Advanced Variance Reduction Methods and Their Implementation

Friday March 27, 2009
Nuclear Engineering and Radiological Sciences
University of Michigan

Douglas E. Peplow
Radiation Transport & Criticality Group
Nuclear Science & Technology Division
Oak Ridge National Laboratory
NUCLEAR SYSTEMS
ANALYSIS, DESIGN,
AND SAFETY

- Radiation shielding
- Radiation transport
- Reactor physics
- Criticality safety
- Nuclear data and codes
- Thermal hydraulics
- Material and fuel irradiation
- Advanced/Space reactors
- Information/Systems analysis
- Reactor/Facility safety
- Risk assessment
- Regulatory support
- System instrumentation and controls
- Enrichment technology

FUELS, ISOTOPES,
AND NUCLEAR
MATERIALS

- Nuclear fuels
- Heavy element production
- Stable/radioactive isotopes
- Medical isotope development
- Separations science and technology
- Nuclear process and equipment design
- Robotics
- Remote handling
- Chemical engineering

Challenging Applications
Driving
Methods Development
**Radiation Protection (RP) Factors**

**Goal:**
Compute the RP factors for armored vehicles from nuclear weapon & radiation dispersal device detonations

**Challenges:**
1. Scatter from air and ground more important than direct radiation
2. Huge difference in scales
3. Extensive user time to develop models
4. Extensive user & computational time to develop effective VR parameters

---

**Dose Rates in a PWR Facility**

**Goal:**
Compute dose rates throughout an entire full-scale commercial PWR facility.

**Challenges:**
1. Facility is very large and very-well shielded
2. Model development is very time consuming
3. Sponsor requested MCNP-based solution
4. Answers-everywhere for such a large problem is considered impossible with MC
Site Boundary Dose

**Goal:**
Determine boundary of controlled area for Independent Spent Fuel Storage Installation (ISFSI).
Limit is 25 mrem/year.

**Challenges:**
1. Need the dose rate everywhere to ensure compliance
2. Need low uncertainties everywhere, independent of the dose rate
3. Problem is very large spatially

---

Radiation Doses in Urban Environment

**Goal:**
Model nuclear blast/RDD in a city to aid emergency response planners

**Challenges:**
1. Requires enormous computational resources to achieve high-fidelity results
2. Models are still in their infancy
Active Interrogation Systems

Goal:
Scan cargo offshore, at ports, at weigh stations
Detect fissionable material as small as 20 kg U

Challenges:
1. Easily concealed
   - Encased in shielding
   - Hidden in a mixed materials
     - Steel
     - Food products
2. Huge Volume of Goods

Active Interrogation

- Source strength is limited
- Large stand-off distances
- Large amounts of shielding
  - Hydrogenous material
    preferentially shields neutrons
  - High-Z (proton number) material
    preferentially shields photons
- Eventual designs will probably employ
  a mix of source types and a mix of
detectors
Criticality Accident Alarm Systems

Goal:
Determine detector responses in different locations of a building for a given a criticality accident

Challenges:
1. Thick Shielding
2. Large Buildings
3. Criticality Calculation/Shielding Calculation

Methods and Implementation

Hybrid MC/DO Methods
SCALE 6
ADVANTG (MCNP)
Variance Reduction

- Changing the sampling routines to optimize the simulation to get more particles to do something

- Traditional methods:
  - Rely on knowing the expected results
  - Require trial and error
  - Multiple methods may work against each other
  - May require several iterations
  - Typically involve many steps
  - May require specialized MC codes

Variance Reduction

- What is desired:
  - Tell MC code what tally/tallies to calculate
  - The MC code figures out the best way to do that

- Importance map (weight windows)
  - If we knew how “important” a given particle is as a function of \((\vec{r}, E, \Omega)\), then weight window target values can be assigned, using roulette and splitting to control particle weight
  - Importance is the solution to the adjoint equation, using the tally location as the spatial component of the adjoint source and the tally response function as the energy component of the adjoint source
A Bit of Review

