Variance Reduction for Multi-physics Analysis of Moving Systems

Chelsea D'Angelo

Preliminary Exam

Feb. 2, 2018



Introduction

Shutdown Dose Rate (SDR) Analysis



- Fusion Energy Systems (FES)
 - Burning plasma, D-T fusion
 - ${}_{1}^{2}H + {}_{1}^{3}H \rightarrow {}_{2}^{4}He + {}_{0}^{1}n$
- Neutrons penetrate deeply into system components, causing activation
- Radioisotopes persist long after shutdown
- Important to quantify the dose caused by decay photons

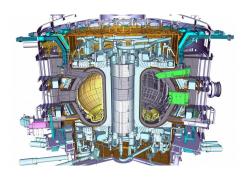
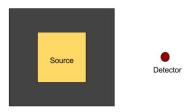


Figure: Cutaway view of ITER drawing.

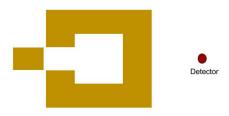


- FES are designed with modular components
 - Can move during maintenance procedure
- Interested in SDR at a particular location
- SDR will change as a function of the activated component's position over time





- FES are designed with modular components
 - Can move during maintenance procedure
- Interested in SDR at a particular location
- SDR will change as a function of the activated component's position over time



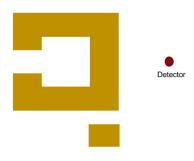


- FES are designed with modular components
 - Can move during maintenance procedure
- Interested in SDR at a particular location
- SDR will change as a function of the activated component's position over time





- FES are designed with modular components
 - Can move during maintenance procedure
- Interested in SDR at a particular location
- SDR will change as a function of the activated component's position over time





- FES are designed with modular components
 - Can move during maintenance procedure
- Interested in SDR at a particular location
- SDR will change as a function of the activated component's position over time



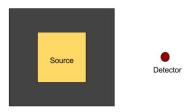


- FES are designed with modular components
 - Can move during maintenance procedure
- Interested in SDR at a particular location
- SDR will change as a function of the activated component's position over time





- FES are designed with modular components
 - Can move during maintenance procedure
- Interested in SDR at a particular location
- SDR will change as a function of the activated component's position over time



Goal



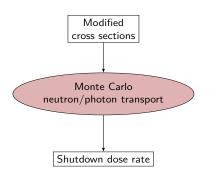
Optimize the calculation of the **shutdown dose rate** at a particular location as activated components are **moving** around the facility.

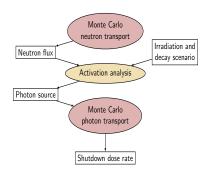
SDR Solution Methods



Direct 1-Step Method (D1S)

Rigorous 2-Step Method (R2S)





Monte Carlo Radiation Transport



- Monte Carlo (MC) analysis of FES is:
 - Accurate for large, complex models
 - Challenging due to the highly attenuating structural materials
 - Results scored in regions that have low particle flux, have higher statistical uncertainty

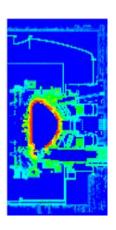


Figure: Photon source in ITER tokamak building.

Error in MC Calculations



(1)

• Uncertainty in MC calculations:

$$\Re = \frac{\sigma_{\overline{x}}}{\overline{x}}$$

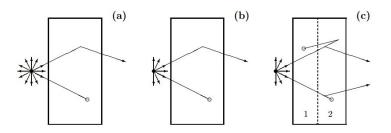
$$\sigma_{\overline{x}} \propto rac{1}{\sqrt{N}}$$

- To decrease statistical uncertainty:
 - Increase number of histories, N
 - Use variance reduction (VR) techniques

MC Variance Reduction Techniques



- Techniques to modify particle behavior
 - Goal: preferentially sample events that will contribute to results of interest
- Statistical weight of particles is adjusted to keep playing a fair game
- Types
 - Modified Sampling: source direction and energy biasing
 - Population Control: geometry and energy splitting/rouletting



Hybrid Deterministic/MC VR Methods



- Use **deterministic** estimate of the adjoint flux, Ψ^+ , to generate **Monte Carlo** VR parameters
- Adjoint flux can define the importance of regions of phase space to the detector response
- Define detector response function to be the adjoint source

