Investigation of Clustering in MCNP6 Monte Carlo Criticality Calculations

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Monte Carlo Methods, Codes, & Applications (XCP-3) X Computational Physics Division
Introduction

• Monte Carlo
  – Simulate particle behavior
  – Tally event occurrences to estimate physical results
  – Must have enough particles to cover phase space of the problem

• The undersampling problem
  – Not enough particles to cover phase space
  – All MC results are questionable, possibly wrong
  – How can you diagnose the absence of coverage?
  – The cure: Run more particles in the simulation
  – Questions: How many? How do you know it's enough?

• Clustering
  – For criticality problems
    • Iterations using next-generation fission source
    • Convergence assessment depends on fission source coverage
  – In some problems, repeated iterations lead to clustering
Sutton’s Model Problem & Shannon Entropy
Sutton’s Model Problem

- **Recent references**
  - T.M. Sutton & A. Mittal, “Neutron Clustering in Monte Carlo Iterated-Source Calculations”, ANS MCD 2017, Jeju, S. Korea, April 16-20, 2017

- **Model problem for clustering investigations**
  - Homogeneous box
  - 400 x 400 x 400 cm³
  - reflecting boundary conditions
  - One-speed: \( \Sigma_T = 1.0, \Sigma_S = 0.6, \Sigma_C = 0.2, \Sigma_F = 0.2, \nu = 2.4, f(\mu) = \frac{1}{2} \)

- **Exact solution**: uniform distribution of fission sites throughout volume of box
  - Start with initial source guess = exact solution, uniform in volume
  - Shannon entropy for exact uniform source distribution: \( H_{\text{exact}} = \log_2(N_S) \), where \( N_S \) is the number of grid-cells in Shannon entropy mesh

  - For a 10 x 10 x 10 Shannon entropy mesh, \( H_{\text{exact}} = \log_2(100) = 9.966 \)

  - Can compare actual \( H_{\text{src}} \) for calculations that vary some of the problem parameters to \( H_{\text{exact}} \), as an indicator of clustering in this model problem
Clustering vs Neutrons/cycle

1000 neutrons/cycle

10,000 neutrons/cycle

100,000 neutrons/cycle

Cycle 1  Cycle 1000  Cycle 2000  Cycle 3000  Cycle 4000
Clustering and Shannon Entropy

- **Shannon entropy vs cycle**

  - For this model problem (running 5000 cycles)
    - Visual inspection of plots of fission source points
    - MCNP determination of $H_{ave}$ for the last half of the problem

  \[
  H_{ave} < 0.7 \, H_{exact} \quad \text{corresponds to severe clustering}
  \]
  \[
  H_{ave} > 0.7 \, H_{exact} \quad \text{corresponds to some or no clustering}
  \]
H vs Varying Parameters

Higher density
Larger size ➜ lower H, more clustering
Small neuts/cycle Smaller mfp

Note that cases with same ρL or same mfp/L have identical clustering
That is, 2*ρ and .5*L (or .5*mfp and .5*L) does not change clustering
(Remember that this is an infinite medium, no leakage)
A Simple Physical Approach

• For the original problem
  – $\lambda = 1.00$ cm
  – $l_F = 2.23$ cm, RMS distance from birth to fission site (from mcnp6)
  – $L = 400$ cm

  – So,
    If a single neutron “covers” a volume $(4\pi/3 \cdot l_F^3)$, and for this problem total volume = $L^3$

max coverage for

  1,000 neuts $\sim$ 0.073% of volume - severe clustering
  10,000 neuts $\sim$ 0.73% of volume - some clustering
  100,000 neuts $\sim$ 7.3% of volume - no clustering

define $f_H^{\text{max}} = \text{max fraction of H volume covered, } N \cdot (4\pi/3 \cdot l_F^3)/V_H$

(assumes no overlap of spheres, so can be >100%)
Clustering and Shannon Entropy (more)

- **Shannon entropy**
  - Used to diagnose convergence of iterated fission source
    - Superimpose coarse mesh, \( N_S = m \times m \times m \) bins
    - For each iteration, tally \( N \) fission neutrons in bins
    - Normalize to get \( \{ p_k, \; k=1,\ldots,N_S \} \), coarse global PDF
    - Then,
      \[
      H = - \sum p_k \log_2(p_k), \quad \text{note: } 0 \log_2(0) = 0
      \]
      Uniform particle distribution \( \Rightarrow \max H: \quad H_{\max} = \log_2(N_S) \)
      All neutrons at same point \( \Rightarrow \min H: \quad H_{\min} = 0 \)
  
- Plot \( H \) vs cycle, converged when \( H \) is asymptotically constant

  - **Fundamental assumption:**
    \( N >> N_s \), enough neutrons to get reliable \( p_k \) tallies

- **Clustering reduces the computed Shannon entropy**
  - If \( N \) is small, coverage is not sufficient for reliable \( p_k \) tallies
  - If \( N \sim N_s \) or \( N < N_s \), \( H_{\max} = \log_2(N) \), wrong!
Clustering and Shannon Entropy  (more)