• Forward Transport Equation

\[ H \phi(\vec{r}, E, \Omega) = Q(\vec{r}, E, \Omega) \]

\[ H = \Omega \cdot \nabla + \Sigma(\vec{r}, E) - \int d\Delta \Sigma'(\vec{r}', E', \Omega' \rightarrow \Omega) \]

• Solve for flux, then compute detector response

\[ R = \iint \sigma_\text{det}(\vec{r}, E) \phi(\vec{r}, E) \, dE \, d\vec{r} \]

• Adjoint Transport Equation

\[ H^+ \Phi(\vec{r}, E, \Omega) = Q^+(\vec{r}, E, \Omega) \]

\[ H^+ = -\Omega \cdot \nabla + \Sigma(\vec{r}, E) - \int d\Delta \Sigma'(\vec{r}', E', \Omega' \rightarrow \Omega') \]

• Solve for adjoint flux using \( q^+(\vec{r}, E) = \sigma_a(\vec{r}, E) \), then compute

\[ R = \iint q(\vec{r}, E) \phi^+(\vec{r}, E) \, dE \, d\vec{r} \]

Using Importances

• If the true importances are known, then there is no need for the MC calculation

• If the approximate importances are known, then weight windows can be used for a MC game:

\[ \overline{w}(\vec{r}, E) = \frac{c}{\phi^+(\vec{r}, E)} \]
CADIS Methodology

Consistent Adjoint Driven Importance Sampling

Biased source and importance map work together

- Solve the adjoint problem using the detector response function as the adjoint source.
  \[ q^+ (\vec{r}, E) = \sigma_d (\vec{r}, E) \]

- Weight window targets are inversely proportional to the adjoint flux (measure of importance of the particles to the response).
  \[ \overline{w}(\vec{r}, E) = \frac{c}{\phi^+ (\vec{r}, E)} \]

- We want source particles born with a weight matching the weight window targets
  \[ w_0 (\vec{r}, E) \equiv \frac{q(\vec{r}, E)}{\hat{q}(\vec{r}, E)} = \overline{w}(\vec{r}, E) \]

- So the biased source needs to be
  \[ \hat{q}(\vec{r}, E) = \frac{q(\vec{r}, E)}{\overline{w}(\vec{r}, E)} = \frac{1}{c} q(\vec{r}, E) \phi^+ (\vec{r}, E) \]

- Since the biased source is a pdf, solve for \( c \)
  \[ c = \int \int q(\vec{r}, E) \phi^+ (\vec{r}, E) d\vec{r} dE \]
CADIS Methodology - Summary

- Define the adjoint source
  \[ q^+(\vec{r}, E) = \sigma_d(\vec{r}, E) \]
- Solve for the adjoint flux
- Find \( c \)
  \[ c = \int \int q(\vec{r}, E) \phi^+(\vec{r}, E) d\vec{r} dE \]
- Construct weight windows and biased source
  \[ \bar{w}(\vec{r}, E) = \frac{c}{\phi^+(\vec{r}, E)} \]
  \[ \hat{q}(\vec{r}, E) = \frac{1}{c} q(\vec{r}, E) \phi^+(\vec{r}, E) \]

Example – Spent Fuel Cask

Calculate dose rate at six different detector locations

Emission probability (/MeV) vs Energy (MeV)
Example – Spent Fuel Cask

• For detector 3: compute adjoint fluxes

Adjoint neutron fluxes (n/cm²/s) for groups 5 (0.9–1.4 MeV), 10 (0.58–3.0 keV), and 19 (0.8–1 eV) calculated by Denovo

Example – Spent Fuel Cask

• Compute target weights, biased source weights

Neutron target weights from the importance map and source weights (at birth) for neutron group 5 (0.9 to 1.4 MeV).
Example – Spent Fuel Cask

- Biased source

Biased source sampling probability (neutrons/cm²) for neutron groups 5 (0.9–1.4 MeV), 10 (0.58–3.0 keV), and 19 (0.8–1 eV).