Forward:

$$H\Psi(\overrightarrow{r}, E, \widehat{\Omega}) = q(\overrightarrow{r}, E, \widehat{\Omega})$$

$$H = \widehat{\Omega} \cdot \nabla + \sigma_t(\overrightarrow{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\overrightarrow{r}, E' \to E, \widehat{\Omega}' \to \widehat{\Omega})$$
(2)

Adjoint:

$$H^{+}\Psi^{+}(\overrightarrow{r},E,\widehat{\Omega})=q^{+}(\overrightarrow{r},E,\widehat{\Omega}) \tag{3}$$

$$H^{+} = -\widehat{\Omega} \cdot \nabla + \sigma_{t}(\overrightarrow{r}, E) - \int_{0}^{\infty} dE' \int_{4\pi} d\Omega' \sigma_{s}(\overrightarrow{r}, E \to E', \widehat{\Omega} \to \widehat{\Omega}')$$

Hybrid Deterministic/MC VR Methods: CADIS



Consistent Adjoint Driven Importance Sampling (CADIS)

- Use the adjoint flux, Ψ^+ , to generate MC source and transport biasing parameters
- Biased source:

$$\widehat{q}(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{\Psi^{+}(\overrightarrow{r}, E, \widehat{\Omega})q(\overrightarrow{r}, E, \widehat{\Omega})}{R}$$
(4)

• Weight window lower bounds:

$$w_{I}(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{R}{\Psi^{+}(\overrightarrow{r}, E, \widehat{\Omega})(\frac{\alpha+1}{2})}$$
 (5)

Variance Reduction for SDR Analysis



VR for **photon** transport

- Straightforward
- Can use CADIS method to direct photons towards detector
 - Flux-to-dose-rate conversion factors define adjoint source

VR for **neutron** transport

- More complicated
- Biasing function needs to capture
 - 1 Potential of regions to become activated
 - Potential to produce photons that will contribute to the SDR
- Can use CADIS if we can construct adjoint source that will fulfill these criteria

Variance Reduction for SDR Analysis: MS-CADIS



Multi-Step (MS)-CADIS

- VR method to optimize the initial radiation transport step of a coupled, multi-step process
 - Relies upon biasing function that represents importance of particles to final response of interest

Generalized MS-CADIS



• System of coupled, multi-physics:

$$Primary: H\phi(u) = q(u) \tag{6}$$

Secondary:
$$L\psi(v) = b(v)$$
 (7)

Adjoint identities:

$$\langle \phi^+, q \rangle = \langle \phi, q^+ \rangle \tag{8}$$

$$\langle \psi^+, b \rangle = \langle \psi, b^+ \rangle \tag{9}$$

 MS-CADIS requires a representation of the relationship between primary and secondary physics:

$$b(v) = \langle \sigma_b(u, v), \phi(u) \rangle \tag{10}$$

Generalized MS-CADIS



• Response to secondary physics:

$$R_{final} = \langle \omega_R(v), \psi(v) \rangle \tag{11}$$

• Set ω_R as adjoint source and invoke adjoint identity:

$$R_{final} = \langle \omega_R, \psi \rangle = \langle b, \psi_R^+ \rangle \tag{12}$$

• Substitute Eq. 10:

$$R_{final} = \langle \langle \sigma_b(u, v), \phi(u) \rangle, \ \psi_R^+(v) \rangle$$
 (13)

Generalized MS-CADIS



• Switch the order of integration

$$R_{final} = \langle \langle \sigma_b(u, v), \psi_R^+(v) \rangle, \ \phi(u) \rangle$$
 (14)

• Set response of primary physics equal to final response of the system and invoke the adjoint identity to solve for q^+ :

$$R_{final} = \left\langle \left\langle \sigma_b(u, v), \psi_R^+(v) \right\rangle, \ \phi(u) \ \right\rangle = \left\langle q(u), \phi_R^+(u) \right\rangle \tag{15}$$

MS-CADIS adjoint primary source:

$$q^{+}(u) \equiv \langle \sigma_b(u, v), \psi_R^{+}(v) \rangle \tag{16}$$





Groupwise **T**ransmutation (GT)-CADIS

- Implementation of MS-CADIS specifically for SDR analysis
- Provides method to calculate optimal adjoint neutron source, q_n^+ , by first calculating, T, a term that relates the neutron flux to photon source

Moving Geometries and Sources



MCNP6 Moving Objects

- Update in future version of MCNP6
- Allows movement of objects, sources, delayed particles during single simulation
- Available for native MCNP geometry descriptions (not mesh)

