Monte Carlo Methods for Efficient Reactor Analysis

Bojan Petrovic
Nuclear & Radiological Engineering / Medical Physics
G.W. Woodruff School
Georgia Institute of Technology

Oak Ridge National Laboratory, Oak Ridge, TN
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Bojan Petrovic

- Since August 2007: Georgia Tech Professor, Nuclear & Radiological Engineering / Medical Physics
  - Reactor physics, transport theory, shielding
  - Monte Carlo methods for reactor analysis
  - Advanced reactor design
  - Computational medical physics
  - Methods development, numerical simulations

  - Advanced reactor design (IRIS, LMR-AMTEC, …)
  - Advanced fuels and fuel cycle
  - Nondestructive waste characterization
  - SNM detection
  - Methods development, numerical simulations
Research group

• Jordan McKillop, M.S. student
  – Variance reduction in MC shielding problems (using MAVRIC/SCALE)

• James Nathaniel, M.S. student
  – Shielding, sensitivity studies using Sn

• Bo Shi, Ph.D. student
  – Improved convergence/diagnostics of MC criticality simulations

• Jeff Ryckman, Ph.D. student
  – Simulations and variance reduction in computational medical physics (proton therapy)

• Vito Memoli, (“part-time” - visiting Ph.D. student from Politecnico di Milano)
  – Fast reactor analysis

• Ph.D. student starting next semester
  – MC depletion, error propagation
Outline/intent of today’s talk

- Use of Monte Carlo for reactor analysis
- Present several ongoing research projects
- Identify areas for possible collaboration
Monte Carlo methods for simulation of nuclear systems

- Potentially most accurate
- Computationally intense; inherently: $(1/\sigma) \sim N^2$
- Traditionally used for benchmarking/reference
- Strong interest to make MC practical for routine use

DRIVERS:
- Current reactors: improved safety and/or margin, which translates into economic benefit
- Advanced reactors: complex designs require improved methods to accurately model without extensive testing
- Benchmarking of new methods

ENABLERs:
- Steady increase in computational power
- Improved methods
Monte Carlo methods in reactor analysis

Increasingly more challenging:

SHIELDING (FIXED SOURCE)
• Localized/discrete detector(s)
• Flux/dose distribution “everywhere”

CRITICALITY SIMULATIONS
• Critical systems (reactor)
• Criticality safety

CRITICALITY SIMULATIONS WITH DEPLETION
• Reactor, fuel depletion

INCLUDING CONTROL/FEEDBACK
• Criticality
• Feedback
Monte Carlo methods in reactor analysis

SHIELDING (FIXED SOURCE)

- Requires many histories
- Independent histories; determining uncertainty/convergence in principle “straightforward”
- Localized/discrete detector(s)
  - Automated variance reduction needed – reasonably well understood – e.g. CADIS
- Flux/dose distribution “everywhere”
  - Automated global variance reduction needed – e.g. FW-CADIS

CRITICALITY SIMULATIONS [additional “external loop”]

- Slow/false source convergence
- Stationarity diagnostics
- Underestimated uncertainty (correlated batches)
- Difficult to accelerate
- Critical systems (reactor) [depletion/feedback]
- Criticality safety [loosely coupled, undersampling]

CRITICALITY SIMULATIONS WITH DEPLETION [additional “external loop”]

- Reactor, fuel depletion
  - Uncertainty estimation and propagation

PLUS CONTROL/FEEDBACK [additional “external loop”]

- Computer resources
- Tools (couple to T/H, variable temperature cross sections, ….)
Ongoing research projects at Georgia Tech

1) SHIELDING (FIXED SOURCE)
   • Flux/dose distribution “everywhere”
     Using MAVRIC sequence in SCALE6 (FW-CADIS) to analyze IRIS

2) CRITICALITY SIMULATIONS
   Source convergence / improved stationarity diagnostics

3) CRITICALITY SIMULATIONS WITH DEPLETION
   Uncertainty estimation and propagation

