Comparison of MCNP-based Transport Codes for Subcritical Calculations

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Abstract

Several Monte-Carlo-based particle transport codes have been developed to attempt to correctly simulate subcritical systems; in this work, MCNP5 with an internally developed list-mode multiplication patch, MCNPX, MCNP-DSP and MCNPX-PoliMi were compared. Of particular interest is the ability to generate list-mode data (the time and location of neutron absorption events within the detector(s)), which can then be used in a variety of subcritical calculational methods to determine various system parameters. All of the codes except MCNP-DSP compare well in performing subcritical calculations and are capable of producing list-mode data. There is a significant difference between the k-eigenvalue calculations (KCODE) and the inferred k determined using the modified fixed-source coupled with the Hansen-Dowdy formalism of the Feynman variance method. This difference is primarily due to the lack of accounting for the statistical fluctuations in the behavior of time-dependent systems of the former method, and the difference increases with increasing subcriticality.

Background

- **Nuclear Criticality Safety Program (NCSP) Integral Experiments (IE) Element:**
  - "…provide a sustainable infrastructure and a systematic, interactive process to assess, design, perform, and document integral criticality safety-related benchmark quality experiments to support safe, efficient fissionable material operations."
  - Provides support for:
    - Stockpile stewardship program
    - Emergency response and counter terrorism program
    - Non-proliferation and arms control program
    - Global Nuclear Energy Partnership

- **NCSP Analytical Methods (AM) Element:**
  - "…provide for the development and maintenance of state-of-the-art analytical capability for the processing of nuclear data from the Evaluated Nuclear Data File (ENDF) and the radiation transport analysis needed to predict system k-effective values."

Introduction

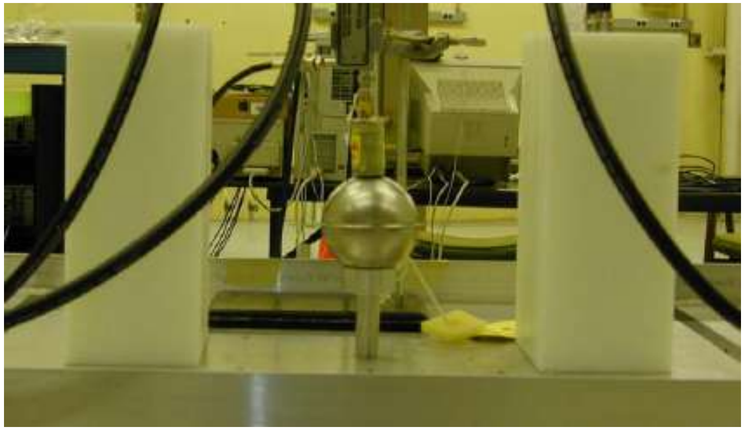
- **Research funded by DOE NCSP**
  - Collaboration between IE program element, the AM program element, LANL and UNLV
- **Need for a MC-based transport code to accurately simulate subcritical systems**
  - List-mode data generation is desirable
  - Change in fission physics is necessary
- **Several codes have either been specifically developed to meet this criteria or contain some capability to perform these calculations:**
  - MCNP5 v.1.60 w/ internally developed multiplication patch
  - MCNPX v.2.7.0 (w/PTRAC)
  - MCNPX-PoliMi (patch for MCNPX v.2.7.0)
  - MCNP-DSP

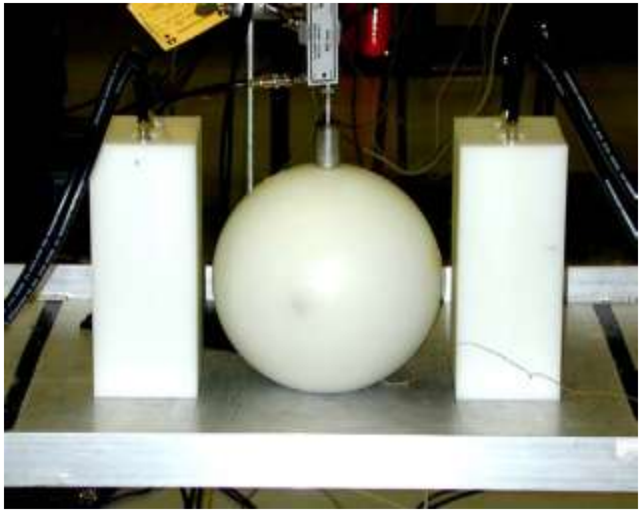
What do we want to compare?

