Variance Reduction for Multi-physics Analysis of Moving Systems

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Preliminary Exam

Feb. 2, 2018

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Motivation

Shutdown Dose Rate (SDR) Analysis

- Fusion Energy Systems (FES)
  - Burning plasma, D-T fusion
  - ${}^2_1H + {}^3_1H \rightarrow {}^4_2He + {}^1_0n$
- Neutrons penetrate deeply into system components, causing activation
- Radioisotopes persist long after shutdown
- Important to quantify the dose caused by decay photons

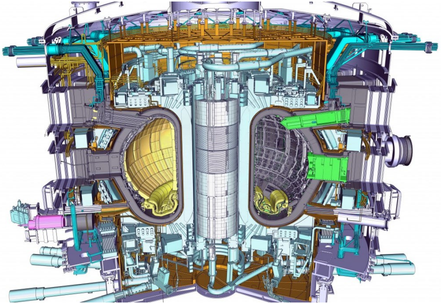
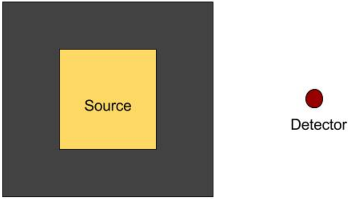


Figure 1 : Cutaway view of ITER drawing.

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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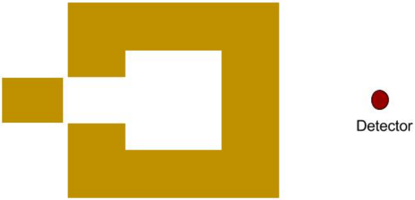

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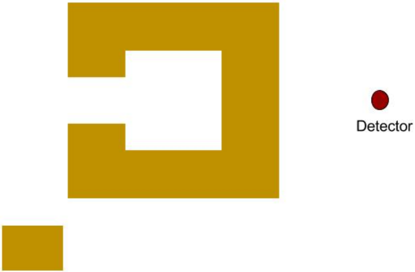

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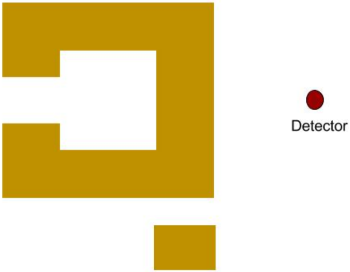

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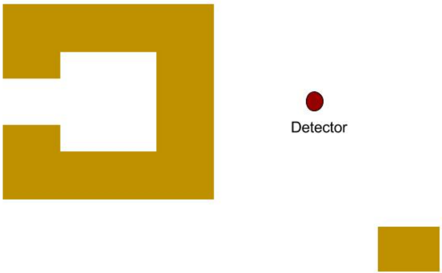

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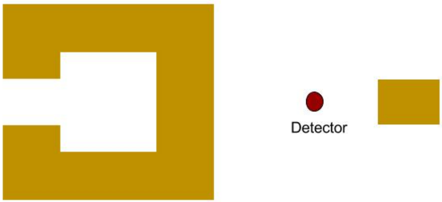

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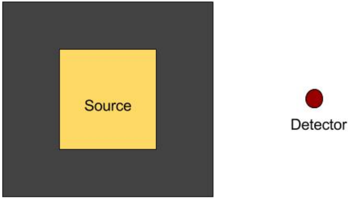


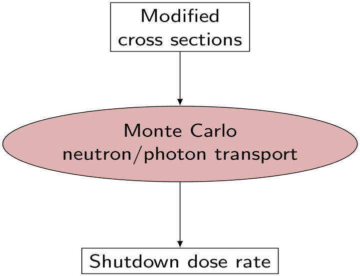
Goal

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

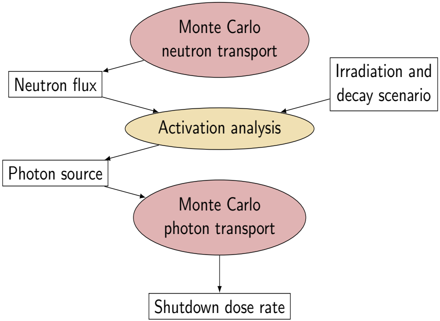
Literature Review

SDR Solution Methods

Direct 1-Step Method (D1S) [1]



Rigorous 2-Step Method (R2S) [2]



Monte Carlo Radiation Transport

- Monte Carlo (MC) method [3]:
  - Stochastic method
  - Simulate 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

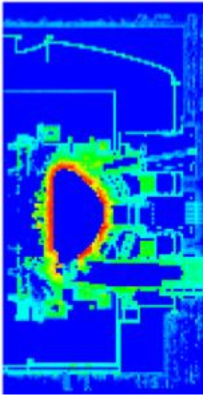


Figure 2 : Photon source in ITER tokamak building.

