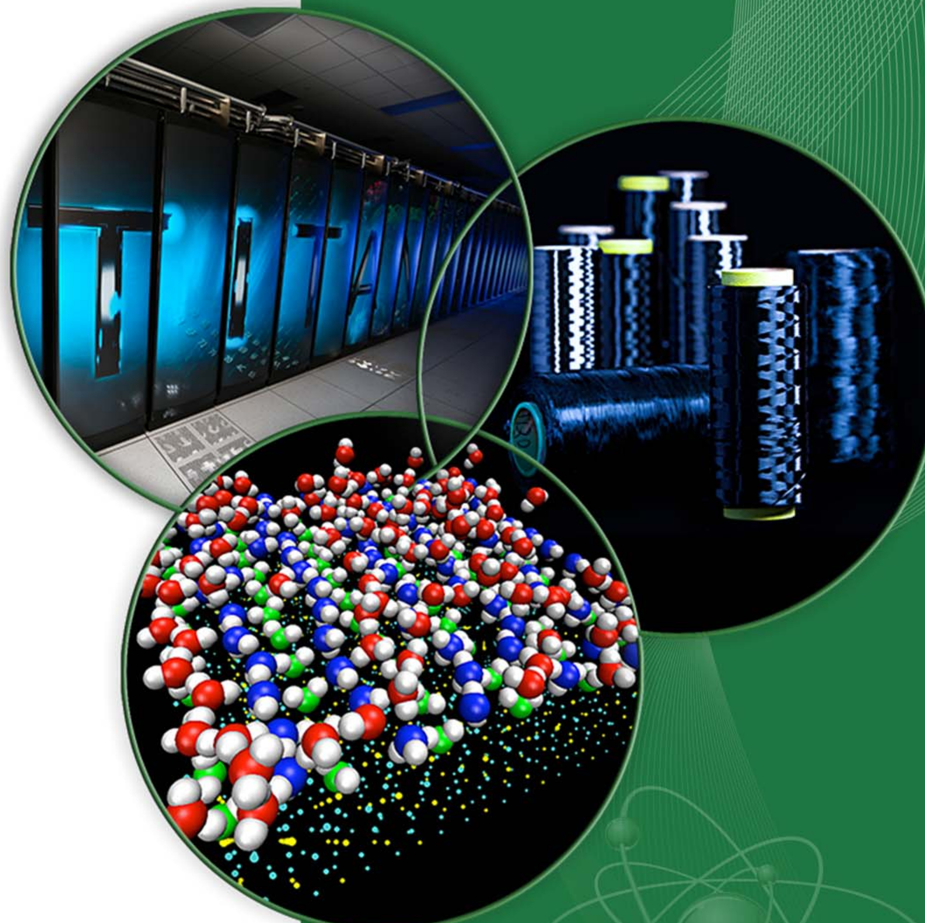
Shielding Capabilities in SCALE 6.2

Monaco/MAVRIC



Douglas E. Peplow
Tuesday, Sept. 26, 2017

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ORNL is managed by UT-Battelle
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Monaco/MAVRIC Shielding Tools

SCALE 6.2

- Replaces MORSE and SAS sequences
  - Introduced with SCALE 6 (Jan 2009)
  - Significant improvements in SCALE 6.1 (Jun 2011)
- Monaco – Monte Carlo transport
  - Based on MORSE/KENO physics
  - SCALE General Geometry Package (SGGP), same as KENO-VI
- MAVRIC – Sequence of Denovo and Monaco
  - Monaco with Automated Variance Reduction using Importance Calculations
  - SCALE sequence which:
    - Computes cross sections
    - Performs a Denovo adjoint calculation, forms importance map and biased source distribution
    - Runs Monaco
- Focus – make it easy on the user

Changes from SCALE 6.1 to 6.2

- Areas of significant change
  - Continuous energy treatment
    - physics, dose responses, tallies
  - More/better links to ORIGEN for source terms
    - Read spectrum from binary concentration file
    - Read in photon lines/intensities from ORIGEN data
  - Improved statistical tests on tallies
  - New statistical tests for mesh tallies
  - Improvements on linking with Denovo
    - Macromaterials for better deterministic models
    - Denovo – more parameters, double precision output
  - Improved link with KENO-VI for CAAS Problems
  - MAVRIC Utilities – for post-processing

SCALE 6.2

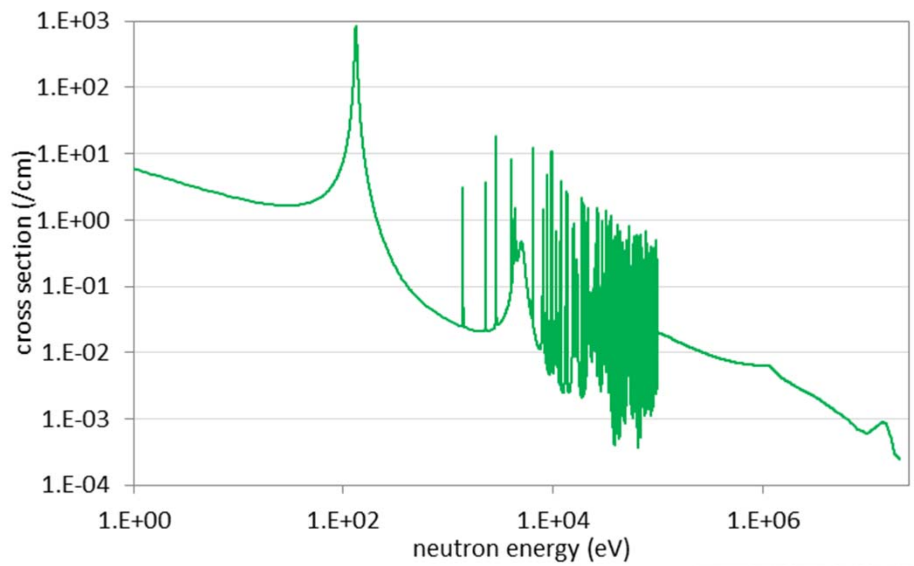
Monaco – fixed-source Monte Carlo

- Multi-group (MG) cross sections
- Continuous-energy (CE) cross sections NEW!

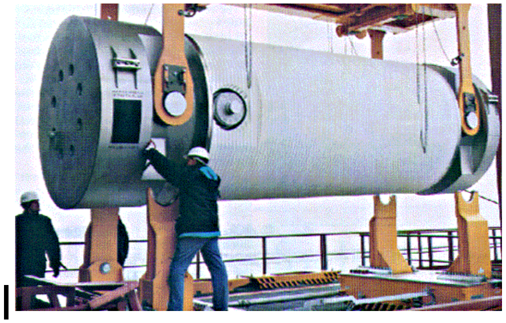
	n	p	libname
ENDF/B-VII.0	238		xn238v7
	27	19	xn27g19v7
	200	47	xn200g47v7
ENDF/B-VII.1	56		xn56v7.1
	252		xn252v7.1
	999		xn999v7.1
	28	19	xn28g19v7.1
	200	47	xn200g47v7.1

	libname
ENDF/B-VII	ce_v7.0_endf.xml
ENDF/B-VII.1	ce_v7.1_endf.xml

(n,γ) in steel



Monaco – Sources



- Define re-usable distributions
  - Built-in distributions
    - Watt spectrum, cosine, exponential
    - MG fission neutron distributions
    - Read an ORIGEN binary concentration (*.f71) file Improved !
    - Look up discrete gammas from ORIGEN library NEW!
  - User-defined distributions
    - Binned histogram
    - Point/value function pairs
    - Discrete lines NEW!
  - Display distributions in ChartPlot, run sampling tests
- Include any number of neutron and photons sources
  - Uses defined distributions for energy, space and angle

