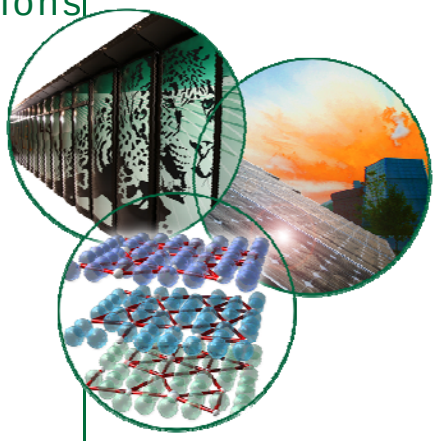
Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Calculations of Distributions & Multiple Localized Quantities



Presented by:

Douglas E. Peplow

John C. Wagner, Edward D. Blakeman
and Douglas E. Peplow
Radiation Transport & Criticality Group
Nuclear Science & Technology Division

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OAK RIDGE NATIONAL LABORATORY
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Overview

- Introductory Remarks
- Motivation for Work
- Theory
  - CADIS
  - FW-CADIS
- Implementation
- Applications & Results
  - Distributions
  - Multiple localized quantities
- Summary & Conclusions

Introductory Remarks

- Monte Carlo (MC) is becoming (or has become) the most widely used method for radiation transport simulations
- Conventional wisdom – Transport Methods:
  - Use deterministic methods where detailed information is needed throughout the problem space
  - Use MC methods everywhere else
- Users are increasingly pushing against this "conventional wisdom" and applying MC to calculate detailed distributions; motivated by:
  - Analysis/design needs
  - Increases in available computational resources
  - Enhancements in code features (e.g., mesh tally capability)
- However, for truly challenging applications, the conventional wisdom has held
- Which leads to the question:
  - "Can one effectively optimize the MC calculation of detailed distributions?"

Introductory Remarks

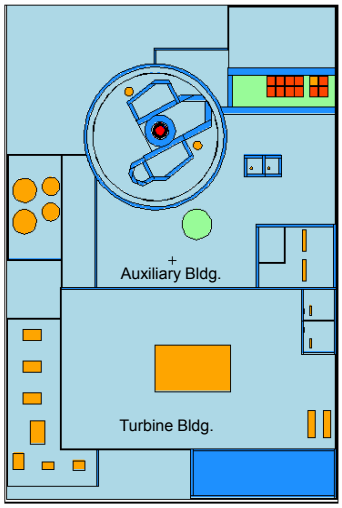
- Conventional wisdom – Variance Reduction:
  - VR techniques focus computational efforts on a specific part of the problem, at the expense of other parts of the problem
  - Very useful/powerful for optimization of single or multiple "similar" responses
  - Hard to use (where automated VR capability is not available)
  - Not very useful for optimization of distributions or multiple "dissimilar" quantities
- In this work, we present a method for optimization of distributions and multiple localized quantities that challenge some (certainly not all) of these conventional beliefs
- Examples of analysis needs:
  - Distributions – results everywhere or over a significant range of the problem space, e.g., space- and/or energy-dependent flux, dose, reaction rate distributions
  - Multiple localized quantities –results in multiple regions of problem space, e.g., response at multiple spatial locations, energy spectrum at one or few locations

Motivation for Work

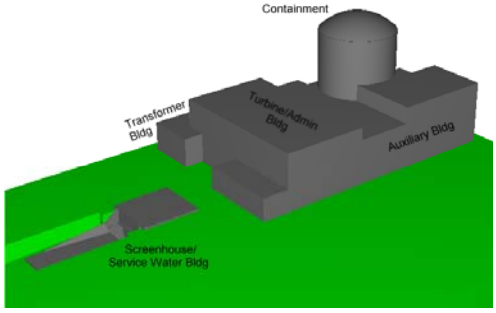
- General:
  - Want the benefits of MC for analyses that require calculation of detailed information throughout a problem
- Specific:
  - Asked (by DTRA) to calculate dose rates through an entire PWR facility – using MC

