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Variance Reduction for Multi-physics Analysis of Moving Systems

Chelsea D'Angelo

Preliminary Exam

Feb. 2, 2018



WISCONSIN
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① Literature Review

SDR Analysis

MC VR Techniques

GT-CADIS Demonstration

Moving Geometries and Sources

② Proposal

TGT-CADIS: VR for SDR Analysis of Moving Systems

③ Implementation Plan

Software

TGT-CADIS Workflow

④ Experiment

⑤ Progress

Stepwise geometry tool

DAGMC update

⑥ Final Thoughts

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

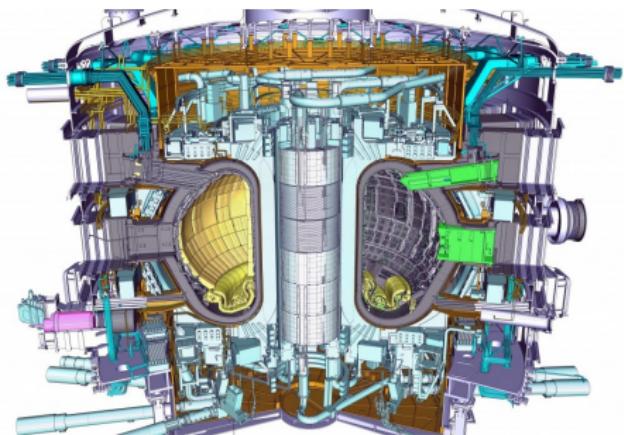
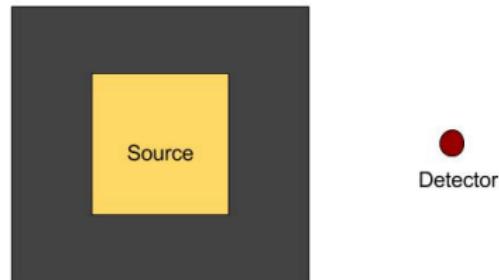


Figure 1 : Cutaway view of ITER drawing.

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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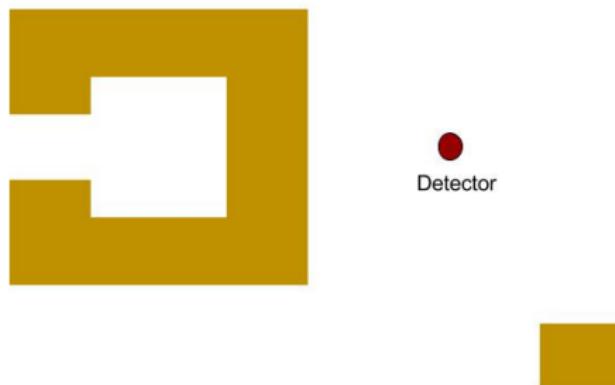
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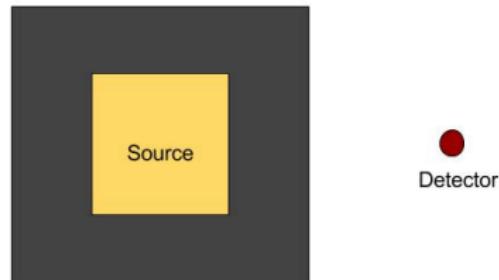
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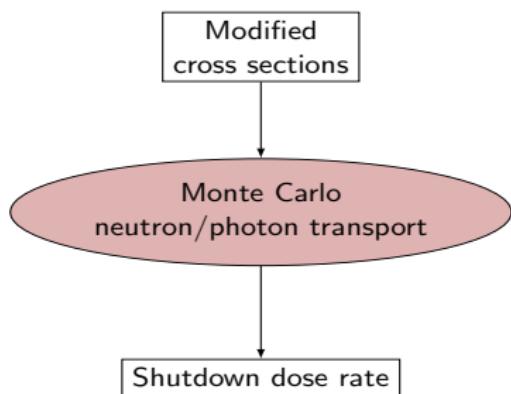


Optimize the calculation of the **shutdown dose rate** at a particular location when activated components are **moving** around the facility.

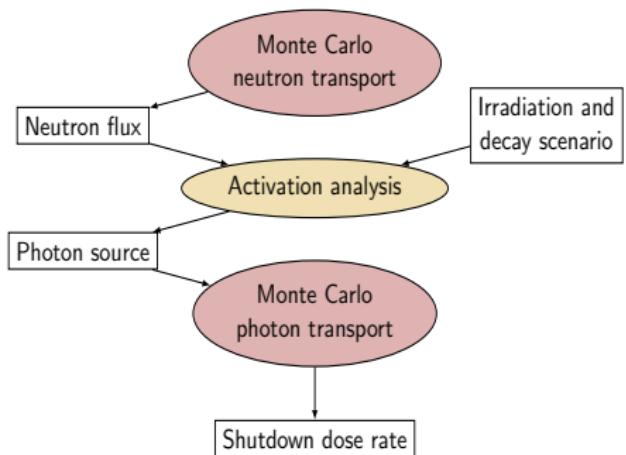
Literature Review

SDR Solution Methods

Direct 1-Step Method (D1S) [1]



Rigorous 2-Step Method (R2S) [2]



Monte Carlo Radiation Transport

- Monte Carlo (MC) solution method [?]
 - Simulates random particle walks through phase space
 - Score quantities of interest in discrete regions of phase space
 - Accurate for large, complex models
 - Challenged in highly attenuated regions
 - Results scored in regions that have low particle flux, have higher statistical uncertainty

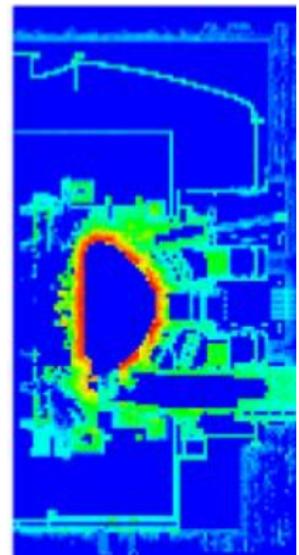


Figure 2 : Photon source in ITER tokamak building.



Error in MC Calculations

- Uncertainty in MC calculations:

$$\mathfrak{R} = \frac{\sigma_{\bar{x}}}{\bar{x}} \quad (1)$$

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

- Efficiency in MC calculations:

$$FOM = \frac{1}{\mathfrak{R}^2 t_{proc}} \quad (2)$$

- To decrease 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
- Adjust statistical weight of particles to keep playing a fair game
- Types
 - **Modified Sampling:** source biasing
 - **Population Control:** splitting/rouletting

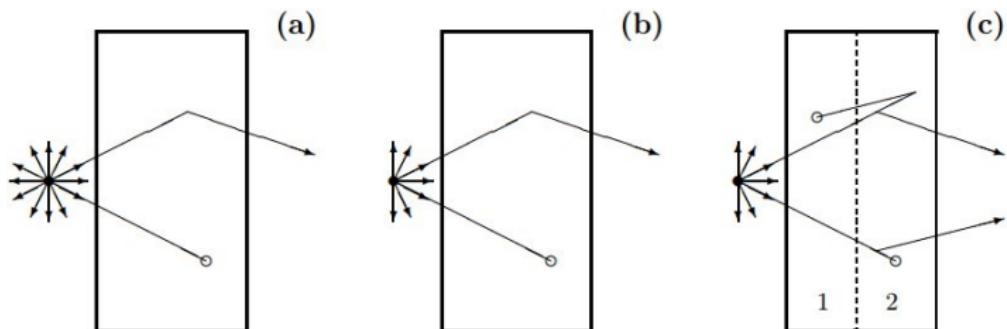


Figure 3 : a) analog b) source biasing c) splitting/roulettting [3]



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 adjoint source to be detector response function

Forward:

$$H\Psi(\vec{r}, E, \hat{\Omega}) = q(\vec{r}, E, \hat{\Omega}) \quad (3)$$

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

Adjoint:

$$\langle \Psi^+, H\Psi \rangle = \langle \Psi, H^+\Psi^+ \rangle \quad (4)$$

$$H^+\Psi^+(\vec{r}, E, \hat{\Omega}) = q^+(\vec{r}, E, \hat{\Omega}) \quad (5)$$

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



Consistent Adjoint Driven Importance Sampling (CADIS)

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

$$\hat{q}(\vec{r}, E, \hat{\Omega}) = \frac{\Psi^+(\vec{r}, E, \hat{\Omega}) q(\vec{r}, E, \hat{\Omega})}{R} \quad (6)$$

- Weight window lower bounds:

$$w_l(\vec{r}, E, \hat{\Omega}) = \frac{R}{\Psi^+(\vec{r}, E, \hat{\Omega})(\frac{\alpha+1}{2})} \quad (7)$$



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



Multi-Step (MS)-CADIS [5]

- 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:

$$\text{Primary} : H\phi(u) = q(u) \quad (8)$$

$$\text{Secondary} : L\psi(v) = b(v) \quad (9)$$

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

- Adjoint identities:

$$\langle \phi^+, q \rangle = \langle \phi, q^+ \rangle \quad (10)$$

$$\langle \psi^+, b \rangle = \langle \psi, b^+ \rangle \quad (11)$$



Generalized MS-CADIS

- Response to secondary physics:

$$R_{final} = \langle \omega_R(v), \psi(v) \rangle \quad (12)$$

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

$$R_{final} = \langle \omega_R, \psi \rangle = \langle b, \psi_R^+ \rangle \quad (13)$$