- **Code capabilities**
  - What tools and abilities does each code bring to the table?
  - How is it different from the mainstream codes?
- **KCODE calculations**
  - Basis of comparison of the physics used in each code
- **Modified fixed source calculations**
  - Does the code produce list-mode data?
  - What physics have been changed?
- **Modified fixed source calculations with varying window widths**
  - Does the code start to deviate from expected results?
- **Reduce/eliminate effect of data variances/discrepancies**
  - Use same data for all codes
- **Must model all components of system correctly**
  - Difficult!

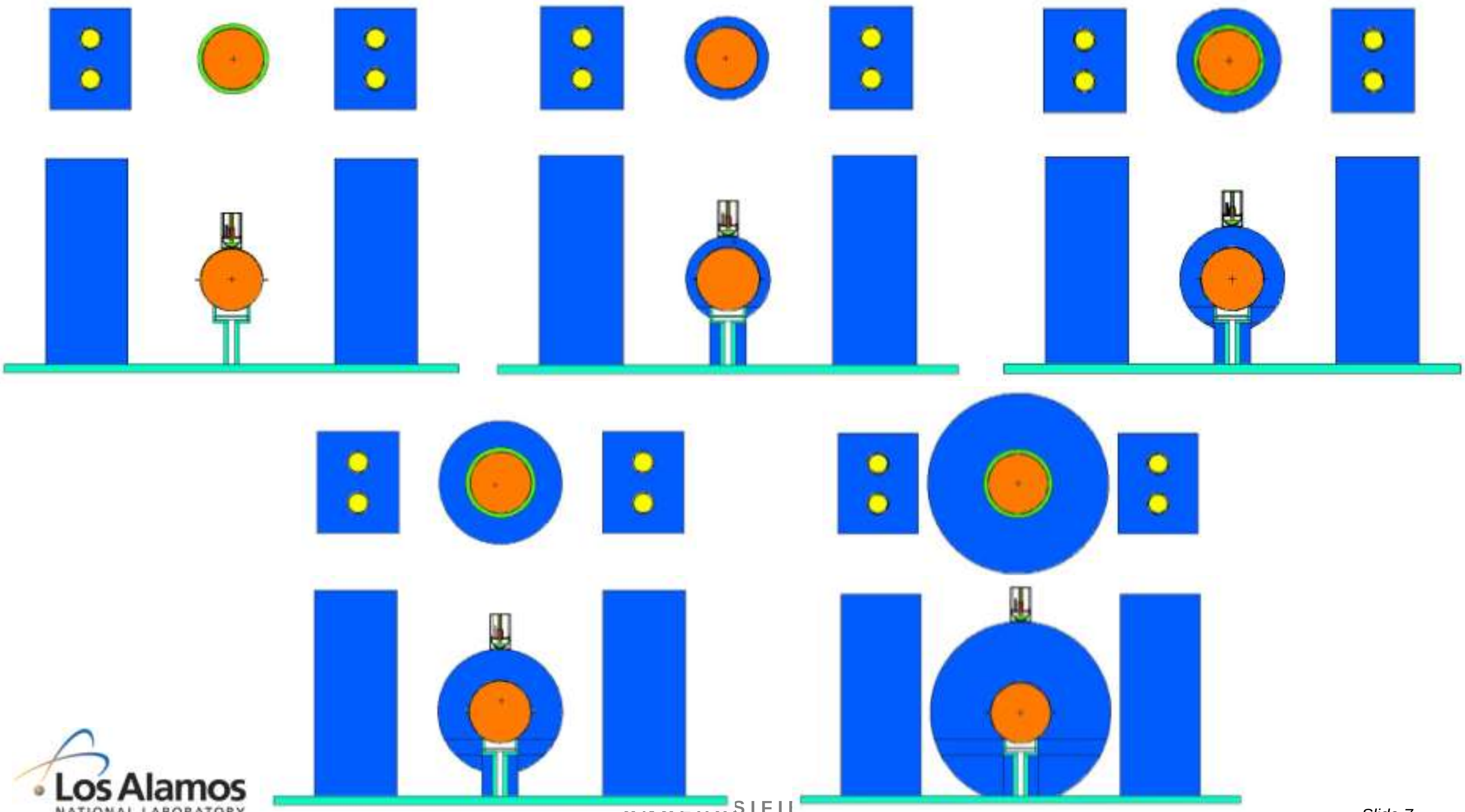
Experiment

- **Models based on ICSBEP benchmark report SUB-PU-MET-FAST-001 (Valentine, 2003)**
  - Los Alamos plutonium sphere, aka “BeRP (beryllium-reflected plutonium) ball”
  - Five different measurement configurations
    - Bare
    - 0.5”, 1”, 1.5” and 3” HDPE-reflected
  - Two He-3 detectors
    - each containing two He-3-filled tubes surrounded by HDPE
    - Placed 12.7cm from center on opposite sides of the BeRP ball





MCNP Models



Code Comparison

- **Current mainstream code (MCNP5 v.1.60):**
  - Rely upon average values for parameters such as nubar
  - Do not correlate fission sources in time and location
  - No energy or angle correlations

- **Modified codes:**
  - Utilize full fission probability distribution
  - Run total number of starting fission events
  - Run in analog mode
  - Require a modified source definition
  - Output some form of list-mode data

MCNP5 v.1.60 w/Multiplication Patch

- **Modifications**
  - New, separate source and tally routines
  - Request list-mode data with a tally modifier on a cell flux tally
  - Uses a full fission probability distribution
    - Lestone or Terrell
  - Can model multiple starting sources/reaction types
    - E.g., SF & (α,n)

- **Limitations**
  - Must run in analog mode when performing multiplication calculation

- **Can be run in MPI mode**

- **To be integrated into MCNP6**

MCNP5 v.1.60 Sample Output