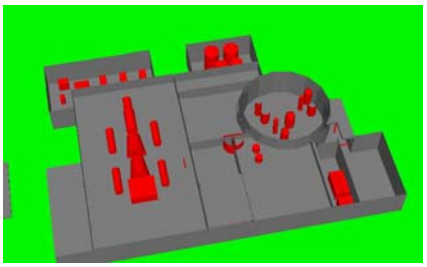
Dose Rates Throughout a PWR Facility

Large scales, massive shielding
Difficult to calculate dose rates

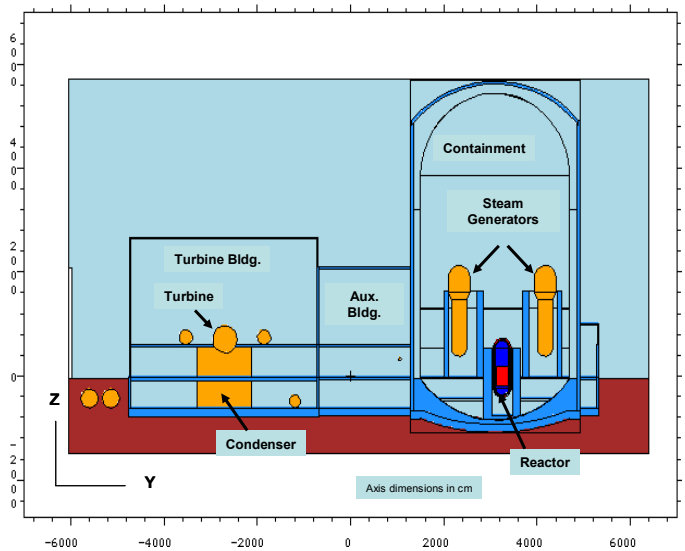


85 × 125 × 70 m





Dose Rates Throughout a PWR Facility



Theory – Adjoint Methodology

- The goal of most "traditional" MC simulations is to calculate the response at some location

$$R = \int_{4\pi} d\Omega \int_{V} dV \int_{E} dE \; \psi(\vec{r}, E, \hat{\Omega})\, \sigma_d(\vec{r}, E, \hat{\Omega})$$

- From the forward and adjoint equations, the adjoint property, and letting the adjoint source be equal to the detector response function, $\boldsymbol{\sigma_d}$, one can derive an alternate formulation for response

$$R = \int_{4\pi} d\Omega \int_{V} dV \int_{E} dE \; \psi^{+}(\vec{r}, E, \hat{\Omega})\, q(\vec{r}, E, \hat{\Omega})$$

- From this one can show that the adjoint function has physical significance as a measure of the importance of a particle to some objective function (e.g., the detector response)

Theory - Adjoint Methodology

- Recognizing the physical meaning of the adjoint function, numerous works have successfully utilized adjoint data for MC VR (for localized quantities)
- Further recognizing the advantages associated with deterministically generated adjoint functions, much work has been done to develop and automate methods based on deterministic importance functions
- Many of these works are discussed in the following review paper:
  - "Monte Carlo Variance Reduction with Deterministic Importance Functions," ***Progress in Nuclear Energy*** 42(1), 25-53 (2003).

Theory – CADIS

- CADIS – Consistent Adjoint Driven Importance Sampling
  - Given an objective function, $\boldsymbol{\sigma_d}$, and the corresponding adjoint importance function, CADIS provides consistent relationships for calculating source & transport biasing parameters based on Importance Sampling
  - Biased source is given by:

$$\hat{q}(\vec{r},E)=\frac{\phi^{+}(\vec{r},E)\,q(\vec{r},E)}{\int_V dV\int_E dE\,\phi^{+}(\vec{r},E)\,q(\vec{r},E)}=\frac{\phi^{+}(\vec{r},E)\,q(\vec{r},E)}{R}$$

    - numerator is the detector response from a given space-energy element
    - denominator is the total detector response
    - the ratio is the relative contribution from each space-energy element to the total detector response

Theory – CADIS

- Applying the weight conservation requirement

$$w(\vec{r},E)\ \hat{q}(\vec{r},E) = \ w_o\, q(\vec{r},E)$$

- The statistical weights are given by

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

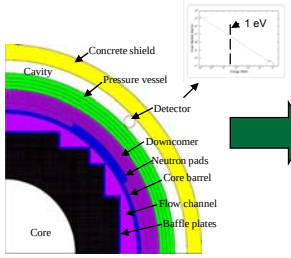
- For use with a weight window technique, the weights can be scaled to calculate lower-weight bounds, w_l

$$w_\ell(\vec{r},E) = \frac{w}{\left(\frac{c_u+1}{2}\right)} = \frac{R}{\varphi^{+}(\vec{r},E)\left(\frac{c_u+1}{2}\right)}, \quad where \ \ c_u = \frac{w_u}{w_\ell}$$

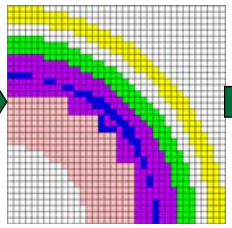
CADIS

- Consistent – CADIS provides source biasing parameters and weight windows such that source particles are started with weights that are within the weight windows
- Has been implemented and automated in:
  - MAVRIC sequence in SCALE 6 (available from RSICC)
  - ADVANTG code (based on MCNP)
- Both codes are used at ORNL for simulations of real applications
    - Ex-vessel detector response
    - Dose rate in a variety of environments
    - DPA to HFIR vessel; shielding design studies for lunar reactor
    - Analysis of shielding penetrations
    - SNM detection simulations
    - Nuclear well-logging tool simulations
  - Resulting in considerable experience with the method and its implementation

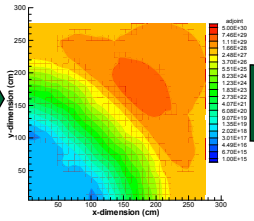
CADIS Example: PWR Ex-Vessel Thermal (^{10}B) Detector Response



