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Title: Investigation of Clustering in MCNP6 Monte Carlo Criticality Calculations

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Expert Group meeting

Advanced Monte Carlo Techniques

Paris, June 2017

LA-UR-17-

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 occurences 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?**

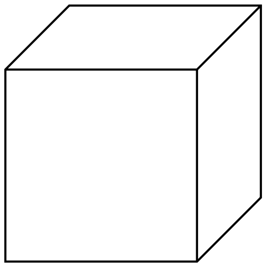
- **Clustering**
  - **For criticality problems**
    - Iterations using next-generation fission source
    - Convergence assessment depends on fission source coverage
  - **In some problems, repeated iterations lead to clustering**

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
  - A. Zoia, E. Dumonteil, "Neutron clustering: spatial fluctuations in multiplying systems at the critical point", ANS MCD 2017, Jeju, S. Korea, April 16-20, 2017

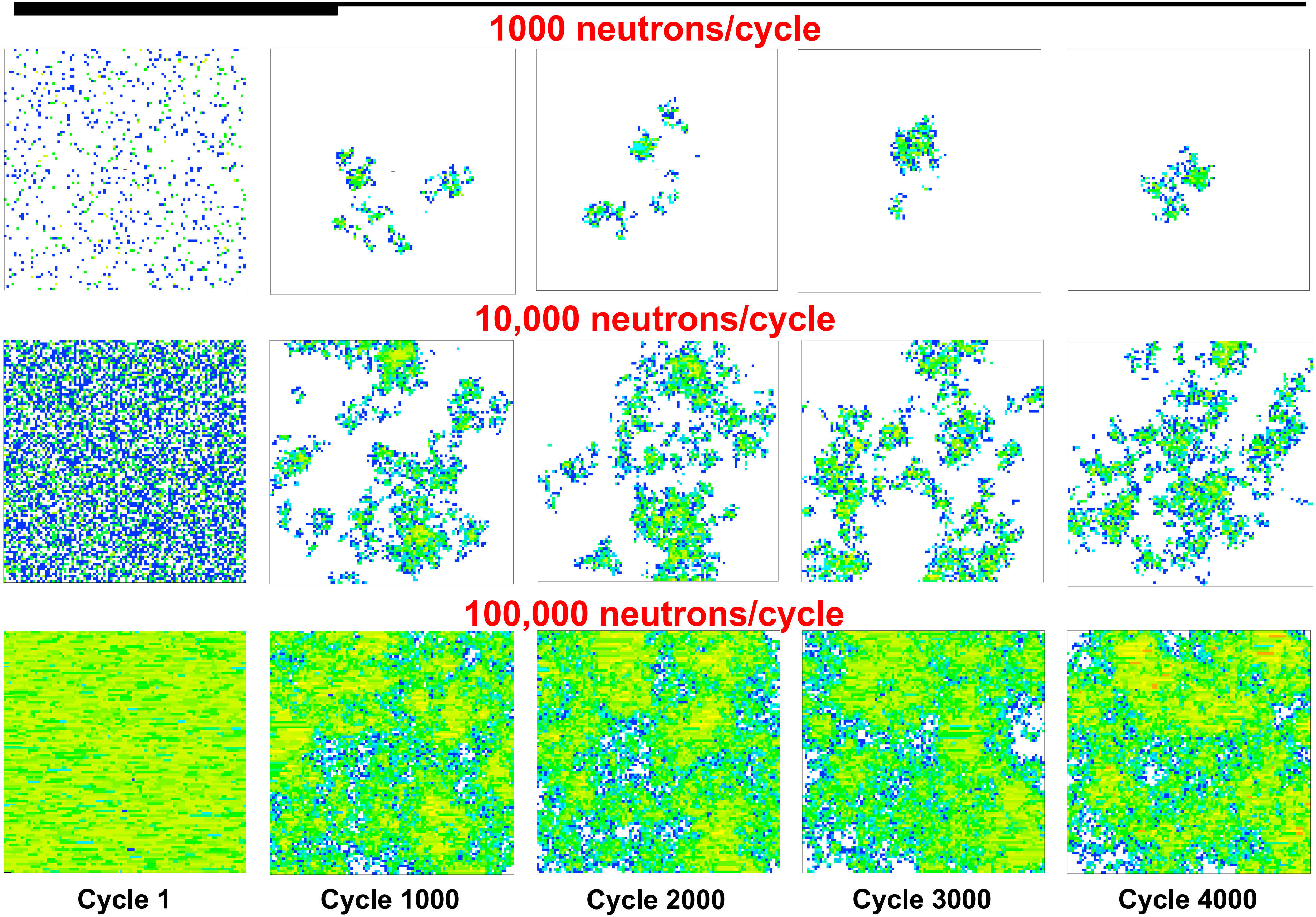
- **Model problem for clustering investigations**



  - Homogeneous box
  - 400 x 400 x 400 cm^3
  - reflecting boundary conditions
  - One-speed: $\Sigma_T = 1.0$, $\Sigma_S = 0.6$, $\Sigma_C = 0.2$, $\Sigma_F = 0.2$, $\nu = 2.4$, $f(\mu) = ½$

