Improved Hybrid Modeling of Spent Fuel Storage Facilities

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Contents

1. Executive Summary

This work developed a new computational method for improving the ability to calculate the neutron flux in deep-penetration radiation shielding problems that contain areas with strong streaming. The "gold standard" method for radiation transport is Monte Carlo (MC) as it samples the physics exactly and requires few approximations. Historically, however, MC was not useful for shielding problems because of the computational challenge of following particles through dense shields. Instead, deterministic methods, which are superior in term of computational effort for these problems types but are not as accurate, were used.

Hybrid methods, which use deterministic solutions to improve MC calculations through a process called variance reduction, can make it tractable from a computational time and resource use perspective to use MC for deep-penetration shielding. Perhaps the most widespread and accessible of these methods are the Consistent Adjoint Driven Importance Sampling (CADIS) and Forward-Weighted CADIS (FW-CADIS) methods. For problems containing strong anisotropies, such as power plants with pipes through walls, spent fuel cask arrays, active interrogation, and locations with small air gaps or plates embedded in water or concrete, hybrid methods are still insufficiently accurate.

In this work, a new method for generating variance reduction parameters for strongly anisotropic, deep-penetration radiation shielding studies was developed. This method generates an alternate form of the adjoint scalar flux quantity, $\phi^{\dagger}_{\Omega}$, which is used by both CADIS and FW-CADIS to generate variance reduction parameters for local and global response functions, respectively. The new method, called CADIS-Ω, was implemented in the Denovo/ADVANTG software. Results indicate that the flux generated by CADIS-Ω incorporates localized angular anisotropies in the flux more effectively than standard methods. CADIS-Ω outperformed CADIS in several test problems. This initial work indicates that CADIS-Ω may be highly useful for shielding problems with strong angular anisotropies. This is a benefit to the public by increasing accuracy for lower computational effort for many problems that have energy, security, and economic importance.

2. Accomplishments

The main accomplishments in this project have been

- Completion of method implementation as well as testing and documentation. The method is available in software that can be obtained through RSICC.
- All small test problems were constructed and executed with all versions of the software.
- Our large spent fuel shielding cask computational model was completed in two code formats and shared with ORNL for use.
- Publication of our first initial results in a peer-reviewed conference, PHYSOR: `http://munkm.github.io/papers/munk_physor16.pdf`
- Established a set of anisotropy metrics and used them to quantify performance.
- Developed a suite of scripts to facilitate test execution and results plotting, as documented here: `https://github.com/munkm/thesiscode`.
- Completion of the PhD of Dr. Madicken Munk [1].
- Adoption of the developed method for use in other research projects.

We accomplished nearly all of the goals outlined in the project. We have yet to complete the full-scale cask model analysis. Two students are conducting these calculations now. One journal article is in preparation that documents the results from Dr. Munk's dissertation. A second journal article will be published that includes the full cask model results. Thus, all work originally proposed in the project will be completed.

3. Project Activities

In this project, we developed a variance reduction method for computational neutral particle transport to improve the ability to design and operate systems in which particle streaming is important, such as monitoring systems for interim used fuel installations. We implemented the method in Exnihilo [2], MCNP [3], and ADVANTG [4], which makes our new tool widely available and easily usable. These innovative analysis tools will enable next generation nuclear material management for existing and future U.S. nuclear fuel cycles, minimizing proliferation and terrorism risk.

Storage casks are particularly challenging for radiation transport calculations because they are characterized by dense shields followed by streaming paths to the detectors. The impact of streaming is amplified in arrays of casks because detectors can only see rear casks through air paths between front casks. Deterministic methods suffer from ray effects between the casks and detectors, making solutions unreliable. Monte Carlo methods are challenged by getting particles out of the cask into the region of interest, and can therefore require unreasonably large calculation times to achieve acceptable statistical uncertainties in the computed tallies.

This report describes current technology in subsection 3.1 and the mathematics of our new method in subsection 3.2. This is followed by a short overview of the results and outcomes from this work in subsection 3.3. Full details and all results can be found in Reference [1].