Monte Carlo model



Deterministic model



Adjoint data

Calculate VR Parameters

Source biasing

$$\hat{q}(\vec{r},E) = \frac{\phi^{+}(\vec{r},E)\,q(\vec{r},E)}{\int_V \int_E q(\vec{r},E)\phi^{+}(\vec{r},E)\,drdE},$$

Transport biasing (weight windows)

$$w_t(\vec{r},E) = \frac{R}{\phi^{+}(\vec{r},E)\left(\frac{c_u+1}{2}\right)}$$

Results

CASE	CPU TIME TO ACHIEVE RE=1% (h)	SPEEDUP
No VR	8.86E+4 (10.1 yrs)	1
Manual VR	13.6	6500*
ADVANTG	**1.02**	**87000**

* Required ~3 weeks by an experienced MC practitioner using all applicable MCNP4C VR capabilities

Theory – Global Variance Reduction

- Global VR Goal:
  - ***Uniform statistical uncertainty in calculated quantities, e.g., space- and energy-dependent flux***
- Suggested (***Cooper and Larsen, NS&E, 2001***) that to achieve uniform statistical uncertainty, one wants uniformly distributed MC particles throughout the system
- Sounds reasonable… how do we get that?

Theory – Global Variance Reduction

- ***Cooper and Larsen, NS&E, 2001***
  - The physical particle density, $n(\vec{r})$, is related to the MC particle density, $m(\vec{r})$, by the average weight $\overline{w}(\vec{r})$.

$$n(\vec{r}) \propto \overline{w}(\vec{r})\ m(\vec{r}) \qquad\qquad m(\vec{r}) \propto \frac{n(\vec{r})}{\overline{w}(\vec{r})}$$

  - For uniform relative uncertainties, make $m(\vec{r})$ constant. So, the average weights need to be proportional to the physical particle density, $n(\vec{r})$, or the estimate of forward flux $\phi(\vec{r})$

$$w(\vec{r}) = \frac{\phi(\vec{r})}{\max(\phi(\vec{r}))}$$

  - Shown to be effective for some test problems

Theory – Global Variance Reduction

- ***Can we develop an adjoint importance function that represents the importance of particles to achieving the desired objective, i.e., uniformly distributed MC particles?***

- First, we cast the problem of calculating MC particle density into our traditional response formulation:

$$R = \int_{4\pi} d\Omega \int_V dV \int_E dE\ \psi(\vec{r}, E, \hat{\Omega})\, \sigma_d(\vec{r}, E, \hat{\Omega})$$

- Since the physical particle density, $n(\vec{r}, E, \hat{\Omega})$, is related to the Monte Carlo particle density, $m(\vec{r}, E, \hat{\Omega})$, by the average weight $\overline{w}(\vec{r}, E, \hat{\Omega})$.

$$n(\vec{r}, E, \Omega) \propto \overline{w}(\vec{r}, E, \Omega)\, m(\vec{r}, E, \Omega)$$

- The total MC particle density can be approximated by

$$R = \int_{4\pi} d\Omega \int_V dV \int_E dE\ \psi(\vec{r}, E, \hat{\Omega}) \left[\frac{1}{\overline{w}\ (\vec{r}, E, \hat{\Omega})\, v} \right]$$

Theory – Global Variance Reduction

- Recall:
  - For uniform relative uncertainties, we want to make the MC particle density constant
  - To achieve this, the average weights need to be proportional to the physical particle density, i.e.,

$$m \approx cont. \qquad \overline{w} \propto n \qquad \overline{w}\,\nu \propto \psi$$

- By substituting the forward flux for $\overline{w}\,\nu$ in the expression for R

$$R = \int_{4\pi} d\Omega \int_V dV \int_E dE\ \psi(\vec{r}, E, \hat{\Omega}) \left[\frac{1}{\psi(\vec{r}, E, \hat{\Omega})} \right]$$

and recognizing that by defining the adjoint source as:

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

We can calculate an adjoint importance function that represents the importance of particles to achieving the desired objective, i.e., uniformly distributed MC particles, which should correspond to approximately uniform relative uncertainties

