LA-UR-16-27301
Approved for public release; distribution is unlimited.

Title: MCNP: Simulating Correlated Data in Fission Events

Author(s): Rising, Michael Evan

Intended for: Advances in Nuclear Nonproliferation Technology and Policy Conference (ANTPC), 2016-09-25/2016-09-30 (Santa Fe, New Mexico, United States)

Issued: 2016-09-23

MCNP®: Simulating Correlated Data in Fission Events

2016 ANS ANNTP Workshop

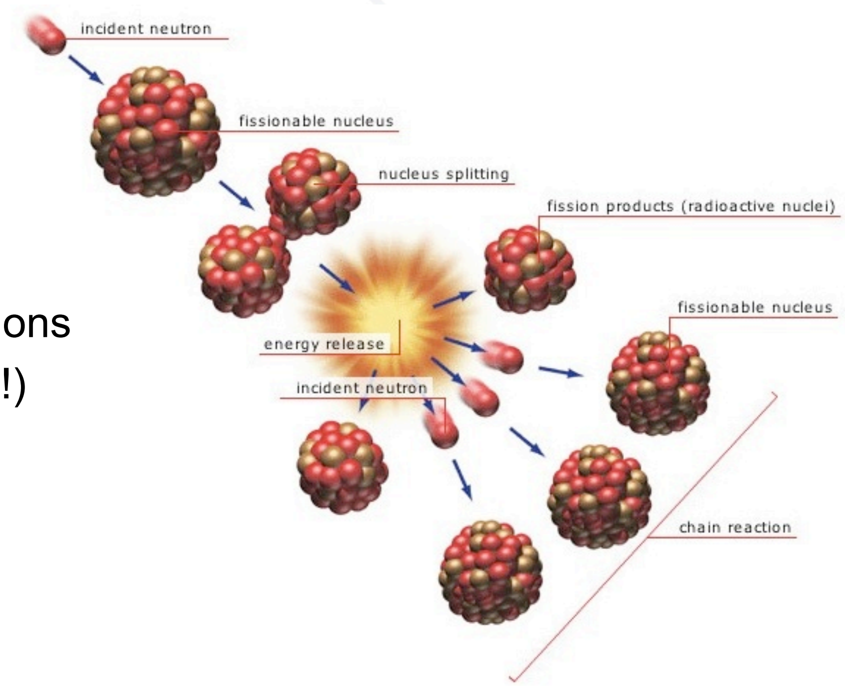
Michael E. Rising
XCP-3 Division, Los Alamos National Laboratory

11 August 2016

UNCLASSIFIED

Outline

- Introduction
- Background
- MCNP Fission Physics Options
  - Default
  - FMULT Card
  - Current LLNL Fission Library / CGM Options
  - FREYA / CGMF Options (Available Soon!)
- Simple Simulation Results
  - MCNP model
  - Comparisons Between Options
  - Neutron and Gamma-ray Correlations
- Example SNM Simulations



Introduction

- Application of interest
  - Global security and nuclear nonproliferation
  - Detection of special nuclear material (SNM)
  - Warhead measurement campaign (WMC)
  - Passive and active interrogation techniques
  - Coincident neutron and photon leakage
- Key issues
  - Average nuclear data quantities are insufficient
  - Cannot predict correlated signatures of shielded SNM
- Approach to obtain predictive capability
  - Use transport code MCNP for modeling neutrons and photons
  - Need microscopic fission event information
  - Fission event generators are under development
  - Implement in MCNP and compare to experiments

Background

- In tabulated nuclear data libraries (i.e. ENDF/B-VII.1):
  - Average secondary neutron and photon information can be available
    - Average multiplicity, $\bar{\nu}$
    - Average spectrum, $\chi(E)$
    - Average energy-angle spectrum, $\chi(E,\theta)$
  - Generally, high-dimensional distributions of secondary particles are unavailable
    - Multiplicity distribution, $P(\nu)$
    - Multiplicity-dependent emission spectra, $\chi(\nu,E)$
    - Multiplicity-dependent energy-angle emission spectra, $\chi(\nu,E,\theta)$
    - Neutron-neutron, neutron-photon and photon-photon correlations
    - Too much data to measure, evaluate and tabulate!
- Default MCNP uses average quantities
  - In some cases, consider this a nuclear data "variance reduction" technique
  - Good for integral quantities, like flux and effective multiplication
  - Bad for studying detailed particle emission physics

MCNP Fission Physics Options

- In nature, a fission event will emit a number of neutrons and gamma rays with some probability distribution, $P(E,\nu)$

- In MCNP, by default
  - The average neutrons emitted is used, $\bar{\nu}(E)$
  - Bounded integer sampling scheme:
    - If $\bar{\nu} = 2.2$,
    - Then, $P(\nu = 2) = 80\%$ and, $P(\nu = 3) = 20\%$
  - Preserves expected value

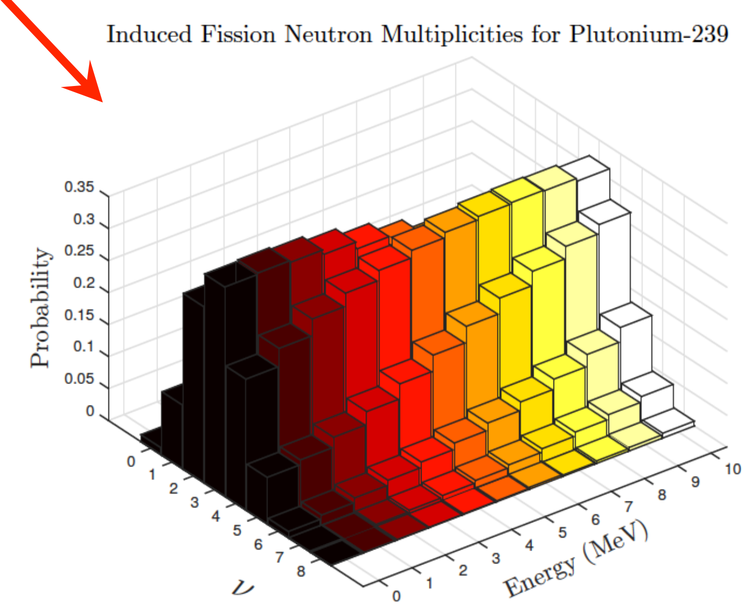


Figure take from: M. Ortega, M.S. Thesis, University of New Mexico, NM.