- ψ_R^+ represents importance function for R_{final}
- Set primary response to final response and apply adjoint identity:

$$R_{final} = \langle q^+, \phi \rangle = \langle q, \phi_R^+ \rangle \quad (14)$$

- Solving for q^+ requires this unique relationship:

$$b(v) = \langle \sigma_b(u, v), \phi(u) \rangle \quad (15)$$

Generalized MS-CADIS

- Substitute Eq. 15 and set primary response equal to secondary :

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

- Switch the order of integration

$$R_{final} = \langle q^+(u), \phi(u) \rangle = \langle \langle \sigma_b(u, v), \psi_R^+(v) \rangle, \phi(u) \rangle \quad (17)$$

- MS-CADIS adjoint primary source:

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

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

Generalized MS-CADIS

- MS-CADIS adjoint primary source:

$$q^+(u) \equiv \langle \sigma_b(u, v), \psi_R^+(v) \rangle \quad (19)$$

- Apply MS-CADIS to coupled neutron-photon physics:

- $q^+(u) \equiv q_n^+(E_n)$
- $\psi^+(v) \equiv \phi_\gamma^+(E_\gamma)$
- 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 [6]

Groupwise Transmutation (GT)-CADIS

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

$$q_n^+(E_n) = \langle T(E_n, E_\gamma), \phi_\gamma^+(E_\gamma) \rangle \quad (20)$$

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

$$q_\gamma(E_\gamma) = \langle T(E_n, E_\gamma), \phi_n(E_n) \rangle \quad (21)$$

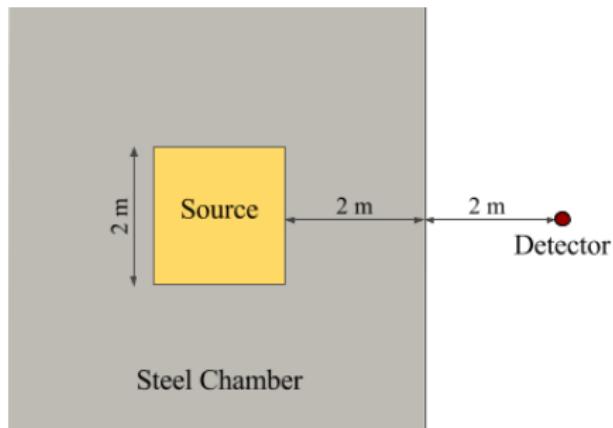
- Calculate by performing single-energy-group irradiations of each material and recording the resultant photon emission densities

$$T_{g,h} = \frac{q_{\gamma,h}(\phi_{n,g})}{\phi_{n,g}} \quad (22)$$

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 Demonstration: Adjoint Photon Transport

GT-CADIS workflow

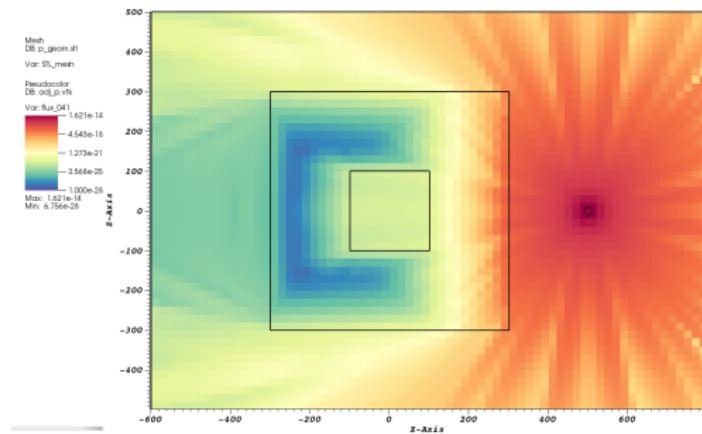
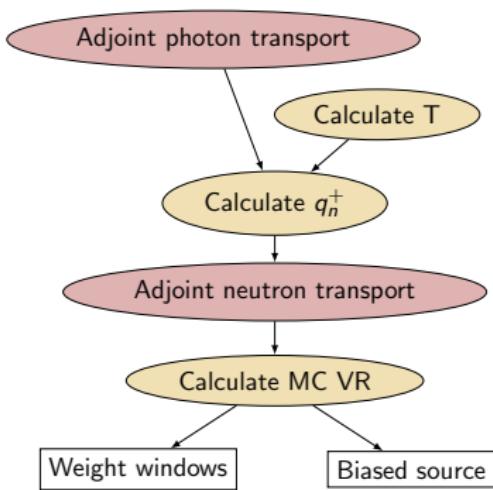


Figure 4 : Adjoint photon flux used to generate adjoint neutron source according to the GT-CADIS method.

GT-CADIS Demonstration: Adjoint Neutron Transport

GT-CADIS workflow

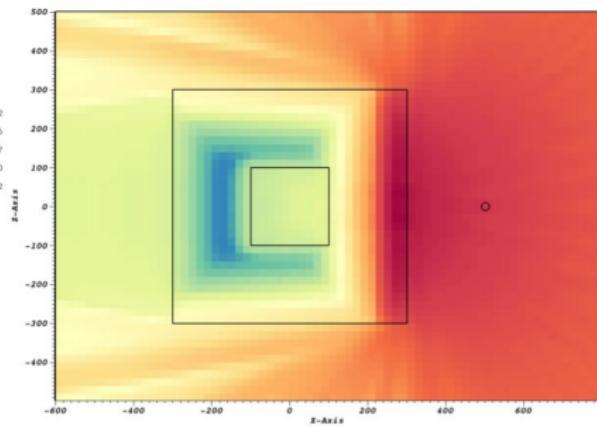
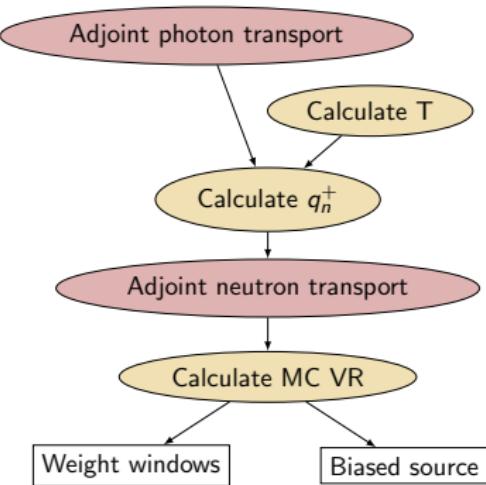


Figure 5 : GT-CADIS adjoint neutron flux. Functions as importance map.

GT-CADIS Demonstration: VR Parameters

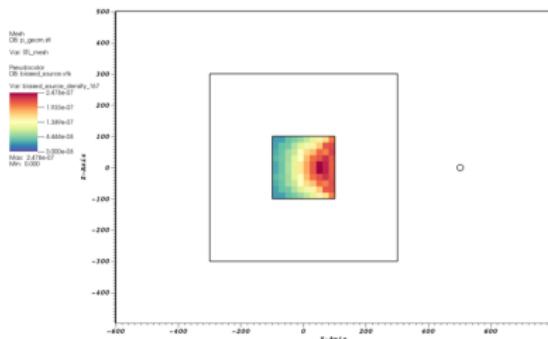


Figure 6 : Biased neutron source generated with GT-CADIS method.

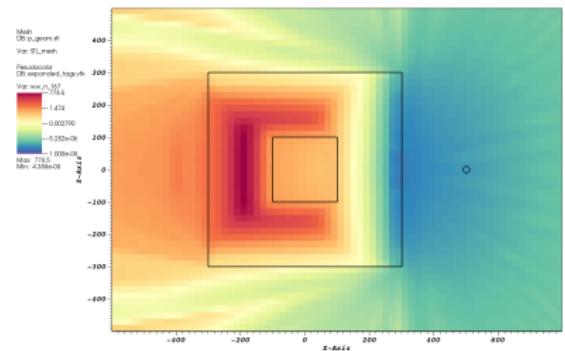


Figure 7 : Weight window mesh generated with GT-CADIS method.

GT-CADIS Demonstration: Forward Neutron Flux

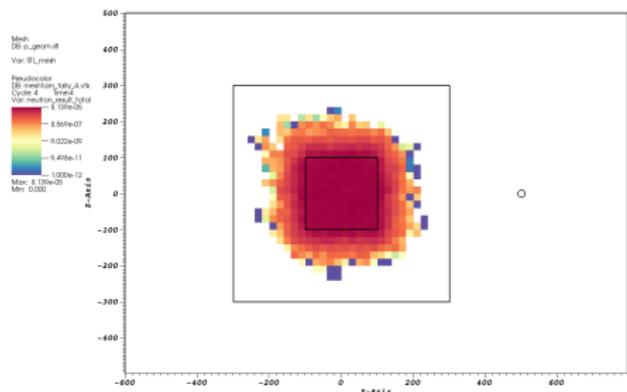


Figure 8 : Neutron flux resulting from analog MC simulation.