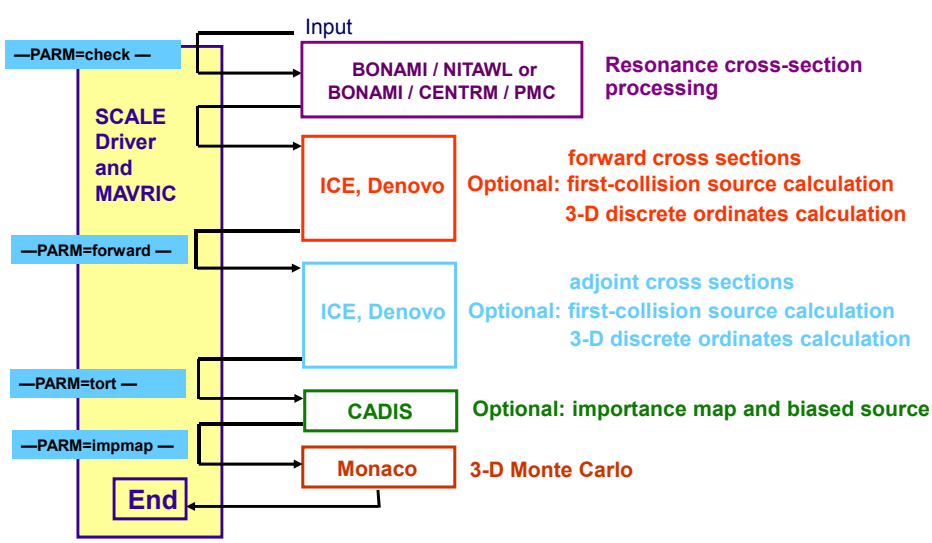
Theory – Global Variance Reduction

- Physically, this corresponds to weighting the adjoint source with the inverse of the forward flux
- Hence, where the forward flux is low, the adjoint source will be high, and vise versa
- Once the adjoint source is determined, the standard CADIS methodology is used
  - Hence, we refer to the method as ***Forward-Weighted CADIS***
- The method requires:
  - A forward solution (for adjoint source weighting)
  - An adjoint solution (for determining biasing parameters)
  - Both can be automated

Theory – FW-CADIS

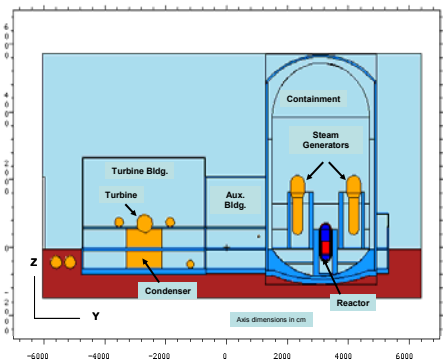
- It can be shown that the adjoint source can be defined to optimize MC for global and semi-global quantities, e.g.,
- For space- and energy dependent flux: $q^{+}(\vec{r},E)=\dfrac{1}{\phi(\vec{r},E)}$
- For total flux: $q^{+}(\vec{r},E)=\dfrac{1}{\int\phi(\vec{r},E')dE'}$
- For response, e.g., dose: $q^{+}(\vec{r},E)=\dfrac{\sigma_d(\vec{r},E)}{\int\phi(\vec{r},E')\sigma_d(\vec{r},E')dE'}$

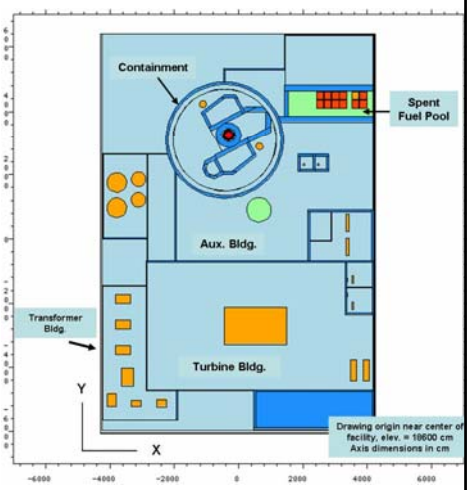
Implementation (SCALE 6/MAVRIC)



Application – dose dist. in PWR facility

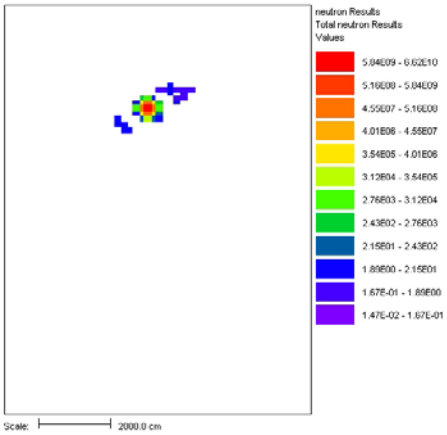
- MCNP model – full PWR facility, including containment, auxiliary, turbine, and transformer buildings
  - Model extent: 85 × 125 × 70 m
- Sources modeled: reactor core, spent fuel pool, coolant activation



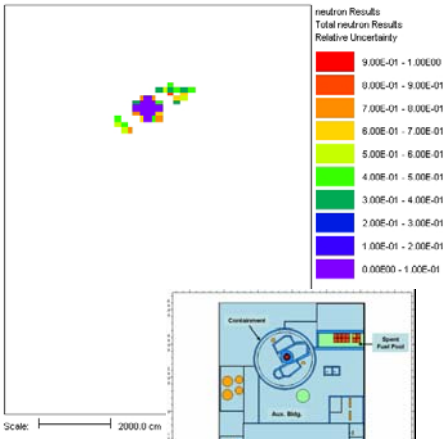


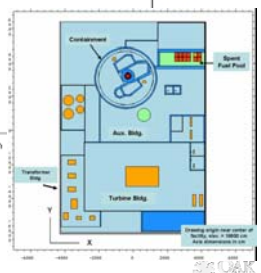
Results – Simulation not feasible with "standard" Monte Carlo (MCNP)