Moving Geometries and Sources



Mesh Coupled implementation of R2S (MCR2S)

- Capability that allows components to move before photon transport step
- Transformations are applied to copies of moving components
- Original component still in original location, set to void material

Review

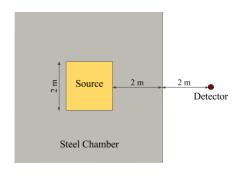


- MC method is most accurate way to obtain detailed particle flux distributions
 - Use MC codes for both neutron and photon transport steps of R2S
 - Need to use VR methods to optimize the transport calculations
- GT-CADIS, an implementation of MS-CADIS, has proven to optimize the neutron transport step of R2S
- MCNP6 and MCR2S have developed some capabilities for performing transport on moving geometries

Demonstration

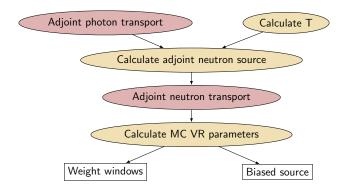


- Geometry
 - Steel chamber
 - 2m x 2m x 2m central cavity
- Source
 - Volume source in central cavity
 - 13.8-14.2 MeV neutrons
- Detector
- Calculate SDR
- 2m away from chamber





GT-CADIS workflow





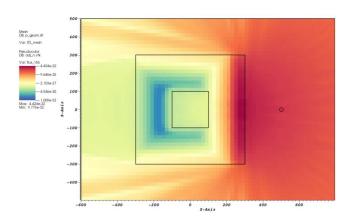


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.





Figure: Demo model.

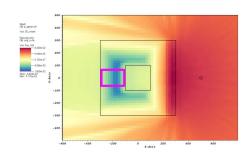


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.





Figure: Demo model.

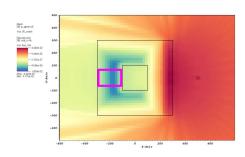


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.





Figure: Demo model.

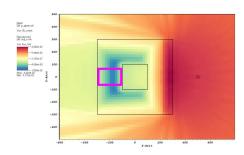


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.



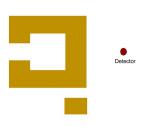


Figure: Demo model.

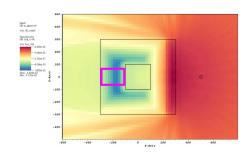


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.



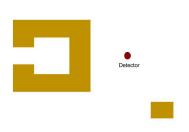


Figure: Demo model.

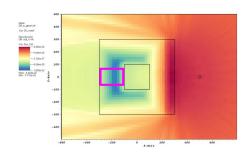


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.





Figure: Demo model.

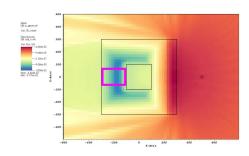


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.

GT-CADIS Demonstration



GT-CADIS importance map is insufficient for moving systems.

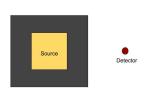


Figure: Demo model.

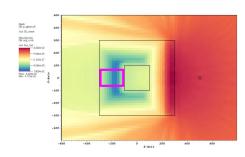


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.

Proposal

VR for Multi-physics Analysis of Moving Systems

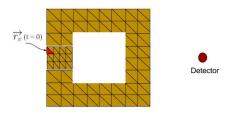


- MS-CADIS optimizes initial radiation transport step in a coupled, multi-step process
- Movement during secondary step changes the construction of the adjoint primary source

Need to derive new adjoint source

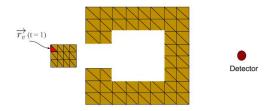


- Geometry movement during secondary physics effects the construction of the adjoint primary source
- Score adjoint secondary flux in discrete volume elements
 - Adjoint flux in volume element v at time t: $\psi^+(\overrightarrow{r}_v(t),t)$
 - Position of volume element v at time t: $\overrightarrow{r}_{v}(t)$
- Integrate over time



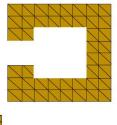


- Geometry movement during secondary physics effects the construction of the adjoint primary source
- Score adjoint secondary flux in discrete volume elements
 - Adjoint flux in volume element v at time t: $\psi^+(\overrightarrow{r}_{\nu}(t),t)$
 - Position of volume element v at time t: $\overrightarrow{r}_{v}(t)$
- Integrate over time





