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# AN AUTOMATED DETERMINISTIC VARIANCE REDUCTION GENERATOR FOR MONTE CARLO SHIELDING APPLICATIONS

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# AN AUTOMATED DETERMINISTIC VARIANCE REDUCTION GENERATOR FOR MONTE CARLO SHIELDING APPLICATIONS

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**SUMMARY**
As part of a larger project to upgrade the shielding capabilities in the SCALE code system, efforts have been initiated to independently develop and demonstrate generalized automated variance reduction. Initial efforts have developed a prototypic utility code for automated variance reduction based on existing Monte Carlo and discrete ordinates codes and proven methodologies. This prototypic utility code represents the first step in this effort and will be used for testing and refining the implementation of existing methodologies and investigating alternative methodologies, before attempting to integrate an automated variance reduction capability into SCALE. This paper describes the utility code and a demonstration of its effectiveness on a standard nuclear well-logging problem. The computational efficiencies achieved are very encouraging when compared to both stochastic and manual approaches for developing variance reduction, and the process seems to be well-suited for automation in a future SCALE shielding analysis sequence.

**I. INTRODUCTION**
The Monte Carlo method is considered to be the most accurate method available for solving complex radiation transport problems. However, due to its nature of simulating individual particles and inferring the average behavior of the particles in the system from the average behavior of the individually simulated particles, the Monte Carlo method is very computationally intensive for deep-penetration. Hence, for many traditional radiation shielding problems, as well as medical and nuclear well-logging applications, the computer time required by analog Monte Carlo is still considered exorbitant and/or prohibitive. Therefore, for difficult problems in which the probability that a particle contributes to the region of interest (tally) is small, some effective means of variance reduction must be used.

Unfortunately, the use of variance reduction methods is not straightforward, and the effective use of variance reduction methods for difficult problems often requires a significant amount of time and effort. In practice, a manual iterative process[1] is performed to develop the variance reduction parameters, converging to some acceptable level of calculational efficiency. A further difficulty lies in the statistical convergence of Monte Carlo results and the potential for biased results due to the misuse of variance reduction techniques.

Responding to these difficulties, a number of strategies (both deterministic and stochastic) for determining variance reduction parameters have been proposed and developed. For example, Booth and Hendricks[2] developed an automated stochastic importance estimation technique called the forward-adjoint generator, which has since become known as the weight-window generator (WWG) because it estimates importances to be used with the weight-window technique. The weight-window technique, which is a standard feature in the MCNP Monte Carlo code,[3] is a space and energy-dependent facility by which particle splitting and Russian roulette are applied in an effort to focus computer time on particles that are most likely to contribute to the response or interest (tally). The importance is estimated as the ratio of the total score due to particles (and their progeny) entering a space-energy interval to the total weight entering the space-energy interval in a Monte Carlo calculation.

To accurately estimate the importance of a space-energy interval, a sufficient number of particles must pass through that space-energy interval and proceed to contribute to the response of interest. For many challenging shielding problems, this condition is difficult to meet within a reasonable amount of computer time, and as a result, either no importance estimate or an unreliable importance estimate may be generated for each space-energy interval. For problems where this approach is viable, an iterative application of the WWG is used to obtain and/or refine the importance estimates.

Alternatively, a number of researchers have utilized deterministic methods for generating importances, particularly for difficult shielding applications. These efforts have generally been based on the recognition that the adjoint function (i.e., the solution to the adjoint Boltzmann transport equation) has physical significance as a measure of the importance of a particle to some objective function (e.g., the response of a detector). It is this physical interpretation that makes the adjoint function well suited for use as an importance function for biasing Monte Carlo calculations.

