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CONVERGENCE TIME AND FIDELITY IN MONTE CARLO SHIELDING

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ABSTRACT

This paper explores the relationship between Monte Carlo convergence time, the fidelity of the Monte Carlo model, the fidelity of the importance model, and the complexity of the case being simulated. It is shown how importance functions reduce run time and add model build time. Convergence time is studied and an equation developed based on theory and eight MCNP cases. Convergence accelerates dramatically with the addition of energy to the usual spatially dependent importances. Other primary determinants of time reduction are shield depth and dimensions required (a measure of complexity.) The equation predicts the benefits of the use of various levels of fidelity (i.e. detail) in the importance function and shows that with the use of spatial and energy dependent importance functions a 25 TVL shield calculation can probably be converged in a day of computer time on a 2GHz PC. A 9 TVL shield can be converged in a minute.

Key Words: importance function, variance reduction, weight windows, Monte Carlo

1 INTRODUCTION

"How much time is needed to converge a Monte Carlo shielding model? How much detail must be modeled to avoid bias? Will this level of detail add too much build time and run time? Will an importance function help or hurt? How much detail must the importance function include? What's the most complex problem that can be solved in a one day run?" These are questions asked every day by Monte Carlo shielding engineers.

This paper explores the relationship between Monte Carlo convergence time, the fidelity of the Monte Carlo model, the fidelity of the importance model, and the complexity of the case being simulated. The eight cases presented here are static shielding problems. Future users will want to attack more challenging dynamic problems which will require significant calculational acceleration. The equation presented here can help answer these questions.

All the examples in this paper are based on the MCNP Monte Carlo radiation transport code, Reference 6. Users can run the code in analog mode, i.e. without variance reduction techniques. Or, they can run with a variance reduction technique such as weight windows, which is based on the inverse of the importance function, also known as the adjoint flux. Thus, $ww(\underline{r},E) = C / I(\underline{r},E)$.

Once a model has been built and a run made, the convergence time, T_C, can be predicted by the use of the Figure of Merit, FOM. The relation between T_C and FOM is:

T_C (minutes) = 1/(RE^2*FOM).

RE is the relative error. Thus a figure of merit of 1 predicts 100 minutes required to converge the problem to plus or minus 10% at the one sigma level. In this paper convergence always means achieving RE=0.1.

Unfortunately, for many shielding problems T_C can be upwards of weeks, months, and even years. The most common methods to accelerate these calculations include parallel processing, switching to deterministic methods, and variance reduction. Parallel processing can reduce time by a factor of ten to fifty using existing software on existing systems, but, users must play with motherboards, compilers, and operating systems. Deterministic methods are well known but require users to process cross-sections, avoid voids, and struggle with streaming rays. This paper is about one particular method of variance reduction implemented in MCNP; weight windows.

Of all the variance reduction techniques in MCNP this author finds that weight windows is the most generally useful for shielding problems. It is a form of Importance sampling, which is also known as transport biasing. It uses an importance function to control splitting and rouletting and thereby reduce the convergence time.

1.1 Run Time versus Importance

T_C, the length of time required to converge a Monte Carlo shield simulation is determined almost entirely by the availability and accuracy of an importance function, I(). Table I gives two examples from Reference 2. Note the enormous reduction in run times with the use of importances.

Table I. Monte Carlo Convergence Time			
Case	Description	no I()	accurate I()
5a/b	Photon Dose from SNF Cask	14 hours	<1 min.
2a/c	Damage to Reactor Shroud	½ year	5 min.

One might always want to use an importance function except that as many days or weeks as it takes to build the Monte Carlo model, it can take more to generate the importance function. In the SNF case, it can take two weeks to build the model, therefore, it may be just as efficient to let it run overnight as to generate and use an importance function. There is no choice with the Shroud example.

Software exists that can generate importances. The computer code A3MCNP, Reference 2, generates importances automatically using Discrete Ordinates. MCBEND, Reference 8, does so stochastically within the Monte Carlo code. ATTILA, Reference 9, useful because of its variable mesh, is not automated.

1.2 Complexity and Fidelity

Complexity describes physical reality. Fidelity describes the detail included in the Monte Carlo model and also in the importance model. Time addresses both engineering and computer run time.