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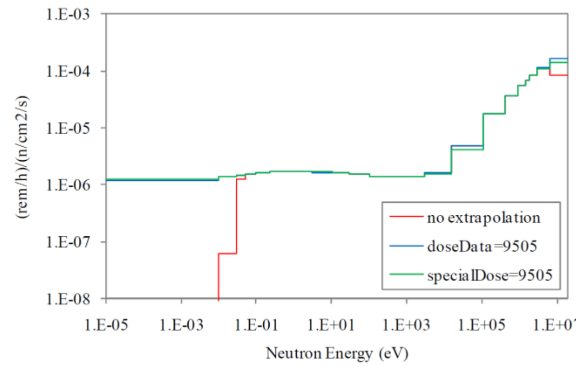
Monaco Responses

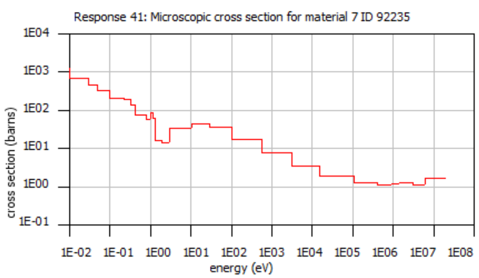
- Built-in responses
  - Flux-to-dose rate conversion factors

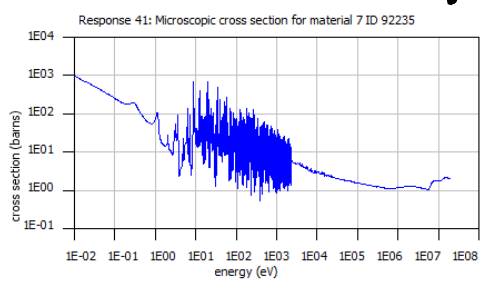
Response	Neutron Energy Range (MeV)		Photon Energy Range (MeV)	
Henderson conversion factors	0.01	18	0.01	10
Claiborne-Trubey conversion factors			0.02	16
ANSI standard (1977) flux-to-dose-rate factors	2.5E-08	20	0.01	15
ANSI standard (1991) flux-to-dose-rate factors	2.5E-08	14	0.01	12
ICRU-44 Table B.3 (air) Kerma	2.5E-08	29		
ICRU-57 Table A.21 (air) Kerma			0.01	10
Ambient dose equivalent (ICRU-57)	1.0E-09	20.1	0.01	10
Effective dose (ICRU-57)	1.0E-09	18	0.01	10

Improved !

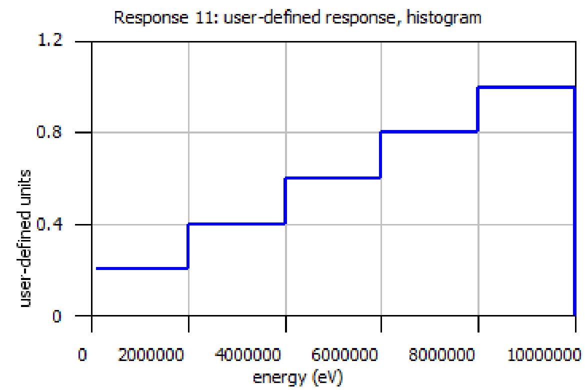


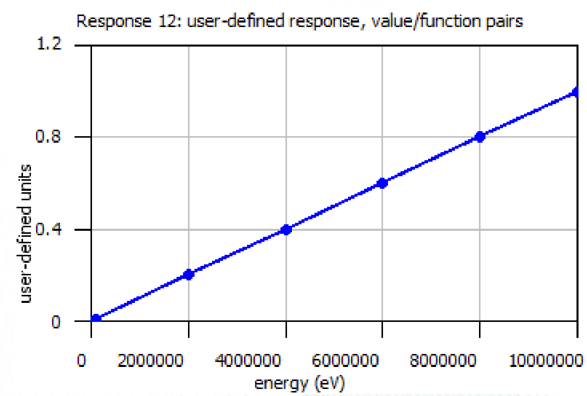
  - Reaction rates from cross-section library





- User-defined responses
  - Binned histogram
  - Point/value function pairs





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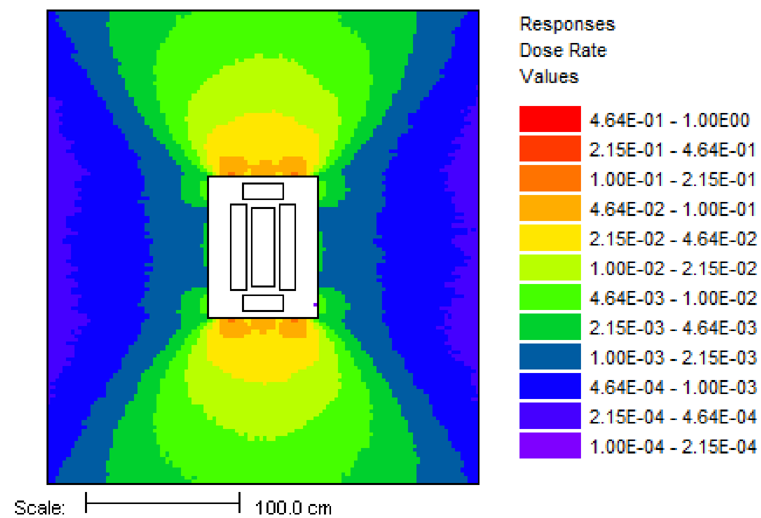
Monaco - Tallies

- Basic tally types – for flux
  - Region tally
  - Point detector
  - Mesh Tally
- Add any number of responses
- Energy binning
  - automatic in MG
  - User-specified in CE NEW!

```
Final Tally Results Summary
 ============================

Neutron Point Detector 2.  example point detector
                         average      standard     relat      FOM     stat checks
    tally/quantity        value       deviation    uncert    (/min)   1 2 3 4 5 6
    ------------------  -----------  -----------  -------  --------  -----------
    uncollided flux     5.28059E-03  3.15856E-06  0.00060
    total flux          9.76163E-01  1.06422E-03  0.00109  8.39E+04  X X X X X X
    response 1          7.55800E-05  8.63873E-08  0.00114  7.64E+04  X X X X X X
    ------------------  -----------  -----------  -------  --------  -----------

 Neutron Region Tally 4.  example region tally
                         average      standard     relat      FOM     stat checks
    tally/quantity        value       deviation    uncert    (/min)   1 2 3 4 5 6
    ------------------  -----------  -----------  -------  --------  -----------
    total flux (tl)     9.75719E-01  5.54774E-05  0.00006  3.09E+07  X X X X X X
    total flux (cd)     0.00000E+00
    response 1          7.55800E-05  8.63873E-08  0.00114  7.64E+04  X X X X X X
    ------------------  -----------  -----------  -------  --------  -----------
```

