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NNSA Office of Nonproliferation Research and Development
Simulation, Algorithms, and Modeling (SAM) Program

A Multisensor Fusion Approach to the Model-Based Solution of Inverse Radiation Transport Problems

FY2009 Summary of Accomplishments

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Introduction

Characterization of unknown radiation sources requires solution of the radiation transport problem in the inverse sense. The capability to solve inverse transport problems on the basis of gamma spectroscopic analysis has been under development for over a decade and has reached a reasonable level of maturity. (See, for example, Mattingly and Mitchell 2008 and the references therein.) The key features of Sandia's inverse solver are

- It uses one-dimensional (1D) radiation transport models of the source to synthesize an estimate of the gamma spectrum. Deterministic radiation transport methods are used to maintain acceptable fidelity while maximizing the speed.
- It compares that estimate to the measured gamma spectrum using a chi-squared error metric.
- It uses iterative optimization of the transport model variables (e.g., the dimensions of the 1D layers) to solve for an optimal model of the source configuration.

However, an inverse solution based upon the gamma spectrum alone is relatively poorly constrained. Gammas are rapidly attenuated by dense, high atomic number (high Z) materials. Consequently, special nuclear materials (SNM) tend to be self-shielding: gammas that are externally observable from thick SNM generally emerge from a thin outer layer of the material. As a result, in general the gamma spectrum can only be used to solve for features near the source's external surface (e.g., SNM surface area).

In addition to being self-shielding, though, SNM is generally also self-multiplying: neutrons can initiate fission chain reactions in SNM, and those chain reactions can substantially increase the neutron population. Furthermore, neutrons tend to penetrate SNM more easily than gammas; neutrons are generally rapidly attenuated by low-Z materials, which tend to be transparent to gammas.

Neutron observables, however, lack a gamma spectrum's specificity to the source's isotopic composition. In other words, neutron observables do not impart many degrees of freedom to the inverse problem. Consequently, though neutron observables may be used to solve for the source's bulk configuration (e.g., SNM mass), by themselves they too only weakly constrain the inverse solution.

Due to the complementary characteristics of photon and neutron transport, an inverse solution based upon simultaneous analysis of gamma and neutron observables tends to be better constrained than a solution obtained by analysis of either observable alone.

Very recently, in a previous SAM project, Sandia implemented a method to rapidly and accurately synthesize neutron multiplicity counting statistics from deterministic neutron transport calculations. (See Mattingly and Varley 2008 or Mattingly and Varley 2007 for details.) This development enabled the simultaneous analysis of gamma spectrometry and neutron multiplicity observables in Sandia's inverse transport solver.

However, several issues prevent the widespread practical use of this approach:

- Computation of neutron multiplicity statistics via deterministic transport is orders of magnitude faster than calculations using Monte Carlo methods, but it is still too slow for some inverse problems.
- Actual measurements to validate the calculations used by the inverse solver are scarce, and obtaining new measurements is prohibitively expensive.
- There is no rigorous, systematic way to weight the two observables in the computation of the error metric used by the inverse solver.

The current SAM project addresses each of these issues. The end result will be a validated, practical implementation of an inverse transport solver that uses gamma spectrometry and neutron multiplicity observables to characterize source configuration.

Objectives

The principal goal of this project is to develop, implement, and test methods to rapidly and accurately solve inverse radiation transport problems via iterative forward modeling of gamma spectrometry and neutron multiplicity observables. The three primary objectives that will enable that goal to be achieved are:

- ***Develop and test methods to accelerate deterministic neutron transport calculations of neutron multiplicity statistics.*** Deterministic numerical solution of the neutron transport equation discretizes the problem domain. There are numerous alternative approximations for the spatial, spectral, directional, and temporal dependence of the transport medium properties, transport operators, and the neutron population. Some of these approximations can be applied to accelerate the solution of the forward and adjoint neutron transport equations. In general, more approximate methods are capable of obtaining a solution faster than higher fidelity approximations. However, these faster solution techniques can introduce error into the calculations and therefore cause the inverse solver to converge on an incorrect solution. Alternative solution techniques will be tested for computational speed and accuracy applied to neutron multiplicity calculations. The study will find a balance that minimizes solution time while maintaining an acceptable level of accuracy in the inverse solution.