MCNP Fission Physics Options

- FMULT option within MCNP turns on neutron multiplicity sampling and allows the user to,
  - Modify spontaneous fission average multiplicity and yield rate
  - Change Watt energy spectrum parameters for spontaneous fission
  - Provide Gaussian FWHM width for spontaneous and induced fission multiplicity distributions
  - Select a sampling algorithm and data source
- Does not handle fission gamma ray emission
- Each neutron emitted,
  - Direction is isotropic and independently sampled
  - Energy is sampled independently from the same energy distribution (uncorrelated)

1fission multiplicity data.

zaid	width	watt1	watt2	yield	sfnu
90232	1.079	.800000	4.00000	6.00E-08	2.140
92232	1.079	.892204	3.72278	1.30E+00	1.710
92233	1.041	.854803	4.03210	8.60E-04	1.760
92234	1.079	.771241	4.92449	5.02E-03	1.810
92235	1.072	.774713	4.85231	2.99E-04	1.860
92236	1.079	.735166	5.35746	5.49E-03	1.910
92238	1.230	.648318	6.81057	1.36E-02	0.048
93237	1.079	.833438	4.24147	1.14E-04	2.050
94236	0.000	.000000	0.00000	0.00E+00	0.080
94238	1.115	.847833	4.16933	2.59E+03	0.056
94239	1.140	.885247	3.80269	2.18E-02	2.160
94240	1.109	.794930	4.68927	1.02E+03	0.063
94241	1.079	.842472	4.15150	5.00E-02	2.250
94242	1.069	.819150	4.36668	1.72E+03	0.068
95241	1.079	.933020	3.46195	1.18E+00	3.220
* 96242	1.053	.887353	3.89176	2.10E+07	0.021
96244	1.036	.902523	3.72033	1.08E+07	0.015
96246	0.000	.000000	0.00000	0.00E+00	0.015
96248	0.000	.000000	0.00000	0.00E+00	0.007
97249	1.079	.891281	3.79405	1.00E+05	3.400
98246	0.000	.000000	0.00000	0.00E+00	0.001
98250	0.000	.000000	0.00000	0.00E+00	0.004
98252	1.207	1.180000	1.03419	2.34E+12	0.002
98254	0.000	.000000	0.00000	0.00E+00	0.000
100257	0.000	.000000	0.00000	0.00E+00	0.021
102252	0.000	.000000	0.00000	0.00E+00	0.057

* = used in problem.

See MCNP6 User's Manual, Los Alamos National Laboratory, LA-CP-14-00745 (2014).

MCNP Fission Physics Options

- MCNP6.1.1 contains two (low-energy) event generators:
- LLNL Fission Library[1]
  - Spontaneous, neutron-induced and photo-fission
  - Fission Reaction Event Yield Algorithm (FREYA)[2] isotopes:
    - Spontaneous: ^{238}U, ^{240}Pu, ^{244}Cm and ^{252}Cf
    - Neutron-induced: ^{233}U, ^{235}U and ^{239}Pu
  - When available, FREYA generates secondary neutrons and photons
- Cascading Gamma-ray Multiplicity (CGM)[3] - LANL
  - Generates secondary particles from a variety of reactions
  - No fission! (CGMF under active development)

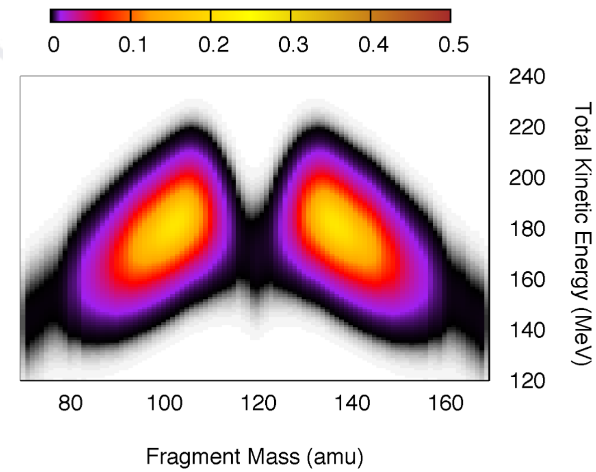
[1] J.M. Verbeke, C. Hagmann, and D. Wright, Lawrence Livermore National Laboratory, UCRL-AR-228518 (2014).

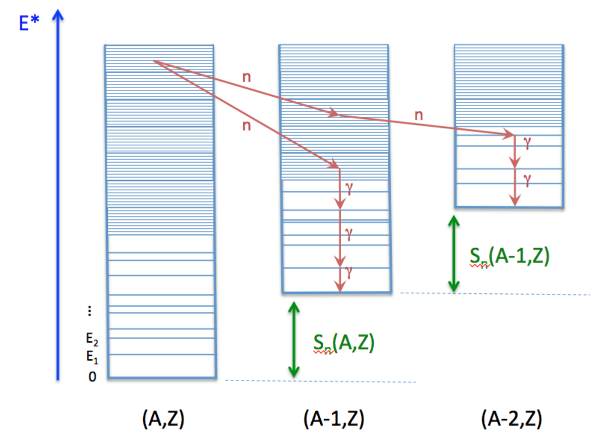
[2] R. Vogt and J. Randrup, *Phys. Rev. C*, vol. 84, pp. 044612-1-14 (2011).

[3] T. Kawano, P. Talou, M.B. Chadwick, and T. Watanabe, *J. Nucl. Sci. Tech.*, 47 (5), 462-69 (2010).

MCNP Fission Physics Options

- CGMF is a superset of CGM with an added fission reaction capability
- Fission fragments are sampled from a joint probability distribution function of mass (A), charge (Z) and total kinetic energy (TKE)
- Uses Hauser-Feshbach statistical theory of nuclear reactions
- Neutron / photon competition is treated during evaporation from fission fragments
- Monte Carlo is used to sample each step in the de-excitation process

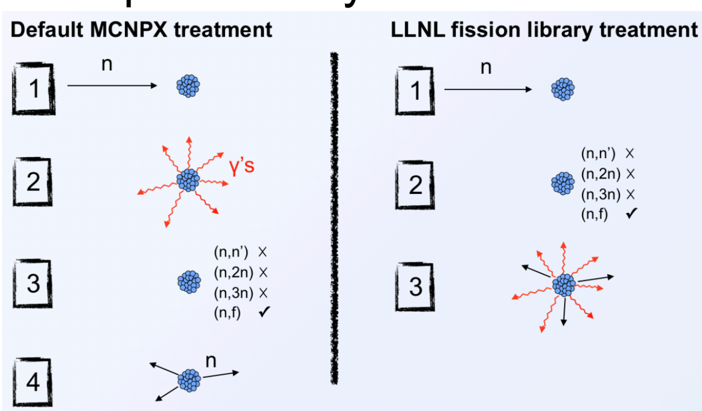


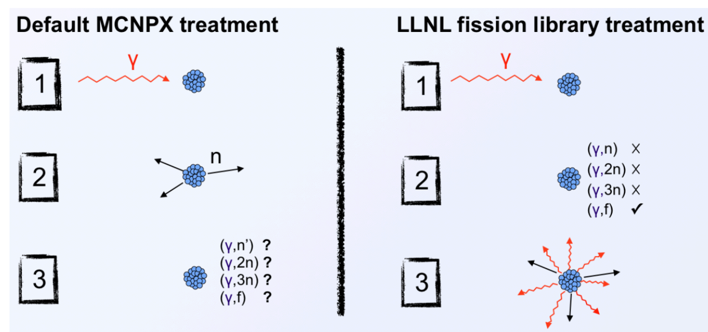


[4]B. Becker, P. Talou, T. Kawano, Y. Danon, and I. Stetcu, *Phys. Rev. C*, 87, 014617 (2013).