Early work[4,5] developed simplified, problem-specific tools with notable success. One of the earliest efforts[4] in this area was by Tang and Hoffman, which used two-dimensional (2-D) discrete ordinates adjoint functions to bias multi-group Monte Carlo calculations. The work was extended to include automation of the biasing procedure for spent fuel cask dose calculations using one-dimensional (1-D) adjoint functions, culminating in the SAS4 shielding analysis sequence[6] of the SCALE code package.[7]

A number of more recent efforts[8-11] have applied multi-dimensional adjoint functions and/or approximate adjoint functions with varying degrees of success and addressed issues associated with automating the biasing procedure.

As the methodology has matured and been demonstrated, it has become apparent that automated variance reduction will become an important feature for Monte Carlo shielding codes. Consequently, as part of a larger project to upgrade the shielding capabilities in SCALE, which includes the development of a new continuous-energy Monte Carlo code based on KENO VI geometry[7] and point-wise cross-section data from AMPX,[12] efforts have been initiated to independently develop and demonstrate generalized automated variance reduction. To this end, initial efforts have developed a prototypic utility code for automated variance reduction based on existing Monte Carlo and discrete ordinates codes and proven methodologies. This prototypic utility code will be used for testing and refining the implementation of existing methodologies and investigating alternative methodologies, before attempting to integrate a general, multi-dimensional automated variance reduction capability into SCALE. Other areas that may be explored include approaches for angular biasing, optimization of problems with multiple regions of interest (tallies), and automated variance reduction for eigenvalue problems.

The remainder of this paper describes the prototypic utility code, ADVANTG (Automated Deterministic VAriaNce reducTion Generator), that automates the generation of variance reduction parameters for MCNP shielding calculations. The methodology employed is reviewed in the following section, followed by a description of the ADVANTG code and a demonstration of its usage on a standard nuclear well-logging problem.

## II. VARIANCE REDUCTION METHODOLOGY

The variance reduction approach in ADVANTG is based on the previously developed and proven CADIS (Consistent Adjoint Driven Importance Sampling) methodology,[8] which provides consistent relationships for calculating source and transport biasing parameters based on importance sampling. This methodology is utilized to calculate space- and energy-dependent source biasing parameters and weight-window values.

The biased source distribution, $\hat{q}(\vec{r},E)$, is given by the following relation

$$\hat{q}(\vec{r},E) = \frac{\phi^{+}(\vec{r},E)\, q(\vec{r},E)}{R} = \frac{\phi^{+}(\vec{r},E)\, q(\vec{r},E)}{\int_V \int_E \, q(\vec{r},E)\phi^{+}(\vec{r},E)\, drdE},$$

where $\phi^{+}(\vec{r},E)$, $q(\vec{r},E)$, and $R$ are the scalar adjoint function, the unbiased source, and the detector response, respectively. The numerator is the detector response from space-energy element $(d\vec{r}\ , dE)$, and the denominator is the total detector response, $R$. Therefore, the ratio is a measure of the relative contribution from each space-energy element to the total detector response.

For transport biasing, the weight window technique is employed. The weight-window technique provides a means for assigning space- and energy-dependent importances and applying geometric splitting/roulette and energy splitting/roulette, while at the same time controlling weight variations. The weight-window technique requires weight window lower bounds $w_\ell$, and the width of the window is controlled by the input parameter $c_u$, which is the ratio of upper and lower weight-window bounds $(c_u = \frac{w_u}{w_\ell})$. The space- and energy-dependent weight window lower bounds $w_\ell$ are given by[8]

$$w_\ell(\vec{r}, E) = \frac{w}{\left(\frac{c_u + 1}{2}\right)} = \frac{R}{\phi^+(\vec{r}, E)\left(\frac{c_u + 1}{2}\right)}.$$

In MCNP, the default value for $c_u$ is 5. Because the calculational efficiency has been observed to be fairly insensitive to small deviations in this parameter, the default value was employed throughout this work. Note that because the source biasing parameters and weight window lower bounds are consistent, the source particles are started with statistical weights $(w(\vec{r}, E) = \frac{q(\vec{r}, E)}{\hat{q}(\vec{r}, E)})$ that are within the weight windows, as desired. This is an important advantage of the CADIS methodology because it eliminates the incompatibility between source and transport biasing that has been problematic in other approaches due to poor calculational efficiency and/or false convergence.[13,14] For example, if the statistical weights of the source particles are not within the weight windows, the particles are immediately split or rouletted in an effort to bring their weights into the weight window. This results in unnecessary splitting/rouletting and a corresponding degradation in computational efficiency. Furthermore, for problems in which the adjoint function varies significantly within the source region (space and/or energy), the source biasing is very effective for improving calculational efficiency.