- ***Implement and validate high fidelity Monte Carlo neutron transport calculations of neutron multiplicity statistics.*** Ideally, deterministic neutron multiplicity calculations would be tested against measurements. However, although literally thousands of neutron multiplicity measurements of SNM in diverse configurations have been performed in the past, the experimental conditions of only a few of those measurements were sufficiently documented for benchmark purposes. Consequently, we will have to rely in part on synthetic data for validation. Monte Carlo is an alternative method for numerical solution of the neutron transport equation, and although it is comparatively slow, it employs relatively few approximations. Throughout most of the numerical radiation transport community, Monte Carlo methods are regarded as having the highest fidelity, and their accuracy for simulating fundamental radiation transport phenomena has been previously validated against hundreds of benchmark measurements. Monte Carlo methods specifically designed to produce high fidelity simulations of neutron multiplicity measurements will be implemented and tested against benchmark measurements. The validated Monte Carlo code will be used to generate synthetic data to test deterministic calculations for cases where insufficient measured data are available.
- ***Develop a systematic approach to combining the analysis gamma spectrometry and neutron multiplicity observables in the solution of inverse radiation transport problems.*** Gamma spectrometry and neutron multiplicity observables do not contribute equal degrees of freedom to the inverse problem, and they are not independent of one another. Random and systematic variations in measurement conditions can potentially produce correlated experimental errors in both observables. More significantly, however, changes in transport model variables induce correlated variations in the computed observables. These variations are strongly correlated both internal to each observable (i.e., the model errors are auto-correlated) and between observables (i.e., the model errors are also cross-correlated). The experimental and model error covariances dictate the dimensionality and topography of the inverse solution space and provide a systematic method to combine the analysis of both observables. The auto- and cross-correlation of experimental and modeling errors in gamma spectrometry and neutron multiplicity observables will be evaluated, and the effect of accounting for error covariance in the inverse solution will be characterized.

Accomplishments

This project is being executed as a partnership between Sandia National Laboratories, the University of Florida (UF), and the University of Michigan (UM). UF is leading the development of accelerated deterministic radiation transport methods for neutron multiplicity calculations. UM is leading the implementation of high fidelity Monte Carlo neutron multiplicity simulations. Sandia is leading the multivariate statistical analysis of experimental and computed gamma spectrometry and neutron multiplicity observables. Sandia is also assisting its university partners by providing benchmark measurements of SNM to validate their codes, and Sandia is guiding their developments using its own implementation as a baseline for performance. Sandia is also coordinating efforts at all three institutions.

Several significant accomplishments were realized in FY2009.

Deterministic Radiation Transport

The University of Florida developed a platform that will be used for evaluation of alternative methods for accelerating deterministic neutron multiplicity calculations. PENTRAN[1], UF's three-dimensional (3D) parallel-execution radiation transport solver, will be used to evaluate the impact on speed and accuracy of numerous alternative solver options and cross-section generation schemes. Several supporting codes and databases were developed this year to work with PENTRAN to support UF's study.

- UF's code GMIX was originally designed to generate neutron cross-section mixtures and source terms from a transport model's material specification. UF extensively augmented GMIX to also generate neutron multiplicity moments for all spontaneously fissioning and fissile nuclides, which are necessary for the simulation of neutron multiplicity measurements.
- UF developed a new neutron cross-section library, Alpha79, to use as a baseline for comparison against the current speed and accuracy obtained using Sandia's Kynea3 library. Sandia and UF jointly tested several revisions to Alpha79. The latest revision, Alpha79j, reproduces the accuracy obtained with Sandia's Kynea3 library, so it is an adequate baseline for testing future collapsed libraries.
- UF performed a series of adjoint neutron transport calculations to estimate the energy-dependent neutron detection efficiency of the Los Alamos NPOD neutron multiplicity counter (which was used in several benchmark measurements by Sandia). Sandia used UF's adjoint transport estimate of detection efficiency to verify its Monte Carlo and empirical models of the detector's response function, which are central to Sandia's implementation of neutron multiplicity simulations.
- UF developed and tested a new code, YGROUP, designed to compute the Feynman-Y neutron multiplicity statistic from PENTRAN forward and adjoint neutron transport solutions. YGROUP is an implementation of Sandia's technique for computing neutron multiplicity statistics, so it provides the basis for testing different transport solver options and cross-section generation schemes for speed and accuracy relative to the baseline performance obtained using Sandia's

