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Title:

MCNP CALCULATIONS FOR THE OECD/NEA SOURCE CONVERGENCE BENCHMARKS FOR CRITICALITY SAFETY ANALYSIS

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OECD/NEA Working Party on Nuclear Criticality Safety,
Expert Group on Source Convergence Analysis
Paris, France, 19 September 2001

Los Alamos
NATIONAL LABORATORY

Abstract

MCNP Calculations for the OECD/NEA Source Convergence Benchmarks for Criticality Safety Analysis

FB Brown, RC Little, A Sood, DK Parsons, TA Wareing

Improper source convergence can lead to non-conservative estimates of the k-effective for various fissionable configurations, such as the “Whitesides problem”, spent fuel casks, spent fuel storage pools, and fuel processing systems. To improve the robustness of criticality safety analyses with respect to source convergence the OECD/NEA has established an expert group to investigate the long-standing problem of source convergence for certain classes of nuclear criticality safety problems.

Under the guidance of the Working Party on Nuclear Criticality Safety, the major assignments of the Expert Group include:

- Developing criticality safety benchmark problems which exhibit convergence problems.

- Testing fission source algorithms for vulnerability to slow convergence.

- Developing criteria to measure convergence reliability.

- Developing source convergence guidelines for the nuclear criticality safety analysts.

- Exploring and evaluating methods to detect source convergence.

- Publishing the results.

To support this international effort to improve the understanding of criticality calculations, members of the Expert Group have specified and calculated a set of four source convergence benchmark problems using a variety of standard Monte Carlo computer codes. This report documents the calculations performed at Los Alamos National Laboratory using the MCNP Monte Carlo code. Results are presented for the four benchmark calculations, as well as for a number of additional supporting calculations performed with both Monte Carlo and deterministic codes.

Source Convergence Benchmark

Calculations with MCNP

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Benchmark Calculations with MCNP

Benchmark 1 — Checkerboard Storage of Assemblies — FB Brown

Benchmark 2 — Pincell Array with Irradiated Fuel — A Sood

Benchmark 3 — Three Thick 1D Slabs — RC Little & DK Parsons

Benchmark 4 — Array of Interacting Spheres — RC Little & TA Wareing

OECD/NEA Working Party on Nuclear Criticality Safety
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Paris, France — 19 September 2001

Benchmark 1
Checkerboard Storage of Assemblies

MCNP Calculations

Forrest Brown

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Outline

- Problem description
- Results for 36 cases
- Additional results

- MCNP input
- MCNP k-eigenvalue strategy

Benchmark 1 — Checkerboard Storage of Assemblies

Contact: Forrest B. Brown
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fbrown@lanl.gov

Code: **MCNP4C2**

Method: continuous-energy Monte Carlo

Geometry: exact, as specified

Cross-sections: ENDF/B-VI, processed by NJOY into MCNP library

Computer: SGI Origin-2000, using 4-10 processors

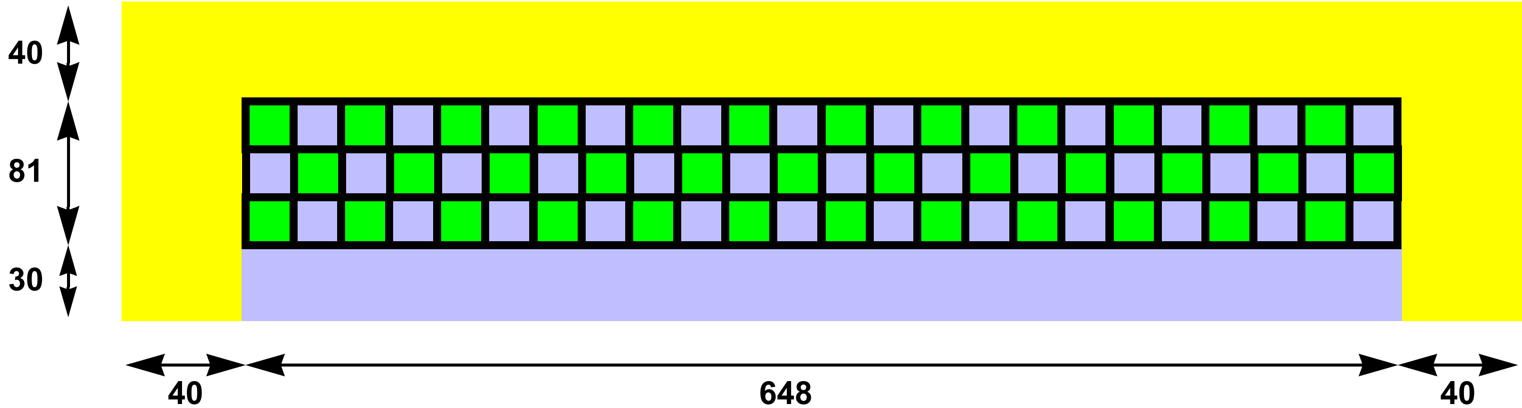
Date: August, 2001

Benchmark 1 — Checkerboard Storage of Assemblies

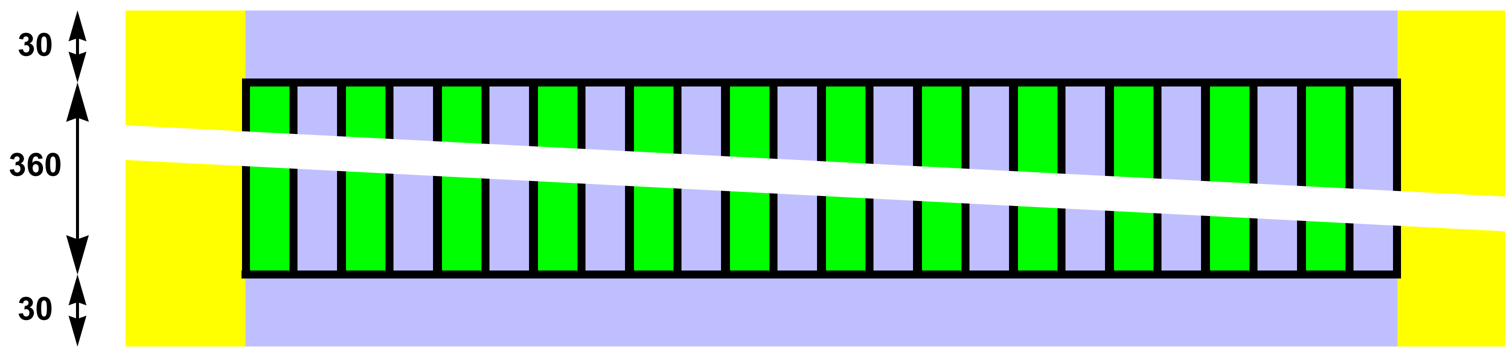
Material Compositions		MCNP Cross-sections	
Fuel			
U238	2.2380e-2	92238.60c,	endf-VI.2
O	4.6054e-2	8016.60c	
U235	8.2213e-4	92235.60c,	LANL-proposed endf-VI.2
Water			
H	6.6706e-2	1001.60c,	with $S(\alpha,\beta)$ lwtr.01t
O	3.3353e-2	8016.60c	
Zirconium			
Zr	4.2910e-2	40000.60c,	natural Zr, endf-VI.1
Iron			
Fe	8.3770e-2	26000.55c,	natural Fe, rmccs
Concrete			
H	5.5437e-3	1001.60c,	with $S(\alpha,\beta)$ lwtr.01t
C	6.9793e-2	6000.60c,	natural C
Si	7.7106e-3	14000.60c,	natural Si
Ca	8.9591e-3	20000.60c,	natural Ca
O	4.3383e-2	8016.60c	

Benchmark 1 — Checkerboard Storage of Assemblies

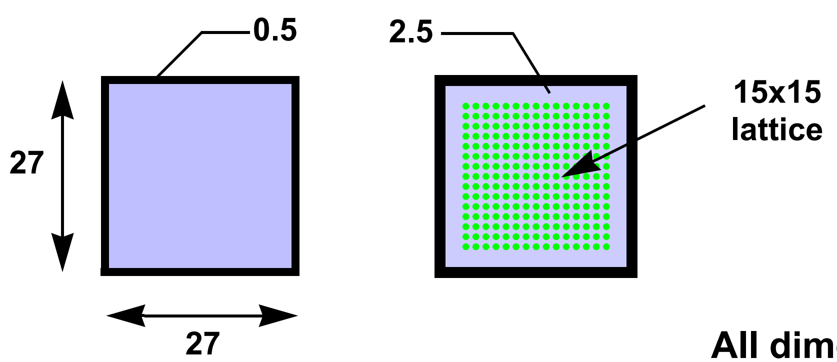
Top View



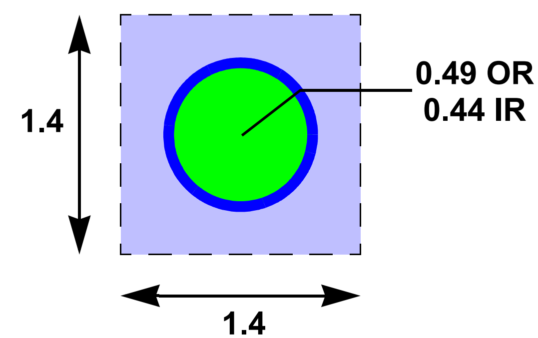
Side View



Element Details



Pin Cell



All dimensions in cm

Benchmark 1 — K-effective Results

Cases	Total Generations	Skipped Generations	Histories / Generation					
			1000	2000	5000	10000	20000	50000
Uniform								
1, 13, 25	520	20	0.88008 (114)	0.87818 (70)	0.87996 (53)			
2, 14, 26	540	40	0.87892 (114)	0.87843 (70)	0.88019 (53)			
3, 15, 27	600	100	0.87813 (114)	0.87871 (79)	0.88032 (44)			
37, 38, 40	1100	100				0.87998 (26)	0.88059 (18)	0.88046 (9)
39, 41	1100	100					0.88064 (18)	0.88125 (9)
42	5500	500				0.88192 (9)		
43	9055	500				0.88192 (1)		
Location (1,1)								
4, 16, 28	520	20	0.88044 (106)	0.87862 (79)	0.88069 (53)			
5, 17, 29	540	40	0.88100 (106)	0.87939 (79)	0.88127 (53)			
6, 18, 30	600	100	0.88203 (106)	0.88131 (79)	0.88256 (44)			
Location (23,3)								
7, 19, 31	520	20	0.87817 (114)	0.87871 (79)	0.87799 (44)			
8, 20, 32	540	40	0.87880 (114)	0.87915 (79)	0.87838 (44)			
9, 21, 33	600	100	0.88060 (115)	0.87987 (79)	0.87889 (44)			
Location (12,2)								
10, 22, 34	520	20	0.87729 (114)	0.87859 (79)	0.87750 (57)			
11, 23, 35	540	40	0.87790 (114)	0.87938 (79)	0.87832 (53)			
12, 24, 36	600	100	0.87935 (114)	0.88003 (79)	0.87893 (53)			

Benchmark 1 — Observations

- Cases 1-36 were specified for Benchmark 1

K-effective Results

- MCNP4C2 performs 10 statistical tests on Keff results — all 36 cases passed
- Comparison to MCNP reference (90 M histories): Keff = 0.88192 (1)

— **With no corrections to σ:**

Agreement within 1-σ:	3 / 36
Agreement within 2-σ:	8 / 36

— **With MacMillan corrections to σ, using various dominance-ratios:**

	0.900	0.990	0.999
Agreement within 1-σ:	6 / 36	11 / 36	30 / 36
Agreement within 2-σ:	10 / 36	27 / 36	32 / 36

— General trend:
+ More histories/generation ⇒ better agreement
+ More skipped generations ⇒ better agreement
+ Should use >10K histories/generation, skip >500 generations

Benchmark 1 — Observations

Fission Distribution

- MCNP4C2 performs 10 statistical tests on selected tallies, which for these problems applied to the fuel element fission rates:

  — Cases 1-3, 13-15, 25-27 with **uniform initial source** in fuel pins **passed** all of the MCNP statistical tests

  — Other cases (4-12, 16-24, 28-36) with initial **source in one fuel element failed** at least some of the MCNP statistical tests

  + all failed the test for "*no zero bins*"
  + all failed the test for "*all relative errors < .1*"

- Converged fission distribution, from MCNP reference case (90 M histories):

37084	11171	4239	1494	871	615	354	413	235	120	13	4	
	15225	5659	2253	958	587	426	321	246	143	50	4	7
7972	5226	2118	891	466	264	237	173	108	43	9	3	

(normalized to sum = 100000)

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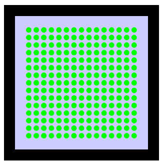
Benchmark 1 — Additional Results

All calculations: 100 settle cycles, 1000 active cycles, 5000 starters

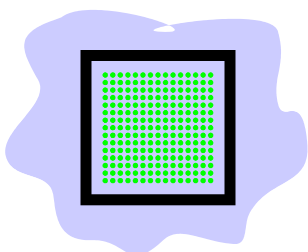
Infinite Lattice of Fuel Elements



Keff = 1.11695 (29)

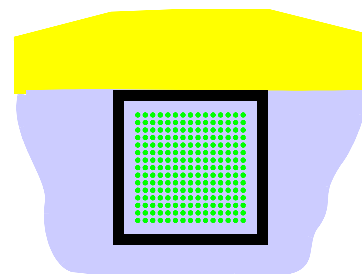
MCNP reference for Benchmark 1
Keff = 0.88192 (1)

Single Fuel Element, surrounded by water



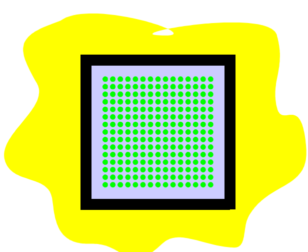
Keff = 0.85779 (34)

Single Fuel Element, water 3 sides, concrete 1 side



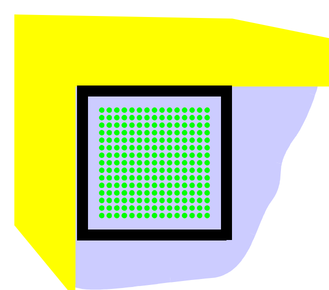
Keff = 0.86817 (34)

Single Fuel Element, surrounded by concrete



Keff = 0.90390 (34)

Single Fuel Element, water 2 sides, concrete 2 sides



Keff = 0.88017 (35)

```
Benchmark 1 -- case= 37
c     =======================================================
c     =====> OECD/NEA Source Convergence Benchmark 1 (FBB)
c     =====>   Starters:      10000
c     =====>   Skipped gens:  100
c     =====>   Total gens:    1100
c     =====>   Start source:  uniform in fuel
c     =======================================================
c
c     =======================================================
c     =====> Cell cards
c     =======================================================
c     =====> Fuel pin, clad, water  unit cell
1     1  0.06925613  -1        u=1         $ fuel
2     2  0.042910     1 -2     u=1         $ clad
3     3  0.100059     2        u=1         $ water
c     =====> fuel lattice, infinite array of pins in water
4     0              -3        u=2  lat=1  fill=1
c     =====> fuel element
5     0              -4        u=3  fill=2  $ fuel lattice
6     3  0.100059     4 -5     u=3          $ water gap
7     4  0.083770     5        u=3          $ steel
c     =====> water element
8     3  0.100059    -5        u=4          $ water
9     4  0.083770     5        u=4          $ steel
c     =====> element lattice, infinite
10    0              -6        u=5  lat=1   fill= 1:24 1:3 0:0
        3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4
        4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3
        3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4 3 4
c     =====> full model
11    0              -7        fill=5     $ lattice of elements
12    3  0.100059    -8                   $ water, top
13    3  0.100059    -9                   $ water, bottom
14    3  0.100059    -10                  $ water, side
15    5  0.0725757   -11                  $ concrete, left
16    5  0.0725757   -12                  $ concrete, right
17    5  0.0725757   -13                  $ concrete, side
18    0               14                  $ outer void
c     =======================================================

c     =======================================================
c     =====> surface cards
c     =======================================================
c     =====> pin cell
1     RCC  0. 0. 0.  0. 0. 360.  0.44
2     RCC  0. 0. 0.  0. 0. 360.  0.49
3     RPP  -.7 .7  -.7 .7    0. 360.
c     =====> fuel & water elements
4     RPP  -10.5 10.5  -10.5 10.5   0. 360.
5     RPP  -13.  13.   -13.  13.    0. 360.
6     RPP  -13.5 13.5  -13.5 13.5   0. 360.
c     =====> full model
c     =====>   for ease in numbering the lattice elements,
c     =====>   pick the lower-left corner to be (13.5,13.5),
c     =====>   not (0,0). This shifts all other surfaces.
7     RPP  13.5 661.5   13.5  94.5    0. 360. $ box, elements
8     RPP  13.5 661.5   13.5  94.5  360. 390. $ water, top
9     RPP  13.5 661.5   13.5  94.5  -30.   0. $ water, bottom
10    RPP  13.5 661.5  -16.5  13.5  -30. 390. $ water, side
11    RPP -26.5  13.5  -16.5 134.5  -30. 390. $ concrete,left
12    RPP 661.5 701.5  -16.5 134.5  -30. 390. $ concrete,right
13    RPP  13.5 661.5   94.5 134.5  -30. 390. $ concrete, side
14    RPP -26.5 701.5  -16.5 134.5  -30. 390. $ outer boundary
c     =======================================================

c     =======================================================
c     =====> data cards for problem
c     =======================================================
kcode   10000    1.0  100  1100
imp:n    1 16r  0
c     =====> initial source guess
sdef erg=d1    cel=d2    x=d3    y=d4    z=d5
sp1  -3 .988 2.249      $ Watt spectrum, thermal u235 fission
sp2  D 1. 35r
si2  L    11:10(1 1 0):-5:4:1   11:10(3 1 0):-5:4:1
          11:10(5 1 0):-5:4:1   .....
          11:10(21 3 0):-5:4:1  11:10(23 3 0):-5:4:1
sp3  C 0. 1.
si3  H -10.5 10.5     $ sample x
sp4  C 0. 1.
si4  H -10.5 10.5     $ sample y
sp5  C 0. 1.
si5  H    0. 360.     $ sample z
c     =====> material cards
m1   92238 2.2380e-2   92235 8.2213e-4  8016 4.6054e-2  $ fuel
m2   40000 4.2910e-2                                    $ Zr
m3    1001 6.6706e-2    8016 3.3353e-2                  $ water
mt3   lwtr
m4   26000 8.3770e-2                                    $ Fe
m5    1001 5.5437e-3  6000 6.9793e-3 14000 7.7106e-3 $ concrete
     20000 8.9591e-3  8016 4.3383e-2
mt5   lwtr
c     =====> tallies:
f4:n  (1<4<5<10[  1 1 0,   3 1 0,   5 1 0,   7 1 0,   .....
                 17 3 0,  19 3 0,  21 3 0,  23 3 0 ]<11) T
fm4   0.06925613 1 -6
```

MCNP K-Eigenvalue Strategy

Initial source points:

- N points sampled with user-specified energy, space, angle distributions

For each generation:

- Renormalization: Total starting weight is N, number of starters may vary
- Histories:

At collisions, the probability of producing a fission neutron is $p = \frac{1}{K} \frac{\nu \Sigma_f}{\Sigma_t} \cdot W,$

where W = weight entering collision,
K = previous generation estimate of Keff

For n = floor(p), with probability p-n, n sites are banked
otherwise n+1 sites are banked

Keff estimators: collision, absorption, track-length, combined estimators

- Statistical Analysis: Many checks on results & uncertainty -- see below

Correlation & Monte Carlo Eigenvalue Calculations

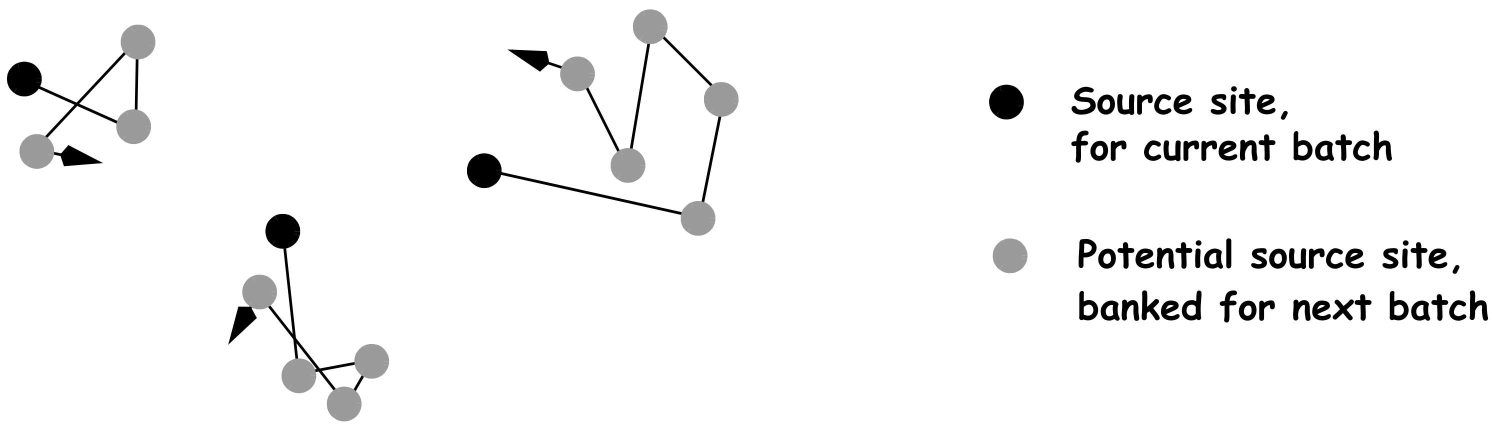
Successive batches are not independent

- Source for current batch depends on histories in last batch, ...