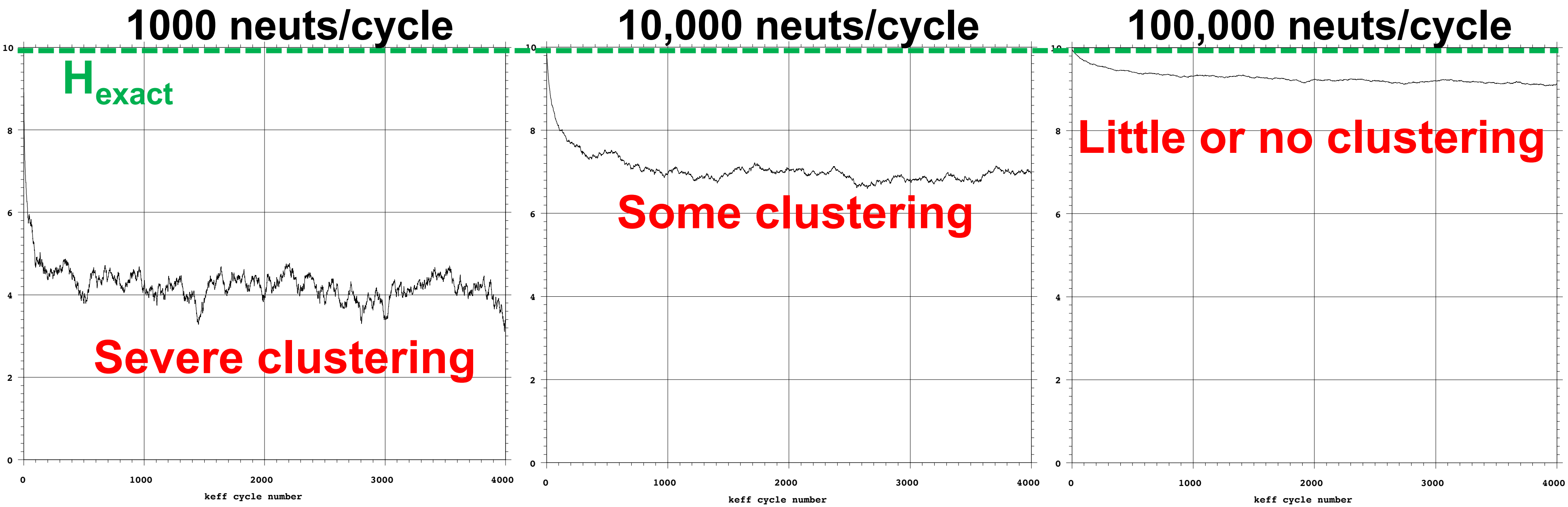
  - **Exact solution**: uniform distribution of fission sites throughout volume of box
    - Start with initial source guess = exact solution, uniform in volume
    - Shannon entropy for exact uniform source distribution: $\mathbf{H_{exact} = log_2(N_S)}$, where N_s is the number of grid-cells in Shannon entropy mesh
    - **For a 10 x 10 x 10 Shannon entropy mesh,** $\mathbf{H_{exact} = log_2(100) = 9.966}$
    - Can compare actual H_{src} for calculations that vary some of the problem parameters to H_{exact}, as an indicator of clustering in this model problem

Clustering vs Neutrons/cycle



Clustering and Shannon Entropy

- **Shannon entropy vs cycle**

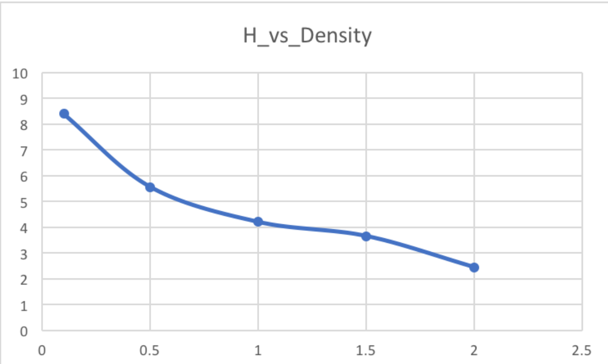


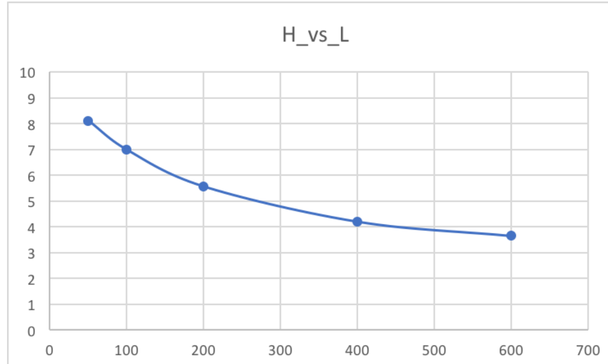
– **For this model problem (running 5000 cycles)**
  - Visual inspection of plots of fission source points
  - MCNP determination of H_{ave} for the last half of the problem

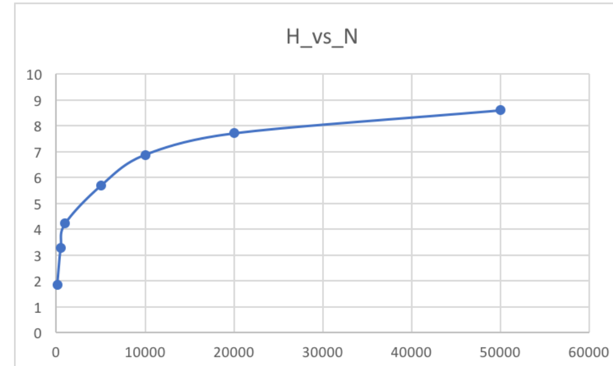
$H_{ave} < 0.7\ H_{exact}$ corresponds to **severe** clustering

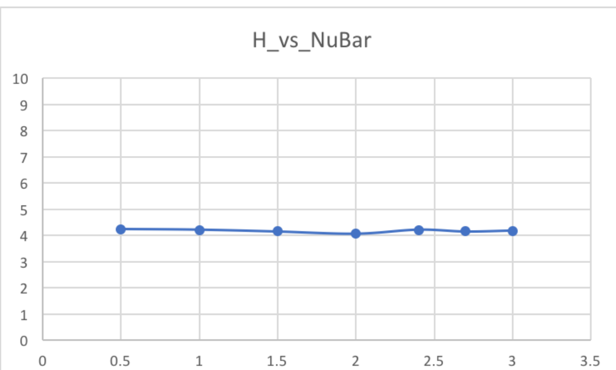
$H_{ave} > 0.7\ H_{exact}$ corresponds to **some or no** clustering

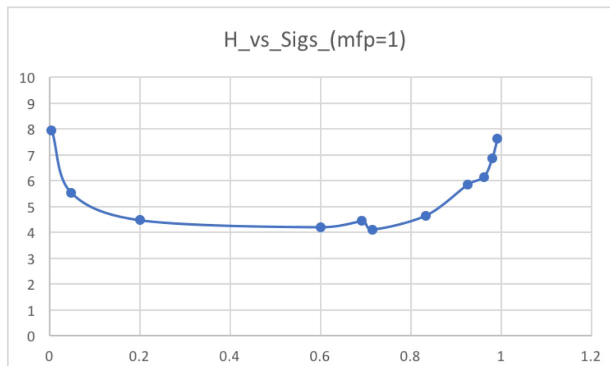
H vs Varying Parameters











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
  - λ = 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 $(4\pi/3 \cdot \ell_F^3)$,
    and for this problem total volume = L^3

    max coverage for

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

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

    (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 x m x m bins**
    - For each iteration, tally **N fission neutrons** in bins
    - Normalize to get **{ p_k, k=1,...,N_s }**, coarse global PDF
    - Then,

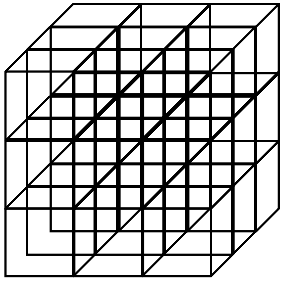
      $H = - \text{Sum } p_k \log_2(p_k)$, note: $0 \log_2(0) = 0$

