CAAS Modeling with SCALE

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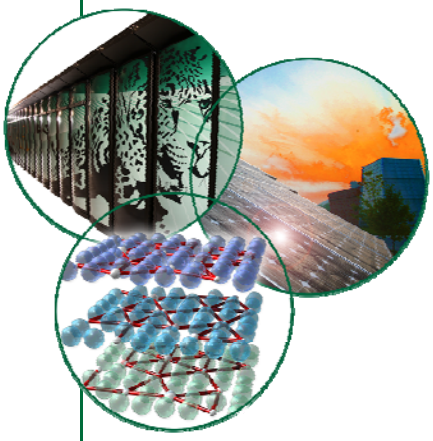

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CAAS Problems

- Criticality accident alarm systems are difficult problems because they consist of
  - Criticality calculation
  - Deep penetration shielding calculation
  - May require "answer everywhere"
- Past approaches include
  - Point source, point-kernel, one-dimensional
  - Build-up factors
  - Three-dimensional discrete ordinates
  - Very long 3-D Monte Carlo

Capabilities in SCALE 6

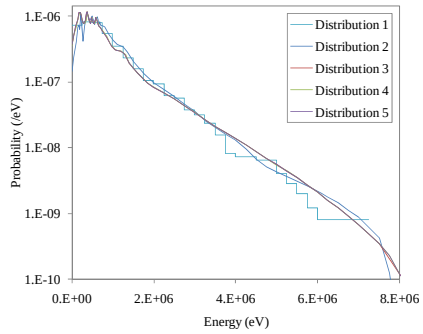
- KENO Family of Criticality Codes
  - KENO-Va Simple geometries, multi-group
  - KENO-VI Quadratic solid geometry, multi-group
  - KENO-CE Quadratic solid geometry, cont. energy
- MAVRIC Shielding Sequence
  - Hybrid method: uses approximate DO adjoint to form weight windows and biased source for detailed MC (uses the CADIS method)
  - Monaco Functional Module: fixed source MC, same geometry and cross sections (MG) as KENO-VI
  - Forward-weighted CADIS for "answer everywhere"

CAAS Capability in SCALE 6

- Step One – KENO-VI (MG) calculation
  - Standard criticality problem
  - Include as much detail as required
  - New option to save the fission distribution, $f(\vec{r},E)$, as a mesh-based source
- Step Two – MAVRIC shielding calculation
  - Use mesh-based fission source
  - Optionally add fission photons
  - Include building-level details and fine details near critical assembly
  - Use CADIS or FW-CADIS to calculate detector responses

Fission Photons

- 22 isotopes in ENDF/B-VII.0
- 5 distributions
- Multipliticity: 6.31 to 8.18



Californium 98											Cf250 1	Cf251 1
Berkelium 97												
Curium 96							Cm242 5				Cm248 1	
Americium 95							Am241 3		Am243 5			
Plutonium 94						Pu239 4	Pu240 4	Pu241 1	Pu242 5	Pu243 1		
Neptunium 93					Np237 2							
Uranium 92	U232 1	U233 4	U234 1	U235 2	U236 1	U237 1	U238 1	U239 1	U240 1	U241 1		

KENO-VI Calculation

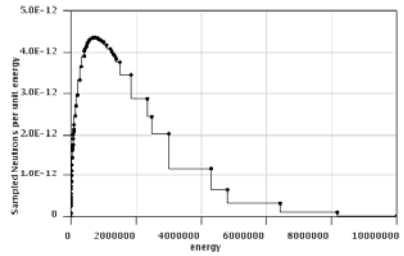
- CSAS6 Sequence
  - User supplies mesh grid and
  - Sets a flag to save fission source $f(\vec{r},E)$