- Spatial correlation between batches can be important for:

  — Large reactors, with small leakage
  — Heavy-water moderated or reflected reactors

Computed variances are (usually) too small, due to batch-to-batch correlation



Approximate Corrections for Correlation

During the Monte Carlo calculation:

- Compute statistics in the "usual" manner: $\bar{x},\ \tilde{\sigma}_{\bar{x}}^2$

- Also compute batch-to-batch correlation coefficient, lag-1: $R_{x,1}$

Approximate corrections for correlation (~1972)

- To be conservative, corrections are applied only if they **increase** the variance

- Macmillan's prescription:

$$\sigma_{\bar{x}}^2 \approx \tilde{\sigma}_{\bar{x}}^2 \cdot \left[1 + \frac{2R_{x,1}}{1-\rho}\right]$$

- Gast's prescription

$$\sigma_{\bar{x}}^2 \approx \tilde{\sigma}_{\bar{x}}^2 \cdot \left[1 + \frac{10 \cdot R_{x,1}^2}{1-R_{x,1}}\right]$$

ρ = dominance ratio

$\tilde{\sigma}_{\bar{x}}^2$ = "apparent" variance

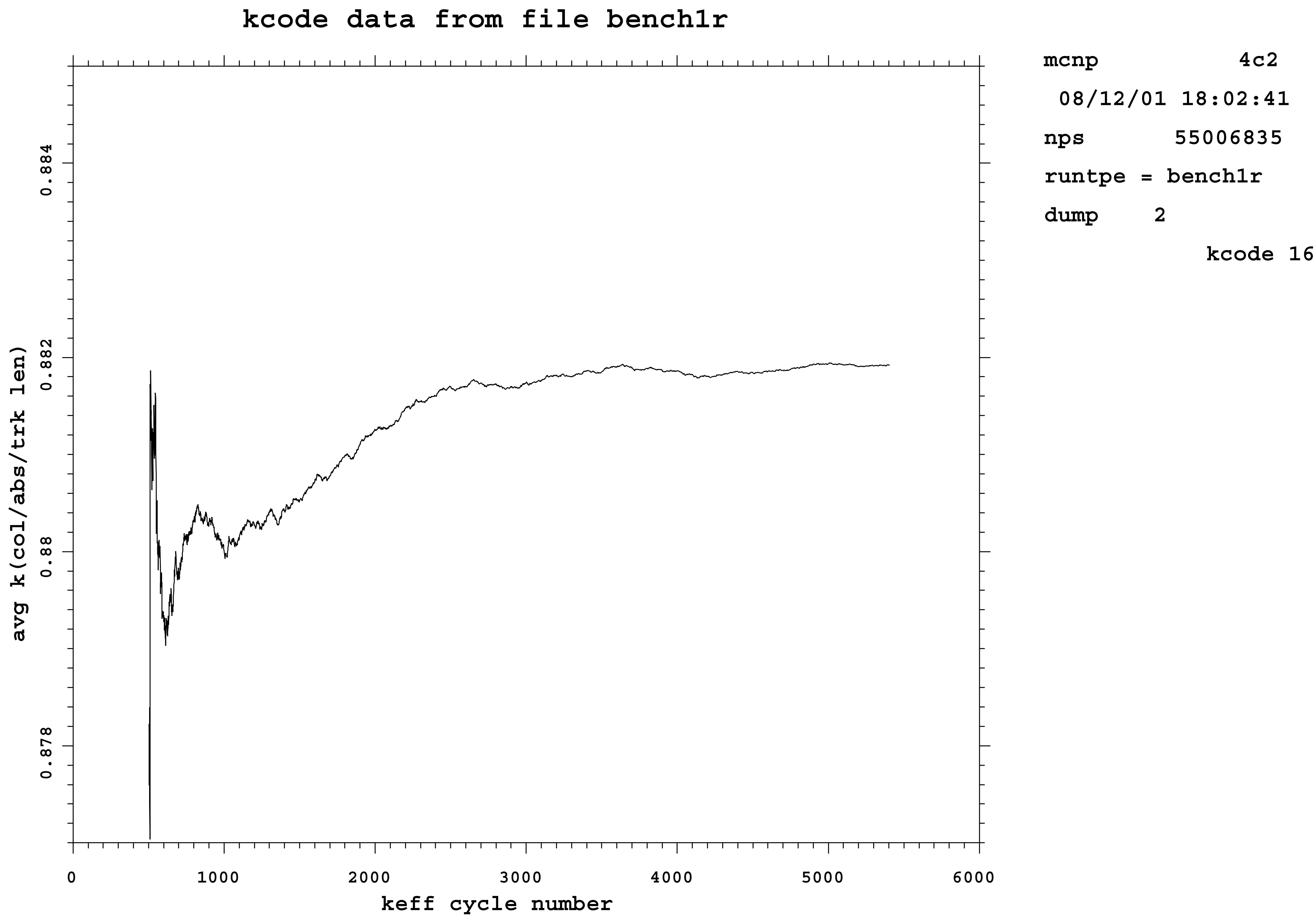
$R_{x,1}$ = serial correlation coeff., lag-1 in batch x's

References

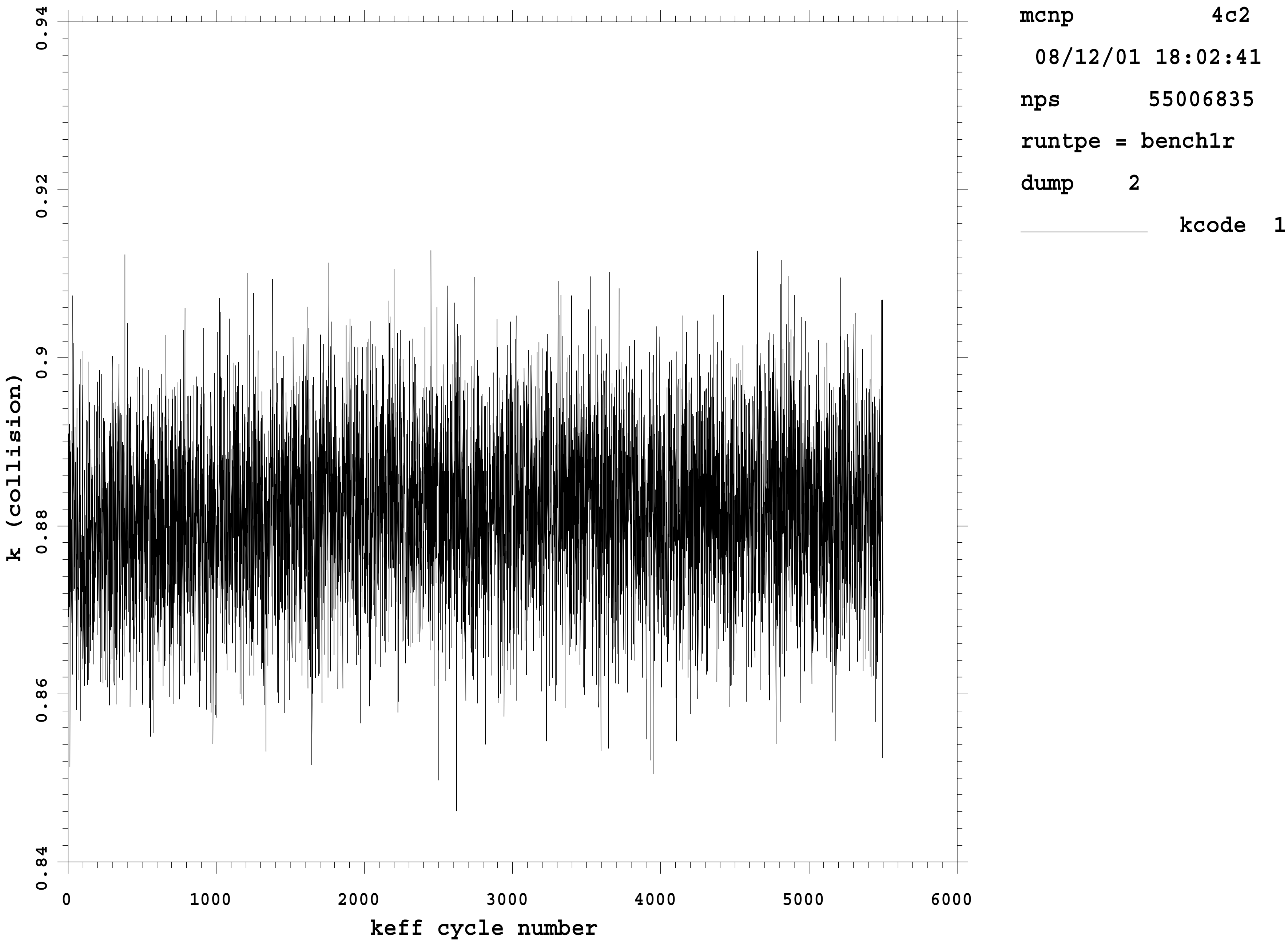
D. B. MacMillan,
"Monte Carlo Confidence Limits for Iterated-Source Calculations",
Nucl. Sci. Eng., **50**, 73-75 (1973).

R. C. Gast & N. R. Candelore,
"Monte Carlo Eigenfunction Strategies and Uncertainties",
ANL-75-2, 162-187 (1974).

MCNP Reference Case — Cumulative Keff(combined) vs Cycle



MCNP Reference Case — Keff(collision) vs Cycle



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Paris, France — 19 September 2001

Benchmark 2
Pincell Array with Irradiated Fuel

MCNP4C2 Calculations

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Los Alamos National Laboratory
<asood@lanl.gov>

Overview

- Problem description
- Summary of Criticality Convergence Features of MCNP
- Results
- Observations

Benchmark 2 — Pincell Array with Irradiated Fuel

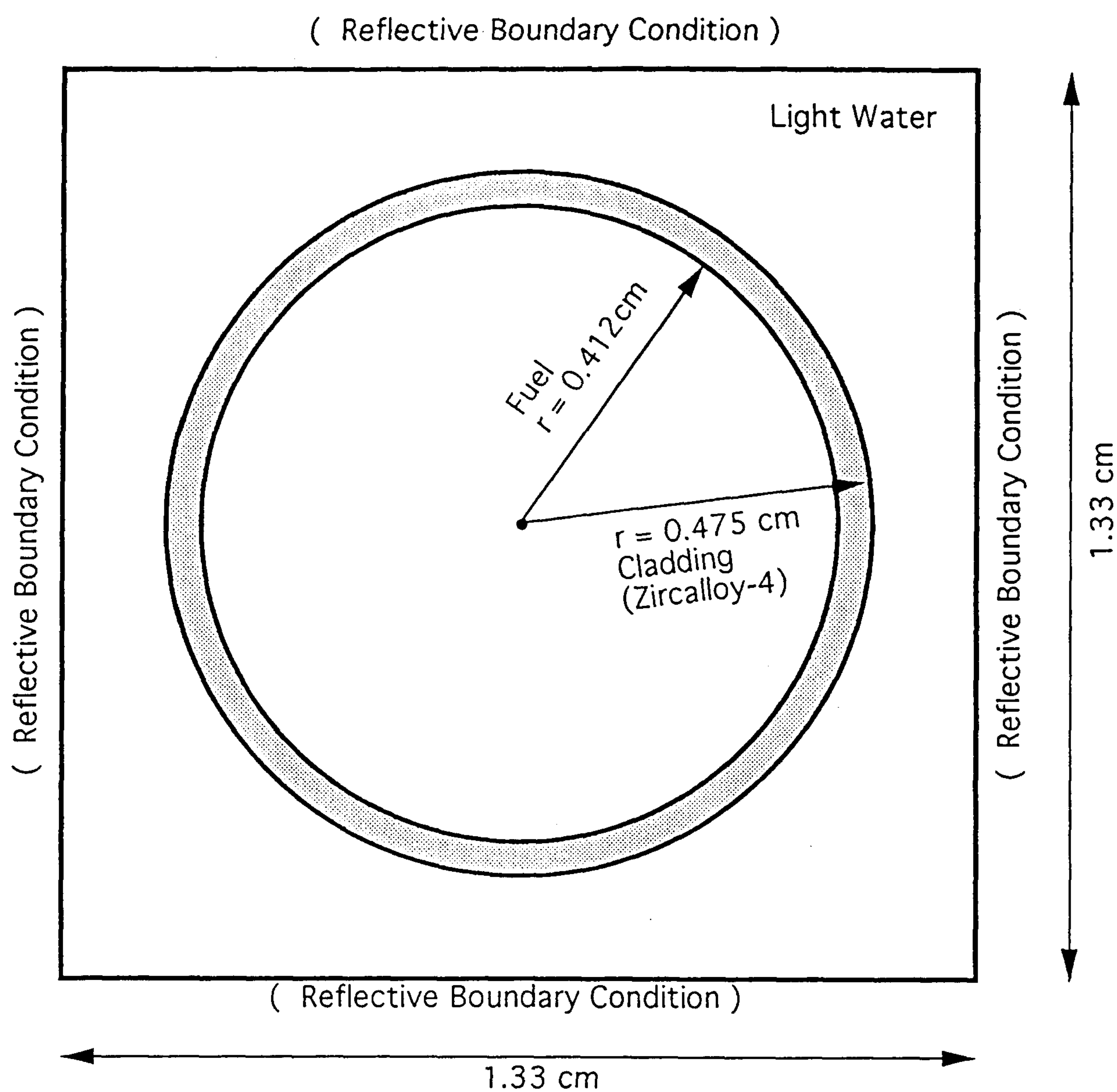
Contact:	Avneet Sood LANL, X-5 505-667-2119 asood@lanl.gov
Code:	**MCNP4C2**
Method:	continuous-energy Monte Carlo
Geometry:	exact, as specified
Cross-sections:	mixture of ENDF/B-V and ENDF/B-VI,
Computer:	SGI Origin-2000, using 4-10 processors
Date:	September, 2001

Benchmark 2 — Pincell Array with Irradiated Fuel

Material Compositions	MCNP Cross-sections
Fuel	
Fresh Fuel EU45 4.5%	LANL-proposed endf-VI.2
Fresh Fuel EU40 4.0%	LANL-proposed endf-VI.2
UO2 (natural)	LANL-proposed endf-VI.2
Irradiated fuel	ENDF-V
B21G 21.57 GWD/MTU	Mo-95,Ru-101,Rh-103,Sm-147,
B24G 24.023 GWD/MTU	Sm-149,Sm-150,Sm-151,Sm-152,
B30G 30.58 GWD/MTU	Nd-143,Nd-145
B40G 40.424 GWD/MTU	ENDF-VI.2
B55G 54.605 GWD/MTU	all other isotopes
Water	LANL-proposed endf-VI.2
	S(α,β) lwtr.01t (300 K)
Cladding and Endplug	
Zircalloy-4	ENDF-V -- Cr, Fe
	ENDF-VI.2 -- Zr

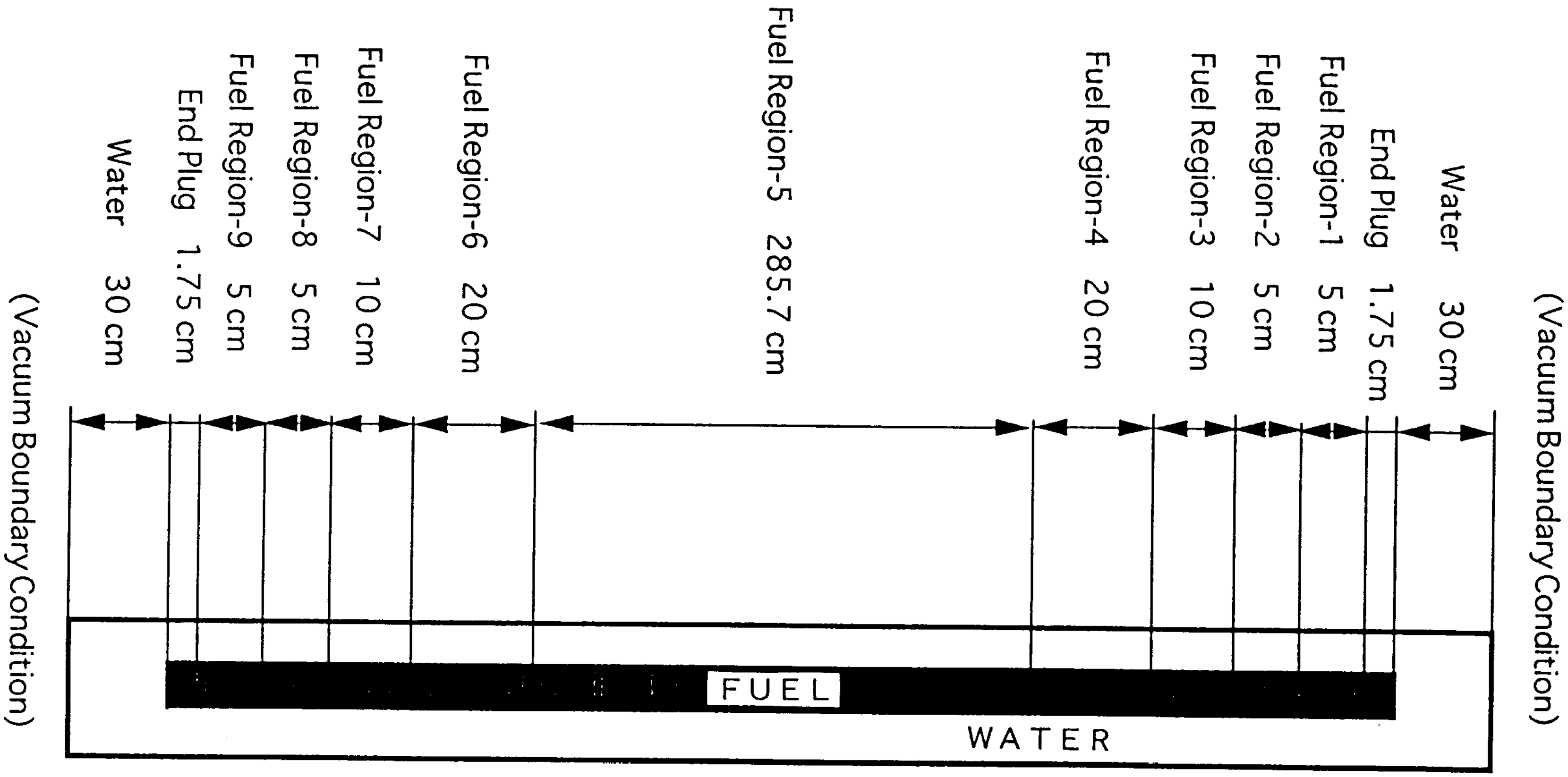
Benchmark 2 — Pincell Array with Irradiated Fuel

Top View



Benchmark 2 — Pincell Array with Irradiated Fuel

Side View:



Summary of Criticality Convergence Features of MCNP

keff Results Summary Table

Batched keff Tables

keff Results by Cycle, including plots

keff Results by Number of Cycles Skipped, including plots

keff Results Summary Table

Single page summary of calculations

Problem ID, definitions, termination

Were all fissionable cells sampled? - warnings

Normality checks of keff cycle data - warnings

Any trends in last 10 cycles?