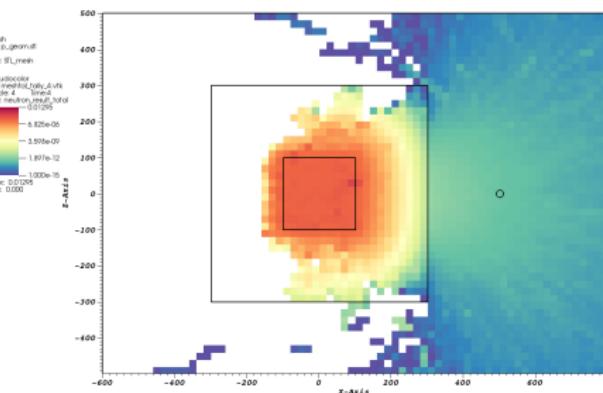


Figure 9 : Neutron flux resulting from MC simulation using GT-CADIS biased source and weight window mesh.

GT-CADIS Demonstration: Forward Photon Source

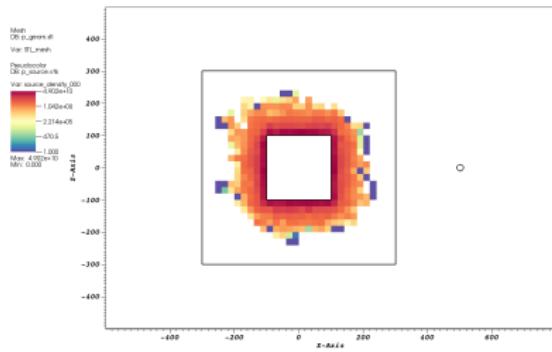


Figure 10 : Photon source generated by ALARA activation calculation using the analog MC neutron transport result.

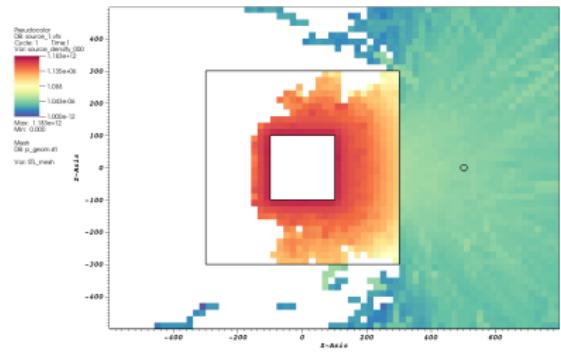


Figure 11 : Photon source generated after ALARA activation calculation using the GT-CADIS optimized neutron transport result.

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

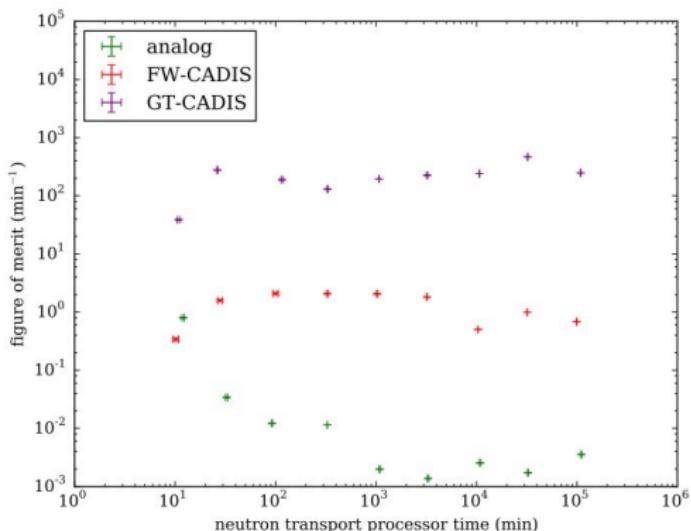


Figure 12 : FOM as function of neutron transport processor time. [?]

GT-CADIS Demonstration

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

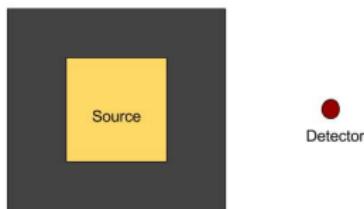


Figure 13 : Demo model.

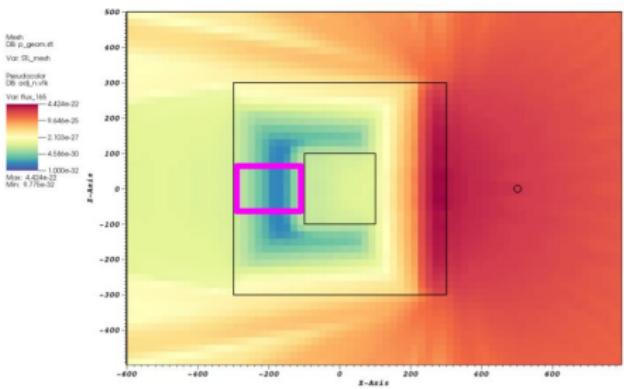


Figure 14 : GT-CADIS adjoint neutron flux. Functions as importance map.

GT-CADIS Demonstration

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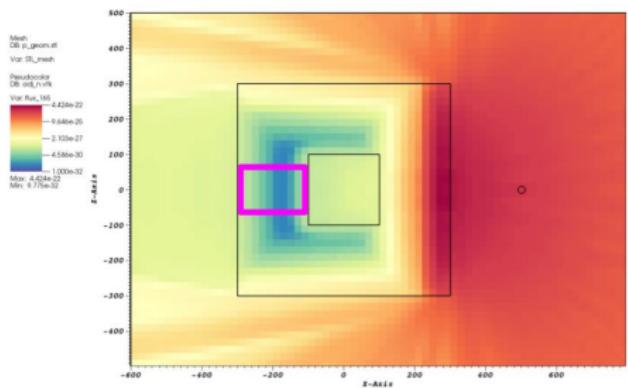


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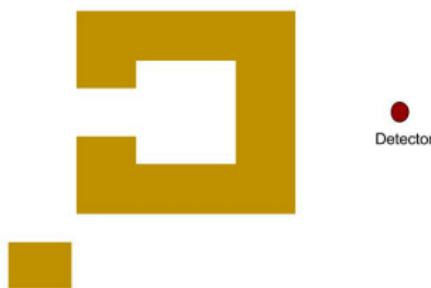


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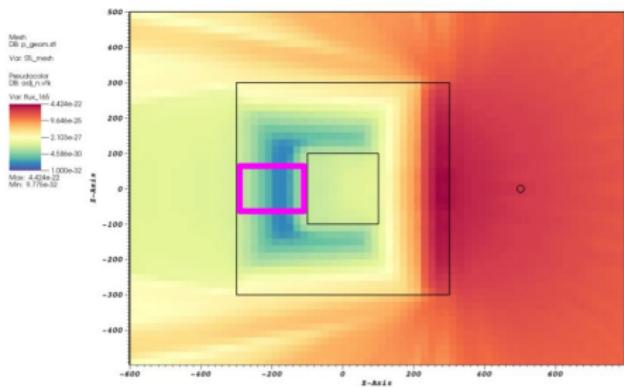


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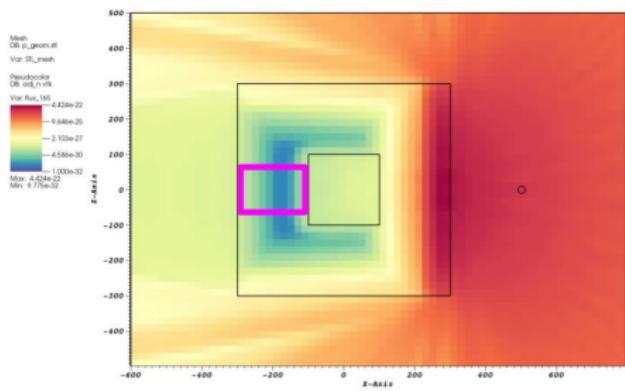


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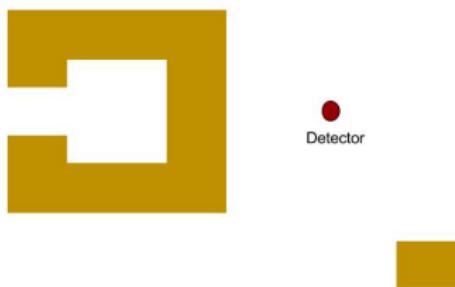


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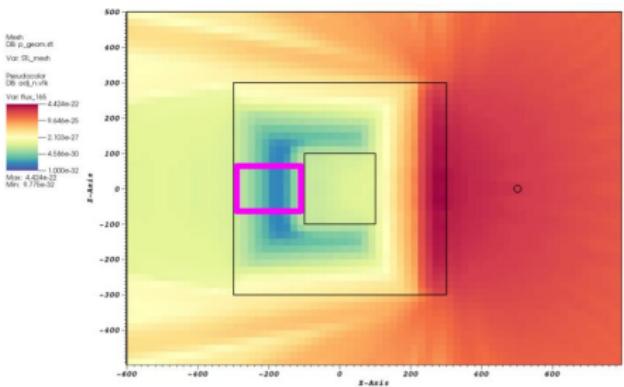


