# Forward-Weighted CADIS Method for Global Variance Reduction


**John C. Wagner**

**Edward D. Blakeman**

**Douglas E. Peplow**

Radiation Transport & Criticality Group
Nuclear Science & Technology Division


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## Overview

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- **Motivation for Work**
- **Theory**
  - CADIS
  - FW-CADIS
- **Implementation**
- **Example Results**
- **Summary & Conclusions**

## Introductory Remarks

- Monte Carlo (MC) is becoming 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 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 results of a method for optimization of global and semi-global quantities that challenge some (certainly not all) of these conventional beliefs
- VR Terminology
  - Global VR – calculate results everywhere, e.g., flux distributions
  - Semi-global VR – calculate results in select ranges or locations, e.g., response at multiple spatial locations, energy spectrum at one or few locations

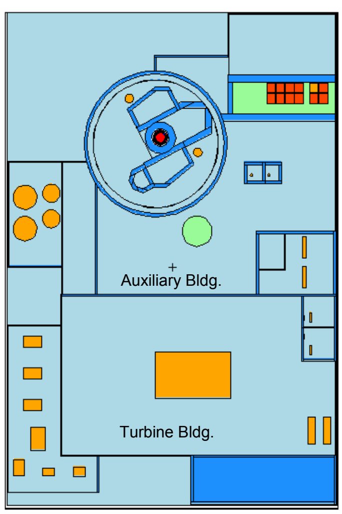
## Motivation for Work

- **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**

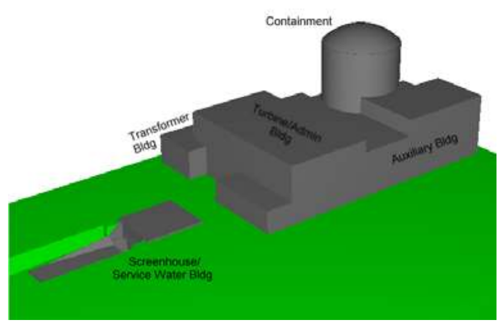


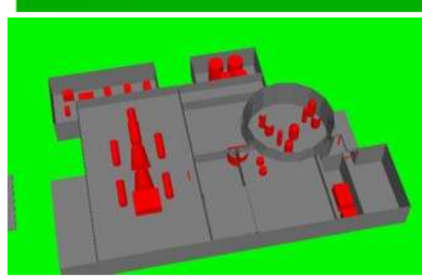
## Dose Rates Throughout a PWR Facility

**Large scales, massive shielding**
**Difficult to calculate dose rates**

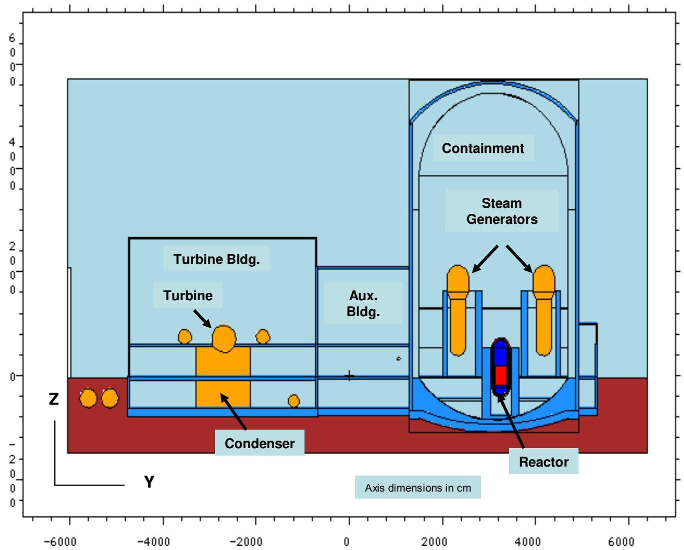



**85 × 125 × 70 m**



# 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, $\sigma_d$, 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 reviewed in the following 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, $\sigma_d$, 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 are scaled to calculate lower-weight bounds, $w_l$**

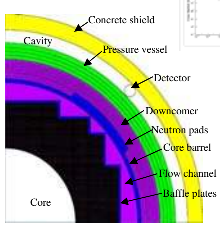
$$w_\ell(\vec{r},E) = \frac{w}{\left(\frac{c_u+1}{2}\right)} = \frac{R}{\phi^{+}(\vec{r},E)\left(\frac{c_u+1}{2}\right)} \quad where \;\; c_u = \frac{w_u}{w_\ell}$$