Final boxed answer for combined keff (>30 active)

All 7 keff estimate results

Batched keff Table

Useful in examining cycle-to-cycle correlation in spatial source distribution

Collapsed cycle data by increasing batch size

Reports new keff averages, std. dev., and confidence intervals

Normality checks performed on batched results

keff Results by Cycle

List of 3 keff estimates and combined keff by cycle with std. dev.

FOM printed for combined keff

Largest/smallest active cycle results reported for each estimator

Plotted combined keff by cycle with std. dev.
User can visually detect trends in final answer.

keff Results by Number of Cycles Skipped

Reports keff, std. dev., combined keff,
and confidence intervals by cycles skipped

Normality checks on each

Cycle number of minimum std. dev. for
combined keff is listed

Combined keff for first and second half
of calculation compared -- warnings

Plotted combined keff by cycles skipped.
User can visually detect trends

Benchmark 2 — K-effective Results

Problem	keff	Std. Dev.
Case 1-1	1.34253	0.00006
Case 1-2	1.34223	0.00007
Case 1-3	1.34093	0.00006
Case 2-1	1.05324	0.00006
Case 2-2	1.05322	0.00006
Case 2-3	1.05271	0.00007

Benchmark 2 — Case 1-1 Fission Fraction Results

Case 1-1

Fuel Region	Fission Fraction	Rel. Err.
1	0.018755	0.00091
2	0.020270	0.00091
3	0.051246	0.00061
4	0.094811	0.00042
5	0.035885	0.00033
6	0.39925	0.00024
7	0.21574	0.00033
8	0.085150	0.00042
9	0.078897	0.00052

Benchmark 2 — Observations

K-effective Results

- 100000 neutrons/cycle, 1000 active cycles -- LONG SIMULATION TIME!
- MCNP4C2 performs 10 statistical tests on Keff results — warnings were given!

— **Problem 1-1**:

no trends visible in keff or in skipped cycles
small changes in confidence interval for batched results (0.00001)
minimum std. dev. occurs with 18 inactive cycles
1st and 2nd halves look normally distributed at 68% conf. level

— **Problem 1-2**:

*no trends visible in keff; visible trends in skipped cycles
small changes in confidence interval for batched results (0.00002)
*minimum std. dev. occurs with 227 inactive cycles
1st and 2nd halves look normally distributed at 68% conf. level

— **Problem 1-3**:

*Upward trend visible in keff; no visible trends in skipped cycles
small changes in confidence interval for batched results (0.00002)
minimum std. dev. occurs with 23 inactive cycles
*1st and 2nd halves look normally distributed at 99% conf. level

Benchmark 2 — Observations

K-effective Results - continued

— **Problem 2-1:**

no trends visible in keff or in skipped cycles
*some estimators are normally distributed at 99% confid. level
small changes in confidence interval for batched results (0.00001)
minimum std. dev. occurs with 53 inactive cycles
*1st and 2nd halves look normally distributed at 99% conf. level

— **Problem 2-2:**

*no trends visible in keff; visible trends in skipped cycles
*absorption estimator not normally distribued at 99% confid. level
small changes in confidence interval for batched results (0.00002)
minimum std. dev. occurs with 76 inactive cycles
1st and 2nd halves look normally distributed at 95% conf. level

— **Problem 2-3:**

*Upward trend visible in keff; no visible trends in skipped cycles
small changes in confidence interval for batched results (0.00002)
batched results not normally distributed at 99% conf. level
*minimum std. dev. occurs with 278 inactive cycles
*1st and 2nd halves not normally distributed at 99% conf. level

Benchmark 2 — Observations

Fission Distribution

- MCNP4C2 performs 10 statistical tests on selected tallies, which for these problems applied to the fuel element fission rates:
  - Cases 1-1: missed 1 statistical test -- FOM not constant
  - Cases 1-2: missed 1 statistical test -- trends in last half of answer
  - Cases 1-3: missed 4 statistical test -- trends in last half of answer
  - Cases 2-1: passed all statistical tests
  - Cases 2-2: missed 6 statistical tests -- large relative error, slope, etc
  - Cases 2-3: missed 5 statistical tests -- trends in last half of answer

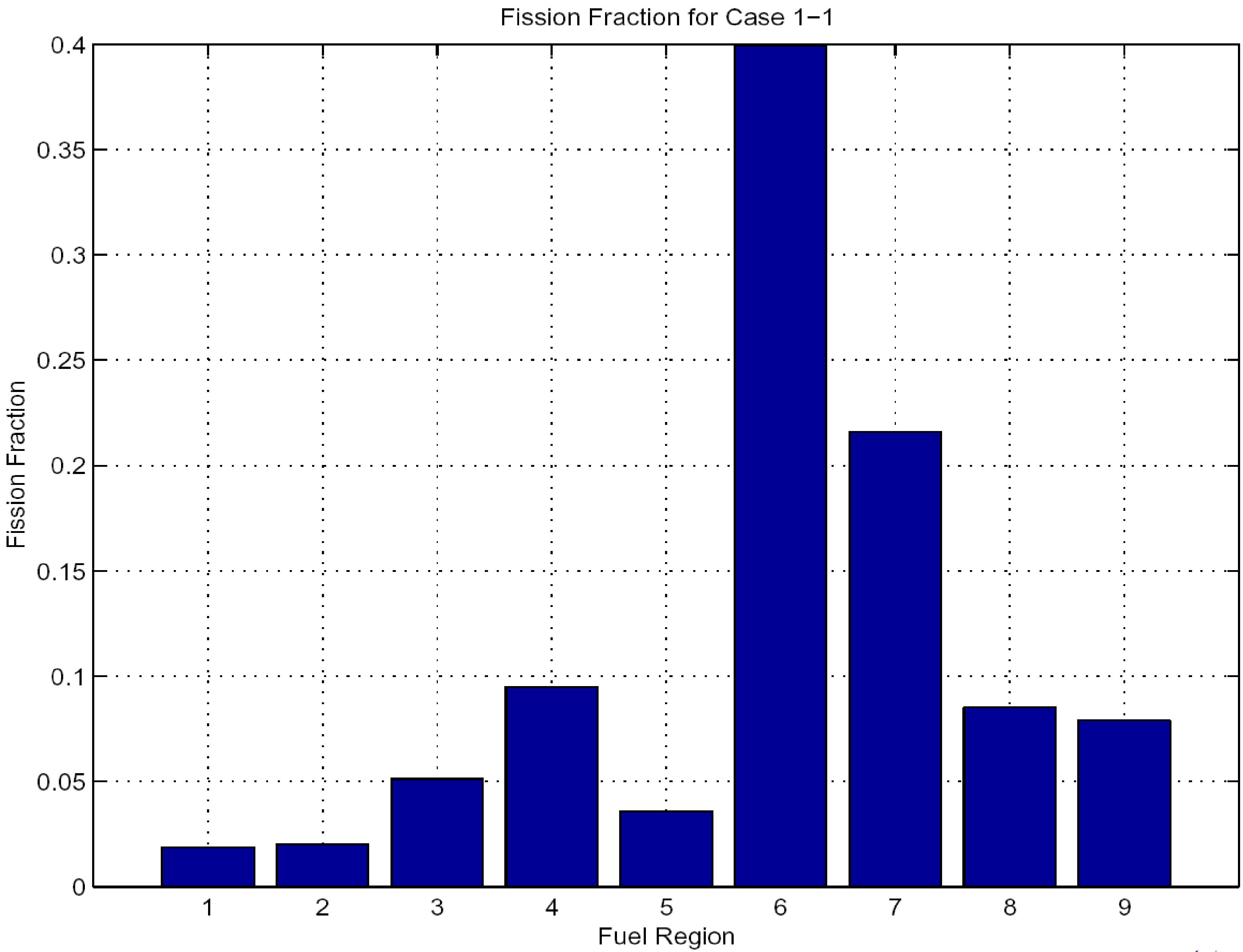
Date:	September 2001
Institution:	MCNP Team, Diagnostic Applications Group (X-5), Los Alamos National Laboratory
Contact person:	Avneet Sood
E-mail address:	asood@lanl.gov
Voice phone number:	505.667.2119
FAX phone number:	505.665.3046
Problem name:	OECD/NEA Source Convergence Benchmark 2: Pincell array with irradiated fuel
Case name:	Case 1_1
Code name:	MCNP4C2
Code type:	Monte Carlo
Cross Section Library:	ENDF-V and ENDF-VI
Starting source:	uniform volume sampling in fuel region
nskip:	200 inactive cycles
ngen:	1000 active cycles
nhist:	100000 histories per cycle
ngensh:	1
final k-eff estimate:	1.34253
final est. uncert. (1 sigma):	0.00006

Fuel Region	Volume (cm^3)	Sigma_f*flux (fissions/cm^3)	Rel. Err.	Flux (neut/cm^3)	Rel. Err.
1	2.66633E+00	8.9753e-03	9.0000e-04	5.1087e-02	6.0000e-04
2	2.66633E+00	9.7004e-03	9.0000e-04	6.8213e-02	5.0000e-04
3	5.33267E+00	1.2262e-02	6.0000e-04	8.6154e-02	4.0000e-04
4	1.06653E+01	1.1343e-02	4.0000e-04	7.8145e-02	3.0000e-04
5	1.52354E+02	3.0054e-04	3.0000e-04	1.1089e-02	3.0000e-04
6	1.06653E+01	4.7766e-02	2.0000e-04	3.2914e-01	1.0000e-04
7	5.33267E+00	5.1621e-02	3.0000e-04	3.6253e-01	2.0000e-04
8	2.66633E+00	4.0749e-02	4.0000e-04	2.8673e-01	3.0000e-04
9	2.66633E+00	3.7757e-02	5.0000e-04	2.1482e-01	3.0000e-04

Fission fractions averaged over all active generations:

Fuel Region	Fission Fraction	Relative Error
1	1.8755e-02	9.0906e-04
2	2.0270e-02	9.0906e-04
3	5.1246e-02	6.1351e-04
4	9.4811e-02	4.2000e-04
5	3.5885e-02	3.2619e-04
6	3.9925e-01	2.3748e-04
7	2.1574e-01	3.2619e-04
8	8.5150e-02	4.2000e-04
9	7.8897e-02	5.1614e-04

Case 1-1



Fission Fraction for Case 1−1
Fission Fraction
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
1
2
3
4
5
6
7
8
9
Fuel Region

Date:	September 2001
Institution:	MCNP Team, Diagnostic Applications Group (X-5), Los Alamos National Laboratory
Contact person:	Avneet Sood
E-mail address:	asood@lanl.gov
Voice phone number:	505.667.2119
FAX phone number:	505.665.3046
Problem name:	OECD/NEA Source Convergence Benchmark 2: Pincell array with irradiated fuel
Case name:	Case 1_2
Code name:	MCNP4C2
Code type:	Monte Carlo
Cross Section Library:	ENDF-V and ENDF-VI
Starting source:	uniform volume sampling in fuel region
nskip:	200 inactive cycles
ngen:	1000 active cycles
nhist:	100000 histories per cycle
ngensh:	1
final k-eff estimate:	1.34223
final est. uncert. (1 sigma):	0.00007

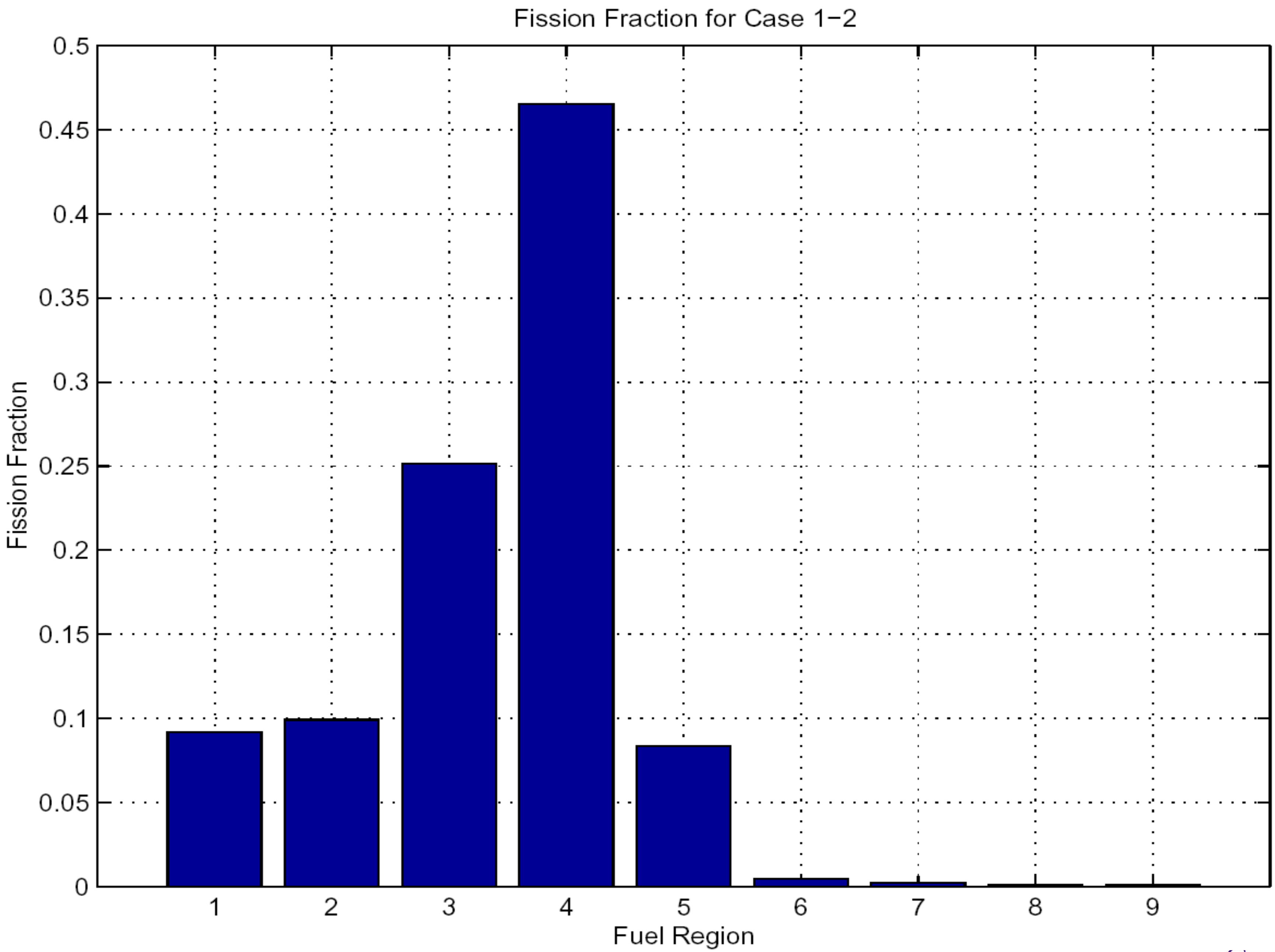
Fuel Region	Volume (cm^3)	Sigma_f*flux (fissions/cm^3)	Rel. Err.	Flux (neut/cm^3)	Rel. Err.
1	2.66633E+00	1.8909e-02	4.0000e-04	2.6308e-01	3.0000e-04
2	2.66633E+00	2.0387e-02	4.0000e-04	3.5128e-01	2.0000e-04
3	5.33267E+00	2.5822e-02	2.0000e-04	4.4409e-01	2.0000e-04
4	1.06653E+01	2.3911e-02	2.0000e-04	4.0341e-01	1.0000e-04
5	1.52354E+02	3.0061e-04	3.0000e-04	1.1090e-02	3.0000e-04
6	1.06653E+01	2.3334e-04	2.0000e-03	4.0674e-03	1.5000e-03
7	5.33267E+00	2.5209e-04	2.7000e-03	4.4662e-03	1.8000e-03
8	2.66633E+00	1.9900e-04	3.9000e-03	3.5459e-03	2.5000e-03
9	2.66633E+00	1.8385e-04	4.2000e-03	2.6503e-03	2.9000e-03

Fission fractions averaged over all active generations:

Fuel Region	Fission Fraction	Relative Error
1	9.1980e-02	4.1820e-04
2	9.9166e-02	4.1820e-04
3	2.5121e-01	2.3429e-04
4	4.6524e-01	2.3429e-04
5	8.3553e-02	3.2387e-04
6	4.5401e-03	2.0037e-03
7	2.4524e-03	2.7028e-03
8	9.6797e-04	3.9019e-03
9	8.9428e-04	4.2018e-03

Case 1-2

Case 1-2



Fission Fraction for Case 1−2
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
Fission Fraction
1
2
3
4
5
6
7
8
9
Fuel Region

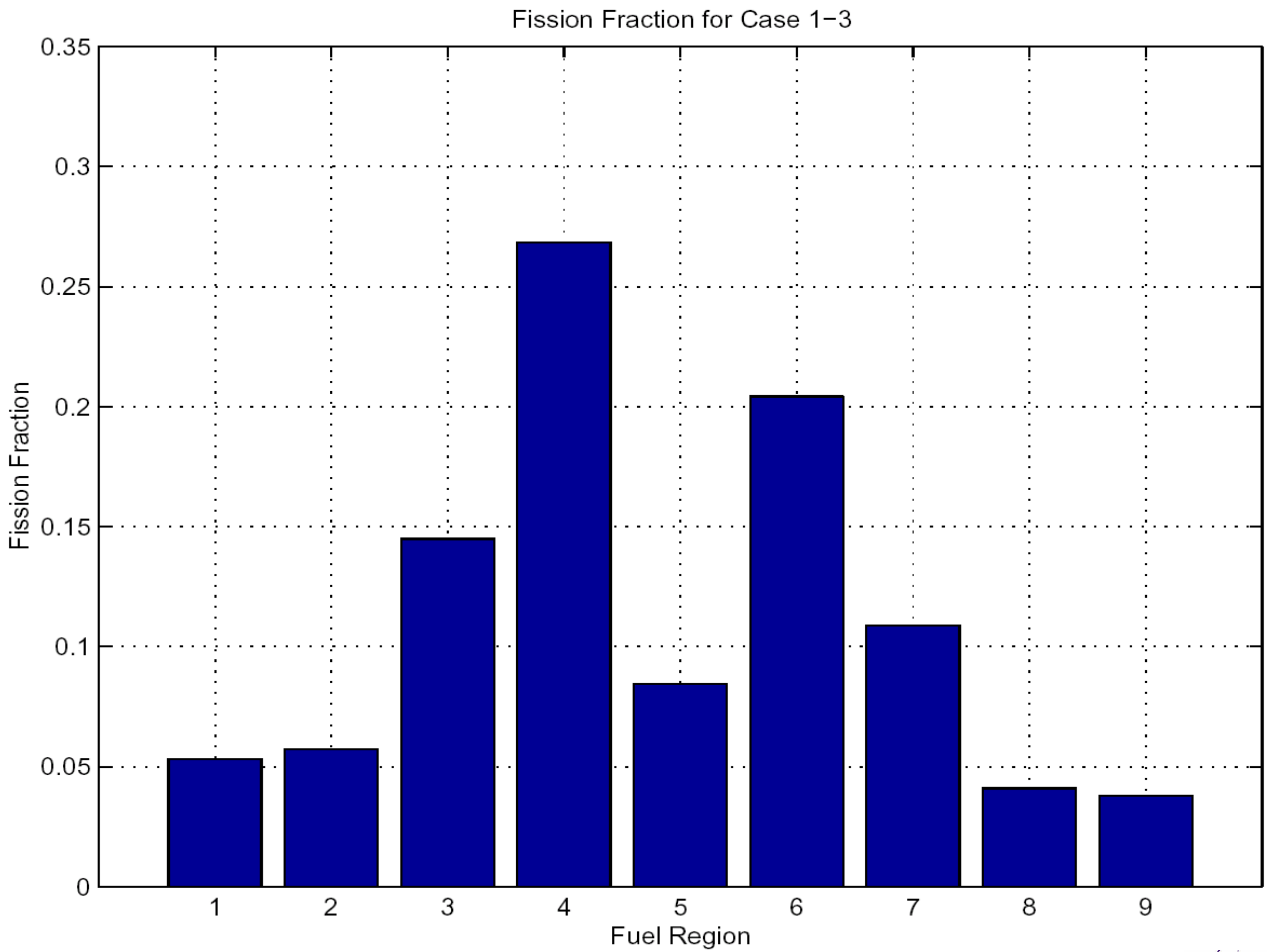
Date:	September 2001
Institution:	MCNP Team, Diagnostic Applications Group (X-5), Los Alamos National Laboratory
Contact person:	Avneet Sood
E-mail address:	asood@lanl.gov
Voice phone number:	505.667.2119
FAX phone number:	505.665.3046
Problem name:	OECD/NEA Source Convergence Benchmark 2: Pincell array with irradiated fuel
Case name:	Case 1_3
Code name:	MCNP4C2
Code type:	Monte Carlo
Cross Section Library:	ENDF-V and ENDF-VI
Starting source:	uniform volume sampling in fuel region
nskip:	200 inactive cycles
ngen:	1000 active cycles
nhist:	100000 histories per cycle
ngensh:	1
final k-eff estimate:	1.34093
final est. uncert. (1 sigma):	0.00006