Example – Spent Fuel Cask

- Speed up is significant (Six separate calcs)

Results

<table>
<thead>
<tr>
<th>detector</th>
<th>Analog Monaco 5164 min</th>
<th>MAVRIC 543 min</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.54E-04 ± 24.0%</td>
<td>7.07E-04 ± 0.7%</td>
</tr>
<tr>
<td>2</td>
<td>6.97E-03 ± 5.9%</td>
<td>7.77E-03 ± 0.5%</td>
</tr>
<tr>
<td>3</td>
<td>1.55E-02 ± 2.0%</td>
<td>1.54E-02 ± 0.4%</td>
</tr>
<tr>
<td>4</td>
<td>4.57E-04 ± 4.7%</td>
<td>4.27E-04 ± 0.7%</td>
</tr>
<tr>
<td>5</td>
<td>1.36E-02 ± 0.9%</td>
<td>1.35E-02 ± 0.2%</td>
</tr>
<tr>
<td>6</td>
<td>2.91E-03 ± 1.2%</td>
<td>2.91E-03 ± 0.2%</td>
</tr>
</tbody>
</table>

\[ FOM = \frac{1}{T \sigma^2} \]

Speed up

<table>
<thead>
<tr>
<th>detector</th>
<th>Monaco</th>
<th>MAVRIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>8759</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1880</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>372</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>298</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>176</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>305</td>
</tr>
</tbody>
</table>
Implementation: ADVANTG

• ADVANTG
  – Based on John C. Wagner’s Dissertation
  – MCNP4C3 and TORT
  – Source must be a list of points
  – Does single particle CADIS only
  – Use final wwinp and biased source with any MCNP/X

Implementation: ADVANTG (cont’d)

• ADVANTG 2.0
  – Generates material specs and map using MCNP-5.1.40 mod
  – Uses Denovo for $S_N$ flux estimates
  – Provides cuboid and spherical source regions
  – Neutron, photon, and coupled problems
  – CADIS and FW-CADIS methods
**Denovo – \( S_N \) Transport**

Denovo is a new parallel \( S_N \) transport code
- 3D regular grids
- GMRES (with DSA – preconditioning) within-group solver
- Transport, Two-Grid accelerated Gauss-Seidel for multigroup
- Koch-Baker-Alcouffe (KBA) parallel domain-decomposition
- Parallel, first-collision source
- 5 different spatial differencing schemes
  - Weighted-Diamond (with and without linear-zero flux fixup)
  - Theta-Weighted-Diamond
  - Step-characteristics
  - Linear-Discontinuous Finite Element
  - Trilinear-Discontinuous Finite Element
- Multiple input front-ends including Python
- High-performance parallel I/O using HDF5

---

**Denovo Doses in Urban Environment**

Doses for a 1KT event (\( 1\times10^{23} \) neutrons)
**Implementation: MAVRIC in SCALE 6**

- **Input**
  - BONAMI / NITAWL or BONAMI / CENTRM / PMC
  - Optional: adjoint cross sections
  - Resonance cross-section processing
  - 3-D discrete ordinates calculation
  - Optional: importance map and biased source
- **End**
  - 3-D Monte Carlo

---

**Monaco – Multi-Group Shielding**

- **Based on MORSE**
- **Same XS and geometry as KENO-VI**
- **Flexible, friendly user input**
  - Source description is separable: space, energy, direction
  - Region tallies, mesh tallies, point detector tallies
  - Integrates fluxes with response functions (dose)
- **Variance Reduction capabilities**
  - Weight windows based on region/energy
  - Mesh-based weight windows
- **Future**
  - Parallel, Continuous Energy, more user features
CADIS – Consistent Adjoint Driven Importance Sampling

- Provides consistent relationships for calculating source & transport biasing parameters
- Eliminates the incompatibility between source & transport biasing that has been problematic in other approaches
- Large speed-up for source/detector problems
- Described in more detail in:
  - *Progress of Nuclear Energy*, 42(1), 2003

Review...