[1] PENTRAN stands for "**p**arallel **e**nvironment **n**eutral-particle **tran**sport."

solver options and the Alpha79 library. YGROUP also implements three different methods for collapsing cross-sections:

  - Flat weighting: energy groups in the collapsed library are simply algebraic sums of neighboring groups in the fine-structure library.
  - Reaction rate weighting: neighboring groups in the fine-structure library are weighted according to a reaction rate (e.g., induced fission) when they are summed to construct the collapsed library.
  - Contributon weighting: energy groups in the collapsed library are obtained by a weighted sum of neighboring groups in the fine-structure library. The weighting function is a forward-adjoint inner product, where the adjoint represents neutron importance to a functional (e.g., detector count rate), so that the summation emphasizes the energy regions that contribute substantially to, e.g., detector response.

- UF has tested several libraries collapsed from Alpha79j. They have been able to produce collapsed libraries that roughly halve the computational time (by reducing the number of energy groups by a factor of 2). Preliminary tests of these libraries show that they can estimate the Feynman-Y as accurately as the fine-structure Alpha79j library.

See Attachment 1 for more details on this year's accomplishments in deterministic radiation transport. Development and testing of alternative solver options and cross-section libraries will continue into FY2010.

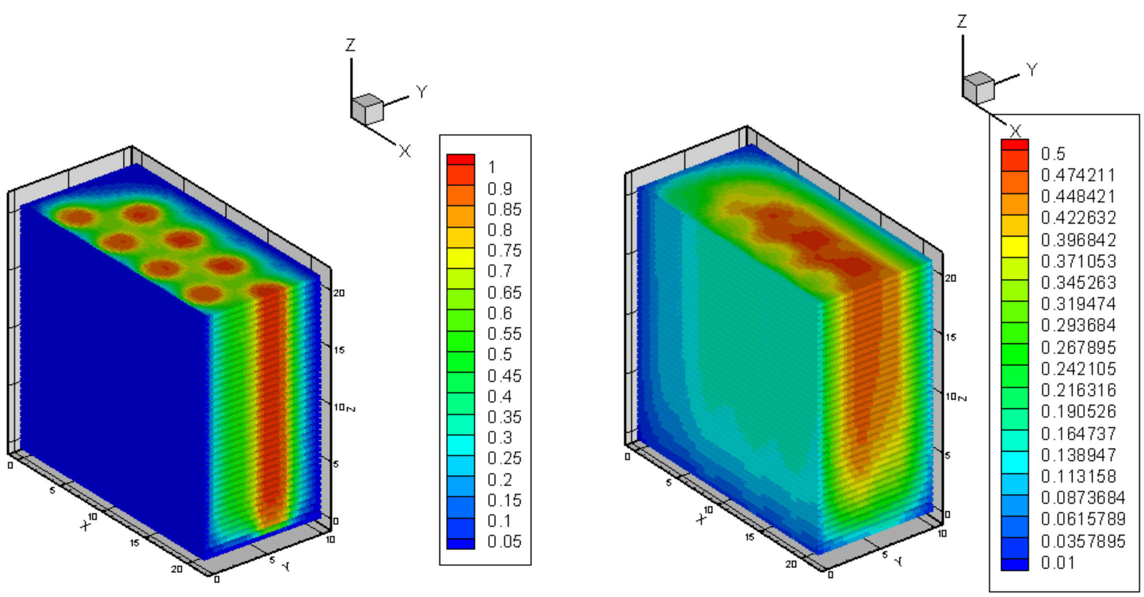

Figure 1: PENTRAN calculation of adjoint scalar flux in the Los Alamos NPOD multiplicity counter for thermal neutrons (left) and fast neutrons (right). The adjoint flux represents the importance of neutrons to the detector response.