Fuel Region	Volume (cm^3)	Sigma_f*flux (fissions/cm^3)	Rel. Err.	Flux (neut/cm^3)	Rel. Err.
1	2.66633E+00	1.0904e-02	5.0000e-04	1.5158e-01	4.0000e-04
2	2.66633E+00	1.1726e-02	5.0000e-04	2.0213e-01	3.0000e-04
3	5.33267E+00	1.4873e-02	3.0000e-04	2.5583e-01	2.0000e-04
4	1.06653E+01	1.3784e-02	2.0000e-04	2.3262e-01	2.0000e-04
5	1.52354E+02	3.0356e-04	3.0000e-04	1.1205e-02	3.0000e-04
6	1.06653E+01	1.0488e-02	3.0000e-04	1.7709e-01	2.0000e-04
7	5.33267E+00	1.1181e-02	4.0000e-04	1.9180e-01	3.0000e-04
8	2.66633E+00	8.4061e-03	6.0000e-04	1.5014e-01	4.0000e-04
9	2.66633E+00	7.7616e-03	6.0000e-04	1.1159e-01	4.0000e-04

Fission fractions averaged over all active generations:

Fuel Region	Fission Fraction	Relative Error
1	5.3102e-02	5.1352e-04
2	5.7106e-02	5.1352e-04
3	1.4486e-01	3.2204e-04
4	2.6851e-01	2.3175e-04
5	8.4474e-02	3.2204e-04
6	2.0431e-01	3.2204e-04
7	1.0891e-01	4.1678e-04
8	4.0938e-02	6.1132e-04
9	3.7800e-02	6.1132e-04

Case 1-3



Los Alamos NATIONAL LABORATORY

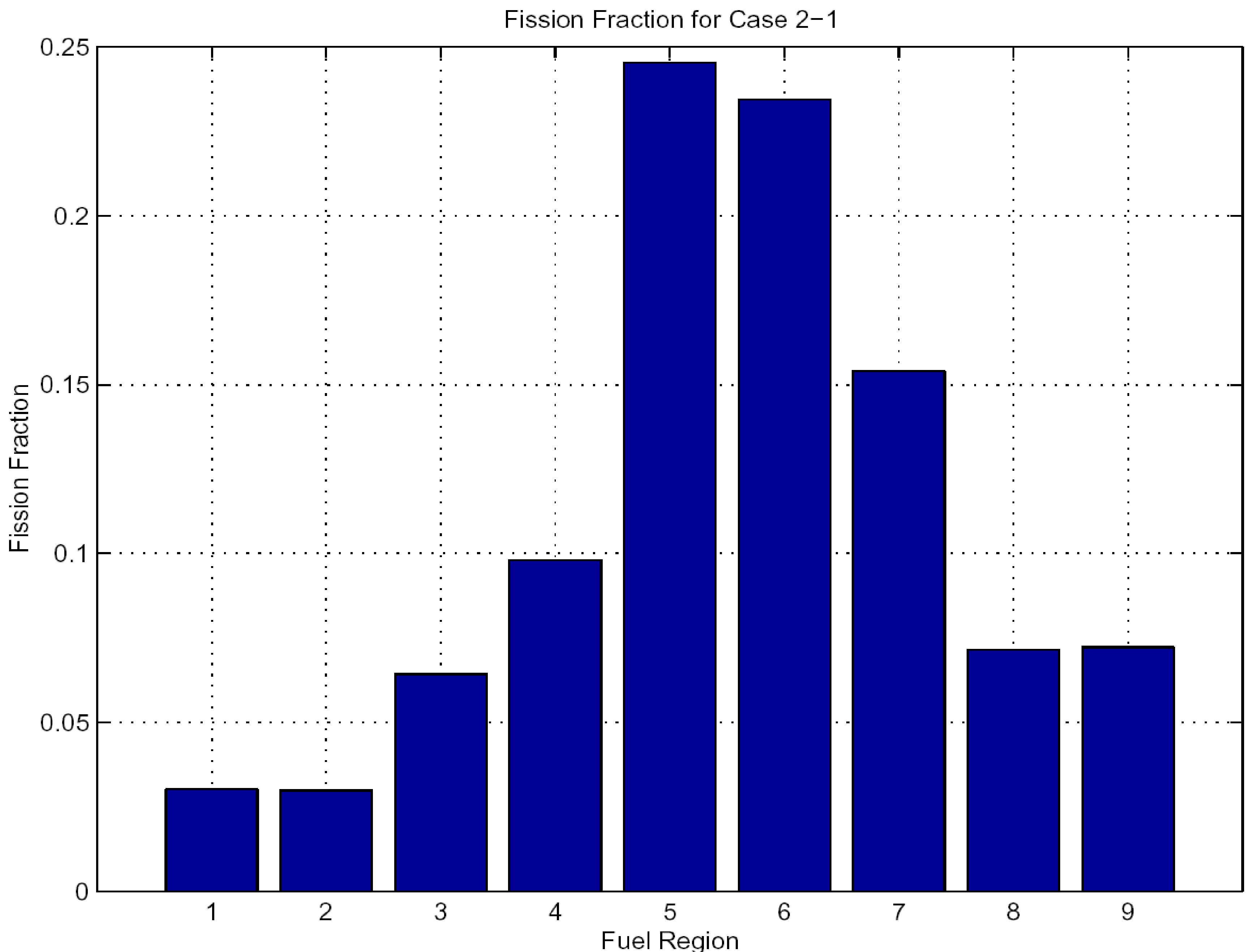
Date: September 2001
Institution: MCNP Team, Diagnostic Applications Group (X-5), Los Alamos National Laboratory
Contact person: Avneet Sood
E-mail address: asood@lanl.gov
Voice phone number: 505.667.2119
FAX phone number: 505.665.3046
Problem name: OECD/NEA Source Convergence Benchmark 2: Pincell array with irradiated fuel
Case name: Case 2_1
Code name: MCNP4C2
Code type: Monte Carlo
Cross Section Library: ENDF-V and ENDF-VI
Starting source: uniform volume sampling in fuel region
nskip: 200 inactive cycles
ngen: 1000 active cycles
nhist: 100000 histories per cycle
ngensh: 1
final k-eff estimate: 1.05324
final est. uncert. (1 sigma): 0.00006

Fuel Region	Volume (cm^3)	Sigma_f*flux (fissions/cm^3)	Rel. Err.	Flux (neut/cm^3)	Rel. Err.
1	2.66633E+00	4.4698e-03	8.0000e-04	7.8073e-02	5.0000e-04
2	2.66633E+00	4.4202e-03	8.0000e-04	9.8097e-02	5.0000e-04
3	5.33267E+00	4.7628e-03	5.0000e-04	1.1137e-01	4.0000e-04
4	1.06653E+01	3.6306e-03	4.0000e-04	9.2234e-02	3.0000e-04
5	1.52354E+02	6.3539e-04	2.0000e-04	1.8167e-02	2.0000e-04
6	1.06653E+01	8.6776e-03	3.0000e-04	2.2049e-01	2.0000e-04
7	5.33267E+00	1.1394e-02	3.0000e-04	2.6655e-01	2.0000e-04
8	2.66633E+00	1.0571e-02	5.0000e-04	2.3473e-01	3.0000e-04
9	2.66633E+00	1.0694e-02	5.0000e-04	1.8697e-01	3.0000e-04

Fission fractions averaged over all active generations:

Fuel Region	Fission Fraction	Relative Error
1	3.0199e-02	8.0982e-04
2	2.9864e-02	8.0982e-04
3	6.4358e-02	5.1556e-04
4	9.8118e-02	4.1929e-04
5	2.4530e-01	2.3622e-04
6	2.3452e-01	3.2527e-04
7	1.5397e-01	3.2527e-04
8	7.1423e-02	5.1556e-04
9	7.2254e-02	5.1556e-04

Case 2-1



Fission Fraction for Case 2−1
Fission Fraction
Fuel Region
0.25
0.2
0.15
0.1
0.05
0
1
2
3
4
5
6
7
8
9

Date:	September 2001
Institution:	MCNP Team, Diagnostic Applications Group (X-5), Los Alamos National Laboratory
Contact person:	Avneet Sood
E-mail address:	asood@lanl.gov
Voice phone number:	505.667.2119
FAX phone number:	505.665.3046
Problem name:	OECD/NEA Source Convergence Benchmark 2: Pincell array with irradiated fuel
Case name:	Case 2_2
Code name:	MCNP4C2
Code type:	Monte Carlo
Cross Section Library:	ENDF-V and ENDF-VI
Starting source:	uniform volume sampling in fuel region
nskip:	200 inactive cycles
ngen:	1000 active cycles
nhist:	100000 histories per cycle
ngensh:	1
final k-eff estimate:	1.05322
final est. uncert. (1 sigma):	0.00006

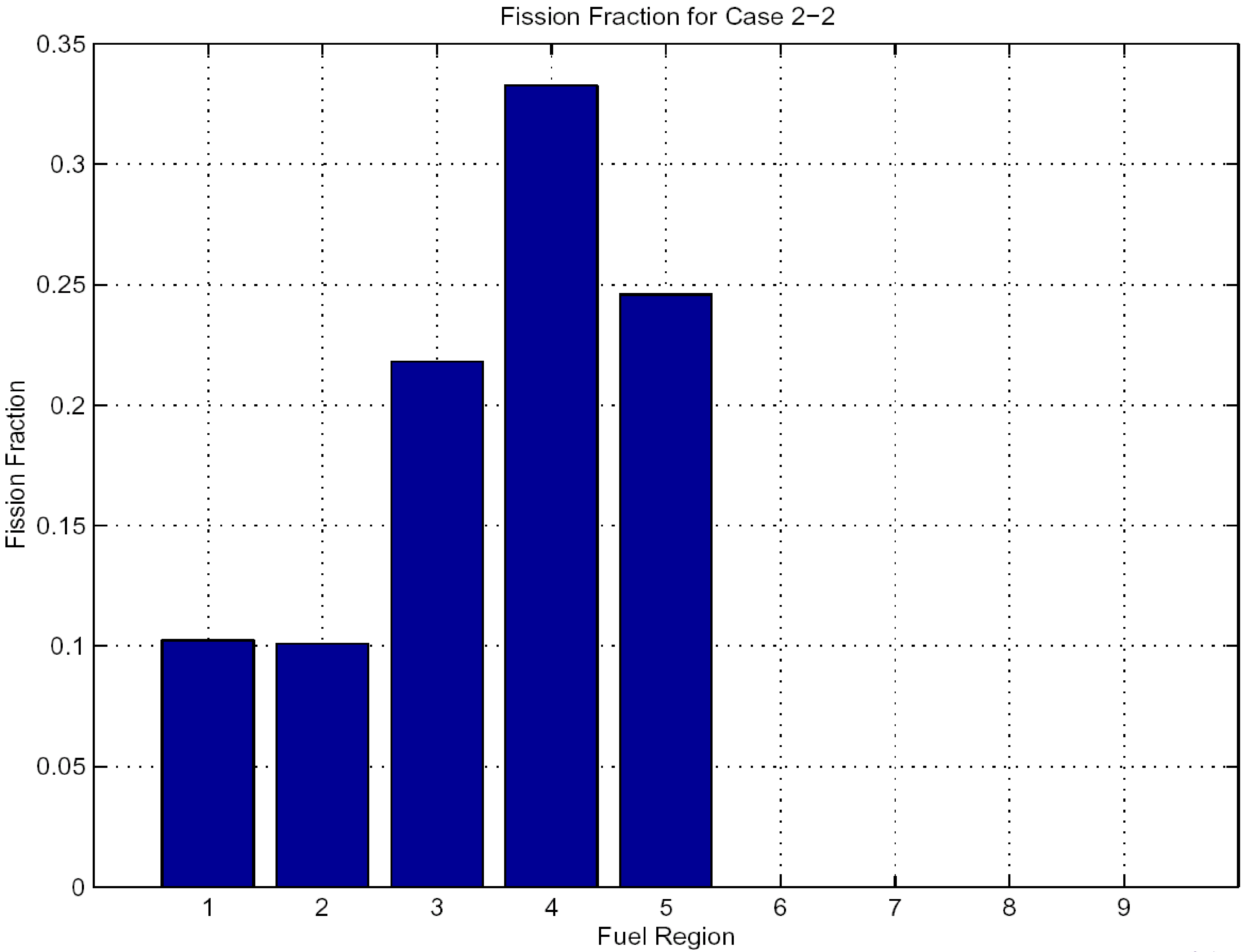
Fuel Region	Volume (cm^3)	Sigma_f*flux (fissions/cm^3)	Rel. Err.	Flux (neut/cm^3)	Rel. Err.
1.	2.66633E+00	1.5151e-02	4.0000e-04	2.6478e-01	3.0000e-04
2.	2.66633E+00	1.4952e-02	4.0000e-04	3.3221e-01	2.0000e-04
3.	5.33267E+00	1.6131e-02	3.0000e-04	3.7738e-01	2.0000e-04
4.	1.06653E+01	1.2306e-02	2.0000e-04	3.1259e-01	1.0000e-04
5.	1.52354E+02	6.3708e-04	2.0000e-04	1.8214e-02	2.0000e-04
6.	1.06653E+01	1.2237e-07	7.1700e-02	3.3150e-06	5.4100e-02
7.	5.33267E+00	1.0422e-07	1.0240e-01	2.7669e-06	7.3700e-02
8.	2.66633E+00	1.1761e-07	1.4310e-01	2.4484e-06	9.0400e-02
9.	2.66633E+00	1.1340e-07	1.5300e-01	1.9085e-06	1.0320e-01

Fission fractions averaged over all active generations:

Fuel Region	Fission Fraction	Relative Error
1.	1.0238e-01	4.1765e-04
2.	1.0103e-01	4.1765e-04
3.	2.1800e-01	3.2316e-04
4.	3.3262e-01	2.3331e-04
5.	2.4597e-01	2.3331e-04
6.	3.3073e-06	7.1700e-02
7.	1.4084e-06	1.0240e-01
8.	7.9468e-07	1.4310e-01
9.	7.6624e-07	1.5300e-01

Case 2-2

Case 2-2



Fission Fraction for Case 2−2
Fission Fraction
Fuel Region
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
1
2
3
4
5
6
7
8
9

Date:	September 2001
Institution:	MCNP Team, Diagnostic Applications Group (X-5), Los Alamos National Laboratory
Contact person:	Avneet Sood
E-mail address:	asood@lanl.gov
Voice phone number:	505.667.2119
FAX phone number:	505.665.3046
Problem name:	OECD/NEA Source Convergence Benchmark 2: Pincell array with irradiated fuel
Case name:	Case 2_3
Code name:	MCNP4C2
Code type:	Monte Carlo
Cross Section Library:	ENDF-V and ENDF-VI
Starting source:	uniform volume sampling in fuel region
nskip:	200 inactive cycles
ngen:	1000 active cycles
nhist:	100000 histories per cycle
ngensh:	1
final k-eff estimate:	1.05271
final est. uncert. (1 sigma):	0.00007

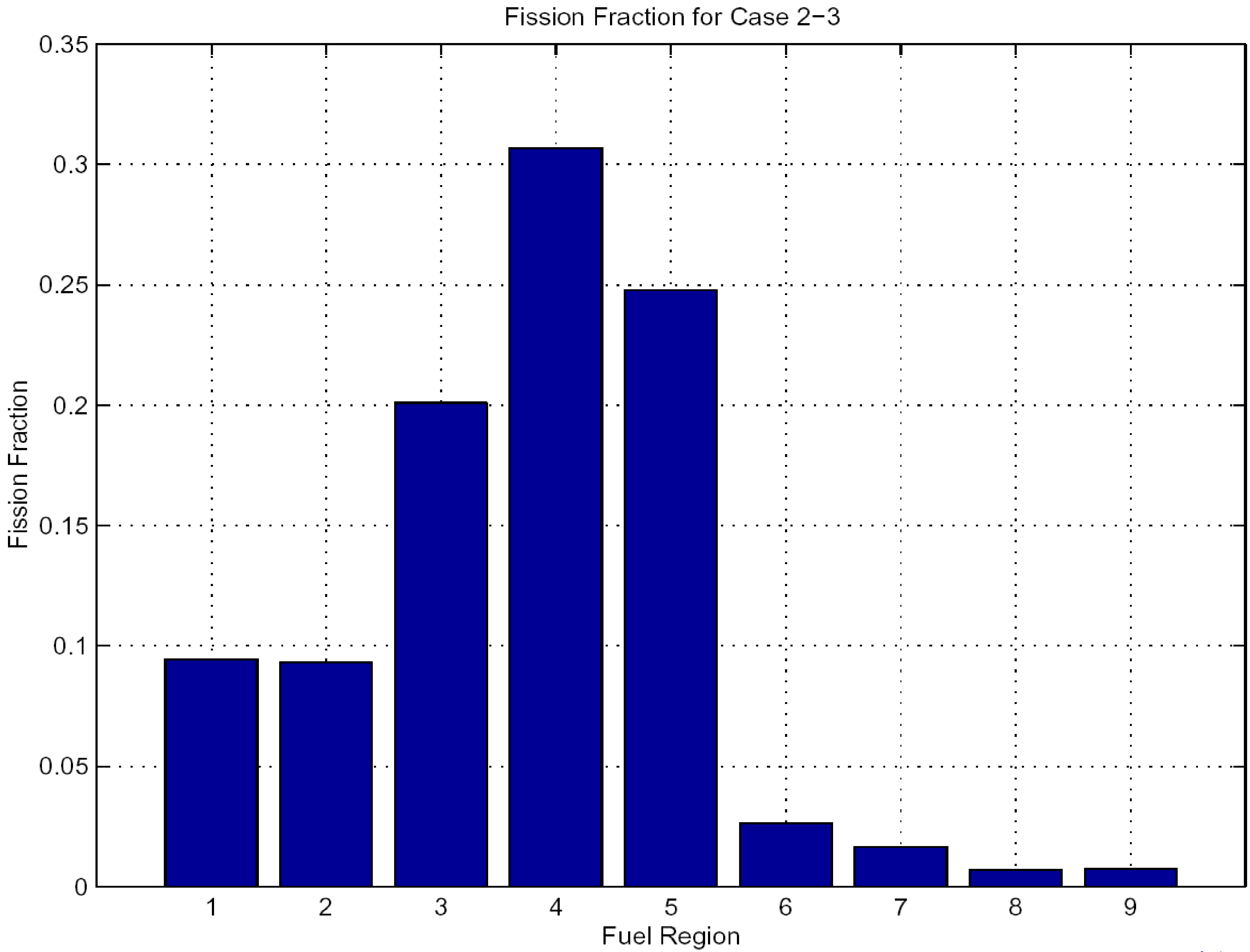
Fuel Region	Volume (cm^3)	Sigma_f*flux (fissions/cm^3)	Rel. Err.	Flux (neut/cm^3)	Rel. Err.
1	2.66633E+00	1.3953e-02	4.0000e-04	2.4381e-01	3.0000e-04
2	2.66633E+00	1.3771e-02	4.0000e-04	3.0593e-01	2.0000e-04
3	5.33267E+00	1.4860e-02	3.0000e-04	3.4765e-01	2.0000e-04
4	1.06653E+01	1.1342e-02	2.0000e-04	2.8815e-01	1.0000e-04
5	1.52354E+02	6.4107e-04	2.0000e-04	1.8330e-02	2.0000e-04
6	1.06653E+01	9.7884e-04	8.0000e-04	2.4904e-02	6.0000e-04
7	5.33267E+00	1.2223e-03	1.1000e-03	2.8567e-02	7.0000e-04
8	2.66633E+00	1.0248e-03	1.5000e-03	2.4158e-02	9.0000e-04
9	2.66633E+00	1.0664e-03	1.6000e-03	1.9048e-02	1.1000e-03