- Analog Monte Carlo tallies tend to have relative uncertainties inversely proportional to flux
  - Low flux areas are the hardest to converge
  - Computation time is controlled by worst uncertainty

- Biasing (typically weight windows) helps move particles to areas of interest
  - Spend more time on “important” particles
  - Sacrifice results in “unimportant” areas
  - Different biasing for different tallies

- CADIS (weight windows and biased source) is very effective for source-detector type problems
Mesh Tallies/Multiple Tallies

- Monte Carlo is used to calculate many tallies
  - Mesh tally - answers everywhere
  - Wide range in relative uncertainties
- Many applications need mesh tallies
  - Dose rate maps
  - Activation of surrounding materials
  - Burn up of fuel pins in reactors

- Need to compute mesh tallies/multiple tallies with similar uncertainties in a single MC calculation

Gamma Ray Litho-Density Log

- Problem Description from
  

- Source: Cs-137, 2.7 Ci
- Detectors: NaI
  - Near: 2x2 at 20 cm
  - Far: 4x4 at 40 cm
- Borehole: 20 cm diam
- Tool: 10 cm diam
### How To Improve Uncertainties

- **Weight windows/biased source with CADIS**
  - Calculate adjoint fluxes from an adjoint source at one of the detector locations
    \[ q^-(\vec{r}, E) = \sigma_j(\vec{r}, E) \]
  - Estimate of response
    \[ R = \int \int \phi^+(\vec{r}, E) q(\vec{r}, E) \, d\vec{r} \, dE \]
  - Create importance map
    \[ \overline{w}(\vec{r}, E) = \frac{R}{\phi^+(\vec{r}, E)} \]
    
    and consistent biased source
    \[ \hat{q}(\vec{r}, E) = \frac{1}{R} q(\vec{r}, E) \phi^+(\vec{r}, E) \]
    \[ w_0(\vec{r}, E) = \frac{R}{\phi^+(\vec{r}, E)} \]
  - Run the forward Monte Carlo
Discrete Ordinates Mesh

$49 \times 43 \times 59 = 124,313$

CADIS – for Near Detector

<table>
<thead>
<tr>
<th>Calculation</th>
<th>Minutes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adjoint DO</td>
<td>7</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>126</td>
</tr>
</tbody>
</table>

Total Photon Flux

Relative Uncertainty

Results

Near $1.54 \times 10^3$ (±0.5%)
Far 0.00
**CADIS – for Far Detector**

**Total Photon Flux**

<table>
<thead>
<tr>
<th>Calculation</th>
<th>Minutes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adjoint DO</td>
<td>7</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>124</td>
</tr>
</tbody>
</table>

**Relative Uncertainty**

Results

- **Near**: $3.10 \times 10^3 \pm 65%$
- **Far**: $5.59 \times 10^1 \pm 0.3%$

**How To Improve Uncertainties**

- **CADIS works**
  - Improves the FOM for that detector
  - At the expense of tracking particles deep into the formation
  - At the expense of the other detector

- **How to get both detectors simultaneously?**

- **Try adjoint source in both detectors**
How To Improve Uncertainties

• Adjoint source in both detectors:
  – Recall that the adjoint source locations act like particle attractors in the MC.
  – MC particles will tend to go to the “easiest” source location.
  – Need to put more adjoint source in the far detector so that the same number of particles get to each.
• How much adjoint source strength to put into the far detector relative to the near?
• Ratio needs to be same as ratio of the responses!

