Working Title: Monte Carlo Analysis of Dynamic Systems

by

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Abstract

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Eloquent summary of my work.

1 INTRODUCTION

The successful completion of this project will provide the workflow and tools necessary to efficiently calculate quantities of interest resulting from coupled, multi-physics processes in dynamic systems. Â The MC physics code will be modified to implement rigid-body transformations on the CAD-based geometry. MS-CADIS, a VR method for coupled, multi-physics problems, will be adapted to incorporate dynamics. Â An experiment will be contrived to demonstrate the limitations of existing VR methods as they apply to dynamic problems and verify the efficacy of this new method. Â Given these objectives, the following chapters will include background and theory relevant to VR methods in coupled, multi-physics systems. Â Chapter no. will provide an introduction to computational radiation transport and specifically the VR methods used in MC calculations. Â Chapter no. will discuss SDR analysis and the VR methods specific to these calculations. Â Chapter no. will introduce radiation transport in dynamic systems, discuss how they are handled now and how motion affects VR in coupled multi-physics problems like SDR calculations. Â Finally, chapter no. will discuss the progress that has been made towards this new methodology and outline a proposal of the work to be done.

The rapid design iteration process of complex nuclear systems has long been aided by the use of computational simulation. Traditionally, these simulations involve radiation transport in static geometries. However, in certain scenarios, it is desirable to investigate dynamic systems and the effects caused by the motion of one or more components. For example, Fusion Energy Systems (FES) are purposefully designed with modular components that can be moved in and out of a facility after shutdown for maintenance. To ensure the safety of maintenance personnel, it is important to accurately quantify the shutdown dose rate (SDR) caused by the gammas emitted by structural materials that became activated during the device operation time. This type of analysis requires neutron transport to determine the neutron flux, activation calculation to determine the isotopic inventory, and finally a photon transport calculation to determine the SDR. While MC calculations are revered to be the most accurate method for simulating radiation transport, the computational expense of obtaining low error results in systems with heavy shielding can be prohibitive. However there are techniques, known as variance reduction (VR) methods, that can be used to increase the computational efficiency. There are several types of VR methods, but the basic theory is to artificially increase the simulation of events that will contribute to the quantity of interest such as flux or dose rate. One class of VR techniques relies upon a deterministic estimate of the adjoint solution of the transport equation to formulate biasing parameters used in the MC transport. The adjoint flux has physical significance as the importance of a region of phase space to the objective function.

The purpose of this work is to create a methodology for the efficient calculation of quantities of interest in dynamic, geometrically complex nuclear systems. For cases involving coupled multi-physics analysis, such as SDR calculations, a new hybrid deterministic/MC VR technique will be proposed. This new method will adapt the Multi-Step Consistent Adjoint Driven Importance Sampling (MS-CADIS) method to dynamic systems. The basis of MS-CADIS is that the importance function used in each step of the problem must represent the importance of the particles to the final objective function. As the spatial configuration of the materials changes, the probability that they will contribute to the objective function also changes. In the specific case of SDR calculations, the importance function for the neutron transport step must capture the probability of materials to become activated and subsequently emit photons that will make a significant contribution to the SDR. This new VR method will also take advantage of the Groupwise Transmutation (GT)-CADIS method which is an implementation of MS-CADIS that optimizes the neutron transport step of SDR calculations. GT-CADIS generates an adjoint neutron source based on certain assumptions and approximations about the transmutation network. To adapt this method for dynamic systems, the adjoint neutron source will be calculated at each time step and then averaged in order to generate the biasing functions for the neutron transport step.

2 LITERATURE REVIEW

2.1 SDR calculations

Shutdown dose rate (SDR) calculations are necessary to quantify the potential dose to personnel working in facilities exposed to intense radiation fields like fusion energy systems (FES). The dose rate is caused by decay photons that are emitted by materials irradiated by neutrons. Therefore, these calculations involve a neutron transport step, then an activation analysis to determine the decay photon spectrum for a specific irradiation and decay scenario, and finally a photon transport step to determine the dose rate. One methodology for calculating the SDR is known as the Rigorous Two Step (R2S) method. This method relies on a MC code for both neutron and photon transport and a nuclear inventory code for activation analysis. The goal of the neutron transport step is to determine the neutron flux discretized by space and energy. This neutron flux along with an irradiation and decay scenario of interest are used as input into a nuclear inventory code. This code will give the photon flux as a function of decay time which is then used as the source for the photon transport step. A photon flux tally fitted with flux-to-dose-rate conversion factors is used during this step to determine the final SDR [4].