MCNP Fission Physics Options

- FREYA is LLNL's fission event generator
- In MCNP6, it is accessible through LLNL Fission Package
- The LLNL Fission Package includes more tabulated and fitted data used for lesser known isotopes FREYA can't presently handle
- FREYA uses a Monte Carlo Weisskopf approach
  - Neutrons emitted by sampling from Weisskopf spectrum
  - After neutrons are done emitting, gamma rays are emitted from residual energy
- Computationally more efficient than Monte Carlo Hauser-Feshbach





MCNP Fission Physics Options

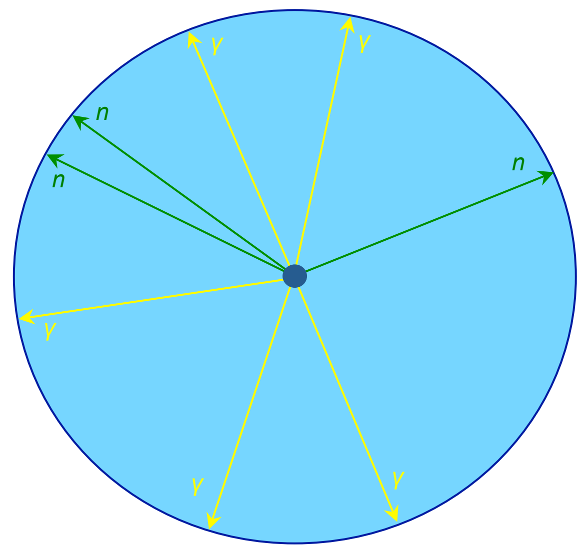
- How do users access these models in MCNP?
- FMULT data card with method keyword
  - method = 5 → LLNL Fission Library
  - method = 6 → FREYA
  - method = 7 → CGMF
- If FREYA/CGMF cannot handle a specific spontaneous or neutron-induced fission isotope, the LLNL Fission Library is used
- If the LLNL Fission Library cannot handle a specific spontaneous or neutron-induced fission isotope, the default FMULT parameters are used
- Some additional information printed to output file:

```
warning.  Using FMULT, not CGMF, for spontaneous fission of  98250.
```

```
* = this isotope was used in the simulation, but the nuclear data came from **CGMF + LLNL fission library.
**  CGMF handles neutron-induced (n,f) fission of Pu-239.
    The remaining (n,f) nuclear data will come from the LLNL fission library.
```

Simple Simulation Results

- Useful test problem to tabulate secondary multiplicity, energy and angular distributions
  - Point source at origin of sphere
  - Force immediate collision from source
  - Secondary particles stream to sphere
  - Tallies on sphere surface



- Two simple cases
  - Spontaneous fission of ^{252}Cf
  - Neutron-induced fission of ^{239}Pu
  - Tallied mean values:
    - Multiplicity, $\overline{\nu}_n$ & $\overline{\nu}_\gamma$
    - Energy, $\overline{\chi}_n$ & $\overline{\chi}_\gamma$

Simple Simulation Results

- MCNP ^{252}Cf spontaneous fission input files

Default MCNP

```
Test of spontaneous fission multiplicity
c
1   1  -1e-10  -1   imp:n=1
99  0            1   imp:n=0

1  so  .001

m1   98252  1
sdef par=-sf
c
fmult 98252 method=3 data=3 shift=1
c
nps    1000000
mode   n p
totnu  no
cut:n  2j 0 0
c
*f11:n  1
f111:n  1
c
*f21:p  1
f211:p  1
```

LLNL Fission Library

```
Test of spontaneous fission multiplicity
c
1   1  -1e-10  -1   imp:n=1
99  0            1   imp:n=0

1  so  .001

m1   98252  1
sdef par=-sf
c
fmult 98252 method=5
c
nps    1000000
mode   n p
totnu  no
cut:n  2j 0 0
c
*f11:n  1
f111:n  1
c
*f21:p  1
f211:p  1
```

method=6 → FREYA
method=7 → CGMF

Simple Simulation Results

- Spontaneous Fission ^{252}Cf:

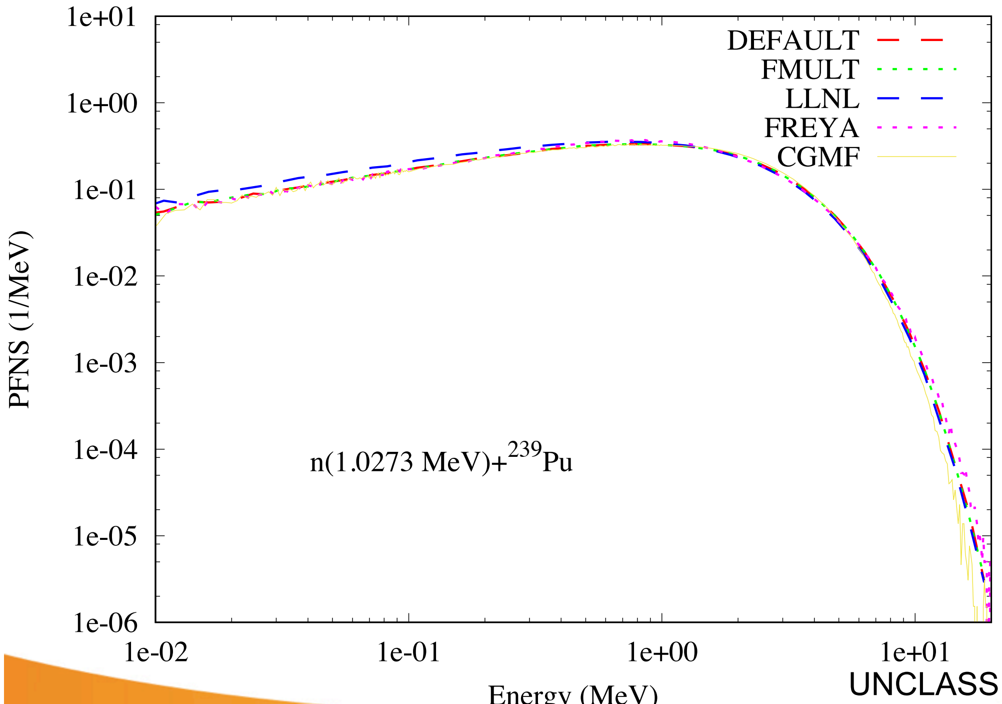
Quantity	Default	LLNL	FREYA	CGMF
$\bar{\nu}_n$	3.7566(11)	3.7725(11)	3.7507(12)	3.8818(13)
$\bar{\nu}_\gamma$	N/A	8.3150(33)	6.8814(30)	8.6780(33)
$\bar{\chi}_n$	2.1293(8)	2.1292(8)	2.2302(10)	2.0983(8)
$\bar{\chi}_\gamma$	N/A	0.8983(3)	0.7105(2)	0.8131(3)

