Variance Reduction for Multi-physics Analysis of Moving Systems

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Preliminary Exam

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Introduction

Shutdown Dose Rate (SDR) Analysis

- Fusion Energy Systems (FES)
  - Burning plasma, D-T fusion
  - ${}_1^2H + {}_1^3H \rightarrow {}_2^4He + {}_0^1n$
- Neutrons penetrate deeply into system components, causing activation
- Radioisotopes persist long after shutdown
- Important to quantify the dose caused by decay photons

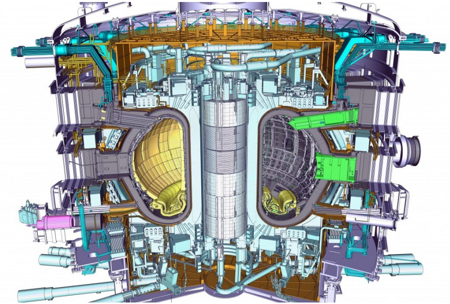
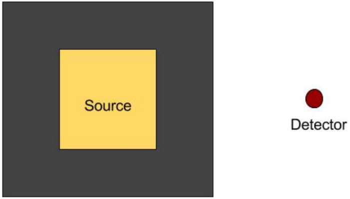


Figure: Cutaway view of ITER drawing.

SDR Analysis: Movement After Shutdown

- 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



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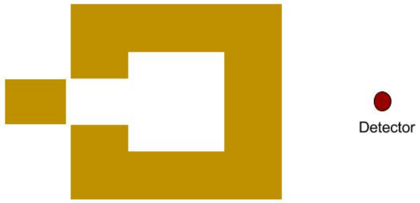

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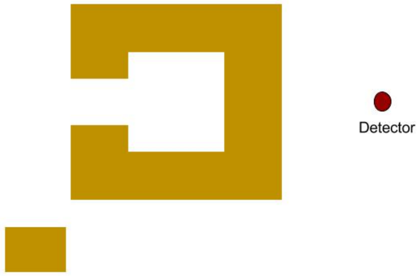

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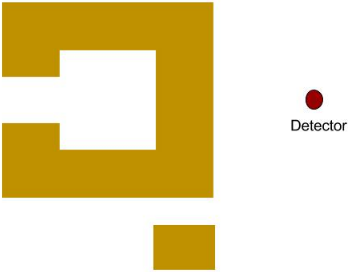

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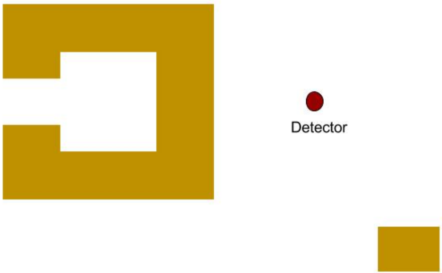

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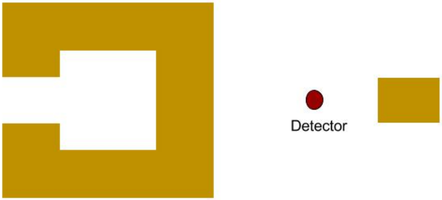
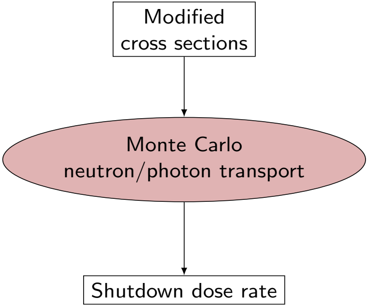


Goal

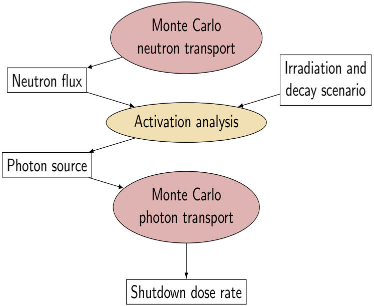
Optimize the calculation of the **shutdown dose rate** at a particular location as activated components are **moving** around the facility.

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

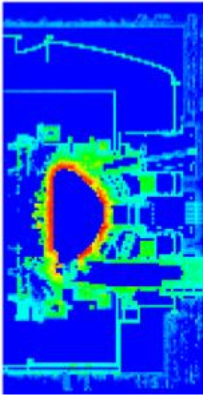


Figure: Photon source in ITER tokamak building.

Error in MC Calculations

- Uncertainty in MC calculations:

$$\Re = \frac{\sigma_{\overline{x}}}{\overline{x}} \tag{1}$$

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

- 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

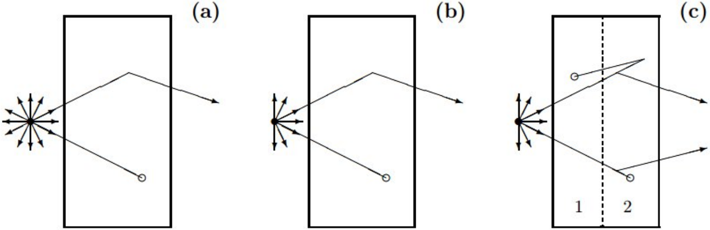


Figure: a) Analog b) Source biasing c) Splitting/rouletting

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:

$$H\Psi(\overrightarrow{r}, E, \widehat{\Omega}) = q(\overrightarrow{r}, E, \widehat{\Omega}) \tag{2}$$

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

Adjoint:

$$\langle \Psi^+, q \rangle = \langle \Psi, q^+ \rangle \tag{3}$$

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

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

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:

$$\widehat{q}(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{\Psi^+(\overrightarrow{r}, E, \widehat{\Omega}) q(\overrightarrow{r}, E, \widehat{\Omega})}{R} \tag{5}$$