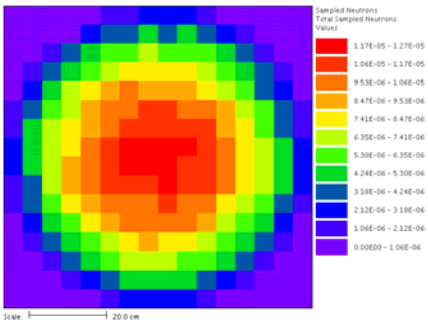
```
'-----------------------------------------------
' Parameters Block
'-----------------------------------------------
read parameters
    ...
    cds=yes
end parameters

'-----------------------------------------------
' Grid Block - mesh grid for source
'-----------------------------------------------
read grid 1
    xmin=-10.0  xmax=10.0  numXcells=10
    ymin=-10.0  ymax=10.0  numYcells=10
    zplanes -10 -8 -6 -4 -2 -1 0 1 2 4 6 8 10 end
end grid
```

KENO-VI Calculation

- Output
  - Multiplication k_{eff}
  - Neutrons per fission $\bar{\nu}$
  - Fission source distribution

JAERI STACY $UO_2(NO_3)_2$
leu-sol-therm-020





MAVRIC Calculation

- Use the KENO-VI generated fission source
  - To optionally add fission photons, the user specifies the ZAID and the value for $\bar{\nu}$

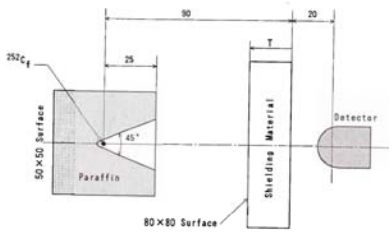
```
'-----------------------------------------------
' Source Block – for 1e18 fissions
'-----------------------------------------------
read sources
    src 1
        meshSourceFile="fissionSource.msm"
        origin x=280 y=300 z=100
        strength=2.6e18
        fissPhotonZAID=92235 nu-bar=2.6
    end src
end sources
```

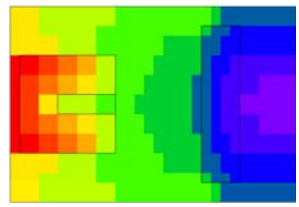
- Use automated variance reduction (importance map and biased source) to optimize detector response FOM

CADIS Methodology

Consistent Adjoint Driven Importance Sampling

An importance map and biased source are developed that optimize the calculation of a specific tally.





- Ali Haghighat and John C. Wagner, "Monte Carlo Variance Reduction with Deterministic Importance Functions," *Progress in Nuclear Energy* 42(1), 25-53, (2003).

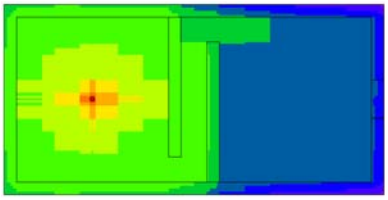
CADIS Methodology in MAVRIC

- Nearly automatic – user supplies only
  - Mesh grid (coarse) for the discrete ordinates calculations
  - Adjoint source, which corresponds to the tally to optimize

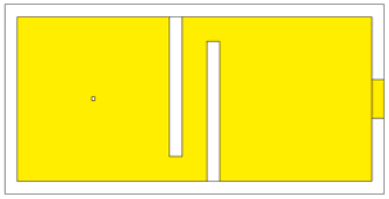
Define the adjoint source	$q^+(\vec{r},E)=\sigma_d(\vec{r},E)$
Solve for the adjoint flux	$\phi^+(\vec{r},E)$
Estimate detector response	$c=\iint q(\vec{r},E)\,\phi^+(\vec{r},E)\,d\vec{r}dE$
Construct weight windows	$\overline{w}(\vec{r},E)=\dfrac{c}{\phi^+(\vec{r},E)}$
Construct biased source	$\hat{q}(\vec{r},E)=\dfrac{1}{c}q(\vec{r},E)\,\phi^+(\vec{r},E)$

Optimizing Multiple Tallies

- In order to calculate multiple tallies (or a mesh tally), calculate the adjoint flux from multiple adjoint sources.