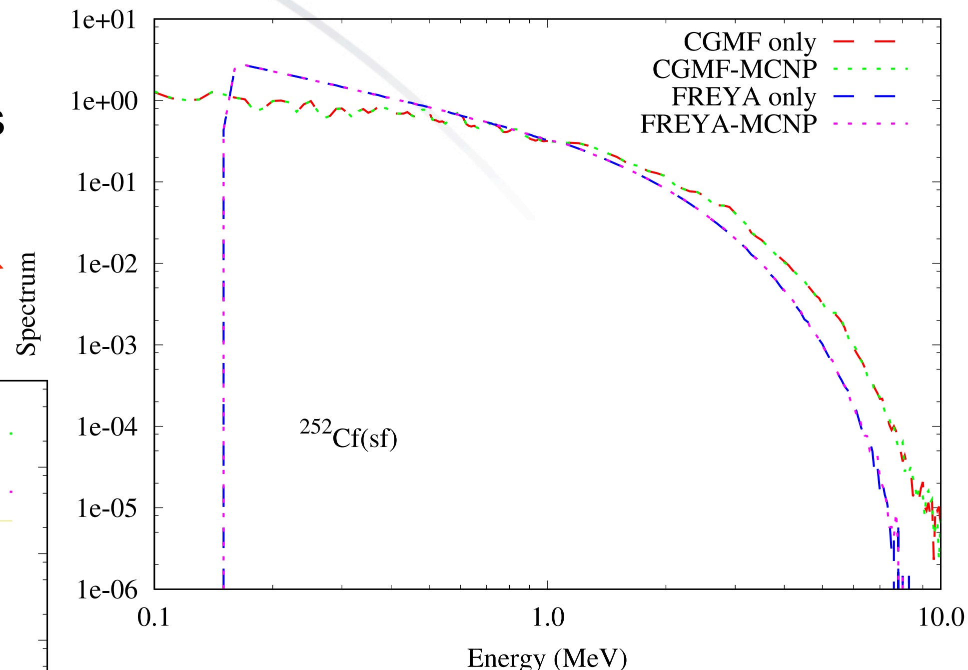
- Neutron-Induced Fission n(1.0273 MeV)+^{239}Pu

Quantity	Default	FMULT	LLNL	FREYA	CGMF
$\bar{\nu}_n$	3.0126(27)	3.0130(30)	3.0137(27)	3.0066(10)	3.2591(13)
$\bar{\nu}_\gamma$	7.7917(23)	7.7917(23)	7.3069(73)	6.7726(29)	8.2737(32)
$\bar{\chi}_n$	2.1392(21)	2.1381(21)	2.0358(20)	2.0782(10)	2.0882(9)
$\bar{\chi}_\gamma$	0.8662(4)	0.8662(4)	0.8985(9)	0.7407(3)	0.8895(3)

Simple Simulation Results

- Multiplicity and Energy Distributions
  - Energy, $\chi_n(E)$ & $\chi_\gamma(E)$

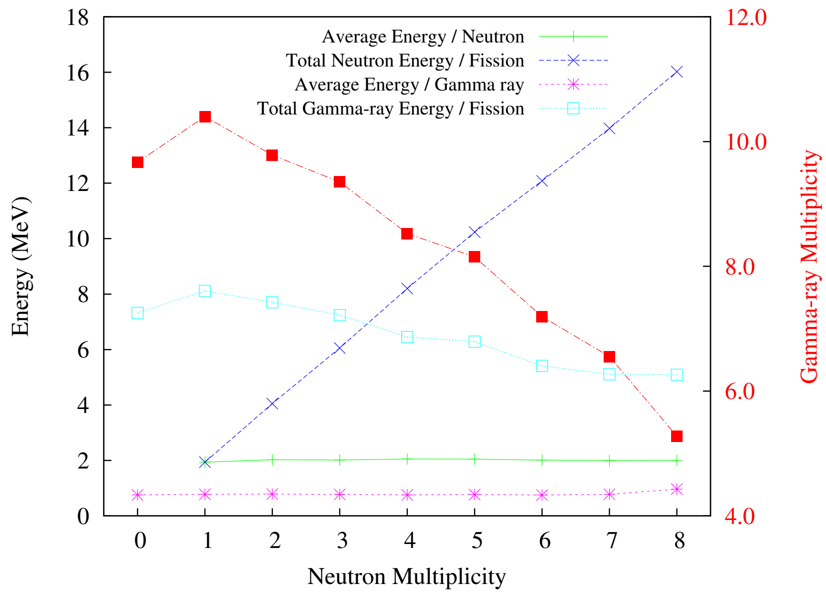


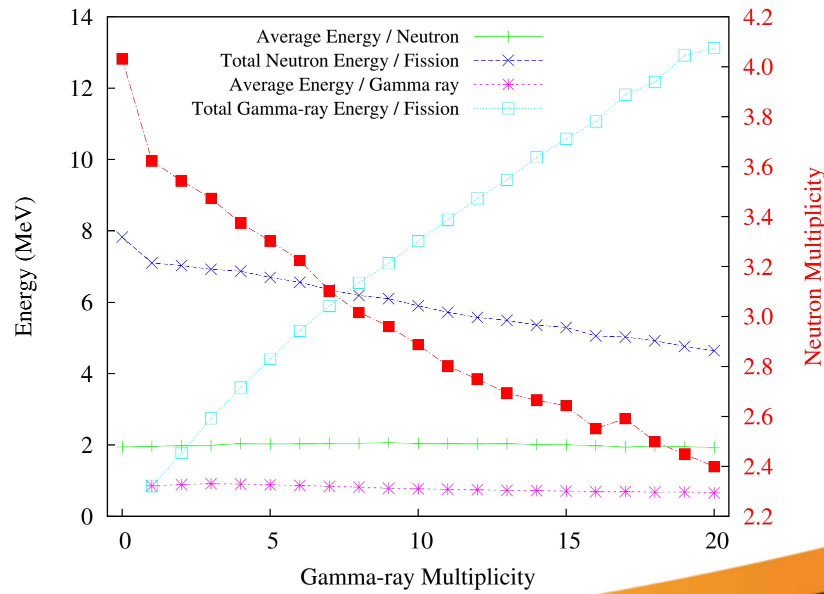


UNCLASSIFIED

Simple Simulation Results

- Multiplicity and Energy Distributions
  - Multiplicity, $P(\nu_n)$ & $P(\nu_\gamma)$
- Neutron – gamma ray energy and multiplicity correlations
- This physics needs to be validated with experiment!