Fission fractions averaged over all active generations:

Fuel Region	Fission Fraction	Relative Error
1	9.4344e-02	4.1675e-04
2	9.3117e-02	4.1675e-04
3	2.0096e-01	3.2200e-04
4	3.0675e-01	2.3170e-04
5	2.4768e-01	2.3170e-04
6	2.6474e-02	8.0851e-04
7	1.6529e-02	1.1062e-03
8	6.9293e-03	1.5046e-03
9	7.2106e-03	1.6043e-03

Case 2-3

Case 2-3


Fission Fraction for Case 2−3
Fission Fraction
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
1
2
3
4
5
6
7
8
9
Fuel Region

Benchmark 3
Three Thick 1D Slabs

MCNP Calculations

Robert C. Little

Diagnostics Applications Group (X-5)
Los Alamos National Laboratory
<rcl@lanl.gov>

D. Kent Parsons

Primary Design & Assessment (X-4)
Los Alamos National Laboratory
<dkp@lanl.gov>

Outline

- Problem description
- Results
- MCNP input
- Plots
  - — Onedant Results: K-effective vs Asymmetry
  - — Onedant Results: Fission Fractions vs Asymmetry
  - — Onedant & MCNP: K-effective for 30 cm Reflector
  - — Onedant & MCNP: K-effective for 20 cm Reflector
  - — Onedant & MCNP: K-effective for 10 cm Reflector
- Onedant & MCNP Results

Benchmark 3 — Three Thick 1D Slabs

Contact: Robert C. Little
LANL, X-5
505-665-3487
rcl@lanl.gov

Code: **MCNP4C2**

Method: continuous-energy Monte Carlo

Geometry: exact, as specified

Cross-sections: ENDF/B-VI, processed by NJOY into MCNP library

Computer: Sun workstation

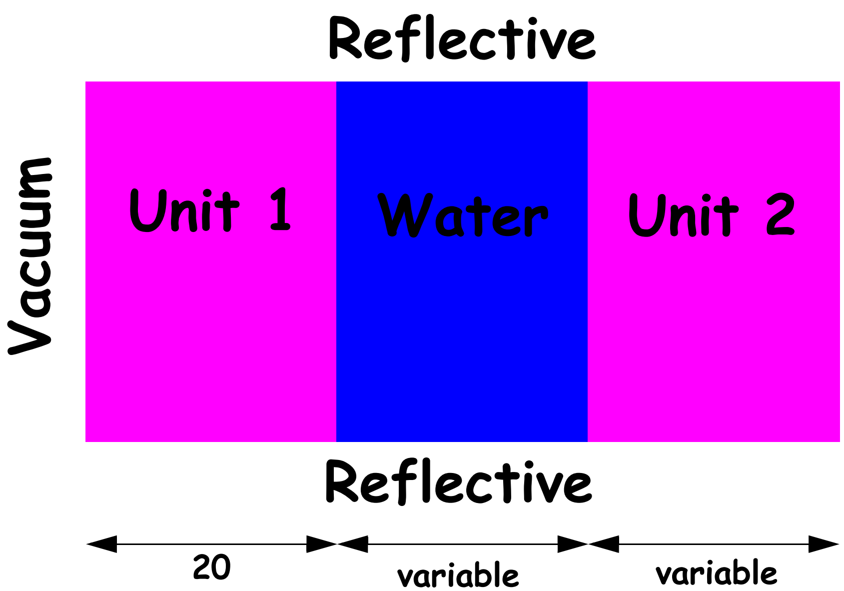
Date: August, 2001

Benchmark 3 — Three Thick 1D Slabs

Material Compositions		MCNP Cross-sections	
Uranyl Solution			
U235	7.6864e-5	92235.60c,	LANL-proposed endf-VI.2
U238	6.8303e-4	92238.60c,	endf-VI.2
O	3.7258e-2	8016.60c	
H	5.9347e-2	1001.60c,	with $S(\alpha,\beta)$ lwtr.01t
N	2.1220e-3	7014.60c	
Water			
H	6.6706e-2	1001.60c,	with $S(\alpha,\beta)$ lwtr.01t
O	3.3353e-2	8016.60c	

Benchmark 3 — Three Thick 1D Slabs

Case	Unit 1	Unit 2	Water
	----------Thickness----------		
1	20	20	30
2	20	18	30
3	20	15	30
4	20	12	30
5	20	20	20
6	20	18	20
7	20	15	20
8	20	12	20
9	20	20	10
10	20	18	10
11	20	15	10
12	20	12	10



2000 neutrons/generation
50 generations skipped before tallies
550 active generations
uniform initial source distribution

All dimensions in cm

MCNP Continuous-Energy Results for 12 Cases

F1 = fraction of fission neutrons in slab 1

Case	T1	T2	T3	k_{eff}	Std Dev	F1
1	20	30	20	0.91890	0.00060	0.42155
2	20	30	18	0.91731	0.00061	0.95262
3	20	30	15	0.91674	0.00061	0.98654
4	20	30	12	0.91638	0.00063	0.99273
5	20	20	20	0.92641	0.00059	0.45389
6	20	20	18	0.91900	0.00062	0.83481
7	20	20	15	0.91772	0.00059	0.93144
8	20	20	12	0.91587	0.00060	0.96340
9	20	10	20	0.97089	0.00056	0.48885
10	20	10	18	0.95683	0.00057	0.61508
11	20	10	15	0.94182	0.00057	0.74493
12	20	10	12	0.93467	0.00058	0.83132

Additional MCNP Calculations with One Fissile Region Only

30 cm H_2O

Case	T1	T2	T3	k_{eff}	Std Dev	F1
1	20	30	20	0.91890	0.00060	0.42155
2	20	30	18	0.91731	0.00061	0.95262
2L	20	30	0	0.91648	0.00061	1
2R	0	30	18	0.87143	0.00061	0
3	20	30	15	0.91674	0.00061	0.98654
3R	0	30	15	0.78929	0.00060	0
4	20	30	12	0.91638	0.00063	0.99273

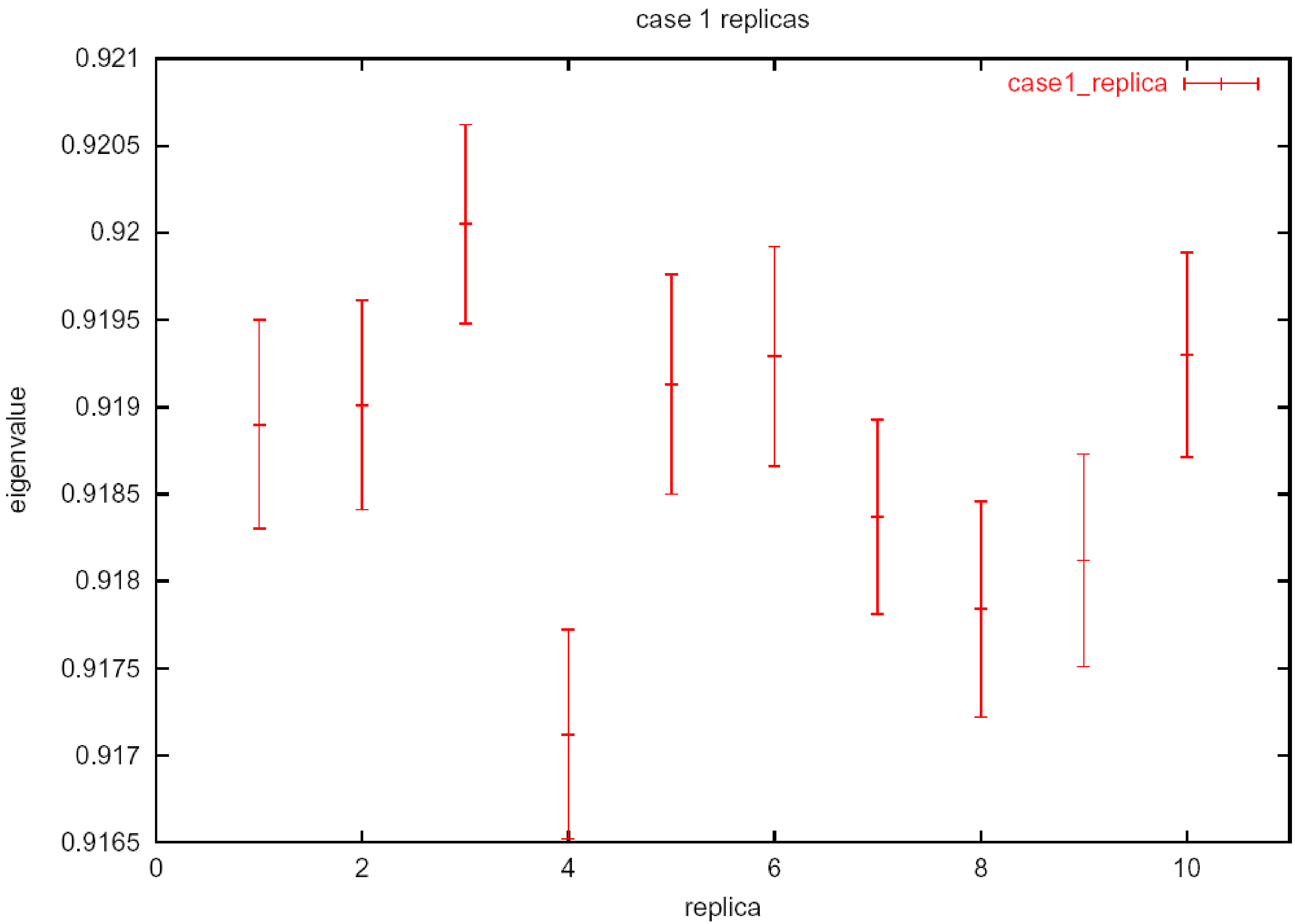
Focus on the Symmetric Cases

Case	T1	T2	T3	k_{eff}	Std Dev	F1
1	20	30	20	0.91890	0.00060	0.42155
2	20	30	18	0.91731	0.00061	0.95262
3	20	30	15	0.91674	0.00061	0.98654
4	20	30	12	0.91638	0.00063	0.99273
5	20	20	20	0.92641	0.00059	0.45389
6	20	20	18	0.91900	0.00062	0.83481
7	20	20	15	0.91772	0.00059	0.93144
8	20	20	12	0.91587	0.00060	0.96340
9	20	10	20	0.97089	0.00056	0.48885
10	20	10	18	0.95683	0.00057	0.61508
11	20	10	15	0.94182	0.00057	0.74493
12	20	10	12	0.93467	0.00058	0.83132

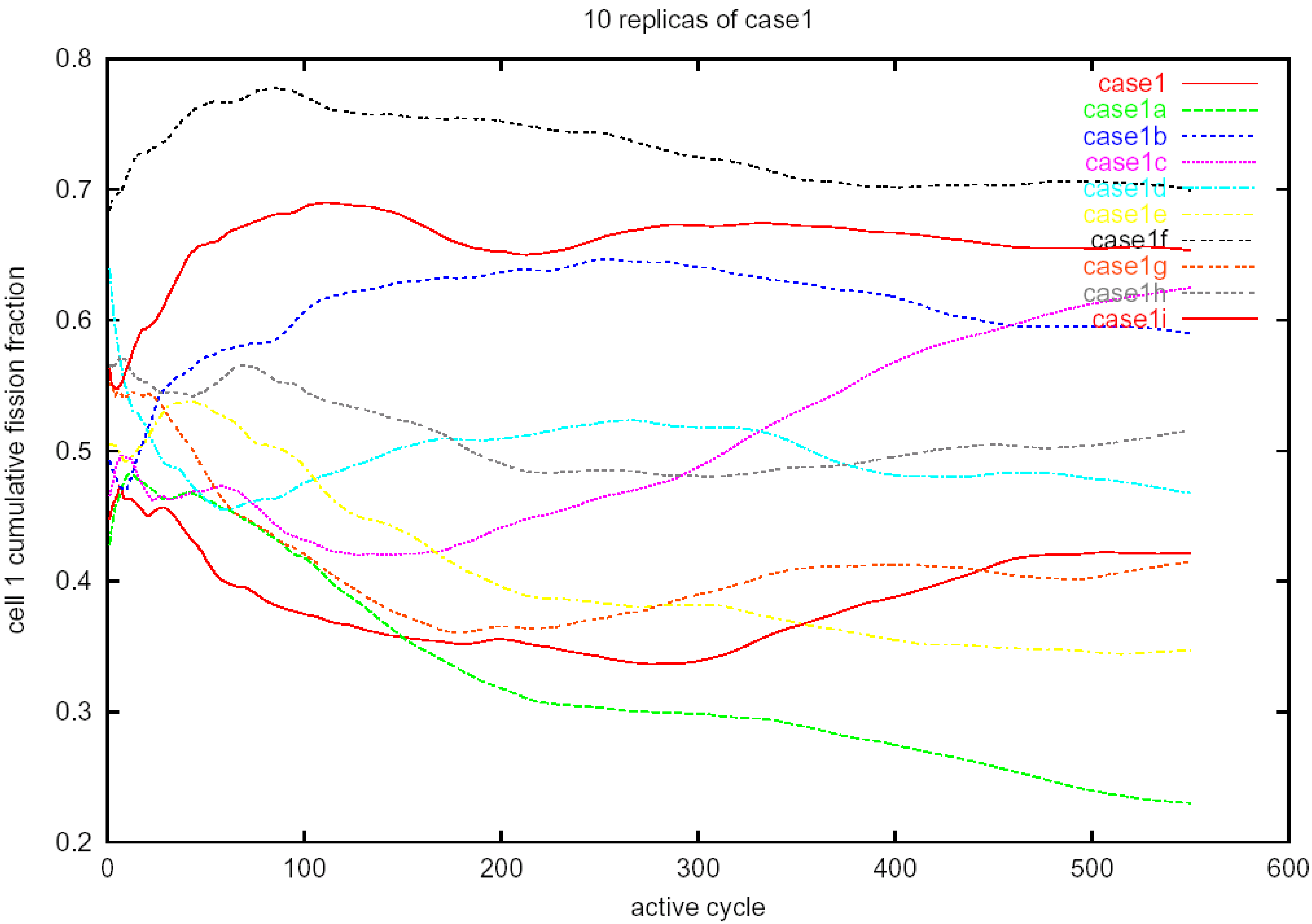
10 Replicas of Case 1 Were Calculated

Case	T1	T2	T3	k_{eff}	Std Dev	F1
1	20	30	20	0.91890	0.00060	0.42155
1A	20	30	20	0.91901	0.00060	0.23027
1B	20	30	20	0.92005	0.00057	0.58971
1C	20	30	20	0.91712	0.00060	0.62459
1D	20	30	20	0.91913	0.00063	0.46762
1E	20	30	20	0.91929	0.00063	0.34748
1F	20	30	20	0.91833	0.00056	0.69936
1G	20	30	20	0.91784	0.00062	0.41487
1H	20	30	20	0.91812	0.00061	0.51532
1I	20	30	20	0.91930	0.00059	0.65373

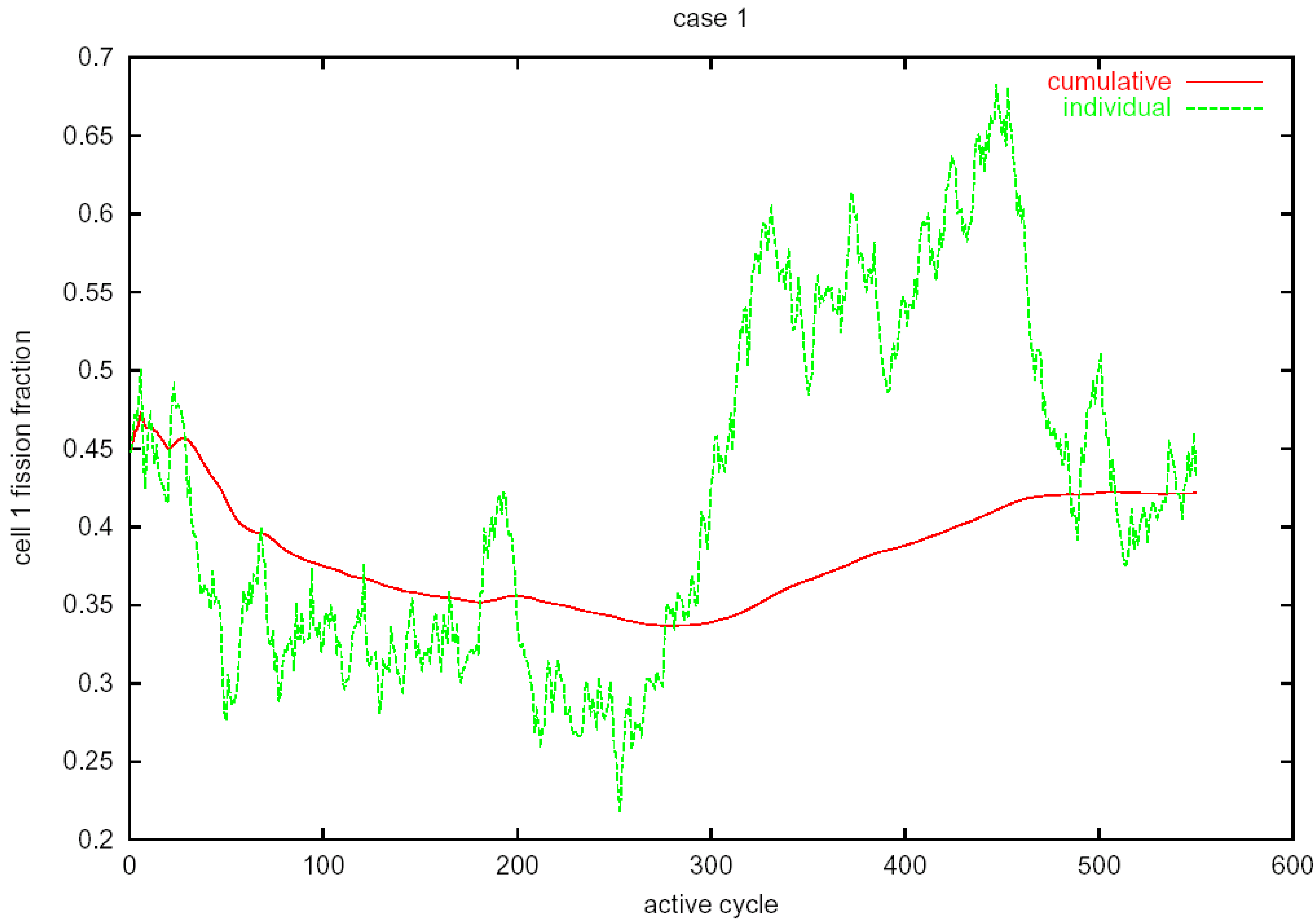
MCNP: K-effective for 10 Replicas of Case-1