Cell #	Time
35	12792666206.51392
53	26726868933.31010
53	1030157422.58655
41	24131693466.17297
47	13850822270.88635
41	13380726238.07623
35	16140226533.41064
47	5847947933.72676
41	15567770564.15230
47	17698370151.90875
53	23547499824.55188
47	3171604385.66092
47	15105209957.54287
47	18776006683.05566
41	9002389760.93181
41	22140811653.53840
35	16211796461.24377

- **Time given in shakes (10^{-8} seconds)**
- **Correct list-mode data format obtained**

MCNPX v.2.7.0

- **Modifications**
  - Can generate list-mode data if PTRAC is used along with a neutron capture tally
    - PTRAC records the time from the fission event to the capture in the detector
  - Uses a full fission probability distribution (Gaussian) if spontaneous fission is enabled in the source definition
    - Terrell

- **Limitations (when using PTRAC)**
  - Must run in analog mode when performing a neutron capture tally
  - PTRAC file can be very large

MCNPX v.2.7.0 Sample Output

Gen #	Time	Cell #	Particle #
1	0.00000E+00	0	3
1	9.59795E+03	-41	2
1	0.00000E+00	0	1
2	0.00000E+00	0	1
3	0.00000E+00	0	2
3	0.00000E+00	0	1
4	0.00000E+00	0	4
4	0.00000E+00	0	3
4	0.00000E+00	0	2
4	0.00000E+00	0	1
5	0.00000E+00	0	4
5	0.00000E+00	0	3
5	0.00000E+00	0	2
5	0.00000E+00	0	1
6	0.00000E+00	0	2

- **Time is in the incorrect format**
- **Extra data columns present**
  - Remove extra columns, flip time and cell columns

MCNPX-PoliMi

- **Modifications**
  - Correct neutron and gamma multiplicities
  - Correlation between neutron interaction and gamma production
  - Uses a full fission probability distribution
    - Terrell, Zucker & Holden, or Gwin (U-235 only)
  - Conservation of energy for each interaction
  - Output file contains list mode data
    - records the time from the fission event to the capture in the detector
  - Angular distribution of prompt neutrons from fission
  - Neutron energy correlated with fission multiplicity
- **Limitations**
  - Must run in analog mode
  - No delayed neutrons
  - No multigroup cross sections
  - No MPI or continue-run capabilities