## III. DEVELOPMENT OF ADVANTG

As this work was a first step toward developing and demonstrating an independent automated variance reduction capability, it has made use of existing codes that are not a part of the SCALE package. As development and integration into SCALE proceeds, these codes will be replaced with codes that are a part of the SCALE package.

In the meantime, the prototypic utility code, ADVANTG, is essentially a deterministic WWG for MCNP that also generates consistent source biasing parameters. The input for using ADVANTG is very similar to that required for using the MCNP mesh-based statistical WWG,[3] and ADVANTG outputs weight window values to the MCNP WWINP file, which may be read and utilized by the standard (unmodified) version of MCNP. As indicated in the flowchart shown in Figure 1, ADVANTG automatically generates input files for material cross-section processing based on the GIP code[15] and 3-D (x-y-z or r-θ-z) discrete ordinates adjoint calculations with the TORT code.[15] Following the GIP and TORT calculations, ADVANTG reads the standard TORT binary output file and the MCNP unbiased source to output the weight window values and biased source definition cards.

The spatial mesh and energy group boundaries for the TORT calculation are taken directly from the MCNP WWG MESH and WWGE cards,[3] and materials are assigned to meshes based on mesh center coordinates. Although previous studies [8,16,17] have confirmed that the effectiveness of the adjoint function for variance reduction is not overly sensitivity to mesh fidelity, the capability to generate 2-D color plots of the spatial mesh and material specifications for any (and all) axial plane(s) is available.

Another aspect of automating discrete ordinates calculations is automating the cross-section mixing/processing, which requires the generation of an input file for an applicable code. In this work, we have employed the GIP code and it is assumed that an appropriate multi-group library is available. The atom densities and material mixture specifications, in terms of ZAIDs (isotope identifiers), are taken directly from the MCNP input. For the specification of material mixtures in GIP, the