2.2 Analog Monte Carlo Calculations

To quantify the dose rate, we need to know the flux of photons produced by the decaying radionuclides in the activated components. The activation is caused by neutron irradiation. We need to know what the neutron flux looks like in every region of phase space.

We need a detailed distribution of the neutron flux throughout all regions of phase space. The neutron distribution along with and irradiation and decay scheme of interest can then be input for a nuclear inventory code to generate the photon emission density. This photon emission density is used as a source for the photon transport step which ultimately produces the photon flux in every region. The photon flux coupled with a flux-to-dose-rate conversion factor will give us the dose rate.

There are two ways to solve the Boltzmann transport equation: deterministically and stochastically. The most optimal way to perform accurate, full-scale analysis of FES is through Monte Carlo radiation transport *need source*. In general, Monte Carlo (MC) calculations rely on repeated, random sampling to solve mathematical problems. The MC method can be applied to radiation transport by solving the Boltzmann transport equation through the simulation of random particle walks through phase space. In analog operation mode (i.e. no variance reduction), the source particle's position, energy, direction and subsequent collisions are sampled from probability distribution functions (PDFs). Quantities of interest such as flux can be scored, or tallied, by averaging particle behavior in discrete regions of phase space.

Radiation transport simulations in geometries that have thick shielding, such as FES, become challenging for MC codes. The particles have lots of interactions (absorption and scattering) in the shielding regions. This results in low particle fluxes in these discrete regions of phase space.

The statistical error is a function of the relative error, R, which is defined as

$$R = \frac{S_{\overline{x}}}{\overline{x}} \tag{2.1}$$

where $\overline{x}$ is the average of the tally scores, and $S_{\overline{x}}$ is the standard deviation of the tally scores. For a well behaved tally, R is proportional to $1/\sqrt{N}$ where N is the number of tally scores [3].

To reliably predict results in these regions, many particle histories need to be simulated which may require large amounts of computer time [1].

MC calculation efficiency is measured by a quantity known as the figure of merit (FOM). The FOM is a function of relative error, R, and computer processing time, T, as given by

$$\mathrm{FOM} = \frac{1}{R^2 T} \tag{2.2}$$

It is desirable to have a high FOM because it means that less computation time is needed to achieve a reasonably low error, less than 0.1 according to the MCNP manual [3]. The relative error is inversely proportional to N. VR methods aim to increase the FOM by increasing N and decreasing $S_{\overline{x}}$ by sampling from biased PDFs; this effectively forces more collisions in regions of phase space that are important to the tally of interest.

2.3 VR Methods

Certain MC calculations require the use of variance reduction methods in order to complete or improve the efficiency of the calculation. This is accomplished by preferentially sampling trajectories that are likely to contribute to the tallies of interest. In order to compensate for this biased sampling, the particle statistical weight is adjusted accordingly. The relationship between the particle statistical weight, w, and the PDF that governs particle behavior is as follows

$$w_{\mathrm{biased}} \mathrm{pdf}_{\mathrm{biased}} = w_{\mathrm{unbiased}} \mathrm{pdf}_{\mathrm{unbiased}} \tag{2.3}$$

One of the earliest and still commonly used methods of VR is particle splitting and rouletting. This is particularly useful in deep penetration simulations, like FES. Generally speaking, to increase the number of particle histories that can contribute to tallies of interest, it is desirable to split particles as the enter more important regions and roulette particles as the enter less important regions. This requires assigning an importance, I, to every region in the geometry and adjusting the weight, w, of the new particles. When a particle moves from a region A to a region B, the ratio of importances is calculated. If region B is more important than region A such that $I_B/I_A \geqslant 1$, the particle with original weight w_0 is split into $n = I_B/I_A$ particles, each with weight w_0/n. If instead region B is less important than region A such that $I_B/I_A < 1$, the particle will undergo roulette. The particle will survive with a probability n and weight w_0/n [2]. The weight window method in MCNP utilizes both splitting and rouletting. A weight window is a region of phase-space that is assigned an upper and lower bound. The windows can be assigned to cells in the geometry, on a superimposed mesh, and to energy bins. When a particle enters a weight window, its weight is assessed; if its weight is above the upper bound or below the lower bound, it is either split or rouletted, respectively.