$D(\vec{r},E)$

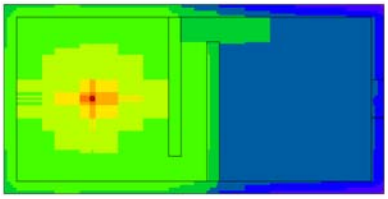


$q^{+}(\vec{r},E)$

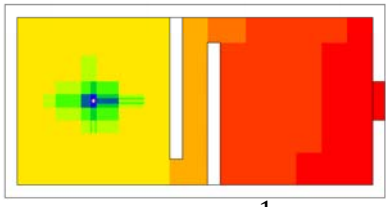
- To compute more uniform relative uncertainties in the tallies (or across a mesh tally), weight each adjoint source inversely by the expected tally values

Optimizing Multiple Tallies

- In order to calculate multiple tallies (or a mesh tally), calculate the adjoint flux from multiple adjoint sources.



$D(\vec{r},E)$



$$q^{+}(\vec{r},E) \propto \frac{1}{D(\vec{r},E)}$$

- To compute more uniform relative uncertainties in the tallies (or across a mesh tally), weight each adjoint source inversely by the expected tally values

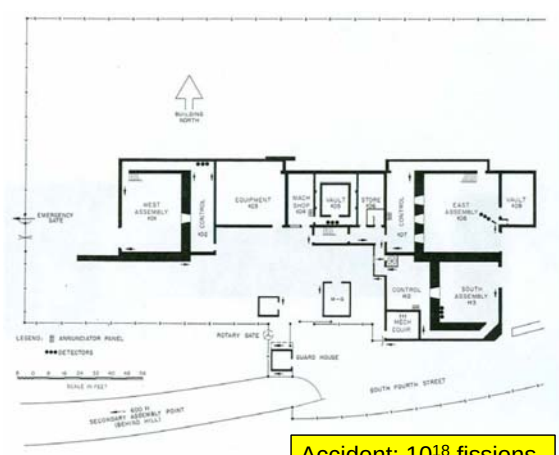
Forward-Weighted CADIS

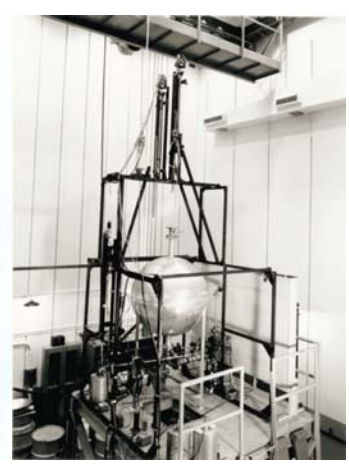
FW-CADIS in MAVRIC

Estimate the forward flux	$\phi(\vec{r},E)$
Define the adjoint source	$q^{+}(\vec{r},E)=\dfrac{\sigma_d(\vec{r},E)}{\iint \sigma_d(\vec{r},E)\,\phi(\vec{r},E)\,d\vec{r}\,dE}$
Solve for the adjoint flux	$\phi^{+}(\vec{r},E)$
Estimate "detector" response	$c=\iint q(\vec{r},E)\,\phi^{+}(\vec{r},E)\,d\vec{r}dE$
Construct weight windows	$\overline{w}(\vec{r},E)=\dfrac{c}{\phi^{+}(\vec{r},E)}$
Construct biased source	$\hat{q}(\vec{r},E)=\dfrac{1}{c}q(\vec{r},E)\,\phi^{+}(\vec{r},E)$

Example Problem

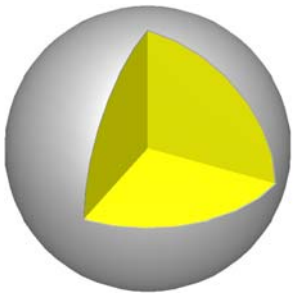
- Simulation of u233-sol-therm-008 experiment in the Oak Ridge Critical Experiments Facility





Accident: 10^{18} fissions

KENO-VI Model



```
'uranyl nitrate
    u-233  1 0.0 3.3441E-05 end
    u-234  1 0.0 5.2503E-07 end
    u-235  1 0.0 1.0184E-08 end
    u-238  1 0.0 2.5474E-07 end
    th-232 1 0.0 1.4756E-07 end
    n      1 0.0 7.4943E-05 end
    h      1 0.0 6.6357E-02 end
    o      1 0.0 3.3469E-02 end

'type 1100 aluminum
    al     2 0.0 5.9881E-02 end
    mn     2 0.0 1.4853E-05 end
    fe     2 0.0 1.0958E-04 end
    cu     2 0.0 5.1364E-05 end
    si     2 0.0 2.1790E-04 end
```