Neutron dose rate



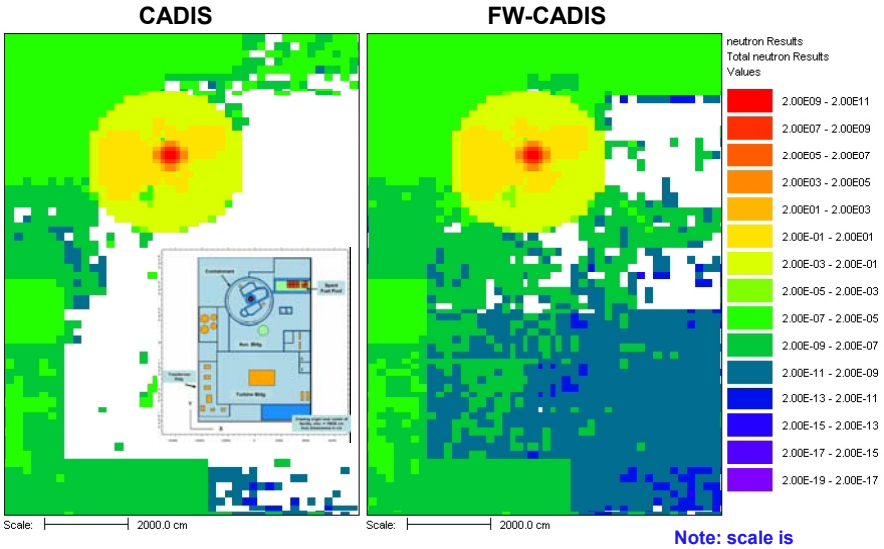
Relative error





- 1E+10 particle histories; 25 CPU days
  (results from 5E+10 history run look similar)
- Particles cannot escape the containment

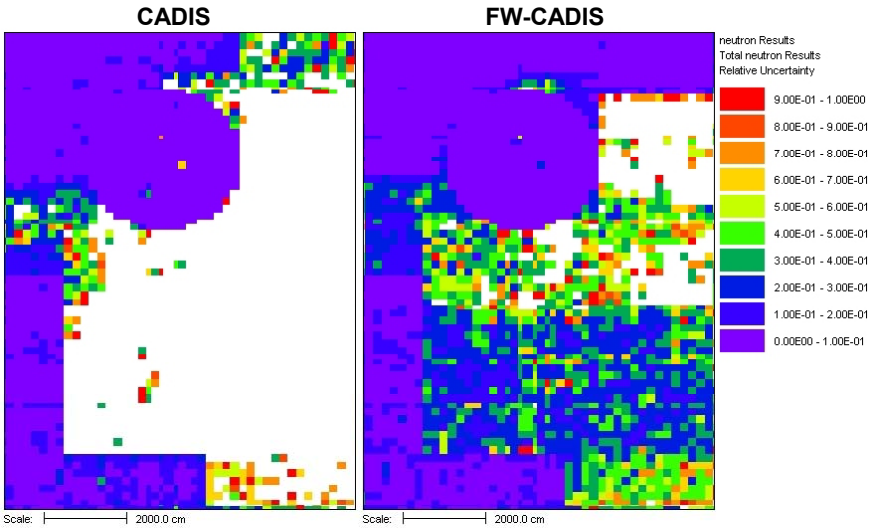
Simulation enabled – FW-CADIS/ADVANTG-MCNP