Error in MC Calculations

- Uncertainty in MC calculations:

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

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

- Efficiency in MC calculations:

$$FOM = \frac{1}{\Re^2 t_{proc}} \tag{2}$$

- 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

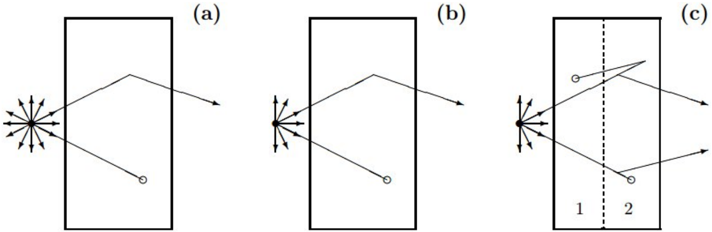


Figure 3 : a) analog b) source biasing c) splitting/rouletting [4]

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:

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

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

Adjoint:

$$\langle \Psi^+, H\Psi \rangle = \langle \Psi, H^+\Psi^+ \rangle \tag{4}$$

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

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

Hybrid Deterministic/MC VR Methods: CADIS [5]

Consistent Adjoint Driven Importance Sampling (CADIS)

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

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

- Weight window lower bounds:

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

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

Variance Reduction for SDR Analysis: MS-CADIS

Multi-**S**tep (MS)-CADIS [6]

- VR method to optimize the initial radiation transport step of a coupled, multi-step process
- When applied to SDR analysis, MS-CADIS will optimize the neutron transport step of R2S

Generalized MS-CADIS

- System of coupled, multi-physics:

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

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

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

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

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- Adjoint identities:

$$\langle \phi^{+}, q \rangle = \langle \phi, q^{+} \rangle \tag{10}$$

$$\langle \psi^{+}, b \rangle = \langle \psi, b^{+} \rangle \tag{11}$$

Generalized MS-CADIS

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

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- Solving for q^+ requires this unique relationship:

$$b(v) = \langle \sigma_b(u, v), \phi(u) \rangle \tag{15}$$

Generalized MS-CADIS

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

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

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- MS-CADIS adjoint primary source:

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

Generalized MS-CADIS

- MS-CADIS adjoint primary source:

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

- Apply 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: $\sigma_b(u,v) \equiv T_{n,\gamma}(E_n, E_\gamma)$

Groupwise **T**ransmutation (GT)-CADIS [7]

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

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

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

$$q_\gamma(E_\gamma) = \langle T(E_n, E_\gamma), \phi_n(E_n) \rangle \tag{21}$$

Variance Reduction for SDR Analysis: GT-CADIS

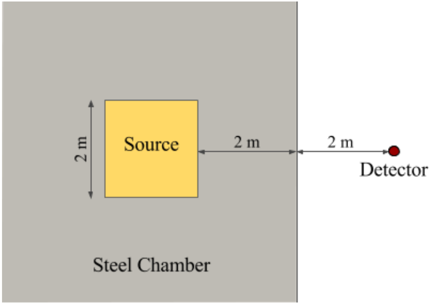
Groupwise **T**ransmutation (GT)-CADIS [7]

- Calculate T:
  1. Irradiate each material with neutrons from a single energy group, g
  2. Record resulting photon emission in each energy group, h

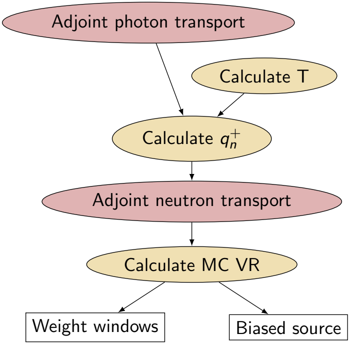
$$T_{g,h} = \frac{q_{\gamma,h}(\phi_{n,g})}{\phi_{n,g}} \tag{22}$$

GT-CADIS Demonstration: Problem Description

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



GT-CADIS workflow



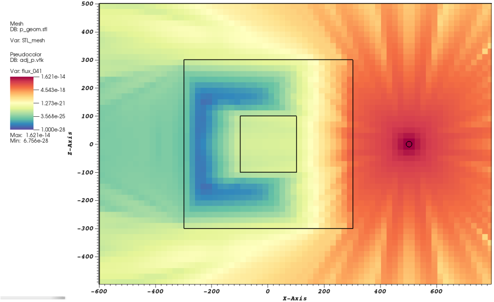
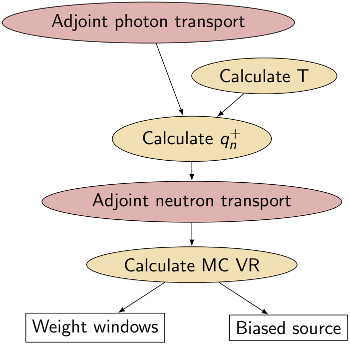