Monte Carlo Radiation Transport

The University of Michigan implemented Monte Carlo simulation of neutron multiplicity measurements. MCNP-PoliMi is a modification of MCNP4 designed for accurate simulation of neutron and photon time-correlation measurements. The code will be used to generate synthetic data to test the accuracy of alternative deterministic transport solution techniques when actual experimental data is unavailable. This year focused on developing tools to use MCNP-PoliMi for simulating neutron multiplicity experiments and validating the results obtained with the code.

- MCNP-PoliMi logs simulated detection events in a list-mode text file that records the particle type (neutron or photon), the interaction type (scatter or absorption), the energy deposited, and the position and time of the interaction. Sandia and UM developed post-processors that accumulate the neutron multiplicity distribution from the MCNP-PoliMi event log. The post-processors also compute statistics of the distribution like the mean, variance, and Feynman-Y.
- MCNP-PoliMi was modified by the Polytechnic of Milan (the code's original authoring institution) to correctly simulate the scattering of thermal neutrons by low-Z materials. The correct treatment of thermal neutron scattering is critical to the accurate simulation of most neutron multiplicity counting instruments because these instruments generally incorporate low-Z materials to enhance detection efficiency.
- UM and Sandia constructed MCNP-PoliMi models of benchmark measurements Sandia conducted at the Nevada Test Site (NTS) in January 2009. The models were constructed to simulate benchmark measurements of a californium point source and the Los Alamos BeRP ball, an unclassified sphere of weapons-grade plutonium metal. The calculations were compared to the measurements to validate MCNP-PoliMi.
- During validation of MCNP-PoliMi, a critical logic error in the original MCNP4 code was identified. The error caused neutrons produced by induced fission to be incorrectly distributed in direction, which in turn introduced significant errors into the neutron multiplicity simulations. The error was corrected by the Polytechnic of Milan, and a new version of MCNP-PoliMi was released.

See Attachment 2 for more details on this year's accomplishments in Monte Carlo radiation transport. Validation of MCNP-PoliMi will continue into FY2010.

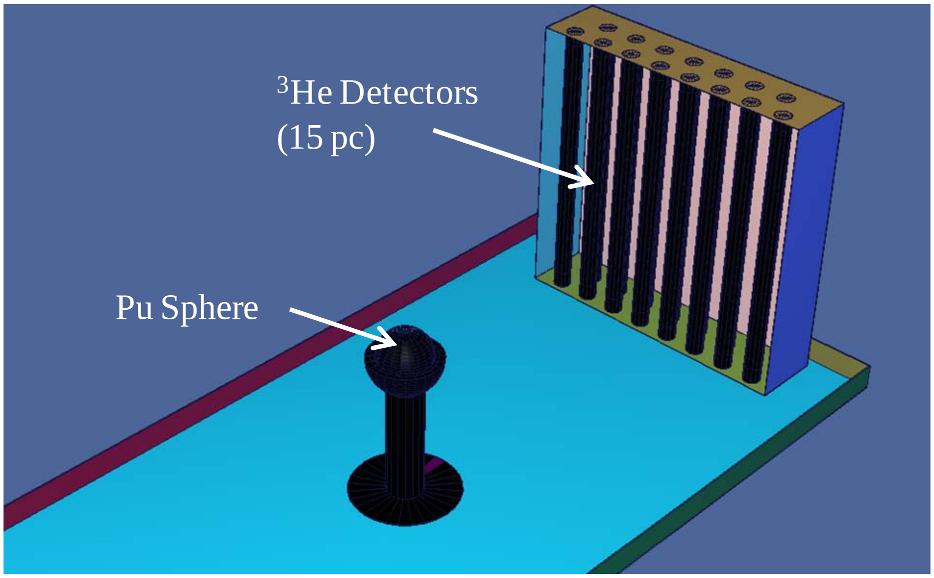

Figure 2: MCNP-PoliMi model of a benchmark measurement of the Los Alamos BeRP ball plutonium source using the NPOD multiplicity counter. Models such as the one shown were used to validate MCNP-PoliMi against experiments.