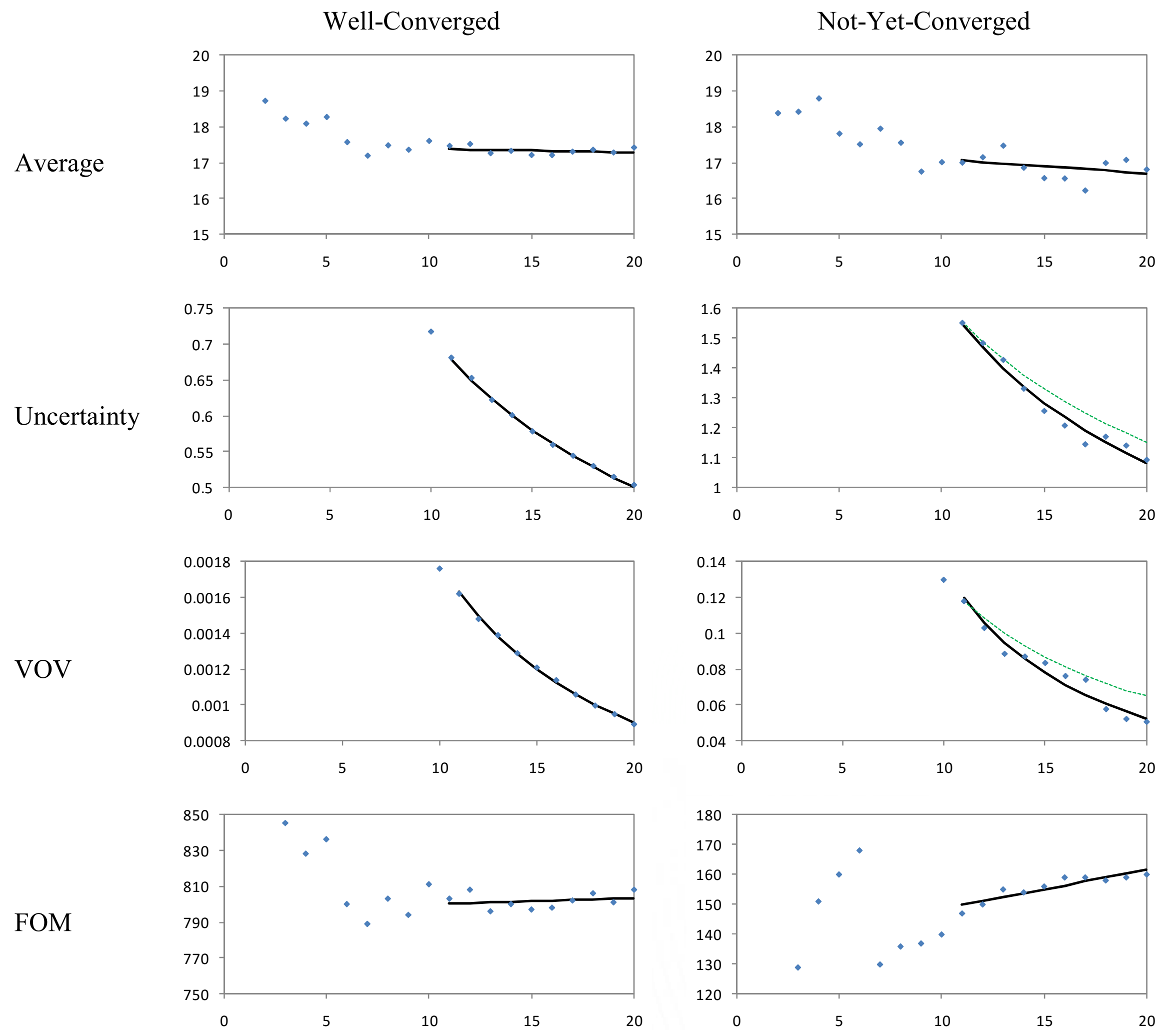


- Statistical tests for convergence Improved !
- Statistical tests for mesh tally convergence NEW!

Statistical Checks – Reg. and Point Det.

	Quantity/Test	Goal	Within
1.	mean relative slope of linear fit	= 0.00	±0.10
2.	standard deviation exponent of power fit	= -0.50	$R^2 > 0.99$
3.	relative uncertainty final value	< 0.05	
4.	relative VOV exponent of power fit	= -1.00	$R^2 > 0.95$
5.	relative VOV final value	< 0.10	
6.	figure-of-merit relative slope of linear fit	= 0.00	±0.10

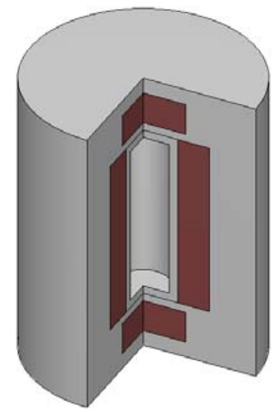
Improved !

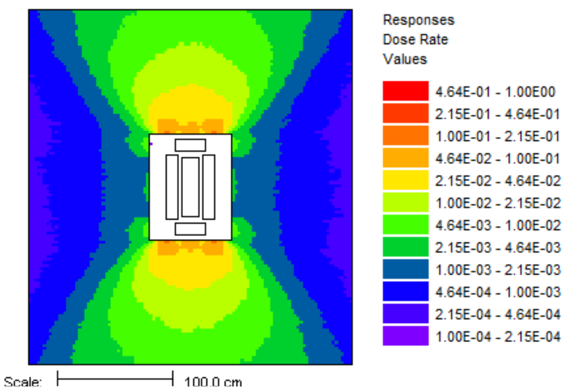


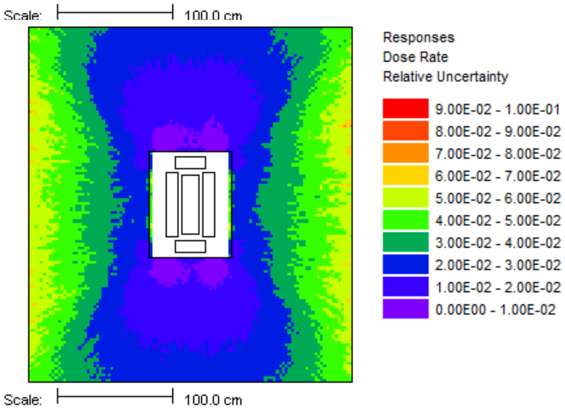
Statistical Checks – Mesh Tallies

NEW!

	Quantity	Test	Goal	Within
1.	ζ, fraction with score	relative slope of linear fit	= 0.00	±0.10
2.	$\bar{r}$, mean relative uncertainty	exponent of power fit	= -0.50	$R^2 > 0.99$
3.	variance of $\bar{r}$	exponent of power fit	= -1.00	$R^2 > 0.95$
4.	figure-of-merit	relative slope of linear fit	= 0.00	±0.10







problem.out

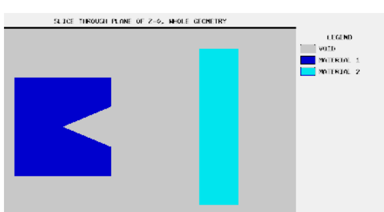
```
Photon Mesh Tally 1.

                      zeta     mean     var of     FOM     passed
tally/quantity        value   rel unc   rel unc   (/min)   1 2 3 4
------------------   ------  --------  --------  --------  -------
flux, bin 0          0.8221  2.78E-01  1.01E-09  1.43E-02  X - - -
tot flux, bin 0      0.9870  6.43E-02  5.60E-10  2.67E-01  X X X X
resp 5/bin 0         0.9870  5.22E-02  2.80E-10  4.06E-01  X X X X
------------------   ------  --------  --------  --------  -------
```