2.4 Automated VR Techniques

VR techniques require the user to have a priori knowledge of the problem physics in order to assign importance parameters. Many techniques have been developed over the years to automate the selection and assignment of these parameters to reduce the time and expertise required by the user.

One class of VR techniques, known as hybrid deterministic/MC methods, is based upon the solution to the adjoint Boltzmann transport equation having physical significance as the measure of importance of a particle to some specified objective function. Because deterministic solutions to the transport equation require much less computation time, they are useful as an estimate of particle flux throughout phase space which can then be used to determine importance of specific regions. To demonstrate the use of the adjoint solution as an importance function, we will first start with the linear, time-independent Boltzmann transport equation shown below

$$H\Psi = q \tag{2.4}$$

where Ψ is the angular flux, q is the source of particles, and the operator H is given by

$$H = \widehat{\Omega} \cdot \nabla + \sigma_t(\vec{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E' \to E, \widehat{\Omega}' \to \widehat{\Omega}) \tag{2.5}$$

where σ_t is the total cross-section and σ_s is the differential scattering cross-section. The adjoint identity states that

$$\langle \Psi^+, H\Psi \rangle = \langle \Psi, H^+\Psi^+ \rangle \tag{2.6}$$

where $\langle \cdot \rangle$ refers to the integration over space, energy, and angle and the adjoint operator H^+ is given by

$$H^+ = -\widehat{\Omega} \cdot \nabla + \sigma_t(\vec{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E \to E', \widehat{\Omega} \to \widehat{\Omega}') \tag{2.7}$$

The identity can also be written as

$$\langle \Psi^+, q \rangle = \langle \Psi, q^+ \rangle \tag{2.8}$$

As mentioned, the adjoint solution to the transport equation will be used as an importance function therefore we need to solve

$$H^+\Psi + = q^+ \tag{2.9}$$

which requires the thoughtful selection of an adjoint source q^+. To demonstrate the physical significance of the adjoint, we will consider the detector response, R

$$R = \langle \Psi, \sigma_d \rangle \tag{2.10}$$

where σ_d is a detector response function. If we choose the adjoint source to be equivalent to the detector response function,

$$q^+ = \sigma_d \tag{2.11}$$

and substitute this into Eq. 2.10 and Eq. 2.8

$$R = \langle \Psi, q^+ \rangle = \langle \Psi^+, q \rangle \tag{2.12}$$

the adjoint flux Ψ^+ represents the importance of a region to σ_d. This final relation allows us to know the response R for any source q once the adjoint flux Ψ^+ for a detector of interest is known.

The Consistent Adjoint Driven Importance Sampling (CADIS) method is one of the hybrid deterministic/MC VR techniques that uses the adjoint solution to formulate source and transport biasing parameters for MC transport. More specifically, CADIS determines the parameters for source biasing and the weight window lower bounds in a consistent manner. The response, or tally, of interest in a transport calculation can be represented by the following equation

$$R = \int_V d\overrightarrow{r} \int_E dE \int_{4\pi} d\widehat{\Omega} \sigma_d(\overrightarrow{r}, E, \widehat{\Omega}) \Psi(\overrightarrow{r}, E, \widehat{\Omega}) \tag{2.13}$$

and in terms of the adjoint flux,

$$R = \int_V d\overrightarrow{r} \int_E dE \int_{4\pi} d\widehat{\Omega} q(\overrightarrow{r}, E, \widehat{\Omega}) \Psi^+(\overrightarrow{r}, E, \widehat{\Omega}) \tag{2.14}$$

The MC solution of the response relies upon the sampling of the particle source distribution, $q(\overrightarrow{r}, E, \widehat{\Omega})$, represented by a PDF. In an effort to decrease the variance, it is possible to sample from a biased PDF which is given by

$$\widehat{q}(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{\Psi^+(\overrightarrow{r}, E, \widehat{\Omega}) q(\overrightarrow{r}, E, \widehat{\Omega})}{R} \tag{2.15}$$

This biased PDF represents the contribution of particles from phase-space $(\vec{r}, E, \hat{\Omega})$ to the total detector response, R. As previously mentioned, when sampling from a biased PDF, the particle weight needs to be adjusted to eliminate systematic bias.