A measure of complexity is the number and range of dimensions needed to simulate reality without bias. A reactor is more complex because the model requires three spatial dimensions,

whereas a point source is less complex because one spatial dimension is required. A thick shield is more difficult to model than a thin shield because the range of distance is greater in the former than the latter. A 12 TVL (tenth value layer) shield is almost impossible to model whereas a 3 TVL shield takes a few minutes of run time.

Fidelity is the level of detail put into the model. A high fidelity reactor model might explicitly include each fuel rod and might calculate the neutron and photon energy spectrum at the pressure vessel surface. A low fidelity model lumps all fuel together and might calculate fast neutron fluence at the vessel. A low fidelity model of a highly complex reality is probably biased.

The time to build and the time to run a model increases with fidelity. The author's Monte Carlo experience has been that the total time for all runs in a project is roughly three times the time to make the final fully converged runs. This is because there are many short runs made at the beginning of the project that are not run to completion or perfect convergence, but are used for scoping. debugging and sensitivity studies.

1.3 Total Time

The following thought experiment is based on the author's experience. Table II-A estimates the time to build an MC model and the associated I() model. Cell (a) is for a simple Monte Carlo model of a point source and 2 foot thick shield. Cell (b) assumes an importance function is used. Cell (c) is a high fidelity model of a reactor for an np (neutron photon) leakage calculation plus a high fiedlity importance model.

Table II-B below is the Monte Carlo run time in minutes. The higher the fidelity of the importance function the less time the MC calculation takes. Table II-C is the run time to generate the importance function in minutes. Note that run time increases with both the fidelity of the importance model and the fidelity of the Monte Carlo model.

Table II-D is the total run time in hours including both the runs to generate the importance function and the runs to generate the Monte Carlo answers. Note that the times have been multiplied by three as discussed in section 1.2 above.

Table II-E above makes the critical point. You can have too much as well as too little fidelity in the importance calculation. For a low complexity case a low/no fidelity MC model is adequate. Note how cell (d) in Table II-E gives the lowest time. Notice also that using the highest fidelity importance quadruples the time. For a high complexity reality and it's high fidelity MC model, a medium fidelity I() model is shortest, see cell (e). In each of the three MC cases, low, medium and high, choosing the highest fidelity importance function would add two to three weeks to total time. In none of these cases does the highest fidelity importance function lead to the shortest total time. In general the fidelity of the importance function may be less than the fidelity of the Monte Carlo model.

1.4 The Best Fidelity

Many users find their way to an adequate fidelity by starting with a low fidelity MC model and no I(). If it doesn't converge they add detail to the model and maybe generate a low fidelity importance function. If that doesn't converge they escalate again, stopping when they can get an answer out of a run that comes close to converging in three days, accepting the results because they've run out of time and budget.

Table II-A Build Time (hours)				
		MC Model Fidelity		
		low	medium	high
I() Model Fidelity	high	160	200	(c) 280
	medium	120	160	240
	low	(b) 80	120	200
	none	(a) 40	80	160

Table II-B MC Run Time (minutes)				
		MC Model Fidelity		
		low	medium	high
I() Model Fidelity	high	1	5	50
	medium	5	50	100
	low	10	100	6000
	none	60	1000	100000

Table II-C I() Run Time (minutes)				
		MC Model Fidelity		
		low	medium	high
I() Model Fidelity	high	100	300	1000
	medium	50	150	300
	low	20	50	100
	none	0	0	0

Table II-D Run Time (hours) x 3				
		MC Model Fidelity		
		low	medium	high
I() Model Fidelity	high	5	15	53
	medium	3	10	20
	low	2	8	305
	none	3	50	5000

Table II-E Total Time (hours)		
MC Model Fidelity		
low	medium	high
165	215	333
123	170	(e) 260
82	128	505
(d) 43	130	5160

Others, go for the highest fidelity Monte Carlo model and importance function, wasting lots of time, when much less detail would have adequately solved the problem.

