LA-UR-14-27061

Use of Fission Data in MCNP6

Michael James

FIESTA 2014 Workshop

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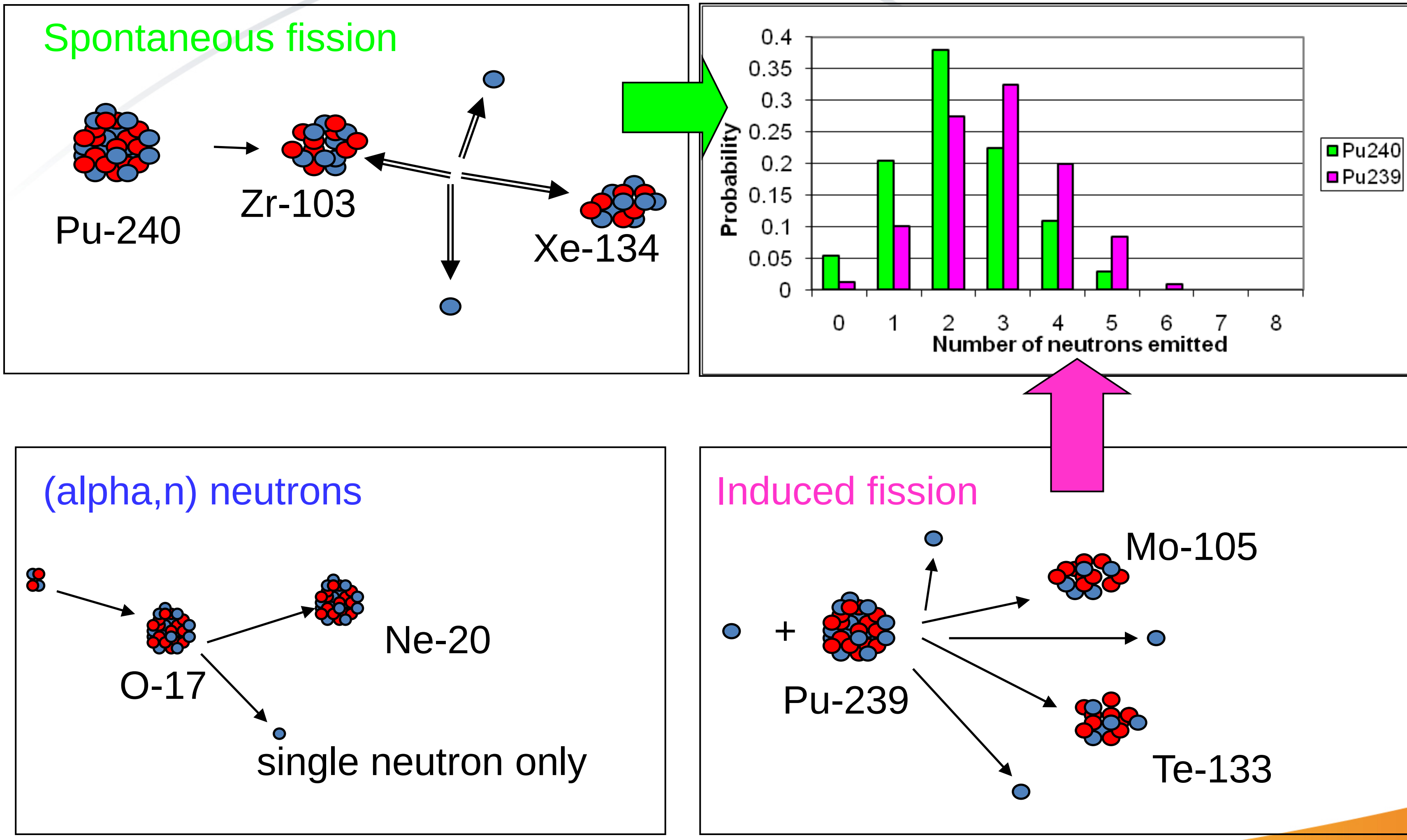
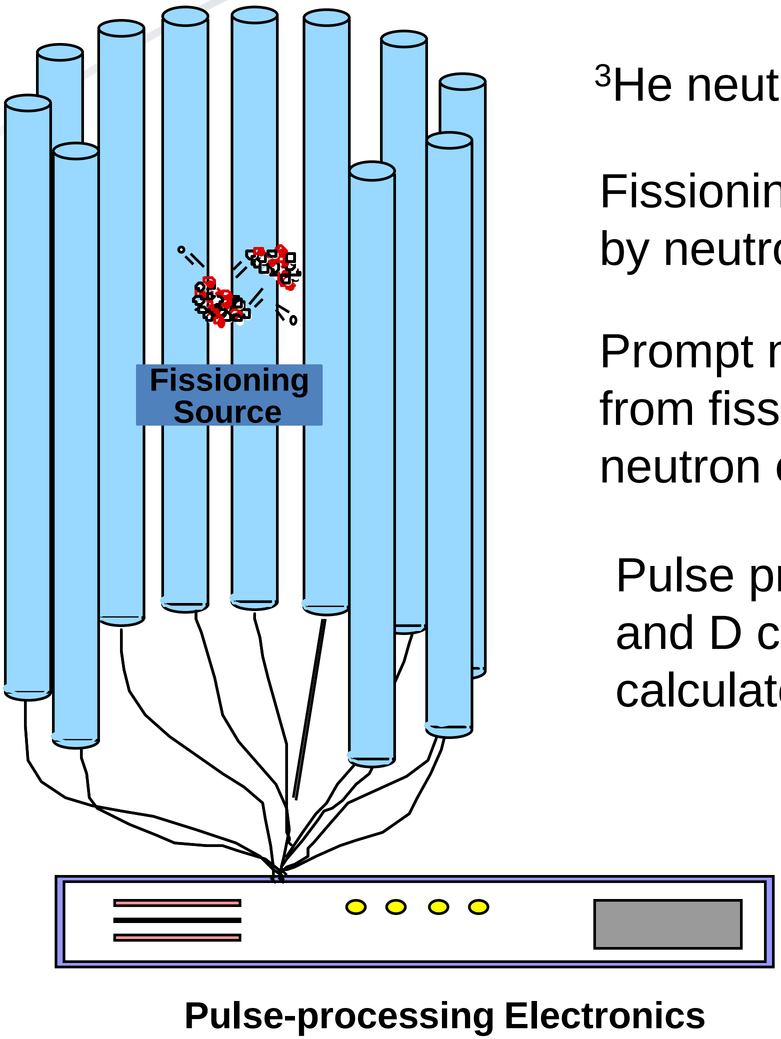
Outline

- Introduction
- Detection - Fission multiplicity
- Detection - Delayed particles
- Burnup – Fission yields, Q value
- Summary

Neutron Signatures



Passive Neutron Counter



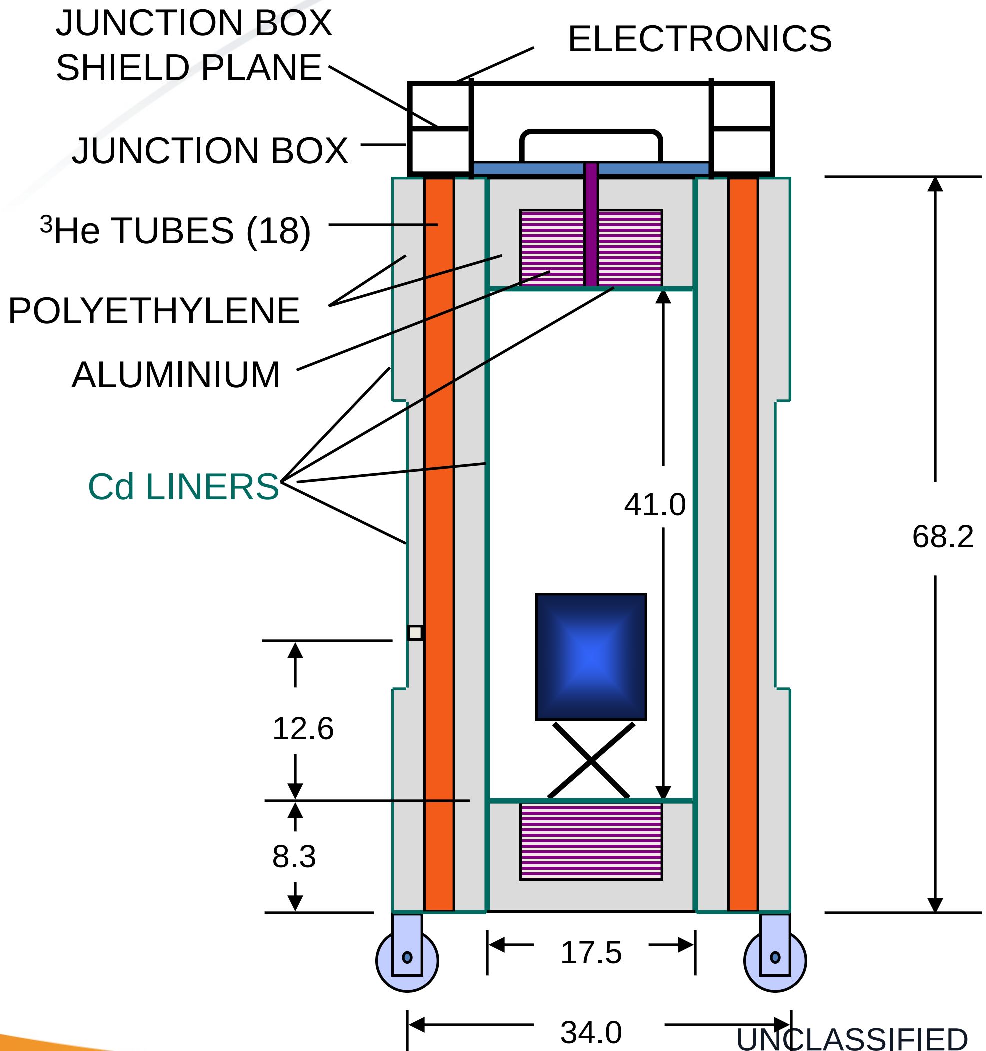
^{3}He neutron detectors

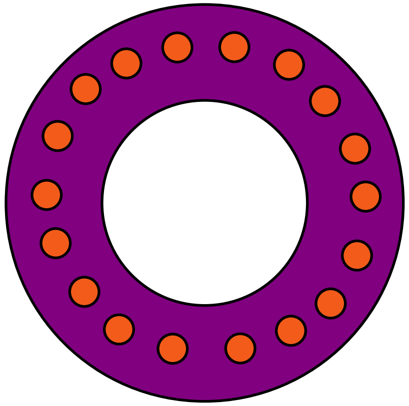
Fissioning source surrounded by neutron detectors