MCNPX-PoliMi Sample Output

- **Sample output:**

particle number	projectile type	interaction type	target nucleus	cell number of collision event	energy deposited in collision (MeV)	time (shakes)	collision position (x, y, z)			WGT	generation number	number of scatterings	code
18	1	-99	2003	58	0.20624	1.019	-26.28	-2.29	1.84	1	0	1	0
12	1	0	2003	58	2.42073	1.026	-24.51	-2.54	6.18	1	0	1	0
15	1	-99	2003	58	1.42718	1.053	-25.15	-3.17	2.34	1	0	1	0
11	1	-99	2003	40	0.78974	1.169	25.25	2.97	5.92	1	0	1	0
9	1	-99	2003	46	0.17272	1.347	25.11	-2.11	-0.4	1	0	2	0
6	1	-99	2003	58	0.24532	1.386	-25.13	-3.12	3.31	1	0	2	0
10	1	-99	2003	58	0.54088	1.739	-25.97	-3.35	3.84	1	0	3	0
11	1	0	2003	40	0.88908	2.357	25.15	2.62	6.67	1	0	2	0
6	1	0	2003	46	0.76822	2.448	24.46	-2.39	3.08	1	0	3	0
14	1	0	2003	40	1.123	3.166	25.54	2.49	3.19	1	0	1	0
7	1	-99	2003	58	0.13075	3.696	-25.86	-2.69	0.28	1	0	7	0
10	1	0	2003	52	0.79333	3.746	-24.31	2.13	6.52	1	0	8	0
15	1	0	2003	40	0.7702	4.228	24.91	2.77	3.62	1	0	6	0
17	1	0	2003	40	0.78207	4.959	24.72	2.05	2.06	1	0	7	0

- **Time is in the incorrect format**
- **Extra data columns present**
  - Remove extra columns, flip time and cell columns

MCNP-DSP

- **Modifications:**
  - Output given in data blocks of detector responses
  - Correlation between neutron interaction and gamma production
  - Six calculation modes
  - Angular distribution of prompt neutrons from fission
  - Uses a full fission probability distribution
    - Terrell or Zucker & Holden
- **Limitations:**
  - Based on outdated version of MCNP
    - Cannot use anything later than ENDF6
  - Doesn't generate list-mode data
  - Limited to four detector volumes plus one external source
  - No MPI or continue-run capabilities

MCNP-DSP Sample Output

- **Sample output:**

```
Detector Triggered Multiplicity
Neutron
Detector #  2
Value       Triggered          Random
    0             220            9776
    1             223               0
    2             223               0
    3             223               0
    4             223               0
    5             223               0
    6             223               0
    7             223               0
    8             222               1
    9             218               4
   10             218               0
   11             216               2
   12             216               0
   13             215               1
   14             215               0
   15             213               2
   16             212               1
```

- **Not list-mode data**
  - In this case, DSP has provided a multiplicity distribution as requested in the secondary input file
  - Time-distribution of counts was determined in secondary input file

Simulations

- **All simulations were run:**
  - Using the same geometry and material cards
  - With ENDF/B-VI.0
  - Using the same measurement parameters
    - no dead time
    - 300 second measurement time
      - 39424551 SF events (nps)
    - 512 μs gate width
    - Pu-240 as primary SF isotope
      - 5.954 wt%
    - Pu-239 as primary IF isotope
  - Running only neutrons (gammas are turned off)
- **KCODE and fixed source calculations were run using each code**
  - DSP cannot run KCODE or standard MCNP tallies