3.1. Original Technology

Cutting-edge variance reduction methods that speed up Monte Carlo calculations often use deterministic solutions to make weight window maps. Perhaps the most widespread and accessible of these methods are the Consistent Adjoint Driven Importance Sampling (CADIS) [5–7] and Forward-Weighted CADIS (FW-CADIS) [8–10] methods. These methods create consistently-biased source distributions and weight window targets using a coarse determinstic solution for the adjoint scalar flux, $\phi^\dagger$, as a measure of the importance.

In general, we are interested in finding some response, R, characterized by some response function $f(\mathbf{r}, E)$ in some volume V_f:

$$R = \int_E \int_{V_f} f(\mathbf{r}, E)\phi(\mathbf{r}, E) dV dE \; , \tag{1}$$

where $\phi(\mathbf{r}, E)$ is the forward scalar flux, which describes how neutrons flow from the source $q(\mathbf{r}, E)$ to contribute to the response. Note that the adjoint scalar flux, $\phi^\dagger(\mathbf{r}, E)$, represents how each part of phase space contributes to the adjoint "source" ($q^\dagger(\mathbf{r}, E)$, which can be set as the response of interest). Thus, $\phi^\dagger$ represents the expected contribution of a source particle to the desired response.

With this in mind, we can create variance reduction parameters for use in MC. We coarsely and quickly perform a deterministic calculation to get $\phi^\dagger(\mathbf{r}, E)$. Equations (2) describe the biasing parameters generated by CADIS and FW-CADIS (jointly referred to as FW/CADIS).

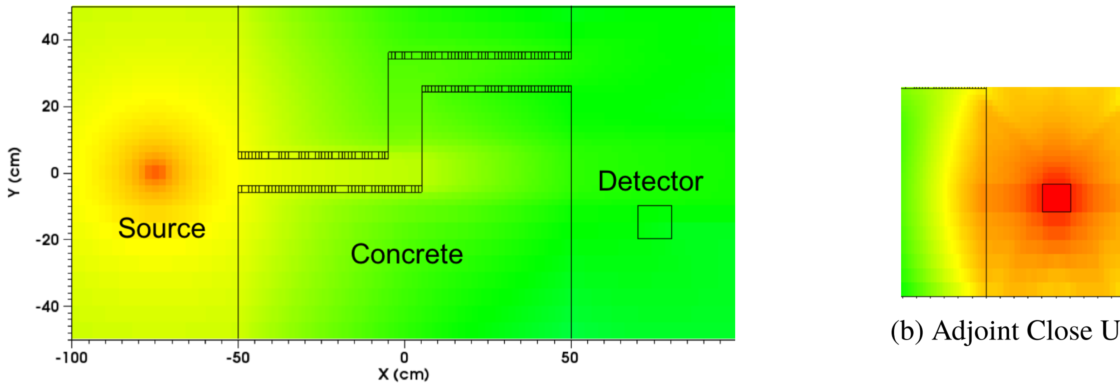
$$\hat{q}(\vec{r}, E) = \frac{\phi^\dagger(\vec{r}, E) q(\vec{r}, E)}{\iint \phi^\dagger(\vec{r}, E) q(\vec{r}, E) dE d\vec{r}} = \frac{\phi^\dagger(\vec{r}, E) q(\vec{r}, E)}{R} \; , \tag{2a}$$

$$w_0(\vec{r}, E) = \frac{q}{\hat{q}} = \frac{R}{\phi^\dagger(\vec{r}, E)} \; , \tag{2b}$$

$$\hat{w}(\vec{r}, E) = \frac{R}{\phi^\dagger(\vec{r}, E)} \; , \tag{2c}$$

where $\hat{q}$ is the biased source distribution, w_0 is the starting weight of the particles, $\hat{w}$ is the target weight of the particles, and R is the response of interest. For the standard implementations, these items are a function of space and energy only.