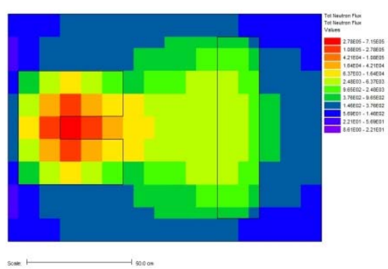
problem.mt1.resp5.out

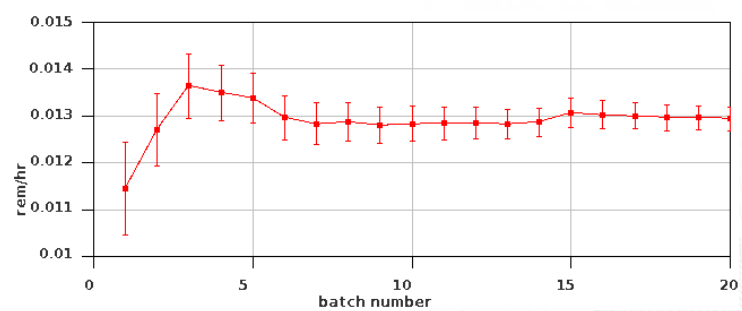
```
Mesh Tally Statistical Checks - relative variance density function
    (fits are over the last half of the simulation)

quantity                  check                      goal    actual    R**2  pass
----------------------    ----------------------    -----  --------  ------  ----
1 fraction with score     rel slope of linear fit    0.00    0.0000           yes
2 mean rel. uncert.       exponent of power fit     -0.50   -0.4922  0.9997   yes
3 var. of rel. uncert.    exponent of power fit     -1.00   -1.0114  0.9999   yes
4 figure-of-merit (FOM)   rel slope of linear fit    0.00   -0.0159           yes
----------------------    ----------------------    -----  --------  ------  ----
```

Monaco

- Output
  - Provides feedback for checking input
    - Distributions and responses make *.chart files
    - Grid geometries and cylindrical geometries ( ) make *.3dmap files
    - Geometry *.png files (like Keno)
  - Tallies
    - Summarized in main SCALE output file
    - Details saved in files (energy groups, convergence details)
  - Java Viewers replaced by Fulcrum
    - ChartPlot
    - MeshFileViewer





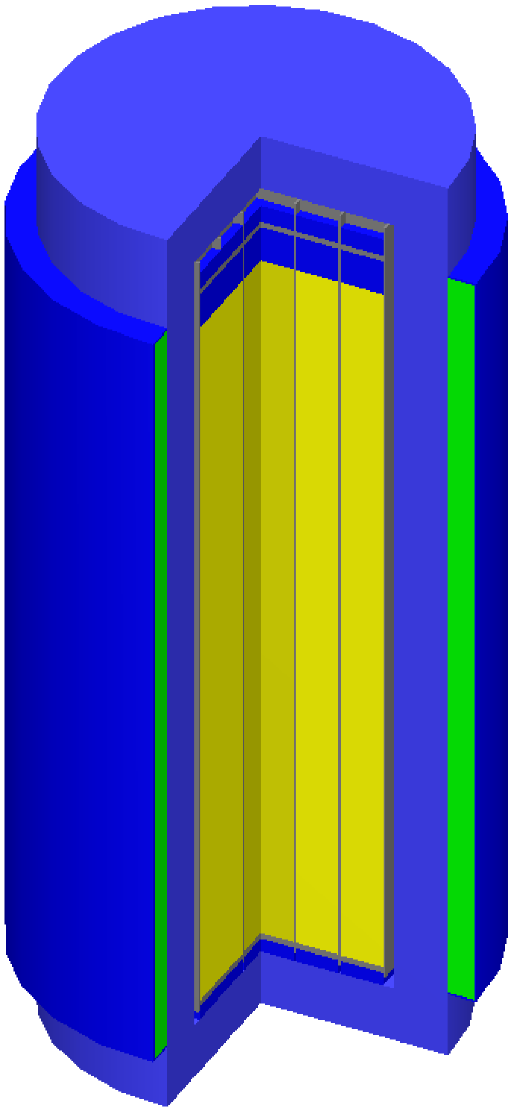


MAVRIC – Automated Variance Reduction

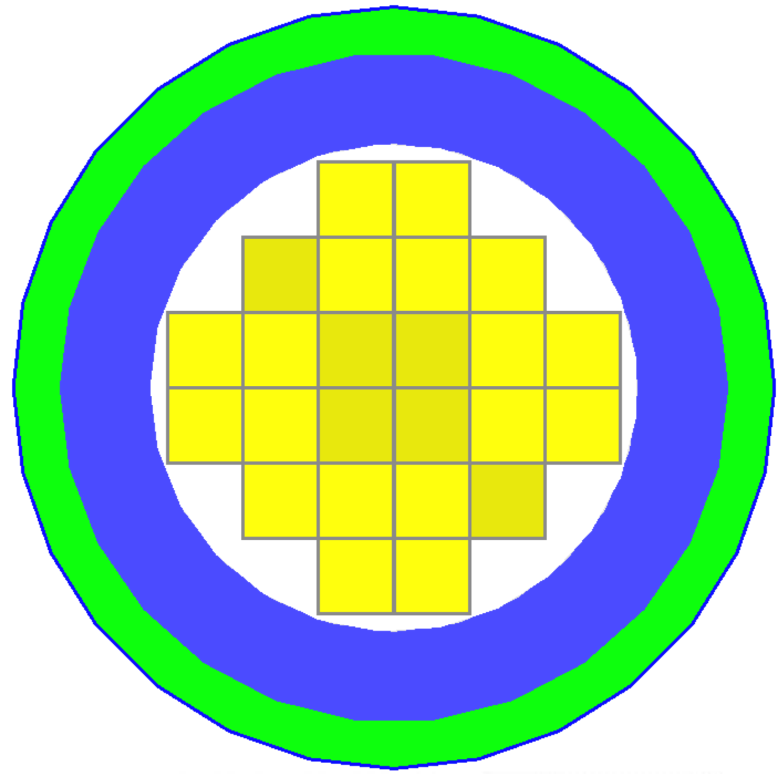
- Variance reduction parameters for Monte Carlo are often difficult to compute
- MAVRIC is designed to automate variance reduction
  - Use Denovo deterministic solution to create an importance map and a consistent biased source(s)

- Methods
  - CADIS
    - Optimizes a single response in a single tally
    - Requires an adjoint deterministic calculation
  - FW-CADIS
    - Optimizes several tallies or a mesh tally
    - Requires 1 forward and 1 adjoint deterministic calculation