Prompt multiple neutron emission from fission detected as coincidence neutron events

Pulse processing electronics count the S and D count rates, which are used to calculate the mass of fissioning isotopes

HLNCC


JUNCTION BOX
SHIELD PLANE
ELECTRONICS
JUNCTION BOX
³He TUBES (18)
POLYETHYLENE
ALUMINIUM
Cd LINERS
41.0
68.2
12.6
8.3
17.5
34.0

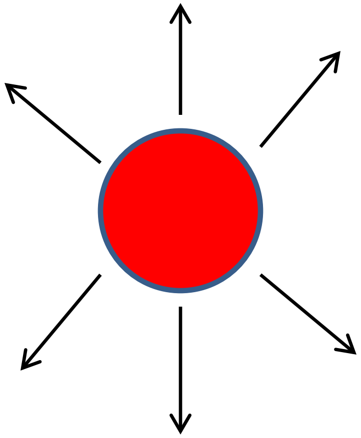


Multiplicity Treatments in MCNP

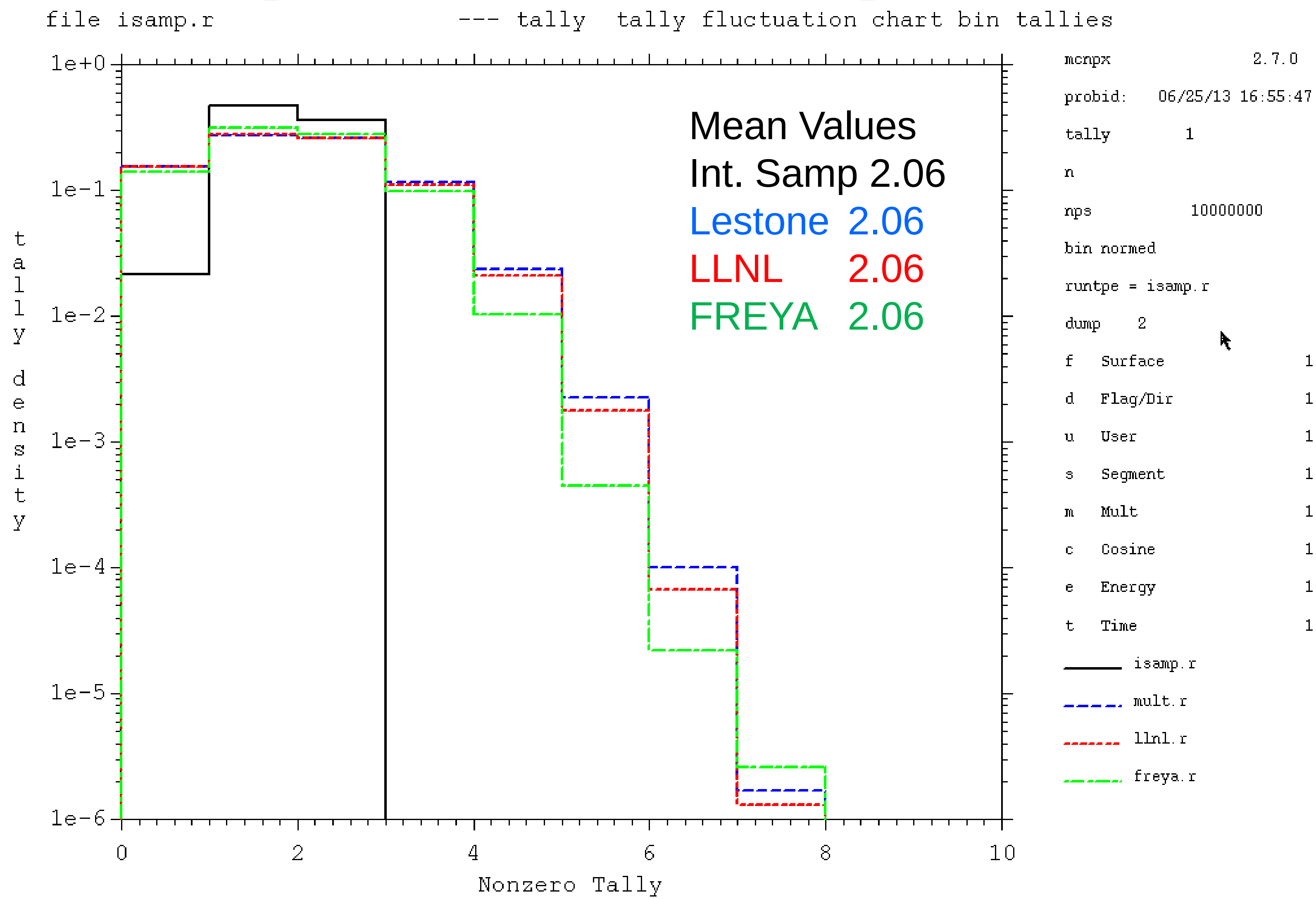
- Several options for simulating fission multiplicity have been added to MCNP in the last few years.
  - Spontaneous multiplicities from Enslinn (LA-13422)
  - Induced multiplicities from Lestone (LA-UR-05-0288)
  - LLNL Fission Library (UCRL-AR-228518)
- Invoked with FMULT card
  - "All or nothing" approach - the chosen multiplicity model is applied to all fissions (SF and Induced).

Fission Multiplicity Treatments in MCNP

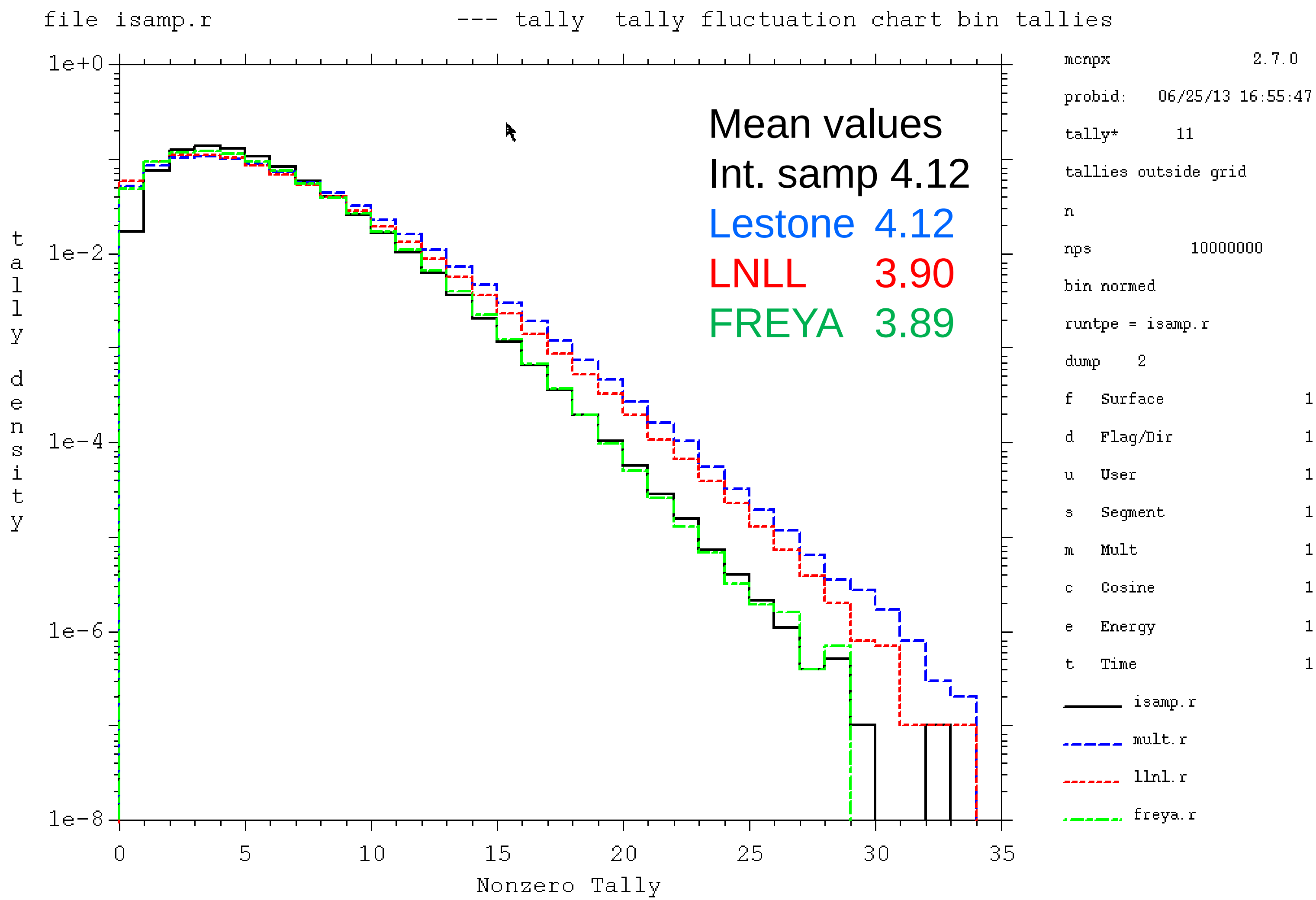
- Start a thermal neutron in U-235
- 83.7% Fissions
- All results use the Tally Probability Density Function to compare history scores (modified to score in integer values).
- Run neutron source in sphere with 1st interaction (lca 7j -2).
- Tally crossings (F1) and energy of crossings (*F11) on sphere surface.
- Neutron multiplicities should agree overall for most physics.
- Total Neutron Energy per Fission should show higher "tail" for uncorrelated treatments. Large multiplicity values sample from same energy functions resulting in higher energy totals.
- Compare Integer sampling, default multiplicity treatment (Lestone), LLNL library and FREYA.