Multivariate Statistical Analysis

Sandia characterized covariance in gamma spectrometry and neutron multiplicity experimental and modeling errors. Experimental errors occur due to variations in radiation emission, transport, and detection. These errors are principally random. Modeling errors occur due to incorrect estimation of the variables in the model used to fit the experiment during an inverse solution. These errors are principally systematic. Characterization of the covariance between errors, both experimental and modeling, will be used to develop a rigorous approach to combining the analysis of gamma spectrometry and neutron multiplicity measurements.

- The covariance between experimental errors in the gamma spectrum was characterized using synthetic data (measurement of an adequate number of gamma spectrum replicates is impractical). It was shown that correlated errors do result when the instrument inadequately compensates for instrument drift. However, the majority of spectrometers are capable of holding their calibration for short-dwell measurements, and techniques to compensate for drift in post-processing are generally effective at eliminating these errors. Aside from calibration drift errors, it was observed that variations are largely uncorrelated between channels in the gamma spectrum.[2]
- The covariance between experimental errors in the Feynman-Y neutron multiplicity statistic was characterized using measurements of plutonium conducted at NTS this January. It was shown that random variations in the Feynman-Y are very highly correlated between channels.[3] This high degree of correlation occurs because the Y is the ratio of two statistics (the mean and

[2] The channels in a gamma spectrum represent different photon energies.
[3] The channels in the Feynman-Y represent different counting times.

variance), which are accumulated by summation over the entire neutron multiplicity distribution.

- Preliminary characterization of the cross-covariance between experimental errors in the gamma spectrum and the Feynman-Y was conducted using a combination of synthetic gamma spectral data and measured neutron multiplicity data. As expected, the initial characterization reveals no strong correlation between experimental errors in the two observables.
- An analysis of the correlation between model errors arising from systematic errors in model variables was conducted, and a method to compute the model *error* covariance matrix by forward propagation of the model *variable* covariance matrix was developed. This analysis of covariance was implemented in an inverse solver employing a standard Levenberg-Marquardt minimizer and the GADRAS radiation transport and gamma spectrometer response kernels.
- The inverse solver was used to study the effect of including model error covariance in the minimization metric. To date two example problems have been studied to characterize the topography of the inverse solution space. The first example exhibited high correlation between modeling errors, which resulted in a solution that was nearly degenerate. The second example exhibited modeling errors that were more nearly independent, which resulted in a tightly constrained solution. The solver will be extended to include the GADRAS neutron multiplicity counter response kernel in the near future.

See Attachments 3 and 4 for more detail on this year's accomplishments in multivariate statistical analysis. Characterization of inverse solution space topography will continue in FY2010.

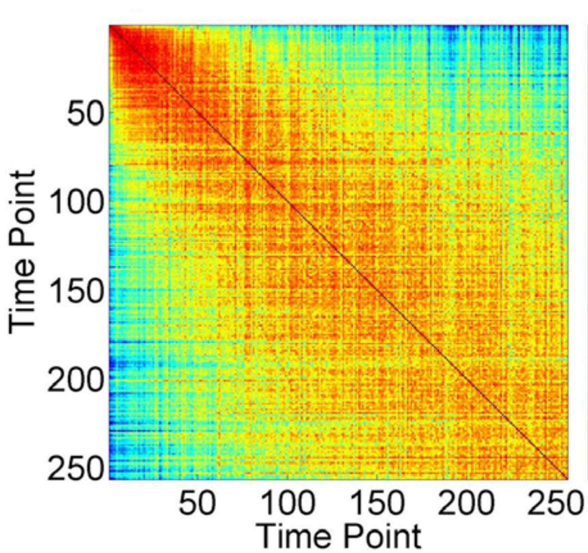

Figure 3: Channel-wise correlation matrix for the Feynman-Y neutron multiplicity statistic. Individual channels in the Feynman-Y are strongly cross-correlated, so the observable contributes only a small number of degrees of freedom to the problem solution.