- Weight window lower bounds:

$$w_l(\overrightarrow{r}, E, \widehat{\Omega}) = \frac{R}{\Psi^+(\overrightarrow{r}, E, \widehat{\Omega})(\frac{\alpha+1}{2})} \tag{6}$$

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
  2. 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
- When applied to SDR analysis, MS-CADIS will optimize the neutron transport step of R2S

Generalized MS-CADIS

- System of coupled, multi-physics:

$$Primary : H\phi(u) = q(u) \tag{7}$$

$$Secondary : L\psi(v) = b(v) \tag{8}$$

$$b(v) = f(\phi(u))$$

- Adjoint identities:

$$\langle \phi^{+}, q \rangle = \langle \phi, q^{+} \rangle \tag{9}$$

$$\langle \psi^{+}, b \rangle = \langle \psi, b^{+} \rangle \tag{10}$$

Generalized MS-CADIS

- Response to secondary physics:

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

- Define $b^+ \equiv \omega_R$ and apply adjoint identity:

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

  - ψ_R^+ represents importance function for R_{final}

- Set primary response to final response and apply adjoint identity:

$$R_{final} = \langle q^+, \phi \rangle = \langle q, \phi_R^+ \rangle \tag{13}$$

- Solving for q^+ requires this unique relationship:

$$b(v) = \langle \sigma_b(u, v), \phi(u) \rangle \tag{14}$$

Generalized MS-CADIS

- Substitute Eq. 14 and set primary response equal to secondary :

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

- Switch the order of integration

$$R_{final} = \langle q^{+}(u), \phi(u) \rangle = \Big\langle \ \langle \sigma_b(u,v), \psi_R^{+}(v) \rangle, \ \phi(u) \ \Big\rangle \tag{16}$$

- MS-CADIS adjoint primary source:

$$q^{+}(u) \equiv \langle \sigma_b(u,v), \psi_R^{+}(v) \rangle \tag{17}$$

- Prompt photon production: $\sigma_b(u,v) \equiv \sigma_{n,\gamma}(E_n, E_\gamma)$

Generalized MS-CADIS

- MS-CADIS adjoint primary source:

$$q^{+}(u) \equiv \langle \sigma_b(u, v), \psi_R^{+}(v) \rangle \tag{18}$$

- Apply MS-CADIS to coupled neutron-photon physics:
  - $q^{+}(u) \equiv q_n^{+}(E_n)$
  - $\psi^{+}(v) \equiv \phi_\gamma^{+}$
  - Prompt photon production: $\sigma_b(u, v) \equiv \sigma_{n,\gamma}(E_n, E_\gamma)$
  - Delayed photon production: $\sigma_b(u, v) \equiv T_{n,\gamma}(E_n, E_\gamma)$

Variance Reduction for SDR Analysis: GT-CADIS

Groupwise Transmutation (GT)-CADIS

- Implementation of MS-CADIS specifically for SDR analysis
- Provides method to calculate optimal adjoint neutron source, q_n^+:

$$q_n^+(E_n) = \langle T(E_n, E_\gamma), \phi_\gamma^+(E_\gamma) \rangle \tag{19}$$

- $T(E_n, E_\gamma)$
  - Approximation of the transmutation process
  - Solution exits when SNILB criteria are met
  - Defined by this relationship:

$$q_\gamma(E_\gamma) = \langle T(E_n, E_\gamma), \phi_n(E_n) \rangle \tag{20}$$

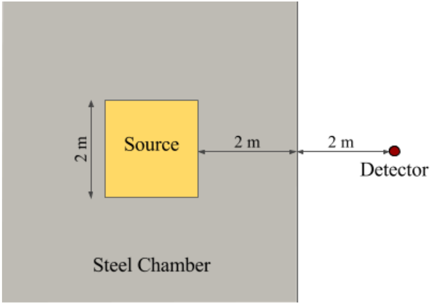
- Calculate by performing single-energy-group irradiations of each material and recording the resultant photon emission densities

$$T_{g,h} = \frac{q_{\gamma,h}(\phi_{n,g})}{\phi_{n,g}} \tag{21}$$

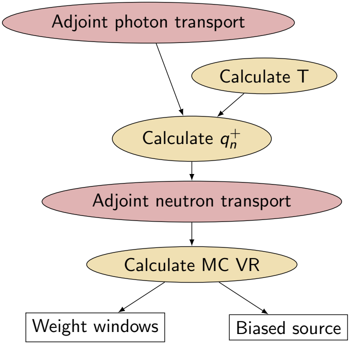
Demonstration

GT-CADIS Demonstration: Problem Description

- 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



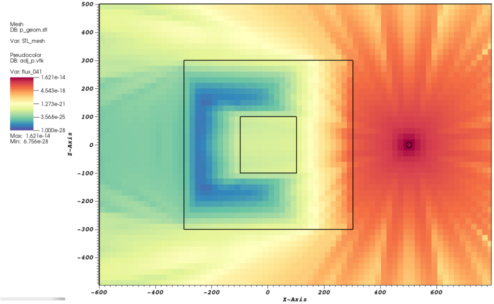
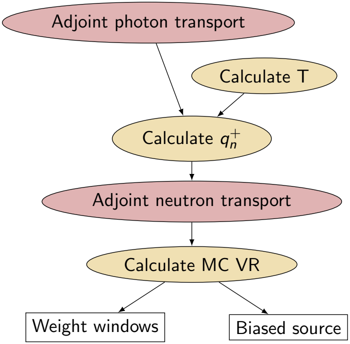


Figure: Adjoint photon flux used to generate adjoint neutron source according to the GT-CADIS method.