Neutron Multiplicity

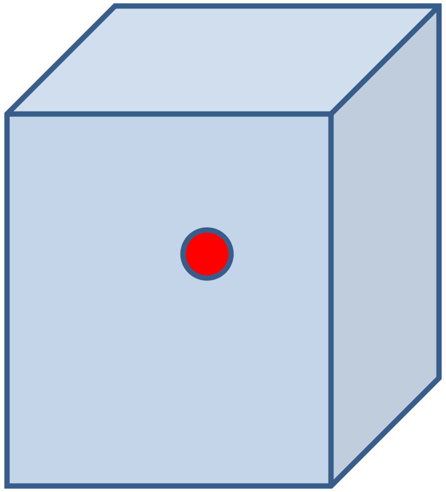


Total Neutron Energy per fission



Angular Correlation

- Place source in cube, run 1st interaction (lca 7j -2).
- Tally on opposite faces and adjacent faces.
  - 3 tallies on opposite facets (1.1+1.2, 1.3+ 1.4, 1.5+1.6)
  - 3 tallies on adjacent facets (1.1+1.5, 1.2+1.4, 1.3+1.6)
- If neutron emissions correlate along vector line, then opposite faces should see higher neutron counts/multiplicities.



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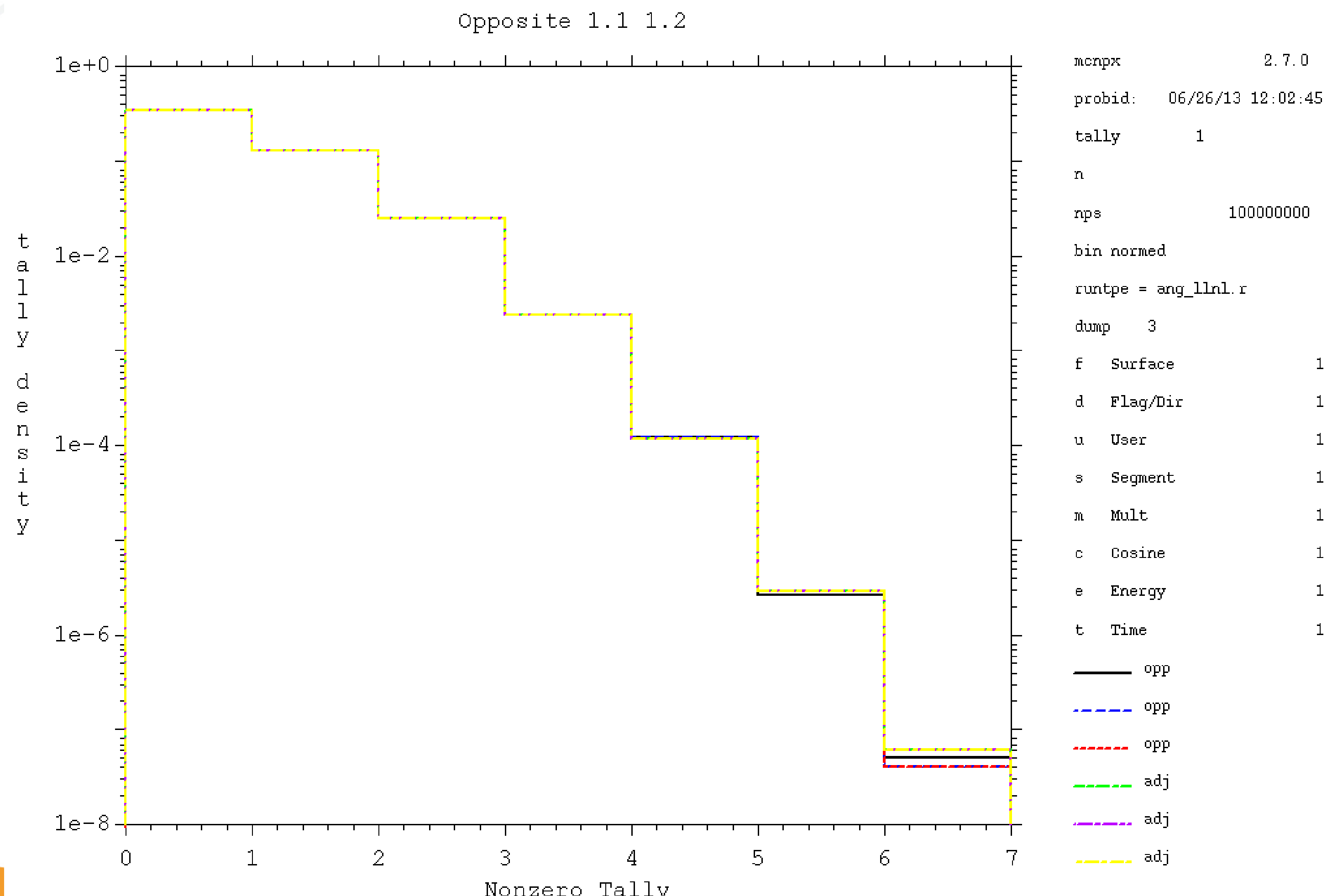
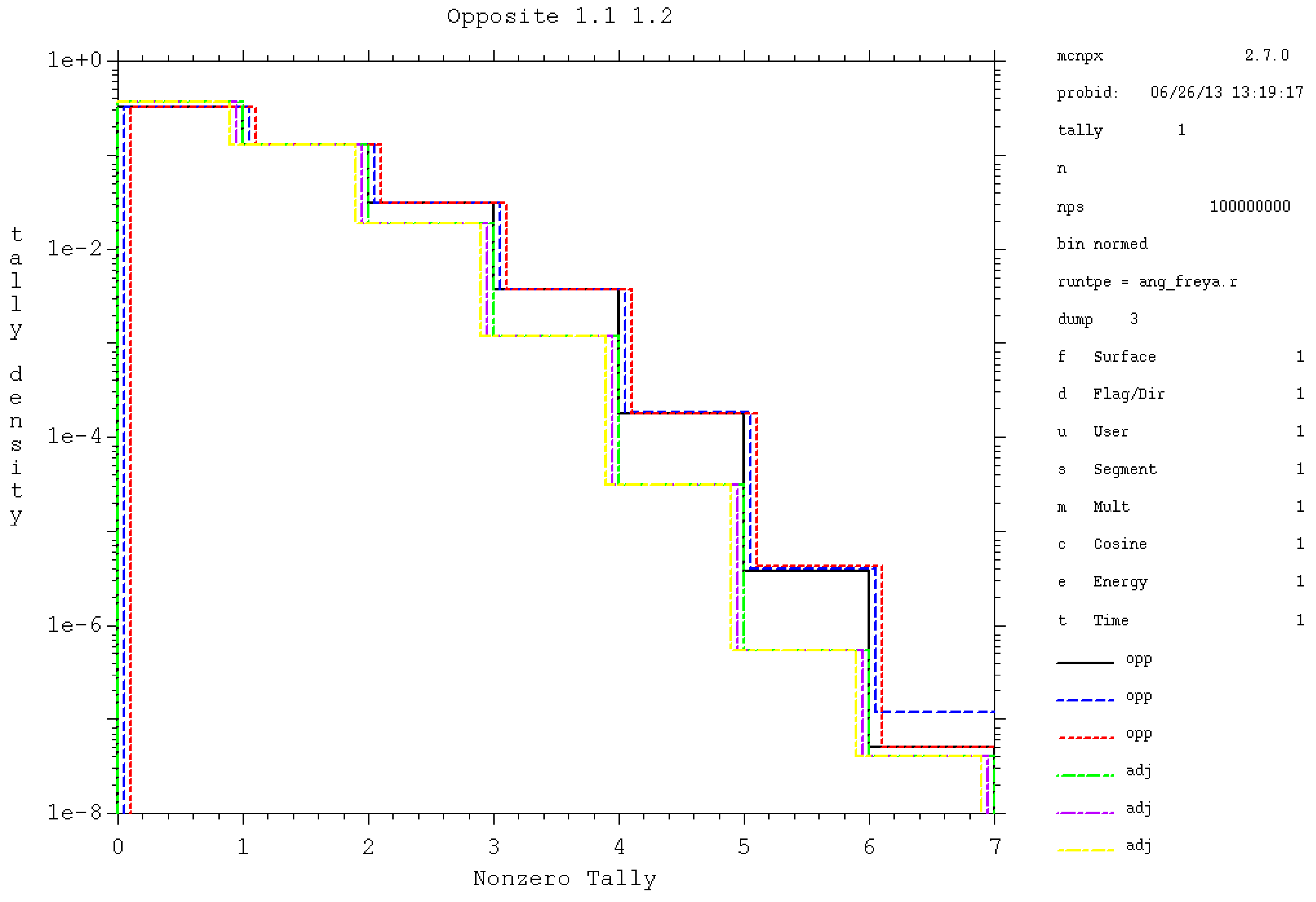
LLNL Fission Library

LLNL is isotropic and uncorrelated, all tallies are identical.