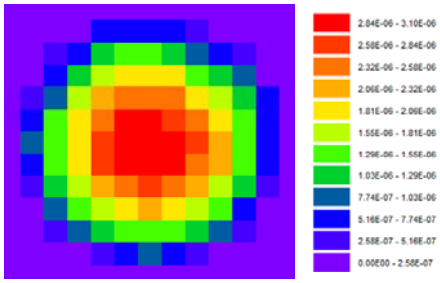
```
sphere 21  61.011
sphere 22  61.786
media 1 1  21     vol=951290.2363
media 2 1  22 -21 vol=36714.09735
```

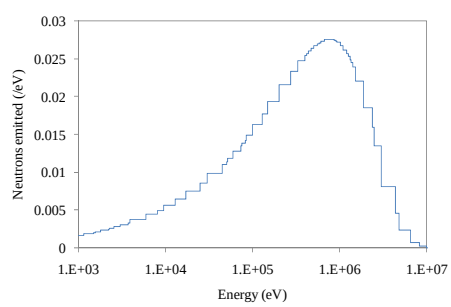
```
read gridGeometry 1
    xplanes -61.011 -55 -45 -35 -25 -15 -5 5 15 25 35 45 55 61.011 end
    yplanes -61.011 -55 -45 -35 -25 -15 -5 5 15 25 35 45 55 61.011 end
    zplanes -61.011 -55 -45 -35 -25 -15 -5 5 15 25 35 45 55 61.011 end
end gridGeometry
```


KENO-VI Results

- Five minute calculation

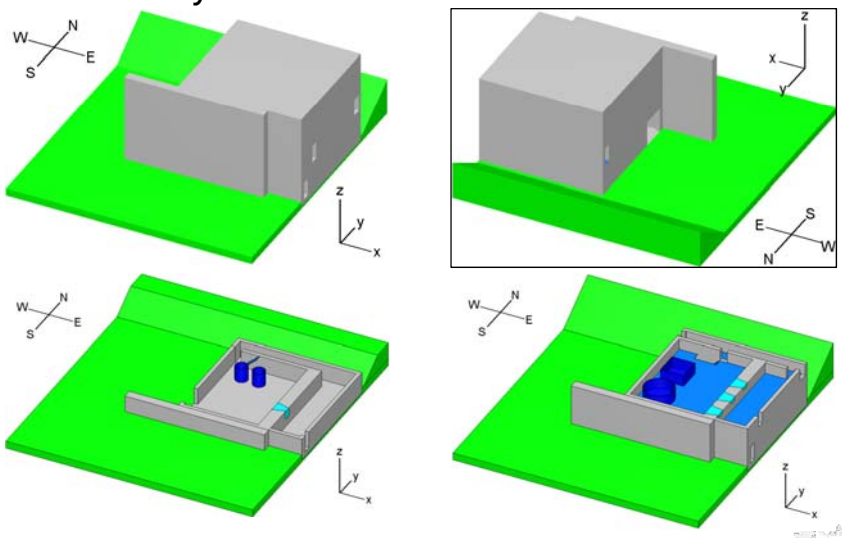
Quantity		Value	Uncertainty
k_{eff}	best estimate system k-eff	1.00204	0.00050
$\bar{\nu}$	system nu bar	2.49719	5.63E-07





