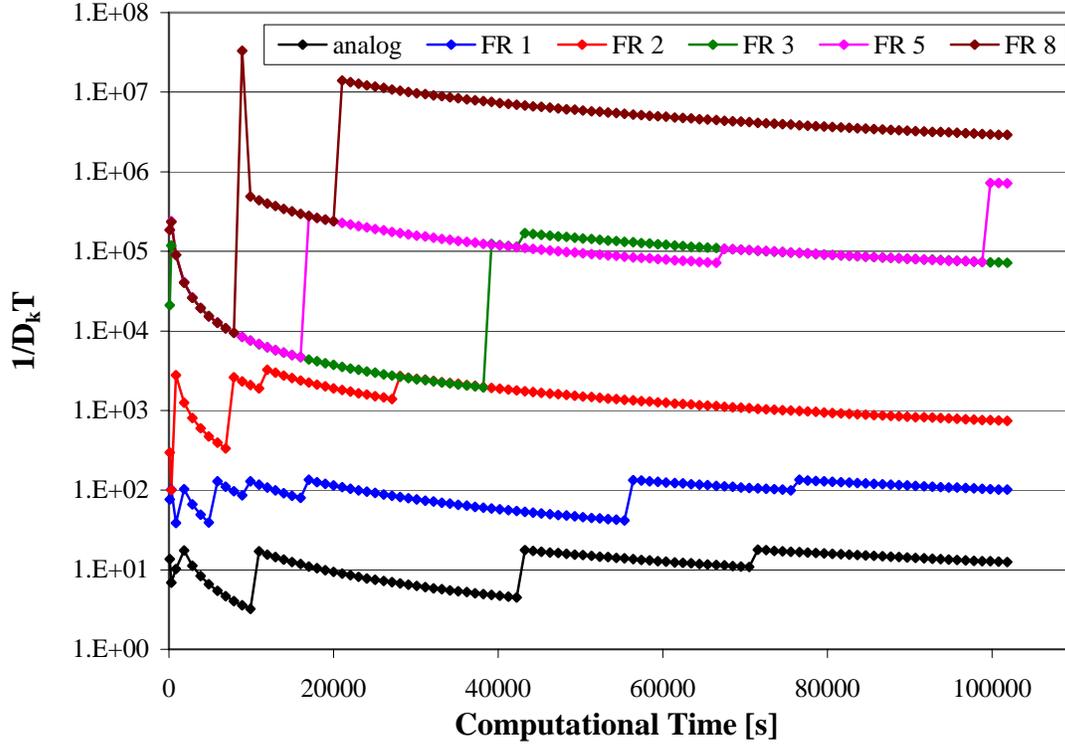


Figure 4. The detection limit based figure of merit is shown for the analog case and 5 different forced reaction (FR) variance reduction parameters.

In particular, it can be shown that a figure of merit, $1/D_k R^2 T$, is constant for the analog case. In regions where D_k is constant, this FOM is constant since R^2 behaves as $1/T$. Consider how D_k and R^2 vary across a jump in the detection limit:

$$\begin{aligned} \frac{D_k^-}{D_k^+} &\equiv \frac{Y_i}{Y_{i+1}} = \frac{N_{i+1}}{N_i} = \frac{T_{i+1}}{T_i} \\ \frac{R_-^2}{R_+^2} &\equiv \frac{R_i^2}{k^2} = k^2 \frac{T_i}{T_{i+1}} \frac{1}{k^2} = \frac{T_i}{T_{i+1}}, \\ \therefore D_k^- R_-^2 &= D_k^+ R_+^2 \end{aligned} \quad (13)$$

where D_k^- and D_k^+ are the detection limit on the left and right of the jump, respectively, and R_-^2 and R_+^2 are the squares of the relative errors on the left and right of the jump, respectively. Thus, for analog problems this FOM is constant across a jump in the detection limit as well as during the periods where the detection limit does not change.

