Review of Hybrid Radiation Transport Methods, Codes, and Applications at Oak Ridge National Laboratory

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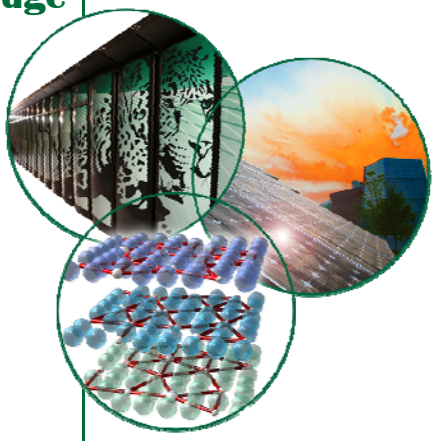

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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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Overview

- Introductory Remarks / Motivation
- Hybrid Methods (Automated Variance Reduction)
  - CADIS – optimization of single tally
  - FW-CADIS – optimization of distributions or multiple tallies
- Code Implementation
  - SCALE
  - ADVANTG
- Applications
- Current Development Activities
- Summary Remarks

Introduction – Hybrid Methods

- Hybrid methods attempt to use the best attributes of Monte Carlo (MC) & deterministic methods in a complementary manner
- In this discussion, the Hybrid Methods *use fast, approximate* (deterministic) *calculations to speed-up highly accurate (MC) simulations*
- How does it work?
  - Calculate 3-D adjoint function with a deterministic code
  - Calculate variance reduction (VR) parameters based on adjoint function
  - Utilize the VR parameters in the MC simulation
  - Automate above steps (key to usefulness!)

Introduction – Previous Works

- Recognizing the physical meaning of the adjoint function, numerous works have developed methods to use adjoint data for MC VR (for localized quantities)
- Recognizing the potential advantages, much work has been done to develop and automate methods based on deterministic importance functions
  - Advantages include:
    - Substantial computational speed-ups
    - Substantial reduction in requirements for user time, effort, and expertise
    - Improved computational reliability; reduced likelihood of biasing solution
- Numerous efforts have shown the benefits and demonstrated the feasibility of automated stochastic- and deterministic-based VR
- 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)

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Consistent Adjoint Driven Importance Sampling

- **Objective – optimization of a single tally in a MC calculation**
- **Relationships for calculating consistent source & transport biasing parameters**
- **Biased source:**

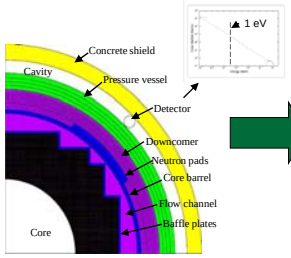
$$\hat{q}(\vec{r},E)=\frac{\phi^{+}(\vec{r},E)\,q(\vec{r},E)}{\int_V dV\int_E dE\,\phi^{+}(\vec{r},E)\,q(\vec{r},E)}=\frac{\phi^{+}(\vec{r},E)\,q(\vec{r},E)}{R}$$

- **Weight targets:**

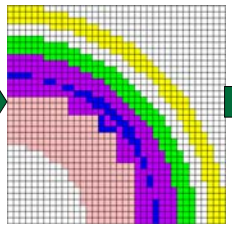
$$w(\vec{r},E)=\frac{q(\vec{r},E)}{\hat{q}(\vec{r},E)}=\frac{R}{\phi^{+}(\vec{r},E)}$$

- **Unique feature is the consistency, which ensures particles start within the weight window interval**

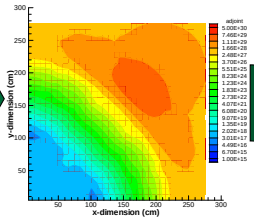
CADIS Example: PWR Ex-Vessel Thermal (^{10}B) Detector Response



Monte Carlo model



Deterministic model



Adjoint data

VR Parameters

Source biasing

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

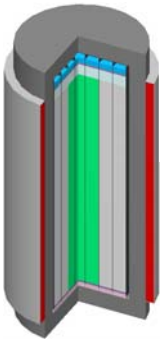
Transport biasing (weight windows)