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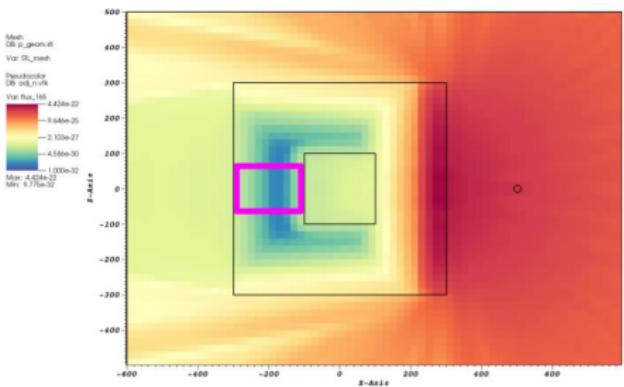


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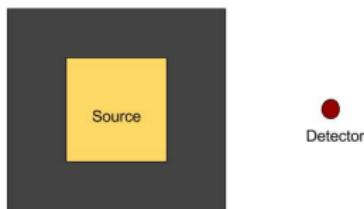


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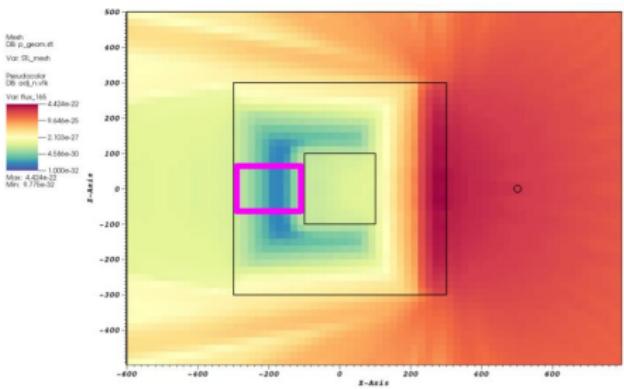


Figure 14 : GT-CADIS adjoint neutron flux. Functions as importance map.

Moving Geometries and Sources

MCNP6 Moving Objects [7], [8]

- 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)[9]

- 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

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

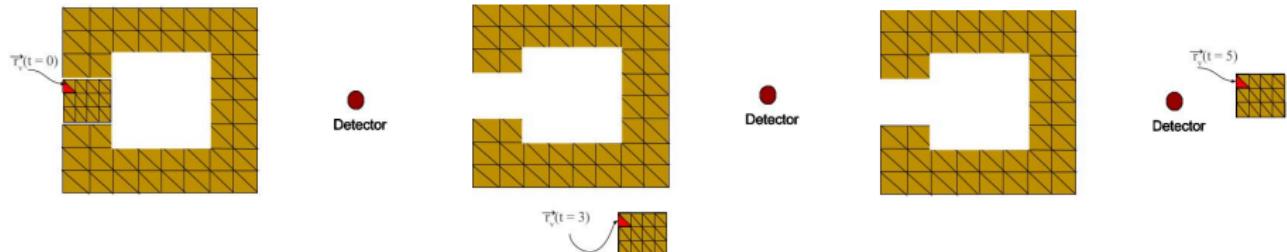
- Movement after shutdown, during photon transport, changes the construction of the adjoint primary source

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 : $\phi_{\gamma}^{+}(\vec{r}_v(t), t)$
 - Position of volume element v at time t : $\vec{r}_v(t)$
- Integrate over time

$$q_n^{+} = \frac{\int_t \phi_{\gamma}^{+}(\vec{r}_v(t), t) T_v(t) dt}{\int_t dt} \quad (23)$$



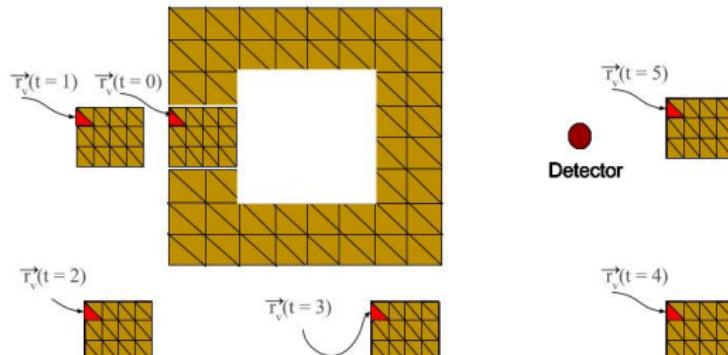
TGT-CADIS: Adjoint Neutron Source

- Calculate coupling term, T , for each volume element

$$T_{v,g,h} = \frac{q_{\gamma,v,h}(\phi_{n,v,g})}{\phi_{n,v,g}} \quad (24)$$

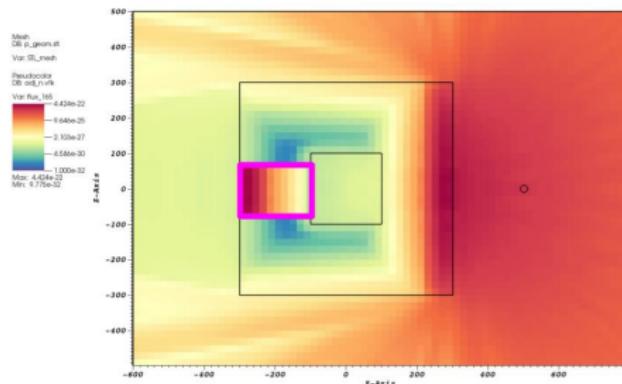
- Combine with adjoint photon flux in each volume element

$$q_{n,v,g}^+ = \frac{\sum_{t_{mov}} (\sum_h T_{v,g,h} \phi_{\gamma,v,h,t_{mov}}^+) \Delta t_{mov}}{t_{tot}} \quad (25)$$