GT-CADIS workflow



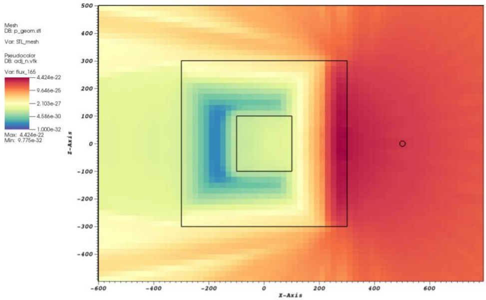


Figure: GT-CADIS adjoint neutron flux. Functions as importance map.

GT-CADIS Demonstration: Variance Reduction Parameters

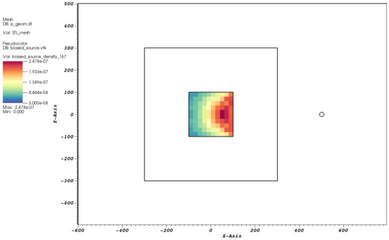


Figure: Biased neutron source generated with GT-CADIS method.

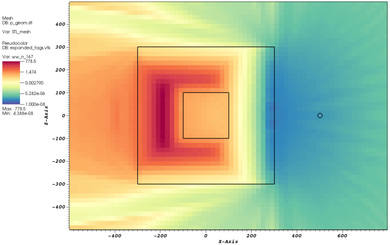


Figure: Weight window mesh generated with GT-CADIS method.

GT-CADIS Demonstration: Forward Neutron Flux

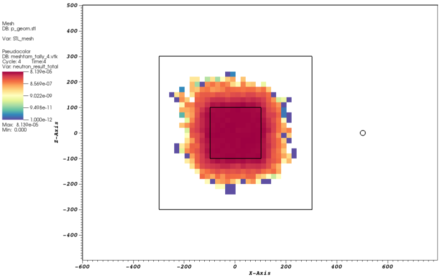


Figure: Neutron flux resulting from analog MC simulation.

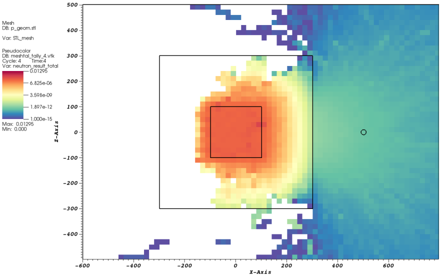


Figure: Neutron flux resulting from MC simulation using GT-CADIS biased source and weight window mesh.

GT-CADIS Demonstration: Forward Photon Source

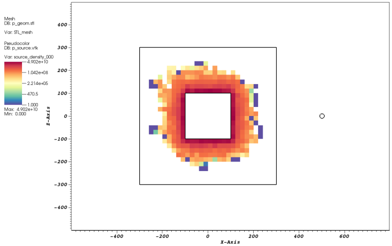


Figure: Photon source generated by ALARA activation calculation using the analog MC neutron transport result.

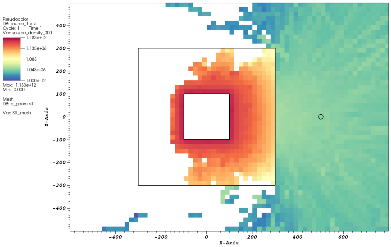


Figure: Photon source generated after ALARA activation calculation using the GT-CADIS optimized neutron transport result.

GT-CADIS Speedups

- VR parameters produced by GT-CADIS method result in much faster convergence of the neutron transport flux in comparison to analog and FW-CADIS methods

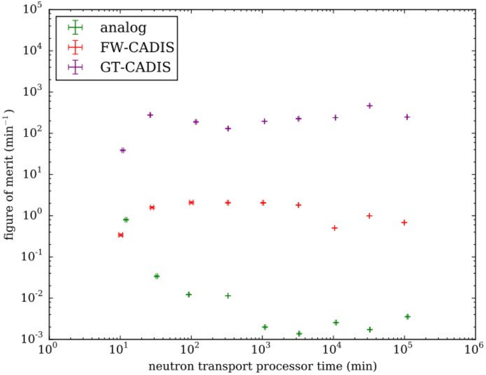


Figure: FOM as function of neutron transport processor time

GT-CADIS Demonstration

GT-CADIS importance map is **insufficient** for moving systems.

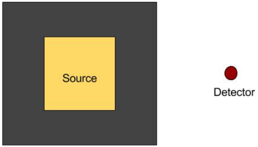
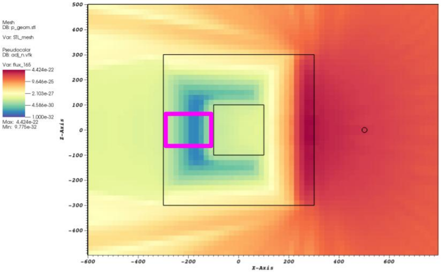


Figure: Demo model.