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

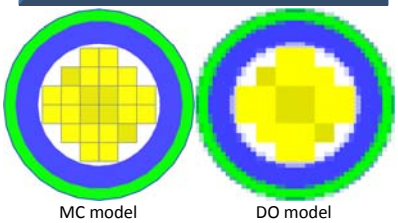
Case	CPU Time (h)[A]	Speedup
No VR	8.86E4 (10.1 yrs)	-
Manual VR[B]	13.6	6500
CADIS	1.02	87000

[A] Time to achieve ≤ 1% RE
[B] Required 3 weeks by an experienced Monte Carlo practitioner

CADIS Example: Spent Fuel Cask

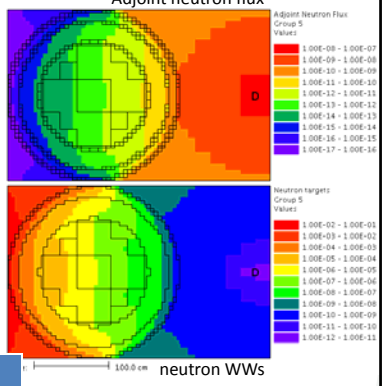


Calculate total dose rate (neutron and photon) two meters from the surface of a TN-24P storage cask loaded with *two types* of assemblies.



MC model DO model

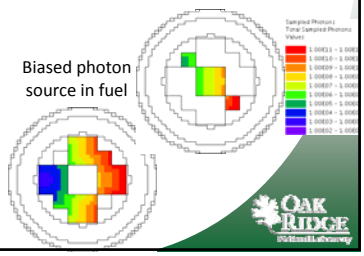
Adjoint neutron flux



neutron WWs

Dose	Analog		CADIS (1 calc, 24 min)
	neutron calc (900 min)	photon calc (903 min)	
Neutron	3.84E-4 (3.0)	n/a	3.74E-3 (1.5)
Photon	3.02E-4 (0.7)	5.17E-3 (39.0)	8.01E-3 (0.9)
Total	5.17E-3 (39.0)		8.38E-3 (0.9)
SPEEDUP of a factor of 93,000			

Biased photon source in fuel



Forward Weighted CADIS method

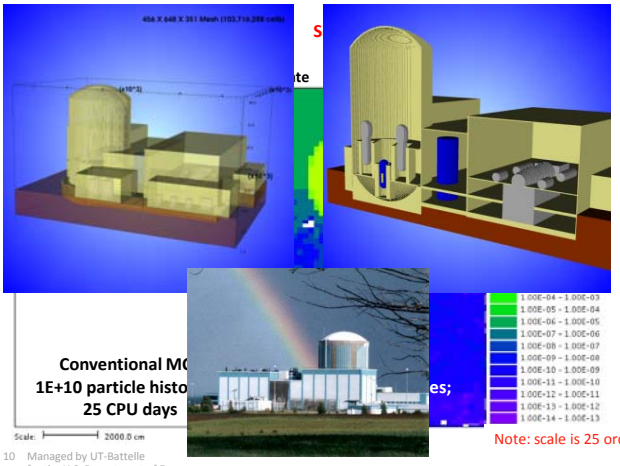
- **Objective –** ***Uniform statistical uncertainty in calculated quantities, e.g., space- and energy-dependent flux***
- **Involves determining a function that represents the importance of particles to achieving uniform MC particle density, which is related to statistical uncertainty, throughout all or part of the problem phase-space**
- **Calculation of this importance function involves weighting of the adjoint source with information from a forward solution**
  - **Where the forward flux/response is low, the adjoint importance will be high, and vise versa**
- **To calculate response, such as dose rate, over a mesh tally, the adjoint source is defined as:**