Calculations

- **The list-mode data were analyzed using a LANL-developed script that utilizes the Hansen-Dowdy formalism of the Feynman variance technique**
- **Several values were compared:**
  - **System eigenvalue** (*k*) as calculated using KCODE
  - **Inferred *k***
  - **Net multiplicity** (M_{net}) – weight of leaked neutrons + captured neutrons per starting particle
  - **Leakage multiplicity** (M_L) – ratio of number of neutrons that leak out of the system per starting particle
  - **Total multiplicity** (M_T) – ratio of total number of neutrons that are produced per starting particle
- **The inferred *k* was determined using the calculated total multiplicity in the equation:**

$$k = 1 - \frac{1}{M_T}$$

In-house Post-Processing Script

- **Sample PP Output:**

```
...
The first moments are 3.92402937517173 +/- 0.00291732301296148
The second moments are 20.3847751550081 +/- 0.0291864736218494
The third moments are 127.071685181171 +/- 8.03521692926335e-05
The fourth moments are 914.668781797360
Average deadtime = 0
Ymu = 0.270828564472513
Yu = 0.270828564472513
Yu1 = 0.270828564472513
Correction = 1
First multiplication is 5.74390148726517
##################################################
The efficiency is 0.00394760637529606
The randoms ratio is 0.00154240164021351
The transmission ratio is 0.996440822885869
The total multiplication is 5.74390148726517
The leakage multiplication is 3.9412189221044
The calculated SNM mass is 8082.40107258589 grams
```

Results – Keff and Multiplication comparison

Code	KCODE	St Dev	1/(1-k)	inferred k	Mnet	ML	MT	% Difference
BeRP Ball - Bare Case								
MCNP5 w/patch	0.77791	0.00006	4.5027	0.82407	3.191	3.9041	5.6841	5.93%
MCNPX v 2.7.0	0.77787	0.00005	4.5019	0.82558	3.167	3.9347	5.7334	6.13%
MCNPX-PoliMi	0.77783	0.00006	4.5021	0.82573	8.276	3.9376	5.7381	6.16%
MCNP-DSP	---	---	---	0.91860	7.293	7.0603	12.2846	---
BeRP Ball - 0.5in HDPE Reflected Case								
MCNP5 w/patch	0.82624	0.00006	5.7551	0.86762	4.019	5.0634	7.5539	5.01%
MCNPX v 2.7.0	0.82621	0.00007	5.7541	0.86868	4.035	5.1013	7.6150	5.14%
MCNPX-PoliMi	0.82634	0.00006	5.7584	0.86756	10.275	5.0615	7.5507	4.99%
MCNP-DSP	---	---	---	0.93030	9.508	8.1677	14.3468	---
BeRP Ball - 1in HDPE Reflected Case								
MCNP5 w/patch	0.86897	0.00008	7.6318	0.90162	5.324	6.6822	10.1648	3.76%
MCNPX v 2.7.0	0.86897	0.00008	7.6318	0.90339	5.362	6.7976	10.3510	3.96%
MCNPX-PoliMi	0.86905	0.00007	7.6365	0.90239	13.340	6.7320	10.2451	3.84%
MCNP-DSP	---	---	---	0.94090	12.927	9.5494	16.9196	---
BeRP Ball - 1.5in HDPE Reflected Case								
MCNP5 w/patch	0.90136	0.00009	10.1379	0.92563	7.052	8.7165	13.4459	2.69%
MCNPX v 2.7.0	0.90143	0.00009	10.1451	0.92774	7.145	8.9596	13.8381	2.92%
MCNPX-PoliMi	0.90151	0.00008	10.1533	0.92677	17.416	8.8467	13.6560	2.80%
MCNP-DSP	---	---	---	0.94355	17.335	9.9757	17.7134	---
BeRP Ball - 3in HDPE Reflected Case								
MCNP5 w/patch	0.93685	0.00008	15.8353	0.95169	11.252	13.2141	20.7001	1.58%
MCNPX v 2.7.0	0.93671	0.00010	15.8003	0.95179	11.169	13.2415	20.7444	1.61%
MCNPX-PoliMi	0.93683	0.00008	15.8253	0.95119	26.660	13.0811	20.4857	1.53%
MCNP-DSP	---	---	---	0.95046	27.190	11.3027	20.1844	---