Work in progress.....
(1) Fixed source (shielding)  
Dose/flux distribution “everywhere”  

Code/Method: MAVRIC/FW-CADIS  
Test problem: IRIS reactor  
(Determining radiation environment throughout the plant)
IRIS – International Reactor Innovative and Secure

- Advanced integral light water reactor
- 335 MWe/module
- Innovative, simple design
- Enhanced Safety-by-Design™
- International team
- Potential for deployment as Grid Appropriate Reactor
- Anticipated competitive economics
- Cogeneration (desalination, district heating, bio-fuel)
- NRC pre-application underway
- Design Certification testing program underway
- Interest expressed by several countries
- Projected deployment target: 2015 to 2017
- Compact design - single building integrates containment, reactor and auxiliary building
IRIS Integral Reactor Vessel

No external primary loops, all primary components inside the vessel

- 8 helical-coil steam generators
- 8 axial flow fully immersed primary coolant pumps
- Internal control rod drive mechanisms
- Integral pressurizer with large volume-to-power ratio

Thick (1.7m) downcomer provides extra shielding compared to loop PWRs
Benefits of (inherent) additional shielding

- Fast neutron fluence to RV drastically reduced (~6 orders of magnitude)
- Practically no embrittlement
- RV surveillance program not needed (O&M cost reduction)
- Strongly reduced activation
- “Cold” outer RV surface
- Reduced dose for maintenance operations
- Reduced dose/simpler ultimate decommissioning
- Vessel could act as sarcophagous for ultimate disposal
IRIS Shielding Analysis - Challenges

- Integral configuration, extra shielding
- Enhanced dose reduction objectives

More complex shielding analysis (~10 orders of magnitude fast flux attenuation to vessel outer surface)

Dose in accessible areas = ?
Dose at CV boundary = ?
Dose in maintenance = ?
Concrete activation = ?
RV fluence = ?
IRIS Shielding Analysis - Approach

- Core physics (Westinghouse) $\rightarrow$ Fission source distribution

MC + $S_N$
- Improved confidence in results
- Exploit advantages of each method

Shielding analysis (employing expertise within the IRIS team)
- Monte Carlo – MCNP + DSA (K. Burn, ENEA)
- Deterministic – 3D TORT (M. Sarotto, M. Ciotti, ENEA)

And

Investigate using SCALE/MAVRIC to facilitate obtaining MC solution over the large domain
IRIS Reactor Vessel + Containment + Building

- Large spatial domain:
  Building – cylindrical, ~50m diameter
- Complex geometry:
  Shields (walls) and cavities

**Focus of MAVRIC studies:**

Obtain an indication of the flux/dose distribution “everywhere” in the containment (initially) and building (later) to guide detailed studies

Initially – use very simplified model(s) to obtain approximate results
Preliminary / Simplified Geometry for Initial Evaluation

- Very simplified geometry, still 14m x 14m x 30m
- Nevertheless, preserved essential features and difficulties of the actual geometry
- Suitable for investigating the capability to generate global flux/dose distributions throughout a large spatial domain
Preliminary Results

>1MeV: flux and relative uncertainties distribution
~15 min adjoint+forward $S_N$
~2 min MC
(on a Dell PC)

radial distribution (at core midplane) – fast flux and uncertainties
Preliminary Results

>1MeV: flux and relative uncertainties distribution

~15 min adjoint+forward $S_N$ + ~2 min MC
Preliminary Results

>1MeV: flux and relative uncertainties distribution

~15 min adjoint+forward $S_N$

~70 min MC (red to green $\rightarrow$ 12 orders of magnitude)

[not bad, but noisy in spite of large voxels]
Preliminary Results

Finer mesh at core and RV boundary

>1MeV: flux and relative uncertainties distribution

\(~18+6\text{ min forward+adjoint }S_N + ~471\text{ min MC} = 8.25\text{ h}\)
Preliminary MAVRIC/FW-CADIS Results of IRIS Shielding Analysis