$$w(\vec{r}, E, \hat{\Omega})\hat{q}(\vec{r}, E, \hat{\Omega}) = w_0 q(\vec{r}, E, \hat{\Omega}) \tag{2.16}$$

Substituting in Eq. 2.15, the corrected particle weight is shown to have an inverse relation to the adjoint flux, or importance function.

$$w(\vec{r}, E, \hat{\Omega}) = \frac{R}{\Psi^+(\vec{r}, E, \hat{\Omega})} \tag{2.17}$$

In the weight window technique, particles are either split or rouletted as they move from region to region based on the ratio of their importances and their weight is updated accordingly. The weights are used for both the source and transport biasing parameters and are derived in a consistent manner. The transport is biased according to the following relationship

$$w(\vec{r}, E, \hat{\Omega}) = w(\vec{r}\,', E', \hat{\Omega}') \left[\frac{\Psi^+(\vec{r}\,', E', \hat{\Omega}')}{\Psi^+(\vec{r}, E, \hat{\Omega})}\right] \tag{2.18}$$

The width of the weight windows is determined by a parameter defined to be the ratio between upper and lower bounds $\alpha = w_u/w_l$. MCNP uses a default value for α and the weight window lower bounds are given by

$$w_l(\vec{r}, E, \hat{\Omega}) = \frac{R}{\Psi^+(\vec{r}, E, \hat{\Omega})(\frac{\alpha+1}{2})} \tag{2.19}$$

2.5 Automated VR for SDR Calculations

There are two transport steps involved in SDR calculations; the initial neutron transport to simulate the irradiation and the subsequent photon transport simulating the decaying gammas. The full-scale simulations in large, complex FES models are very computationally expensive.

The R2S method applied to a full-scale, 3D FES becomes impractical due to the need for accurate space- and energy-dependent fluxes generated by MC codes throughout the geometry. Optimizing the photon transport step can be done through a straightforward application of the CADIS or FW-CADIS method *need source*. An adjoint transport calculation can be performed where the detector response function is set equal to the photon flux tally fitted with flux-to-dose-rate conversion factors and the resulting adjoint flux can be used as an importance function to determine source and transport biasing parameters *need source*. Optimizing the neutron transport step, however, is not as straightforward because the importance function needs to represent the importance of the neutrons to the final quantity of interest[5]. When applied to SDR calculations, the Multi-Step Consistent Adjoint Driven Importance Sampling (MS-CADIS) method aims to increase the efficiency of the neutron transport step using an importance function that captures the potential of regions to become activated and the importance of the resulting decay photons to the final SDR[5].

As shown before in Eq. *need eqn number*, the detector response can be expressed as the integral of the importance function, I, times the source distribution, q

$$R = \int_V \int_E I(\overrightarrow{r}, E) q(\overrightarrow{r}, E) dV dE \tag{2.20}$$

MS-CADIS provides a method to calculate an approximation of this importance function where the response is the final response of the multi-step process. In the case of an R2S calculation, the final response is the SDR caused by the decay photons. The SDR is defined as

$$SDR = \langle \sigma_d(\overrightarrow{r}, E_p), \phi_p(\overrightarrow{r}, E_p) \rangle \tag{2.21}$$

where σ_d is the flux-to-dose-rate conversion factor at the position of the detector and ϕ_p is photon flux. Consider Eq. 2.10 where it was shown that the response R is equal to the product of the flux and adjoint source. If equation 2.20 is taken to have the same form as Eq. 2.21, and the adjoint photon source is set equal to σ_d, the importance function, I, is defined as the solution of the adjoint transport equation, ϕ_p^+ leading to the following relationship

$$SDR = \langle q_p^+(\vec{r}, E_p), \phi_p(\vec{r}, E_p)\rangle = \langle q_p(\vec{r}, E_p), \phi_p^+(\vec{r}, E_p)\rangle \tag{2.22}$$

The goal of MS-CADIS is to develop an importance function that represents the importance of the neutrons to the final SDR, which is done by setting the neutron adjoint identity equal to the photon response in a relationship equivalent to that shown in 2.22

$$SDR = \langle q_n^+\vec{r}, E_n), \phi_n(\vec{r}, E_n)\rangle = \langle q_n\vec{r}, E_n), \phi_n^+(\vec{r}, E_n)\rangle \tag{2.23}$$