A better way would be to make an intelligent first guess at the fidelity required of both MC and I(), based upon the complexity of the problem and previous experience. These would be quantified in an equation. The user could then use the equation to predict time required to build and converge MC and I() models at various levels of fidelity. Of course complexity and fidelity need more quantitative definitions. The present paper focuses on such an equation for Monte Carlo convergence time. Build time and I() convergence time are left for later.

2 MONTE CARLO CONVERGENCE TIME EQUATION

This is an attempt to build an equation for Monte Carlo convergence time in terms of complexity and fidelity. Convergence time, T_C, is the run time required to achieve a sampling error of 10%.

2.1 Important Parameters

Convergence time data were collected from eight MCNP simulations, some personal and some published. These were chosen to cover a wide range of physical and simulation parameters. They are discussed in section 2.2 below. Important physical parameters are listed in Table III. Some of the parameters are continuous, like energy. Some that are non-continuous, like response type, were given numeric values to make the fitting of the equation easier in Section 2.3.

Table III. Physical Parameters	
Parameter	Range
Particle type	n, p, $p_{secondary}$ (called np)
Shield Thickness	5 to 12 TVL
Particle energy range	neutron thermal to 15 photon 0.01 to 5 MeV
Average Collision per Track	n=200, p=30, $p_{secondary}$ = 230
Experimental measurements	no or yes
Response type	uncollided flux (= 2), DPA (= 2) dose rate (= 1) and foil reactions (= 0)

Table IV shows parameters related to the Monte Carlo and the Importance Function simulations. The ranges in the data are given as are the codes for discrete data.

Table IV. Simulation Parameters		
	Parameter	Values
Monte Carlo		
	Spatial Dimensions	1, 2, 3
	Source Bias	analog (=0) or yes (=1)
	Transport Biasing	analog or yes
Importance		
	Generation Method	none = 0, manual = 1, deterministic or Monte Carlo = 2
	Spatial Dimensions	1, 2, 3
	Spatial subdivisions	none = 0, medium = 1, high = 2
	Energy Groups	none = 0, one = 1, many = 2
	Fidelity	none = 0, medium = 0.5, high=1.5

2.2 Eight MCNP Cases

The eight cases that were explored from the author's experience and literature are listed below along with a description of why they were chosen.

Case 1 – This is a simulation of uncollided 2MeV neutron penetration through a concrete shield of two thicknesses, 8 and 11 TVL (Tenth Value Layer.) It is reported in Reference 1. It is included because it studies the relation between error in the importance map and T_C.

Case 2 – Reference 2 presents the simulation of the flux and DPA (metal damage in displacements per atom) to the shroud of an operating BWR. The authors perform their calculations using A^3MCNP and TORT for the importance function. It is included because for this one case they compare analog, course importance mesh, and fine importance mesh simulations.

Case 3 – There are several simulations of reaction rates of activation foils in the cavity of a BWR, a location several TVLs from the targets in Case 2. This was measured and modeled in DORT (Reference 3) and modeled in 2 dimensions in MCNP and again in 3 dimensions (Reference 4.) It is included because it provides an opportunity to compare stochastic and deterministic calculations with foil measurements.

Case 4 – Dose rate from BWR streaming through primary shield penetrations was simulated and measured (Reference 5.) This was included because it is the deepest simulation we have seen, roughly 12 TVL. It also covers the largest range of energies. Specifically fission neutrons scatter down in energy until they undergo thermal activation of Hydrogen and generate 2.2 MeV photons which scatter down in energy to about 10 KeV.

Case 5 – Reference 2 also includes the simulation of photon dose rate in contact with the surface of a vertical spent nuclear fuel cask. The shield depth is substantial, 7 TVL. It is included because it has about the best set of spatial and energy importance map one can expect.

Case 6 – The dose rate at the surface of the concrete vertical spent nuclear fuel cask was calculated by the author using various manual importance maps. It was included in order to compare the effect of changing from one to five energy groups in the importance map.

Case 7 – Is a calculation by the author of neutron and photon dose rates at long distances (up to a Km) in air for an array of 20 spent nuclear fuel casks. The source is from Case 6. It is included here because it covers large distances in air.

Case 8 – Is the same as Case 7, except that the array is much larger, i.e. 140 SNF casks.