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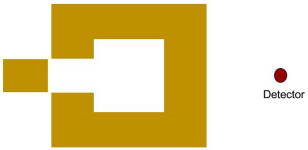

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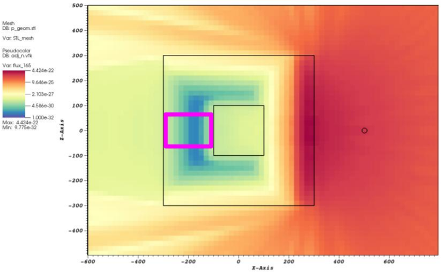

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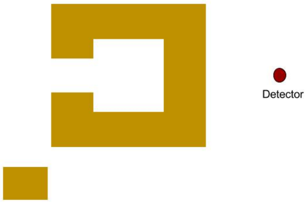

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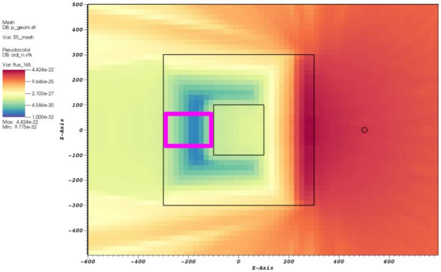

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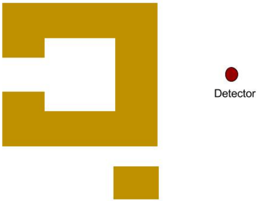

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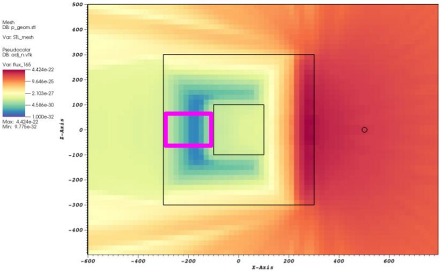

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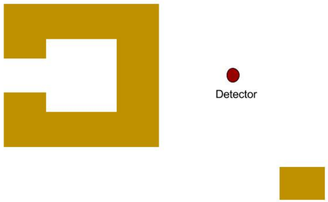

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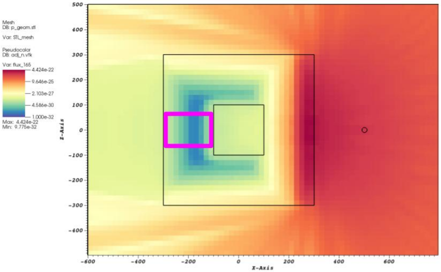

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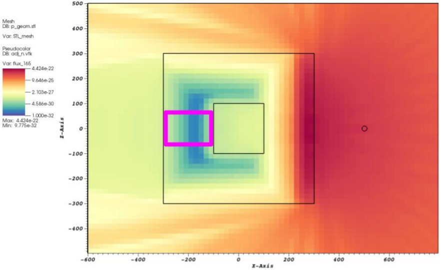

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Moving Geometries and Sources

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 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
- No automated VR for optimizing neutron transport in systems that move after shutdown

Proposal

VR for SDR Analysis of Moving Systems

- GT-CADIS optimizes neutron transport step in static systems

$$q_n^+(E_n) = \langle T(E_n, E_\gamma), \phi_\gamma^+(E_\gamma) \rangle$$

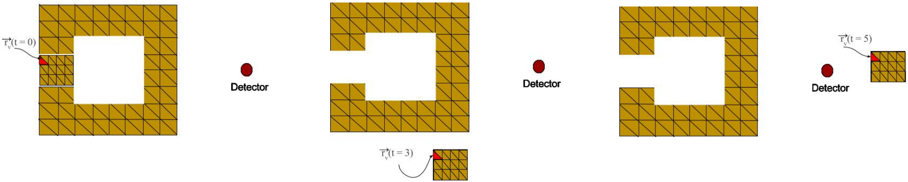
- Movement after shutdown, during photon transport, changes the construction of the adjoint primary source

Derive time-integrated adjoint neutron source

Time-integrated Adjoint Neutron Source

- Score adjoint photon flux in discrete volume elements at each time step
  - Adjoint flux in volume element v at time t: $\phi^+_\gamma(\overrightarrow{r}_v(t), t)$
  - Position of volume element v at time t: $\overrightarrow{r}_v(t)$
- Integrate over time

$$q_n^+ = \frac{\int_t \phi^+_\gamma(\overrightarrow{r}_v(t), t)\, T_v(t)\, dt}{\int_t dt} \tag{22}$$



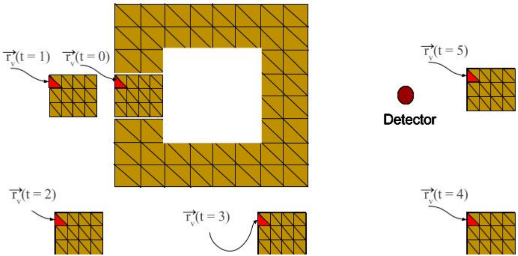
TGT-CADIS: Adjoint Neutron Source

- Calculate coupling term, T, for each volume element

$$T_{v,g,h} = \frac{q_{\gamma,v,h}(\phi_{n,v,g})}{\phi_{n,v,g}} \tag{23}$$

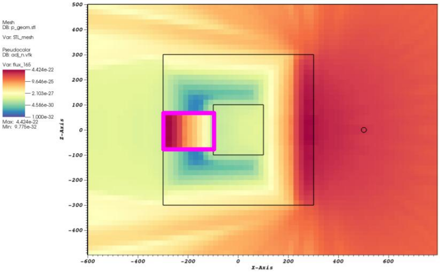
- Combine with adjoint photon flux in each volume element

$$q^{+}_{n,v,g} = \frac{\sum_{t_{mov}} \left(\sum_{h} T_{v,g,h} \phi^{+}_{\gamma,v,h,t_{mov}} \right) \Delta t_{mov}}{t_{tot}} \tag{24}$$