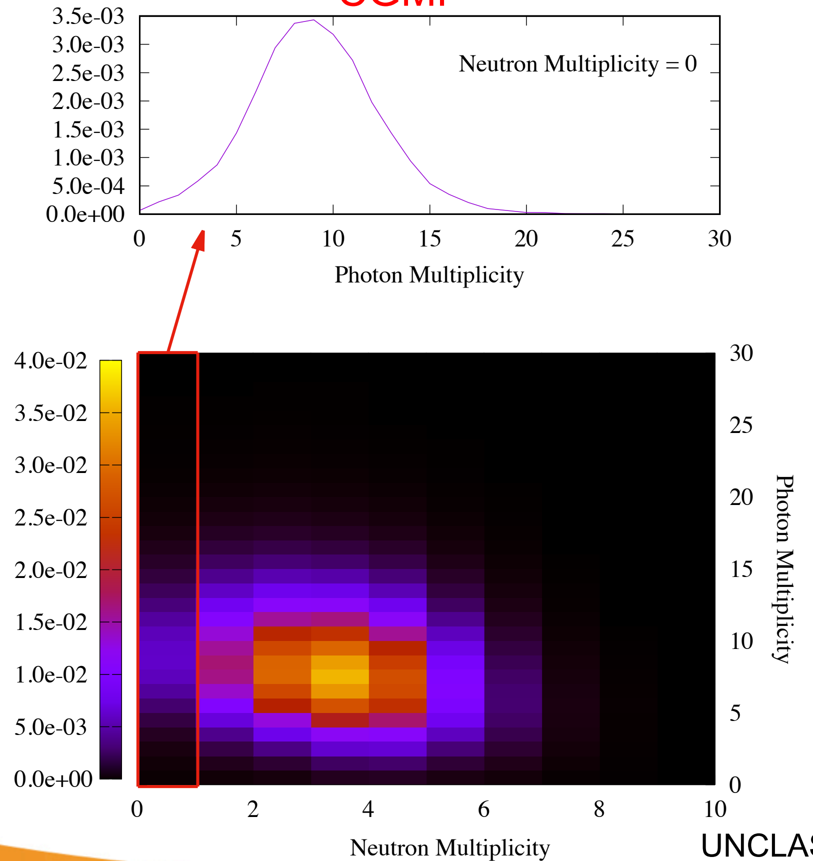


UNCLASSIFIED

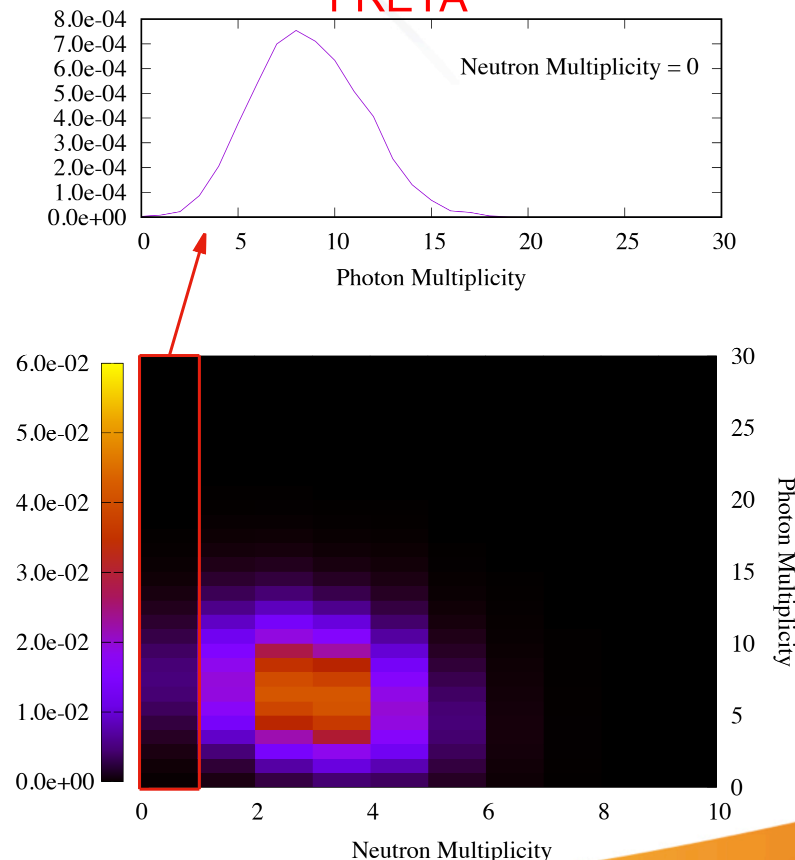
Simple Simulation Results

- Neutron and Gamma Ray Multiplicity

CGMF



FREYA

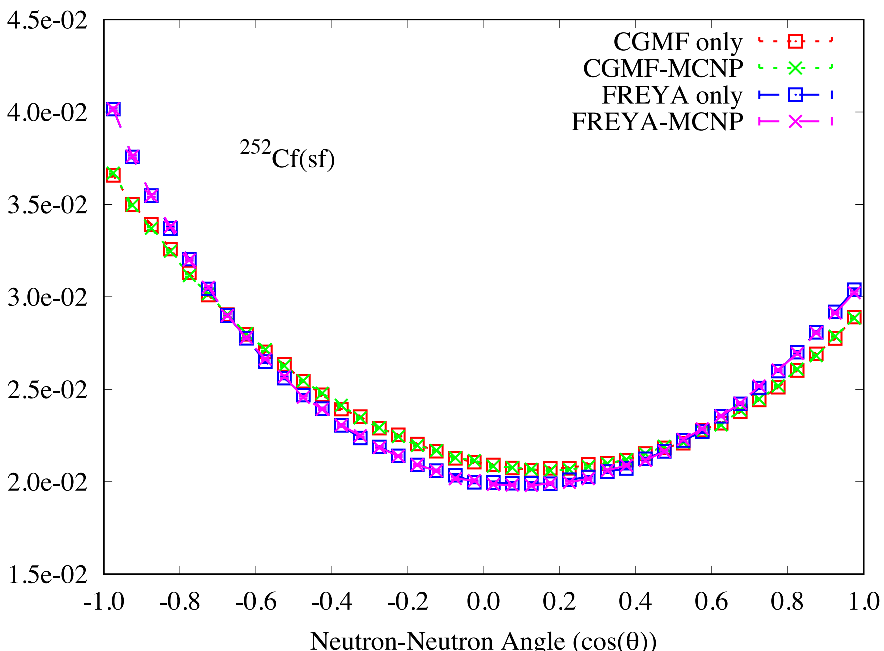


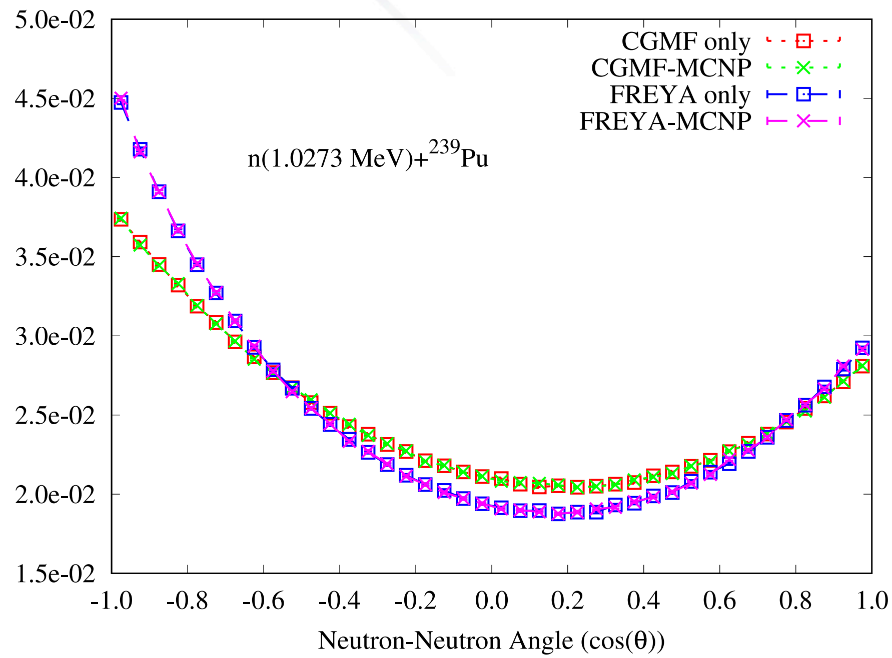
UNCLASSIFIED

Simple Simulation Results

- Default options are isotropic
- Correlations:
  - Multiplicity, $n-n$
  - Angle, $\gamma-\gamma$

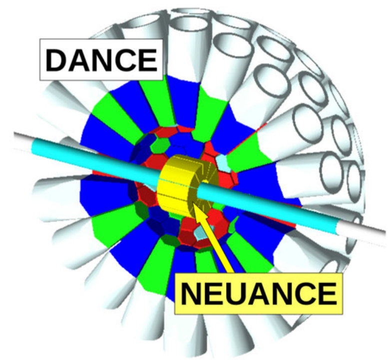
    $n-\gamma$