      Uniform particle distribution ➜ max H: $H_{max} = \log_2(N_S)$

      All neutrons at same point ➜ min H: $H_{min} = 0$

    - 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: $H_{max} = \log_2(N_S)$
    - All neutrons at same point: $H_{min} = 0$

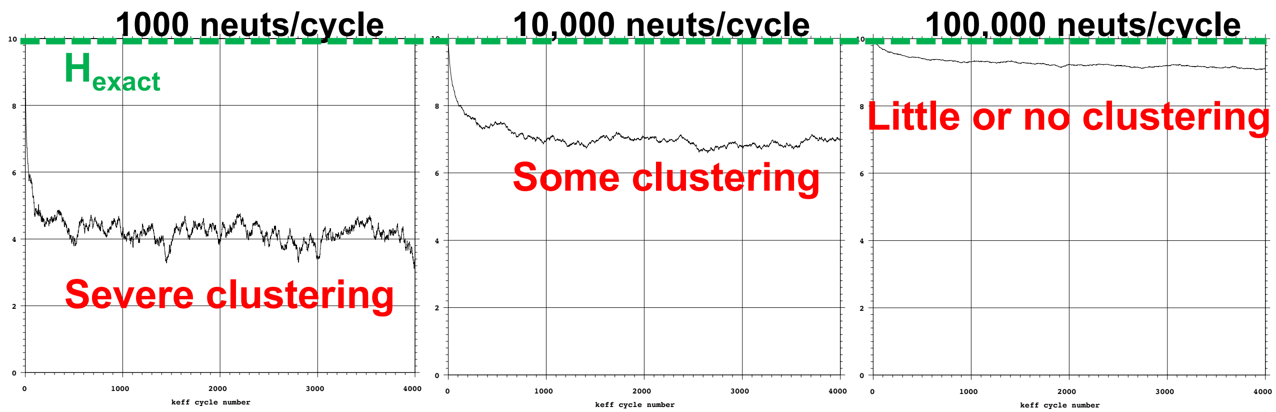
- **Simple example**
  - **10 x 10 x 10 mesh, $N_S = 1000$**
  - **For N = 1,000 neutrons**

1 neut/bin, uniform	**H = 9.97**	
2 neuts/bin, 0 in others	**H = 8.97**	**500 clusters of 2**
4 neuts/bin, 0 in others	**H = 7.97**	**250 clusters of 4**
8 neuts/bin, 0 in others	**H = 6.97**	**125 clusters of 8**
125 neuts/bin, 0 in others	**H = 3.00**	**8 clusters of 125**
250 neuts/bin, 0 in others	**H = 2.00**	**4 clusters of 250**
500 neuts/bin, 0 in others	**H = 1.00**	**2 clusters of 500**
1000 neuts/bin, 0 in others	**H = 0.00**	**1 cluster of 1000**

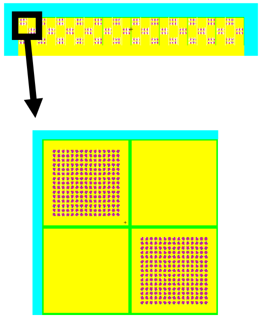
  - **Clustering reduces the computed Shannon entropy**

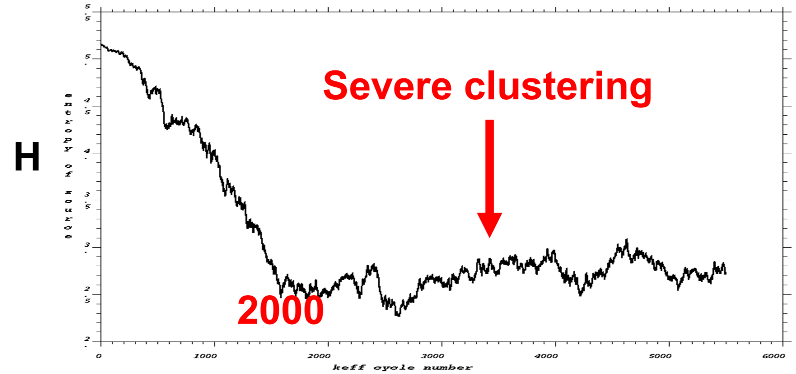
Clustering and Shannon Entropy (more)

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



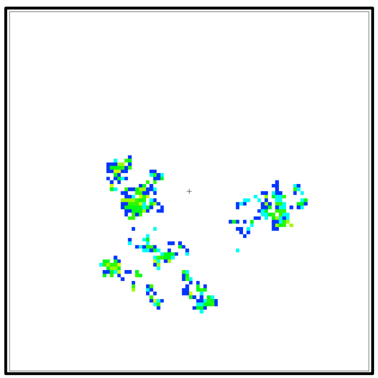
- **Remember the EG-Source-Convergence problem?**





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)



```
=====> file srctp
              nattrib =              10
              npts    =             968
x range:  0.000000000000000E+000   400.000000000000
y range:  0.000000000000000E+000   400.000000000000
z range:  0.000000000000000E+000   400.000000000000

eps    =    25.0000000000000
minpts =              4
npts   =            968

nclust =              4
counts for each cluster:
        1       225
        2       267
        3        94
        4       378
outliers:            4

                2         2 2 2 2
              2 2 2       2 2 2 2
              2         2 2 2 2 2
          3   2         2   2 2
      3   3             2 2
  3 3 3   3 3           2
3 3 3 3         2 2     2
  3 3           2 2 2 2
            2 2 2 2 2 2 2             0 0
        0 2 2 2 2   2 2
            2 2
                2                       1 1     1     1
                                      1 1 1 1   1 1 1 1
        4 4 4                           1 1 1 1 1 1 1
        4 4 4 4 4 4                   1       1 1 1 1   1 1
      4 4 4 4 4 4 4                   1 1 1 1 1 1 1 1   1 1
        4 4 4 4                               1 1 1 1 1 1 1
  4 4   4 4 4 4 4                                 1   1 1
  4 4 4 4     4 4 4                               1
    4 4 4       4
  4 4 4 4 4   4 4
  4 4 4 4
```

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 …..