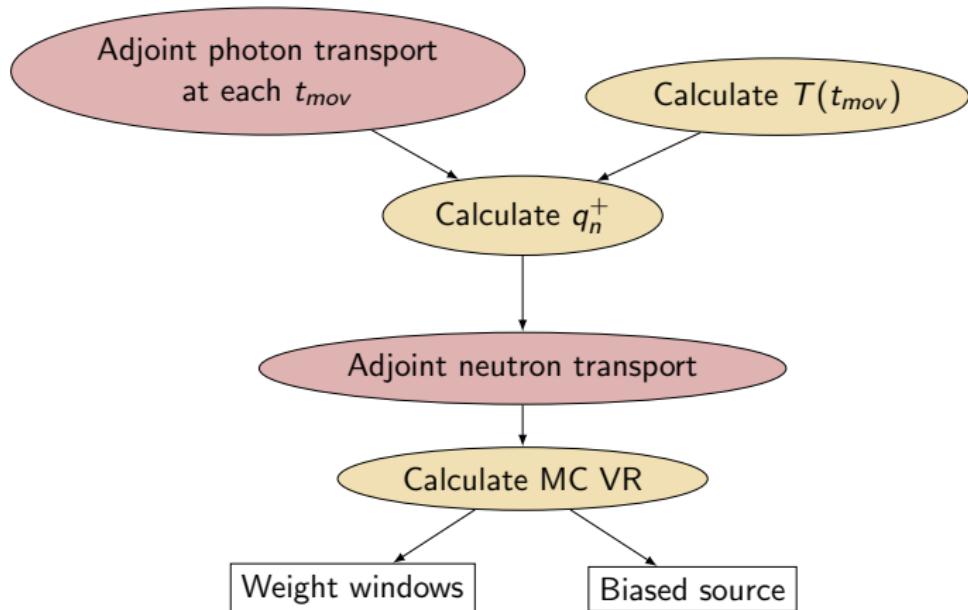
Time-integrated (T)GT-CADIS

- 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



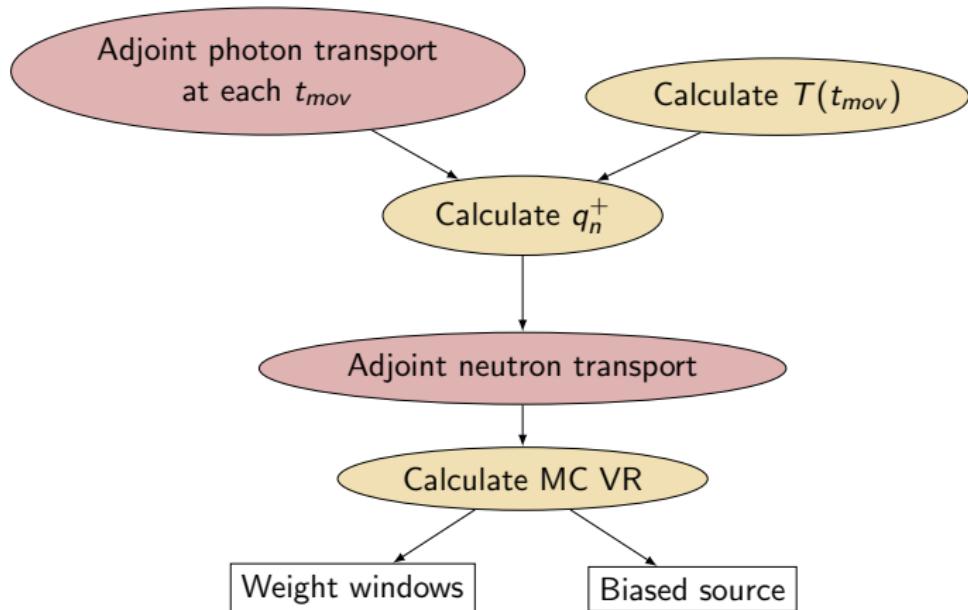
Implementation Plan



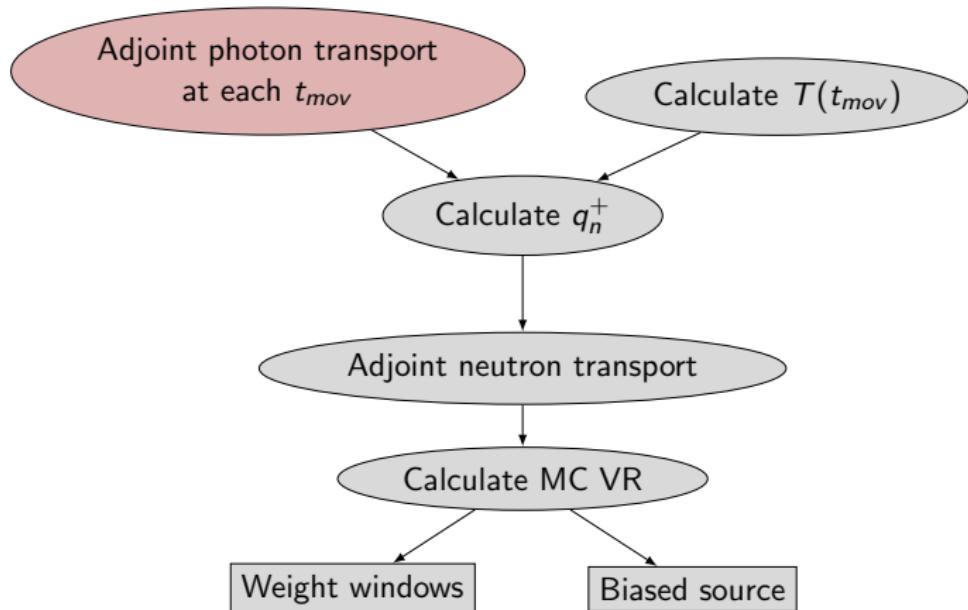
Software

- **PARallel, TIme-Dependent SN** (PARTISN) [10]
 - Deterministic adjoint transport
- **Direct Accelerated Geometry Monte Carlo MCNP** (DAGMCNP) [11]
 - Forward MC transport on CAD geometry
- **Analytic and Laplacian Adaptive Radioactivity Analysis** (ALARA) [12]
 - Activation analysis
- **Python for Nuclear Engineering** (PyNE) [13]
 - Tools to support transport
- **Mesh-Oriented datABase** (MOAB) [14]
 - Moving geometries

Time-integrated (T)GT-CADIS: Workflow

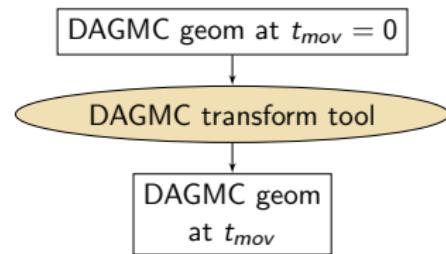
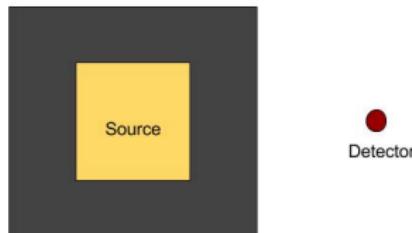


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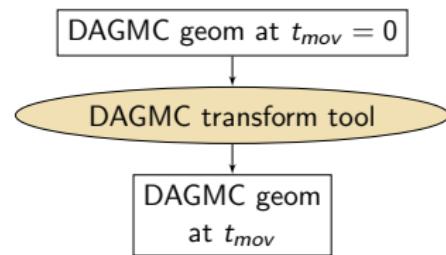
TGT-CADIS: Generate Step-wise Geometries

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



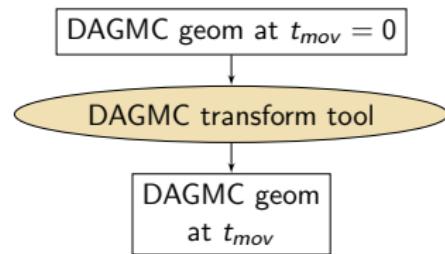
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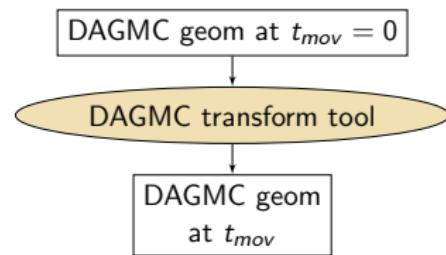
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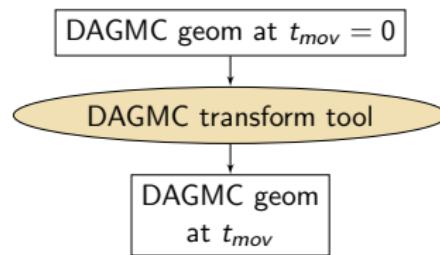
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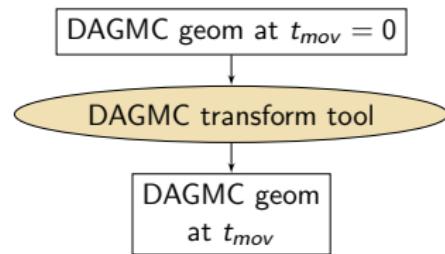
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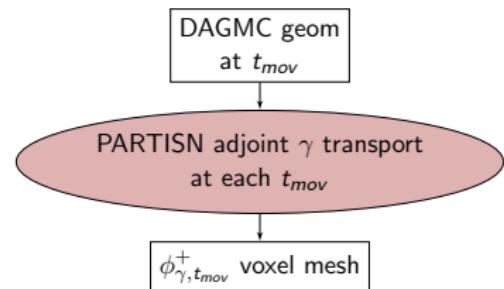
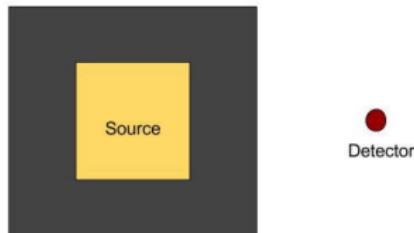


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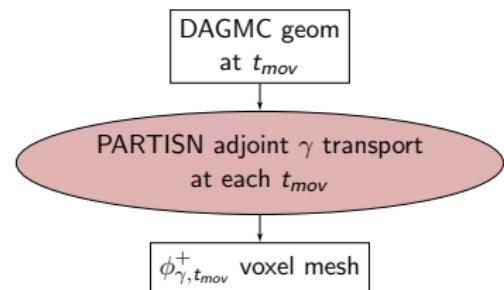
TGT-CADIS: Generate VR Parameters

- Perform adjoint photon transport at each time step



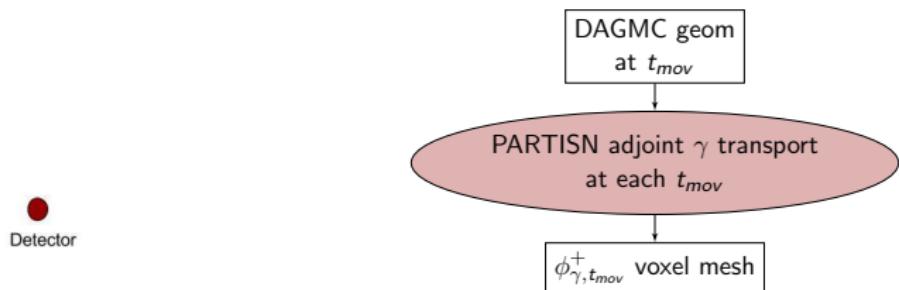
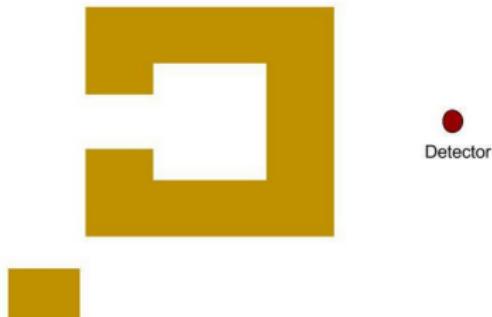
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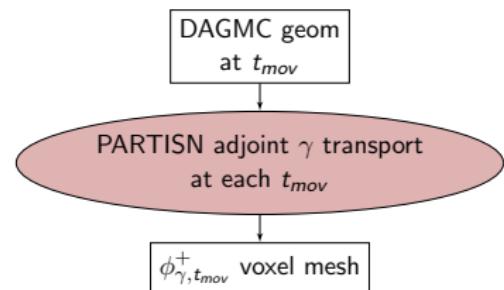
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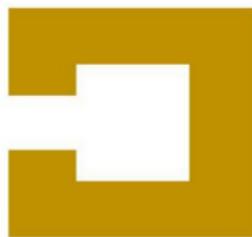
Detector