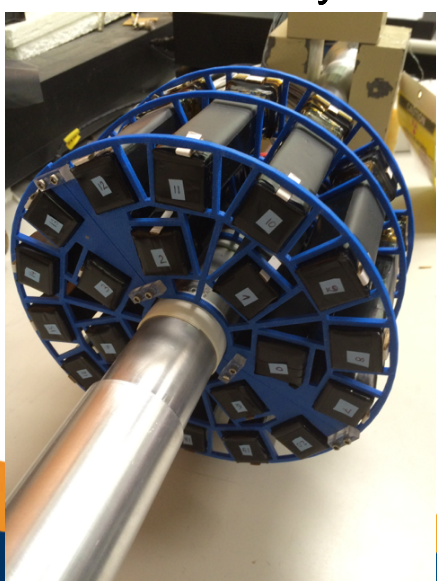


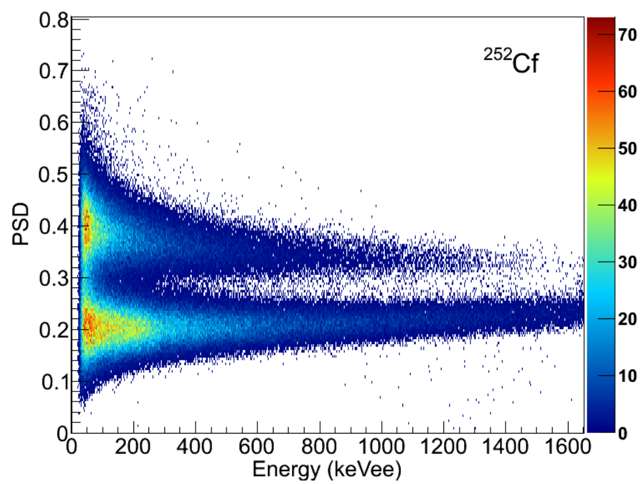


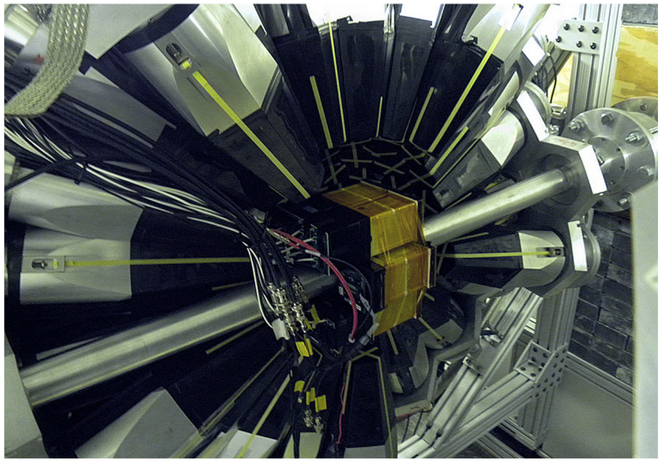
Example SNM Simulations

- Differential Experiment Validation
  - Using differential measurements to validate event-by-event predictions of CGMF/FREYA
  - CNEC student at LANL working on modeling detailed detectors in NEUANCE (M. Pinilla)
  - Using PTRAC and DRiFT to model stilbene
- To make sure CGMF & FREYA are a reflection of reality