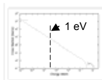


## Theory – CADIS

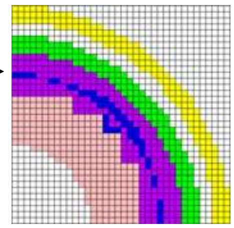
- **The CADIS method**
  - **Provides source biasing parameters and weight windows such that source particles are started with weights that are within the weight windows**
  - **Has been implemented and automated in the ADVANTG code (based on MCNP) and the MAVRIC sequence of SCALE** **(to be released in SCALE 6)**
    - **Both codes are routinely used at ORNL for 3D MC simulations of real applications, e.g.,**
      - **Detector response, dose rate, DPA, total flux, etc.**
    - **Considerable experience with the method**

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

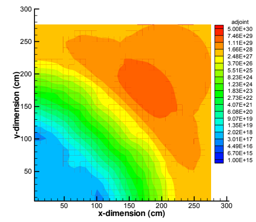



Monte Carlo model



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)**

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

**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 $\overline{w}(\vec{r})$.**

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

  - **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 1-group 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 (from *Cooper and Larsen, NS&E, 2001*):**
  - 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

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

- **By substituting the forward flux for $\overline{w}\,v$ 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 importance will be high, and vise versa**
- **Once the adjoint importance function 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:** $q^{+}(\vec{r},E) = \dfrac{1}{\phi(\vec{r},E)}$

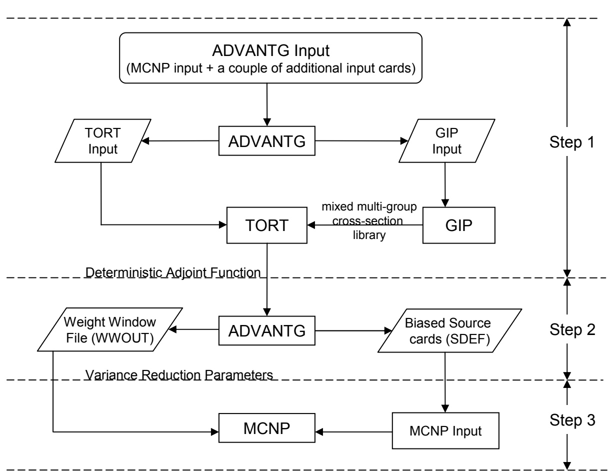
- **For total flux:** $q^{+}(\vec{r},E) = \dfrac{1}{\int \phi(\vec{r},E')dE'}$

- **For response, e.g., dose:** $q^{+}(\vec{r},E) = \dfrac{\sigma_d(\vec{r},E)}{\int \phi(\vec{r},E')\sigma_d(\vec{r},E')dE'}$



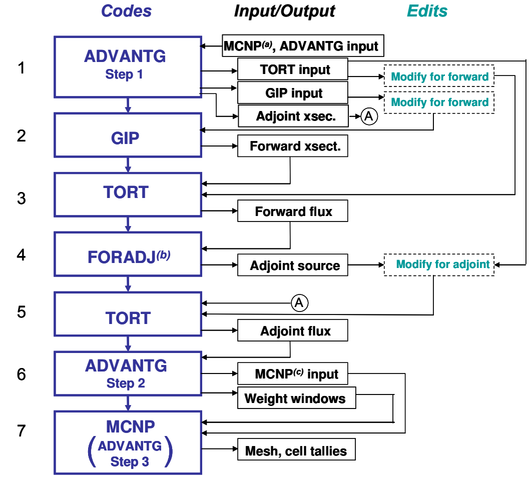
## Implementation (ADVANTG)