>1MeV: flux and relative uncertainties distribution
~18+6 min forward+adjoint $S_N$ + ~471 min MC = ~8.25 h
Useful results (over the ~12 orders of magnitude attenuation)
Initial findings/experience with MAVRIC

• Obtained indication of the global flux/dose distribution in large, deep penetration problem (IRIS – large integral vessel + containment + building)
• Relatively easy to set up and run
• Automated VR
• Obtained global distribution with reasonably reduced uncertainty over the large domain with limited use of both engineering and CPU time

• Further, examining:
  – Impact of Sn solution quality
  – Flux (fast, thermal), dose, activation …..
Impact of $S_N$ solution quality

- Initial results: ~52K meshes, $P_3S_8$
- 100 batches @ 1M
- 18+6+471 min = ~8.25h

- Refined mesh: ~440K meshes, $P_1S_6$
  (reduced $P_L S_N$ to enable finer mesh was necessary on PC)
- 20 batches @ 1M
- 43+17+798 min = ~14.3 h

(Dell Latitude D630 CPU time quoted. About 3x faster on a workstation)
Refined $S_N$ mesh results

$>1$MeV: flux and relative uncertainties distribution

$\sim 43 + 17 + 798 \text{ min} = \sim 14.3 \text{ h}$

Very good performance (covers $>15$ orders of magnitude)
Impact of refined mesh / improved $S_N$

- ~52K meshes, $P_3S_8$
- 100 batches @ 1M
- 18+6+471 min = ~8.25h

- ~440K meshes, $P_1S_6$
- 20 batches @ 1M
- 43+17+798 min = ~14.3 h

- Finer mesh – smoother/better MC convergence
- Less histories ~twice CPU, but more than compensated by gain in variance reduction
Impact of refined mesh / improved $S_N$

~440K meshes, $P_1S_6$, 20 batches @ 1M [43+17+798 min = ~14.3 h]

Forward Gr1 – $S_N$

Relatively accurate $S_N$ (~ within order of magnitude)
[consistent contour levels, defined to cut off below $1\times10^{-12}$]
Impact of refined mesh / improved $S_N$

~52K meshes, $P_3S_8$ 100 batches @ 1M [18+6+471 min = ~8.25h]

- Less accurate $S_N$
- Difference grows to exceed 2 orders of magnitude

ORNL Seminar, April 6, 2009
Impact of refined mesh / improved $S_N$

- ~52K meshes, $P_3S_8$
- 100 batches @ 1M
- 18+6+471 min = ~8.25h

- ~440K meshes, $P_1S_6$
- 20 batches @ 1M
- 43+17+798 min = ~14.3h

- Qualitatively similar, but difference several orders of magnitude upon closer inspection
  (shows same results as previous VG but different contours)
Impact of $S_N$ solution quality

- The approximate shape for $S_N$ flux provides acceleration by orders of magnitude.
- However, VR parameters directly depend on $S_N$ (e.g., adjoint source weighted by inverse forward $S_N$ flux).

- Inaccuracy in $S_N$ flux will lead to equally large region-wise “over/under-population” in MC simulation, requiring longer run time to compensate for weak spots (if we really mean that we need uniform uncertainties throughout).
- The desired MC uncertainty will dictate the optimum trade-off between the speed and accuracy of $S_N$ solution.

- How to maximize the overall efficiency? (difficult to quantify a priori the quality of $S_N$ solution.)
Detailed / group-wise flux distribution and uncertainty

~440K meshes, $P_1 S_6$, 20 batches @ 1M [43+17+798 min = ~14.3 h]

Total flux uncertainty (optimized for)
Detailed/group-wise flux distribution

- Note: MC VR is optimized for integral fast flux (total > 1MeV) distribution
- Group-wise neutron flux distribution?
- Look at the relative uncertainty distribution – is it uniform?