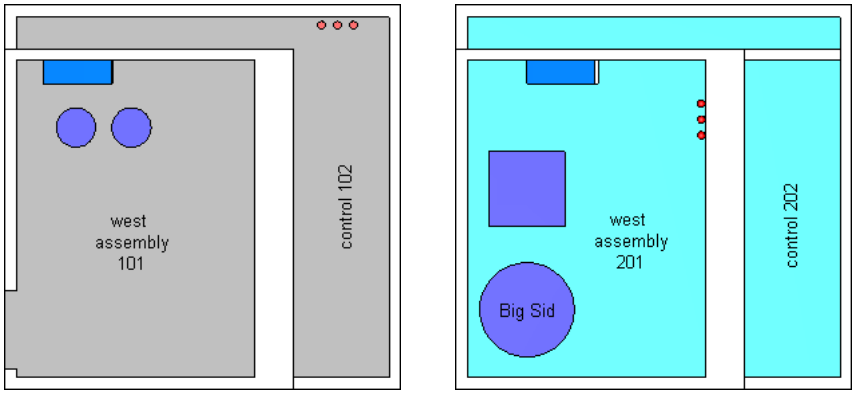
MAVRIC Model

- West Assembly modeled



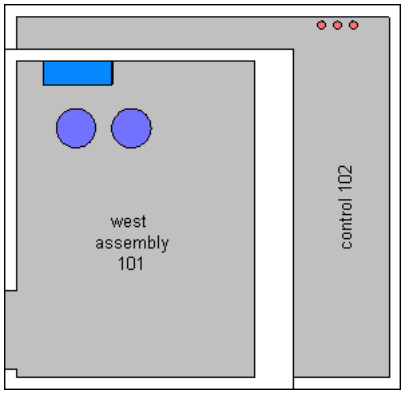
MAVRIC Model

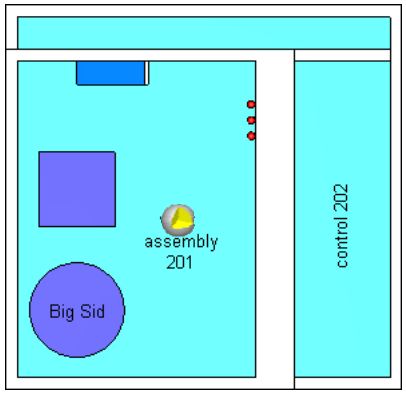
- Detectors on both levels of west assembly



MAVRIC Model

- U233-sol-therm-008 model placed in center of upper level



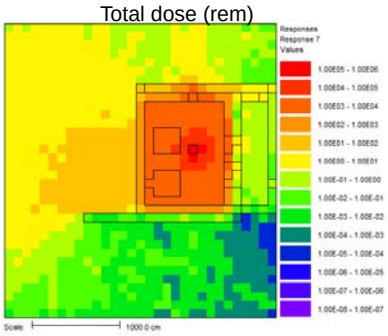


Analog Calculations

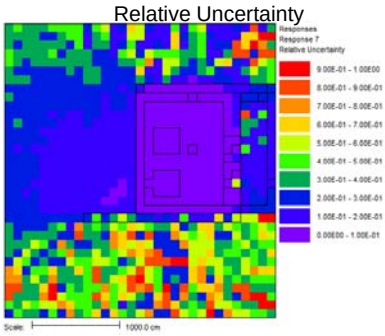
- 7.5 CPU•days
  - Using only implicit capture
  - Neutron dose~10*photon dose
  - Will take too long to get 5% r.u.

Level	Detector	Total Dose Value (rem)	Total Dose Relative Uncertainty
lower	west	2.1	17%
	center	2.0	32%
	east	2.6	29%
upper	south	5.95E+03	4.0%
	center	4.34E+03	4.5%
	north	3.86E+03	4.7%

Total dose (rem)



