Advances in Monte Carlo Methods for Global Reactor Analysis

M&C+SNA 2007
April 15-19, 2007

Bill Martin
Nuclear Engineering and Radiological Sciences
University of Michigan
wrm@umich.edu
Acknowledgements

- Organizers of M&C+SNA 2007
- Helpful discussions with Forrest Brown (LANL) and Kord Smith and others
- All those Monte Carlo methods developers who have been doing the work that I am merely reporting!
This review focuses on Monte Carlo methods for global reactor analysis

- More and more emphasis is being placed on the development of high fidelity methods for analyzing reactor configurations that take into account multi-physics and multi-scale phenomena.
- No attempt to discuss Monte Carlo advances for shielding calculations. This warrants a separate talk.
Rough outline of talk

- Status of Monte Carlo for routine design/analysis of global reactor configurations
- Monte Carlo methods and algorithm development that would contribute to the long range goal of making Monte Carlo methods a production tool for global reactor analysis.
- Monte Carlo and modern computer architectures
Monte Carlo topics

- Adjoint Monte Carlo
- Coupling Monte Carlo to physics modules
- Generation of MGD cross sections
- Global variance reduction
- Hybrid Monte Carlo / deterministic methods
- Monte Carlo depletion
- Performance on advanced computer architectures
- Source convergence
- Stochastic geometry
- Uncertainty quantification
In principle: Monte Carlo can analyze neutronic configurations of arbitrary geometrical complexity, arbitrary physics complexity, and is known to perform efficiently (parallelization efficiency) on all known (production) computer architectures.
Geometric complexity

Very high temperature gas reactor
Geometric complexity – from TRISO microspheres to full core

Coated microsphere: TRISO fuel (< 1 mm dia)

Ceramic coatings (4)

Fuel kernel

PARTICLES  COMPACT  FUEL BLOCK  VHTR CORE
Physics complexity

U238 Capture Cross Section

ENDF Request #6483
Whither Monte Carlo?

In practice: Substantial limitations on Monte Carlo performance due to:

- Sheer size of the problem to be solved
- Slow convergence for global reactor problems
- May be painful to adapt Monte Carlo algorithms to some architectures that are being offered or proposed by computer vendors

Kord Smith’s challenge ….
The Challenge for Monte Carlo
(Kord Smith, Gatlinburg M&C, 2003)

- The problem may be huge:
  - # of fuel assemblies: 200
  - # of axial planes: 100
  - # of pins/assembly: 300
  - # of depletion regions/pin: 10
  - # isotopes to be tracked: 100
  - Total number of tallies: 6 billion

- But the method is slow ....
  - Need 1% statistics on peak powers
  - For an assembly calculation, ~ 1M histories needed to achieve 1% statistics ⇒ ~ 20B histories for 1%
  - But DR = .75 for assembly vs .995 (or worse!) for full core ⇒ ~ 50x longer to converge

5000 h to complete full-core calculation on a 2 GHz PC
Prohibitive run time is the overriding issue that mitigates against Monte Carlo

- Smith’s conclusion: assuming Moore’s Law holds, it would be 2030 before a full core Monte Carlo could be done in less than an hour on a single CPU
- One can glean from Kord’s talk that a deterministic calculation would have taken 1/4 second! Of course, we don’t just do one calculation!
  - 10,000s of 3D steady state calculations
  - 100s of 3D transient calculations
  - 1000s of operational support calculations
- Is there any hope for routine global analysis with Monte Carlo?
- Is the situation that bad? …..
Independent check on Kord’s estimate may be obtained from a talk that was given yesterday ……

HIGH ACCURACY LARGE SCALE MONTE CARLO AND DETERMINISTIC TRANSPORT CALCULATIONS FOR CRITICAL SYSTEMS, S. Langenbuch, A. Seubert, and W. Zwermann

Figure 1. Horizontal cut through one quarter of the VENUS-7 assemblies. Blue pins: MOX fuel; green pins: UO₂ fuel. In assembly 7/0, the central pins for the substitution experiments are displayed in magenta.
Independent estimate of time to complete full core simulation