FREYA

FREYA results show three opposite-surface tallies are larger than three adjacent-surface (curves are displayed with small x-axis offsets for clarity).



Fission Neutron Multiplicity

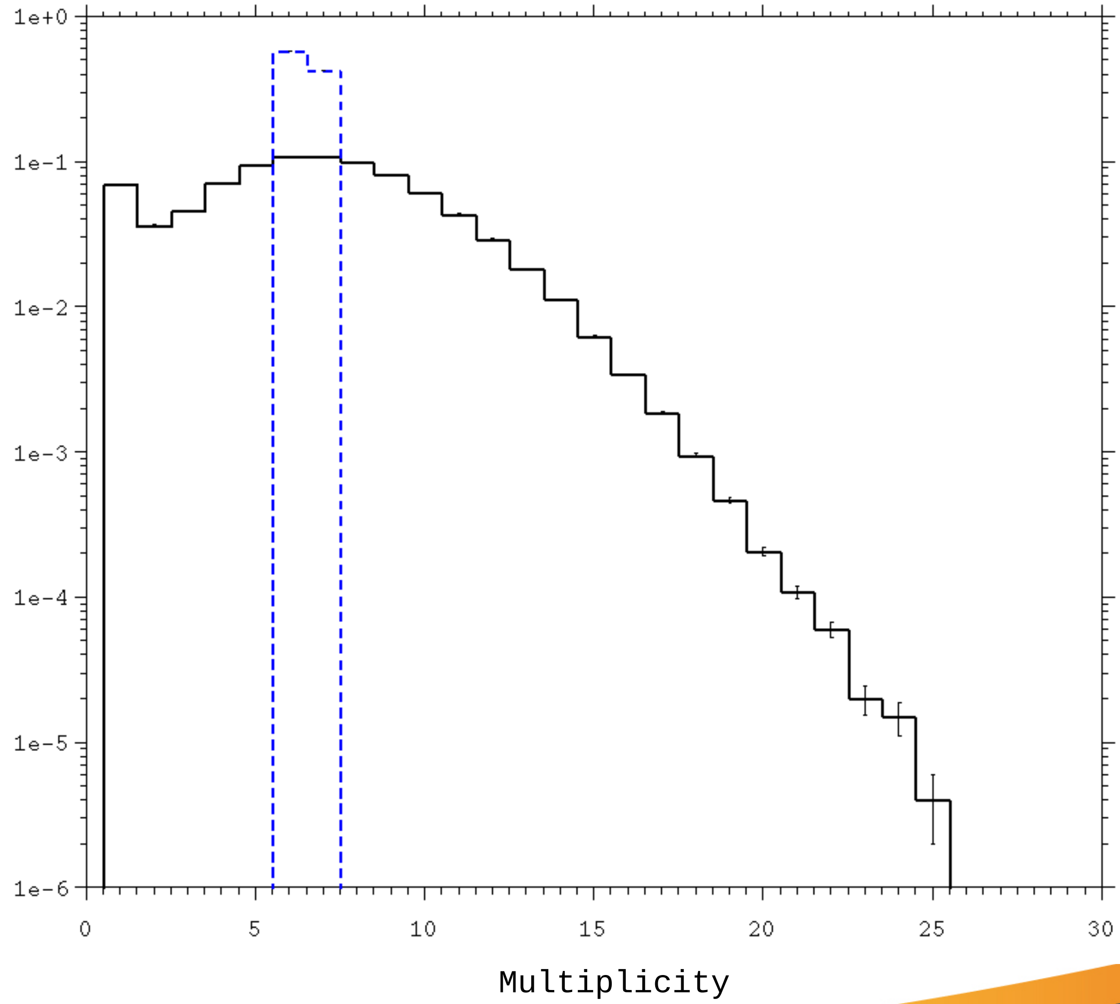
- Standards MCNP6 Treatment is integer sampling.
- Several fission models can be used for multiplicity.
- All emit uncorrelated neutrons in energy and angle.
- Mode detailed physics(CGMF and/or FREYA) would provide better detailed distributions with correlations.

Fission Gamma Multiplicity

- Standard Treatment in MCNP6 is integer sampling.
- LLNL Fission library provides Gaussian distribution.
- Need better model for correlations to preserve spectra/energy and multiplicity?

Fission Gamma Multiplicity

Base fission gamma multiplicity in MCNP6 (blue) compared to LLNL fission model (black).



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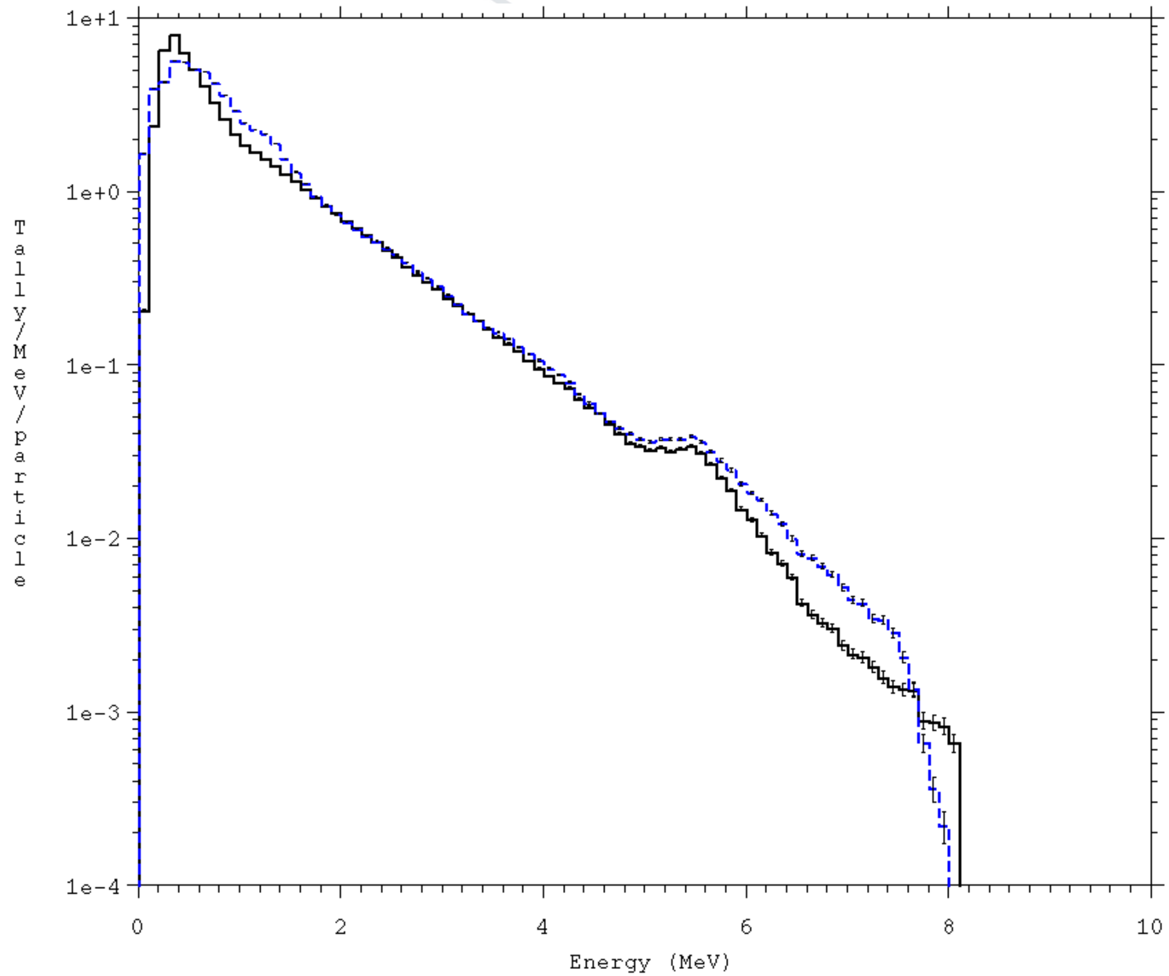
Fission Gamma Multiplicity

Fission gamma spectrum in MCNP6 (blue) compared to LLNL fission model (black).