A Real Problem

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ICSBEP

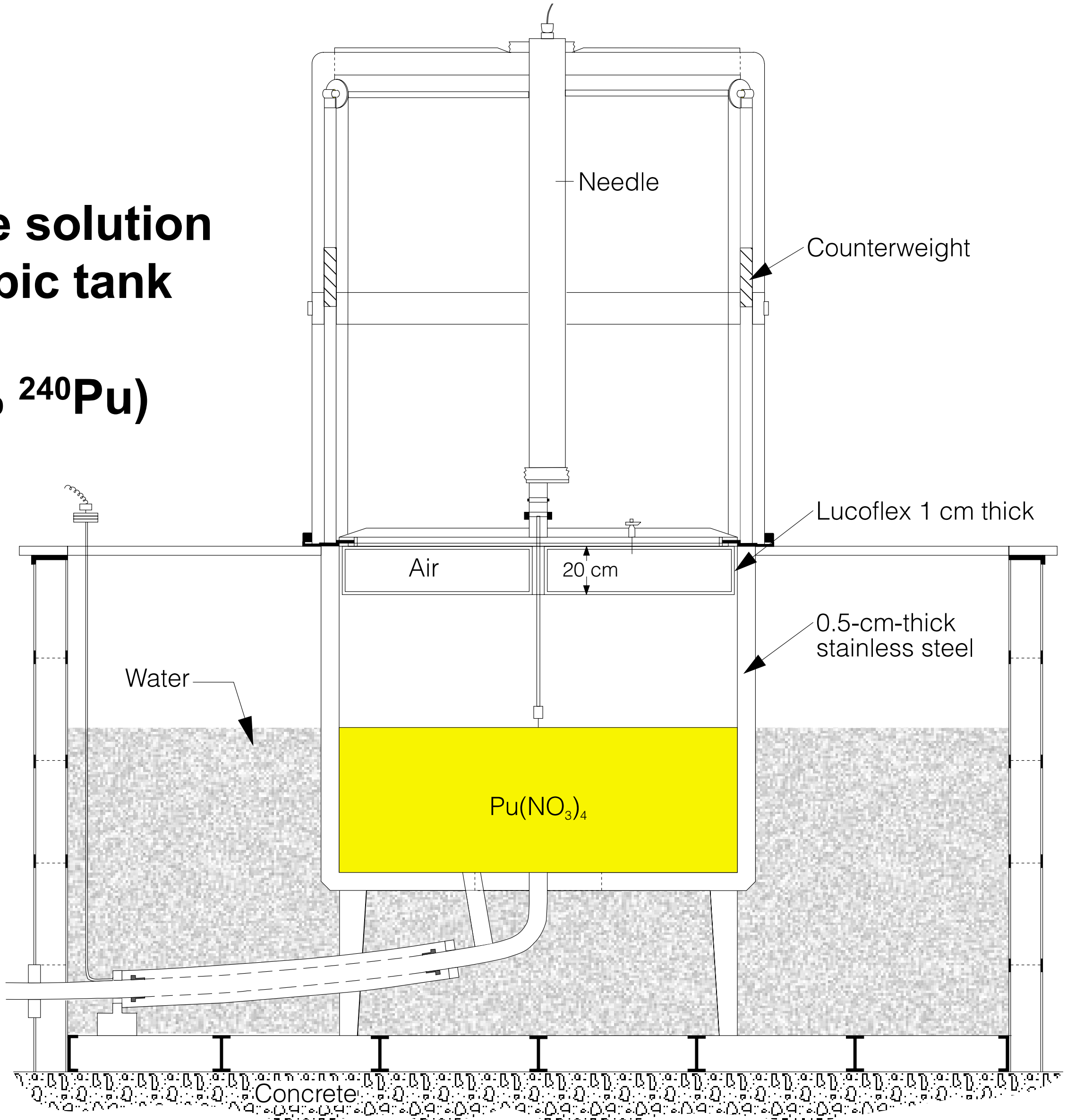
pu-sol-therm-012-13

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(NO3)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
```

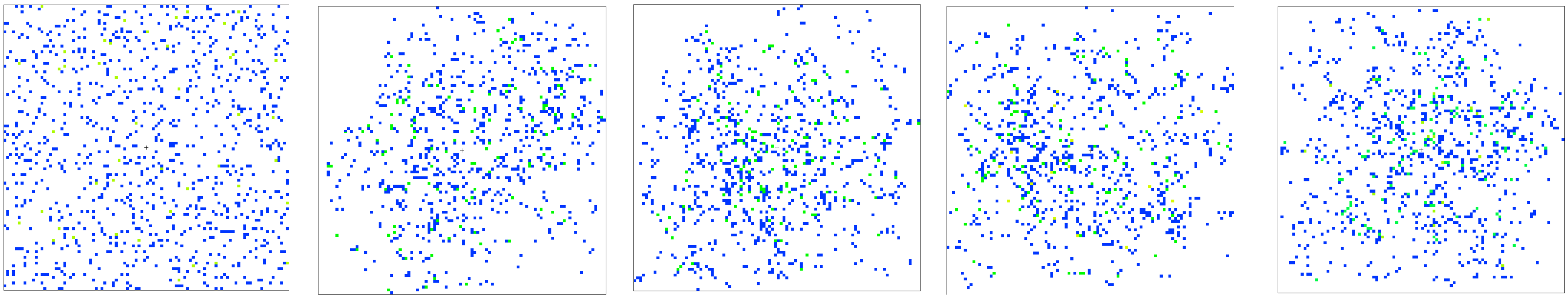


5 sides water reflected experimental configuration

Pu-sol-therm-012 Case 13

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

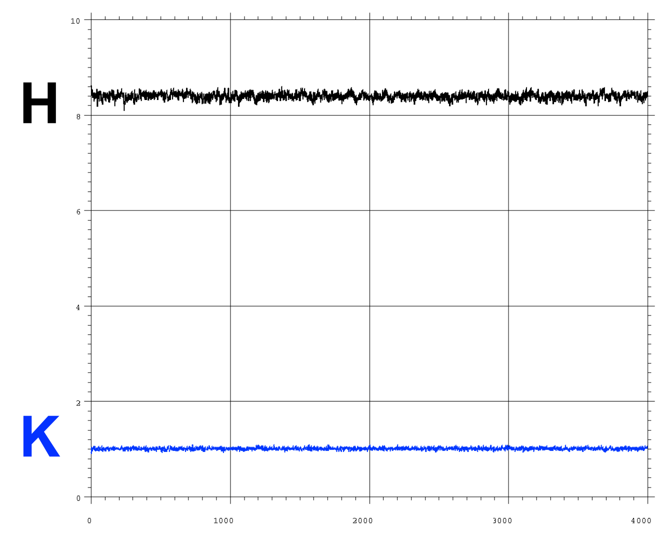
1000 neutrons/cycle



Cycle 1 **Cycle 1000** **Cycle 2000** **Cycle 3000** **Cycle 4000**

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

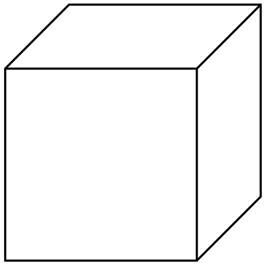
cycles to coalesce to 1 chain = 1228



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)**

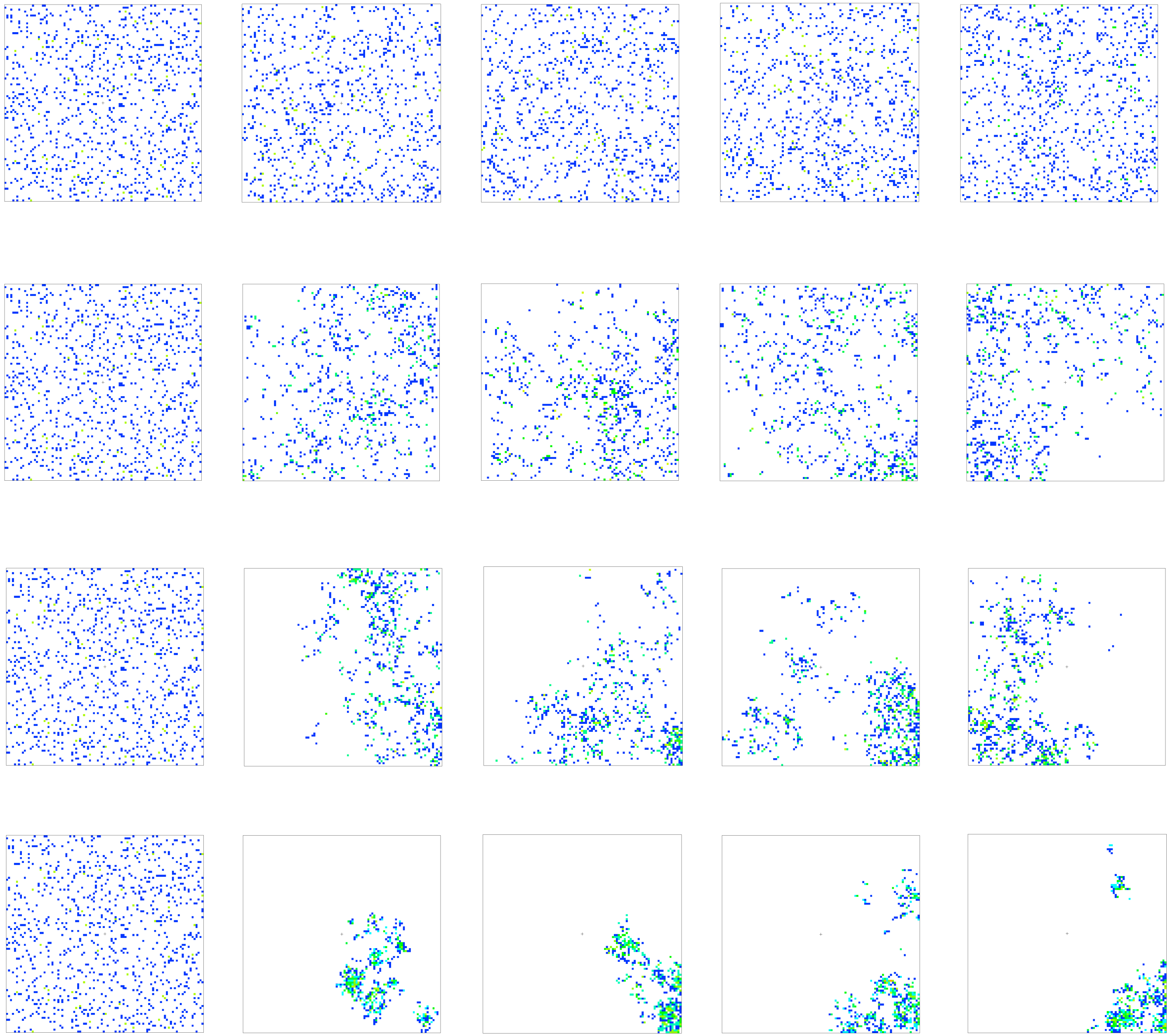
Clustering vs Density (1,000 neuts/cycle)

Density = 0.01
ℓ_F = 114.5 cm
f_H^{max} = 10608%
f_H = 55.2%
ℓ_F/ℓ_{geom} = 44.1%