The above eight cases were modeled at one or more levels of Monte Carlo and Importance fidelity. For each of these a letter was added to the case number. These are all listed in Table V. The log base 10 of the convergence times are shown in the table for each of the cases.

2.3 Equation

In addition to the case data in Table V we know that for a deep penetration problem modeled without importances the convergence time is inversely proportional to P_{EXIT}. This exit probability is the ratio of flux exiting a shield to that entering. Shield thickness expressed as optical thickness TVL is $-\text{Log}(P_{EXIT})$. Therefore, $T_C = k10^{TVL}$, where k is a constant.

Table V. Data Set

Physical					Importance Generation					Monte Carlo		
Case ID	particles	Shield TVL	Response	Measurements	I generation	I Dim	I E groups	I Accuracy	I spatial mesh	Source Bias	Mat. Dim	Log(TC minutes)
1a	n	8	Φu	n	analog	0	0	0	none	n	1	5
1b	n	8	Φu	n	manual	1	1	good	medium	n	1	2
1c	n	8	Φu	n	perfect	1	1	perfect	medium	n	1	0
1d	n	11	Φu	n	analog	0	0	0	none	n	1	8
1e	n	11	Φu	n	manual	1	1	good	medium	n	1	2
1f	n	11	Φu	n	perfect	1	1	perfect	medium	n	1	1
2a	np	6	DPA	0	analog	0	0	0	none	n	3	4
2b	np	8	DPA	0	A3	3	many	0	.3K	y	3	2
2c	np	8	DPA	0	A3	3	many	0	90K	y	3	1
3a	n	7	foil	y	manual	2	1	0	medium	n	2	2
3b	p	11	DR	y	manual	3	1	0	medium	y	3	2
3c	n	7	foil	y	manual	3	1	0	medium	y	3	4
3d	n	7	foil	y	manual	3	1	0	medium	y	3	4
4a	np	12	DR	y	manual	2	1	0	medium	n	2	2
4b	n	11	DR	y	manual	3	1	0	medium	y	3	4
4c	np	12	DR	y	manual	3	1	0	medium	y	3	6
5a	p	6	DR	0	analog	0	0	0	none	y	3	3
5b	p	6	DR	0	A3	3	many	0	10K	y	3	0
6a	p	6	DR	y	manual	2	1	0	medium	y	3	3
6b	n	5	DR	y	manual	2	1	0	medium	y	3	1
6c	p	6	DR	y	manual	2	many	0	medium	y	3	0
7a	p	7	DR	n	manual	3	1	0	medium	y	3	3
8a	p	7	DR	n	manual	3	1	0	medium	y	3	3

It can also be shown that with a perfect importance function $T_C = k_1 TVL$, i.e. is proportional to thickness, which is considerably less. In all cases we assume a single processor 2 GHz PC.

Using these known relations and the data in Table V the log of T_C was explored with least squares regression methods. The F_I parameter was coded based on the data, as defined in the equation below. The parameters F_I, DIM, and TVL had the most effect on T_C. The relation with FI is non linear. After some experimentation the following equation form seemed to give the best fit:

$$T_C = 10^{0.407D + 0.114R_S - 0.964F_I + 0.157R^{(1.5-F_I)}}$$

Where

D = the number of spatial dimensions represented in the model, 1, 2, or 3.
R_S = is the depth of the shield in Tenth Value Layers, TVL.

F_I = Fidelity of the importance function where 0 for analog (no importance function,) 0.5 for spatial importance function, and 1.5 for spatial and energy dependent importance function.

The accuracy of the equation is shown in Figures I-A through C. Figure I-D gives the non-linear relation between T_C and F_I. Table VI gives the calculated to experimental ratios for each case.