Combining these adjoint identities in Eq. 2.22 and 2.23, gives a relationship

$$\langle q_n^+(\vec{r}, E_n), \phi_n(\vec{r}, E_n)\rangle = \langle q_p(\vec{r}, E_p), \phi_p^+(\vec{r}, E_p)\rangle \tag{2.24}$$

In order to solve for the adjoint neutron source, q_n^+, an equation relating the photon source, q_p, to the neutron flux, ϕ_n, is needed. The decay photon source is a result of neutron irradiation and the two quantities can be related by the following definition:

$$q_p(\vec{r}, E_p) = \int_{E_n} T(\vec{r}, E_n, E_p)\phi_n(\vec{r}, E_n)dE_n \tag{2.25}$$

where $T(\vec{r}, E_n, E_p)$ is a quantity that represents the transmutation process. If an adequate T can be found, this photon source can be used to solve for the adjoint neutron source in Eq. 2.24.

$$q_n^+ \vec{r}, E_n) = \int_{E_p} T(\vec{r}, E_n, E_p)\phi_p^+(\vec{r}, E_p)dE_p \tag{2.26}$$

Concentrating on the photon source at a single point, Eq. 2.25 can be expressed as this non-linear function of ϕ_n

$$q_p(E_p) = \int_{E_n} f(\phi_n)dE_n \tag{2.27}$$

The full transmutation process is complex and would be tedious to capture. As the purpose of calculating T is only a step in calculating q_n^+ which will be used to generate our biasing parameters, an approximation of a linear relationship between q_p and ϕ_n will suffice.

2.6 Moving Systems

This section will discuss how systems that involve moving components are currently modeled. Historically, Monte Carlo analysis of dynamic systems is performed using a series of separate calculations with different input files that contain step-wise changes of the geometric position. The moving objects capability in MCNP6 allows for the motion of objects during a single simulation.

MCNP6 Moving Objects Capability

This new capability available in MCNP6 allows for rigid body transformations of objects including rectilinear translations and curvilinear translations and rotations. The objects can move with constant velocity, constant acceleration, or be relocated. Object kinetics are not treated so the user must use caution and supply transformations that will not cause objects to overlap. This capability is currently applicable to MCNP's native geometry format, constructive solid geometry (CSG) and is not available for mesh-based geometries *make sure this is true*.

Sources can also be assigned to moving objects, therefore can move with the same dynamics as other objects in the problem.

This capability also allows for the treatment of secondary particles emitted by objects in motion. The delayed particle's location, direction, energy, and time are stored at the time of fission or activation and then at the time of emission, the object's updated location and orientation are calculated to provide the correct location and orientation of the delayed particle emission at the time of emission.

Should reference presentation on FLUKA simulation w/ moving geom.

3 PROGRESS

3.1 DAGMC Simulations with Geometry Transformations

3.2 Demonstration of GT-CADIS

The GT-CADIS method has proven to be an effective form of VR for calculating the SDR in static FES where the SNILB criteria are met. As it stands, this method will not provide appropriate VR parameters for the cases where there is movement after shutdown. The follow experiment will demonstrate the need for a time-integrated coupling term in order to provide useful VR parameters for dynamic systems.

Problem Description

The geometry chosen is a simplified representation of a fusion energy device. It is composed of a chamber of stainless steel with a central cavity measuring 2m x 2m x 2 m. The walls are 2 m thick. The chamber is surrounded by air and there is helium in the central cavity. A uniform, volumetric source of 14 MeV neutrons was placed in the central cavity. First, the R2S workflow was performed in analog and then the GT-CADIS method was used to generate VR parameters to optimize the neutron transport step of R2S.

Figure 3.1: C

utaway view of the geometry.

Figure 3.2: N

eutron flux and relative error resulting from analog MC simulation.

Figure 3.3: P

hoton flux and relative error resulting from analog MC simulation.

Figure 3.4: A

djoint photon flux used to generate adjoint neutron source.

Results

Discussion

Figure 3.5: B

iased source generated with GT-CADIS method.

Figure 3.6: W

eight window mesh generated with GT-CADIS method.

Figure 3.7: N

eutron flux and relative error resulting from MC simulation using GT-CADIS biased source and weight window mesh.

Figure 3.8: P

hoton flux and relative error resulting from MC simulation using GT-CADIS biased source and weight window mesh.