Figure 4 : Adjoint photon flux

GT-CADIS Demonstration: Adjoint Neutron Transport

GT-CADIS workflow



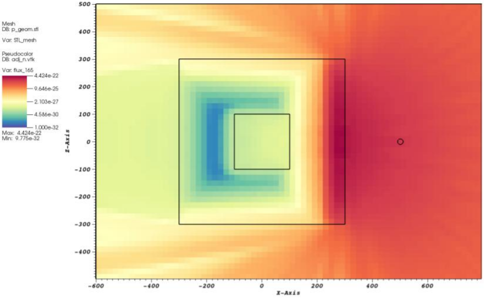


Figure 5 : GT-CADIS adjoint neutron flux. Functions as importance map.

GT-CADIS Demonstration: VR Parameters

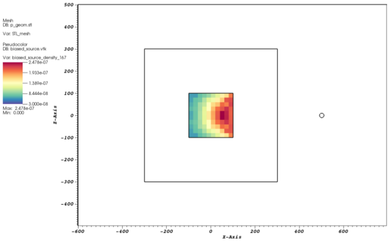


Figure 6 : Biased neutron source generated with GT-CADIS method.

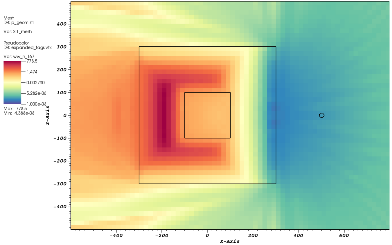


Figure 7 : Weight window mesh generated with GT-CADIS method.

GT-CADIS Efficiency

- 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

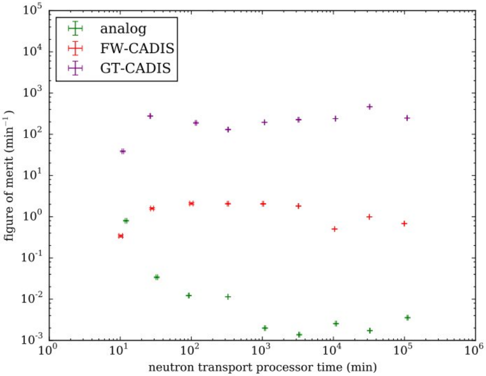


Figure 8 : FOM as function of neutron transport processor time. [8]

GT-CADIS Demonstration

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

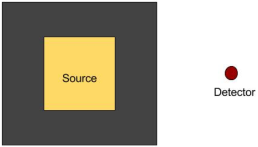


Figure 9 : Demo model.

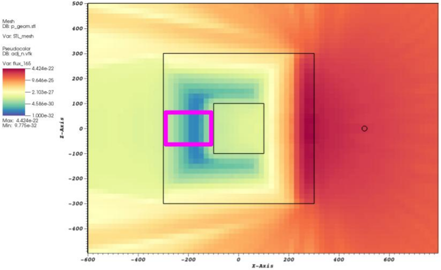


Figure 10 : GT-CADIS adjoint neutron flux. Functions as importance map.

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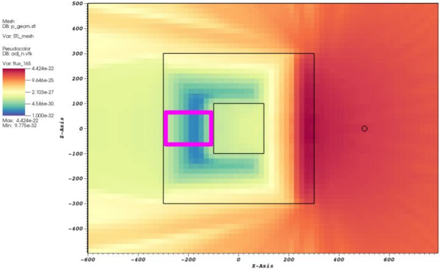

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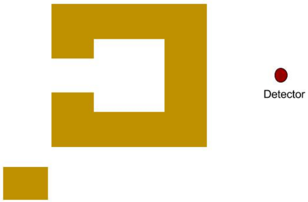

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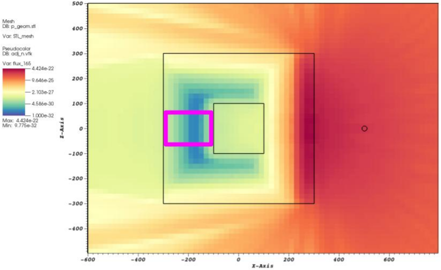

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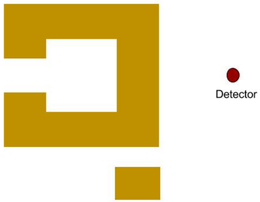

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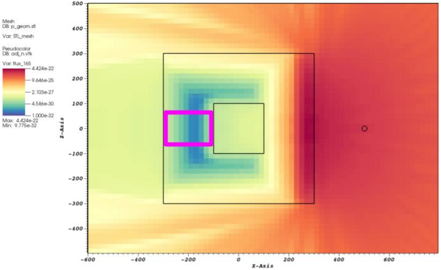