- **~1E+9 particle histories; 20 CPU days**

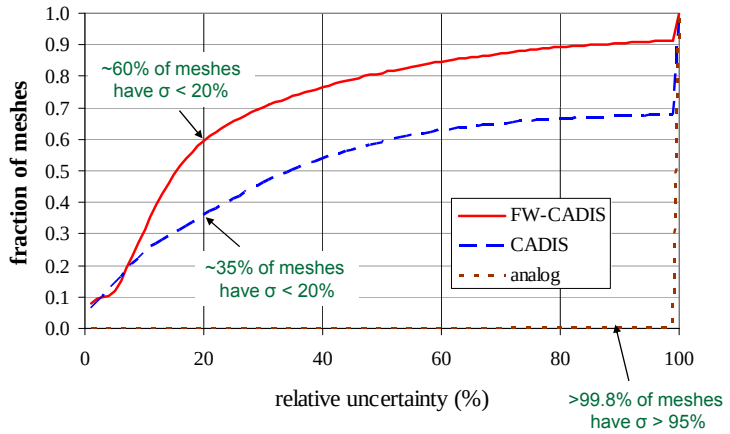
Note: scale is >30 orders of magnitude

Simulation enabled – FW-CADIS/ADVANTG-MCNP



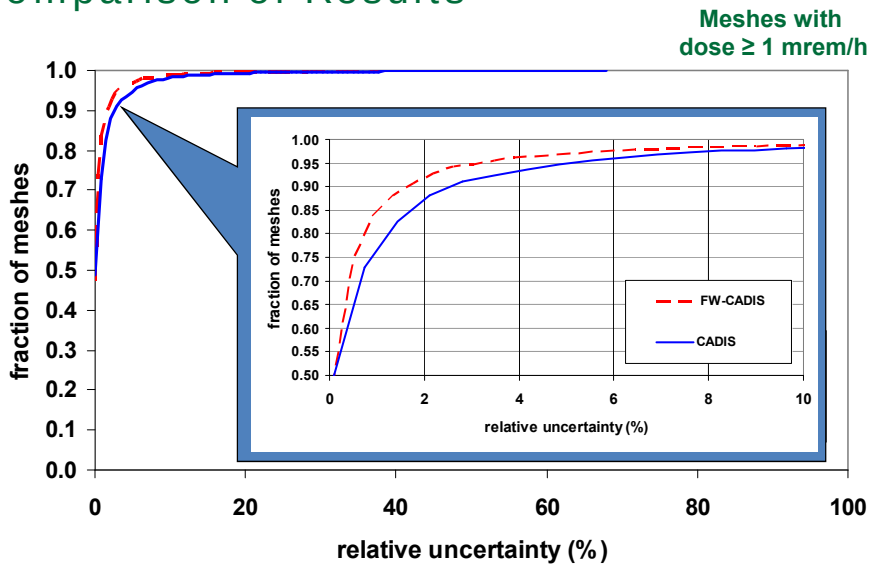
- **~1E+9 particle histories; 20 CPU days**

Comparison of Results



Relative uncertainty histogram comparison for the methods

Comparison of Results

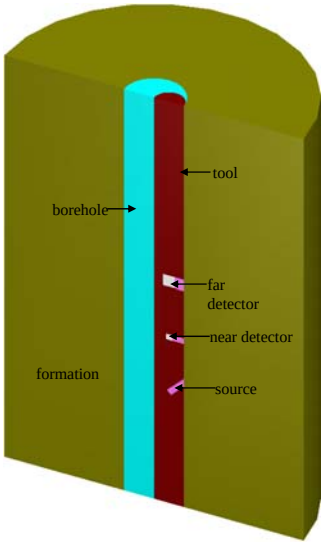


Application – gamma litho-density tool

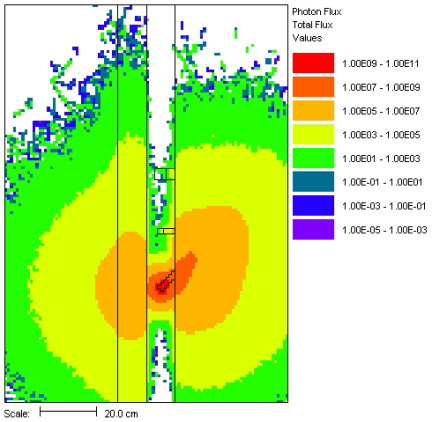
- GOAL: ***obtain uniform statistical uncertainty in multiple detector responses***
- Problem Description from

  Robin P. Gardner and Kuruvilla Verghese, "Monte Carlo Nuclear Well Logging Benchmark Problems with Preliminary Intercomparison Results," *Nuclear Geophysics* 5(4), 429-438 (1991).

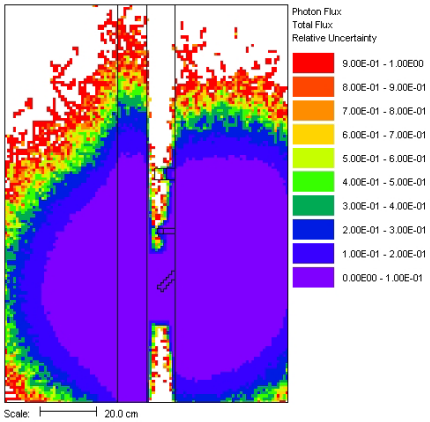
- Source: Cs-137, 2.7 Ci
- Detectors (collimated): NaI
  - Near: 2x2 at 20 cm
  - Far: 4x4 at 40 cm
- Borehole: 20 cm diam
- Tool: 10 cm diam



Gamma Tool – Analog



Total Photon Flux



Relative Uncertainty

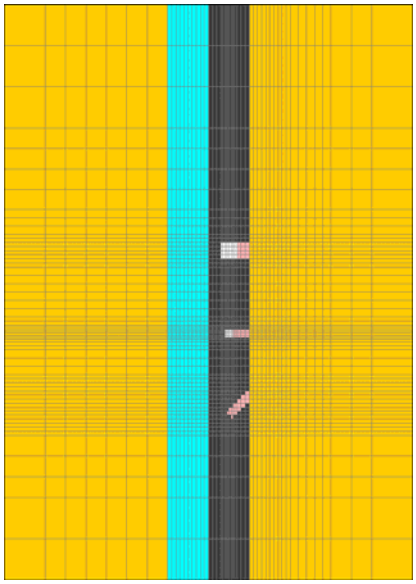
Calculation	Minutes
Monte Carlo	2762

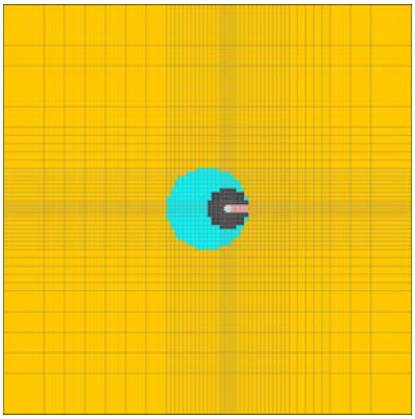
Results

Near 1.49×10^{3} (±8.2%)