Figure 5 shows results for an FOM with this formulation. The results agree with the analytic calculation that FOM is constant for analog case and nearly constant for the variance reduction cases. Even though, this FOM is likely to experience some fluctuations due to the discrete behavior of the detection limit, it can be used in a problem without a target isotope to compare the overall efficiency of different schemes. Most importantly, it is effective at providing an estimate of the necessary computing time for a given modeling technique to achieve a certain overall precision, as indicated by the detection limit.

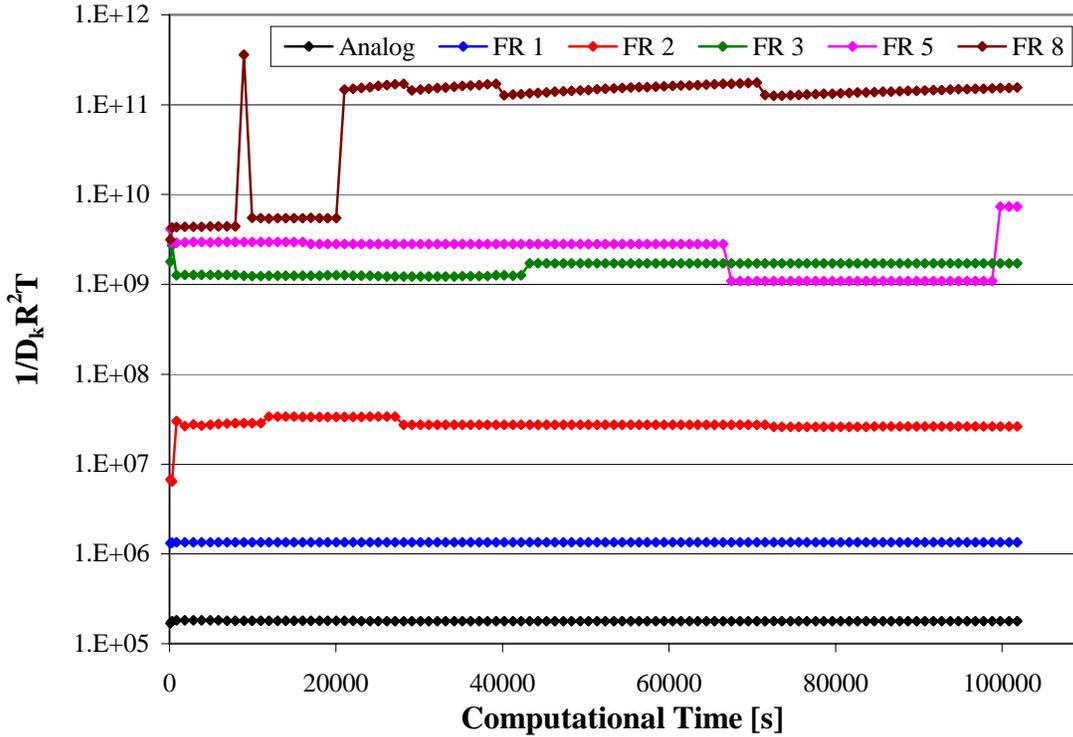


Figure 5. Figure of merit using error corrected detection limit provides a measure of the overall efficiency of the problem with a nearly constant value for a given modeling scheme.

4 CONCLUSIONS

A number of statistical measures can be employed to assess the performance of different Monte Carlo modeling schemes for a given isotopic inventory problem. From these, two valuable figures of merit have been derived that meet the criteria described above: a figure of merit should provide quantitative information about statistical performance, independent of the number of simulated histories, providing guidance on the relationship between computational cost and performance. The FOM based on the relative error of a single tally result ($1/R^2T$) is recommended for the problem with a known target isotope. In these situations, the modeling scheme can be optimized for that single result and the necessary computing time to achieve a target precision can be calculated. However, since many problems do not have readily identified target isotopes, or may have multiple important isotopes, a FOM based on the detection limit, corrected by the relative error, ($1/D_k R^2T$) is useful for assessing the overall efficiency of the problem. With this FOM, the modeling scheme can be optimized against the detection limit and then the necessary computing time to achieve a target detection limit can be calculated.

5 ACKNOWLEDGEMENTS

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