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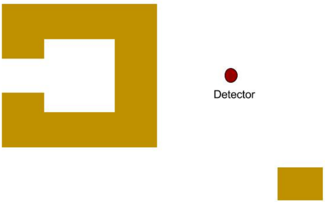

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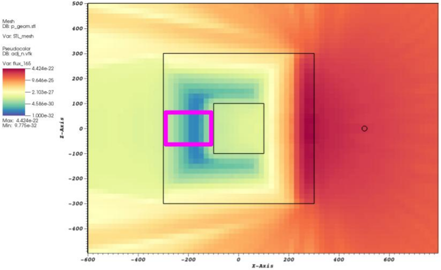

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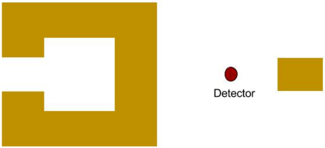

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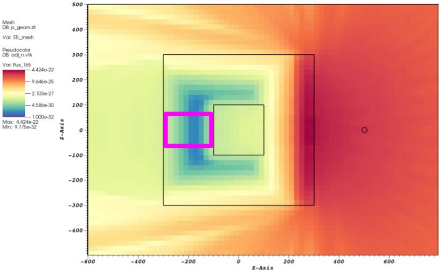

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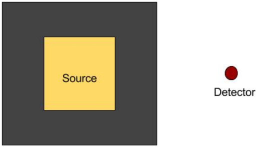

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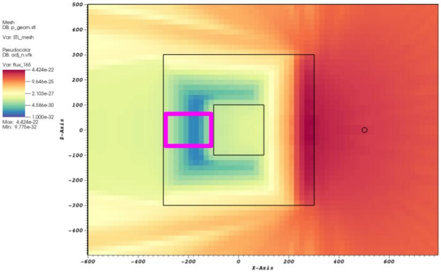

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Moving Geometries and Sources

MCNP6 Moving Objects [9], [10]

- 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)[11]

- 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 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

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

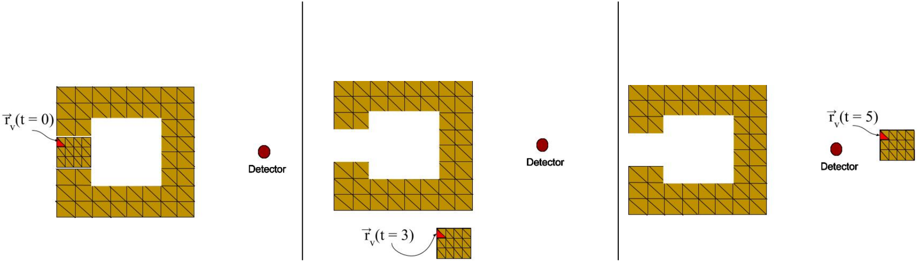
- Movement after shutdown, during photon transport:

Need 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: $\overrightarrow{r}_v(t)$
- Combine with T and integrate over time

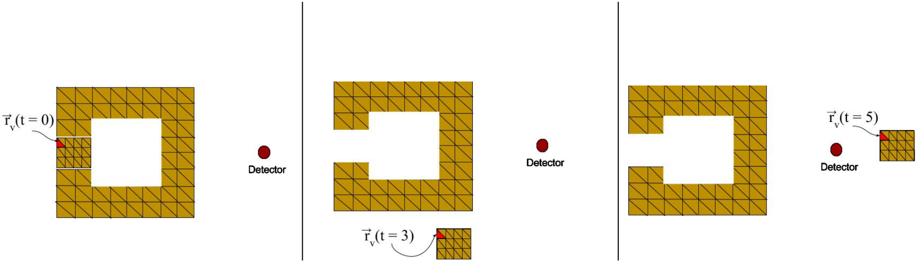
$$q_n^+ = \frac{\int_t \phi_\gamma^+(\overrightarrow{r}_v(t), t)\, T_v(t)\, dt}{\int_t dt} \tag{23}$$



TGT-CADIS: Adjoint Neutron Source

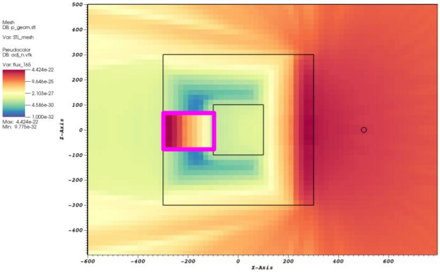
- Discrete form:
  - t_{mov} is the time step
  - Δt_{mov} is the duration of the time step
  - t_{tot} is the total number of time steps