Multiplicity

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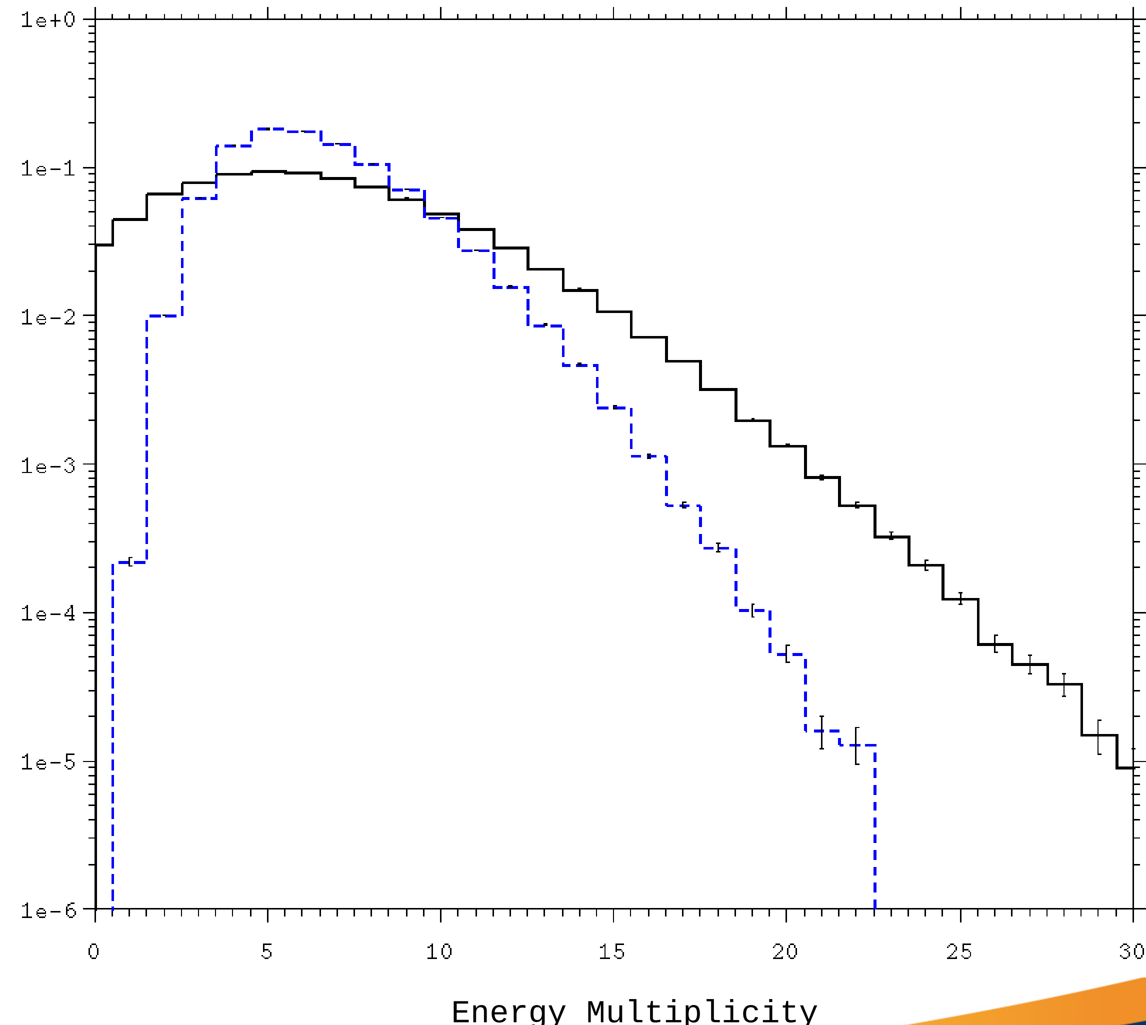
Fission Gamma Multiplicity

Overall Fission gamma energy in MCNP6 (blue) compared to LLNL fission model (black).

Gamma energy/fission:
Default: 6.44
LLNL: 5.83



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Delayed Particle Physics

- The need arose to compute signals from active interrogation scenarios.
- Leverage the existing CINDER code in MCNP to produce time-dependent isotopics.
- Fission sampling uses existing fission product distributions in CINDER (cinder.dat).
- FP Distributions are from
  - Thermal reactor
  - Fast Reactor
  - 14-MeV source
- MCNP can integrate over FP distribution to gather either coarse binwise spectrum of 25 groups or detailed line spectrum.

CINDER90 in MCNP6

- What is there?
  - FP yields for many isotopes at 3 energies
  - Decay information for 3360 isotopes (half-life, branching ratios, decay products)
  - 25 group decay gamma spectra
  - 63 group cross sections for many reactions.
  - Mostly from ENDF/B-VI
  - Photonuclear FP yields from GEF* Code added by NEN-5.

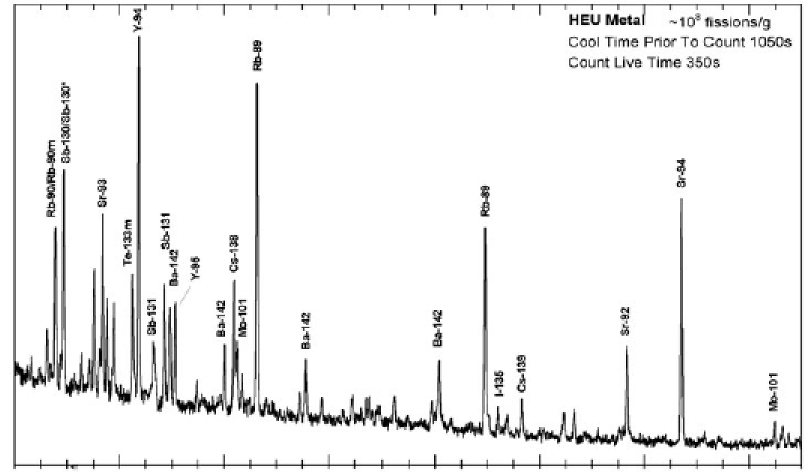
*Schmidt, K. H., Jurado, B., "General Model Description of Fission Observables," CENBG CNRS/IN2P3 Report, France, October (2010).Available at http://www.cenbg.in2p3.fr/GEF

CINDER90 in MCNP6 – cont.

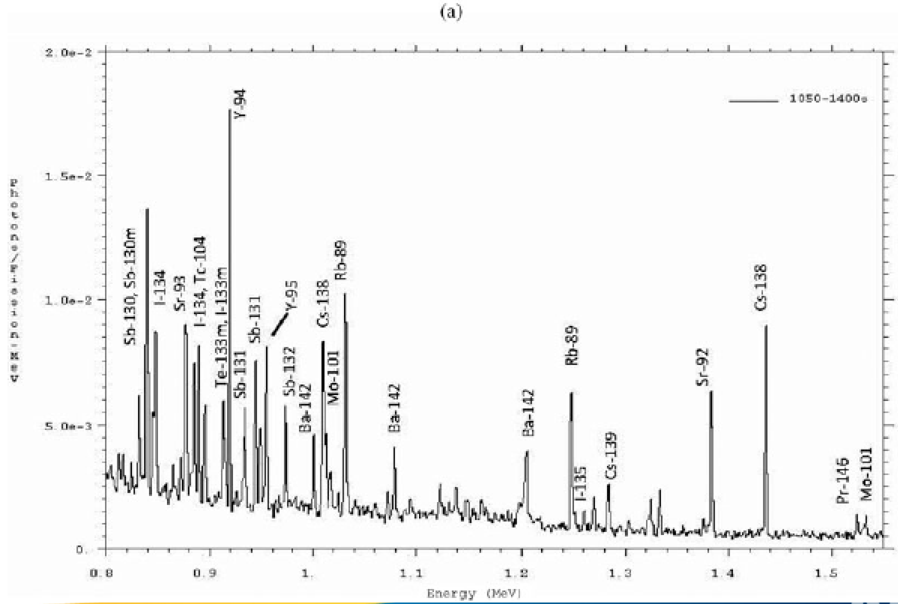
- What is there?
  - Markov chain solver for evolution of isotopes.
  - Post-processing code reports decay gamma spectra at each time step.

Qualitative benchmark of DG

- Compared results to Beddingfield experiments.
- Much of the structure was captured although some differences were also clear.