Relative Uncertainty



Variance Reduction in MAVRIC

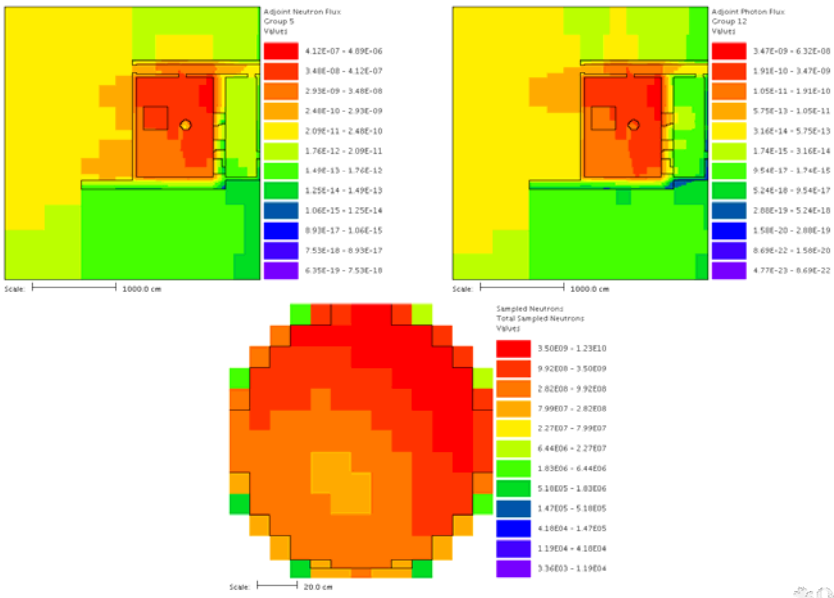
Three calculations, to optimize dose calculation in:

A. Upper level detectors
B. Lower level detectors
C. Mesh tally in and around west assembly bay

For A and B, the CADIS method was used to generate importance maps and biased sources:

Define the adjoint source	$q^{+}(\vec{r},E)=\sigma_d(\vec{r},E)$
Solve for the adjoint flux	$\phi^{+}(\vec{r},E)$
Estimate detector response	$c=\iint q(\vec{r},E)\,\phi^{+}(\vec{r},E)\,d\vec{r}dE$
Construct weight windows	$\overline{w}(\vec{r},E)=\dfrac{c}{\phi^{+}(\vec{r},E)}$
Construct biased source	$\hat{q}(\vec{r},E)=\dfrac{1}{c}q(\vec{r},E)\,\phi^{+}(\vec{r},E)$

A. Upper Level Detectors



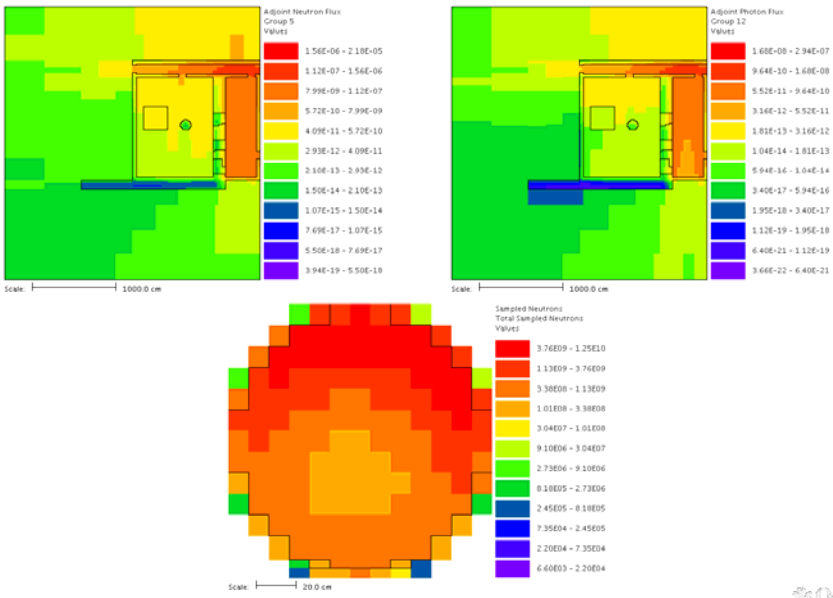
A. Upper Level Detectors

- Using CADIS in MAVRIC
  - 26 minute adjoint DO calculation with Denovo
  - 162 minute forward Monte Carlo calculation with Monaco
    - Using mesh-based weight windows
    - Using mesh-based biased source