• **Shannon entropy**
  \[ H = - \text{Sum} \ p_k \log_2(p_k), \]
  note: \( 0 \log_2(0) = 0 \)

  – For \( N_S = m \times m \times m \) bins, and \( N \) neutrons
    • Uniform particle distribution: \( H_{\text{max}} = \log_2( N_S ) \)
    • All neutrons at same point: \( H_{\text{min}} = 0 \)

• **Simple example**
  – \( 10 \times 10 \times 10 \) mesh, \( N_S = 1000 \)
  – For \( N = 1,000 \) neutrons
    
    | Clusters/Neutrons | H  | Clusters |
    |-------------------|----|----------|
    | 1 neutron/bin, uniform | 9.97 | 500 clusters of 2 |
    | 2 neutrons/bin, 0 in others | 8.97 | 250 clusters of 4 |
    | 4 neutrons/bin, 0 in others | 7.97 | 125 clusters of 8 |
    | 8 neutrons/bin, 0 in others | 6.97 | 8 clusters of 125 |
    | 125 neutrons/bin, 0 in others | 3.00 | 4 clusters of 250 |
    | 250 neutrons/bin, 0 in others | 2.00 | 2 clusters of 500 |
    | 500 neutrons/bin, 0 in others | 1.00 | 1 cluster of 1000 |
    | 1000 neutrons/bin, 0 in others | 0.00 |           |

  – Clustering reduces the computed Shannon entropy
Clustering and Shannon Entropy (more)

- **Shannon entropy & clustering**
  - Clustering leads to erroneously small asymptotic $H$, but how do you diagnose that if you don't know $H_{\text{exact}}$?
  - Clustering leads to jagged, gross variations in asymptotic $H$, which can be observed

- **Remember the EG-Source-Convergence problem?**
Cluster Analysis, Using DBSCAN

• There are many algorithms for identifying clusters
  – Used in image processing, etc.
  – A simple & useful algorithm is DBSCAN (density-based scan)

DBSCAN applied to original problem, with 1000 n/cycle

View from top

4 clusters (in 3D)

Need to choose 2 parameters, eps & minpts

It is not clear how useful the cluster analysis is .....

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****> File mcretp = 10
    npt = 10
    x range: 0.00000000000000E+00 400.000000000000
    y range: 0.00000000000000E+00 400.000000000000
    z range: 0.00000000000000E+00 400.000000000000
    eps = 25.000000000000
    minpts = 4
    npts = 968

clus = 4
counts for each cluster:
1 2 25
2 2 267
3 3 94
4 4 378
outliers: 4
A Real Problem

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ICSBEP
pu-sol-therm-012-13
Pu-sol-therm-012 Case 13

**PU-SOL-THERM-012**

Criticality of plutonium nitrate solution
In a large water-reflected cubic tank

(130 x 130 x 67.46 cm) (19% $^{240}$Pu)

C Pu(NO$_3$)$_4$ Solution
C 13.2 gPu/cc total
C atoms= 1.00306E-01
C
M1 94239  2.47132E-05
   94240  6.26195E-06
   94241  1.85624E-06
   94242  3.74965E-07
   95241  2.01156E-07
   7014   1.37165E-03
   8016   3.53011E-02
   1001   6.35948E-02
   26000  3.55846E-06
   24000  1.14431E-06
   28000  8.11038E-07

5 sides water reflected experimental configuration
Pu-sol-therm-012 Case 13

- Examine source points in fissile solution
- No clustering is evident, even with only 1,000 neutrons/cycle

1000 neutrons/cycle

RMS distance between fissions, \( \ell_F = 13.1 \) cm
Max coverage of \( H_{src} \) volume, \( f_{H_{max}} = 814 \% \)
Fraction of \( H_{src} \) volume with fission, \( f_H = 42 \% \)
\( \ell_F / \text{mean chord length}, \ell_F / \ell_{geom} = 20 \% \)

cycles to coalesce to 1 chain = 1228
Sutton’s Model Problem
Using Solution from
pu-sol-therm-012-13
Model Problem, with pu-sol-therm-012-13 Solution

- **Model problem for clustering investigations**
  - Homogeneous box
  - 400 x 400 x 400 cm$^3$
  - reflecting boundary conditions
  - Material: *fissile solution from pu-sol-therm-012-13*

- **Note that the volume is ~56x larger than pu-sol-therm-012-13**

- **Vary the solution density, 0.01 – 0.25 atoms/cm$^3$, nominal = 0.10 atoms/cm$^3***
  - note that density variation ~ size variation (L)
Clustering vs Density (1,000 neuts/cycle)

Density = 0.01
\[ \ell_F = 114.5 \text{ cm} \]
\[ f_{H_{\text{max}}} = 10608\% \]
\[ f_{H} = 55.2\% \]
\[ \ell_F / \ell_{\text{geom}} = 44.1\% \]