For problems with strong anisotropies in the particle flux, the importance map and biased source developed using the space/energy treatment above may not represent the real importance well enough to



(a) Forward Flux

(b) Adjoint Close Up

Figure 1: Concrete Maze with 10 MeV isotropic point source and NaI detector

sufficiently improve performance in the Monte Carlo calculation. Note that because the *scalar* adjoint flux is used in Eqns. (2), the angular dependence of the importance function is not retained. Thus, no information is retained on how particles move towards the response function. The drawback of this simplification is that, within a given space/energy cell, the map provides the average importance of a particle moving in *any direction* through the cell—excluding information about how particles move *toward* the objective. However, if the angular dependence of the importance function were fully retained, the map would be very large (tens or hundreds of GB) and more costly to use in the Monte Carlo simulation.

An example of missing important angular behavior can be seen in this maze problem. A 10 MeV isotropic point source is next to a concrete maze followed by an NaI detector. This problem has vacuum boundary conditions. In Figure 1a one can see the geometry and forward flux. Figure 1b shows the adjoint flux. We can see that (a) this is representing how areas of phase space contribute to the solution and (b) that no angular information is being captured. In a vacuum system, particles that exit the back of the geometry should not affect the detector. This behavior is being missed by the standard method, and thus not speeding up MC as well as it could.

Interim used fuel installations exhibit strong angular anisotropies, and therefore the ability to simulate them effectively for nuclear material management is limited with current tools. This led us to develop a new method, which we're calling the FW/CADIS-Ω method. In MC without performance improvement, relative error (Re) decreases as the square of time (t). Thus, we measure improving a calculation by using the Figure of Merit (FOM):

$$\text{FOM} = \frac{1}{Re^2 t} \,. \tag{3}$$

?

3.2. CADIS-Ω

To do fast, accurate transport for used fuel monitoring, we need an importance map generated quickly using deterministic methods that captures the impact of angle in the importance information. In this work we build on past methods, but calculate the adjoint scalar flux in a way that has not been done before.

Our new automated hybrid method, which we're calling FW/CADIS-Ω, incorporates angular information into the biasing parameters for FW/CADIS while not explicitly biasing in angle. That is, we generate space- and energy-dependent importance maps that incorporate the flux anisotropy in a more effective way than current implementations without adding the complication of angular weight windows. FW/CADIS-Ω uses Eqns. (2), but generates the adjoint scalar flux differently.

We use the idea of the contributon flux, defined in Eqn. (4), in generating the adjoint scalar flux. Contributons are pseudo-particles that carry "response" from the radiation source to a detector [11–13].

$$\Psi(\vec{r},\ \hat{\Omega}, E) = \psi^{\dagger}(\vec{r},\ \hat{\Omega}, E)\psi(\vec{r},\ \hat{\Omega}, E) \tag{4}$$

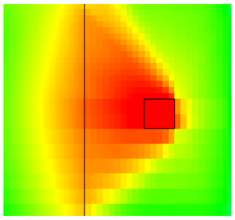
The contributon flux includes both forward and adjoint information, expressing the importance of a particle that is born at a forward source and moves through space towards an adjoint source, contributing to the solution. An importance map made using contributon flux will assign high importance to particles that are created at the forward source and are likely to generate a response in the detector.

In FW/CADIS-Ω, we integrate the contributon flux over angle and divide by the integrated forward angular flux as shown in Eqn. (5). This quantity, which we designate $\phi^{\dagger}_{\Omega}$, is then used in Eqns. (2), just like the standard FW/CADIS methods.

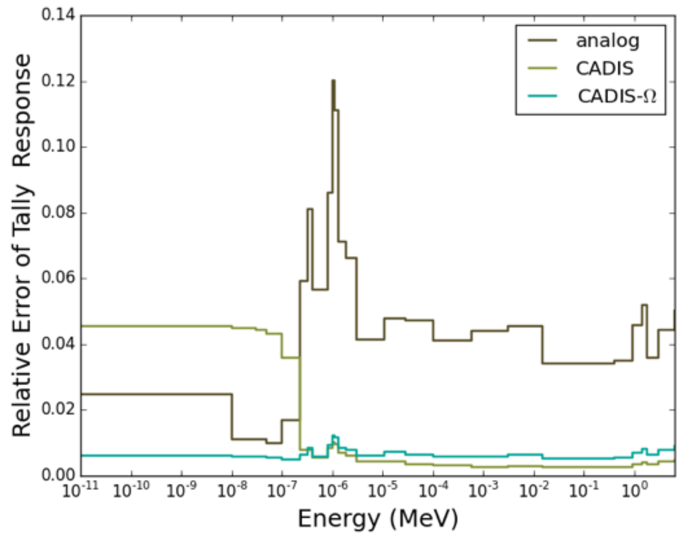
$$\phi^{\dagger}_{\Omega}(\vec{r}, E) = \frac{\int_{4\pi} \psi(\vec{r}, E, \hat{\Omega})\psi^{\dagger}(\vec{r}, E, \hat{\Omega})d\hat{\Omega}}{\int_{4\pi} \psi(\vec{r}, E, \hat{\Omega})d\hat{\Omega}} \tag{5}$$