(a)



Delayed Neutrons

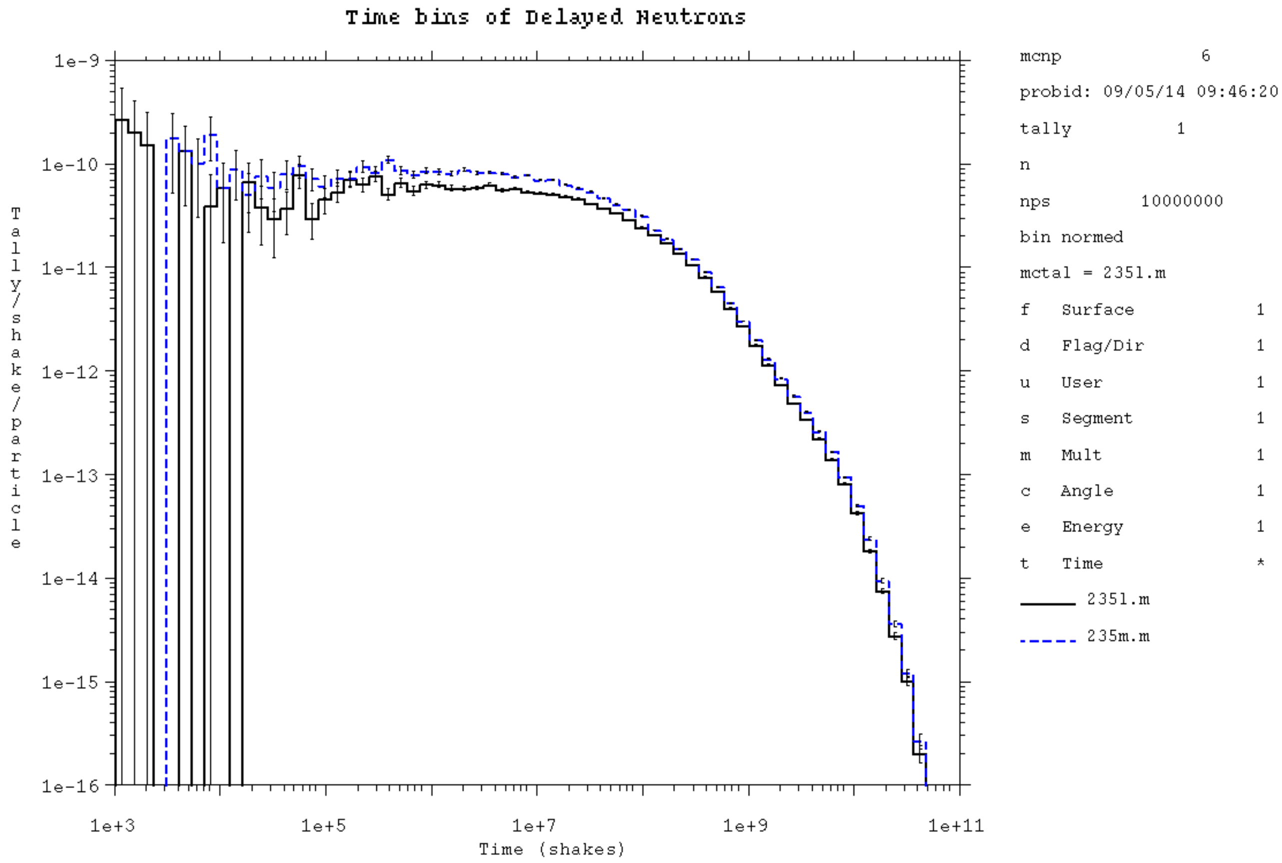
- MCNP has historically done delayed particles using six-group formulation from ENDF and sampling a specified energy spectrum.
- The delayed particle feature allows us to build a custom delayed-neutron precursor from the FP set and sample for time and energy.
- Data files delay_library_v3.dat contains decay neutron information for 279 isotopes.
- This process is much slower!

DN from U-235 Results

DN Fraction:

ENDF: 0.00656

MCNP/CINDER 0.00773



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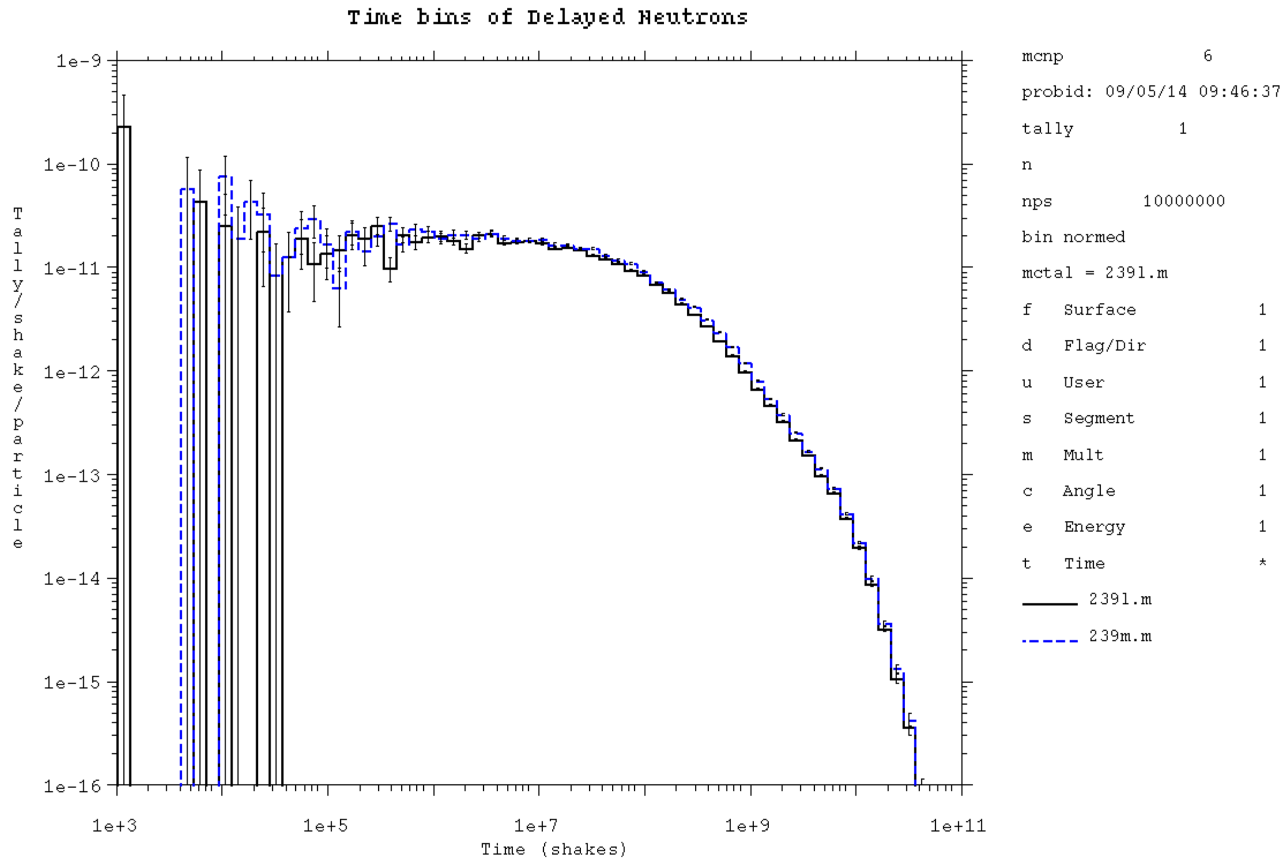
DN from Pu-239 Results

DN Fraction:

ENDF:	0.00226
MCNP/CINDER	0.00257



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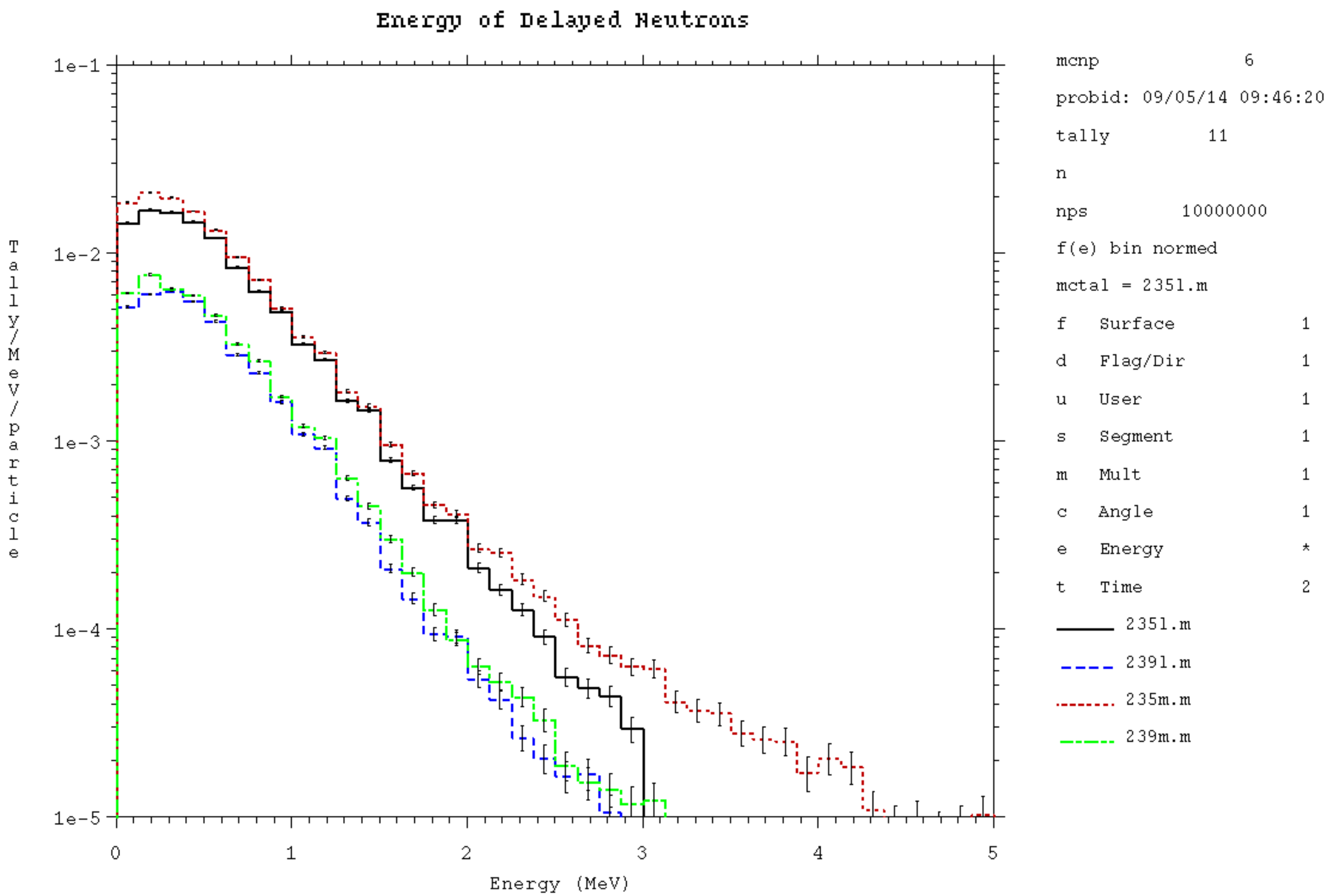
DN Spectra