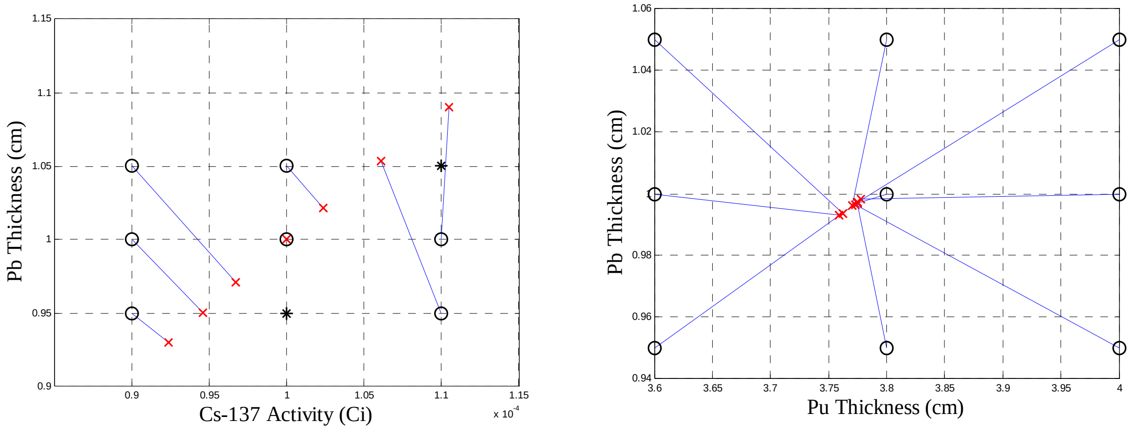

Figure 4: Solution topography for two example problems; the black circles represent initial guesses for model variables, and the red *x*'s represent the final solution for the variables. The problem on the right is degenerate, and the problem on the right possesses a single well-constrained solution

Summary

The principal goal of this project is to develop approximate methods to rapidly solve inverse radiation transport problems for the purposes of characterizing unknown radiation sources. Many classes of inverse transport problem are poorly constrained unless they are solved by simultaneous analysis of gamma spectrometry and neutron multiplicity observables. The tasks executed in this project are designed to implement a practical solution to inverse transport problems on the basis of these two observables. The principal objectives are:

- Develop and test methods to accelerate deterministic neutron transport calculations of neutron multiplicity statistics.
- Implement and validate high-fidelity Monte Carlo neutron transport calculations of neutron multiplicity statistics.
- Develop a systematic approach to combining the analysis gamma spectrometry and neutron multiplicity observables in the solution of inverse radiation transport problems.

This year, significant progress was made:

- A platform for developing accelerated methods to solve forward and adjoint neutron transport problems was constructed and tested.
- A Monte Carlo code to simulate neutron multiplicity measurements was developed and is being validated against benchmark data.
- Analyses of experimental and modeling error covariances were conducted to determine how correlated errors affect the inverse solution topography, which dictates how the two observables should be combined.

Consequently, at the beginning of FY2010, the project is positioned to begin evaluation of different transport acceleration strategies, to validate the results obtained using those approximations, and to systematically combine the analysis of gamma spectrometry and neutron multiplicity measurements.

References

Mattingly, John, and Dean J. Mitchell. "A Framework for the Solution of Inverse Radiation Transport Problems." *IEEE Nuclear Science Symposium Conference Record.* Dresden, Germany, 2008. 1265 - 1270.

Mattingly, John, and Eric S. Varley. *Development and Preliminary Testing of Feynman-Y Synthesis in GADRAS (SAND2007-5427).* Sandia National Laboratories, 2007.