4 PROPOSAL

4.1 Adapt MS-CADIS for Moving Geometries

The MS-CADIS method can be used to generate an adjoint neutron source that can be used to generate biasing parameters that will optimize the neutron transport step of a coupled, multi-step process. In previous studies *need ref*, this method has been shown to decrease the variance in the neutron transport step of the R2S workflow. These studies, however, have only involved static systems with the same geometry used for all transport steps. As seen in section *need number*, it was demonstrated that the variance reduction parameters generated with the GT-CADIS method are insufficient for optimizing the neutron transport step in cases that involve the movement of irradiated components after shutdown. The following section *need number* will discuss a proposed adaptation to the MS-CADIS method that will show the derivation of a time-integrated coupling term.

Generalized MS-CADIS Method

Time-integrated Coupling Term

Apply Time-integrated coupling to GT-CADIS

tet mesh n flux tally -tag tet mesh w transformations source.h5m for each decay time update position run transport

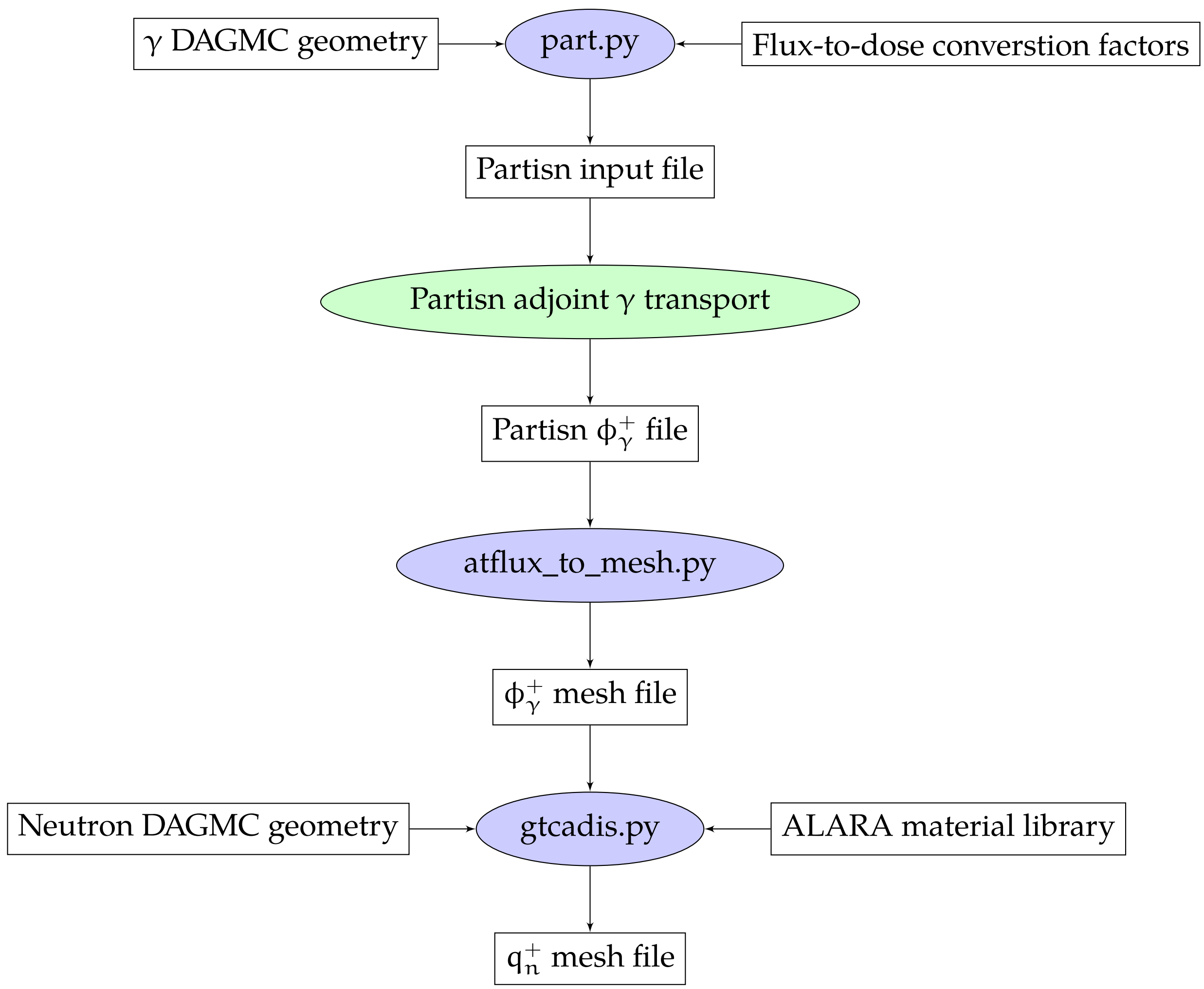

Figure 4.1: Workflow for generating the optimal adjoint neutron source via the GT-CADIS method. Scripts are shown in blue ovals, physics codes in green ovals, and files in white rectangles.