Example Problem: Simplified TN24P Cask

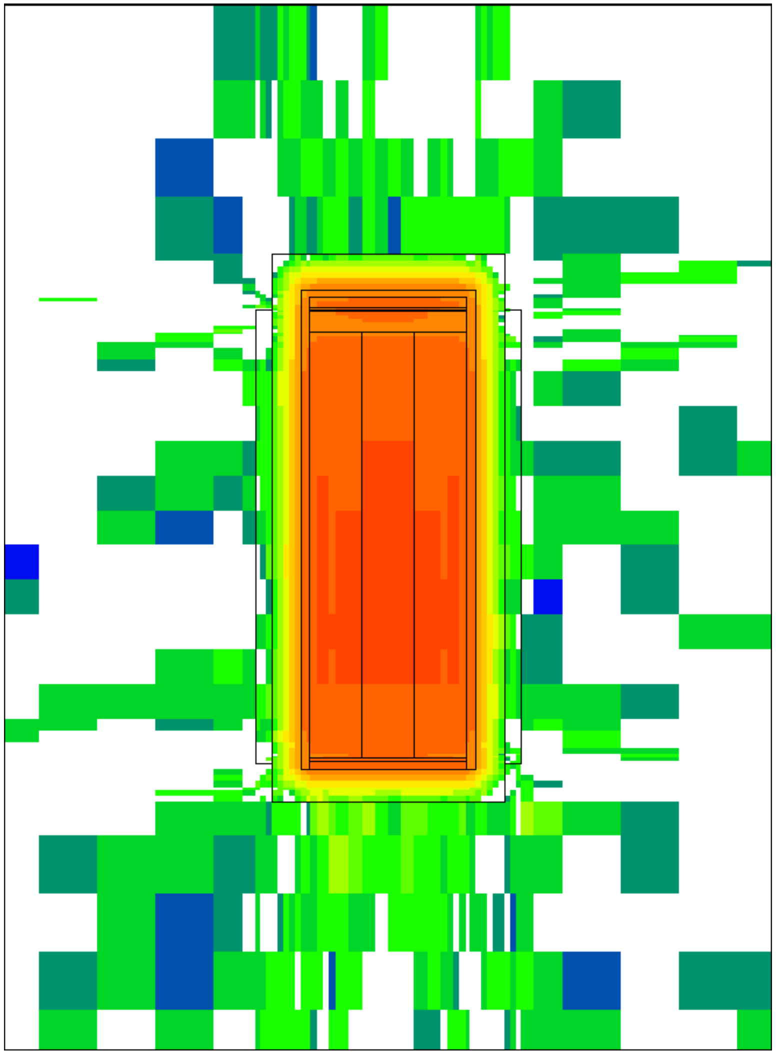


Spent fuel: neutrons and photons
Activated hardware: photons



Objective: Determine dose rates at various points outside of the cask

Analog

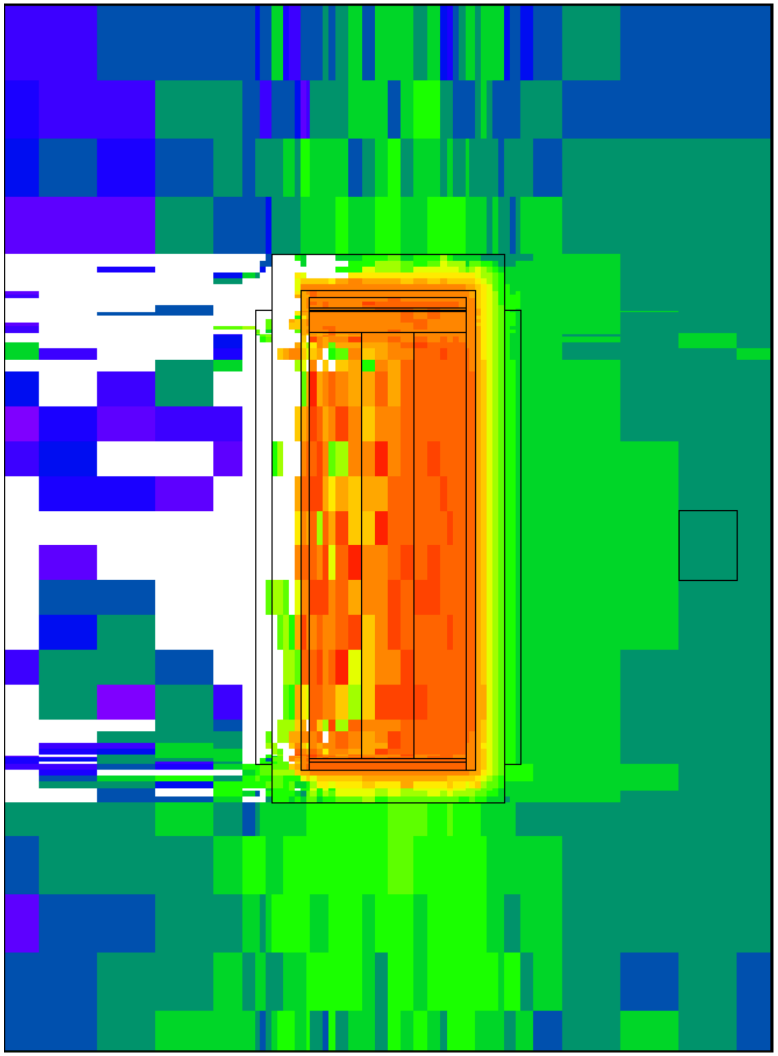


- Analog Monte Carlo
  - Sample a source particle
    - Position
    - Direction
    - Energy
  - Simulate its natural path
    - Distance before interaction
    - Sample possible interactions

Run Time: 100 hours

Can be slow to converge!

CADIS – Accelerate a single tally



Denovo 12 m; Monaco 45 m

Define the adjoint source = response

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

Compute the adjoint flux $\phi^{+}(\vec{r},E)$

Estimate the detector response

$$R = \int_{V_s}\int_E q(\vec{r},E)\,\phi^{+}(\vec{r},E)\,dE\,dV$$

Construct weight windows

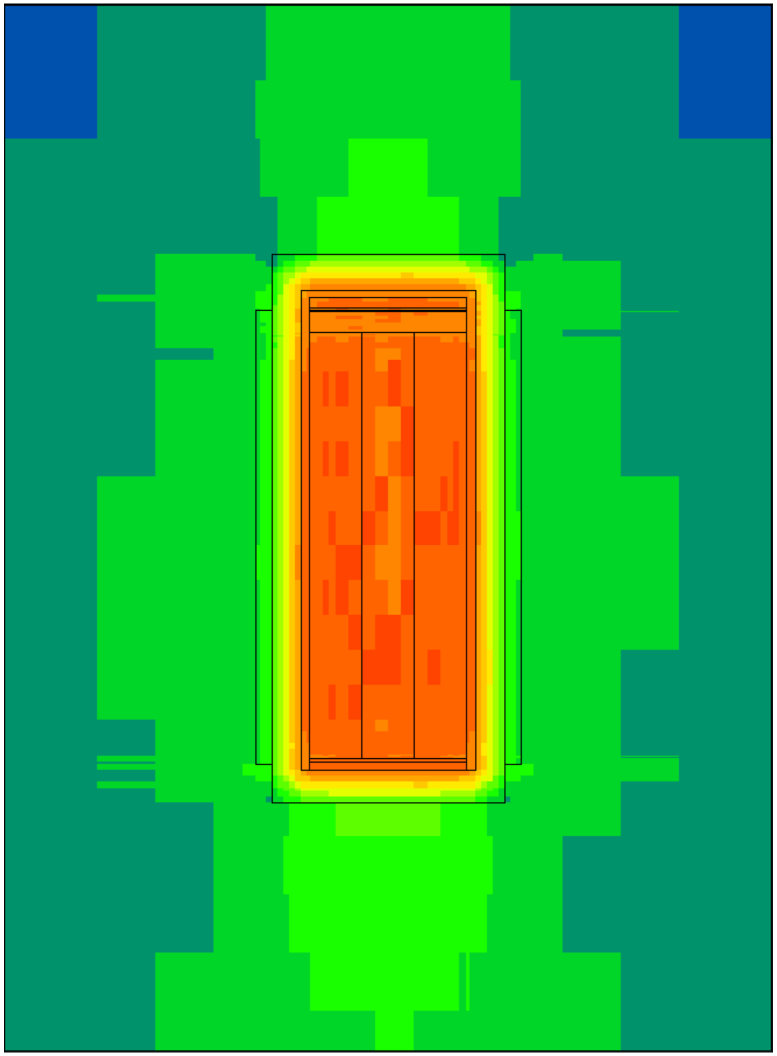
$$\overline{w}(\vec{r},E) = \frac{R}{\phi^{+}(\vec{r},E)}$$

Construct biased source

$$\hat{q}(\vec{r},E) = \frac{1}{R} q(\vec{r},E)\phi^{+}(\vec{r},E)$$

Use in the Monte Carlo

FW-CADIS – multiple tallies or mesh tallies



Denovo 17 m, 13 m; Monaco 90 m

Adjoint source corresponds to the area to be optimized by the Monte Carlo
- more adjoint source in low-flux areas
- less adjoint source in high-flux areas