Far 6.13×10^{1} (±19%)

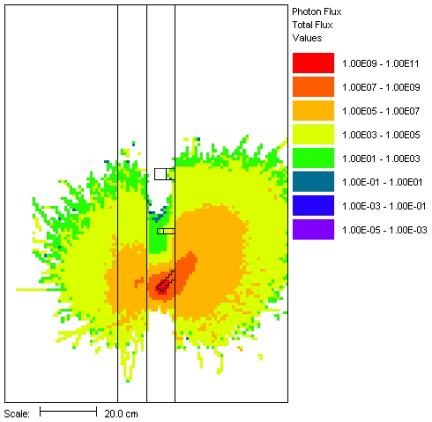
Gamma Tool – Discrete Ordinates Mesh



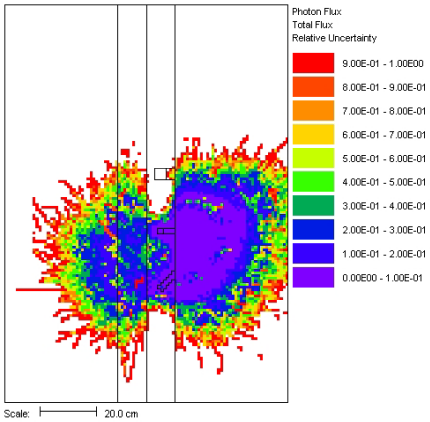


49×43×59 = 124,313

Gamma Tool – CADIS: NEAR Detector



Total Photon Flux



Relative Uncertainty

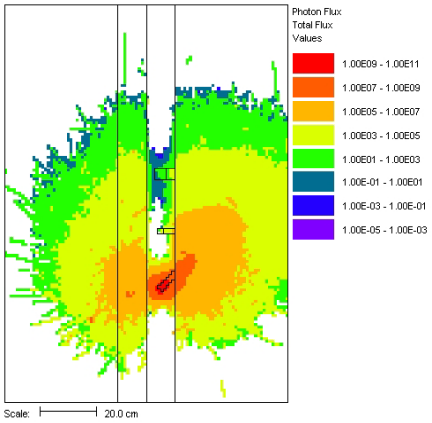
Calculation	Minutes
Adjoint DO	7
Monte Carlo	126

Results

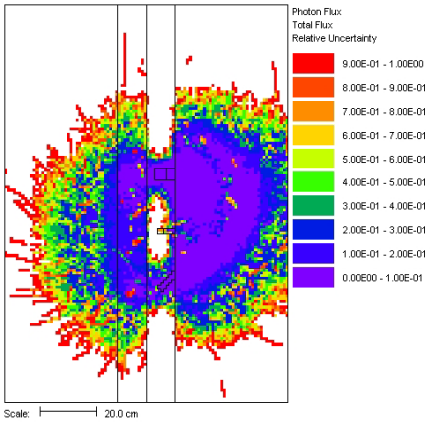
Near **1.54×10^3 (±0.5%)**

Far 0.00

Gamma Tool – CADIS: FAR Detector



Total Photon Flux



Relative Uncertainty

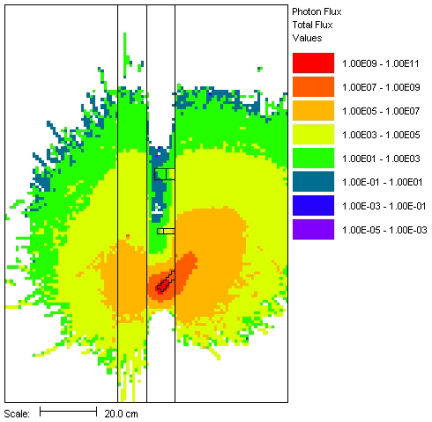
Calculation	Minutes
Adjoint DO	7
Monte Carlo	124

Results

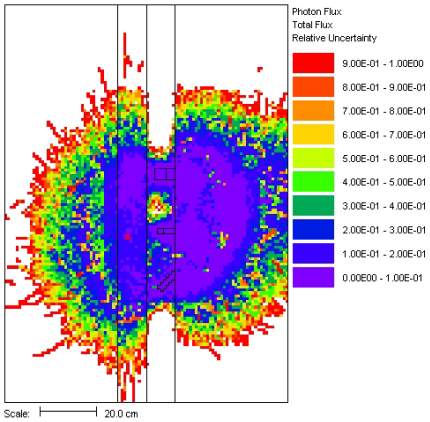
Near 3.10×10^{3} (±65%)