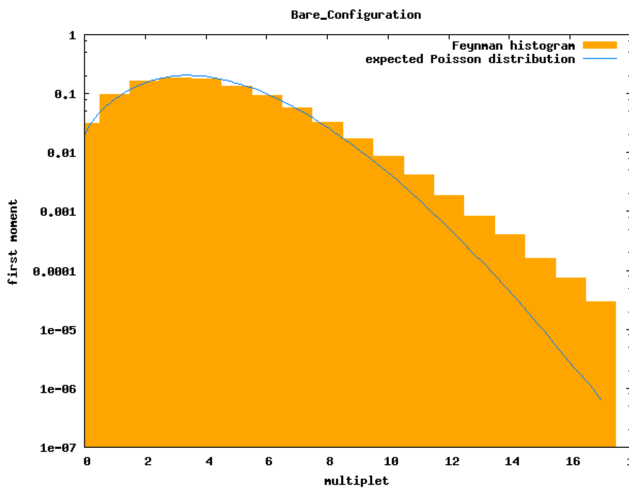
Results – Feynman Window Width Comparison

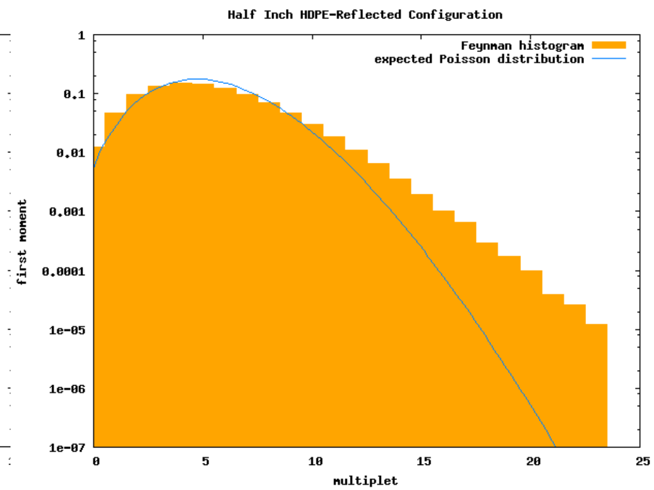
Code	Window Width (μs)	First Moment	Uncertainty	Second Moment	Uncertainty	M_T	M_L
MCNP5p	256	1.950	0.001	6.195	0.008	5.508	3.795
Bare	512	3.899	0.003	20.137	0.029	5.684	3.904
	1024	7.799	0.006	70.857	0.104	5.796	3.974
MCNPX	256	1.960	0.001	6.259	0.009	5.559	3.827
Bare	512	3.920	0.003	20.350	0.029	5.733	3.935
	1024	7.841	0.006	71.579	0.105	5.802	3.977
MCNPX-PoliMi	256	1.957	0.001	6.238	0.009	5.545	3.818
Bare	512	3.913	0.003	20.287	0.029	5.738	3.938
	1024	7.827	0.006	71.351	0.105	5.817	3.986
MCNP5p	256	2.612	0.002	10.470	0.014	7.314	4.914
Half-inch	512	5.224	0.004	34.936	0.048	7.554	5.063
	1024	10.448	0.007	124.833	0.174	7.677	5.140
MCNPX	256	2.632	0.002	10.626	0.014	7.389	4.961
Half-inch	512	5.264	0.004	35.457	0.049	7.615	5.101
	1024	10.528	0.007	126.759	0.177	7.762	5.193
MCNPX-PoliMi	256	2.631	0.002	10.600	0.014	7.320	4.918
Half-inch	512	5.263	0.004	35.397	0.048	7.551	5.061
	1024	10.525	0.007	126.587	0.176	7.688	5.147
MCNP5p	256	3.368	0.002	16.932	0.022	9.759	6.431
1-inch	512	6.735	0.005	57.397	0.078	10.165	6.682
	1024	13.470	0.009	206.356	0.285	10.329	6.784
MCNPX	256	3.407	0.002	17.356	0.023	9.951	6.550
1-inch	512	6.814	0.005	58.809	0.081	10.351	6.798
	1024	13.627	0.009	211.379	0.293	10.531	6.909
MCNPX-PoliMi	256	3.409	0.002	17.321	0.023	9.844	6.483
1-inch	512	6.818	0.005	58.754	0.080	10.245	6.732
	1024	13.635	0.009	211.387	0.292	10.434	6.849