Estimate the forward flux $\phi(\vec{r}, E)$

Estimate the dose rate $R(\vec{r}, E)$

Adjoint source $q^+(\vec{r}, E) = \sigma_d(\vec{r}, E)/R(\vec{r}, E)$

-- *now same as CADIS* --

Compute the adjoint flux $\phi^+(\vec{r}, E)$

Construct weight windows $\overline{w}(\vec{r}, E)$

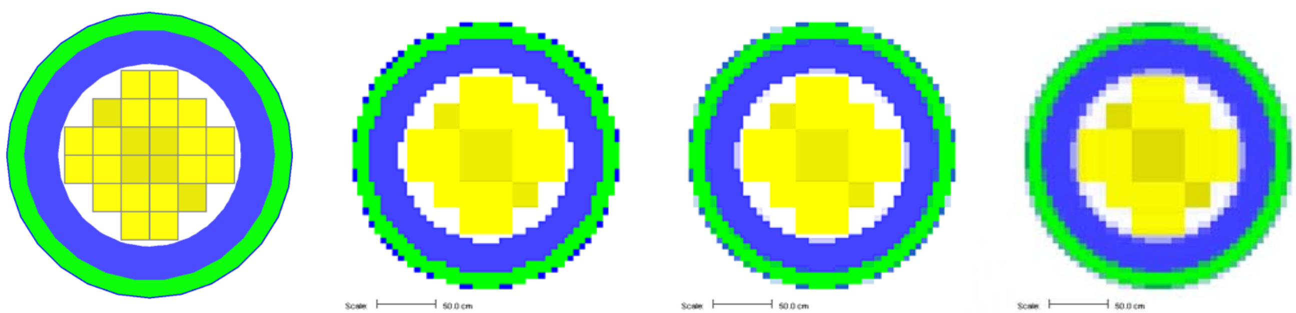
Construct biased source $\hat{q}(\vec{r}, E)$

Use in the Monte Carlo

MAVRIC

- Sequence can be run in parts
  - Go so far, review adjoint calcs, importance maps, biased sources
  - Reuse previously computed files
  - Use MAVRIC to run Denovo (serial)

- More accurate deterministic calcs give higher MC FOM
  - More meshes, more angles, more scattering components…
  - Macromaterials Improved !



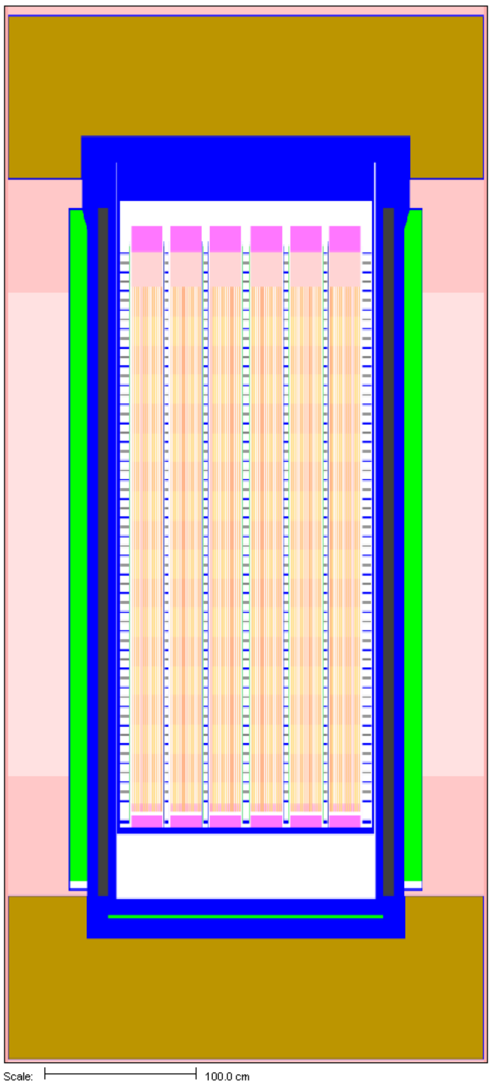
MAVRIC Utilities

NEW!

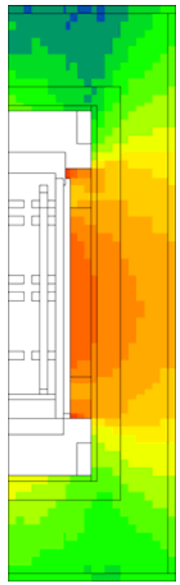
Improved !

- Help the user in post-processing results
- Mesh Tally files (~20)
  - Display overview, add, subtract, multiply, divide, scale, invert
  - Filter (keep values above or below a given value)
  - Find location of minimum or maximum
- Denovo Flux files (~15)
  - Similar to above
- Others
  - Display overviews of other file types
  - Convert importance map to MCNP wwinp file

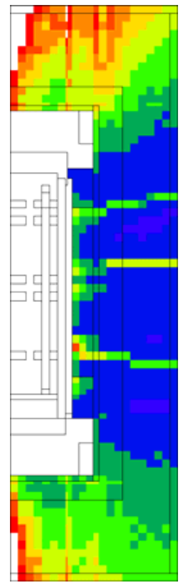
MAVRIC Utilities – UNF Dose Rates



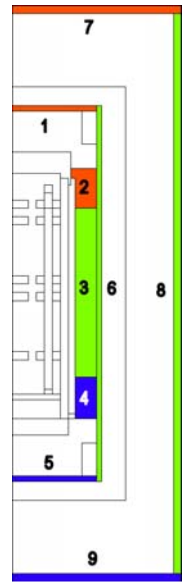
geometry



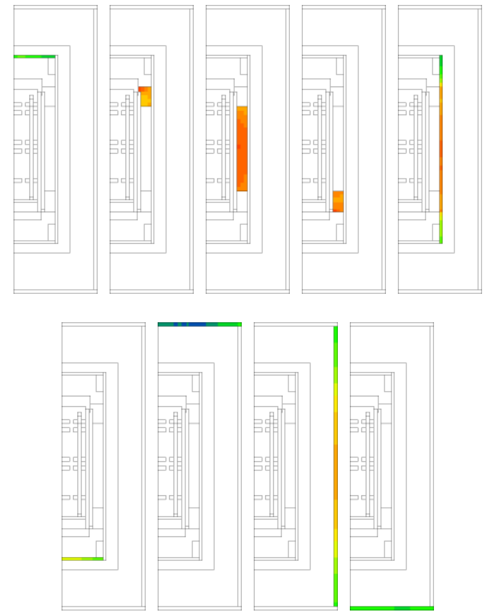
dose mrem/hr



rel unc 0-10%



zones



Location		15 years after last discharge mrem/hr	15 years after last discharge rel. unc.	25 years after last discharge mrem/hr	25 years after last discharge rel. unc.
Cask	Top	0.23	8%	0.16	8%
Cask	Upper Radial	27.78	3%	18.98	3%
Cask	Middle Radial	19.98	14%	12.45	3%
Cask	Lower Radial	85.27	2%	57.50	2%
Cask	Bottom	1.06	7%	0.34	9%
PB	Radial	11.89	2%	7.94	2%
2 m	Top	0.13	6%	0.08	5%
2 m	Radial	4.28	2%	2.77	3%
2 m	Bottom	0.19	10%	0.10	5%