- **CADIS - automated**



# Implementation (ADVANTG)

- **FW-CADIS – no major obstacles, but not yet fully automated**

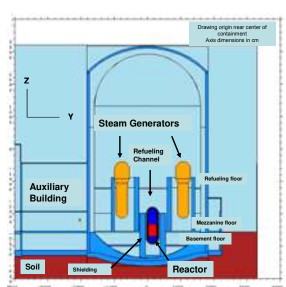


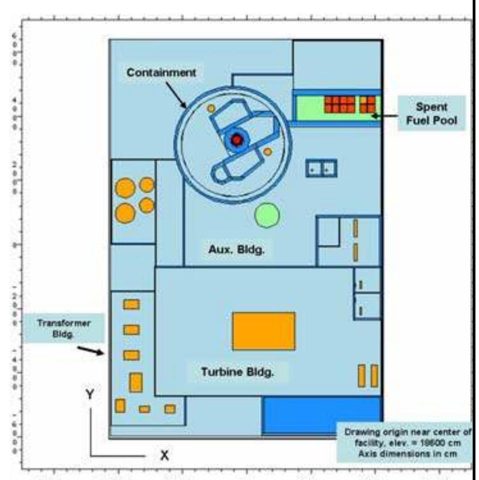

CADIS & FW-CADIS are fully automated in the SCALE MAVRIC sequence



# Application

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

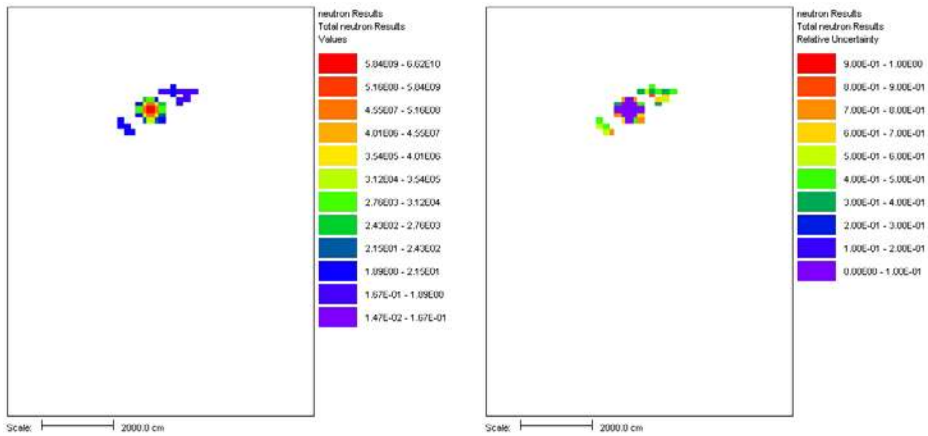


## Example Results – analog

Neutron dose rate

Relative error



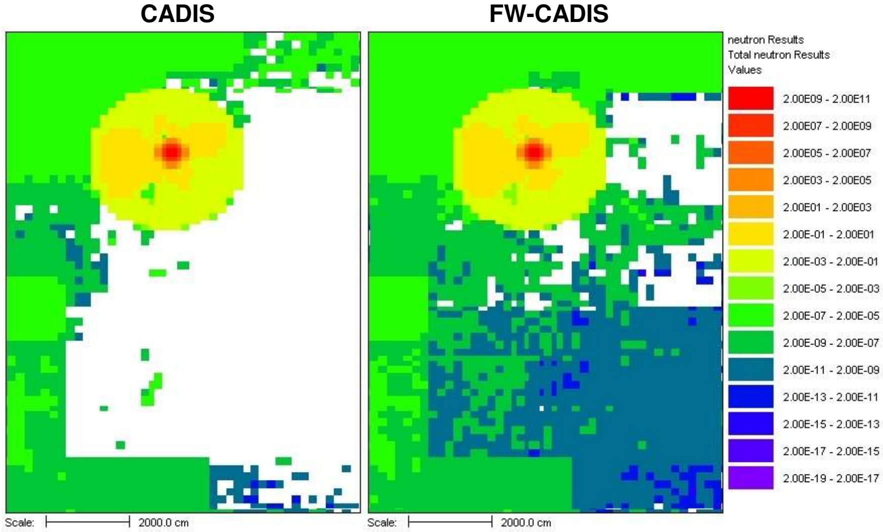

- **1E+10 particle histories; 25 CPU days**



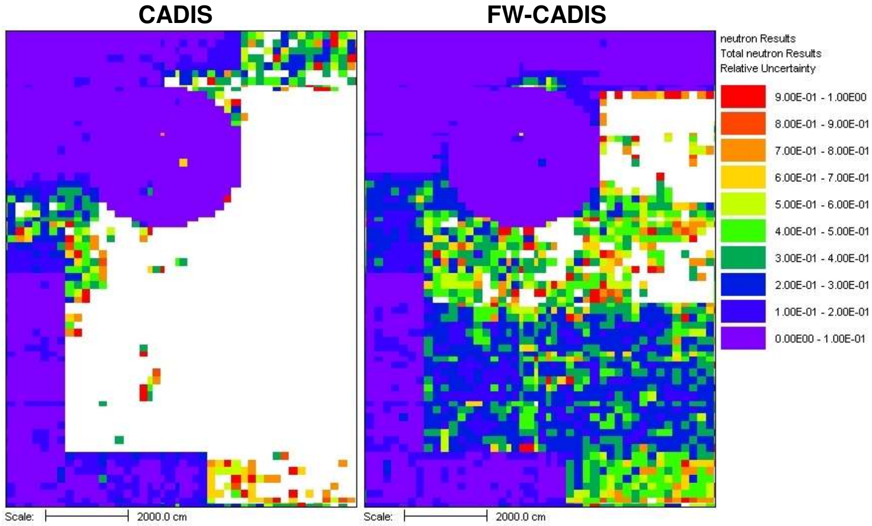
## Example Results – neutron dose rates

CADIS

FW-CADIS