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

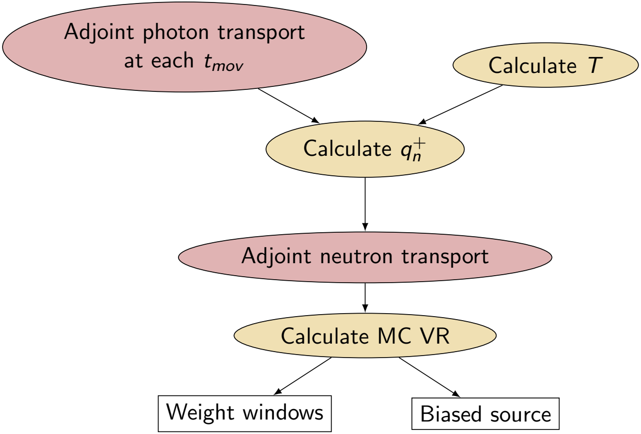


Time-integrated (T)GT-CADIS

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



Time-integrated (T)GT-CADIS: Workflow

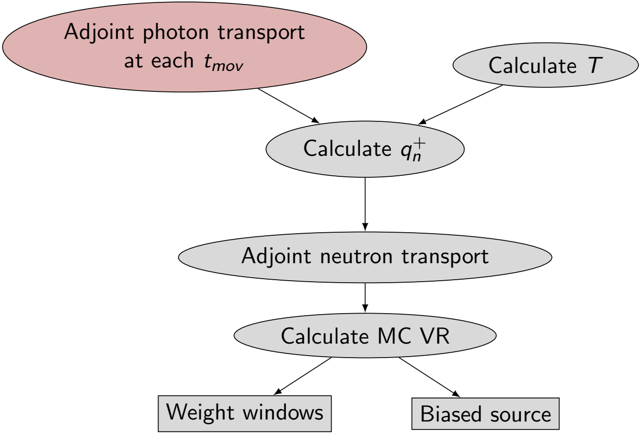


Implementation Plan

Software

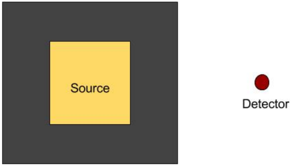
- **PARTISN**: **PAR**allel, **TI**me-Dependent **SN** [12]
  - Deterministic adjoint transport
- **DAGMC**: **D**irect **A**ccelerated **G**eometry [13], **M**onte **C**arlo, **MCNP**: **M**onte **C**arlo **N** **P**article [3]
  - Forward MC transport on CAD geometry
- **ALARA**: **A**nalytic and **L**aplacian **A**daptive **R**adioactivity **A**nalysis [14]
  - Activation analysis
- **PyNE**: **Py**thon for **N**uclear **E**ngineering [15]
  - Tools to support transport
- **MOAB**: **M**esh-**O**riented dat**AB**ase [16]
  - Moving geometries

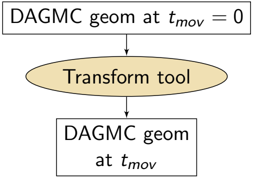
Time-integrated (T)GT-CADIS: Workflow



TGT-CADIS: Generate Stepwise Geometries

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





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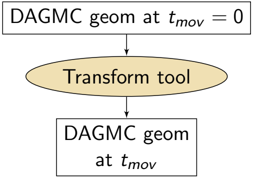

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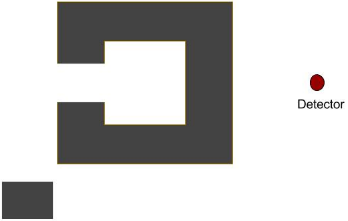

DAGMC geom at $t_{mov} = 0$

↓

Transform tool

↓

DAGMC geom at t_{mov}

TGT-CADIS: Generate Stepwise Geometries

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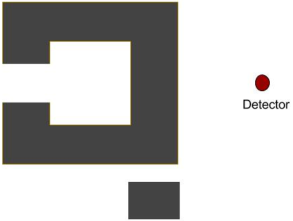

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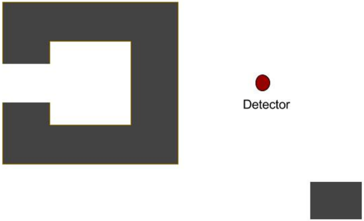

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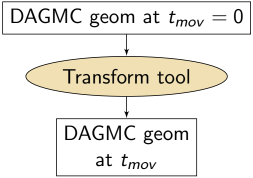
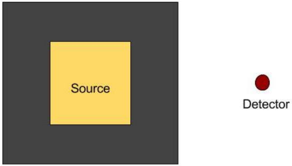
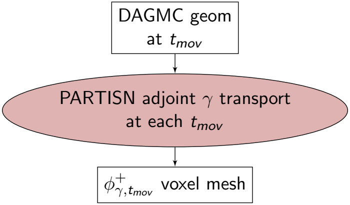