U-235 ENDF
U-235 MCNP/CINDER
Pu-239 ENDF
Pu-239 MCNP/CINDER



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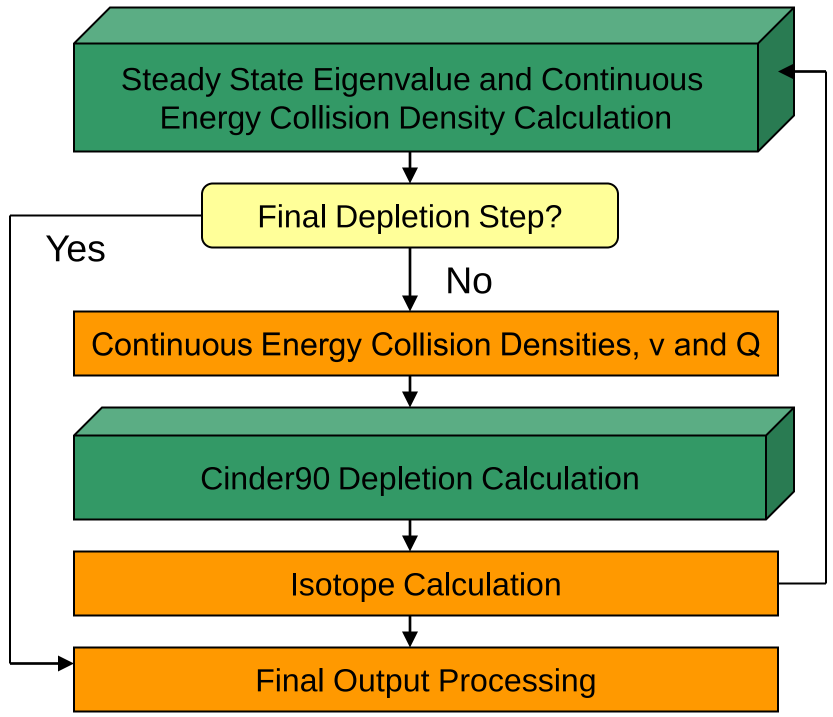
Burnup/Depletion Capability in MCNP6

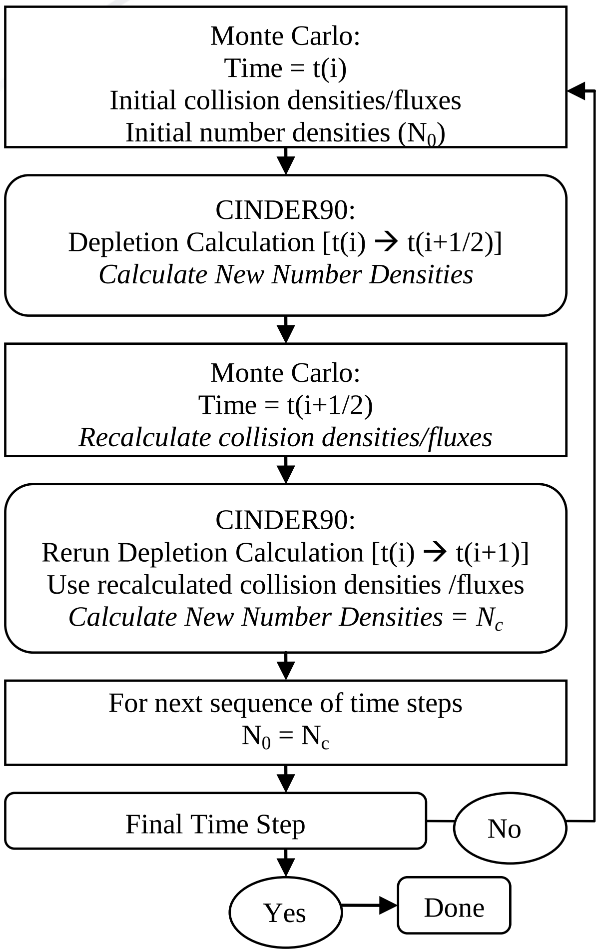
- Show flowchart
- Ability to track isotopic evolution in critical systems.
- Relies on CINDER for data/algorithms.

Monte Carlo Linked Depletion Process

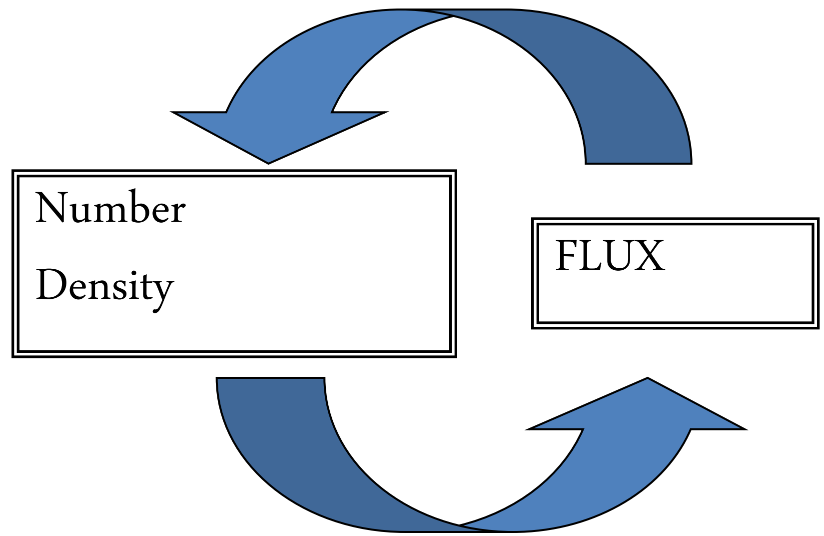


- Steady state Monte Carlo using MCNPX, depletion utilizing CINDER90

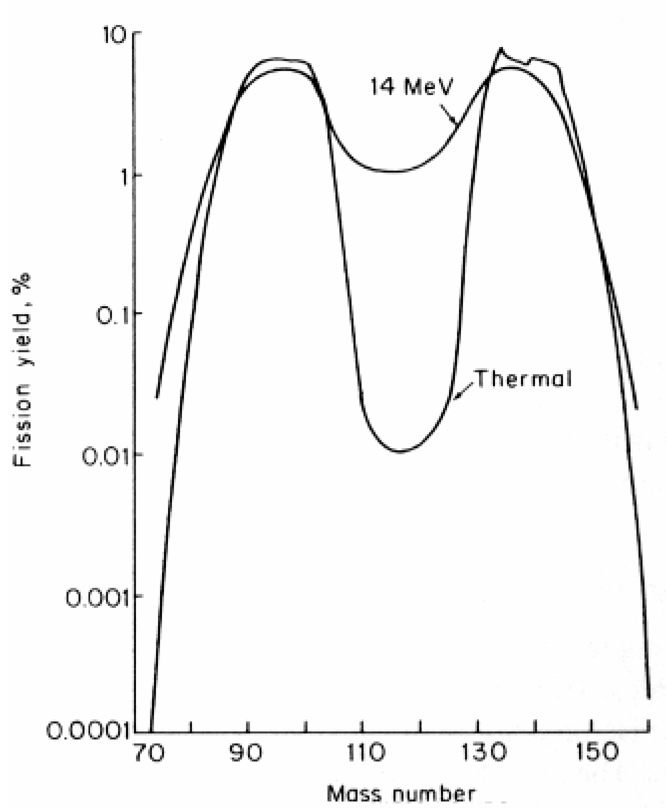
Predictor Corrector



$$N(r,t) = N(r,0)e^{-\sum_{i=0}^{E} \sigma(r,E) \int_{t1}^{t2} \phi(r,t')dt'}$$



FP Yield Energy Dependence



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FP Yield Data Available

Element	Z	A	Thermal	Fast	HE	SF
Th	90	227	x			
Th	90	229	x			
Th	90	232		x	x	
Pa	91	231		x		
U	92	232	x			
U	92	233	x	x	x	
U	92	234		x	x	
U	92	235	x	x	x	
U	92	236		x	x	
U	92	237		x		
U	92	238		x	x	x
Np	93	237	x	x	x	
Np	93	238		x		
Pu	94	238		x		
Pu	94	239	x	x	x	
Pu	94	240	x	x	x	
Pu	94	241	x	x		
Pu	94	242	x	x	x	