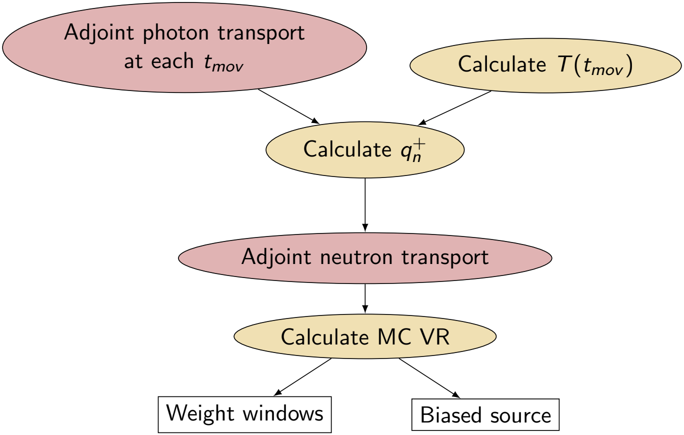
Time-integrated (T)GT-CADIS

- 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

Time-integrated (T)GT-CADIS: Workflow

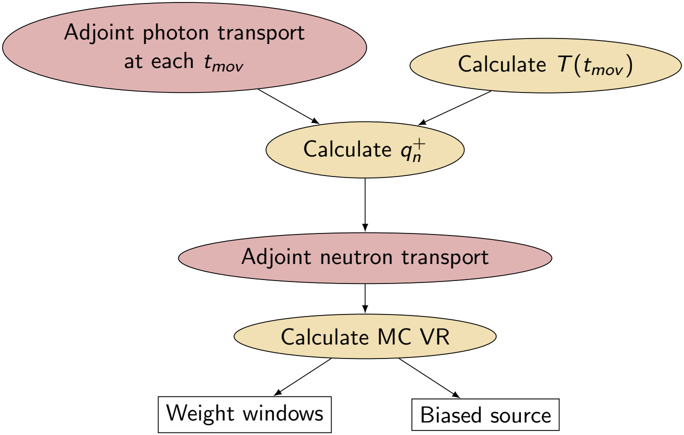


Implementation Plan

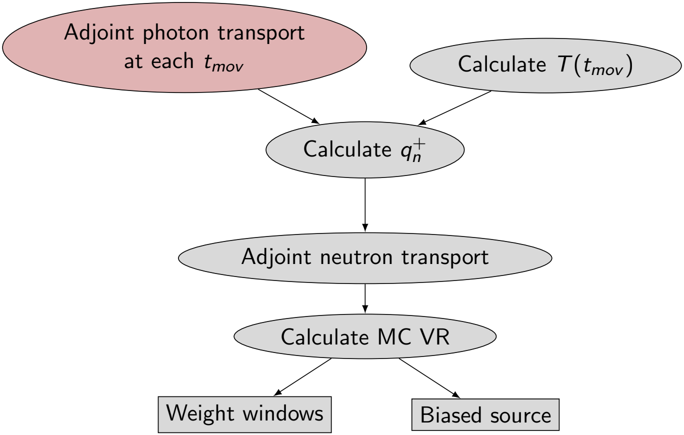
Software

- **PAR**allel, **TI**me-Dependent **SN** (PARTISN)
  - Deterministic adjoint transport
- **D**irect **A**ccelerated **G**eometry **M**onte **C**arlo MCNP (DAGMCNP)
  - Forward MC transport on CAD geometry
- **A**nalytic and **L**aplacian **A**daptive **R**adioactivity **A**nalysis (ALARA)
  - Activation analysis
- **Py**thon for **N**uclear **E**ngineering (PyNE)
  - Tools to support transport
- **M**esh-**O**riented dat**AB**ase (MOAB)
  - Moving geometries

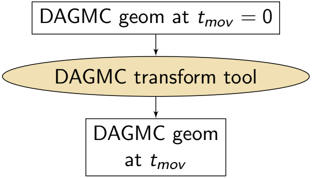
Time-integrated (T)GT-CADIS: Workflow

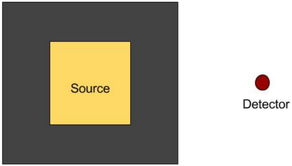


Time-integrated (T)GT-CADIS: Workflow



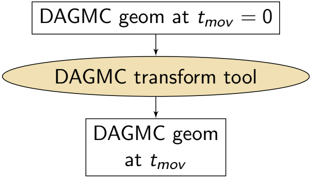
- Generate geometry files at each time step of movement after shutdown





TGT-CADIS: Generate Step-wise Geometries

- Generate geometry files at each time step of movement after shutdown



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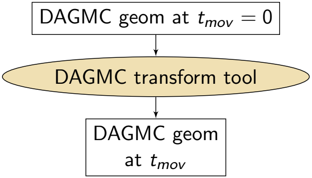
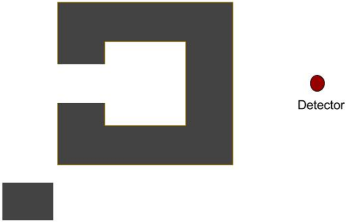




TGT-CADIS: Generate Step-wise Geometries

- Generate geometry files at each time step of movement after shutdown

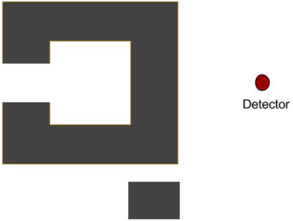
DAGMC geom at $t_{mov} = 0$

↓

DAGMC transform tool

↓

DAGMC geom at t_{mov}



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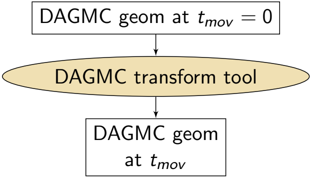