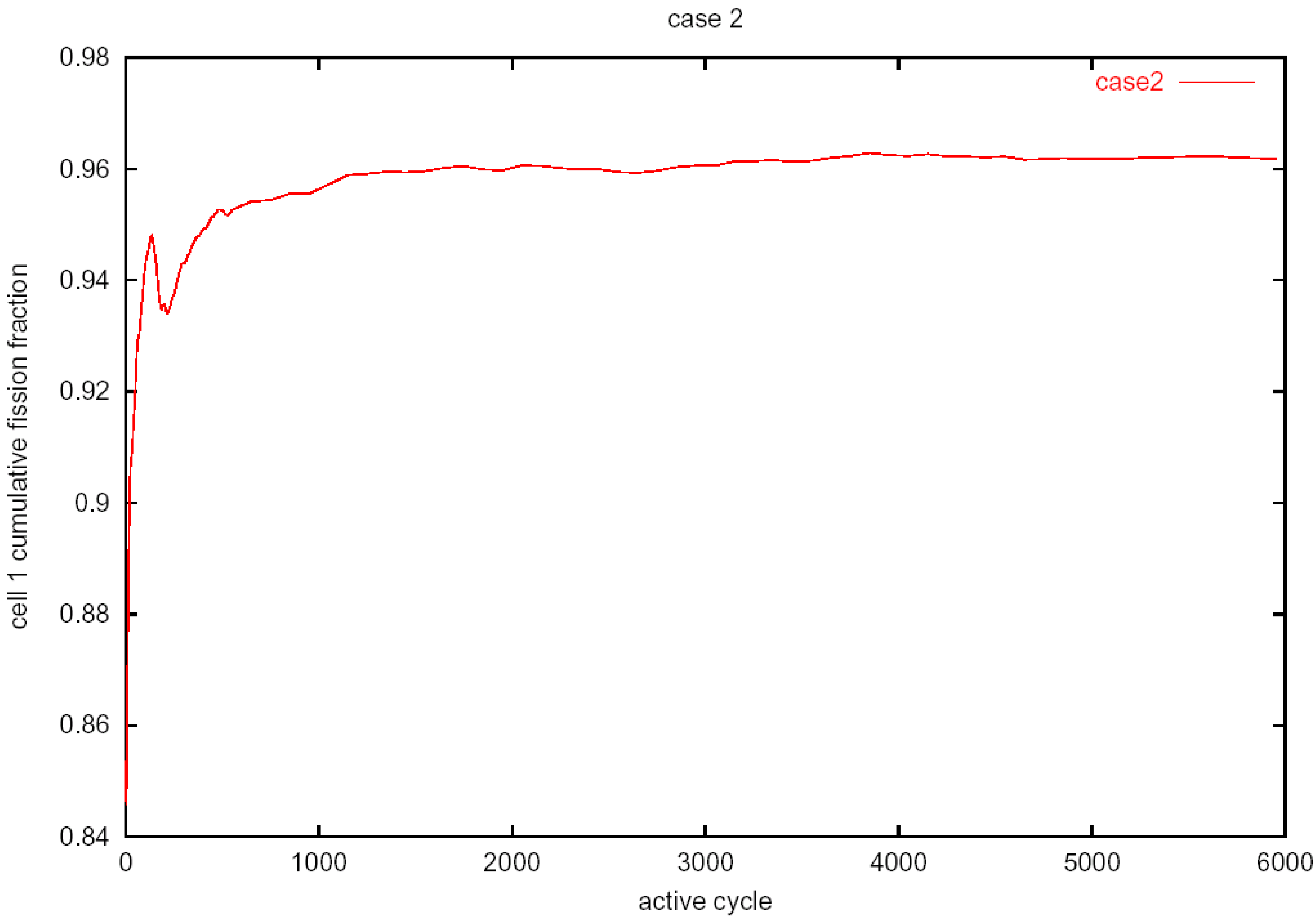
Cell 1 Fission Fraction Convergence for 10 Replicas of Case-1



Cell 1 Fission Fraction Convergence for Case-1



MCNP Reference: Cell 1 Fission Fraction Convergence, Case 2

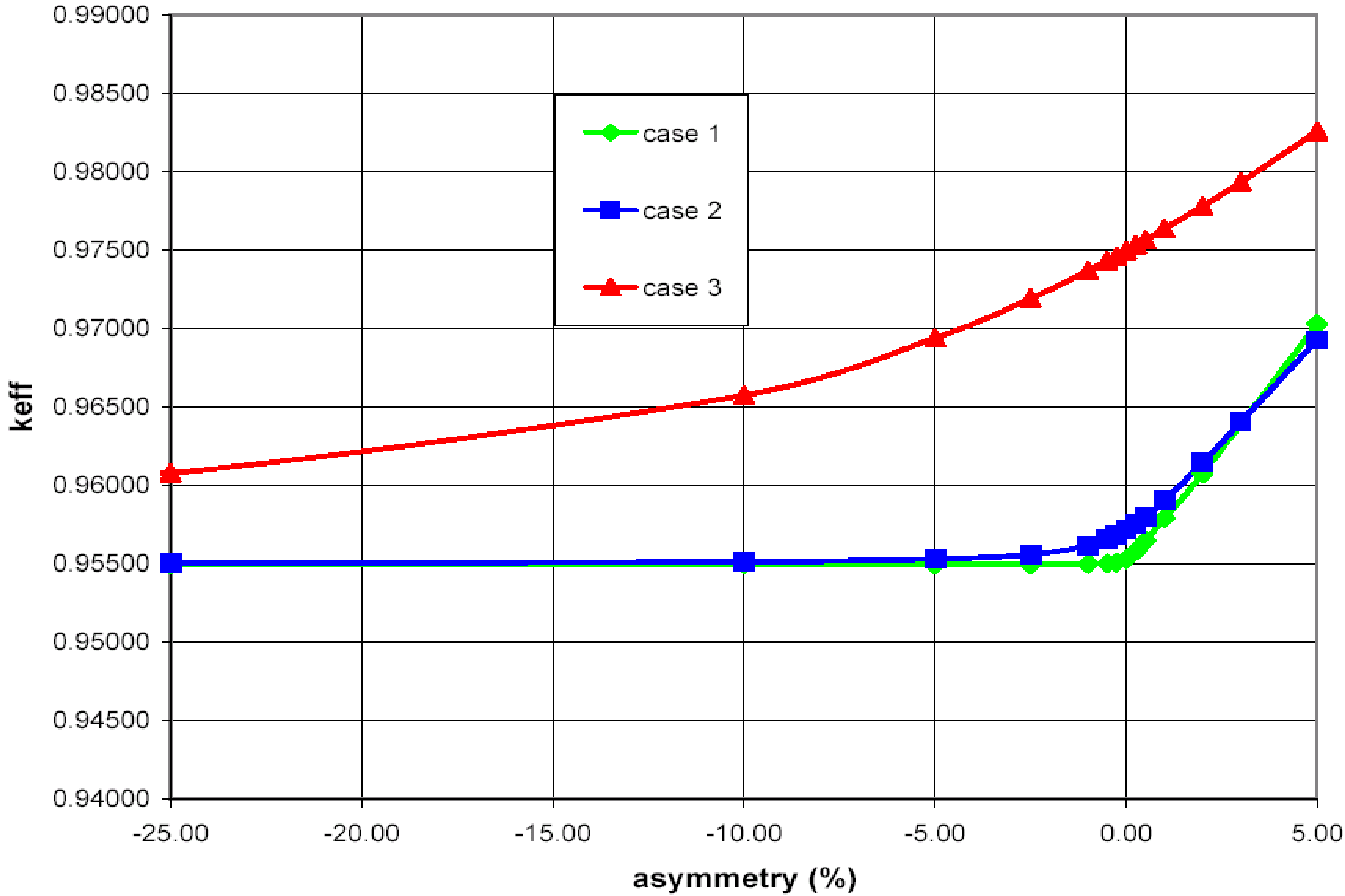


Benchmark 3 — Deterministic Calculations

- Additional supporting calculations were done using **Onedant**

- Onedant:
  - — Sn code, 1D
  - — For consistent comparisons with MCNP, a series of calculations was run with both codes, using **multigroup** cross-sections & **P0 scattering**
  - — Fine mesh: 1 mm mesh spacing
  - — High-order Sn: S96 double-Gauss

Onedant Results: K-effective vs Asymmetry



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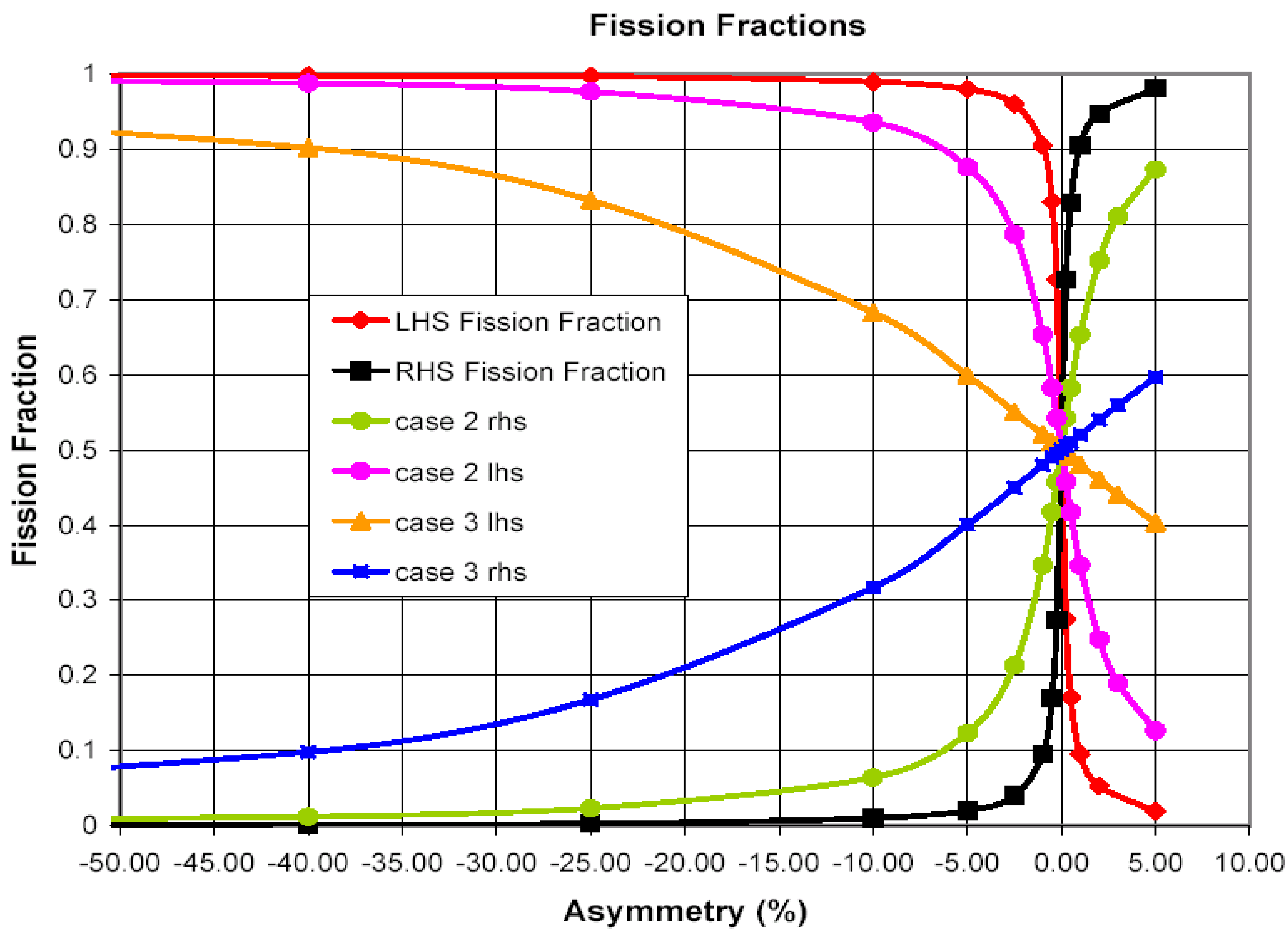
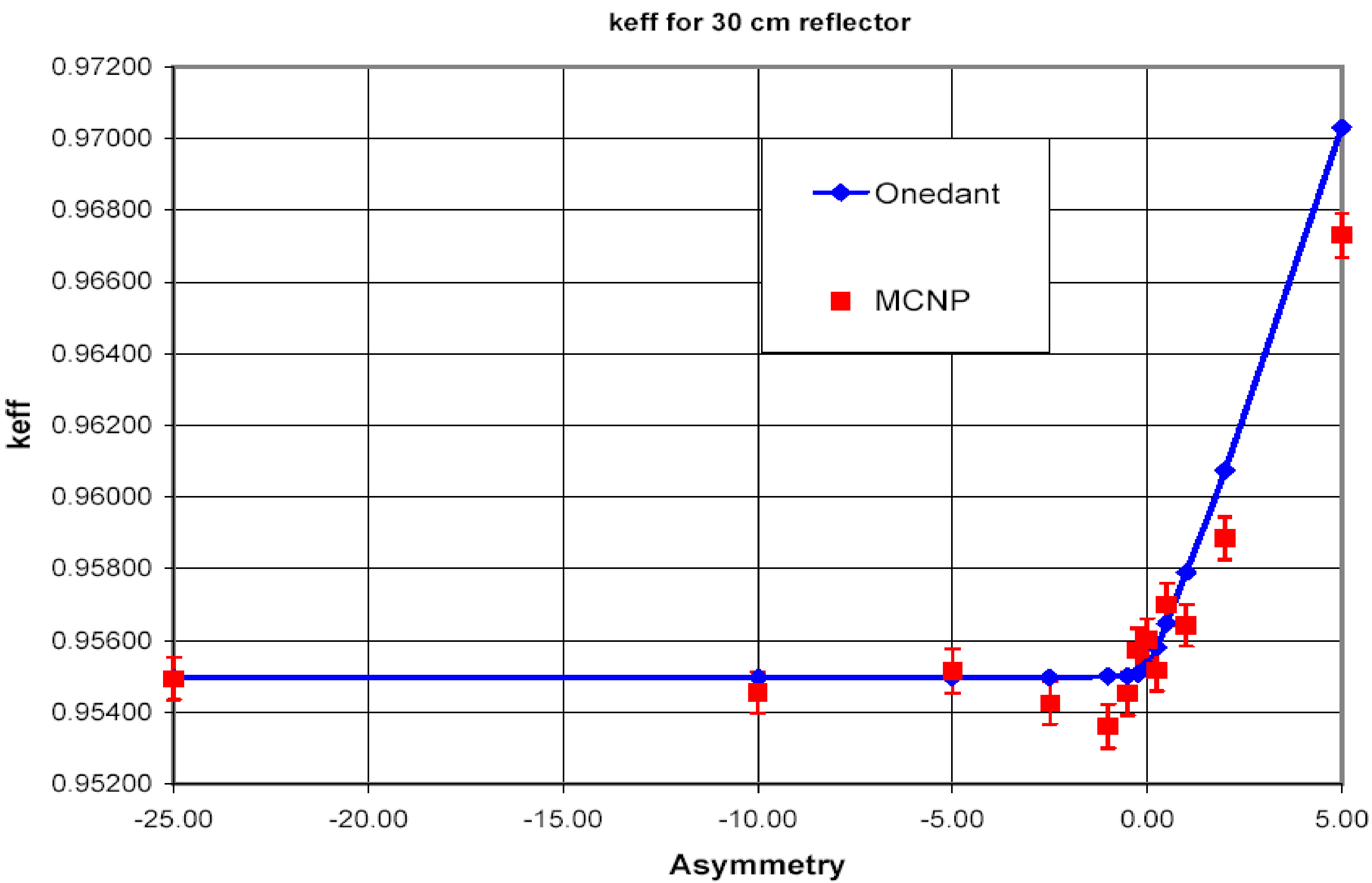
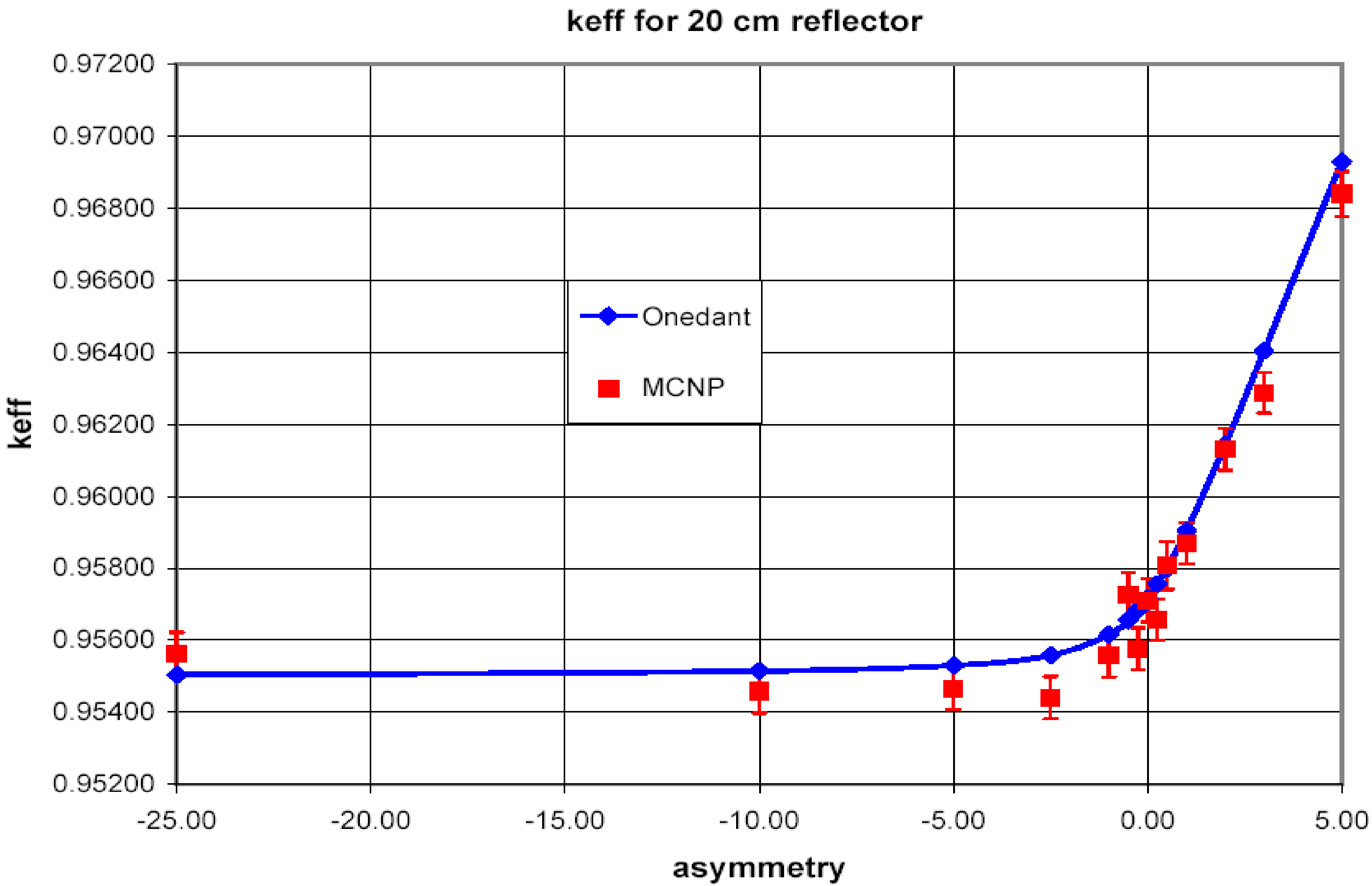
Onedant Results: Fission Fractions vs Asymmetry