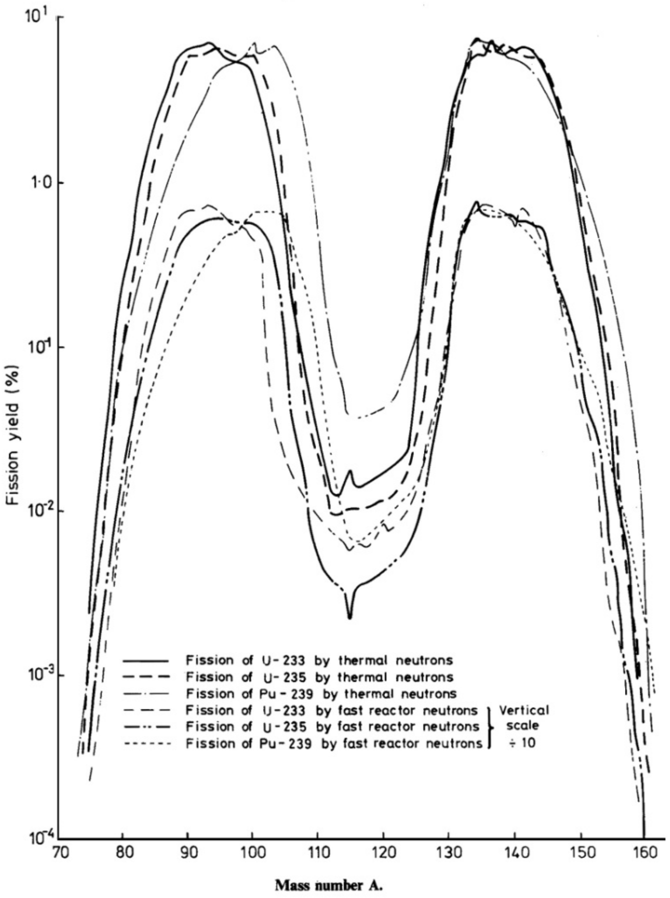
Element	Z	A	Thermal	Fast	HE	SF
Am	95	241	x	x	x	
Am	95	242m	x			
Am	95	243		x		
Cm	96	242		x		
Cm	96	243	x	x		
Cm	96	244		x		x
Cm	96	245	x			
Cm	96	246		x		x
Cm	96	248		x		x
Cf	98	249	x			
Cf	98	250				x
Cf	98	251	x			
Cf	98	252				x
Es	99	253				x
Es	99	254	x			
Fm	100	254				x
Fm	100	255	x			
Fm	100	256				x

- Transmutation chain data for 3400 isotopes
- Fission Yield Data for 1325 isotopes
  - Thermal: 18 isotopes, Fast: 22 isotopes, HE: 11 isotopes, S.F.: 9 isotopes

FP Yield Nuclide Dependence

Open Cinder.dat

- Go to second “#3215"
- 12,13,14 =(n,f) yield sets
- Go to “Fission Yield”



Recoverable Energy per Fission

$$Q_{recoverable} = Q_{prompt} + Q_{delayed} + (\bar{\nu}(E) - k_{eff})*Q_{capture\ \gamma} - Q_{neutrino}$$

- Prompt Q value is usually determined from ENDF tape
  - File 1 MT 458

- Delayed Q value may be estimated assuming local energy deposition
  - Deposited gamma energy may need adjustment
    - 207 of 390 isotopes contain capture gamma data in ENDF VII.0

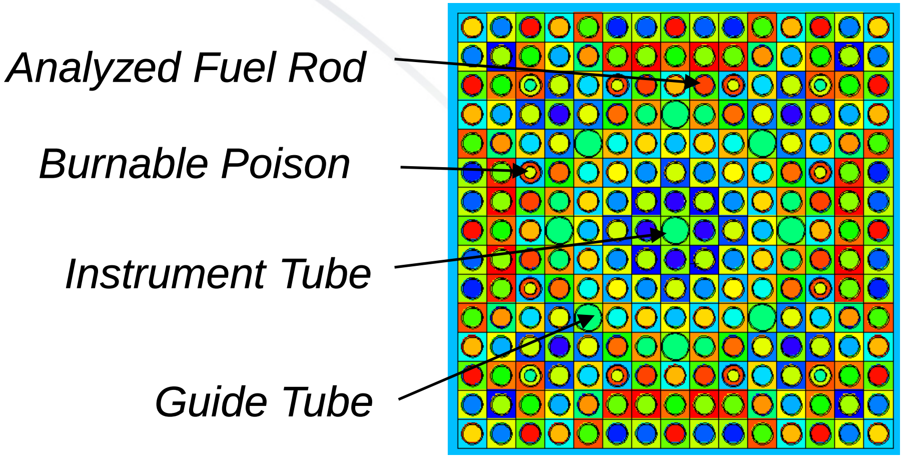
Emitted and recoverable energy for fission of U-235

Form	Emitted Energy (MeV)	Recoverable Energy (Mev)
Fission Fragments	168	168
Fission Product Decay		
γ -rays	8	8
β-rays	7	7
neutrinos	12	--
Prompt gamma rays	7	7
Fission neutrons (kinetic energy)	5	5
Capture γ-rays	**--**	**3-12**
Total	**207**	**198-207**

- Prompt Q not available for all actinides.
  - Qfis array on MCNP is incomplete and ad-hoc (ENDF-VI, JEFF-3.1, ??)
  - Data present for 22 isotopes (64 actinides in ENDF-VII)
- Capture gamma data incomplete.

H. B. Robinson

- 15 X 15 Westinghouse fuel assembly from H. B. Robinson Unit 2
  - ORNL/TM-12667
  - ENDF/B VII.0 temperature dependent library
  - 16.02, 23.8, 28.47, and 31.66 GWD/MTU



Cycle	1	2	3	4
Operating Interval (days)	243.5	243.5	156	156
Downtime (days)	40	64	39	--**
Average Soluble Boron Concentration (ppm)	625.5	247.5	652.5	247.5

** 3936 for Cases A-B or 3637 for Cases C-D

Results

	Case A 16.02 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	3.73	0.42	0.60	2.62
236U	-3.43	-1.76	-1.50	-3.37
238U	0.06	0.12	0.10	0.17
238Pu	-2.69	-3.41	1.50	2.29
239Pu	5.59	0.27	7.00	2.01
240Pu	2.66	3.32	-1.50	4.22
241Pu	7.68	3.57	5.90	7.04
237Np	-3.23	-6.13	6.00	-2.76
99Tc	8.49	10.91	12.40	11.35
137Cs	-3.06	-1.12	0.20	-1.64

	Case B 23.8 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	3.71	-0.58	1.40	4.11
236U	-2.70	-1.90	-2.20	-3.09
238U	-0.60	-0.54	-0.60	-0.53
238Pu	-4.22	-3.86	0.90	0.83
239Pu	2.50	-0.37	7.70	1.31
240Pu	1.62	0.59	-4.20	1.61
241Pu	5.44	2.82	6.00	4.97
237Np	-4.88	-7.31	5.50	-5.55
99Tc	5.70	6.76	8.60	8.34
137Cs	-2.82	-1.88	-0.80	-2.22

Results

	Case C 28.47 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	-3.27	-11.80	-4.90	-2.44
236U	1.84	3.72	2.20	1.24
238U	0.47	0.47	0.50	0.54
238Pu	-11.04	-14.72	-6.50	-7.01
239Pu	-0.64	-9.22	5.30	-1.77
240Pu	2.09	-5.42	-4.90	1.14
241Pu	-5.08	-11.03	0.50	-4.72
237Np	3.03	2.43	14.30	2.45
99Tc	11.45	9.58	14.60	14.94
137Cs	0.11	-0.38	3.90	0.70

	Case D 31.66 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	-0.08	-9.66	3.30	5.98
236U	0.17	1.18	-0.40	-1.51
238U	-0.73	-0.73	-0.80	-0.89
238Pu	-8.58	-10.69	2.60	1.97
239Pu	-0.20	-8.66	12.80	6.00
240Pu	1.32	-6.52	-4.10	2.65
241Pu	-2.56	-8.79	9.10	2.71
237Np	1.58	3.08	18.40	7.91
99Tc	7.79	5.53	11.20	11.90
137Cs	-2.45	-3.09	1.50	-1.44

Notes on Results

- Results
  - **No code best predicts all isotopes at all burnups**
  - Creation and destruction is dictated by spectrum and geometry self-shielding; it is difficult to determine the specific reaction where the methods differ
  - **The difference in data or calculation setup may be generating the largest difference**
- Conclusions on MCNP6 burnup
  - Each actinide and Cs-137 was computed to within a few %
  - Tc-99 was computed to within 12%
- H.B Robinson
  - At 16-28 GWD/MTU → SCALE/SAS2H, MCNPX 2.6.0, MONTEBURNS and MCNP6 produces similar results
  - 31.66 GWD/MTU → MCNP6 produces “superior” results

Issues in Burnup

- Relies on FP data for specific systems.
  - Difficult to generalize to other systems.
- Estimate of Q value/Captured fission energy is limited by incomplete datasets.

Spontaneous Fission Rate of U-235

- “Pet Peeve”
- ENDF, SOURCES4C, CINDER use 1.05e-5 n/s-g (Branching ratio 7.2e-11)
  - Phys Rev C V.23 No. 3 (1981) p.1110
- MCNP6, Ensslin, Wikipedia use 2.99e-4 n/s-g (Branching ratio 2.0e-9)
  - Phys Rev V.86 No. 1 (1952) p.21
- These numbers differ by factor of 30!
- Why?!

Summary

- Historically MCNP used fission cross sections and (integer samping).
- Multiple other kinds of fission data have been incorporated (multiplicity, FP distributions).
- There is a need and interest in adding more fidelity to these datasets/models.