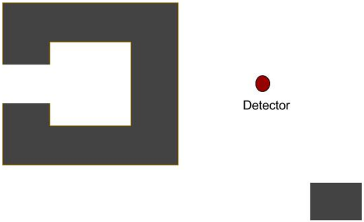

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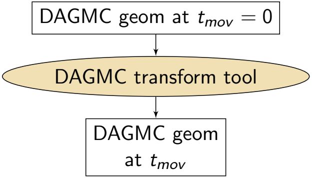
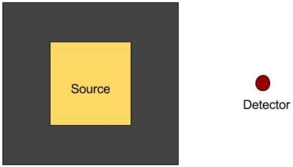
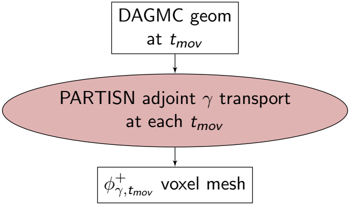


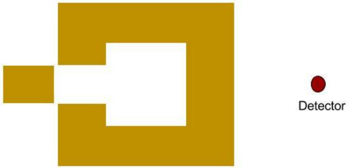
- Perform adjoint photon transport at each time step





TGT-CADIS: Generate VR Parameters

- Perform adjoint photon transport at each time step



DAGMC geom at t_{mov}

↓

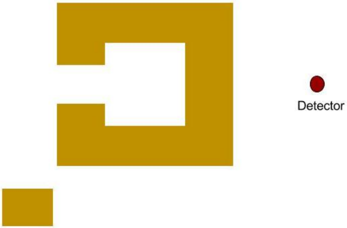
PARTISN adjoint γ transport at each t_{mov}

↓

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

TGT-CADIS: Generate VR Parameters

- Perform adjoint photon transport at each time step



DAGMC geom at t_{mov}

↓

PARTISN adjoint γ transport at each t_{mov}

↓

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TGT-CADIS: Generate VR Parameters

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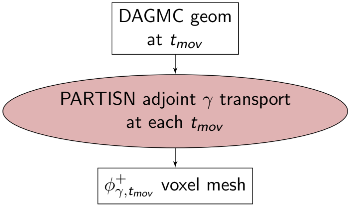

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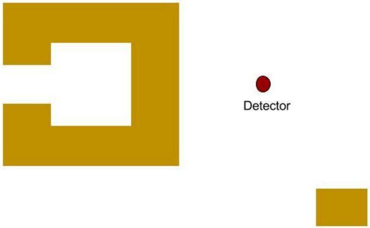

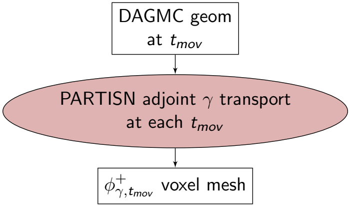

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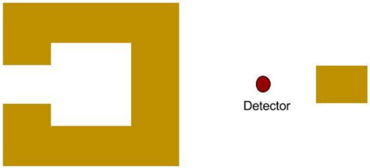


DAGMC geom at t_{mov}

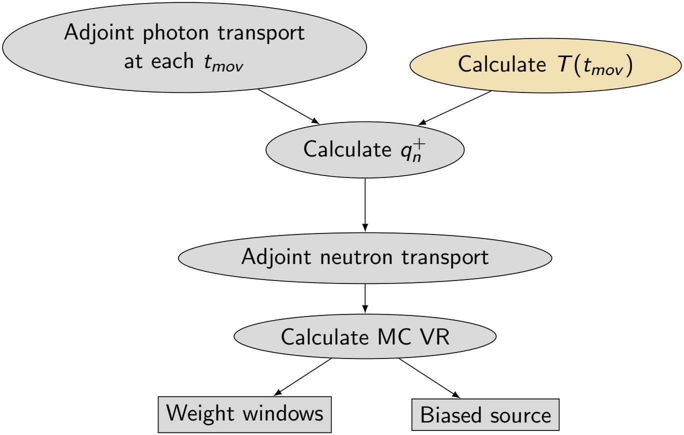
↓

PARTISN adjoint γ transport at each t_{mov}

↓

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

Time-integrated (T)GT-CADIS: Workflow



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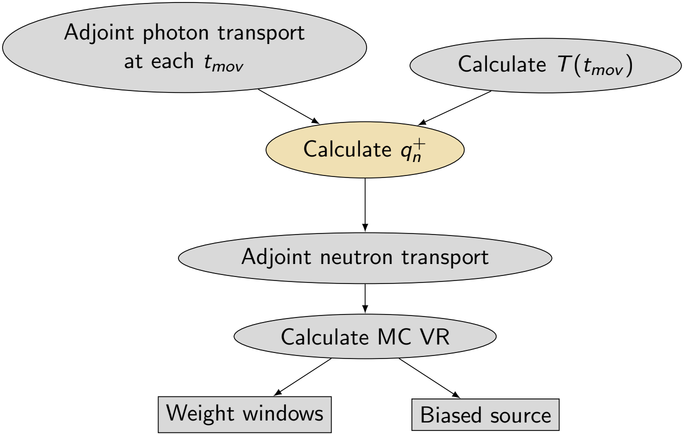
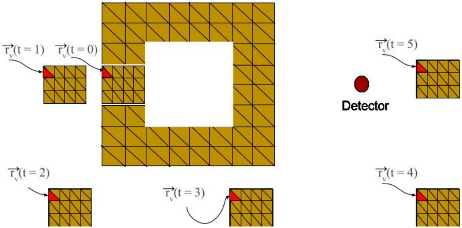
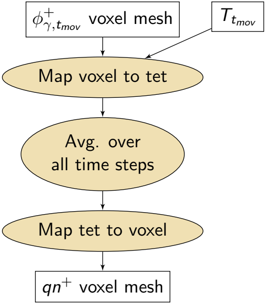
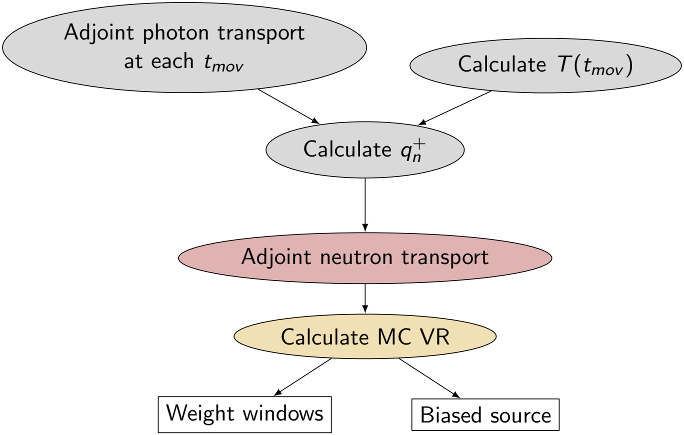