In a strongly anisotropic system, the adjoint scalar flux generated by Eqn. (5) will be influenced by which directions were most prominent in the forward case. We can see this by considering the contributon flux, the numerator of Eqn. (5). Particles in $\phi^{\dagger}_{\Omega}$ include the impact of how the direction they are moving influences the answer, which should allow for more effective Monte Carlo transport when angular effects are important. Note that in an isotropic system, $\phi^{\dagger}_{\Omega}$ will be essentially the same as $\phi^{\dagger}$.

We can see the impact of this newly-defined adjoint flux by looking at the maze problem from Figure 2. Figure 2a shows a close up of the adjoint flux from our new method. In this case it is clear that particles going out the back of the problem are not expected to contribute to the detector. This is the kind of result that makes sense, and demonstrates the appropriate incorporation of angular information. Furthermore, we see in Figure 2b that this is reflected in CADIS-Ω obtaining a lower relative error than either CADIS or analog MC for the same number of particles. Finally, CADIS-Ω obtained a FOM



(a) New Method Adjoint Close Up



(b) Relative Error for Analog, CADIS, and CADIS-Ω

Figure 2: Concrete Maze Comparison

of 145, while CADIS's was only 5.1. This illustrates the type of improvement this project can achieve.

One of the additionally useful items developed in this work is a collection of metrics to characterize anisotropy. Each metric can be used to help us characterize how our method preforms for what types of problems:

- Scalar Contributon Ratio: If the adjoint or forward angular flux is significantly peaked in $\hat{\Omega}$, this will result in a deviation between the numerator and denominator because there will be a multiplicative effect in the angular flux captured in Φ_c and not ϕ_c.

$$M_1 = \frac{\phi^\dagger(\vec{r}, E)\phi(\vec{r}, E)}{\int_{\hat{\Omega}} \psi^\dagger(\vec{r}, \hat{\Omega}, E)\psi(\vec{r}, \hat{\Omega}, E)} = \frac{\phi_c}{\Phi_c}$$

- Adjoint Flux Ratio: metric for comparing which regions have significantly differing bias parameters in standard-adjoint and omega-adjoint situations. This metric will deviate from unity if the forward flux is anisotropic.

$$M_2 = \frac{\phi^\dagger_{\hat{\Omega}}(\vec{r}, E)}{\phi^\dagger(\vec{r}, E)}$$

- Maximum to Average Flux Ratios: the ratio between the maximum and average angular contributon flux in each space-energy voxel. The higher this quantity, the more peaked the contributon flux is in Ω.

$$\psi^c = \psi^\dagger(\vec{r}, E, \hat{\Omega})\psi(\vec{r}, E, \hat{\Omega})$$
$$M_3 = \frac{\psi^c_{\text{max}}}{\psi^c_{\text{avg}}}$$
$$M_4 = \frac{\frac{\psi^c_{\text{max}}}{\psi^c_{\text{avg}}}}{\frac{\psi^\dagger_{\text{max}}}{\psi^\dagger_{\text{avg}}}}$$

- Maximum to Minimum Flux Ratios: this quantity incorporates information about the behavior of the local maximum relative to the local minimum angular flux in each cell. This metric may be more appropriate to describe the anisotropy of the flux in cells where the distribution of flux values are not well reflected by the average flux.

$$M_5 = \frac{\psi^c_{\text{max}}}{\psi^c_{\text{min}}}$$
$$M_4 = \frac{\frac{\psi^c_{\text{max}}}{\psi^c_{\text{min}}}}{\frac{\psi^\dagger_{\text{max}}}{\psi^\dagger_{\text{min}}}}$$

We used the Figure of Merit as well as these metrics to study a large number of test problems.