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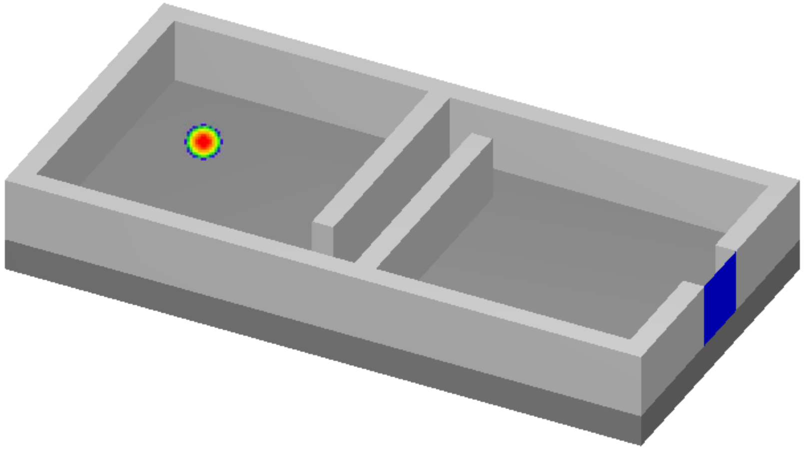
KENO Source for Monaco/MAVRIC

- Developed for modeling criticality accident alarm systems
- KENO-VI Improved !
  - Define a grid geometry
  - Set a flag to store fission density tally
  - Stores $\bar{\nu}$ (neutrons per fission)



- MAVRIC utility
  - Convert fission density into source distribution
- Monaco/MAVRIC
  - Use a ‘meshSource’
  - Specify fission/sec or neutrons/sec

```
src 1
    meshSourceFile=“C:\mydocu~1\caasExample\fissionSource.msm"
            origin x=600 y=650 z=400
    fissions=1.0e17
end src
```

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ORIGEN for Source Energy Distribution

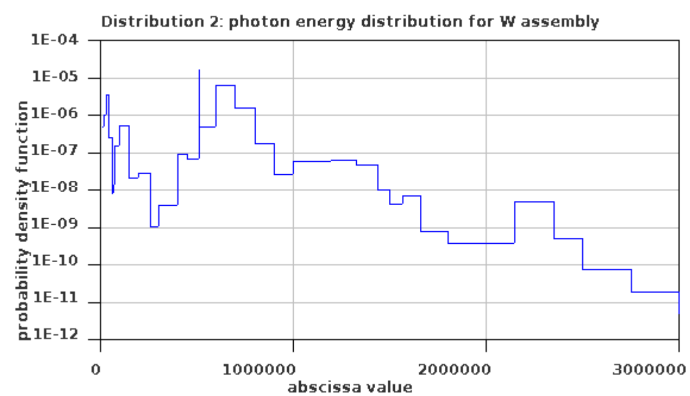
- ORIGEN
  - Set energy bins (n, p, or both)
  - Save a binary concentration (*.f71) file
- Monaco/MAVRIC
  - Define an energy distribution

Improved !

```
distribution 1
    special="origensBinaryConcentrationFile"
    filename="c:\somewhere\reactorFuel.f71"
    parameters C S end
end distribution
```

C – case number

S: 1 – total neutron
2 – spontaneous fission
3 – (α,n)
4 – delayed neutrons
5 – photons

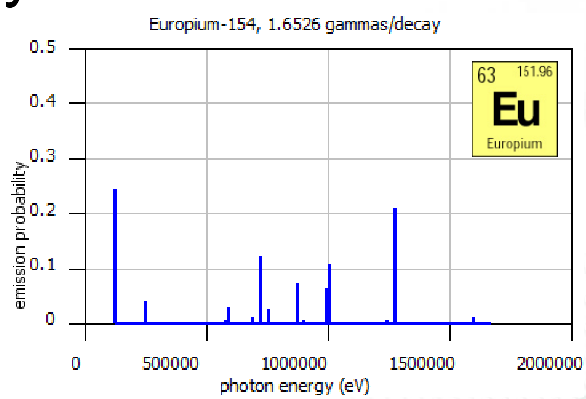


  - This is a histogram
- Or, use ORIGEN data directly

NEW!

  - Discrete distribution

```
distribution 5
   special="origensDiscreteGammas"
   parameters Z A end
end distribution
```



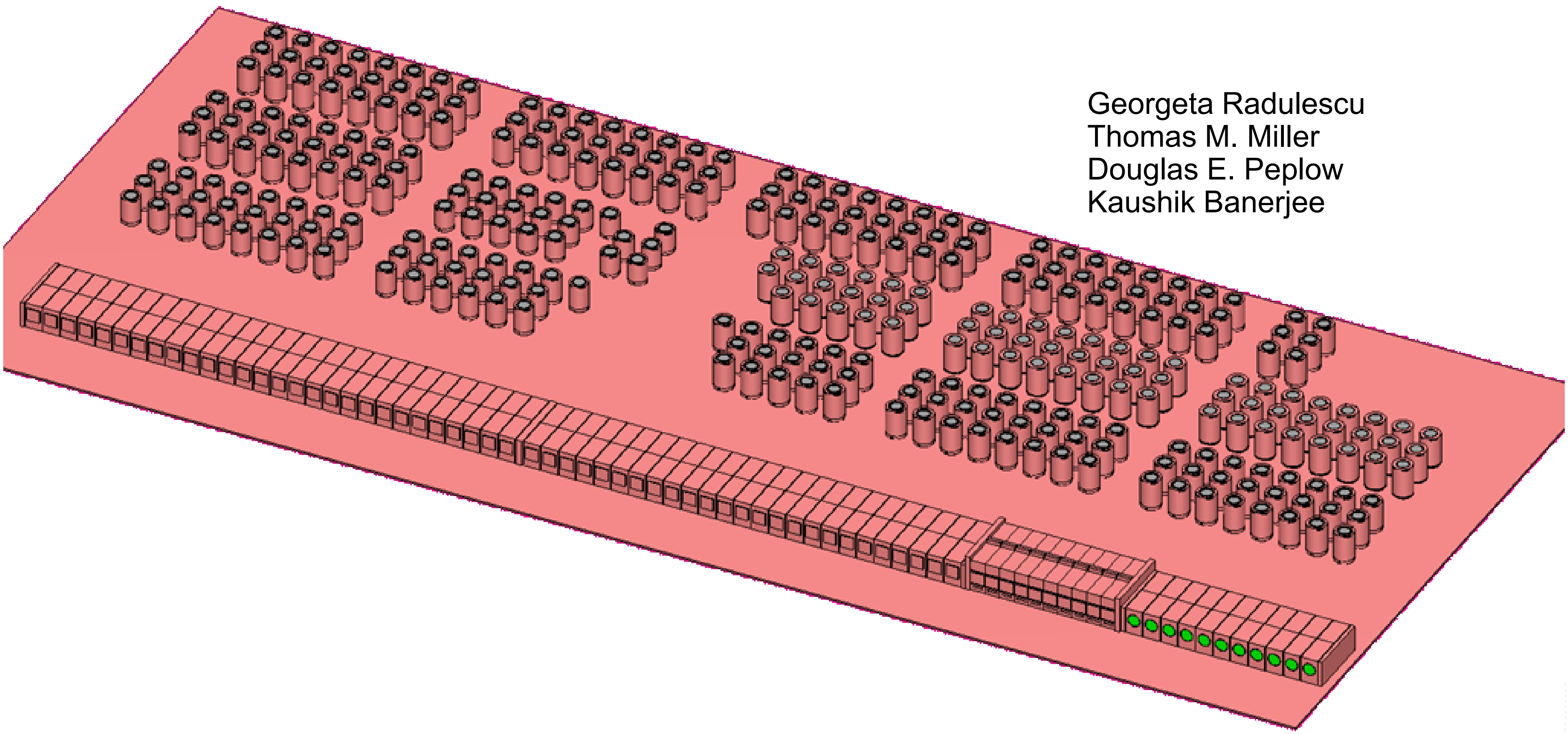
Modern Storage Site

Modern Storage Site

http://wcsstorage.com/resources/

MAVRIC Approach

- Detailed 3D model of Phase I
  - 467 storage casks
  - Vertical and horizontal
- Need dose rate (mrem/yr) at site boundary