Far 5.59×10^{1} (±0.3%)

Gamma Tool – FW-CADIS: Both Detectors



Total Photon Flux



Relative Uncertainty

Calculation	Minutes
Forward DO	6
Adjoint DO	7
Monte Carlo	126

Results

Near 1.54×10^{3} (±0.6%)

Far 5.56×10^{1} (±0.4%)

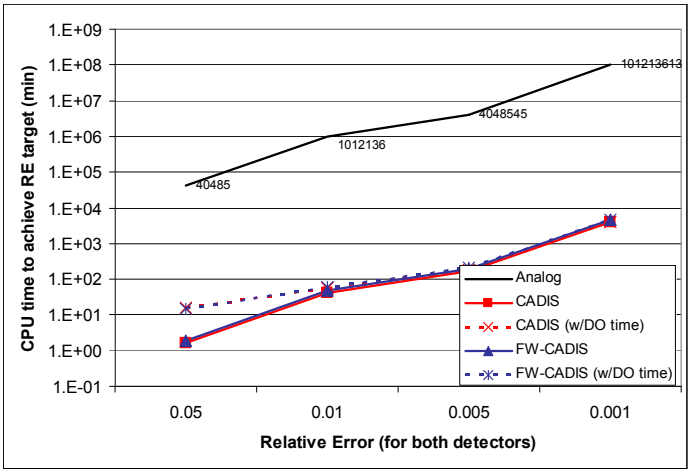
Gamma Tool – Methods Comparison

	Flux in Detector		Time (min)	FOM
Analog				
Near	1.494E+03	8.2%	2762	
Far	6.130E+01	19.1%	2762	
CADIS Near				
Near	1.545E+03	0.5%	133	6461
Far	0.000E+00	0.0%	133	#DIV/0!
CADIS Far				
Near	3.100E+03	65.2%	132	0.3
Far	5.587E+01	0.3%	132	66931
FW-CADIS				
Near	1.543E+03	0.6%	139	3506
Far	5.564E+01	0.4%	139	39236

CPU Time (min) to Achieve RE Targets

	Relative Error Target			
	0.05	0.01	0.005	0.001
Analog				
Near	7341.88	183547	734188	18354699
Far	40485.45	1012136	4048545	1.01E+08
Total	**40485.45**	**1012136**	**4048545**	**1.01E+08**
CADIS Near				
Near	8.26	34.06	114.68	2694.49
CADIS Far				
Far	7.67	21.4	64.32	1437.77
Total	**15.93**	**55.46**	**179**	**4132.26**
FW-CADIS				
Near	14.87	60.43	202.82	4759.27
Far	13.91	36.36	106.52	2351.66
Total	**14.87**	**60.43**	**202.82**	**4759.27**
Speed-up				
Analog/CADIS	**2541**	**18250**	**22618**	**24494**
Analog/FW-CADIS	**2723**	**16749**	**19961**	**21267**

CPU Time to Achieve RE Targets



Summary & Conclusions

- A new hybrid method, FW-CADIS, has been developed and tested for optimizing MC calculations of distributions and multiple quantities
- FW-CADIS requires two approximate solutions (one forward and one adjoint) to generate consistent source biasing and weight window parameters for the MC simulation and does not require any modifications to existing MC codes
- Although additional testing and thorough analysis of results are continuing, all results to-date have been excellent
  - Successfully applied to several problems at ORNL, e.g.,
    - Dose rate distributions, including a full-size spent fuel storage cask array
    - Criticality accident alarm system analyses
    - Detector response in the multiple detectors in well-logging tools
    - Active & passive detection applications
- FW-CADIS should be suitable for a large range of problems, and may be useful for MC depletion calculations

Summary & Conclusions

- Advanced methods for VR, which rely on deterministic solutions, are ***enabling the use of MC for deep-penetration and answers-everywhere applications***
  - CADIS – Consistent Adjoint Driven Importance Sampling, optimization of local quantities
  - FW-CADIS – Forward-Weighted CADIS, optimization of distributions (e.g., mesh tallies), as well as multiple local quantities
- The results of these methods could have significant implications on how MC is used in the future
- CADIS & FW-CADIS available in SCALE 6

Closure – Questions & Discussion

- Acknowledgements:
  - Sponsors: Defense Threat Reduction Agency (DTRA) & NRC
- Contact Info:
  - Douglas Peplow, peplowde@ornl.gov
  - John Wagner, wagnerjc@ornl.gov
- Other related papers at this conference:
  - ***Automated Weight-Window Generation for Threat Detection Applications Using ADVANTG***, 10:45AM, Tuesday Session 10B: Hybrid Methods in Particle Transport I, Room: Saratoga 3
  - ***Criticality Accident Alarm System Modeling with SCALE***, 10:45AM, Thursday, Session 28B: Criticality Safety, Room: Saratoga 3