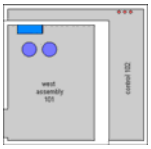
	Neutron		Photon		Total	
Detector	Value (rem)	Relative Uncertainty	Value (rem)	Relative Uncertainty	Value (rem)	Relative Uncertainty
south	4.70E+03	0.9%	676	3.1%	5.38E+03	0.8%
center	3.96E+03	0.9%	601	3.4%	4.56E+03	0.9%
north	3.49E+03	1.0%	469	3.6%	3.96E+03	1.0%

FOM Improvement: ~1300

B. Lower Level Detectors



B. Lower Level Detectors



- Using CADIS in MAVRIC
  - 23 minute adjoint DO calculation with Denovo
  - 900 minute forward Monte Carlo calculation with Monaco
    - Using mesh-based weight windows
    - Using mesh-based biased source

	Neutron		Photon		Total	
Detector	Value (rem)	Relative Uncertainty	Value (rem)	Relative Uncertainty	Value (rem)	Relative Uncertainty
west	6.42	1.5%	0.515	6.1%	6.93	1.5%
center	4.97	1.6%	0.365	5.6%	5.34	1.6%
east	4.28	2.0%	0.286	4.5%	4.57	1.9%

FOM Improvement: 1600-5000

C. Mesh Tally In and Around Building

- In order to obtain a mesh tally with more uniform relative uncertainties, the Forward-Weighted CADIS method is used.

Estimate the forward flux	$\phi(\vec{r},E)$
Define the adjoint source	$q^{+}(\vec{r},E)=\dfrac{\sigma_d(\vec{r},E)}{\iint \sigma_d(\vec{r},E)\,\phi(\vec{r},E)\,d\vec{r}\,dE}$
Solve for the adjoint flux	$\phi^{+}(\vec{r},E)$
Estimate "detector" response	$c=\iint q(\vec{r},E)\,\phi^{+}(\vec{r},E)\,d\vec{r}dE$
Construct weight windows	$\overline{w}(\vec{r},E)=\dfrac{c}{\phi^{+}(\vec{r},E)}$
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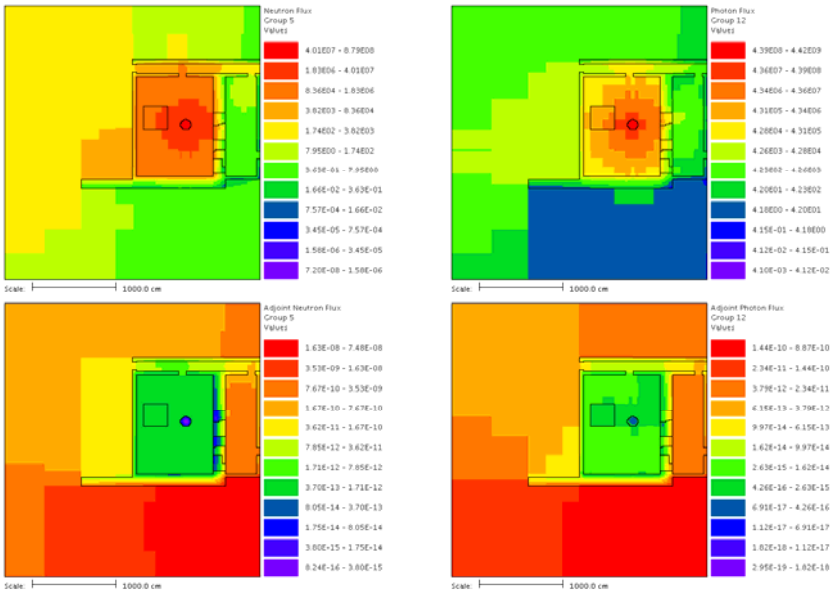
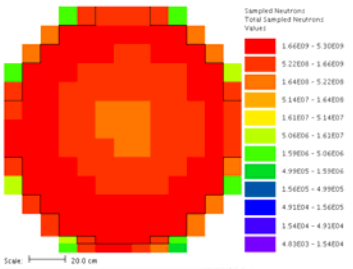
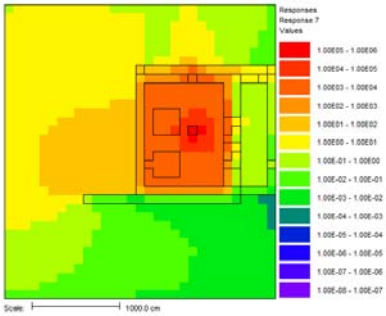
C. Mesh Tally In and Around Building