Figure I-A Equation versus Analog Runs

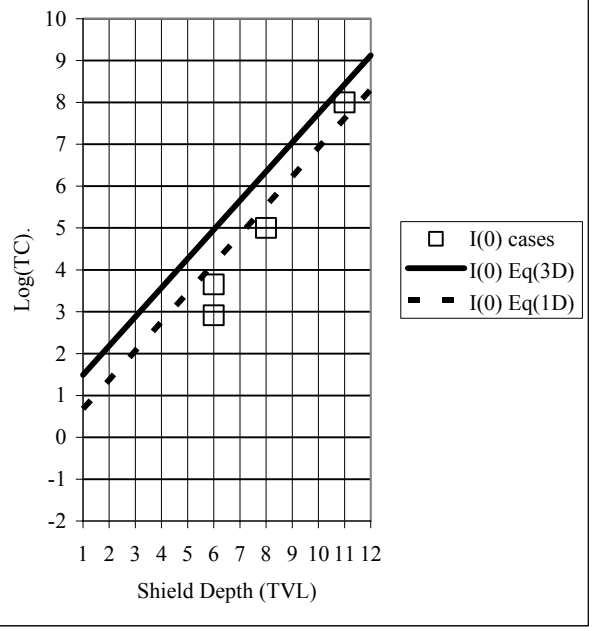

Figure I-B Equation versus I(r) Runs

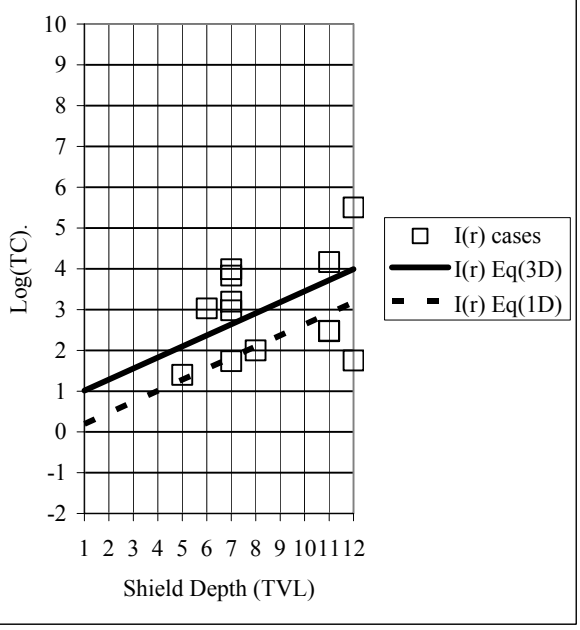

Figure I-C Equation versus I(r,E) Runs

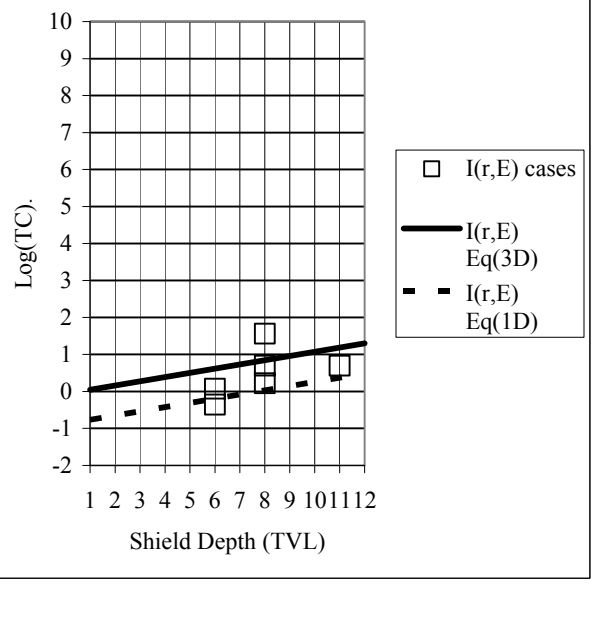

Figure I-D Log(TC) versus FI

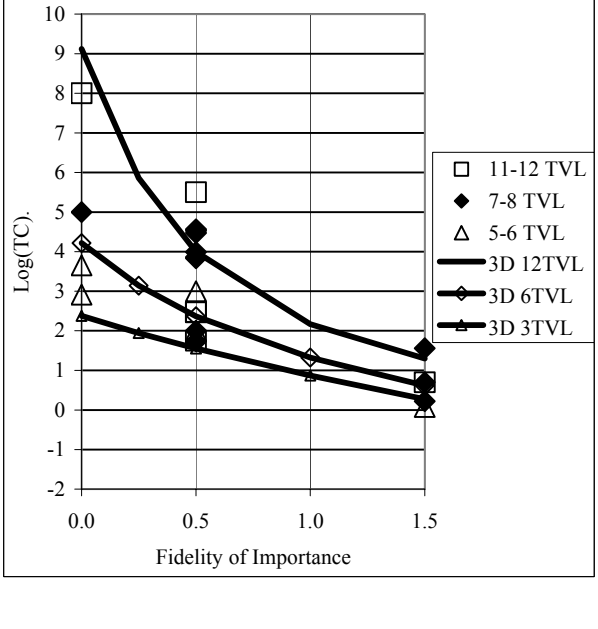

Table VI – Calculated to Experimental Ratios by Case							
ID	case	DIM	Depth TVL	F_I	T_C Calc. (min.	T_C Exp. (min.)	C/E
1a	1D uflux 8	1	8	0	74970	100000	0.7
1b	1D uflux 8	1	8	0.5	124	100	1.2
1c	1D uflux 8	1	8	1.5	1	2	0.6
1d	1D uflux 11	1	11	0	24790839	100000000	0.2
1e	1D uflux 11	1	11	0.5	808	300	2.7
1f	1D uflux 11	1	11	1.5	2	5	0.5
2a	BWR Shroud DPA	3	6	0	16405	4500	3.6
2b	BWR Shroud DPA	3	8	1.5	7	36	0.2
2c	BWR Shroud DPA	3	8	1.5	7	5	1.4
3a	2D BWR cav foils	2	7	0.5	170	54	3.1
3b	BWR cav 3D p1 DR	3	11	0.5	5266	294	17.9
3c	BWR cav foils 3D + cd	3	7	0.5	434	9794	0.0
3d	BWR cav foils 3D	3	7	0.5	434	6798	0.1
4a	2D BWR strmg np DR	2	12	0.5	3850	56	68.4
4b	BWR strmg 3D n DR	3	11	0.5	5266	14612	0.4
4c	BWR strmg 3D np DR	3	12	0.5	9831	318206	0.0
5a	SNF Cask p DR	3	6	0	16405	821	20.0
5b	SNF Cask p DR	3	6	1.5	4	0	9.3
6a	SNF Cask p DR	3	6	0.5	232	1066	0.2
6b	SNF Cask n DR	3	5	0.5	124	25	5.0
6c	SNF Cask p DR	3	6	1.5	4	1	3.5
7a	SNF 20 Casks p	3	7	0.5	434	958	0.5
8a	SNF 140 Casks p	3	7	0.5	434	1562	0.3

2.4 Discussion

The three most important contributors to convergence time are shield depth, fidelity of the importance function and modeled dimensions, in decreasing order. The method of importance generation and the fidelity of the mesh are less important. The fastest times are achieved when the importance function is both spatially and energy dependent.