3.3. Results and Outcomes

The flux can have anisotropy resulting from more than one mechanism. We have identified several separate processes that affect the flux anisotropy. These processes can be grouped into three categories that can overlap in one problem:

- anisotropy in the flux resulting from strongly directional sources,
- anisotropy resulting from strong differences between material properties (this can be due to differences in materials spatially or due to changes in interaction probabilities as a function of energy),
- anisotropy in the flux from algorithmic limitations (ray effects).

There are four primary physical mechanisms by which the flux may be anisotropic: streaming paths, problems with high scattering effects, problems with high material heterogeneity (specifically with materials with strong differences in scattering and absorption probabilities), and problems with monodirectional sources. We created a set of test problems to investigate the new method's performance in all of these areas.

The labyrinth problems have isotropic point sources on the left hand side of the problem emitting a Watt spectrum of neutrons approximating the energy spectrum emitted by that of ^{235}U fission. On the right hand side of the problem there is a NaI detector recording the flux. They are composed of a concrete maze with an air channel through the maze, and then open air channels at either end of the channels. These problems are likely to have ray effects in the air region near the forward source. These problems have strong differences in interaction probabilities between the air and the concrete, thus they will have material heterogeneity. Further, because the concrete is composed of several lighter-mass elements, these will also be highly scattering.

A steel beam embedded in concrete with a NaI detector located on the right hand side of the problem was another challenge problem. Because the particles have preferential flow through the steel and not the concrete, this is functionally a tough streaming problem.

We also used a problem containing rebar in concrete with steel rebar running through the concrete in different directions. In this problem, a NaI detector is used to measure the response on the right hand side of the problem in yellow. The source is both space- and energy-dependent, emitting a Watt spectrum of neutrons characteristic of ^{235}U fission, and is distributed in a 100x160 centimeter plate on the left hand side of the problem. The source is monodirectional in $+x$. This problem will have angular dependence, but preferential flowpaths through the concrete are not directed towards the detector location on the other side of the shielding in some of the rebar. This problem has material heterogeneity both in the concrete and between the concrete and air. This problem is highly scattering from the concrete, and is unlikely to have ray effects without a strong single preferential flowpath through the shield.

Finally, a small application problem relevant to the interests of this project is a radiotherapy room that has concrete walls, a water-based phantom that is being irradiated by a monodirectional source in the room, and a hallway where a therapy technician might walk. Because this problem is primarily air with concrete borders, it will have strong streaming effects in the air. Because of the high fraction of air in this problem, we also anticipate ray effects to occur. While there will be scattering in this problem, it will not be as strong of an effect as other characterization problems.

The performance of CADIS-Ω was characterized and compared against CADIS and a standard, non-biased analog Monte Carlo run for a series of problems. We found that CADIS-Ω does not outperform CADIS for all problems containing anisotropy in the flux. Depending on how and where the flux anisotropy was induced in the problem, CADIS-Ω had the potential to significantly increase the FOM in Monte Carlo. These results were not consistent, and are not entirely predictable.

In comparing the single turn and multiple turn labyrinths, it was observed that more scattering effects decrease the effectiveness of CADIS-Ω. Because more scattering is required to penetrate the multiple turn labyrinth, the performance of CADIS-Ω was poorer. In the single turn labyrinth energy bins that had more isotropy in the flux induced by scattering also were poorer performing for CADIS-Ω.

To add to this complexity, problems with little or no scattering were also difficult for CADIS-Ω to handle. These problems were also problematic for CADIS, as they were generally comprised of "thin" materials to induce streaming effects. As a result, sampling events occurred over several centimeters, which also was over several orders of magnitude in flux change. This resulted in very high relative errors, as observed in the beam facility problem. This was not as problematic in the therapy room example because the problem was bounded by 10 cm of concrete, which allowed for particle scattering rather than leakage.