Litho-Density Log Input File

```plaintext
read importanceMap
  gridGeometryID=1

  \near detector
  adjointSource 1
    boundingBox 6 4 1 -1 21 19
    unit=1 region=2
    responseID=1
    weight=1.00
  end adjointSource

  \far detector
  adjointSource 2
    boundingBox 7 3 2 -2 42 38
    unit=1 region=4
    responseID=1
    weight=27.55
  end adjointSource
end importanceMap
```
Forward Weighted CADIS in MAVRIC

- Perform a forward discrete ordinates calculation
- Estimate the responses $R(r,E)$ everywhere
- Construct the CADIS adjoint source but weight the source strength with $1/R(r,E)$
- Perform the adjoint discrete ordinates calculation
- Create the weight windows and biased source
- Perform the Monte Carlo calculation

Forward-Weighted CADIS

- To get both detectors with same relative uncertainties, the amount of adjoint source in each detector location needs to be inversely proportional to the expected response.

<table>
<thead>
<tr>
<th>For the calculation of:</th>
<th>Use adjoint source:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi(\vec{r}, E)$</td>
<td>$q^+(\vec{r}, E) = \frac{1}{\phi(\vec{r}, E)}$</td>
</tr>
<tr>
<td>$\int \phi(\vec{r}, E) dE$</td>
<td>$q^+(\vec{r}) = \frac{1}{\int \phi(\vec{r}, E) dE}$</td>
</tr>
<tr>
<td>$\int \phi(\vec{r}, E) \sigma_d(\vec{r}, E) dE$</td>
<td>$q^+(\vec{r}, E) = \frac{\sigma_d(\vec{r}, E)}{\int \phi(\vec{r}, E) \sigma_d(\vec{r}, E) dE}$</td>
</tr>
</tbody>
</table>
Litho-Density Log Input File

```plaintext
read importanceMap
gridGeometryID=1
  ' near detector
  adjointSource 1
    boundingBox 6 4 1 -1 21 19
    unit=1 region=2
    responseID=1
  end adjointSource
  ' far detector
  adjointSource 2
    boundingBox 7 3 2 -2 42 38
    unit=1 region=4
    responseID=1
  end adjointSource
forwardWeighting
responseID=1
end importanceMap
```

FW-CADIS – for both Detectors

<table>
<thead>
<tr>
<th>Calculation</th>
<th>Minutes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forward DO</td>
<td>6</td>
</tr>
<tr>
<td>Adjoint DO</td>
<td>7</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>126</td>
</tr>
</tbody>
</table>

Total Neutron Flux

<table>
<thead>
<tr>
<th>Scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 cm</td>
</tr>
</tbody>
</table>

Relative Uncertainty

```
Results
Near 1.54×10^2 (±0.6%)
Far 5.56×10^1 (±0.4%)
```

Two keywords is almost automatic!
**Photon Methods Comparison**

<table>
<thead>
<tr>
<th></th>
<th>Analog</th>
<th>CADIS</th>
<th>FW-CADIS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Near</td>
<td>Far</td>
<td></td>
</tr>
<tr>
<td>Simulation times (min)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Forward dis. ord.</td>
<td></td>
<td></td>
<td>6</td>
</tr>
<tr>
<td>Adjoint dis. ord.</td>
<td>7</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>2762</td>
<td>126</td>
<td>123</td>
</tr>
<tr>
<td>Charged pairs/sec</td>
<td>1.494E+03</td>
<td>1.545E+03</td>
<td>1.543E+03</td>
</tr>
<tr>
<td>Relative uncertainty</td>
<td>8.15%</td>
<td>0.46%</td>
<td>0.61%</td>
</tr>
<tr>
<td>Charged pairs/sec</td>
<td>6.130E+01</td>
<td>5.387E+01</td>
<td>5.564E+01</td>
</tr>
<tr>
<td>Relative uncertainty</td>
<td>19.14%</td>
<td>0.34%</td>
<td>0.43%</td>
</tr>
<tr>
<td>Monte Carlo FOM(^r) ratio</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Near detector</td>
<td>1</td>
<td>6830</td>
<td>3867</td>
</tr>
<tr>
<td>Far detector</td>
<td>1</td>
<td>71821</td>
<td>43278</td>
</tr>
<tr>
<td>Time (min) required for 1%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Near detector</td>
<td>183547</td>
<td>34</td>
<td>60</td>
</tr>
<tr>
<td>Far detector</td>
<td>1012136</td>
<td>21</td>
<td>36</td>
</tr>
<tr>
<td>Time (min) required</td>
<td>For both detectors</td>
<td>1012136</td>
<td>55</td>
</tr>
<tr>
<td>Time improvement</td>
<td>Speed-up over analog</td>
<td>1</td>
<td>18321</td>
</tr>
</tbody>
</table>