There is lots of variation in the C/E data, however the equation works reasonably well over about nine orders of magnitude. Looking at the Figures we are able to answer some of the initial questions. The whole point of the equation is to predict convergence time based on dimensions simulated, shield depth, and importance fidelity. Questions about bias can only be answered with measurements, however, the equations help predict the impact of additional details on convergence time. It is clear that higher fidelity importance functions always reduce convergence time (at least within the limits of this study,) however they add to model build time as shown in section 1.3. Given a day (1440 minutes) to converge, a model Figure 1-A shows a shield with a depth of 3 to 4 TVL can be calculated without an importance function. With a spatial importance function a depth of 9 to 10 TVL can be converged in that time. With energy

included in the importance function, the depth is beyond the 12 TVL limit of this study, probably on the order (by extrapolation) of 25 TVL. Interestingly, an 8 TVL shield can be converged in ten minutes.

3 CONCLUSIONS

In Monte Carlo transport simulation importance functions reduce run time. However, they add build time. Convergence time does not depend on the method of importance function generation but instead improves dramatically with the addition of energy to the usual spatially dependent importances. Other primary determinants of time reduction are shield depth and dimensions required (a measure of complexity.) An equation has been developed based upon theory and eight cases from literature and personal experience. The equation predicts the benefits of the use of various levels of fidelity (i.e. detail) in the importance function.

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