- Performed 3D simulation of Venus critical to within .1% pin power statistics (axial average)
  - 20,000 active cycles and 10,000 neutrons/cycle
  - 200M histories
- ~ 32 h on single processor of Cray XD1 (MCNP4C)
- Scaling to commercial core
  - ~ 45x for 40,000 fuel pins
  - 100x for axial depletion regions
  - .01x due to .1% vs 1%
  - \( \Rightarrow \) 9B histories or ~ 1500 h on Cray XD1 single processor
  - Does not take into account any change to DR

~1500 h to complete full-core calculation on a Cray XD1
Look more carefully at the 2030 challenge

- Key assumption: single CPU
- Since 2003, vendors have been offering multicore processors
  - Essentially an SMP on a chip
  - Apple – now offers dual quad core
  - Intel – working on a 80 core processor
  - By 2030, how many cores? 1000? 10,000?
  - Monte Carlo can easily take advantage of threads
- Assuming Moore’s Law manifests itself as only more cores starting with a quad core today, then a 1500 core processor will occur in $\log_2(375) \times 1.5$ years ~ 12 years or 2019 Q2!
- So we are now at 2019 vs 2030!
Meeting the challenge

- Monte Carlo will always be ceded the role of the benchmark methodology because of its capability to handle complex geometry and complex physics with minimal approximation.

- For Monte Carlo to go beyond a “benchmark only” role and become a routine tool for reactor designers and analysts, improvements need to be made in several areas.

- Monte Carlo’s key advantage – no “operator split” step in energy to create MGD cross section libraries.
  - This step may degrade the high fidelity simulation of resonance absorption and anisotropic energy transfer.
  - This may be important for high fidelity simulation with thermal-hydraulic feedback, especially transients.
Meeting the challenge: Monte Carlo algorithm and methods development

- Accelerate Monte Carlo fission source convergence
- Couple Monte Carlo with deterministic transport methods
- Accommodate large number of spatial zones and a huge number of tallies (due to depletion)
- Coupling of Monte Carlo to other physics modules to account for T/H and structural feedback and other physics feedback mechanisms
- Global variance reduction techniques to speed up criticality problems
- Adapt as needed to new computer architectures
- Propagation of uncertainty especially with depletion
Fission source convergence

- The key impediment to routine use of Monte Carlo for global reactor analysis
- Assumption: Monte Carlo depletion will require 1% statistics on converged power distribution, otherwise propagated errors may be too large. This needs to be quantified and is only assumed here.
- Shannon entropy: recent advance that is key to assessing fission source convergence
- This conference: implemented in a Monte Carlo setting two classical acceleration methods for systems of linear equations:
  - Source extrapolation (Griesheimer/Toth)
  - Wielandt acceleration (Brown)

Fission source convergence cuts across reactor physics, statistics, and acceleration methods for linear systems of equations.
Shannon entropy of the fission source

- Series of recent papers by Taro Ueki and colleagues have resulted in an understanding of the stationarity of the fission source iteration (i.e., convergence) in terms of Shannon entropy.
- Can diagnose retrospectively whether sufficient inactive cycles have been taken to converge the source distribution.
- Previously, nuclear analysts were flying “blind” by paying attention to the convergence of keff rather than the source distribution. This is particularly problematical for DR ≈ 1.
- Difficult to monitor the convergence of a field (fission source distribution) vs a scalar (keff). Shannon entropy has addressed this need by providing a scalar measure of fission source convergence.
- Now a production option in MCNP5.
- This doesn’t speed up the convergence but it is key to realizing it has occurred.
**Shannon entropy of the fission source distribution**

- **Definition:**
  
  \[ H(S) = -\sum_{j=1}^{N_S} p_j \ln(p_j) \]
  
  where \( p_j = \frac{\text{# source particles in bin } j}{\text{# source particles in all bins}} \)
  
  and \( N_S = \text{#bins} \)

- **Properties:**
  
  \[ 0 \leq H(S) \leq \log_2(N_S) \]
  
  For a uniform source: \( H(S) = \log_2(N_S) \)
  
  For a point source (single bin): \( H(S) = 0 \)

**H(S^n) provides a single number to characterize the source distribution for iteration n**
Example

- Example - Fuel Storage Vault (Problem OECD_bench1)

* F. Brown, LA-UR-07-2193
Monte Carlo does very well with complex physics and complex geometry and very poorly with global (keff) calculations where the global distribution is needed (e.g., to deplete).