TGT-CADIS: Generate VR Parameters

- Perform adjoint photon transport at each time step





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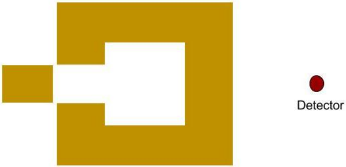

DAGMC geom at t_{mov}

↓

PARTISN adjoint γ transport at each t_{mov}

↓

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

TGT-CADIS: Generate VR Parameters

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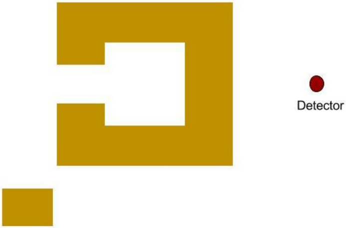

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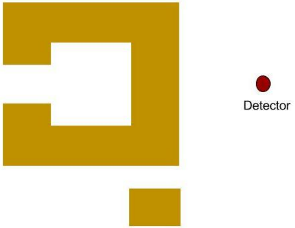

DAGMC geom at t_{mov}

$\downarrow$

PARTISN adjoint γ transport at each t_{mov}

$\downarrow$

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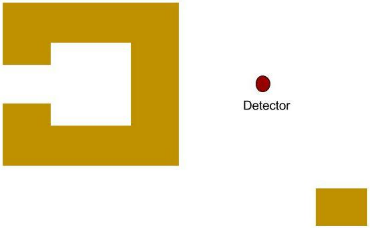

DAGMC geom at t_{mov}

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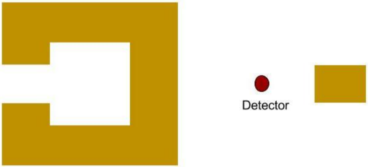

DAGMC geom at t_{mov}

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PARTISN adjoint γ transport at each t_{mov}

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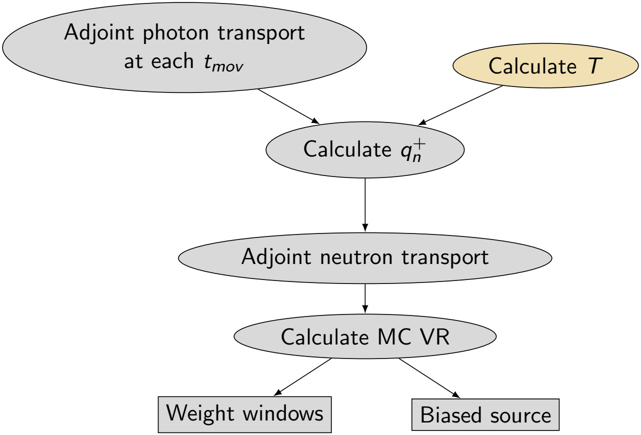
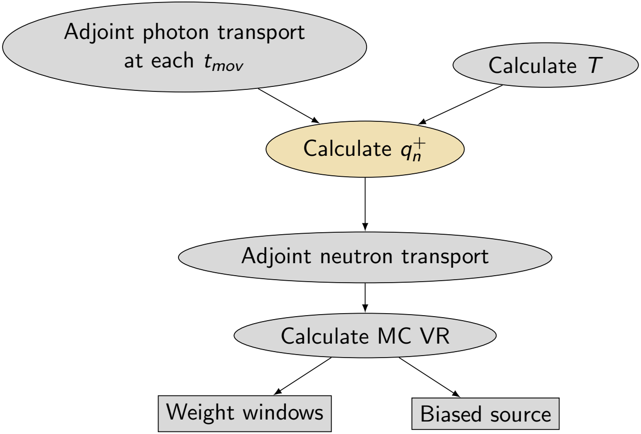
$\phi^{+}_{\gamma,t_{mov}}$ voxel mesh