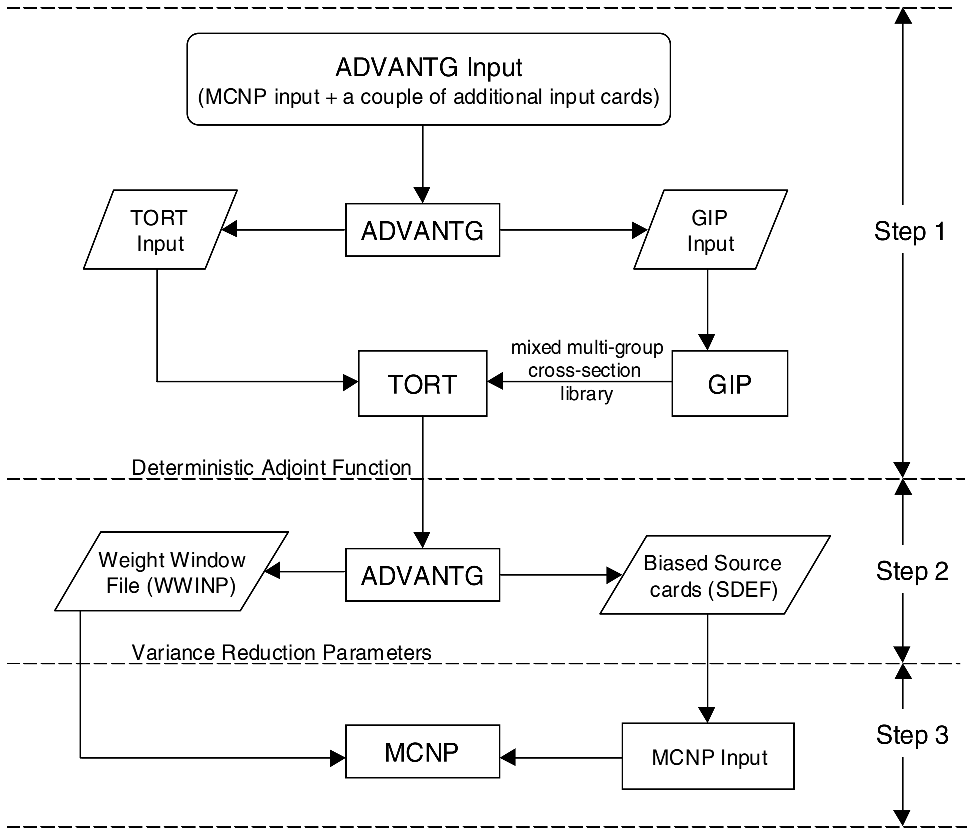


**Figure 1. Automated variance reduction process with ADVANTG utility.**

MCNP ZAIDs are translated into the multi-group library specific component numbers (isotope identifiers). The major difficulty with automating the generation of GIP input files in a general and user-friendly manner lies in this association.

The source for the discrete ordinates adjoint calculation is equivalent to the detector specified in the Monte Carlo input. The detector response function is taken directly from the MCNP input file through the use of a new input keyword.

Finally, there are a number of other input parameters required by TORT in addition to the input associated with the geometry, cross-sections, and source. Suitable default values for these parameters have been defined (e.g., $S_8$ quadrature order, difference scheme, convergence criteria, etc.)

## IV. APPLICATION

A standard nuclear well-logging problem was used to evaluate the implementation and effectiveness of the ADVANTG utility. For the purpose of petroleum exploration, a nuclear well-logging tool, which contains either a neutron or photon source and one or more detectors, is placed in a borehole that contains water and is typically surrounded by a limestone foundation. The response of the detectors to radiation returning from the surrounding formation depends on the material porosity and characteristics. Accurate computer simulation is a very important aspect of this exploratory technique. However, because this technique involves calculating highly precise responses based on radiation that has interacted with the surrounding formation, the transport simulations can be computationally intensive.

The specific problem considered corresponds to test problem 12 from the MCNP test set[3] and is a generic neutron porosity tool in a cylindrical borehole filled with water and surrounded by limestone. In addition to being a relatively challenging problem, this problem was selected for consideration because (1) it has been carefully tuned and optimized by an expert variance reduction practitioner[13,14] – enabling an independent reference of comparison for an expert user, (2) it has been evaluated by others[18] with implementations of automated deterministic-based variance reduction techniques, and (3) it has been used to assess[13,14] the mesh-based stochastic WWG in MCNP.

The problem configuration is shown in Figure 2. The formation consists of limestone with 20% porosity. The tool itself is iron and contains a $^{241}$AmBe source that is modeled as a point source with directional dependence. The tool contains two $^{3}$He detectors with different sizes that are placed at different distances from the source. This evaluation focuses on the detector that is furthest from the source, referred to as the "far detector", because it is the most difficult of the two detectors.

The reference "expert-tuned" input includes 231 cells to facilitate the cell-based weight windows and weight window values are used over 5 energy groups. With the mesh-based weight windows, extraneous cells are not necessary, and thus the model was reduced to 10 cells for all other cases.

First, MCNP calculations were performed without any variance reduction (analog) and with the "expert-tuned" variance reduction to produce reference points for comparison. The "expert-tuned" corresponds directly to test problem 12, with the exception that the WWG was turned off to maximize efficiency. Subsequently, MCNP calculations were performed using mesh-based weight-window values and energy-dependent source biasing parameters generated by ADVANTG. (Note that because this problem involves a point source, the capability for space-dependent source biasing parameters is not applicable, and thus not utilized.)