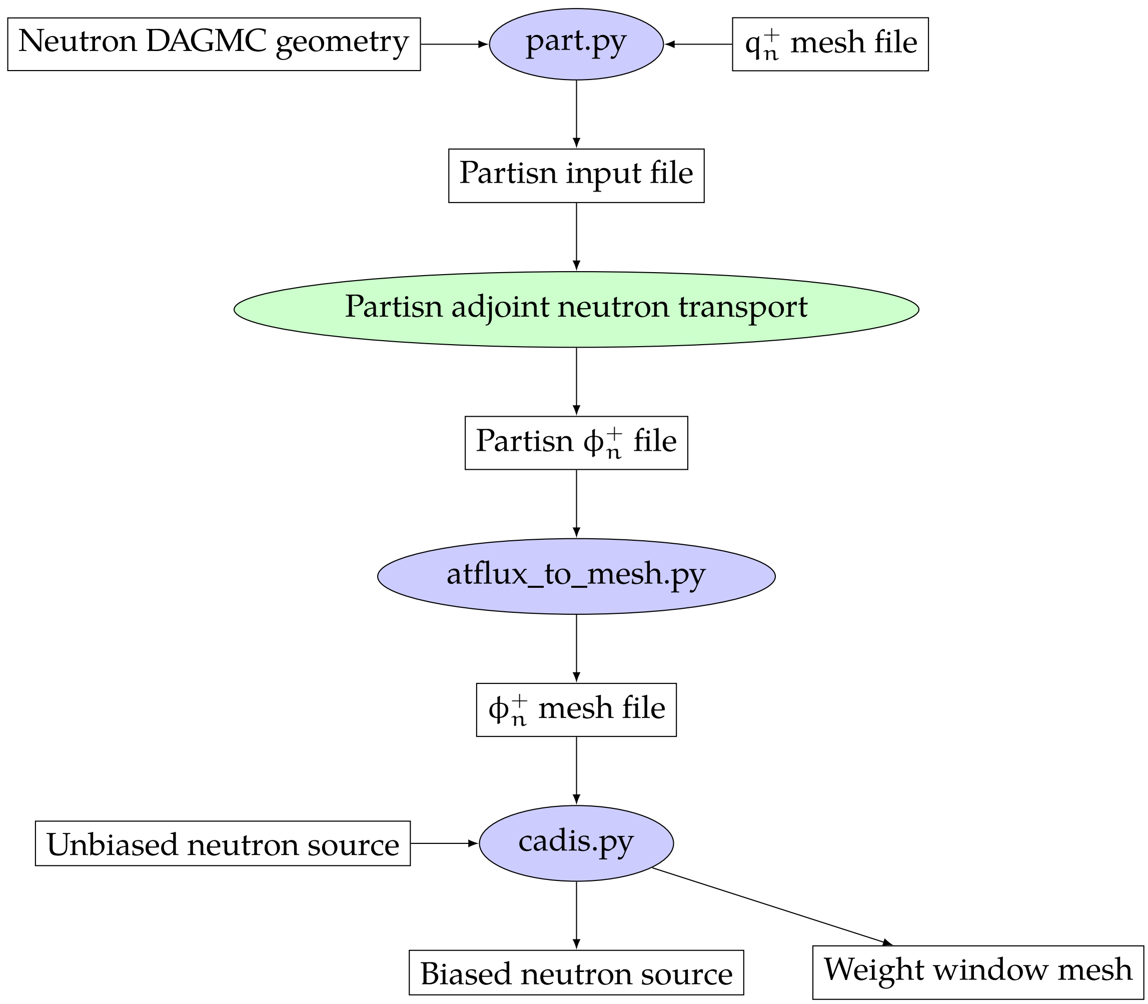

Figure 4.2: Workflow for generating a biased source and weight windows to optimize the neutron transport step. Scripts are shown in blue ovals, physics codes in green ovals, and files in white rectangles.