Density = 0.05
ℓ_F = 26.9 cm
f_H^{max} = 127%
f_H = 35.9%
ℓ_F/ℓ_{geom} = 10.1%

Density = 0.10
ℓ_F = 13.7 cm
f_H^{max} = 16.7%
f_H = 22.9%
ℓ_F/ℓ_{geom} = 5.1%

Density = 0.25
ℓ_F = 5.5 cm
f_H^{max} = 1.1%
f_H = 8.8%
ℓ_F/ℓ_{geom} = 2.1%



Cycle 1 | Cycle 1000 | Cycle 2000 | Cycle 3000 | Cycle 4000

A Real Problem

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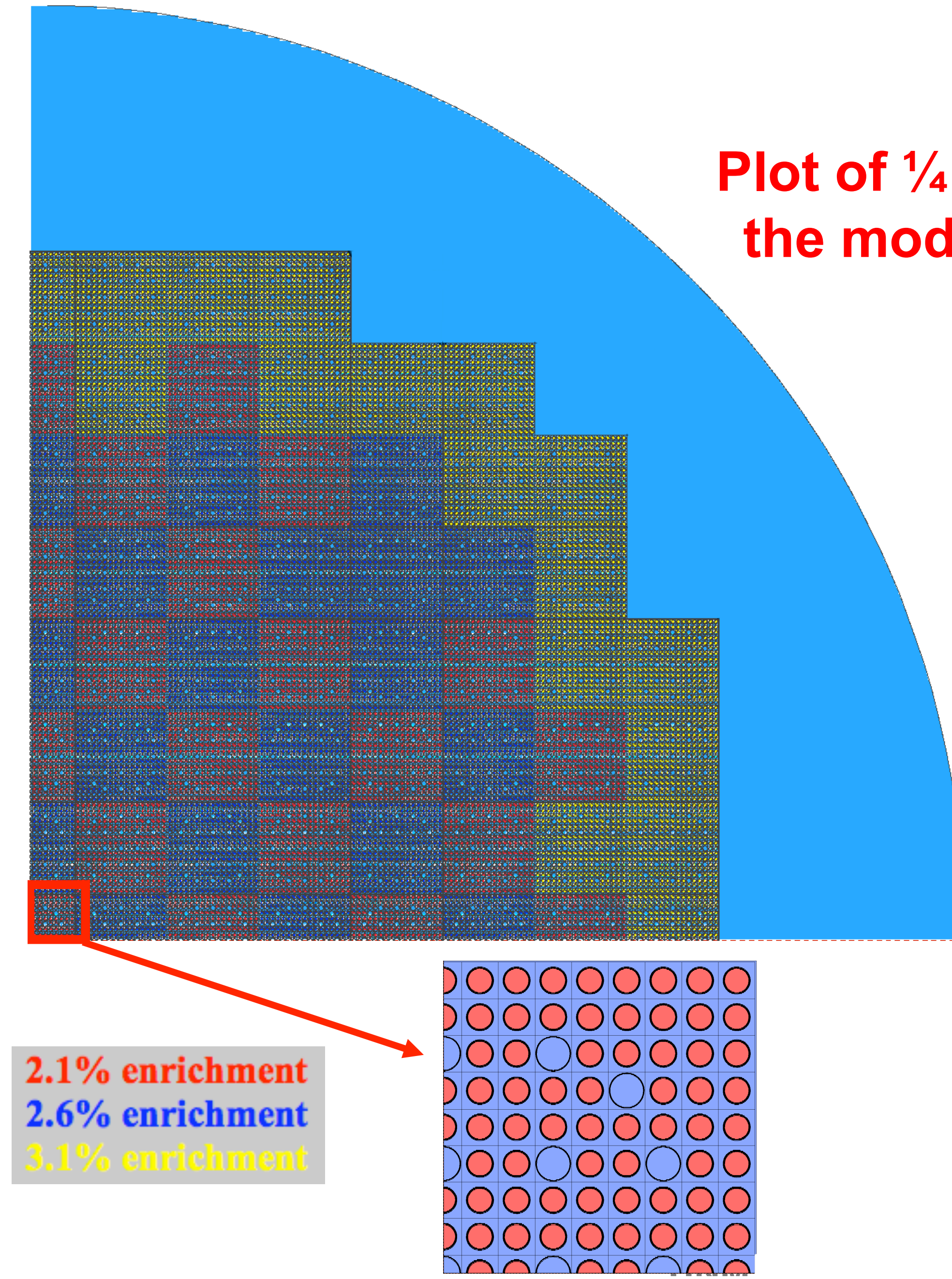
PWR core

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**



PWR2D – Clustering vs Neutrons/cycle

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

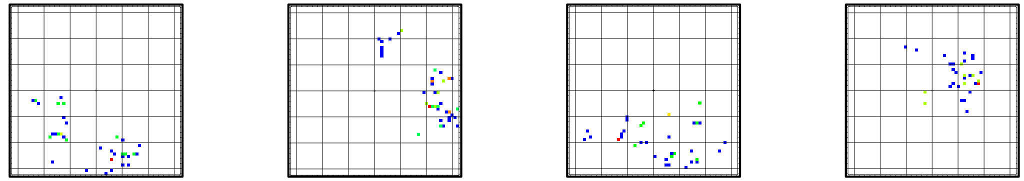
Usually run with 100k neuts/cycle

no clustering in routine calculations

50 neutrons/cycle

ℓ_F = 19.1 cm
f^{max} = 14%
f_H = 1%

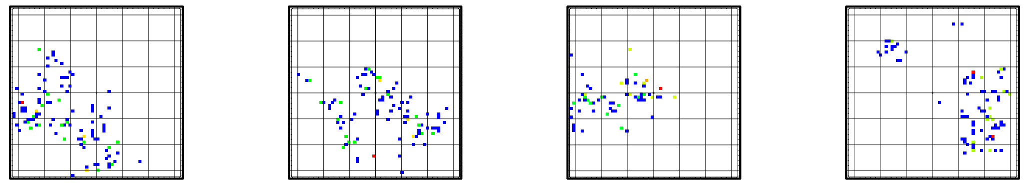
cycles to coalesce to 1 chain = 65



100 neutrons/cycle

ℓ_F = 19.1 cm
f^{max} = 28%
f_H = 2%

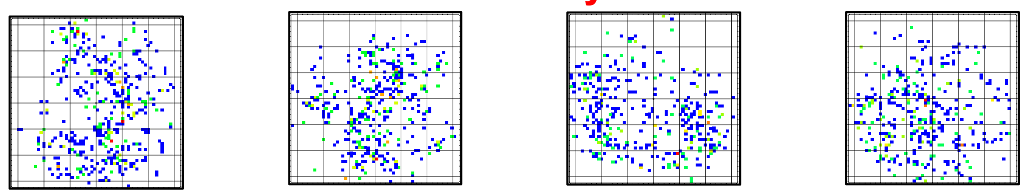