- Map the structured (voxel) mesh to a tetrahedral mesh
- Combine $\phi^{+}_{\gamma,t_{mov}}$ and $T_{t_{mov}}$ and average over time



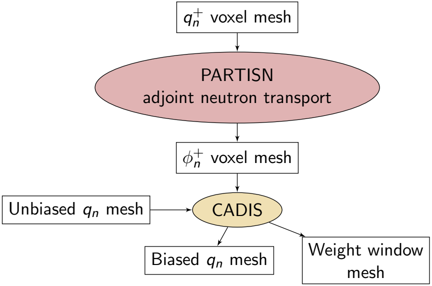


Time-integrated (T)GT-CADIS: Workflow



TGT-CADIS: Generate VR Parameters

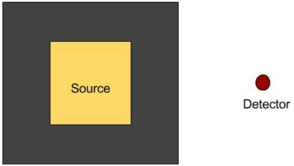
- Perform adjoint neutron transport
- Generate biased source and weight window mesh via CADIS methodology



Experiment

Experiment

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



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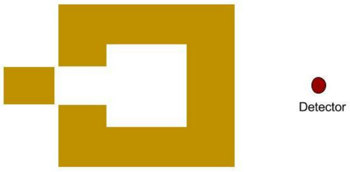

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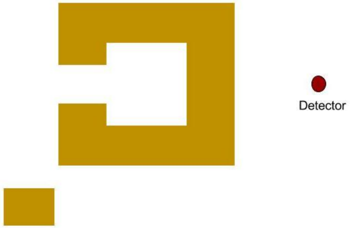

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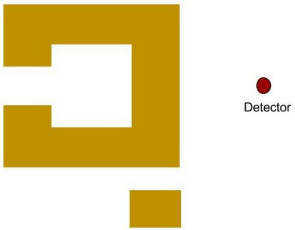

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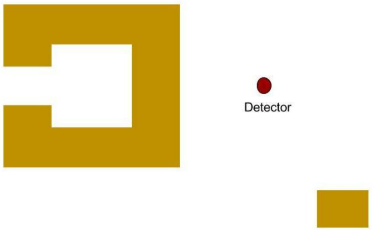

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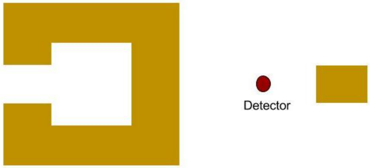
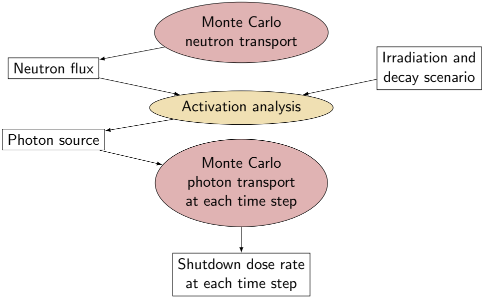


Experiment: Toy Problem

Experimental Steps:

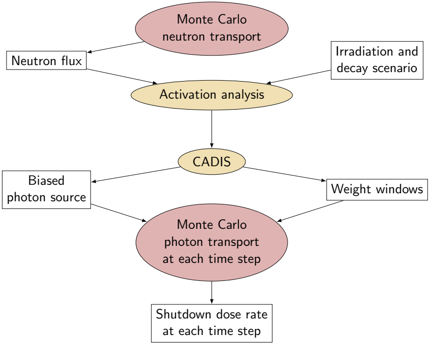
1. No VR



Experiment: Toy Problem

Experimental Steps:

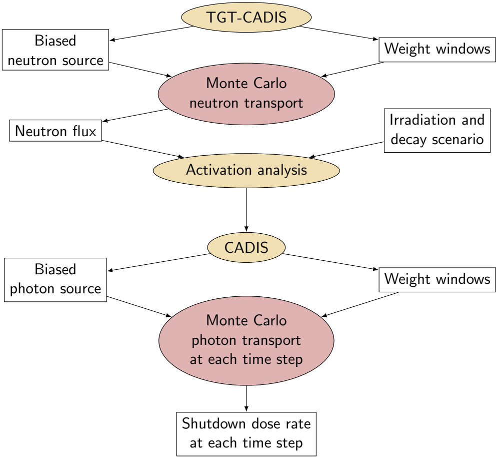
1. No VR
2. Photon VR: CADIS



Experiment: Toy Problem

Experimental Steps:

1. No VR
2. Photon VR: CADIS
3. Neutron and Photon VR: TGT-CADIS, CADIS

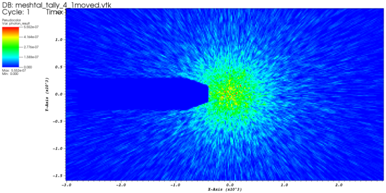


Progress

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

MC Moving Geometry Simulations



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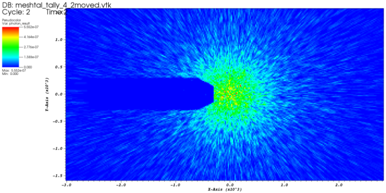