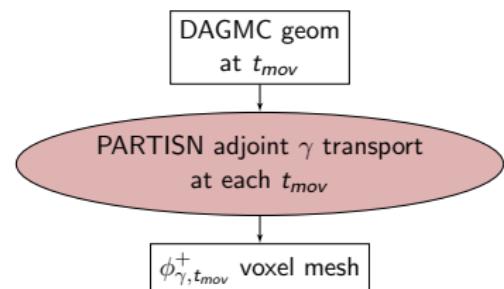
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Detector

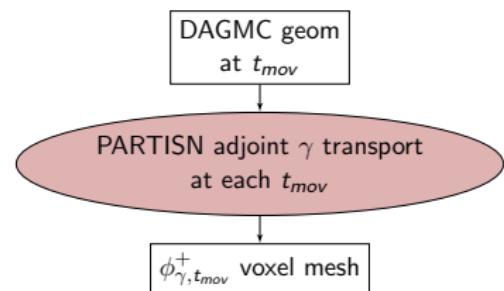


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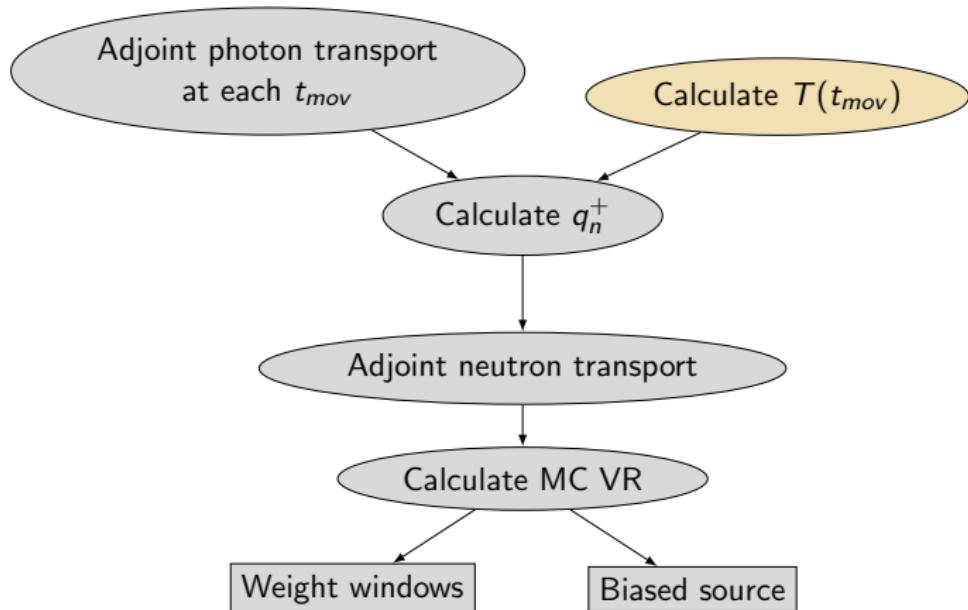
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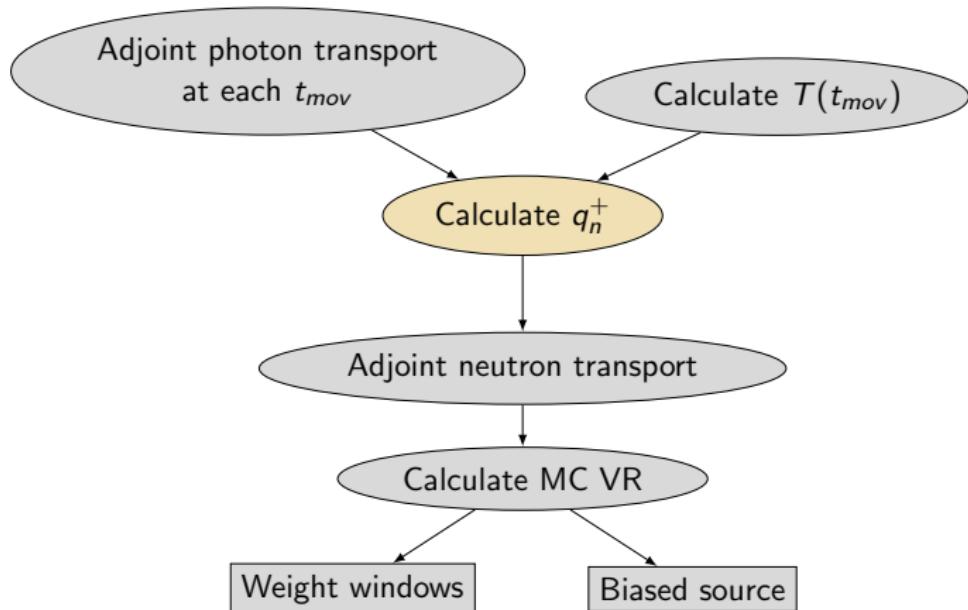
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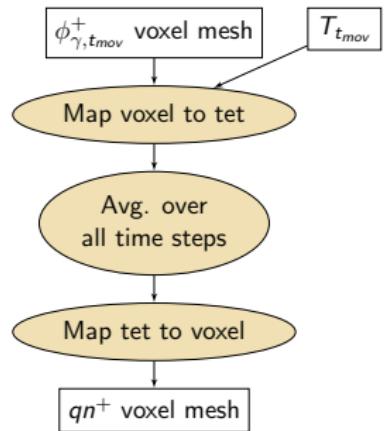
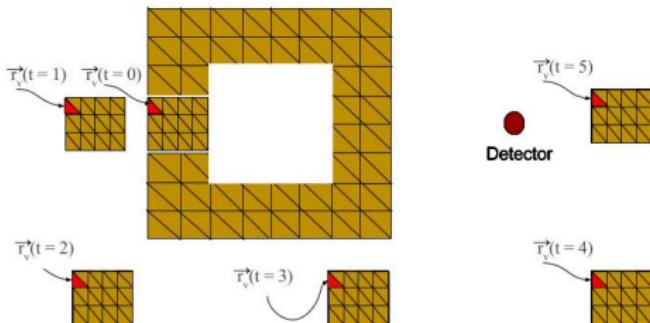
Time-integrated (T)GT-CADIS: Workflow



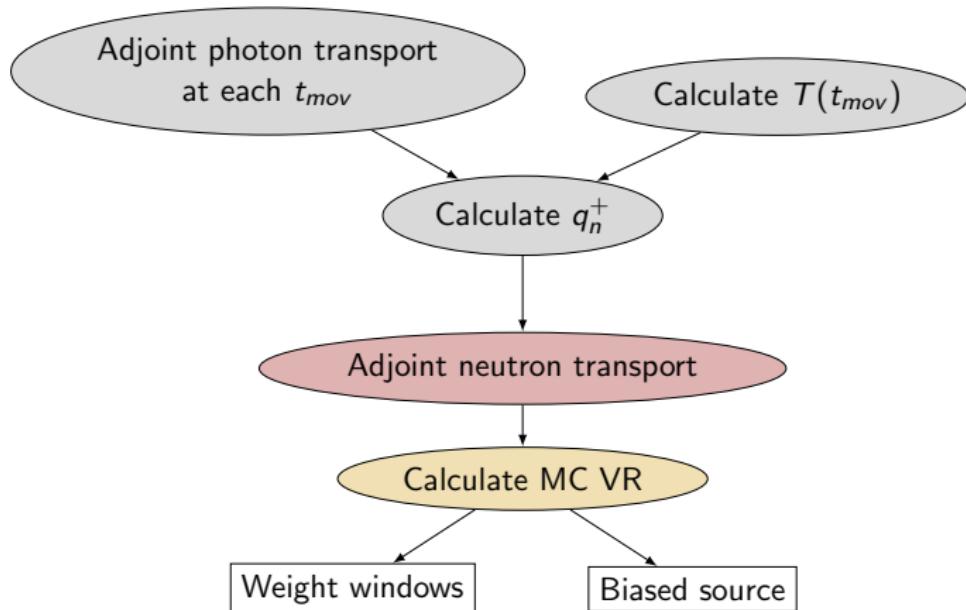
TGT-CADIS: Calculate Adjoint Neutron Source