cycles to coalesce to 1 chain = 91



500 neutrons/cycle

ℓ_F = 19.1 cm
f^{max} = 139%
f_H = 10%

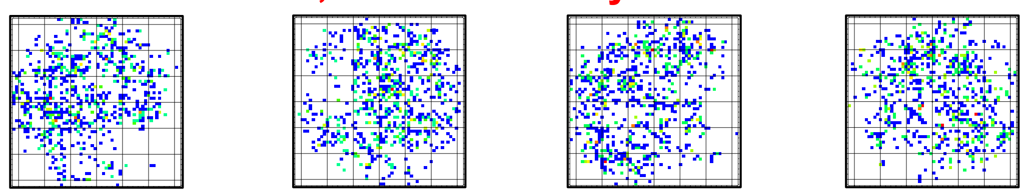
cycles to coalesce to 1 chain = 1061



1,000 neutrons/cycle

ℓ_F = 19.1 cm
f^{max} = 277%
f_H = 18%

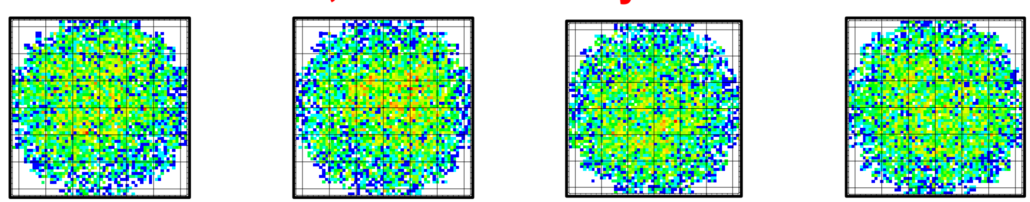
cycles to coalesce to 1 chain = 696



10,000 neutrons/cycle

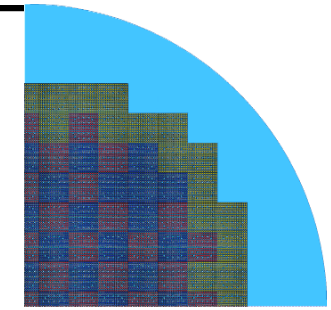
ℓ_F = 19.1 cm
f^{max} = 2775%
f_H = 74%

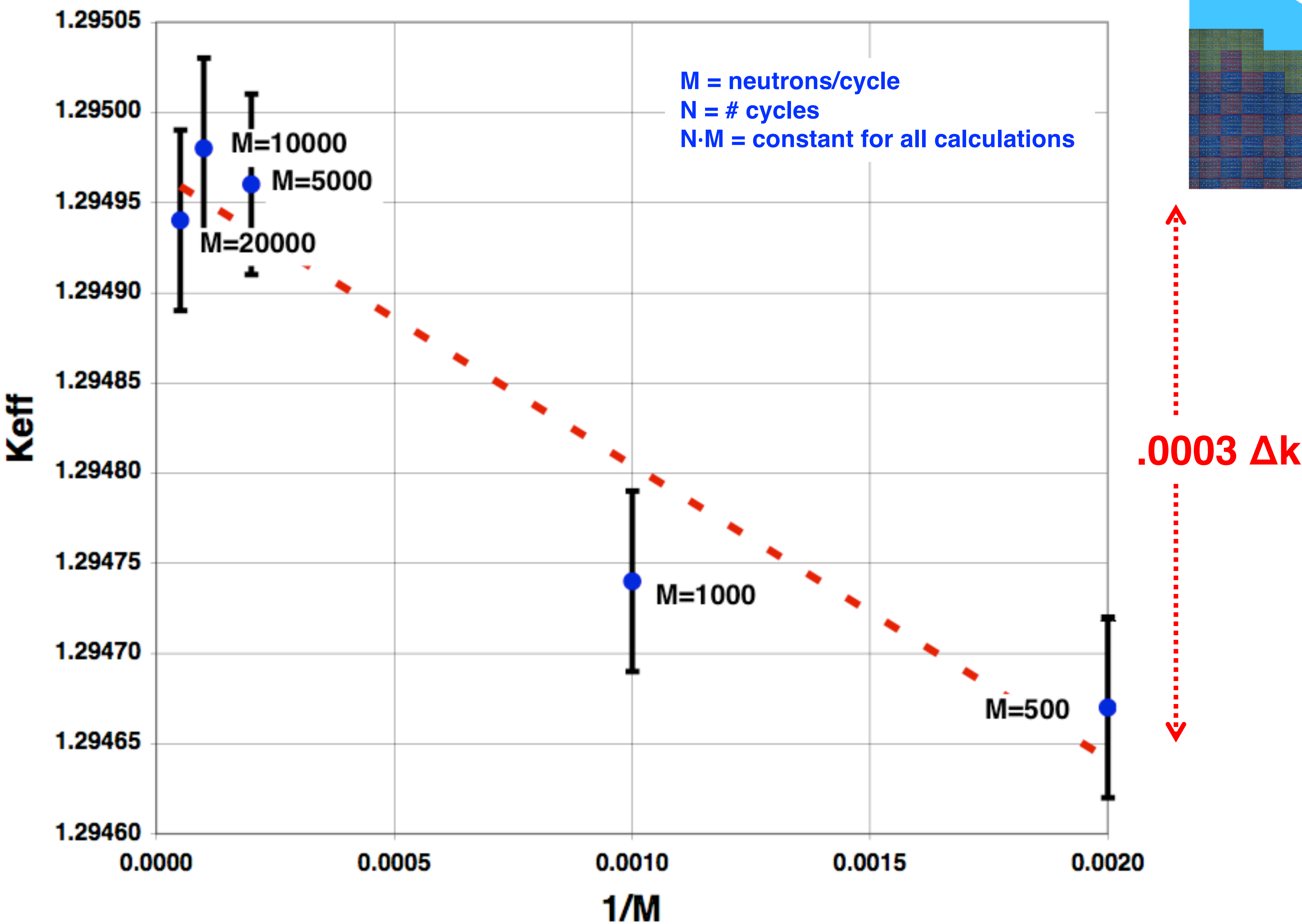
cycles to coalesce to 1 chain = >> 4000



Cycle 1000 Cycle 2000 Cycle 3000 Cycle 4000

Bias in K_{eff} - for 2D ¼-core, from LA-UR-09-05623





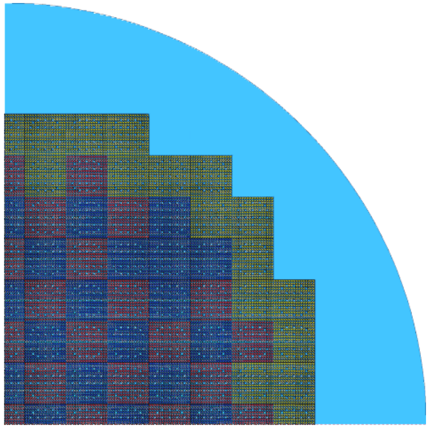
Bias in Tallies - for 2D ¼-core, from LA-UR-09-05623

0.0	-0.5	-0.6	-0.2	-0.3	0.5	0.8								
-0.2	-0.7	-0.8	0.1	0.3	0.7	0.6								
-0.5	-0.7	-0.7	0.0	0.3	0.7	1.0	1.3	1.2	1.6	2.0				
-0.1	-0.7	-0.8	0.2	0.3	0.8	1.1	1.2	1.2	1.3	2.4				
-0.4	-0.6	-0.5	0.0	-0.1	0.2	0.7	0.6	1.4	2.0	1.9	2.7	3.2		