For the ADVANTG cases the weight window mesh boundaries were selected to be consistent with the problem materials boundaries, and the resolution of meshes between material boundaries was varied to evaluate the impact on efficiency. Although it would have been preferable to use a multi-group cross-section library with a fewer number of energy groups (to minimize the time required for the TORT calculations), the 47-group BUGLE96 library[19] was used. Table 1 summarizes the mesh characteristics and computer time for the TORT calculations for the cases considered. The CPU times listed for the TORT calculations are considerably less than the times cited in Ref. 18 for using the mesh-based stochastic WWG.

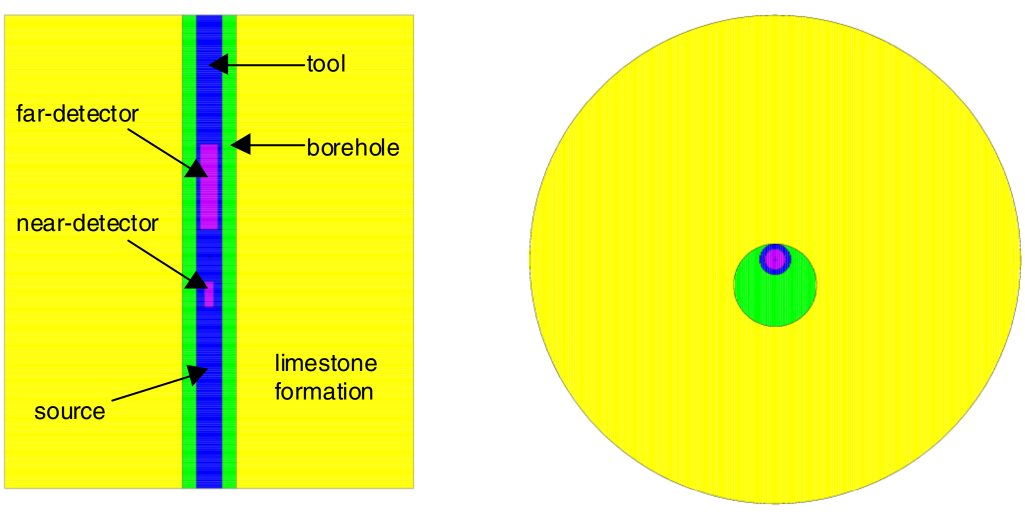


**Figure 2. Radial and axial cross-sectional views of the well-logging problem.**

**Table 1. Mesh characteristics and TORT CPU times for cases considered with ADVANTG**

| Case | No. of spatial meshes used for both the weight windows and the TORT calculation | | | | CPU time for TORT (min) |
|---|---|---|---|---|---|
| | x | y | z | total | |
| 1 | 52 | 52 | 51 | 137904 | 32.8 |
| 2 | 29 | 29 | 26 | 21866 | 5.0 |
| 3 | 21 | 21 | 16 | 7056 | 1.6 |
| 4 | 16 | 15 | 13 | 3120 | 0.8 |

As is common practice, the computational efficiency of each approach was compared using the Figure-Of-Merit (FOM),

$$FOM = \frac{1}{\sigma^2 T},$$

where $\sigma$ and $T$ are the relative statistical error and computer time, respectively. Table 2 provides a summary of the FOM values for the various approaches considered and shows that the ADVANTG cases are notably more efficient than the manually optimized ("expert-tuned") case and a case using the mesh-based WWG. While these improvements in efficiency are significant, the overall efficiency is substantially greater than that indicated in Table 2 when one considers the computer time required by the mesh-based WWG or the user-time required by the expert Monte Carlo variance reduction practitioner. Finally, the total computer time required to achieve results with statistical relative errors of 1% are listed in Table 3. Consistent with the findings of previous studies,[8,16,17] the overall calculational efficiency increased with decreasing spatial-mesh resolution for the cases considered.