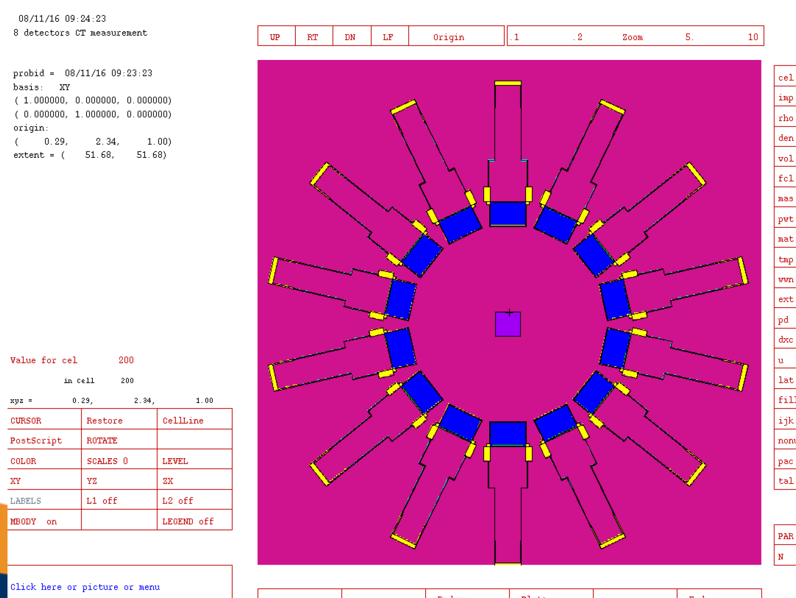


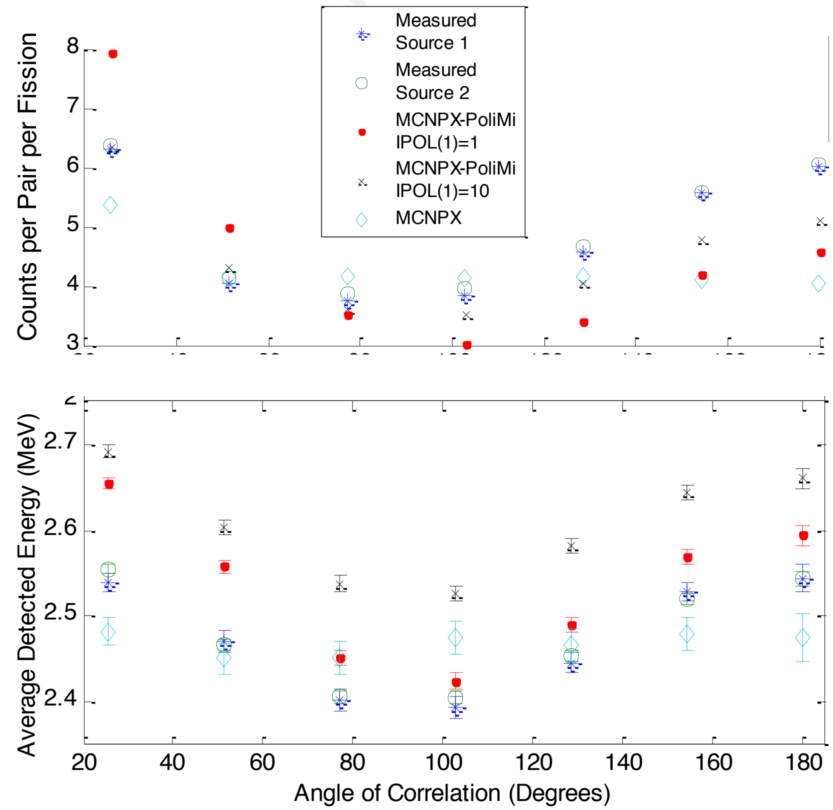


UNCLASSIFIED

Example SNM Simulations

- University of Michigan differential measurements of angular correlations
- Priority is to compare against experimental measurements
- Can compare against other code predictions, like MCNPX-PoliMi