~440K meshes, $P_1S_6$, 20 batches @ 1M
Uncertainty group-by-group (1-5)
Work in progress and future work related to using MAVRIC/SCALE

• Trade-off between $S_N$ and MC
• Detailed (group-wise) distribution
• Practical issues for fast/thermal flux, activation, dose, …
• Detailed IRIS power plant model
• Comparison to MCNP, TORT
(2) Criticality simulations

In search of improved stationarity diagnostics
Monte Carlo criticality simulations

- Slow convergence
- False convergence
- Difficult to establish convergence criteria
- Underestimated statistical uncertainty (correlated histories)
- Under-sampling
- Potentially inaccurate fission source (flux, power) distribution
- Potentially significant reactivity underestimate (NCS)
- Computationally challenging
  (one more implicit level to resolve – eigenvalue/mode)
OECD Benchmark #1 - Spent fuel pool, checkerboard pattern of assemblies (more loosely coupled than core)

EXAMPLE OF A REAL-LIFE APPLICATION WITH POTENTIAL FOR UNDERESTIMATING $K_{eff}$

15x15 FAs, 5%U235
Concrete on 3 sides on the fourth side
Initial source uniform and at different positions
36 prescribed cases
Almost completely decoupled FAs
Extremely slow source convergence
Somewhat similar to an exaggerated case of a large core, checkerboard pattern, with very low-reactivity twice-burnt fuel

Groups/ Codes and basic results Water (Trans. ANS)

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<th>Code</th>
<th>Data</th>
<th>Contributor(s)</th>
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<td>VIM</td>
<td>ENDF/B-V</td>
<td>Roger Blonquist</td>
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</table>
Simple problem to demonstrate source convergence issues  
(B. Petrovic, 2001, Trans. ANS)

Thick slabs (400 cm), alternating, high-low reactivity

PWR-like:
• 40% UO$_2$, 10% Zr, 50% water
• homogeneous mixture
U$_{235}$ enr.: 1% - 2% - 1% - 2% ...

INITIAL SOURCE
Center of 1% U$_{235}$ (low-reactivity) slab

MCNP, 50 generations (cycles)
5,000 neutrons/generation

All 10 statistical checks OK
(no entropy test)
No warnings/indications

Converged to $k \approx 0.91$
CORRECT RESULT IS $k \approx 1.08$!!
Issue – convergence to eigenmode
Bracketing k

HIGH-LOW REACTIVITY ALTERNATING SLABS (200 generations, 20,000 n/gen)

Initial source very different from eigen-distribution if started in low-reactivity slab, but it does not initially impact k

Need to skip more cycles (~100 if start in low reactivity region)

Initial source position
  - High-reactivity slab (black)
  - Low reactivity slab (blue)

Here, k-eff “bracketed” from below/above
But, difficult to bracket in real-life problems

Entropy criterion more likely to detect the unconverged source?
Use of entropy for stationarity diagnostics

- Entropy in Information theory (Shannon Entropy) is a measure of the uncertainty associated with a random variable.
- Introduced into MC criticality simulations to check the stationarity of fission source distribution.

\[ H(S^B) = - \sum_{i=1}^{B} S^B(i) \log_2(S^B(i)) \]

Simple example:
- N-mesh system
  - Uniform source distribution: maximum H;
    \[ P=1/N \]
    \[ H_{\text{max}} = -\frac{N}{N} \log_2\left(\frac{1}{N}\right) = \log_2(N) \]
  - Source in one mesh only: minimum H
    \[ H_{\text{min}} = 0 \]

Entropy diagnostics – examined in many recent studies
Still, it is an integral parameter…..
Entropy diagnostics applied to slab problem

- If the source is initialized in low-reactivity slab
  - 150 cycles
  - Skip 60

- Passes both the k convergence and entropy check…..
  Still with completely incorrect answer k=0.92

Average fission-source entropy for the last half of cycles:
H = 3.77E+00 with population std.dev. = 2.63E-01
Cycle 53 is the first cycle having fission-source entropy within 1 std.dev. of the average entropy for the last half of cycles.
At least this many cycles should be discarded.
Source entropy convergence check passed.