**Table 2. Summary of FOM values for the various variance reduction approaches considered**

| Variance reduction approach | FOM | Ratio [FOM/ analog FOM] |
|---|---|---|
| None (analog) | 6.8 | 1.0 |
| "expert-tuned" | 285 | 41.9 |
| Best case WWG | 170[a] | 25.0 |
| ADVANTG case 1 | 387 | 56.9 |
| ADVANTG case 2 | 502 | 73.8 |
| ADVANTG case 3 | 591 | 86.9 |
| ADVANTG case 4 | 649 | 95.4 |

[a] This value was determined based on scaling FOM values listed in Ref. 13 to the "expert-tuned" FOM value listed above.

As the MCNP mesh-based weight window facilities allow both rectangular and cylindrical geometries, ADVANTG was tested for both geometries. Although the well-logging problem is inherently cylindrical, it was quickly realized (and later discovered to be consistent with the findings of others[13,14]) that the implementation of mesh-based weight windows in cylindrical geometry is notably less efficient than for rectangular geometry. Hence, all results presented herein correspond to rectangular geometry. Finally, note that ADVANTG was also successfully used to (1) separately optimize the calculation for the closer "near-detector" and (2) simultaneously optimize for both detectors. As one would expect, the simultaneous optimization of both detectors could not achieve the FOM values produced by separately optimizing for each detector, but still achieved notably greater efficiencies than those obtained with the "expert-tuned" model.

**Table 3. Resources required to achieve relative statistical errors (σ) of 1% with the various variance reduction approaches considered**

| Variance reduction approach | Number of histories to achieve σ = 0.01 | CPU time for MCNP to achieve σ = 0.01 (min) | CPU time for TORT (min) | Total CPU time (min) |
|---|---|---|---|---|
| None (analog) | 8.5E+7[a] | 1476.0[a] | n/a | 1476.0[a] |
| "expert-tuned" | 2.0E+6 | 34.7 | n/a | 34.7 |
| ADVANTG case 1 | 5.9E+5 | 26.4 | 32.8 | 59.2 |
| ADVANTG case 2 | 6.0E+5 | 19.5 | 5.0 | 24.5 |
| ADVANTG case 3 | 7.3E+5 | 17.0 | 1.6 | 18.6 |
| ADVANTG case 4 | 6.8E+5 | 15.6 | 0.8 | 16.4 |

[a] Estimated based on results from a calculation with 1.0E+7 histories

## V. CONCLUSIONS

A prototypic utility for automated variance reduction, based on deterministic adjoint functions and sound variance reduction methodology, has been independently developed and tested. The computational efficiencies achieved are very encouraging when compared to both stochastic and manual approaches for developing variance reduction, and the process seems to be well-suited for automation in a future SCALE shielding analysis sequence. Based on the work to date, the proposed SCALE shielding sequence will utilize three-dimensional deterministic adjoint functions on a rectangular geometry.

Future work will utilize the prototypic utility code for testing and refining the implementation and investigating alternative methodologies, before attempting integration into SCALE. During the integration process, the utility will be used as a reference for computational efficiency comparisons. Other areas that may be explored include approaches for angular biasing, optimization of problems with multiple regions of interest (tallies), and automated variance reduction for eigenvalue problems.

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## REFERENCES

1. T.E. Booth, “A Sample Problem in Variance Reduction in MCNP,” LA-10363-MS, Los Alamos National Laboratory (1985).

2. T.E. Booth and J.S. Hendricks, “Importance Estimation in Forward Monte Carlo Calculations,” *Nucl. Technol./Fusion*, **5**, 90 (1984).

3. J.F. Briesmeister, Editor, “MCNP — A General Monte Carlo N-Particle Transport Code, Version 4C,” LA-13709-M, Los Alamos National Laboratory (April 2000).

4. J.S. Tang and T.J. Hoffman, “Monte Carlo Shielding Analyses Using an Automated Biasing Procedure,” *Nucl. Sci. Eng.*, **99**, 329 (1988).