—. "Synthesis of the Feynman-Y Neutron Multiplicity Metric using Deterministic Transport." *Annual Meeting of the American Nuclear Society.* Anaheim, California, 2008. 572 - 574.

Attachment 1: University of Florida Report on FY2009 Accomplishments in Deterministic Transport Modeling

Florida Institute of
Nuclear Detection and Security
Nuclear and Radiological Engineering
University of Florida

Year 1 Annual Report: DDTORP Research Program at FINDS/UF

September 2009
By Ce Yi and Glenn Sjoden

DDTORP: Dynamic Deterministic Transport Optimization Research Program
Sponsor Agency: Sandia National Laboratory (PO #875247 Revs 1 to 4)

Attachment 2: University of Michigan Report on FY2009 Accomplishments in Monte Carlo Transport Modeling

A Multisensor Fusion Approach to the Solution of Inverse Radiation Transport Problems

University of Michigan – Year 1 Report

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ABSTRACT
In the course of the present project, the University of Michigan developed and validated high-fidelity Monte Carlo codes for the simulation of neutron multiplicity measurements on special nuclear material (SNM). The development and subsequent validation of these types of Monte Carlo codes relies on the availability of carefully measured data. In this project, we used measurement data obtained by Sandia National Laboratories personnel to enhance and validate the MCNP-PoliMi code system for the simulation of neutron multiplicity measurements of a significant quantity of weapons-grade plutonium metal. The results showed that the MCNP-PoliMi code system is a unique tool for neutron multiplicity analysis.

1.0 INTRODUCTION

The MCNP-PoliMi code system has been used in the past to accurately predict the results of neutron multiplicity measurements using an active well coincidence counter [1]. The goal of this work is to further validate MCNP-PoliMi for neutron multiplicity analysis. The ability of the MCNP-PoliMi code system for the modeling of neutron multiplicity measurements has been previously shown [2]. Measurements of a weapons-grade plutonium sphere with various thicknesses of polyethylene shielding were taken at the Nevada Test Site by Sandia National Laboratories personnel. These measured results were compared to the simulations performed with MCNP-PoliMi. The metric chosen for comparing the simulation to the measured data is the Feynman-Y, which characterizes the deviation of the distribution from that of a Poisson distribution [3].

2.0 MEASUREMENT DESCRIPTION

The measurements were performed on the Los Alamos BeRP (beryllium-reflected plutonium) ball, a 4.483-kg sphere of weapons-grade plutonium metal[2] [4]. The fissile material was reflected by a series of spherical polyethylene shells of varying thickness. These specially designed shells allowed the polyethylene thickness to be set at 0.5, 1.0, 1.5, 3.0, and 6.0 inches. Each shell had

[1] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
[2] The source is referred to as the BeRP ball because one of its first applications was to study the criticality of beryllium-reflected plutonium.

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Attachment 3: Sandia Report on FY2009 Accomplishments in Analysis of Experimental Error Covariance

Chris Stork
Org. 1825
September 7, 2009

Report on FY2009 Activities: A Multisensor Fusion Approach to the Model-Based Solution of Inverse Radiation Transport Problems (Multivariate Statistical Analysis of Gamma and Neutron Signatures)

1. Introduction

This report documents accomplishments made in addressing the two key FY2009 tasks for the Multivariate Statistical Analysis portion of the project, namely (1) characterizing the covariance structure of gamma and neutron signatures for representative source classes, and (2) beginning development of rigorous statistical methods to incorporate covariance information into the inverse transport solution approach. With regard to the first task, the error covariance structures of gamma and neutron signatures for simple one- and two-component systems have been estimated using simulated and experimentally acquired replicate data, and these results will be presented. To address the second task, a statistical framework is being developed to incorporate error covariance information into the chi square criterion used to solve the inverse transport problem. In its current form, this framework includes (a) a covariance matrix related to experimental measurement errors, and (b) a covariance matrix representing systematic biases attributable to computational model (kernel) errors.