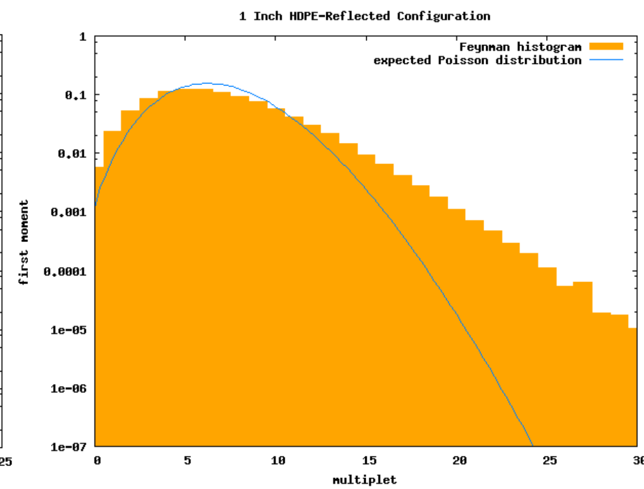
Results – Feynman Window Width Comparison

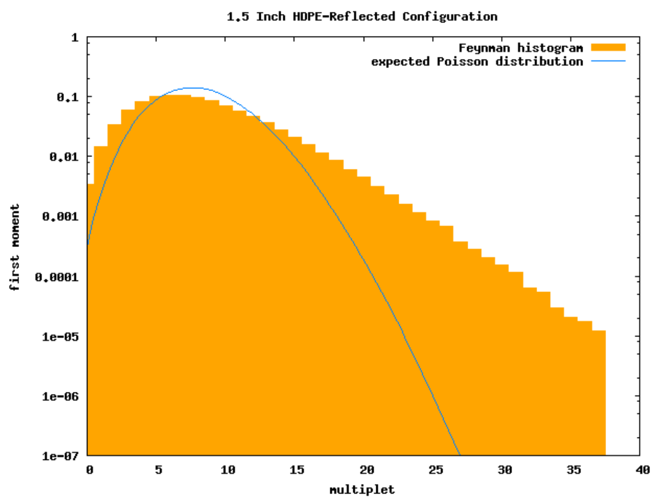
Code	Window Width (μs)	First Moment	Uncertainty	Second Moment	Uncertainty	M_T	M_L
MCNP5p 1.5-inch	256	4.057	0.003	24.383	0.033	12.844	8.343
	512	8.114	0.006	83.595	0.118	13.446	8.716
	1024	16.228	0.011	301.044	0.431	13.766	8.915
MCNPX 1.5-inch	256	4.126	0.003	25.308	0.034	13.211	8.571
	512	8.251	0.006	86.726	0.124	13.838	8.960
	1024	16.503	0.012	311.872	0.452	14.138	9.145
MCNPX-PoliMi 1.5-inch	256	4.127	0.003	25.216	0.034	13.039	8.464
	512	8.254	0.006	86.507	0.123	13.656	8.847
	1024	16.508	0.012	311.544	0.447	13.978	9.046
MCNP5p 3-inch	256	3.962	0.003	23.577	0.032	19.547	12.499
	512	7.924	0.006	82.235	0.126	20.700	13.214
	1024	15.847	0.012	296.026	0.483	21.678	13.820
MCNPX 3-inch	256	3.938	0.003	23.340	0.032	19.586	12.523
	512	7.877	0.006	81.369	0.125	20.744	13.242
	1024	15.754	0.012	292.860	0.480	21.754	13.867
MCNPX-PoliMi 3-inch	256	3.934	0.003	23.216	0.032	19.369	12.389
	512	7.867	0.006	80.935	0.124	20.486	13.081
	1024	15.735	0.012	291.478	0.474	21.457	13.684