5. M.W. Mickael, “A Fast, Automated, Semideterministic Weight Windows Generator for MCNP,” *Nucl. Sci. Eng.*, **119**, 34 (1995).

6. J.S. Tang and M.B. Emmett, “SAS4: A Monte Carlo Cask Shielding Analysis Module Using an Automated Biasing Procedure,” Vol. I, Sect. S4 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*,” NUREG/CR-0200, Rev. 6 (ORNL/NUREG/CSD-2/V2/R6), May 2000. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

7. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 6 (ORNL/NUREG/CSD-2/R6), Vols. I, II, and III, May 2000. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

8. J.C. Wagner and A. Haghighat, “Automated Variance Reduction of Monte Carlo Shielding Calculations Using the Discrete Ordinates Adjoint Function,” *Nucl. Sci. Eng.*, **128**, 186 (1998).

9. K.A. Van Riper, T.J. Urbatsch, P.D. Soran, D.K. Parsons, J.E. Morel, G.W. McKinney, S.R. Lee, L.A. Crotzer, F.W. Brinkley, J.W. Anderson, and R.E. Alcouffe, “AVATAR - Automatic Variance Reduction in Monte Carlo Calculations,” *Proc. Joint. Int. Conf. on Mathematical Methods and Supercomputing in Nuclear Applications*, Saratoga Springs, New York, October 6–10, 1997, Vol. 1, American Nuclear Society.

10. T.M. Shuttleworth, M.J. Grimstone, and S. Chucas, “Application of Acceleration Techniques in MCBEND,” Journal of Nuclear Science and Technology, Supplement 1 (March 2000), *Proc. of Ninth International Conference on Radiation Shielding*, p. 406, Tsukuba, Ibaraki, Japan, October 17–22, 1999.

11. F.X. Giffard, R. Jacqmin, J.C. Nimal, and Y. Peneliau, “Variance Reduction in 3-D Continuous-Energy Monte Carlo Simulations Using Importance Maps Generated by a Deterministic Code,” *Proc. of the Mathematics and Computation, Reactor Physics and*

*Environmental Analysis in Nuclear Applications*, p. 273, Madrid, Spain, September 27–30, 1999.

12. M.E. Dunn and N.M. Greene, "AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications," *Trans. Am. Nucl. Soc.*, **86**, June 2002.

13. J.S. Hendricks and C.N. Culbertson, "An Assessment of MCNP Weight Windows," *Proc. of the PHYSOR 2000 ANS International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium*, Pittsburgh, PA, USA, May 7–12, 2000.

14. C.N. Culbertson and J.S. Hendricks, "An Assessment of MCNP Weight Windows," Los Alamos National Laboratory, LA-13668 (1999).

15. *DOORS 3.2: One, Two- and Three-Dimensional Discrete Ordinates Neutron/Photon Code System*, Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-650.

16. J.C. Wagner, "Acceleration of Monte Carlo Shielding Calculations with an Automated Variance Reduction Technique and Parallel Processing," *Ph.D. Thesis*, The Pennsylvania State University, Nuclear Engineering Dept. (1997).

17. A. Haghighat, H. Hiruta, B. Petrovic, and J.C. Wagner, "Performance of the Automated Adjoint Accelerated MCNP ($A^3$MCNP) for Simulation of a BWR Core Shroud Problem," *Proc. of the International Conference on Mathematics and Computation, Reactor Physics, and Environmental Analysis in Nuclear Applications*, p. 1381, Madrid, Spain, September 27–30, 1999.

18. T.M. Evans and J.S. Hendricks, "An Enhanced Geometry-Independent Mesh Weight Window Generator for MCNP," *1998 ANS Radiation Protection and Shielding Division Topical Conference*, Vol. 1, p. 165, Nashville, TN, April 19–23, 1998.

19. *BUGLE-96: Coupled 47 Neutron, 20 Gamma-Ray Group Cross Section Library Derived from ENDF/B-VI for LWR Shielding and Pressure Vessel Dosimetry Applications*, Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as DLC-185.