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

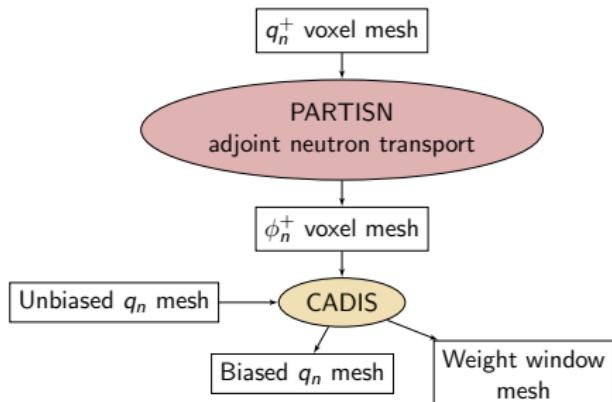


Time-integrated (T)GT-CADIS: Workflow



TGT-CADIS: Generate VR Parameters

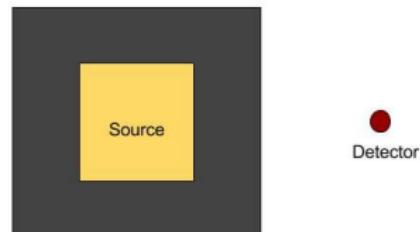
- Perform adjoint neutron transport
- Generate biased source and weight window mesh via CADIS methodology



Experiment

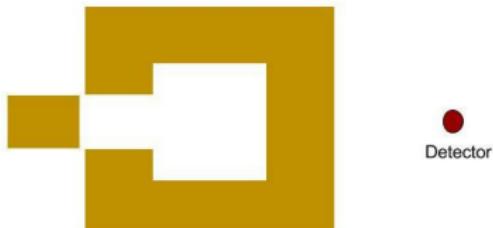
Experiment

- 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



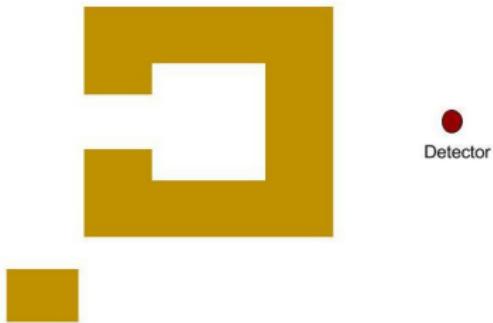
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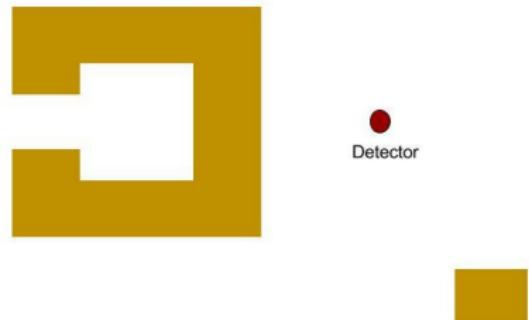
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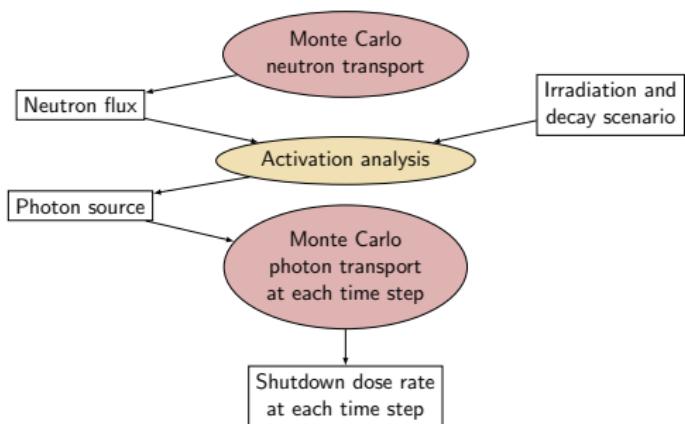
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Experiment: Toy Problem

Experimental Steps:

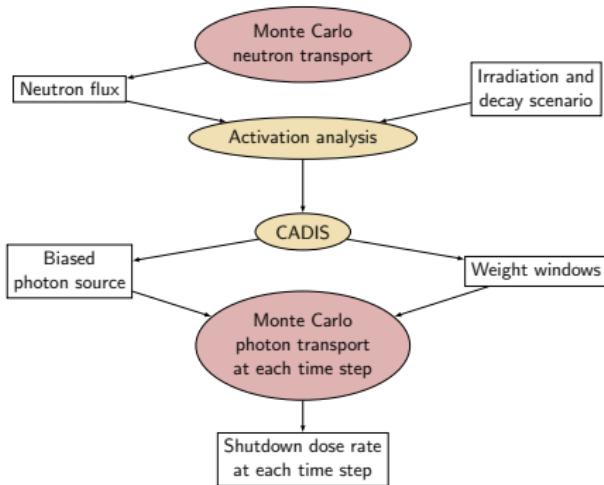
① No VR



Experiment: Toy Problem

Experimental Steps:

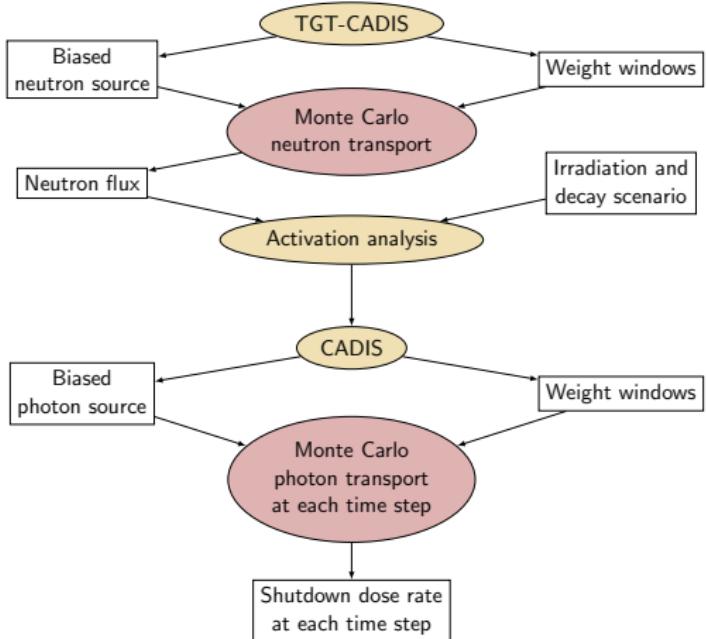
- ① No VR
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CADIS



Experiment: Toy Problem

Experimental Steps:

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



Progress

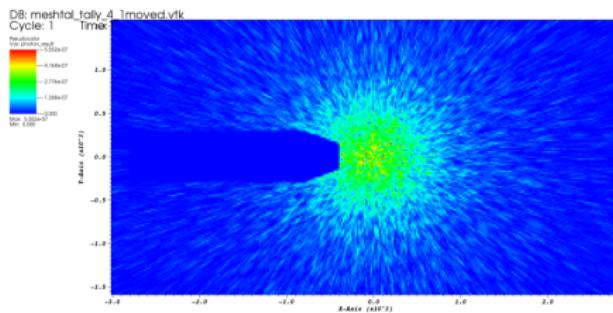


MC Moving Geometry Simulations

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

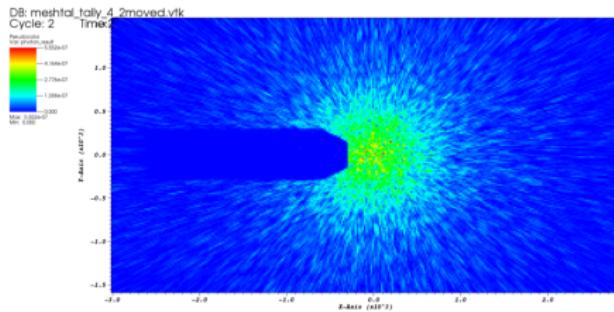
MC Moving Geometry: Stepwise Geometry Tool

- Tool to generate new geometry file at each time step during movement
- Motion data:
 - Time-dependent:
 - Translation or rotation vector
 - Duration of time
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 - Relocation:
 - Translation or rotation distance