Several material variants of the steel beam in concrete problem were run. The results of this small study confirmed that both CADIS and CADIS-Ω obtain poorer FOMs with air than with steel or concrete. In the case of the air variant, the FOMs obtained by CADIS-Ω were generally lower than CADIS, but the relative errors were also better. For all material variants of the steel beam problem, CADIS and CADIS-Ω achieved superior FOMs to the nonbiased analog, but these were an order of magnitude lower for the air variant.

The rebar-embedded concrete problem showed that for problems with geometric complexity, CADIS-Ω can also struggle. Because the rebar in this problem was not always directed in line with the detector tally, particles could more freely move perpendicular to the tally path, crossing out of importance with a preferential flowpath. As a result, in high energy bins the tally relative error was very high for both CADIS and CADIS-Ω. However, CADIS-Ω's performance was poorer. The FOMs obtained by CADIS-Ω in this problem were one to two orders of magnitude smaller than CADIS or the nonbiased analog.

CADIS-Ω achieved lower relative errors than CADIS for many problems, but often this was offset by a very long runtime. The long runtime impacted the FOM. As a result, even though CADIS-Ω achieves a lower relative error for the same particle count, it may be more advantageous to simply run standard CADIS for longer. In a few instances, the runtime for CADIS-Ω is comparable to CADIS. This occurs in the beam and therapy room problems, for example. Although these problems are not the best for either CADIS or CADIS-Ω, there is no caveat to using CADIS-Ω if choosing a hybrid method.

The characterization problems' variations in material and geometric configuration showed that there is no distinct behavior for which CADIS-Ω is universally better. However, in problem geometries where preferential flowpaths are directed towards the tally detector, and where materials provide short mean free paths to interaction or resampling sites, CADIS-Ω is a well-suited method.

The angle-based parametric study provided a number of interesting observations on the performance of the Ω methods. First, the effect of T_{det} does not change the FOM with CADIS-Ω more than CADIS. The hypothesis that I/O requirements would severely impact the FOM for CADIS-Ω was shown to be lower than hypothesized. The FOM change between FOM_{MC} and FOM_{hybrid} was roughly the same for CADIS as CADIS-Ω because the CADIS-Ω runtimes are so much longer than CADIS.

Next, the only consistent region in which CADIS-Ω outperforms CADIS is in high energies. For almost all P_N orders and all quadrature orders, CADIS-Ω achieved lower relative errors and higher FOMs than CADIS. In high energy bins, increasing quadrature order showed a decrease in I_RE, increasing P_N

order did not show a large change in I_RE. In the same bins, I_{FOM} values above unity were observed for both P_N and S_N order, but no trends with changing parameter value were observed.

By including the runtime to calculate the FOM, the comparative performance of CADIS-Ω dropped when compared to using the relative error. Several energy bins in CADIS-Ω–for quadrature orders and P_N orders–achieved better FOMs than CADIS. However no P_N order consistently outperformed the other, while low S_N orders generally achieved better FOMS for CADIS-Ω than CADIS. However, despite the lack of consistent performance for a single P_N order, the raw values obtained with P_N order are promising. With P_N order there were more energy bins that had high I_{FOM} values than with quadrature order.

Another observation was that CADIS-Ω consistently biases particles better than CADIS. For the same number of source particles, CADIS-Ω achieves lower relative error than CADIS for most energy bins with both P_N order and quadrature order. This means that while sampling may be slow, the importance map generated with the Ω flux is generally better at moving particles to the tally region than CADIS.

Based on the results, a number of recommendations can be made based on deterministic solver choice. First, the best P_N order choice is dependent on the energy range in which one is tallying. For low energy regions, P_N order 1 will give the best FOMs relative to CADIS, for intermediate energies P_N 3 is a better choice, and for high energies any P_N order is satisfactory. In general, because lower P_N orders have lower runtimes, these will get the best results for CADIS-Ω the fastest, and have comparatively the best relative errors and FOMs against CADIS. Next, the best S_N order choice is

If one has to choose between varying P_N order and S_N order to improve the importance map for their method, varying S_N order will have a greater impact. This is the case for using either CADIS or CADIS-Ω. However, both methods have a turnarount point at which increasing S_N order does not improve the relative error enough to offset the time increase of the method. For CADIS-Ω, this occurs in bins above S_N 15, and for CADIS it occurs in bins aboe S_N 12. For this type of problem, and using all energy bins in the tally, CADIS-Ω will obtain the best results with a lower P_N order and intermediate S_N orders.