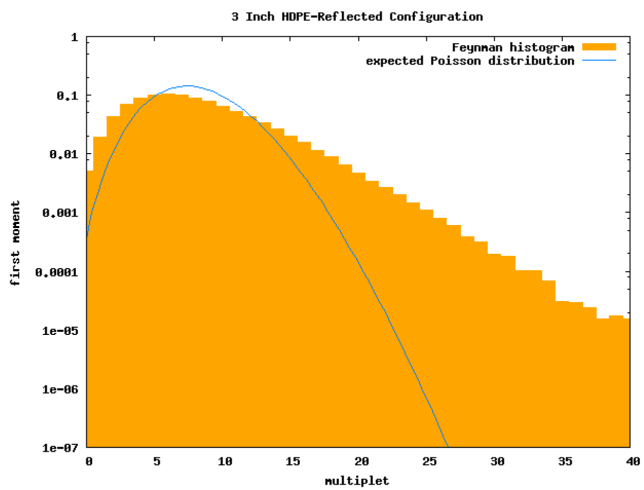
Results – Feynman Histograms











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Summary

- **All of the codes can output some form of list-mode data, except for MCNP-DSP**
- **There are significant differences between the k_{eff} values obtained via KCODE and the modified fixed source methods**
- **MCNP5 w/multiplcation patch, MCNPX w/PTRAC, and MCNPX-PoliMi show good agreement in the inferred *k* calculations for all configurations**
- **Ease of use:**
  - MCNP5 w/patch and MCNPX can be run in MPI mode
  - MCNP5 w/patch output file contains pure list-mode data; output files for MCNPX w/PTRAC and MCNPX-PoliMi required manipulation (e.g., Perl script) to obtain similar format

Future Work

- **Model and compare configurations from other experiments**
- **Compare these results or the simulated results from another configuration to purely experimental results**
  - These experiments have been completed and the data are available for comparison!
- **Include gamma rays in the simulations**

References

- G. ESTES, C. GOULDING, "Subcritical Multiplication Determination Studies," *LA-UR-95-2016*, Los Alamos National Laboratory, Los Alamos, New Mexico (1995).
- C. SOLOMON, "Modifications to the MCNP5 Multiplication Patch", *LA-UR-11-04711*, Los Alamos National Laboratory, Los Alamos, NM (2011).
- A. SOOD, C. SOLOMON, J. HUTCHINSON, W. MYERS, "Direct Calculation of Measured Observables in a Multiplying Subcritical System," *LA-UR-11-01249*, Los Alamos National Laboratory, Los Alamos, New Mexico (2011).
- E. SHORES, B. TEMPLE, "Metallic Plutonium Sphere Multiplication Calculations," LA-UR-08-2357, Los Alamos National Laboratory, Los Alamos, New Mexico (2008).
- X-5 MONTE CARLO TEAM, *MCNP - A General Monte Carlo N-Particle Transport Code, Version 5*, Los Alamos National Laboratory, Los Alamos, NM (2003).
- *MCNPX User's Manual, Version 2.7.0*, Los Alamos National Laboratory, Los Alamos, New Mexico (2011).
- T. VALENTINE, *MCNP-DSP User's Manual*, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2001).
- S. POZZI, et al, *Introduction to MCNPX-PoliMi*, University of Michigan, Ann Arbor, Michigan.
- T. VALENTINE, "Polyethylene-Reflected Plutonium Metal Sphere Subcritical Noise Measurements," *SUB-PU-MET-FAST-001*, International Criticality Safety Benchmark Evaluation Project (2009).
- J. HUTCHINSON, C. SOLOMON, A. SOOD, W. MYERS, M. SMITH-NELSON, "Comparison of Feynman Variance-to-Mean Measurements Using Measured and Simulated Data," *Proc. International Conference on Nuclear Criticality*, Edinburgh, Scotland, September 19–22, 2011, ICNC (2011).
- J. A. THIE, *Power Reactor Noise*, American Nuclear Society, La Grange Park, Illinois, USA (1981).
- M. SMITH-NELSON, K. BUTTERFIELD, W. GEIST, D. MAYO, E. SHORES, B. ROONEY, D. DINWIDDIE, "Neutron Specialist Handbook and Informational Text," *LA-UR-07-6170*, Los Alamos National Laboratory, Los Alamos, New Mexico (2007).