Time-integrated (T)GT-CADIS: Workflow

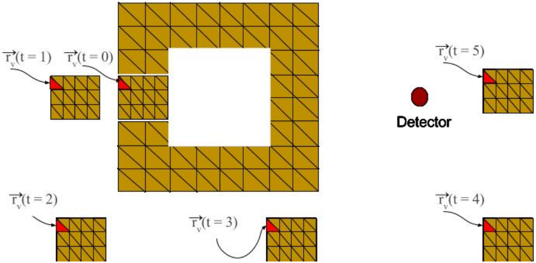


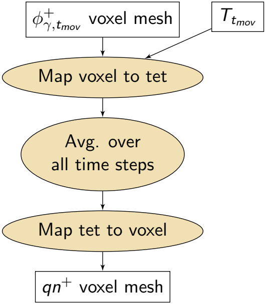
Time-integrated (T)GT-CADIS: Workflow



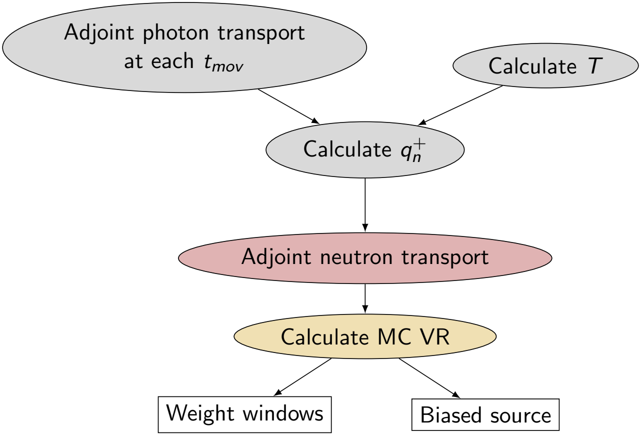
TGT-CADIS: Calculate Adjoint Neutron Source

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



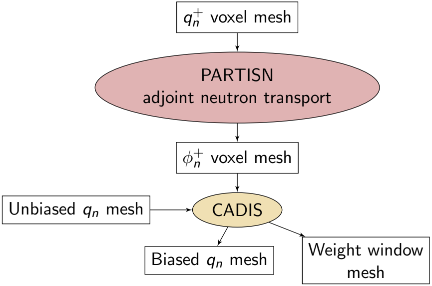


Time-integrated (T)GT-CADIS: Workflow



TGT-CADIS: Generate VR Parameters

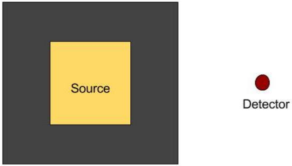
- Perform adjoint neutron transport
- Generate biased source and weight window mesh via CADIS methodology



Experiment

Experiment: Toy Problem

- Assess efficiency of TGT-CADIS
  - Steel chamber with moving component
  - Incrementally add optimization
  - Calculate figure of merit (FOM)



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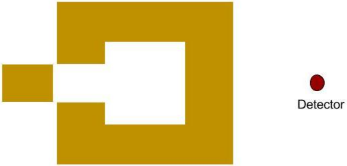

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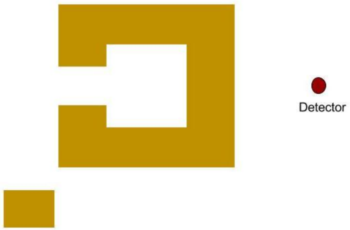

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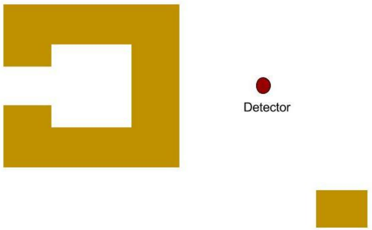

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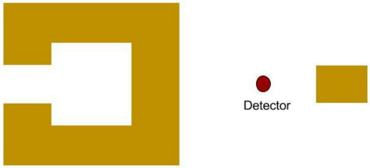
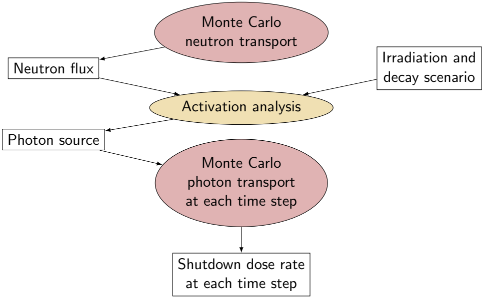


Experiment: Toy Problem

Experimental Steps:

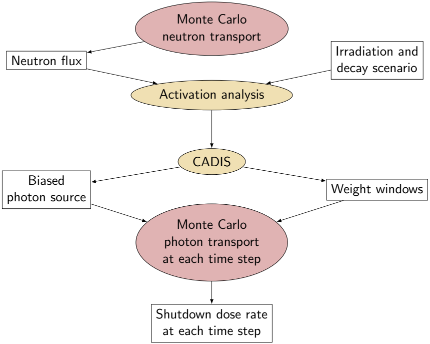
1. No VR



Experiment: Toy Problem

Experimental Steps:

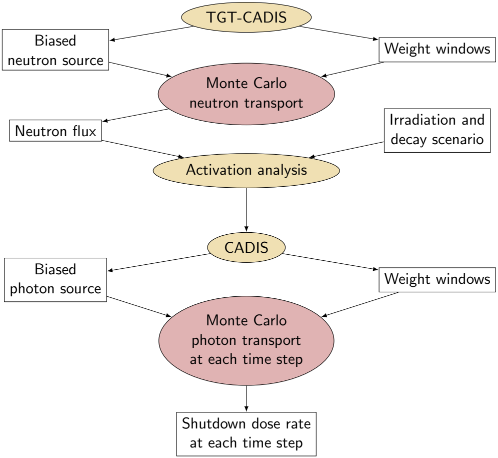
1. No VR
2. Photon VR: CADIS



Experiment: Toy Problem

Experimental Steps:

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



Full-scale Demonstration

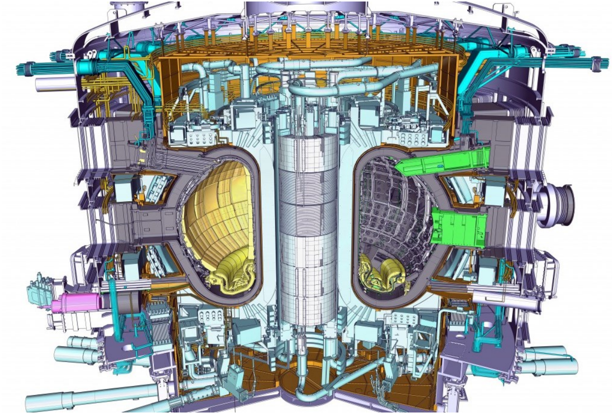


Figure 11 : Cutaway view of ITER drawing.

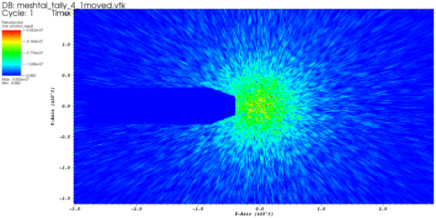
Progress

MC Moving Geometry Simulations

- Capabilities to update position of geometry based on user-defined motion data
  1. Production of step-wise geometry files
  2. DAGMCNP update
- Common functionality:
  - 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
- Motion data:
  - Time-dependent:
    - Translation or rotation vector
    - Duration of time
    - Number of time steps
  - Relocation:
    - Translation or rotation distance



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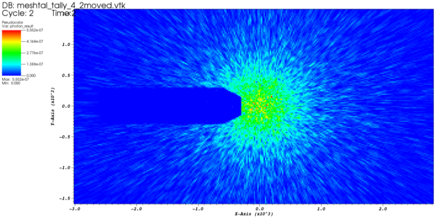

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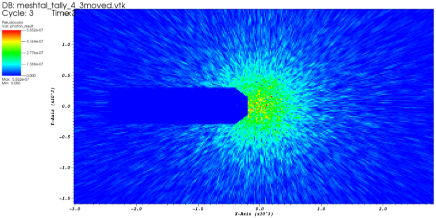

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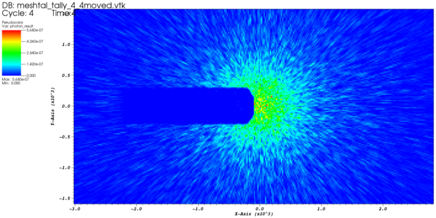

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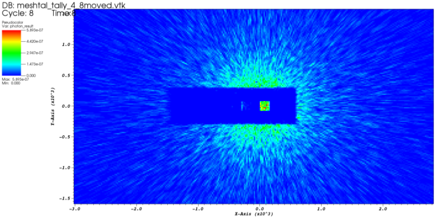

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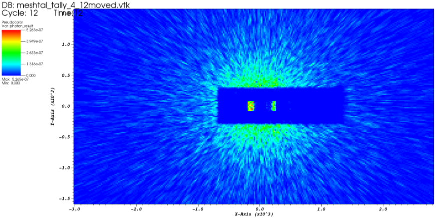

MC Moving Geometry: Stepwise Geometry Tool

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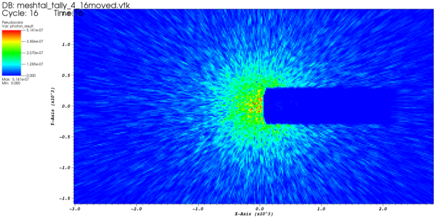

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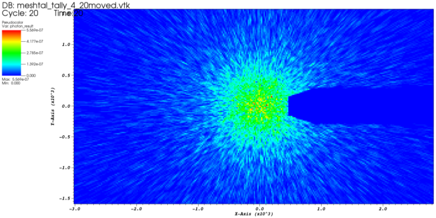

Moving Geometries: DAGMCNP Update

- Functionality to apply MCNP TR(n) card data to DAGMC geometry
- Motion data:
  - Transformation 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 time steps of geometry movement

Limitations

- Geometry movement tools do not treat object kinetics
  - User must be careful to not cause overlap in components
- Can only move components that do not share a surface with any other components

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 optimize SDR analysis in static FES
- **TGT-CADIS** aims to provide the capabilities necessary to **optimize** the calculation of the **SDR** during operations that involve activated components **moving** around the facility

Questions?

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