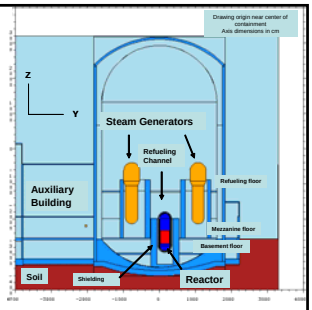
$$q^{+}(\vec{r},E)=\frac{\sigma_d(\vec{r},E)}{\int\phi(\vec{r},E')\sigma_d(\vec{r},E')dE'}$$

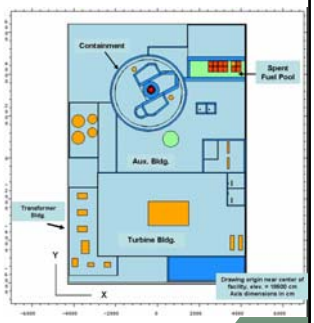
For details, see: "Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Calculations of Distributions and Multiple Localized Quantities," M&C 2009, Saratoga Springs, NY, May 3-7, 2009.

FW-CADIS example: dose throughout a PWR facility

- **Full-scale PWR facility, including containment, auxiliary, turbine, and transformer buildings**
  - **Extent: 85 × 125 × 70 m**
  - **Sources modeled: reactor core, spent fuel pool, coolant activation**







Note: scale is 25 orders of magnitude

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Code Implementation

- The KEY aspect relative to the usefulness of these methods is an implementation that minimizes user time, effort, and overall level of difficulty
- Both methods have been implemented and automated
  - SCALE 6 MAVRIC sequence, which uses the 3-D Monaco MC code
  - ADVANTG code, which prepares VR parameters for MCNP/X
  - Both implementations use the Denovo 3-D discrete ordinates code for deterministic calculations
- Users must provide mesh boundaries and identify the tallies to optimize

MAVRIC first public release, SCALE 6, Feb 2009

Denovo – massively parallel deterministic radiation transport code enabling solutions to enormous nuclear energy applications

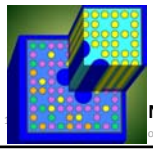
- State of the Art Transport Methods
  - 3-D Discrete Ordinates (SN)
  - Multigroup energy, anisotropic PN scattering
  - 6 spatial discretization algorithms to choose from
- High Performance, Modern, Innovative Solvers
  - GMRES, BiCGStab. or Source Iteration options on within-group solves
  - DSA-preconditioning (SuperLU/ML-preconditioned CG)
  - Transport Two-Grid up-scatter acceleration of Gauss-Seidel MG iteration
  - Parallel first collision approximation
  - Eigenvalue (k_{eff}) and fixed-source problem modes
  - Krylov solvers provided by Trilinos Library

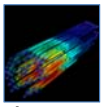
- Parallel Algorithms
  - Koch-Baker-Alcouffe (KBA) wavefront solve
  - Domain replicated & decomposed options for parallel first-collision source
  - Multi-level decompositions in energy and angle under development
  - Parallel I/O for massive problems
- Advanced Visualization and Run-Time Environment
  - Python front-end allows high-degree of flexibility in prescribing input/output
  - Direct connection to SCALE geometry and data
  - HDF5 output directly interfaced with Visit

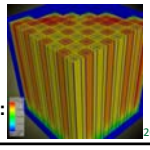
PWR Facility Modeling

Zones	Angles	Groups	State Size (GB)	Output (GB)	Time (m)
103.7M	S_{24}/P_3	27	568.741	83.457	46.97
1,047.8M	S_{24}/P_3	27	5,746.180	843.189	79.43

- **Highlights**
  - Routinely running > 100M cell problems on Cray XT5
  - FY10 ASCR JOULE code
  - 2010 DOE Office of Science INCITE Award
  - Key component of ORNL hybrid (Monte Carlo/deterministic) code/methods development
- **On-going and Future Directions**
  - ORNL LDRD support for development of explicit full-core reactor analyses
  - ORNL LDRD development for hybrid reactor analysis
  - Electron transport for home land security applications

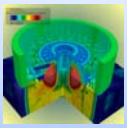






Nuclear Energy: LWR analyses

Fusion: ITER analyses



285M cell, S_{24}/P_3 model of the International Thermonuclear Experimental Reactor (ITER)