Deterministic methods are challenged by complex physics (e.g., due to multigroup approx) and complex geometry (e.g., TRISO fuel) but handle global calculations very efficiently (relative to MC).

Question – is it possible to use deterministic methods for the overall calculation, including the outer iterations for keff, but use Monte Carlo as a “subgrid” method for specific regions of phase space where the deterministic methods don’t perform as well? The Monte Carlo simulation would be a source problem, not an eigenvalue problem.

End result: each method does what it does best.

Michigan: coupling MCNP5 and CPM3 for VHTR analysis.
Accommodate huge demand on memory

- 6 billion tallies $\Rightarrow$ 48 GB memory (others estimate 128 GB!)

- Today’s Monte Carlo codes would be hard pressed to deplete an assembly with only 1 depletion region per pin and 100 isotopes, as this would require 30k tallies and this may exceed the current limits of many production Monte Carlo codes. Full core analysis with pinwise depletion is out of the question.

- MC21, the next generation Monte Carlo code for naval reactors, will accommodate 100s of millions of tallies, as will Mercury, the LLNL next generation Monte Carlo code.
Domain decomposition may help

- The Mercury Monte Carlo code from LLNL utilizes domain decomposition with the ability to replicate domains that have too many particles. This additional flexibility can help with load balance.
- Saving grace for keff calculations – the load balance is reasonably uniform and can be estimated if needed.
- Need to use batch statistics to calculate variance if domain decomposition is used.
High fidelity neutronic analysis for GNEP applications will require consistent physics due to thermal-hydraulic feedback and structural response such as rod bowing.

For steady-state design, specific physics modules coupled at the I/O level may be sufficient. Then it is a matter of having a script (or a very patient human) that interrogates output files and writes input files and manages the sequence of simulations.

For transient analysis, coupling at the I/O level is probably not going to work. Work is needed to examine coupling of time-dependent feedback with Monte Carlo.
Communication between Monte Carlo and physics modules

- Issue – how to communicate information between a Monte Carlo code that predicts histogram quantities and a physics code that may have a continuous representation of the field quantities. This difficulty is compounded by the uncertainty (variance) of the Monte Carlo predictions.

- Potential solution – use functional expansion tallies (Griesheimer et al) to allow the Monte Carlo module to read or write continuous representations of the solution or other field quantities. This does not help the uncertainty issue.

- This has been done with MCNP5 and RELAP/Athena at Michigan for the VHTR using a script that sequentially reads and writes input/output files for MCNP5 and RELAP/Athena. Convergence has been found in 6-10 iterations using a feedback model based on interpolating between bracketing cross section sets using the MCNP5 input processor to “mix” the materials.

- Yesterday, it was reported that Star-CD and MCNP were coupled (Seker et al).
The FET is derived from the property that any well-behaved function can be expressed as a series expansion in a complete set of orthogonal basis functions:

\[
\phi(x) = \sum_{n=0}^{\infty} a_n k_n \psi_n(x)
\]

We then solve for the expansion coefficients using the property of orthogonality:

\[
a_n = \int \phi(x) \psi_n(x) \, dx
\]

The result is an integral that Monte Carlo methods are well suited to evaluate.
If we choose the basis functions such that the lowest order function is unity, then

$$a_0 = \int \phi(x) \psi_0(x) \, dx = \int \phi(x) \, dx$$

Hence the zero-th moment is simply the conventional histogram tally.

So higher order moments of the desired distribution can be estimated and the functional expansion then gives a continuous expression for the quantity of interest not just its average values over a set of bins.