-0.7	-0.9	-0.8	-0.4	0.2	0.5	0.4	1.0	1.2	1.6	2.0	1.6	2.6		
-0.6	-0.3	-0.7	-0.6	-0.6	0.3	0.8	1.1	1.2	1.5	1.1	1.7	1.8		
-0.5	-0.8	-1.0	-0.8	-0.5	0.2	0.8	0.9	1.2	1.2	1.4	1.3	1.9		
-0.5	-0.9	-0.8	-1.0	-0.6	0.2	0.2	0.6	0.9	1.1	0.8	0.7	1.1	0.9	1.5
-0.9	-0.9	-1.1	-1.0	-0.9	-0.1	0.2	0.6	0.8	0.6	0.6	0.6	1.3	1.2	1.1
-1.2	-1.3	-1.2	-1.0	-0.6	-0.5	-0.3	0.2	0.9	0.7	1.1	0.9	1.3	1.2	1.1
-1.3	-1.5	-1.0	-0.9	-0.7	-0.5	-0.6	0.3	0.4	0.5	1.3	1.4	2.1	1.9	1.6
-1.7	-1.5	-1.1	-1.1	-0.6	-0.5	-0.2	-0.1	0.3	0.6	1.0	1.7	2.0	2.1	1.9
-1.5	-1.5	-1.4	-1.0	-1.1	-0.8	0.0	0.1	0.3	0.4	1.0	1.0	1.5	3.1	2.3
-1.6	-1.6	-1.2	-1.2	-0.6	-0.7	-0.4	-0.2	0.1	0.2	0.5	1.6	2.1	2.4	2.3

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

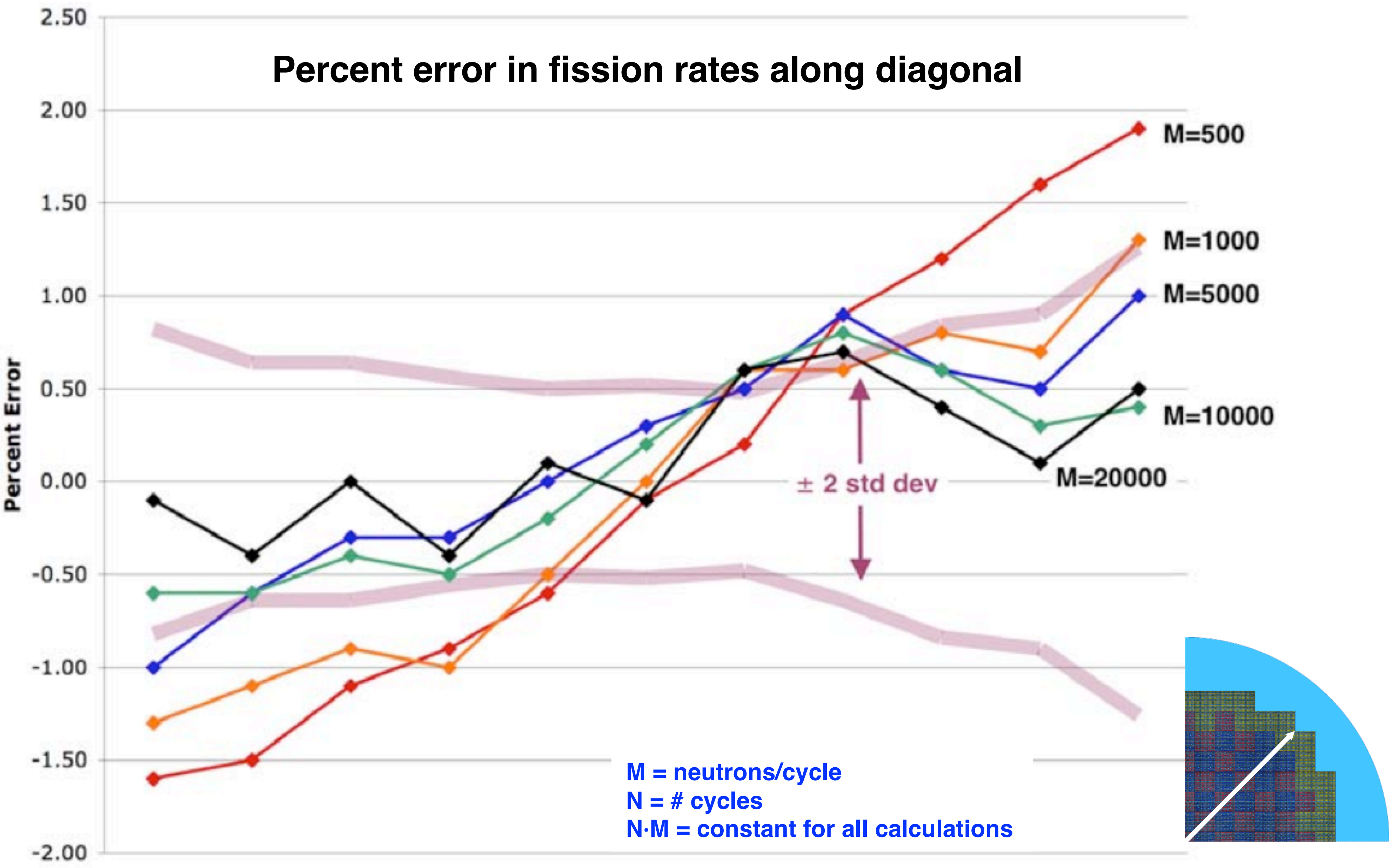
Errors of -1.7% to +3.2%

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

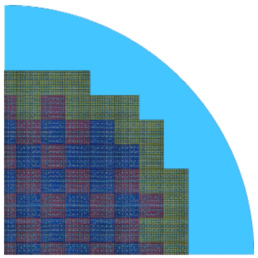


Bias in σ's - for 2D ¼-core, from LA-UR-09-05623