Georgeta Radulescu
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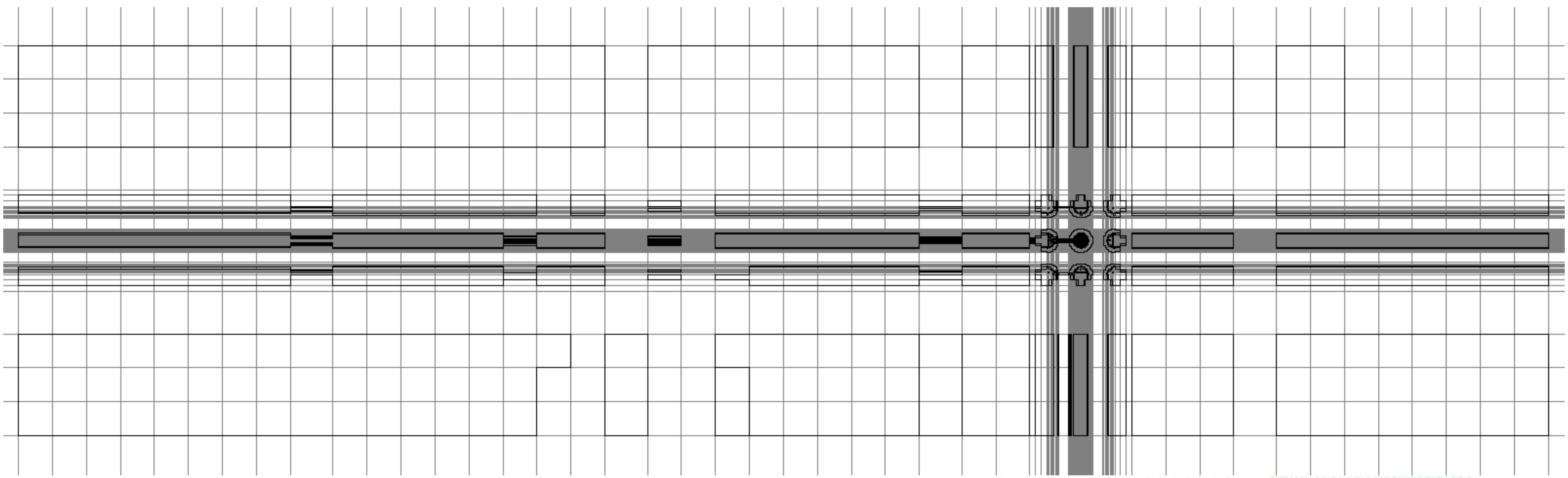
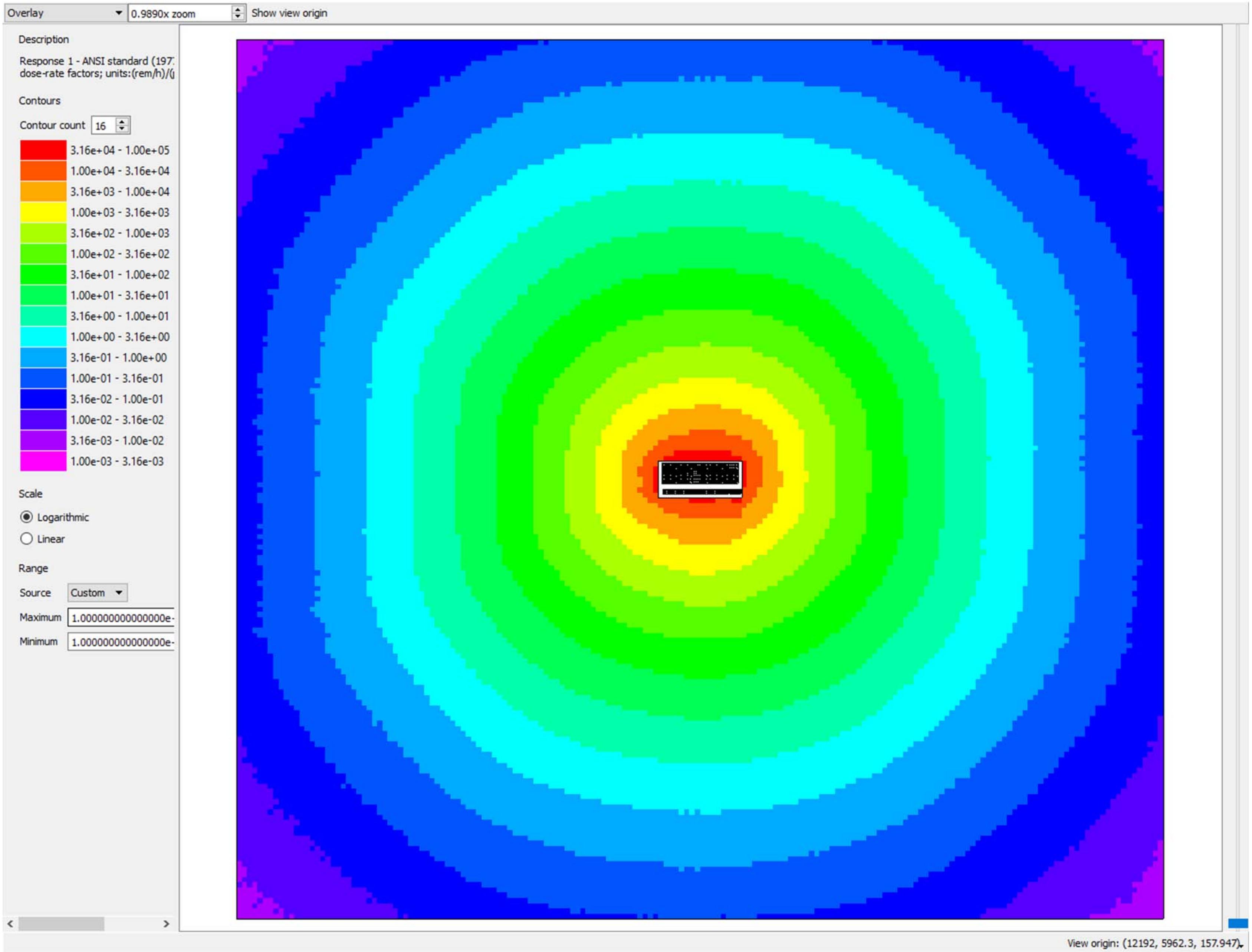
Kaushik Banerjee

MAVRIC Approach

- Monte Carlo will take a long time to sample 467 casks well
- Needs variance reduction - but the Denovo mesh would require an *unbelievable ginormous* amount of memory
- Solution: use full geometry but only consider source in one cask at a time (parallelize on source)
  - Denovo mesh can focus on one cask, with larger meshes far away



Results - Dose rate at ground level



$$\left[\widehat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)\right]\psi\left(\vec{r},\widehat{\Omega},E\right) =$$

$$\int dE \int d\Omega'\,\sigma_s\left(\vec{r},E'\longrightarrow E,\widehat{\Omega}'\cdot\widehat{\Omega}\right)\psi\left(\vec{r},\widehat{\Omega}',E'\right)$$

$$+\,q_{ext}\left(\vec{r},\widehat{\Omega},E\right)$$

scale

Nuclear Systems Modeling & Simulation

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