- Geometry movement during secondary physics effects the construction of the adjoint primary source
- Score adjoint secondary flux in discrete volume elements
 - Adjoint flux in volume element v at time t: $\psi^+(\overrightarrow{r}_v(t),t)$
 - Position of volume element v at time t: $\overrightarrow{r}_{v}(t)$
- Integrate over time

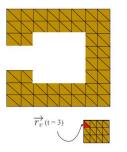








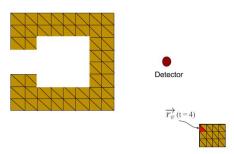
- Geometry movement during secondary physics effects the construction of the adjoint primary source
- Score adjoint secondary flux in discrete volume elements
 - Adjoint flux in volume element v at time t: $\psi^+(\overrightarrow{r}_v(t),t)$
 - Position of volume element v at time t: $\overrightarrow{r}_{v}(t)$
- Integrate over time





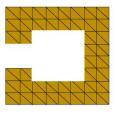


- Geometry movement during secondary physics effects the construction of the adjoint primary source
- Score adjoint secondary flux in discrete volume elements
 - Adjoint flux in volume element v at time t: $\psi^+(\overrightarrow{r}_v(t),t)$
 - Position of volume element v at time t: $\overrightarrow{r}_{v}(t)$
- Integrate over time





- Geometry movement during secondary physics effects the construction of the adjoint primary source
- Score adjoint secondary flux in discrete volume elements
 - Adjoint flux in volume element v at time t: $\psi^+(\overrightarrow{r}_v(t),t)$
 - Position of volume element v at time t: $\overrightarrow{r}_{v}(t)$
- Integrate over time





Time-integrated GT-CADIS



- To apply time-integration to GT-CADIS:
 - Perform adjoint photon transport at each time step of geometry movement
 - 2 Score adjoint photon flux in each volume element, v
 - **3** Integrate over time

Time-integrated Adjoint Neutron Source

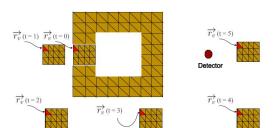


Calculate coupling term, T, for each volume element

$$T_{\nu,g,h} = \frac{q_{\gamma,\nu,h}(\phi_{n,\nu,g})}{\phi_{n,\nu,g}} \tag{17}$$

Combine with adjoint photon flux in each volume element

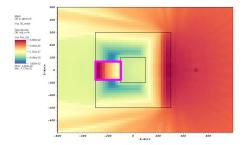
$$q_{n,v,g}^{+} = \frac{\sum_{t_{mov}} \left(\sum_{h} T_{v,g,h} \phi_{\gamma,v,h,t_{mov}}^{+}\right) \Delta t_{mov}}{t_{tot}}$$
(18)



Time-integrated (T)GT-CADIS



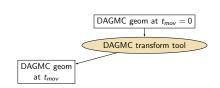
- Perform deterministic adjoint neutron transport using the time-integrated source
- Resultant adjoint neutron flux should look something like this:

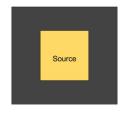


 Use this adjoint neutron flux to generate biasing parameters that will optimize the MC neutron transport step of R2S