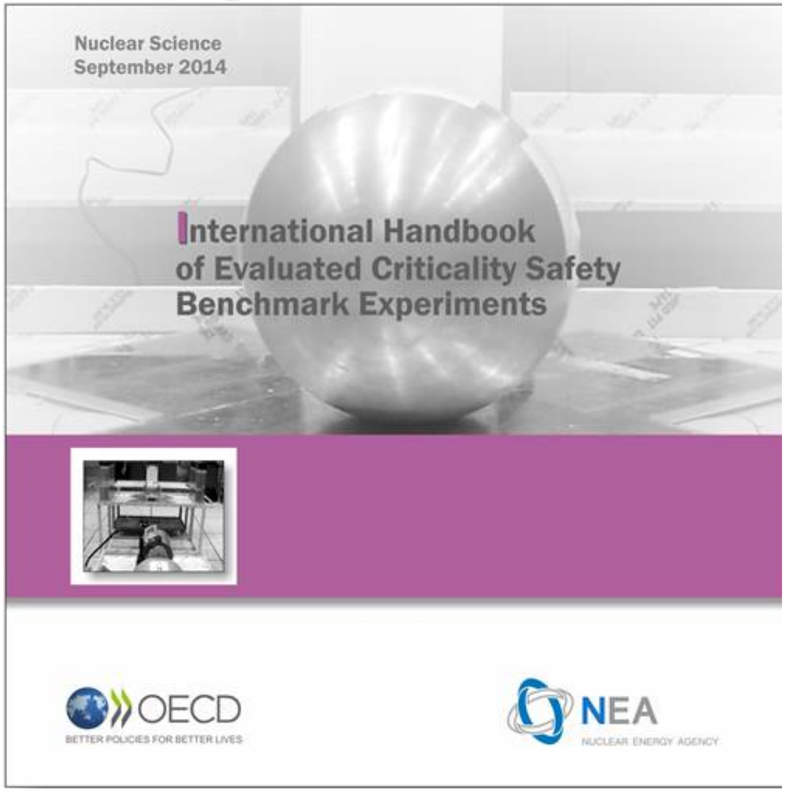




UNCLASSIFIED

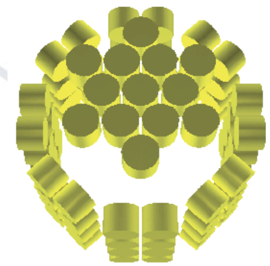
Example SNM Simulations

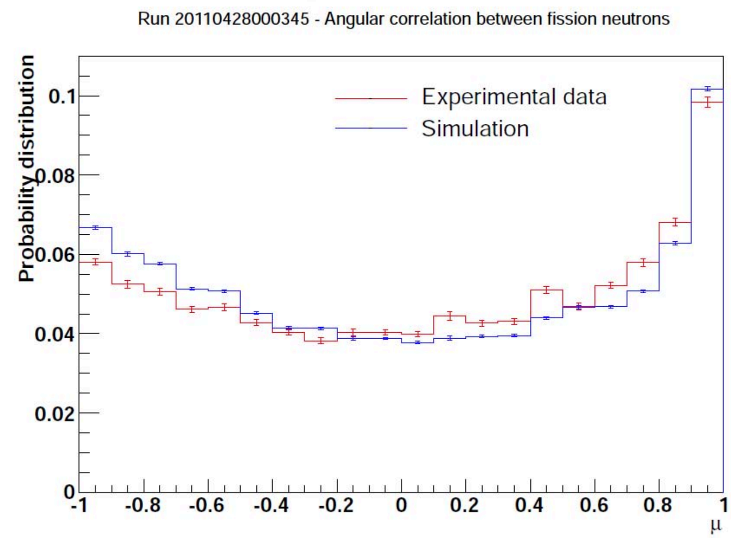
- Integral Experiment Validation
  - Need to compare model prediction to experiment
  - Subcritical work is being done and can be leveraged to validate MCNP6
  - Integral quantities like multiplicity, singlets, doublets, etc. that are sensitive to event generators
  - Can use differential, semi-differential measurements as validation
    - University of Michigan
    - DANCE
    - Nakae, Verbeke, et al.
- To make sure CGMF & FREYA are a reflection of reality

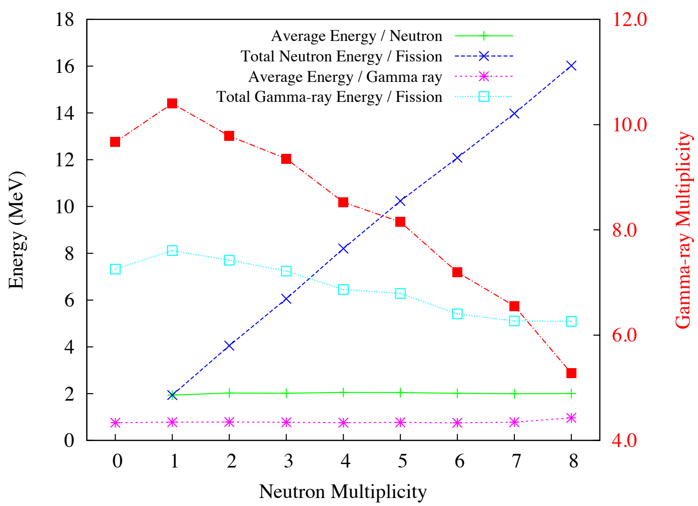


Example SNM Simulations

- Neutron-neutron angular correlations[2]
  - ^{252}Cf SF source in liquid scintillator array
  - Experiment vs. FREYA / LLNL Fission Library







- Neutron-photon energy correlations
  - Thermal neutron-induced fission of ^{239}Pu
  - CGMF (standalone) predictions[7]

[7] M.E. Rising, A. Sood, P. Talou, T. Kawano and I. Stetcu, Los Alamos National Laboratory, LA-UR-14-24979 (2014).

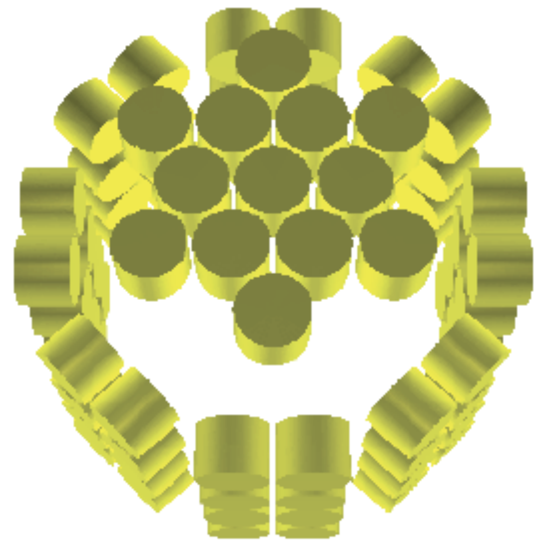
Example SNM Simulations

```
Cf source Birthday-cake liquid scintillator array
c
c CELLS
 17   13   -.874   -17   imp:n,p,h=1   $ scintillator 17
 18   13   -.874   -18   imp:n,p,h=1   $ scintillator 18
...

c
c SURFACES
...

mode n p h   $ transport neutrons, photons, protons
nps 18981035 $ # of neut / sec = 39,761 neuts/s,
c              # of neut in 1801 secs = 71,609,561 neuts.
c              # of fiss in 1801 secs = 71,609,561/3.772690
c                                     = 18,981,035 fiss.
phys:n 1.e8  5j  1  $  keep recoil particle (7th entry)
fmult  98252 method=7
ptrac  file=bin  max=1e9  write=all  type=p,h
       event=col,bnk,ter,sur  filter=17,93,icl
c
```

MCNPX Model Depiction of Liquid Scintillator Detector Array at LLNL[1]



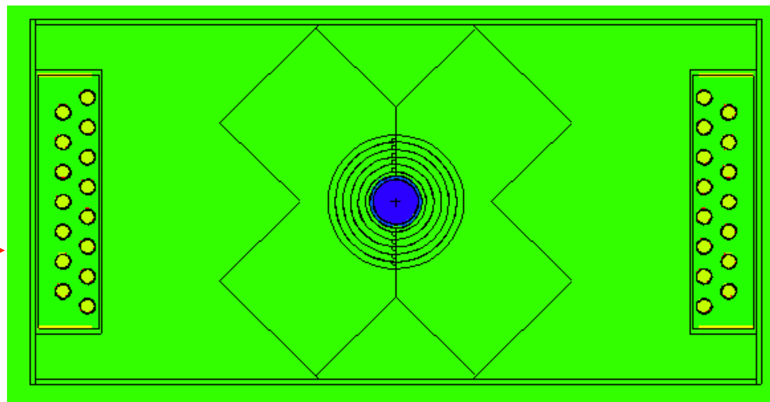
[1]*J.M. Verbeke, C.A. Hagmann, J. Randrup and R. Vogt, Lawrence Livermore National Laboratory, LLNL-PROC-638986 (2013).*

- Use MCNPtools to retrieve proton recoil in detectors

Example SNM Simulations

- Currently, alpha testing new models
  - Students from CNEC and CVT are participating
  - Using simple detector array models
  - Testing list-mode output through PTRAC feature
  - Collaboration with Univ. of Michigan, LLNL & LBNL

- In progress validation models include
  - Separate liquid scintillator arrays at UM, LANL & LLNL
  - Stilbene detector array at LANSCE (NEUANCE / DANCE)
  - Subcritical BeRP ball experiments
  - Criticality validation



Conclusions

- Next version of MCNP 6.2 will contain two new fission event generators
  - FREYA from LLNL/LBNL
  - CGMF from LANL

THANK YOU!