It is also possible to get a continuous expression for the variance.
Using FET for a 2D Flux Tally

Ninth order Legendre expansion tally

MCNP5 20×20 mesh tally

Thermal neutron scalar flux profiles in a fuel pin with 20-million history simulations
Global variance reduction methods

- Conventional wisdom – variance reduction does not work for criticality problems because there are no preferred places to “guide” the neutrons.

- Variational variance reduction (Barrett, Densmore, Larsen) is challenging this belief. This methodology utilizes a functional that employs a low order estimates of the adjoint flux to yield a higher order estimate of the eigenvalue.

- Results have been promising to date but only for multigroup and simple geometries. Also, convergence of the eigenfunction needs to be examined for criticality applications.

- Alternative approach reported yesterday by Christoforou and Hoogenboom to bias collision kernels and transport kernels using approximate adjoint flux.

- More research is needed in this area.
Quantification and Propagation of Uncertainty

- Monte Carlo depletion – introduces uncertainty in the isotopics as well as the random fluctuations due to statistics
- Propagation of uncertainty – more work is needed.
- Effect of cross section uncertainties can be assessed with differential operator sampling but effect of uncertainties across multiple timesteps is a challenge. Ensemble averaging of many simulations is possible but time consuming.
Adapting to new computer architectures

To stay on the performance curve promised by Moore’s Law, Monte Carlo codes must be adapted to run efficiently on new architectures.

To date, Monte Carlo scales well on all architectures:

- Random walks are inherently parallel within a fission source cycle or within a timestep. Parallelizing across particles is natural and allows efficient load balancing without a priori knowledge of the solution.
  - MCNP5 – history-based parallelization with MPI and OpenMP
- For vector architectures, the history-based random walk algorithm can be turned inside out to yield an event-based (or its stack-driven variant) algorithm that results in excellent speedups on vector and parallel-vector architectures
  - RACER – KAPL (event-based)
  - MVP – JAERI (stack-driven)
Architectural trends

- HPC hardware advances are dependent on advances in “consumer” processors and “server” processors.
  - Consumer processors are driven by the game industry and is trending in the direction of cell processors.
  - Server processors are driven by transaction processing and web applications and is moving in the direction of increasing N-core processors.
- Monte Carlo can take advantage of either but it would be very painful for most production Monte Carlo codes to adapt efficiently to cell processors.
What about multi-core processors?

- Dual core and quad core processors are in wide use today. The trend by the chip manufacturers is N-core where N is increasing rapidly.
  - Quad cores are here (Apple dual quad core)
  - Intel is developing an 80-core processor
- Monte Carlo codes which use OpenMP, or “threaded” across histories, can take immediate advantage of multi-core processors.
- MCNP5 is threaded and uses MPI, so it can take full advantage of multiple N-core processors.
What about cell processors?

- The cell processors are essentially attached SIMD processors that function like vector processors.
- The IBM Roadrunner, contemplated for LANL, consists of conventional multi-core processors with attached cell processors.
- Monte Carlo will scale well on cell processors but only if the code has already been “vectorized.” Only RACER (still?) and MVP among well-known production Monte Carlo codes are vectorized (to my knowledge).
- Estimate: many tens (if not 100s!) of person-years to vectorize a conventional Monte Carlo code such as MCNP. By the time it was done, the architects would have moved on to another design. Sigh.
- If HPC architectures move exclusively down the cell processor path (seems unlikely), this could be a limiting factor for using Monte Carlo for routine design/analysis of global reactor configurations.
Conclusions

- Monte Carlo is likely to remain a benchmark analysis tool for the foreseeable future.
- Enabling Monte Carlo to become a production tool competitive with deterministic transport methods will be difficult and may not happen soon.
- This will require substantial advances to accelerate fission source convergence, enable huge numbers of tallies, and allow convenient coupling of stochastic transport with deterministic transport as well as deterministic physics modules. It could also require substantial effort to port to new architectures although this seems unlikely given the trends apparent today.

Monte Carlo will always complement deterministic methods; it will not replace them, at least not before 2019!
Thanks!

Any questions?