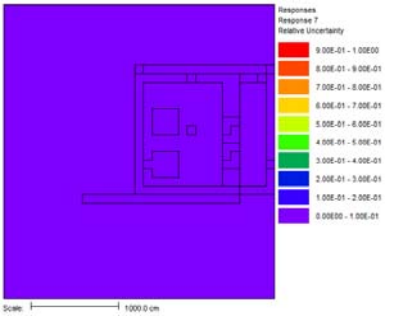


C. Mesh Tally In and Around Building

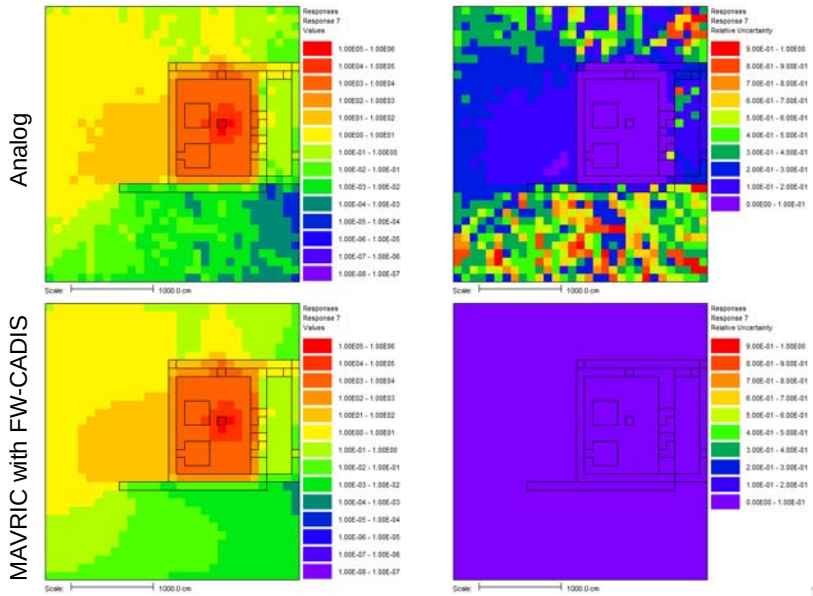
- Using CADIS in MAVRIC
  - 23 minute forward DO calculation
  - 24 minute adjoint DO calculation
  - 900 minute forward MC calculation
    - Using mesh-based weight windows
    - Using mesh-based biased source





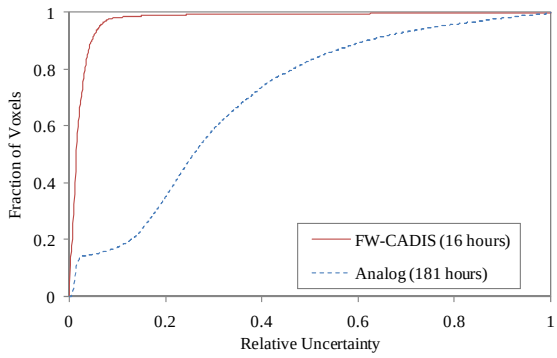


C. Mesh Tally: Compare to Analog



C. Mesh Tally: Compare to Analog

- Create a pdf for relative uncertainty in the mesh tally
  - What fraction of voxels (11594) have less than some level of relative uncertainty?
  - 91% of voxels have less than 5% relative uncertainty



Summary

- New capability in SCALE 6 designed for CAAS problems
- Addresses the difficulties in CAAS problems:
  - Criticality problem and deep-penetration shielding problem
  - Small scale detail for criticality, large scale for shielding
  - Full three-dimensional modeling in both
- Automated Variance Reduction in MAVRIC optimizes calculations for a specific tally – with huge speed-ups
- Future Work for CAAS in SCALE 6
  - Warehouse problems – many fissionable regions
  - Comparisons to measured doses/dose rates