3.4	3.1	2.7	2.7	2.6	2.3	2.7								
3.3	3.7	3.6	3.7	3.7	2.7	2.9								
3.8	3.8	3.9	4.0	3.6	3.3	3.0	2.9	2.5	2.5	2.2				
3.8	3.9	4.2	3.3	3.5	3.4	3.2	3.6	3.0	3.0	2.8				
3.9	3.6	3.5	3.3	3.4	3.4	4.0	3.9	3.5	3.2	3.1	2.5	1.7		
4.1	3.8	3.5	3.2	2.9	2.6	2.9	3.2	3.1	2.8	2.7	1.9	1.7		
3.4	3.4	3.2	3.5	2.6	2.4	2.6	3.0	2.9	2.9	2.8	2.3	2.1		
4.2	3.5	3.4	3.1	2.7	2.3	2.0	2.4	2.5	2.5	2.1	2.3	2.3		
3.9	3.6	3.1	2.9	2.3	1.9	1.9	2.3	2.4	2.9	2.7	2.7	2.2	2.8	2.3
3.7	3.3	3.6	2.4	2.2	2.2	2.5	1.8	2.2	2.6	2.7	2.9	2.5	2.4	2.5
3.0	3.1	3.0	2.2	2.2	2.1	2.4	2.5	2.4	2.6	2.7	2.6	2.7	3.0	2.6
2.9	3.7	3.3	2.6	2.5	2.8	3.0	2.9	3.5	3.2	3.3	3.1	3.1	3.2	3.3
3.2	3.1	2.9	3.1	3.2	3.3	3.5	3.5	3.6	3.9	3.7	3.9	3.5	3.4	2.9
3.4	3.0	3.1	3.6	3.4	3.5	3.9	3.7	4.0	4.3	4.0	4.3	3.8	4.2	3.5
3.5	3.2	2.8	3.5	3.8	3.9	3.9	3.9	4.1	4.1	4.6	4.4	4.7	4.5	3.8

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

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.)**