Implementation Plan

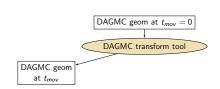


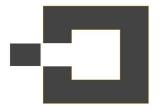






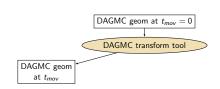








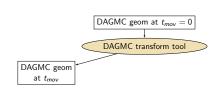








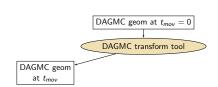










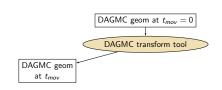










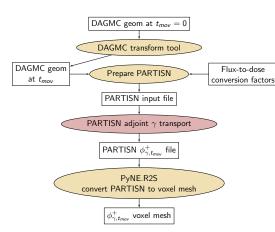








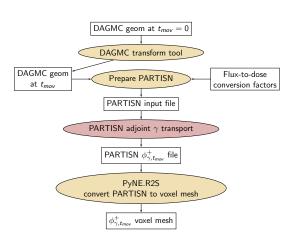






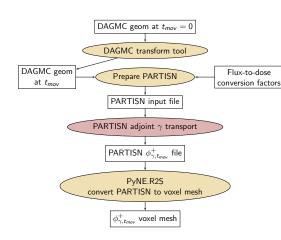






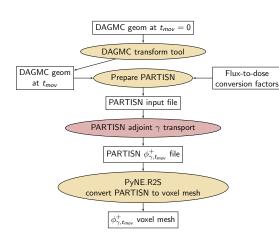








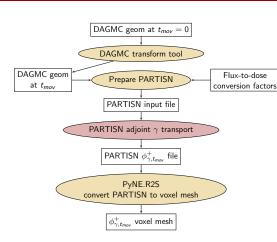




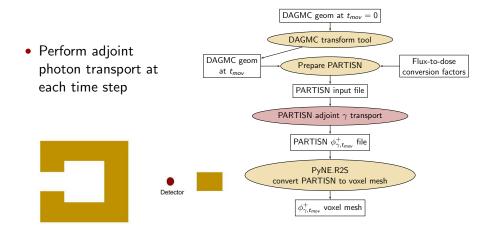










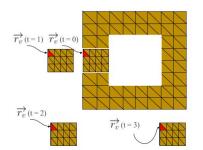


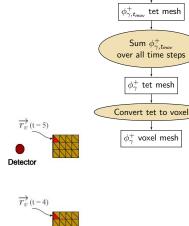


 $\phi_{\gamma,t_{mov}}^+$ voxel mesh

Convert voxel to tet

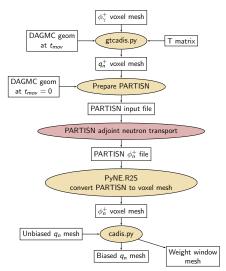
- Map the voxel mesh to a tetrahedral mesh
- Average the adjoint photon flux calculated at each time step







- Calculate T of each voxel
- Calculate adjoint neutron source
- Perform adjoint neutron transport
- Generate biased source and weight window mesh



Experiment

Experiment



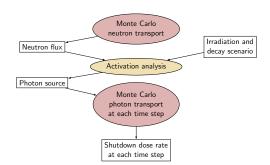
- Toy problem
 - Steel chamber with moving component
 - Incrementally add optimization
 - Calculate figure of merit (FOM) to assess utility of TGT-CADIS method
- Full-scale FES demonstration

Experiment: Toy Problem



Experimental Steps:

No VR

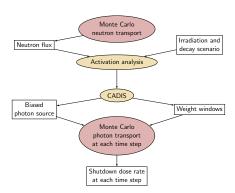


Experiment: Toy Problem



Experimental Steps:

- No VR
- Photon VR: CADIS

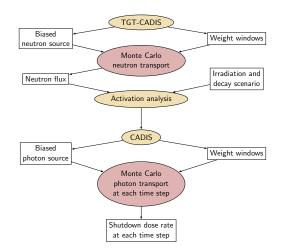


Experiment: Toy Problem



Experimental Steps:

- No VR
- Photon VR: CADIS
- Neutron and Photon VR: TGT-CADIS



Progress

MC Moving Geometry Simulations



- Tools to update position of geometry based on user-defined motion data
 - 1 Production of step-wise geometry files
 - 2 DAGMC update to facilitate on-the-fly geometry transformations
- Motion data:
 - Time-dependent translation or rotation vector, total length of time, number or desired time steps
 - Relocation transform
- Common functionality:
 - Read tag data that specifies type of transformation
 - Identify starting position of each component
 - Update position according to transformation

Conclusions

Assumptions



- Photon transport occurs much faster than geometry movement : reasonable to do quasi-static simulation
- Period of geometry movement is short enough that the photon source will not change appreciably : can use same photon source for all MC calculations

Challenges



- Depending on complexity of model and fidelity of time resolution, can amass large number of CAD geometry files, volume mesh tally files
- Need to optimize this workflow in order to keep file storage at minimum

Summary



- Accurate quantification of the SDR during maintenance procedures is crucial to the design and operation of FES
- GT-CADIS has proven to accurately quantify the SDR in static FES
- TGT-CADIS aims to provide the capabilities necessary to calculate the SDR at various time points during operations that involve activated components moving around the facility



Questions?

TODO



- REFERENCES
- Fig numbers
- FW-CADIS
- Pros/cons deterministic/MC
- Intro DAGMC, MOAB
- Too much detail in Gen. MS-CADIS?
- labels on tet mesh time slices
- Overall alignment/sizing/spacing
- Error propagation
- Add more on moving geom progress, movie
- OBB tree optimization