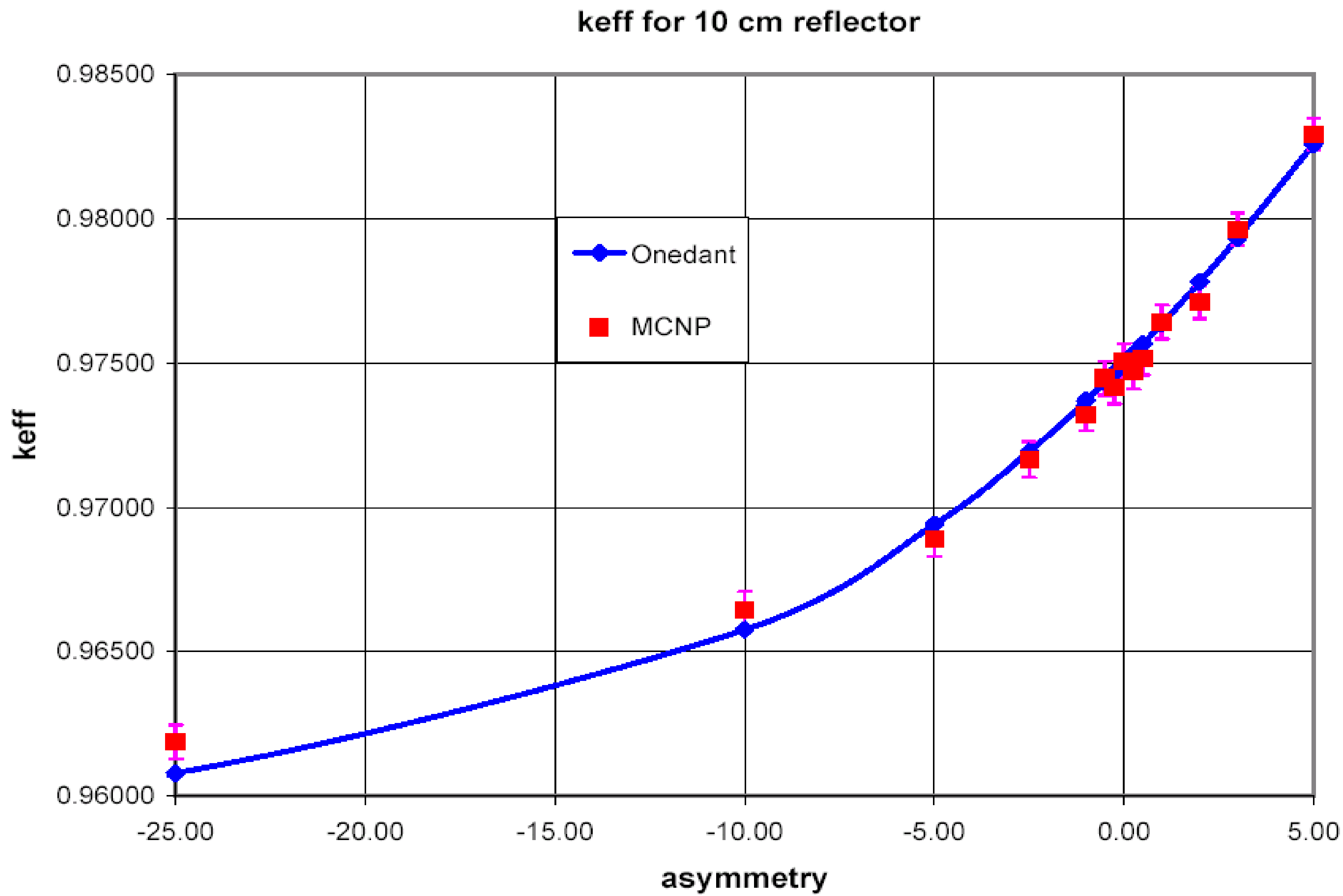
Onedant & MCNP: K-effective for 30 cm Reflector



Onedant & MCNP: K-effective for 20 cm Reflector



Onedant & MCNP: K-effective for 10 cm Reflector



Onedant & MCNP: Results for 30 cm Reflector

name	lhs fuel	rhs fuel	asymmetry percent	onedant			mcnp			
				keff	lhs fission fraction	rhs fission fraction	keff	abs error	lhs fission fraction	rhs fission fraction
dase1d	20	21.00	5.00	0.97031	0.019	0.981	0.96730	0.00061	0.051	0.949
test1p	20	20.40	2.00	0.96074	0.053	0.947	0.95885	0.00060	0.237	0.763
test1q	20	20.20	1.00	0.95790	0.095	0.905	0.95642	0.00058	0.445	0.555
dase1b	20	20.10	0.50	0.95648	0.171	0.829	0.95700	0.00060	0.431	0.569
test1n	20	20.05	0.25	0.95580	0.274	0.726	0.95517	0.00058	0.725	0.275
dase1	20	20.00	0.00	0.95527	0.5	0.5	0.95602	0.00059	0.540	0.460
test1m	20	19.95	-0.25	0.95507	0.726	0.274	0.95574	0.00060	0.388	0.612
dase1a	20	19.90	-0.50	0.95502	0.83	0.17	0.95452	0.00060	0.623	0.377
dase1f	20	19.80	-1.00	0.95500	0.905	0.095	0.95361	0.00061	0.436	0.564
dase1e	20	19.50	-2.50	0.95497	0.96	0.04	0.95426	0.00059	0.816	0.184
dase1c	20	19.00	-5.00	0.95497	0.98	0.02	0.95515	0.00061	0.961	0.039
dase2	20	18.00	-10.00	0.95497	0.99	0.01	0.95455	0.00058	0.980	0.020
dase3	20	15.00	-25.00	0.95496	0.997	0.003	0.95494	0.00059	0.998	0.002
dase4	20	12.00	-40.00	0.95496	0.998	0.002	0.95372	0.00064	0.998	0.002
dase5	20	0.00	-100.00	0.95496	1	0	0.95451	0.00059	1.000	0.000

Onedant & MCNP: Results for 20 cm Reflector

name	lhs fuel	rhs fuel	asymmetry percent	onedant			mcnp			
				keff	lhs fission fraction	rhs fission fraction	keff	abs error	lhs fission fraction	rhs fission fraction
dase1d	20	21.00	5.00	0.96930	0.1265	0.8735	0.96840	0.00062	0.130	0.811
dase1k	20	20.60	3.00	0.96404	0.1895	0.8105	0.96287	0.00056	0.387	0.613
dase1p	20	20.40	2.00	0.96145	0.2483	0.7517	0.96130	0.00058	0.335	0.665
dase1q	20	20.20	1.00	0.95904	0.3467	0.6533	0.95869	0.00057	0.331	0.669
dase1b	20	20.10	0.50	0.95800	0.4175	0.5825	0.95807	0.00066	0.579	0.421
dase1n	20	20.05	0.25	0.95756	0.4576	0.5424	0.95656	0.00057	0.499	0.501
dase1	20	20.00	0.00	0.95716	0.5	0.5	0.95711	0.00061	0.422	0.578
dase1m	20	19.95	-0.25	0.95683	0.5425	0.4575	0.95576	0.00059	0.437	0.563
dase1a	20	19.90	-0.50	0.95655	0.5826	0.4174	0.95726	0.00062	0.552	0.448
dase1f	20	19.80	-1.00	0.95615	0.6534	0.3466	0.95559	0.00061	0.619	0.381
dase1e	20	19.50	-2.50	0.95558	0.7868	0.2132	0.95441	0.00059	0.678	0.322
dase1c	20	19.00	-5.00	0.95530	0.8765	0.1235	0.95465	0.00058	0.782	0.218
dase2	20	18.00	-10.00	0.95514	0.9357	0.0643	0.95458	0.00060	0.941	0.059
dase3	20	15.00	-25.00	0.95504	0.9766	0.0234	0.95564	0.00058	0.979	0.021
dase4	20	12.00	-40.00	0.95501	0.9878	0.0122	0.95498	0.00062	0.988	0.012

Onedant & MCNP: Results for 10 cm Reflector

name	lhs fuel	rhs fuel	asymmetry percent	onedant			mcnp			
				keff	lhs fission fraction	rhs fission fraction	keff	abs error	lhs fission fraction	rhs fission fraction
dase1d	20	21.00	5.00	0.98259	0.403	0.597	0.98293	0.00054	0.396	0.604
dase1k	20	20.60	3.00	0.97934	0.4405	0.5595	0.97963	0.00057	0.433	0.567
dase1p	20	20.40	2.00	0.97781	0.46	0.54	0.97711	0.00058	0.438	0.562
dase1q	20	20.20	1.00	0.97636	0.48	0.52	0.97642	0.00059	0.462	0.538
dase1b	20	20.10	0.50	0.97566	0.49	0.51	0.97516	0.00057	0.479	0.521
dase1n	20	20.05	0.25	0.97532	0.495	0.505	0.97471	0.00061	0.479	0.521
dase1	20	20.00	0.00	0.97498	0.5	0.5	0.97507	0.00060	0.494	0.506
dase1m	20	19.95	-0.25	0.97465	0.505	0.495	0.97417	0.00059	0.492	0.508
dase1a	20	19.90	-0.50	0.97433	0.51	0.49	0.97448	0.00059	0.538	0.462
dase1f	20	19.80	-1.00	0.97370	0.52	0.48	0.97322	0.00056	0.539	0.461
dase1e	20	19.50	-2.50	0.97193	0.55	0.45	0.97166	0.00062	0.561	0.440
dase1c	20	19.00	-5.00	0.96941	0.599	0.401	0.96888	0.00057	0.599	0.401
dase2	20	18.00	-10.00	0.96576	0.683	0.317	0.96644	0.00064	0.677	0.323
dase3	20	15.00	-25.00	0.96079	0.832	0.168	0.96187	0.00059	0.839	0.161
dase4	20	12.00	-40.00	0.95879	0.902	0.098	0.95852	0.00060	0.901	0.099

MCNP Reference Calculations

Reference MCNP calculations (symmetric cases)

100M particles,	~6000 minutes CPU time
Cross-sections:	Multigroup, P0 scatter
Onedant fine mesh:	0.25 mm mesh spacing
High-order Sn:	S96, double Gauss

case	keff (σ)	fine mesh dant keff	(mcnp-onedant) σ	lhs	rhs
30 cm reflector	0.95527 (6)	0.95528	-0.17	0.364	0.636
20 cm reflector	0.95723 (6)	0.95717	1.0	0.492	0.508
10 cm reflector	0.97509 (6)	0.97499	1.7	0.499	0.501

OECD/NEA Working Party on Nuclear Criticality Safety
Expert Group on Source Convergence Analysis
Paris, France — 19 September 2001

Benchmark 4
Array of Interacting Spheres

MCNP Calculations

Robert C. Little

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Los Alamos National Laboratory
<rcl@lanl.gov>

Todd Wareing

Transport Methods (CCS-4)
Los Alamos National Laboratory
<dkp@lanl.gov>

OECD/NEA Source Convergence Benchmark 4

Outline

- Problem Description
- Observations
- Sample MCNP Input File
- Sample Required Output
- Plots
  - K-effective Results
  - Sphere (1,1) Fission Fraction
  - Sphere (3,3) Fission Fraction

Benchmark 3 — Array of Interacting Spheres

Contact: Robert C. Little
LANL, X-5
505-665-3487
rcl@lanl.gov

Code: **MCNP4C2**

Method: continuous-energy Monte Carlo

Geometry: exact, as specified

Cross-sections: ENDF/B-VI, processed by NJOY into MCNP library

Computer: Sun workstation

Date: August, 2001

Benchmark 4 — Array of Interacting Spheres

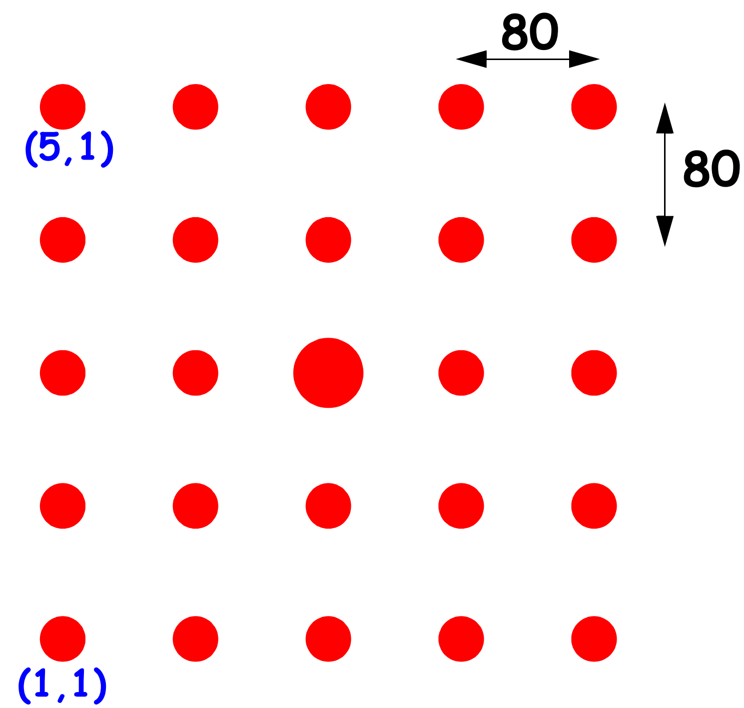
Material Compositions / MCNP Cross-sections

Material	Composition	MCNP Cross-sections	
Highly Enriched Uranium Metal			
U235	4.549e-2	92235.60c,	LANL-proposed endf-VI.2
U238	2.560e-3	92238.60c,	endf-VI.2
Air			
N	4.3250e-5	7014.60c	
O	1.0810e-5	8016.60c	

Benchmark 4 — Array of Interacting Spheres

5 x 5 x 1 Array of Spheres

Case	RN Sequence	Skipped Gen's
1	#1	0
2	#1	200
3	#1	400
4	#2	0
5	#2	200
6	#2	400
...	...	...
298	#100	0
299	#100	200
300	#100	400



125 neutrons/generation
1000 active generations

Center sphere: 10 cm diam.
Other spheres: 8.71 cm diam.

Initial Source:
101 neutrons in center of sphere (1,1)
1 neutron in center of each of the other 24 spheres

All dimensions in cm

Benchmark 4 — Observations

Notes on OECD / NEA Source Convergence Benchmark #4: Array of Interacting Spheres

Written By: Robert C. Little (rcl@lanl.gov; 505.665.3487)
Last Modified: September 6, 2001

Problem Description

Benchmark # 4 is a 5 x 5 x 1 array of highly enriched uranium metal spheres, separated by air. The separation distance is 80 cm. The central sphere has a radius of 10 cm and the other 24 spheres have radii of 8.71 cm. The benchmark was developed by Olivier Jacquet and is adapted from earlier work by Kadotani.

The problem specifications are contrived to emphasize source convergence difficulties. The spatial distribution of starting neutrons is deliberately poor – 101 neutrons in one of the corner spheres and 1 neutron in each of the other 24 spheres. Only 125 starters are used per generation. There are 3 variants required with different numbers of skipped cycles: 0, 200, and 400. Finally, for each of the 3 variants, 100 replicas are run with different random number sequences. For all cases, 1000 active generations were simulated.

Description of Calculations

All calculations were performed with MCNP4C2 (load date 01/20/01) on a SUN Ultra 80. Cross sections are all from the ENDF60 library, which is based on ENDF/B-VI Release 2. MCNP ZAID identifiers are 7014.60c, 8016.60c, 92235.60c, and 92238.60c. A sample input file is shown in Appendix A.

Bounding planes were specified in each dimension at 80 cm perpendicular from the center of the exterior spheres. Neutrons crossing these surfaces were killed. For replica N (N=1,100), the starting random number was chosen to be 1000 * N + 1. The quantity neutron flux times fission cross section times material number density was tallied in each of the 25 spheres. The tally is calculated over all active cycles, not for each individual cycle.

Required Output

The required output for each case is part of the benchmark specification. We have included a sample of such output here as Appendix B. For each of the 300 cases we produced a simple text file with this output. The text files were combined to form one continuous text file and were transmitted electronically to Olivier Jacquet.

The first 12 lines of results for each case include the case number, some summary description, and contact information. The next 4 lines provide the number of skipped generations, the number of active generations, the number of histories per generation, and the number of generations per superhistory. For
MCNP this latter quantity is always 1. The next two lines contain the final k-eff estimate and the one standard deviation absolute (not relative) uncertainty. The values reported here are from the MCNP combined collision / absorption / track-length estimator. For readability we then skip a line. Then we report the individual k-eff estimate for each cycle. For these results we use the MCNP collision estimator. Results are reported for each cycle (inactive or active). We then include another blank line. Finally we report the cumulative fission fraction in each of the 25 uranium spheres. The fractions are derived from the tallies described above multiplied by the cell volumes. The first entry is for sphere 1 (the sphere that dominates the original source distribution), the 13th entry is for the central sphere, etc. These values are cumulative over all active generations and are normalized to 1.

Reference Calculations

To provide a reference result for comparison purposes, an extended calculation was performed. In this case, the initial source was specified to be equal in each of the 25 spheres. 10,000 histories per cycle were simulated. We skipped 1,000 cycles and calculated a total of 6,000 cycles. Therefore we had 50 million active histories in this run. The final combined collision / absorption / track-length estimate of k-eff was 1.11294 with a one sigma absolute standard deviation of 0.00009.

We also have performed eigenvalue calculations for isolated spheres, with radii of 10.0 cm and 8.71 cm. For these runs, all neutrons leaking from the sphere were terminated. We ran 5,000 histories per cycle, skipped 500 cycles, and calculated a total of 2,500 cycles (10 M active histories). The initial source was simply a point in the center of the sphere. For the 10.0-cm sphere, the k-eff was 1.11233 with a one-sigma absolute standard deviation of 0.00019, and for the 8.71-cm sphere, the k-eff was 0.99519 with a one-sigma absolute standard deviation of 0.00019.

Eigenvalue Results

A plot of all 300 eigenvalue results is shown in Figure 1. The results for case 1 with no skipped cycles are in red, for case 2 with 200 skipped cycles are in green, and for case 3 with 400 skipped cycles are in blue. One notes immediately the variation in eigenvalue spread for the different cases. Also, one should compare these results with the reference value of ~ 1.113.

The table below provides some summary information for the eigenvalues for each of the 3 cases. Typical standard deviations reported by MCNP for the individual runs were ~ 0.002. The mean and standard deviation of the mean were calculated from the 100 replica results using the standard formulas that weight the contributions based on the individual uncertainties. The population estimated standard deviation of the mean is calculated from the observed scatter of the population of replica eigenvalues. The ratio of the two standard deviations gives some indication of the Monte Carlo underestimation of the individual eigenvalue uncertainties (assuming, of course, unbiased results).

Case	Skipped Cycles	Minimum k-eff	Maximum k-eff	Mean k-eff	Standard Deviation of the Mean	Population Estimated Standard Deviation of the Mean	Ratio
1	0	1.05756	1.11291	1.09399	0.000218	0.001433	6.6
2	200	1.07862	1.11667	1.10738	0.000195	0.000909	4.7
3	400	1.09798	1.11779	1.11094	0.000188	0.000317	1.7

We have also analyzed the eigenvalue results for each case with respect to the reference value provided above. The deleterious impact of skipping too few cycles is particularly clear in the following table where we provide the percent of replicas for each case that lie within various multiples of a standard deviation from the reference result.

Case	Skipped Cycles	> 5 SD	4-5 SD	3-4 SD	2-3 SD	1-2 SD	< 1 SD
1	0	74	9	3	8	4	2
2	200	24	4	6	12	24	30
3	400	3	2	3	14	36	42

If we compare the magnitude of the replica eigenvalues to the reference result, we find that even when skipping 400 cycles, there is clearly an underestimation of the eigenvalue. It has not been determined from this work how many cycles would need to be skipped for unbiased results (given the unrealistically poor initial source guess).

Case	Skipped Cycles	Percent of Replicas with k-eff < Reference Value	Percent of Replicas with k-eff > Reference Value
1	0	100	0
2	200	88	12
3	400	80	20

MCNP performs several statistical checks on the eigenvalue results and warns the user if the statistical checks fail in some manner. In these calculations, 3 main warning messages arose. The first is "The cycle values do not appear normally distributed at the 99% confidence level." This check is performed for each of the 3 estimators: collision, absorption, and track length. The second warning was "The first and second half values of the combined estimator appear to be different at the 99% confidence level." The third is a warning that "There appears to be an {increasing / decreasing} trend in the combined estimator over the last 10 cycles." The percent of the replica runs for each case flagging these warning messages is indicated in the next Table.