Hybrid methods automated in SCALE

SCALE 6 MAVRIC

- **START** — • **Read and process user Input**
- **Bonami CENTRM PMC** — • **Resonance XS processing (for MG XSs)**
- **Denovo** — • **Forward DO calculation for FW-CADIS** • optional, automated first-collision source
- **Denovo** — • **Adjoint DO calculation for CADIS** • optional, automated first-collision source
- **CADIS** — • **Calculate weight windows and biased source**
- **Monaco** — • **MC Simulation**
- **END** — • **Write output**

Optional steps for hybrid methods

General Usage Observations

- **Mesh boundaries**
  - **If selected to be reasonably consistent with material boundaries, results are not very sensitive**
  - **Failure to capture problem geometry/physics can manifest itself in poor computational efficiency and/or convergence behavior (identified by statistical convergence diagnostics)**
  - **Because the process is automated, creating and utilizing different mesh distributions is a simple matter**
- **Useful features in SCALE**
  - **Visualization tools for viewing and evaluating DO mesh/material map, DO results, mesh-based WWs, and mesh-based biased source**
- **Tally types: results have shown that speedups achieved for track-length estimator and point detector are quite comparable – providing an indication that the methodology is effective for both estimators**

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Speed-ups of 100s to tens-of-thousands observed for many applications with CADIS

Application	Observed speed-up relative to manual VR / analog	Reference(s) (in paper)
PWR cavity dosimetry (MeV reaction rates)	4 / $O(10^4)$	1–3
DPA in BWR core shroud	NA / $O(10^3)$	15
Neutron well-logging tool	2-3 / $O(10^2)$	6, 16
Gamma well-logging tool	NA / $O(10^{3-4})$	6, 16
Dose from single spent fuel storage cask	NA / $O(10^{3-4})$	1, 17, 18
PWR ex-core thermal detector response	~13 / $O(10^4)$	19
Passive threat detection	NA / $O(10^{2-4})$	20
Active-interrogation SNM detection	NA / $O(10^4)$	20
ITER shielding	NA / $O(10^{2-4})$	21, 22
HFIR DPA calculations	NA / $O(10^4)$	23
Criticality accident alarm system analyses	NA / $O(10^{2-3})$	24, 25

FW-CADIS has enabled or greatly accelerated MC simulations for many applications

Application	Reference(s) (in paper)
Dose rate throughout full-scale PWR facility	5, 7, 27
Multiple detector responses in nuclear well-logging tools	6, 16
Site boundary dose rate from an array of spent fuel casks	28, 29
ITER shielding and material heating analysis	21, 22
Dose rates throughout a critical facility	24, 25
Dose rates throughout an urban model from a nuclear weapon detonation	10
Dose rates throughout IRIS reactor containment	30
Dose rates throughout SNS beamline shielding	unpublished

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Current Development Activities

- **Acceleration of reactor and criticality analyses**
  - **Group-wise forward and adjoint fluxes for reactor analyses and sensitivity/uncertainty analyses**
  - **Convergence of the fission source**
  - **Eigenvalue convergence**
- **Acceleration for highly angular-dependent problems**
  - **Active interrogation, beamline shielding**
- **Acceleration of active-interrogation problems**
  - Multi-step CADIS-based approach has been developed and implemented
- **Improvement of use**
  - **Automated/intelligent meshing; improved diagnostics**

Summary

- Hybrid methods at ORNL are enabling the use of MC for deep-penetration and answers-everywhere applications
- Methods are implemented and automated in SCALE 6 (publicly available) and ADVANTG/MCNP
  - Automation/ease-of-use are KEY to usefulness to MC user community
  - Confirmed to give correct (unbiased) answers, where possible
- These methods/codes are having a significant impact on how MC is used at ORNL; significant impact beyond ORNL in the future?
- Current/planned focus:
  - Applications, particularly nuclear security applications
  - Reactor and eigenvalue S/U analyses

Closure – Questions & Discussion

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