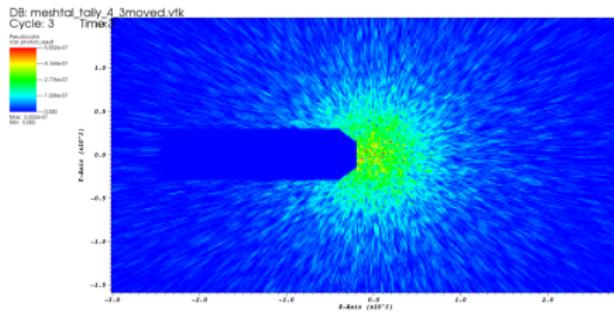
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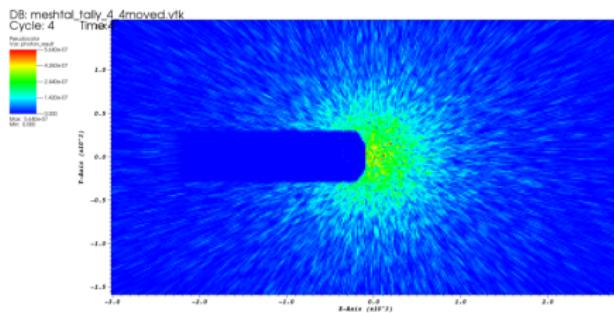
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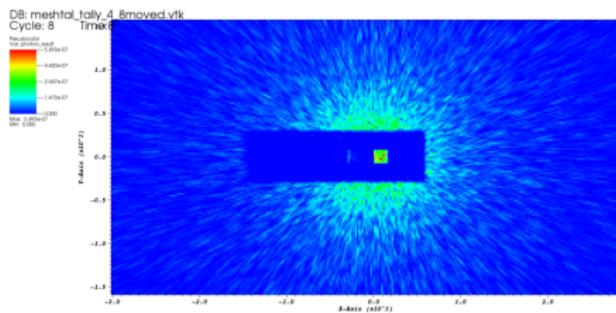
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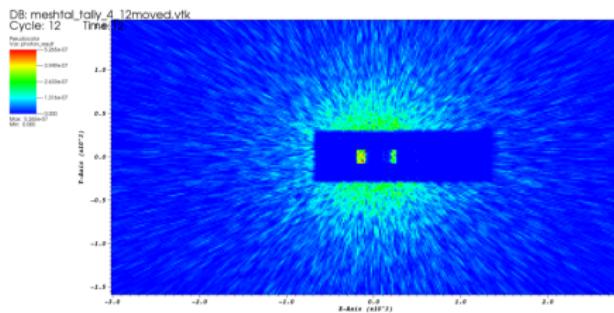
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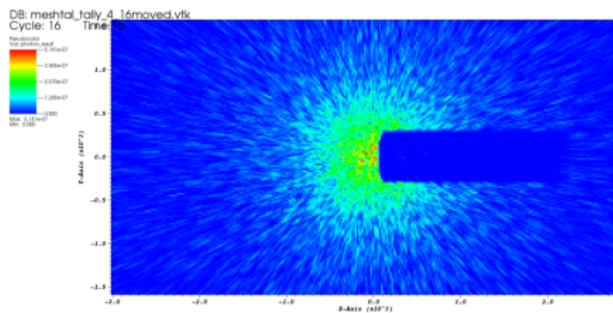
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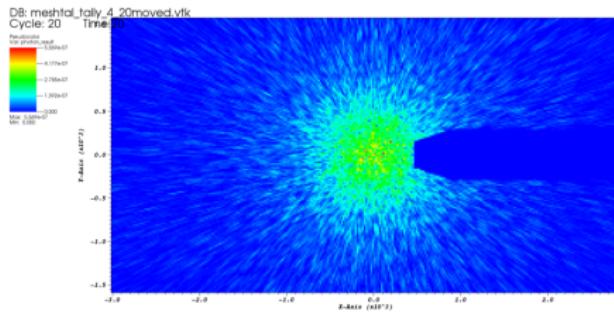
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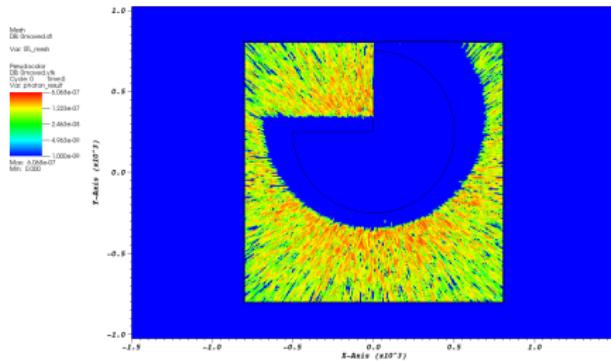
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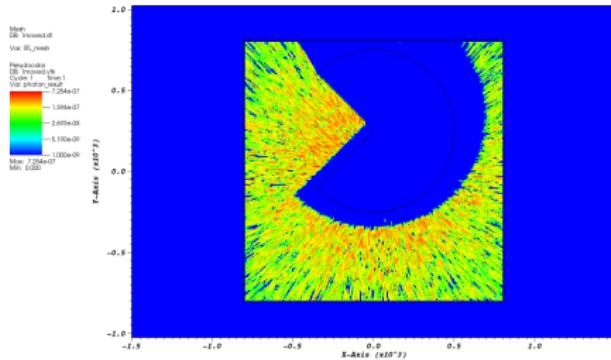
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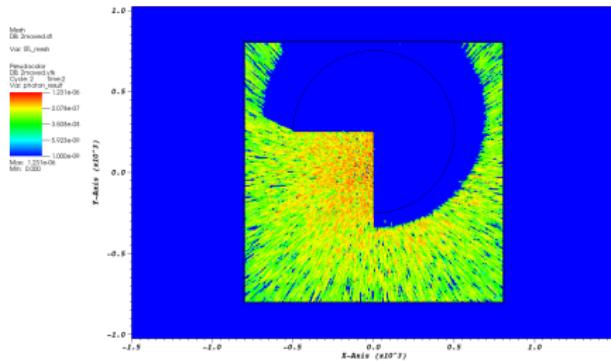
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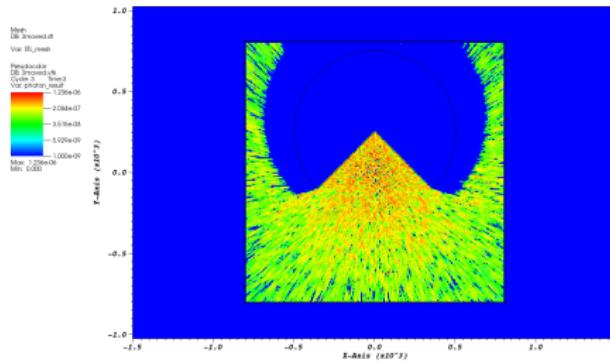
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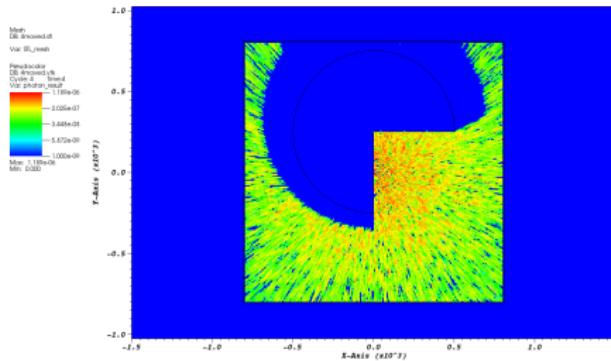
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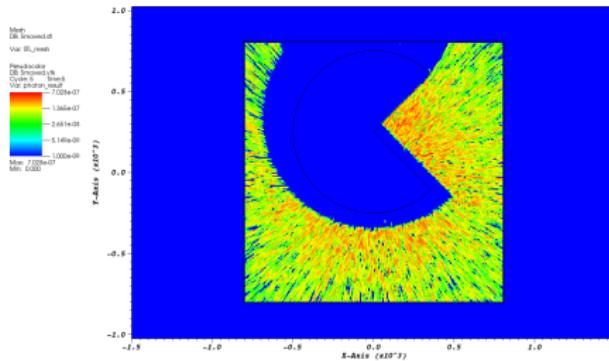
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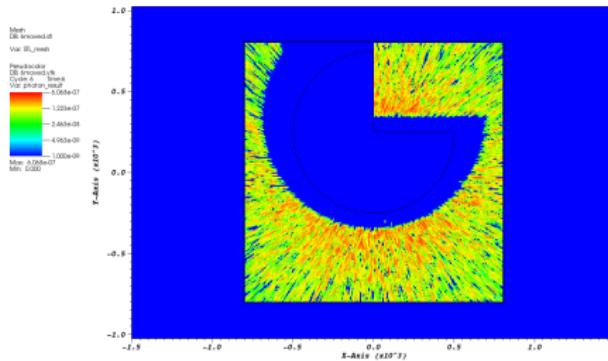
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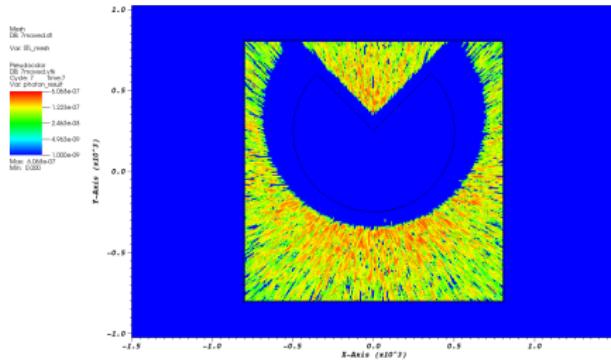
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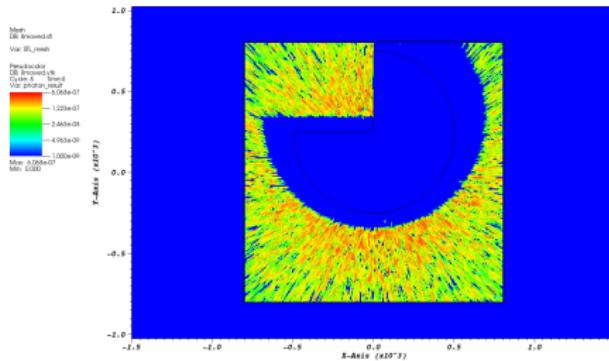
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- Functionality to apply MCNP TR(n) card data to DAGMC geometry
- Motion data:
 - Translation distance
- Separate input file containing transformations for each time step of geometry movement

Final Thoughts



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

- labels on tet mesh time slices
- Overall alignment/sizing/spacing
- Add more on moving geom progress, movie
- OBB tree optimization