Case	Skipped Cycles	Cycle Values Not Normally Distributed	First Half / Second Half Different	Trend in Last 10 Cycles	At Least One Warning Message
1	0	21	81	6	85
2	200	5	35	1	37
3	400	3	13	0	16

For case 1, three of the replicas flagged the warning about "cycle values not normally distributed" for each of the three individual estimators. When this happens, MCNP draws attention to the fact by not printing "boxed" results for the final k-eff. The combined estimators for these 3 runs were 1.06226, 1.07231, and 1.07909. These are some of the worst, but certainly not the absolute worst, k-eff estimates. On the other hand, for the 15 replicas of case 1 with no MCNP eigenvalue warnings, the average k-eff is 1.10704, not great compared to the reference calculation, but much closer than the typical case 1 replica.

Fission Fractions

We will first present fission fraction results from the reference calculation described above. It should be noted, however, that an even longer run is likely necessary to provide true reference fission fractions. Nevertheless, results are given in the following table.

Symmetric Cell ID	Number of Cells	Cells	Average Fission Fraction Per Cell
1	1	13	0.910624
2	4	8, 12, 14, 18	0.011157
3	4	7, 9, 17, 19	0.005783
4	8	2, 4, 6, 10, 16, 20, 22, 24	0.002344
5	4	3, 11, 15, 23	0.000463
6	4	1, 5, 21, 25	0.000254

MCNP errors reported for the number of fissions in each cell are clearly underestimated, likely by a factor of up to several for the outer spheres. We have not as yet analyzed these data however.

The next table provides the average fission fraction over all replicas for each case in 3 specific cells: cell 1, with the artificially high initial source; cell 13, the central sphere; and cell 25, the cell symmetric to cell 1 but all the way on the other side of the array (note that cell 25 also has an artificially high initial source representation, although not nearly as high as cell 1). The reference values from the above table are included for comparison purposes. Once more, we are able to conclude that, using the source specified, skipping 400 cycles is not enough for this problem to be converged. It is also noted that MCNP's statistical checks flagged a trend problem in the fission tallies for each of the 100 replicas in case 1.

Case	Skipped Cycles	Cell 1 Average Fission Fraction	Cell 13 Average Fission Fraction	Cell 25 Average Fission Fraction
1	0	0.089250	0.739715	0.001633
2	200	0.012845	0.862278	0.000655
3	400	0.004325	0.900642	0.000377
Ref		0.000254	0.910624	0.000254

Selected plots of the replica fission fractions are attached. (The values in these plots are actually from the sampled KCODE fission point fractions in each cell, rather than from the tally based fractions described earlier. Therefore, there is an extra degree of stochastic sampling involved in these fractions, and nubar is included here but not in the tally based fractions. These differences do not impact the qualitative conclusions in any manner.)

Deterministic Calculations

Todd Wareing has set up this problem using the deterministic ATTILA code. His initial eigenvalue results are not inconsistent with the Monte Carlo results reported here. We expect more detailed results and analysis in the future.

Appendix A — Sample MCNP Input File

```
OECD/NEA Source Convergence Benchmark 4:Array of Interacting Spheres
c     case = 1
c
c     Benchmark defined by Jacquet (IPSN/DPEA/SEC)
c     Implemented for MCNP by R.C.Little (June 2001)
c
c     Case 1,4,7,...298: 0 skipped generations
c     Case 2,5,8,...299: 200 skipped generations
c     Case 3,6,9,...300: 400 skipped generations
c
c       There are 100 replicas for each number of skipped generations
c         The initial random number is chosen to be (N*1000)+1
c
c           Case:                   1
c           Skipped Generations:    0
c           Total Generations:      1000
c           Initial Random Number:  1001
c
c     Cell Cards
c
c     cells 1-25 are the spheres of uranium metal
c       1-12 and 14-25 are radius 8.71 cm
c       13 has radius of 10.0 cm
1     1 .04805 -1
2     1 .04805 -2
3     1 .04805 -3
4     1 .04805 -4
5     1 .04805 -5
6     1 .04805 -6
7     1 .04805 -7
8     1 .04805 -8
9     1 .04805 -9
10    1 .04805 -10
11    1 .04805 -11
```

```
12   1 .04805 -12
13   1 .04805 -13
14   1 .04805 -14
15   1 .04805 -15
16   1 .04805 -16
17   1 .04805 -17
18   1 .04805 -18
19   1 .04805 -19
20   1 .04805 -20
21   1 .04805 -21
22   1 .04805 -22
23   1 .04805 -23
24   1 .04805 -24
25   1 .04805 -25
c
c    Air -- Inside Box; Outside Spheres
26   2 5.406e-05 26 -27 28 -29 30 -31 1 2 3 4 5 6 7 8 9 10
     11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
c
c    External World (void)
27   0 -26:27:-28:29:-30:31

c
c    Surface Cards
c
c    24 Small Spheres (surfaces 1-12; 14-25)
c    1 Large Sphere (surface 13)
1    s  80  80 0 8.71
2    s 160  80 0 8.71
3    s 240  80 0 8.71
4    s 320  80 0 8.71
5    s 400  80 0 8.71
6    s  80 160 0 8.71
7    s 160 160 0 8.71
8    s 240 160 0 8.71
9    s 320 160 0 8.71
```

```
10   s 400 160 0 8.71
11   s  80 240 0 8.71
12   s 160 240 0 8.71
13   s 240 240 0 10.0
14   s 320 240 0 8.71
15   s 400 240 0 8.71
16   s  80 320 0 8.71
17   s 160 320 0 8.71
18   s 240 320 0 8.71
19   s 320 320 0 8.71
20   s 400 320 0 8.71
21   s  80 400 0 8.71
22   s 160 400 0 8.71
23   s 240 400 0 8.71
24   s 320 400 0 8.71
25   s 400 400 0 8.71
c
c    6 Planes to Bound Box of Air
26   px 0
27   px 480
28   py 0
29   py 480
30   pz -80
31   pz 80

c
c    Material Cards
c
c    M1 - Highly Enriched Uranium Metal
m1   92235 .04549 92238 2.56e-03
c
c    M2 - Air
m2   7014 4.325e-05 8016 1.081e-05
c
c    Miscellaneous Cards
c
```

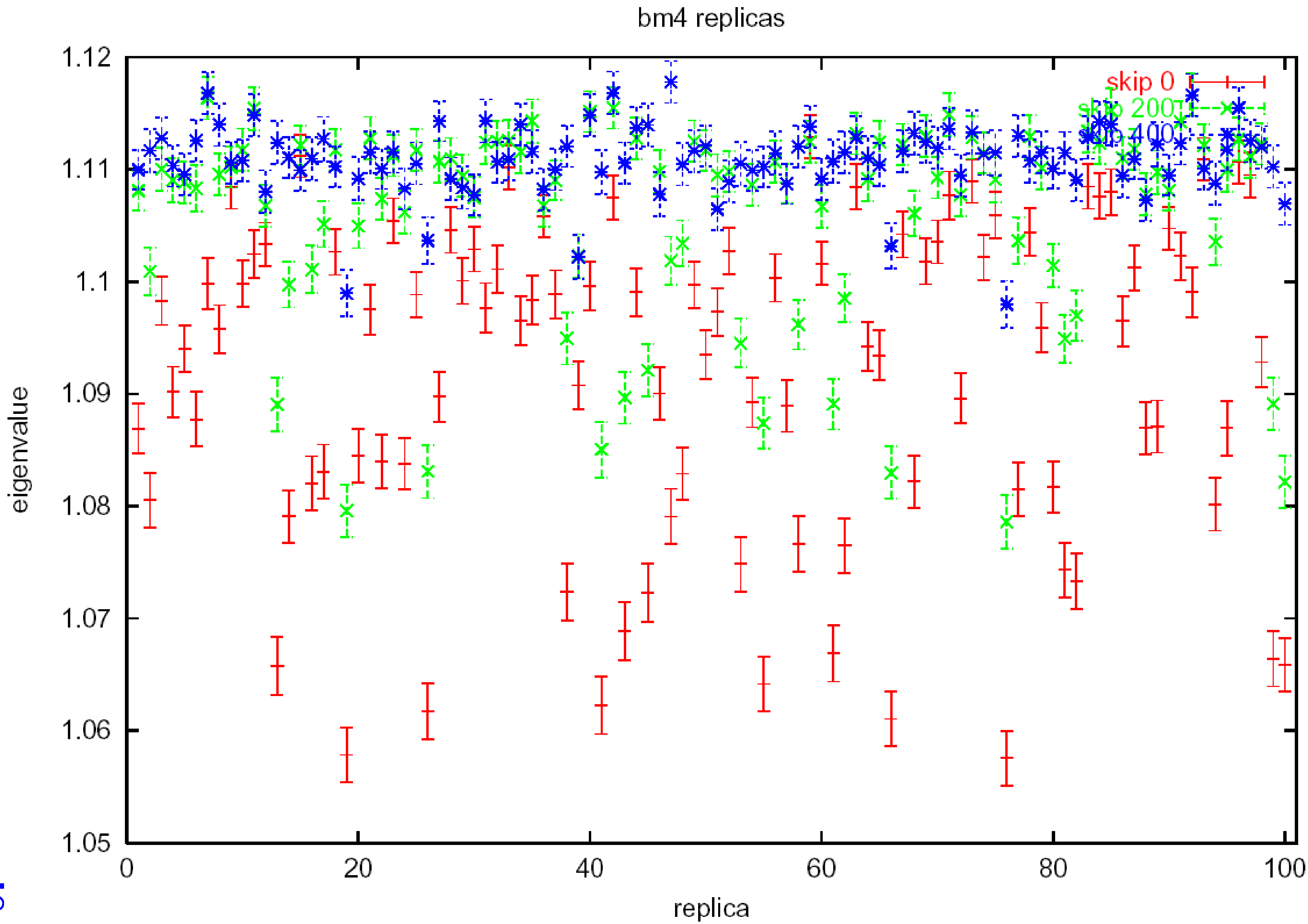
```
mode n
imp:n 1 25r 0
print 130
dbcn 1001
c
c    I chose *not* to print out cumulative source distribution at each cycle
c    prdmp 1
c
c    KCODE Cards
c
c    125 neutrons per cycle
c    initial distribution:
c      101 neutrons in center of sphere # 1
c      1 neutron in center of each of the other 24 spheres
c    initial keff estimate of 1.11 is from preliminary calculations
kcode 125 1.11 0 1000
ksrc 80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
     80 80 0  80 80 0  80 80 0  80 80 0  80 80 0
                80 160 0   80 240 0   80 320 0   80 400 0
     160 80 0  160 160 0  160 240 0  160 320 0  160 400 0
     240 80 0  240 160 0  240 240 0  240 320 0  240 400 0
```

```
     320 80 0  320 160 0  320 240 0  320 320 0  320 400 0
     400 80 0  400 160 0  400 240 0  400 320 0  400 400 0
c
c     tally cards
c
c       f4:n neutron flux tally in each of the 25 spheres
c       multiply the flux tally by the fission cross section (fm -6)
c          to get fission fractions in each sphere
c
f4:n 1 23i 25
fm4  -1 1 -6
```

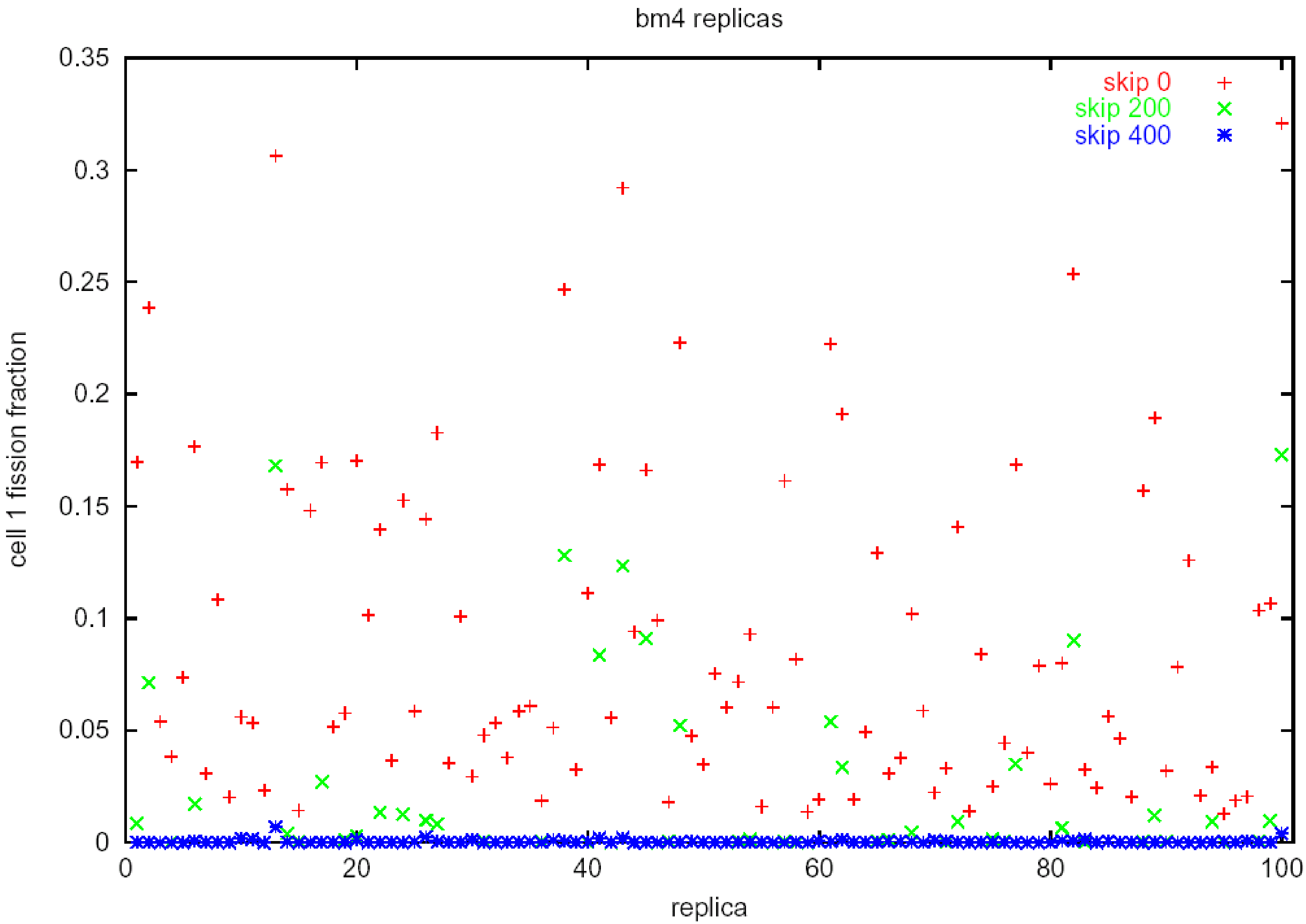
Appendix B — Sample Required Output

```
"Tue Sep  4 14:01:34 MDT 2001"
"LANL, X-5 Group"
"Robert C. Little"
"rcl@lanl.gov"
"505-665-3487"
"505-665-3046 fax"
"Benchmark 4: Array of Interacting Spheres"
"Case 001"
"MCNP4C2"
"Monte Carlo"
"ENDFB/VI"
"source as specified"
0
1000
125
1
1.086930
0.002250

1.27348
1.17438
1.19847
1.00016
1.08043
1.18062
1.00618
1.12912
1.14904
1.02126
snip
snip
snip
1.19187
1.19697
1.24085
1.19474
1.10040
1.06713
1.02940
1.01108
1.05377
1.11250

0.15627
0.00687
0.00060
0.00102
0.00012
0.01886
0.00337
0.01271
0.01055
0.00131
0.00043
0.01470
0.73796
0.00862
0.00033
0.00370
0.00434
0.00977
0.00323
0.00102
0.00070
0.00116
0.00022
0.00193
0.00017
```

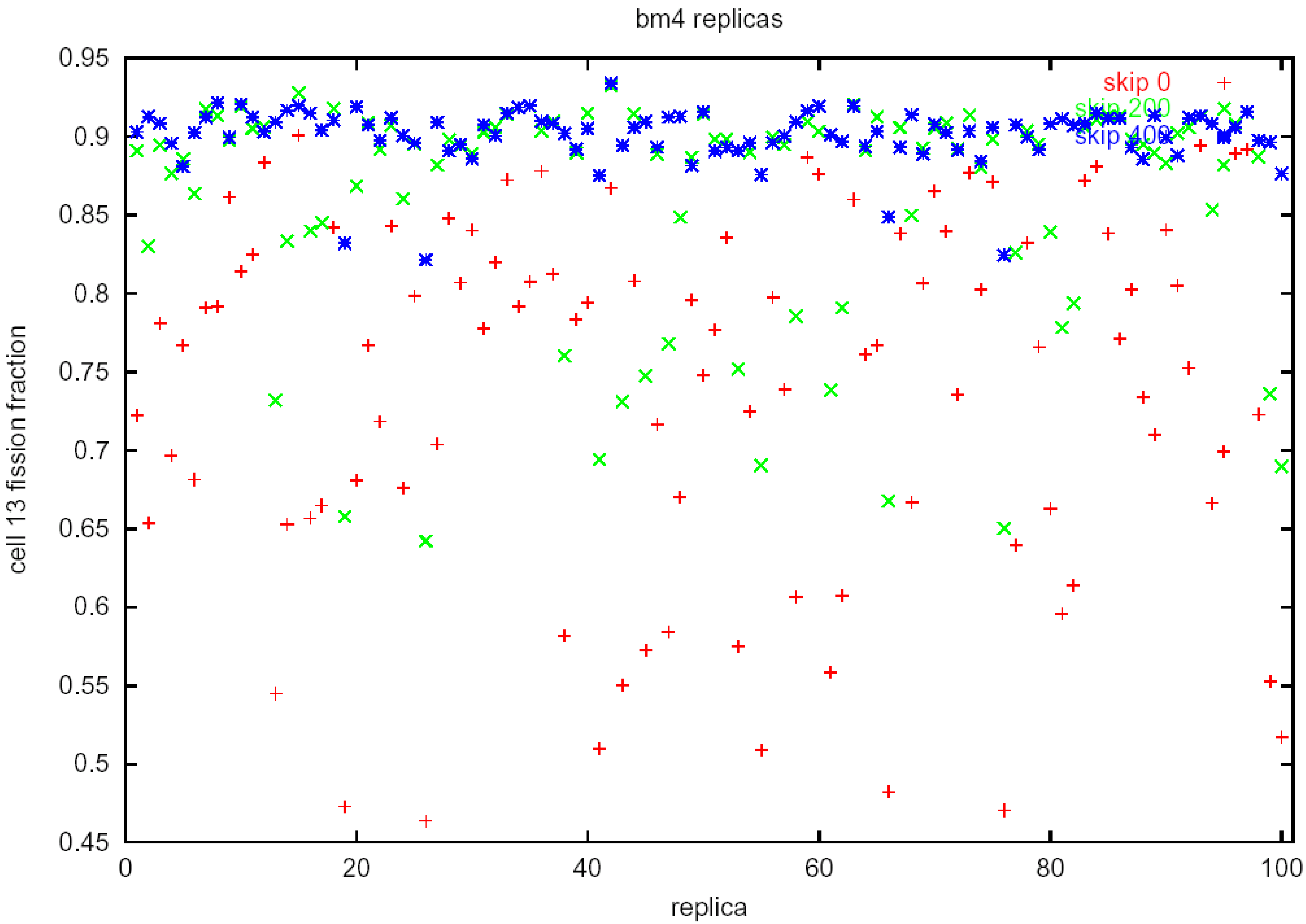
Benchmark 4 — K-effective Results



Benchmark 4 — Sphere (1,1) Fission Fraction Results



Benchmark 4 — Sphere (3,3) Fission Fraction Results



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