The organization of this report is as follows. Section 2 provides a theoretical overview of methods for calculating the covariance structure of gamma and neutron signatures using replicate measurements, and presents a rigorous statistical approach for incorporating covariance information into the inverse transport solution. Section 3 presents the covariance structures of gamma and neutron signatures calculated for simple one- and two-component systems, and investigates the impact of incorporating different variance and covariance terms on the chi square criterion for these systems. Section 4 provides some concluding thoughts.

2. Theory

In this report, scalars are represented by italics, e.g., n. Column vectors are denoted by boldface lowercase letters, e.g., $\mathbf{x}$. All matrices are represented by boldface uppercase letters, e.g., $\mathbf{X}$. Transposition of a matrix or a vector is symbolized by a superscripted 'T', e.g., $\mathbf{X}^{\mathrm{T}}$ and $\mathbf{x}^{\mathrm{T}}$. The inverse of a matrix is represented by a superscripted '-1', e.g., $\mathbf{X}^{-1}$.

Incorporating only variance terms, the normalized chi square criterion can be expressed as

$$Z = \frac{1}{q}\sum_{i=1}^{q}\frac{\left[x_c(i) - x_m(i)\right]^2}{\sigma^2(i)}, \quad (1)$$

Attachment 4: Sandia Report on FY2009 Accomplishments in Analysis of Model Error Covariance

Consideration of the Covariance of Measurement and Modeling Errors when Solving Inverse Radiation Transport Problems

Ed Thomas 9/09/09

Introduction

Currently, comparison of a computed gamma spectrum to a measured gamma spectrum involves a metric of the form, $\chi^2 = \sum_{i=1}^{q} \frac{(\hat{Y}_i - Y_i)^2}{\sigma_i^2}$, where Y_i and $\hat{Y}_i = f(i; \hat{b}_1, \hat{b}_2, \ldots, \hat{b}_p)$ represent the observed and computed spectra at the i^{th} (of q) energy channels [J. Mattingly and D. J. Mitchell, "A Framework for the Solution of Inverse Radiation Transport Problems," Nuclear Science Symposium Conference Record, 2008. NSS '08. IEEE]. The computed spectrum is based on a physics model (f) with estimated model parameters, $\hat{b}_1, \hat{b}_2, \ldots, \hat{b}_p$. The denominator in the sum (σ_i^2) is intended to represent the combined error variances related to measurement and modeling errors specific to the i^{th} channel. Fitting of the computed spectra to measured spectra (via the physics model parameters) is an iterative process with the value of the metric shrinking during the iterative process as the computed spectrum approaches the measured spectrum. The values for the assumed error variances (σ_i^2's) do not change over the iterative process.

The intent here is to outline and demonstrate a method for estimating the parameters of the physics model that utilizes a new metric (and series of models) for comparing the closeness of the computed spectrum to the measured spectrum. The new metric takes into consideration the covariance of the measurement and modeling errors across channels and is of the form, $Z = \frac{1}{q} \cdot D \cdot V^{-1} \cdot D^T$, where $D = (\hat{Y}_1 - Y_1, \hat{Y}_2 - Y_2, \ldots, \hat{Y}_q - Y_q)$ and V is the covariance of the combination of measurement and modeling errors across channels. Unlike the current metric, this metric considers the linked nature of errors across channels.

Statistical Models and Approach

Let $\{Y_i = \mu_i + \varepsilon_i \;\; i = 1,2,\ldots,q\}$ and $\{\hat{Y}_i = \mu_i + \gamma_i \;\; i = 1,2,\ldots,q\}$ represent the observed and computed spectra, respectively. In this representation,

μ_i = true (expected) intensity of the i^{th} energy channel,

ε_i = measurement error of i^{th} energy channel, and

γ_i = model error of i^{th} energy channel.

The mean of the measurement error is assumed to be zero across all channels. The covariance of the measurement error (across channels) is denoted by V_ε.

The model error associated with the computed spectrum can be further decomposed via $\{\gamma_i = m_i + \lambda_i \;\; i = 1,2,\ldots,q\}$, where

m_i = error due to model misspecification (inaccurate model form) and

λ_i = error due to imprecise estimation of the model parameters.

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