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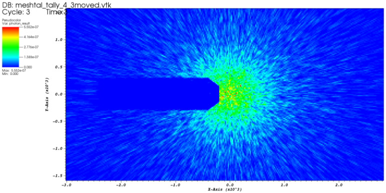

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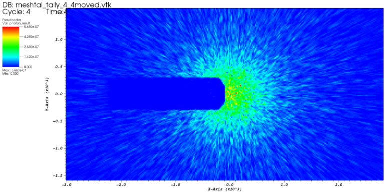

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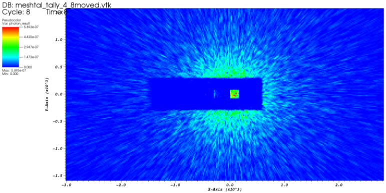

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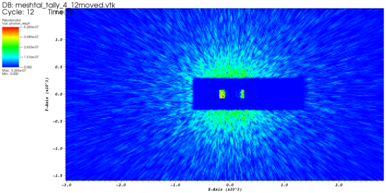

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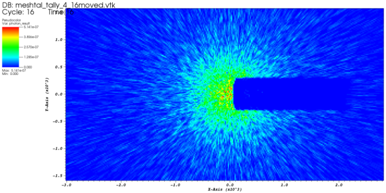

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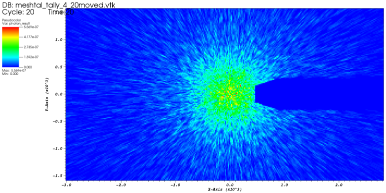

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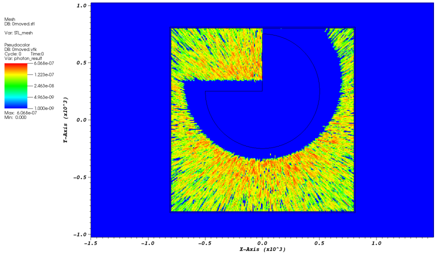

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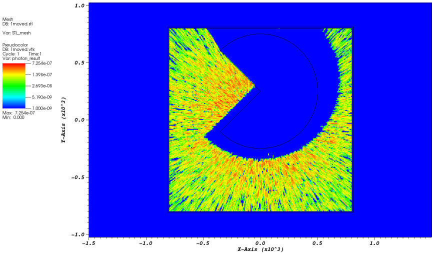

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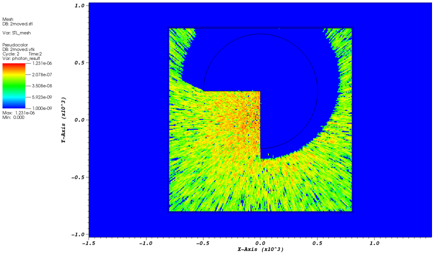
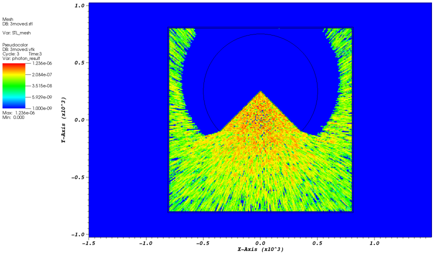


MC Moving Geometry Simulations



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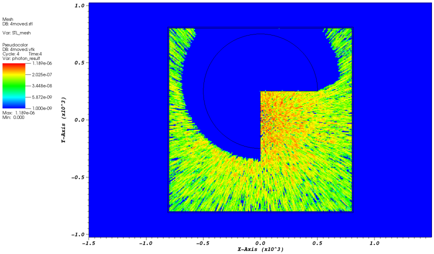

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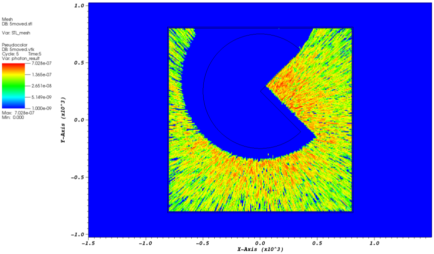

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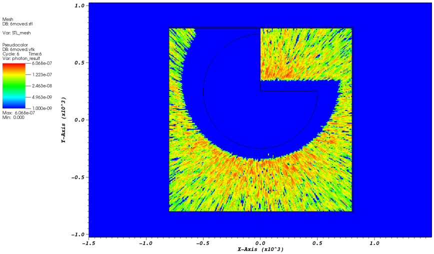

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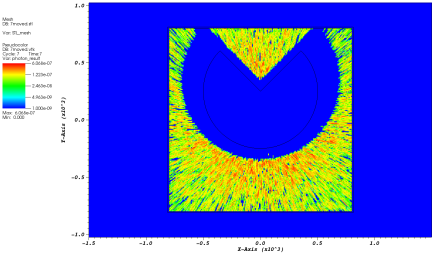

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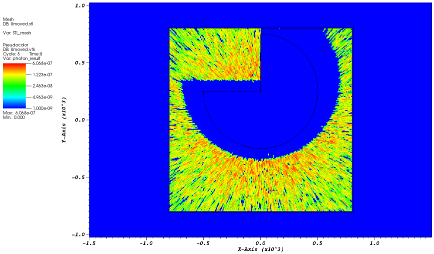

Conclusions

Assumptions

- Photon transport occurs much faster than geometry movement $\therefore$ reasonable to do quasi-static simulation
- Period of geometry movement is short enough that the photon source will not change appreciably $\therefore$ 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