**FW-CADIS for Mesh Tally**

- Mesh tally is just a large set of tallies where we want roughly uniform relative uncertainties
- Instead of two tallies – there are \( I \times J \times K \) tallies
- Adjoint source: the response function divided by the expected forward response in each cell of the mesh tally volume
  - Expected flux
  - Expected total flux
  - Expected dose rate
Importance Map Block Example

For the calculation of:

<table>
<thead>
<tr>
<th>Use adjoint source:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi(\vec{r}, E)$</td>
</tr>
<tr>
<td>$q^-(\vec{r}, E) = \frac{1}{\phi(\vec{r}, E)}$</td>
</tr>
<tr>
<td>$\int \phi(\vec{r}, E) dE$</td>
</tr>
<tr>
<td>$q^-(\vec{r}) = \frac{1}{\int \phi(\vec{r}, E) dE}$</td>
</tr>
<tr>
<td>$\int \phi(\vec{r}, E) \sigma_f(\vec{r}, E) dE$</td>
</tr>
<tr>
<td>$q^-(\vec{r}, E) = \frac{\sigma_f(\vec{r}, E)}{\int \phi(\vec{r}, E) \sigma_f(\vec{r}, E) dE}$</td>
</tr>
</tbody>
</table>

Implementation: ADVANTG

- **ADVANTG 2.0**
  - Generates material specification and material map using MCNP-5.1.40 mod
  - Generates cross sections using GIP
  - Estimates forward flux using Denovo
  - Enfolds forward fluxes and user-specified response to generate adjoint source distribution (multiple response regions are allowed)
  - Estimates adjoint flux using Denovo
  - Generates weight bounds and biased source distribution using CADIS methodology
Implementation: MAVRIC in SCALE 6

- **Input**
  - BONAMI / NITAWL or BONAMI / CENTRM / PMC
  - MAVRIC
  - DENovo

- **Optional: forward cross sections**
  - 3-D discrete ordinates calculation
  - PARM=forward

- **Optional: adjoint cross sections**
  - 3-D discrete ordinates calculation
  - PARM=denovo

- **Optional: importance map and biased source**
  - PARM=impact

- **3-D Monte Carlo**
  - PARM=monaco

Future Challenges
Directional Beam Problem

Goal:
Model active interrogation using a beam source

Problem:
Simplified model of a ship: concentric spheres of homogenized “engine room” material surrounded by air (blue) and water (yellow)
Spherical HEU threat object at the center
14.1MeV neutron beam source in a 2° cone (indicated by black arrow)

Challenge:
Importance map is only function of $\tilde{f}(E)$ so it does not represent the importance of a particle moving directly toward the tally region

---

Directional Beam Problem (cont’d)

- ADVANTG WWs are based on the adjoint scalar flux
- MCNP WWG estimates importance using forward histories
SNS Beamline Shielding

Goals:
- Calculate personnel dose rates outside of beamline
- Calculate scatter background in experimental areas

Challenges:
1. Nearly mono-directional beam
2. Evacuated beamline
3. Thick Shielding
4. Detailed Model

Current MCNP model uses weight windows generator – still slow
Subdividing geometry for importances is extremely time-consuming

Hybrid Methods
1. Need directional information for source in $S_N$ code
2. Adjoint particles need to “flow” up the beamline but cannot since they cannot scatter in vacuum
Summary

• Challenging Applications are Driving the Methods Development
• Hybrid approach is only way to solve these problems