Entropy – a single number (like k).
Two different (not converged) source distributions may have similar entropy
Entropy diagnostics applied to slab problem

- In both cases, entropy initially primarily reflects spreading of the initial delta source, even though very different $k$ (≈0.92 vs 1.08) and distribution.
Entropy bracketing (convergence from above/below)

Similar problem with entropy as with k-eff: deciding when it has converged

Attempt to bracket entropy from above/below – applied to OECD Bench#1
- Uniform source;
- Biased source, upper left lattice position (high reactivity) has 81% of initial source (90% for both X and Y direction)
- Uniform source in lower left lattice position (low reactivity)

Here, seems to provide good indication. Is it useful/practical in general cases?
Collision entropy

• The current use of entropy is based on source sites (“Source Entropy”)

• Introduce “Collision Entropy” (based on the collision sites)
  – The collision rate is related to the flux distribution, and thus can also represent the flux (and source) convergence.
  – Every collision contributes, and since several collisions precede a fission, it could provide a better statistics than the source sites. (However, these events are correlated.)
  – Non-multiplying regions are included in collision entropy, thus could capture more information than source entropy
Collision entropy – example – fissile region

- Homogeneous slab
- 1-group problem
- Width=200 cm in z direction
- $\Sigma_{\text{tot}}=1.000 / \text{cm}$
- $\Sigma_{\text{capt}}=0.084 / \text{cm}$
- $\Sigma_{f}=0.060 / \text{cm}$
- $\Sigma_{s}=0.856 / \text{cm}$, isotropic
- $\nu=2.4$

- 5000 particles/cycle
- 300 total cycles
- Z direction is divided into 40 meshes evenly
- Initial uniform source distribution

- Fissile-only regions, expected to obtain essentially identical results from source and collision entropy
Collision entropy – example – fissile region (cont.)

- In this case, essentially the same (as expected).

<table>
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<th>Source Entropy</th>
<th>Mean Value</th>
<th>σ</th>
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<tbody>
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</table>
Collision entropy – with non– fissile region(s) [work in progress]

- OECD Benchmark#1
  Checkerboard – “half” the space/information not used
  (not clear how much additional information, however)

- Modified 1-group slab problem
  similar to OECD Benchmark#3 (uranyl nitrate slabs separated by water)
(3) Criticality simulations and depletion
MC Depletion

- One additional level of uncertainty
- Difficult to analyze and separate various effects

Project being initiated
- Will employ deterministic with ultra-fine “continuous” library (6,000+ groups) to filter out MC statistical effects
- Collaborative research with Westinghouse

Example of detailed spectrum obtained by deterministic / ultra-fine library
(4) Computational Medical Physics
Proton therapy and secondary (neutron) dose

- Proton therapy - promising treatment modality
- Can adjust depth (Bragg’s peak) to minimize primary dose to healthy tissue
- Can optimize tumor coverage (spread out Bragg’s peak)
- Secondary (neutron) dose to healthy tissue may be of concern
- Simulations - computationally intense
- Developing a methodology for efficient simulations

Thomas F. DeLaney, Hanne M. Kooy, Proton and Charged Particle Radiotherapy, Philadelphia: LWW, 2008
Computational medical physics - proton therapy

- Work in progress: establishing beam-nozzle-patient model

160 MeV proton beam through a 6.9cm thick range shifter

Objective: effective variance reduction for coupled p-n
Summary and Future Work

Work in progress on Monte Carlo methods in reactor analysis, with the objective of making them more practical for routine use:

- Fixed-source MC: Investigating use of MAVRIC/FW-CADIS for global flux/dose distribution in large deep penetration problem:
  - Good results/experience so far
  - Further study in progress (fast-thermal-flux-does-activation; uniform variance for individual fluxes)

- Improved diagnostics for MC criticality
  - Modified entropy
  - Use of different criteria

- MC criticality simulations with depletion
  - Error determination and propagation
  - Supported by “pointwise deterministic” (ultrafine 6,000+ group library)

Computational medical physics:

- Variance reduction for MC coupled proton-neutron-gamma simulations
Thank you for your attention

Questions?