The characterization problems that were run were heavily biased towards low-density streaming to induce anisotropy in the flux. This subset of problems, though highly anisotropic, are not the best for a method so dependent on weight-window type biasing, because particle streaming allowed for particles to cross several orders of magnitude in the flux before re-sampling. This meant that in a high-importance region a particle may split many thousands of times in a new splitting event. Unfortunately, the Ω-methods are not immune to this issue and so suffered the same effects as CADIS, even with positive effects like the reduction of ray effects. Further, with the strong dependence on angle, the Ω-fluxes may have exacerbated this streaming-sampling effect in regions with strong angular dependence around the detector. In a problem like the single turn labyrinth, where the Ω-flux generated a strong line of importance between the exit of the labyrinth and the detector and drastically dropped the importance behind the detector, a particle has much more opportunity to cross several orders of magnitude of importance than it does in CADIS. This is likely what caused CADIS-Ω to take longer in Monte Carlo transport than CADIS in many of the characterization problems.

It should also be noted that while the angle-dependent parametric study revealed how P_N order and quadrature order may affect a problem's results, the best parameter choices for this problem are by no means a prescriptive solution for other problems. Different the characterization problems' results were, depending on the source definition, the material composition of the problem, and the geometric configuration of the problem. Using the deterministic parameter choices that appear the best for the steel beam in concrete may not be the best for, say, a multi-turn labyrinth. From this study we have a good starting point from which to further characterize the method for other application problems.

4. Products

Publications:

- PHYSOR 2016 paper, "FW/CADIS-Ω: AN ANGLE-INFORMED HYBRID METHOD FOR DEEP-PENETRATION RADIATION TRANSPORT" can be found at `http://munkm.github.io/papers/munk_physor16.pdf`
- Madicken Munk's dissertation, "FW/CADIS-Ω: An Angle-Informed Hybrid Method for Neutron Transport", can be found at `http://github.com/munkm/dissertation/thesis.pdf` [1]

Website:

- The GitHub respository that contains code use information, brainstorming, publicly-available details about the cask, process development, and citations `https://github.com/munkm/caskmodels`
- We also have a repository with scripts and plotting tools: `https://github.com/munkm/thesiscode`

Networks or collaborations:

- We have grown the collaboration between ORNL and UCB, with Dr. Munk spending a few months at ORNL learning the codes and building our network.
- The work that we did in this project has formed a tool being used in a new project funded by the DOE-NE NEUP program. The new project is studying reprocessing facilities and is formally in collaboration with Southern Company and informally with Sandia National Laboratory.
- Ms. Vanessa Goss and Ms. Emily Vu are continuing analysis work with the software developed in this project. Ms. Goss will spend the summer at ORNL; Ms. Vu will spend the summer at SNL.
- Ms. Kelly Rowland is completing a PhD developing a related method that is useful for similar problem types.

Technologies or Techniques: As described in the proposal, the new method is our main technique.

Other products:

- The full cask model we created in both SCALE and MCNP formats has been contributed back to ORNL for use by the wider community.
- The new method has been implemented in software (Exnihilo / ADVANTG) that is available through RSICC, so this product is also available to others.

5. Computer Modeling

The details related to computer modeling are included in the Project Activities description and the referenced publications:

- Model description, key assumptions, version, source and intended use;
- Performance criteria for the model related to the intended use;
- Test results to demonstrate the model performance criteria were met (e.g., code verification/validation, sensitivity analyses, history matching with lab or field data, as appropriate);
- Theory behind the model, expressed in nonâĂŘmathematical terms;
- Mathematics to be used, including formulas and calculation methods;
- Whether or not the theory and mathematical algorithms were peer reviewed, and, if so, include a summary of theoretical strengths and weaknesses;
- Hardware requirements; and
- Documentation (e.g., user guide, model code).

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