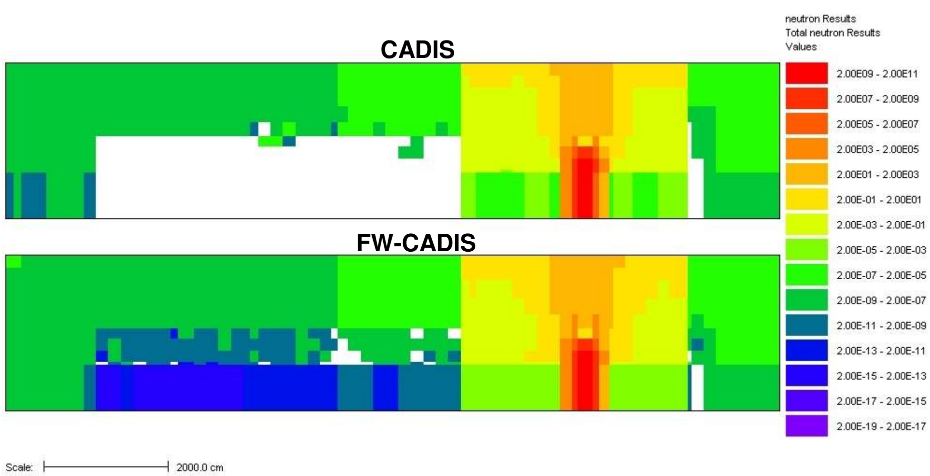


## Example Results – relative errors

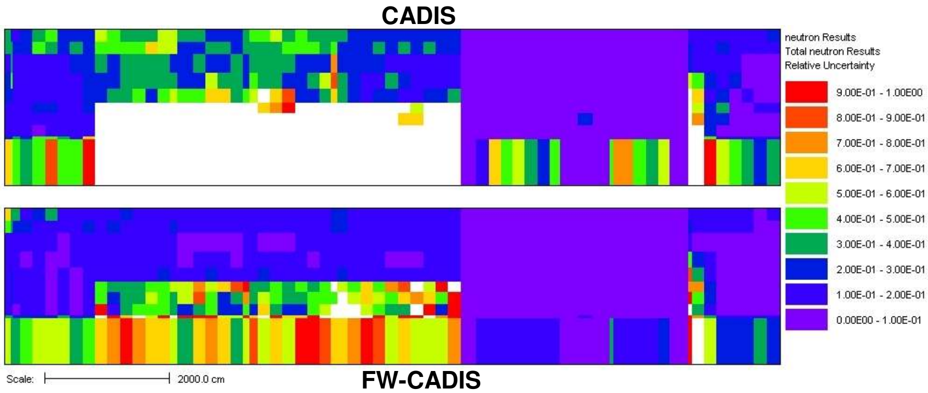





## Example Results – neutron dose rates

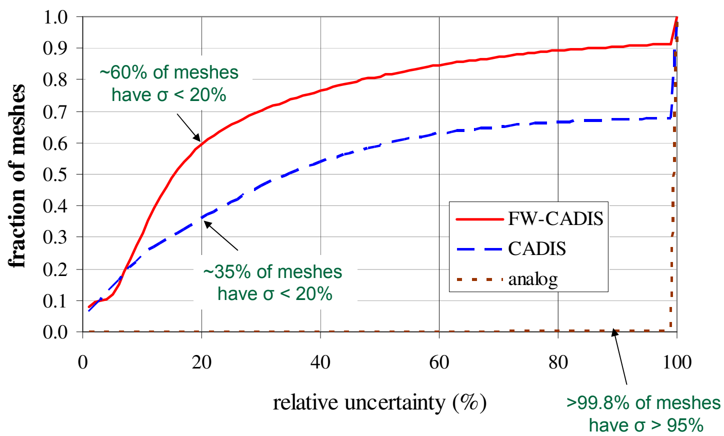


## Example Results – relative errors



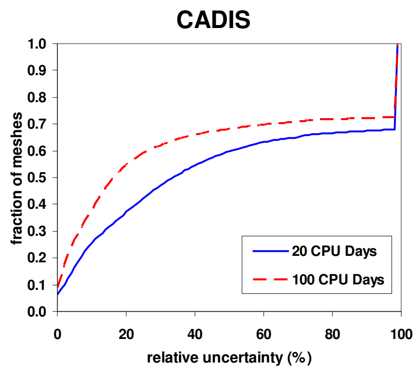


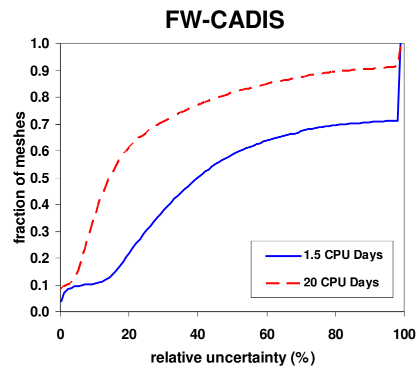

## Comparison of Results




**Relative uncertainty histogram comparison for the methods**

# Comparison of Results

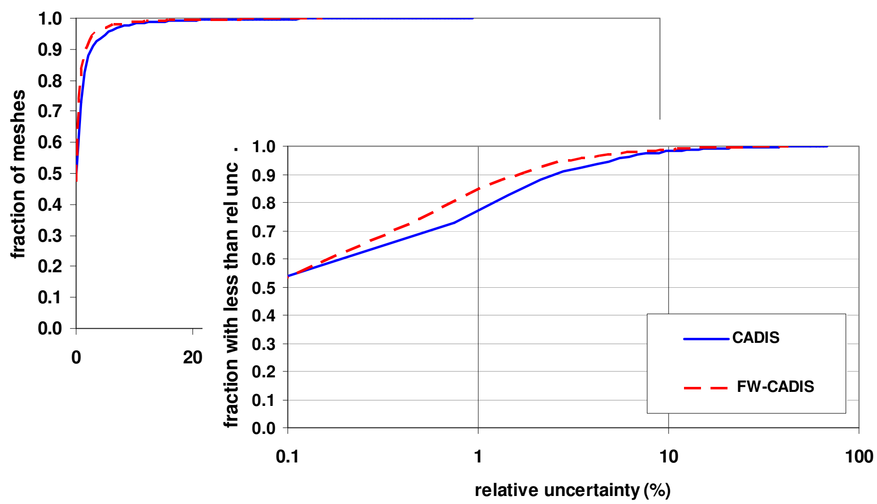



**Comparison of results for different CPU times for the methods**



# Comparison of Results



## Summary & Conclusions

- A new method, FW-CADIS, has been presented for optimization of global and semi-global quantities with MC
- 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 (global)
    - Detector response in the multiple detectors in well-logging tools (semi-global)
    - Spectra at selected locations in a couple of reactor problems
- 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**

## Closure

- **Acknowledgements:**
  - Sponsor: Defense Threat Reduction Agency (DTRA)
  - Co-authors: Ed Blakeman & Douglas Peplow, ORNL
  - Prof. Ed Larsen, University of Michigan

- **Contact Info:**
  - John Wagner, wagnerjc@ornl.gov

- **Questions/Discussion?**