Density = 0.05
\[ \ell_F = 26.9 \text{ cm} \]
\[ f_{H_{\text{max}}} = 127\% \]
\[ f_{H} = 35.9\% \]
\[ \ell_F / \ell_{\text{geom}} = 10.1\% \]

Density = 0.10
\[ \ell_F = 13.7 \text{ cm} \]
\[ f_{H_{\text{max}}} = 16.7\% \]
\[ f_{H} = 22.9\% \]
\[ \ell_F / \ell_{\text{geom}} = 5.1\% \]

Density = 0.25
\[ \ell_F = 5.5 \text{ cm} \]
\[ f_{H_{\text{max}}} = 1.1\% \]
\[ f_{H} = 8.8\% \]
\[ \ell_F / \ell_{\text{geom}} = 2.1\% \]
A Real Problem
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PWR core
Investigation of Clustering in MCNP6 MC Calculations

PWR2D – Realistic PWR Detailed Model

**Nakagawa & Mori model of 2D PWR, realistic**

- 50,952 fuel pins with cladding
- 4,825 water tubes for rods or detectors

Each assembly:
- Explicit fuel pins & rod channels
- 17 x 17 lattice of pins in each assembly
- Enrichments: 2.1%, 2.6%, 3.1%

- ENDF/B-VII.1 nuclear data
- Usually run with 100k neuts/cycle
- For 3D whole-core, reactor was chosen to be 100 cm high, with water above & below

Plot of ¼ of the model

2.1% enrichment
2.6% enrichment
3.1% enrichment
PWR2D – Clustering vs Neutrons/cycle

Whole-core, with fuel in 100 cm axial, 324 x 324 x 100

Usually run with 100k neuts/cycle

no clustering in routine calculations

- $\ell_F = 19.1$ cm
- $f_{\text{max}} = 14\%$
- $f_H = 1\%$

Cycles to coalesce to 1 chain $= 65$

- $\ell_F = 19.1$ cm
- $f_{\text{max}} = 28\%$
- $f_H = 2\%$

Cycles to coalesce to 1 chain $= 91$

- $\ell_F = 19.1$ cm
- $f_{\text{max}} = 139\%$
- $f_H = 10\%$

Cycles to coalesce to 1 chain $= 1061$

- $\ell_F = 19.1$ cm
- $f_{\text{max}} = 277\%$
- $f_H = 18\%$

Cycles to coalesce to 1 chain $= 696$

- $\ell_F = 19.1$ cm
- $f_{\text{max}} = 2775\%$
- $f_H = 74\%$

Cycles to coalesce to 1 chain $= \gg 4000$

50 neutrons/cycle

100 neutrons/cycle

500 neutrons/cycle

1,000 neutrons/cycle

10,000 neutrons/cycle

Cycle 1000

Cycle 2000

Cycle 3000

Cycle 4000
Bias in $K_{eff}$ - for 2D $\frac{1}{4}$-core, from LA-UR-09-05623

$M = \text{neutrons/cycle}$

$N = \# \text{cycles}$

$N \cdot M = \text{constant for all calculations}$

$\Delta k = 0.003$
### Bias in Tallies - for 2D ¼-core, from LA-UR-09-05623

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Percent errors in 1/4-assembly fission rates using 500 neutrons/cycle

**Errors of -1.7% to +3.2%**

**Statistics ~ .1% to .3%**

Reference: ensemble-average of 25 independent calculations, with 25 M neutrons each & 20K neutrons/cycle
Bias in Tallies - for 2D ¼-core, from LA-UR-09-05623

Percent error in fission rates along diagonal

\[ M = \text{neutrons/cycle} \]
\[ N = \# \text{cycles} \]
\[ N \cdot M = \text{constant for all calculations} \]
### Bias in $\sigma$'s - for 2D $\frac{1}{4}$-core, from LA-UR-09-05623

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**True relative errors in 1/4-assembly fission rates, as multiples of calculated relative errors, $\sigma_{\text{TRUE}} / \sigma_{\text{MCNP}}$**

*Calculated uncertainties are 1.7 to 4.7 times smaller than true uncertainties*

Average factor = 3.1
Conclusions, Comments, Suggestions
Conclusions, Comments, Suggestions

• For most practical problems, clustering is not a concern
  – Most problems today: 10k, 100k, or more neutrons/cycle
    • mcnp6.2 will issue warning message if < 10k neuts/cycle
  – For large reactors, it is routine to run very large neuts/cycle, to get more efficient performance on parallel clusters

• For large solution tanks, clustering is a concern
  – Crit-safety practioners will probably not run 100k or 1M neuts/cycle
  – There are some very, very large solution tanks (with very low Keff)
  – But fortunately, Keff result will be conservative, even with clustering
    • Very large solution tank with clustering will be similar to infinite medium problem, with relatively few neutrons leaking. Keff will be overestimated, which is conservative for crit-safety

• Very important to develop a diagnostic for clustering

• Cluster diagnostic for storage racks may be very different from large solution tanks (due to empty space, loose-coupling, etc.)