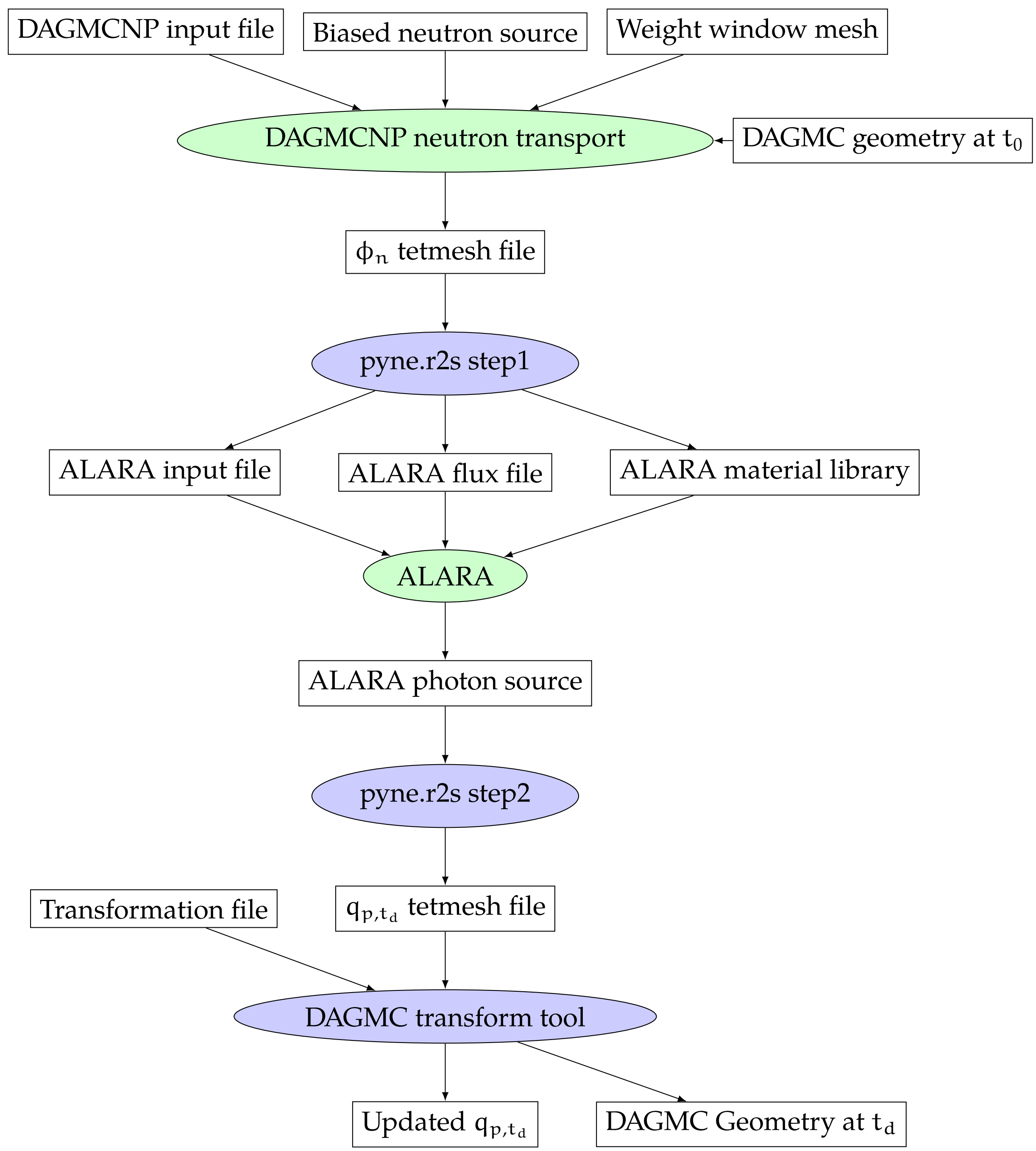

Figure 4.3: R2S workflow for calculating the SDR. This particular flow chart shows the use of a biased source and weight windows to optimize the neutron transport step. Scripts are shown in blue ovals, physics codes in green ovals, and files in white rectangles.

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