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Title: MCNP6.2 Status & Developments: FY16 and early FY17

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MCNP6.2 Status & Developments: FY16 and early FY17

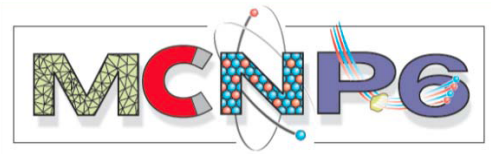
NA-22 Collaboration Meeting
Santa Fe, NM USA

Michael E. Rising
XCP-3 Group, LANL

March 6-7, 2017

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

Outline

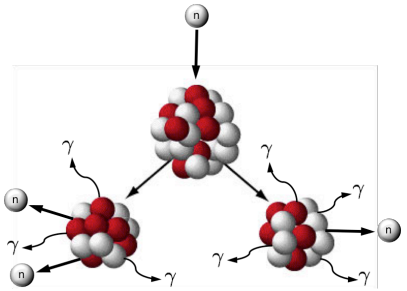


- **What was done in FY16**
  - New models integrated
    - LLNL Fission Library 2.0.1
    - FREYA 2.0
    - CGMF 1.0.9
  - Verification Testing
- **What is being done now**
  - Release of MCNP6.2
  - Validation Testing
- **What will be done in FY17**
  - New MCNP6.2 tools released
  - Code upgrades and modernization
- **What else...**

What was done in FY16
Looking back at previous collaboration meetings

First…

- ✓ Standalone executable for verification
- ✓ Have a user- and developer-friendly interface



Second…

- ✓ Need thermal to 20 MeV for neutron-induced fission
- ✓ Develop and pass all tests with standard configuration and compilers
- ✓ Indicators to users how the model is being used

Third…

- ~ Needs to have validation tests documented and included
- ✓ Further testing on more platforms, configurations, compilers, etc.
- ~ Should be continue-run, MPI-capable and thread-safe
- ✓ Should be tested for performance and memory-usage

What was done in FY16
New models integrated (1)

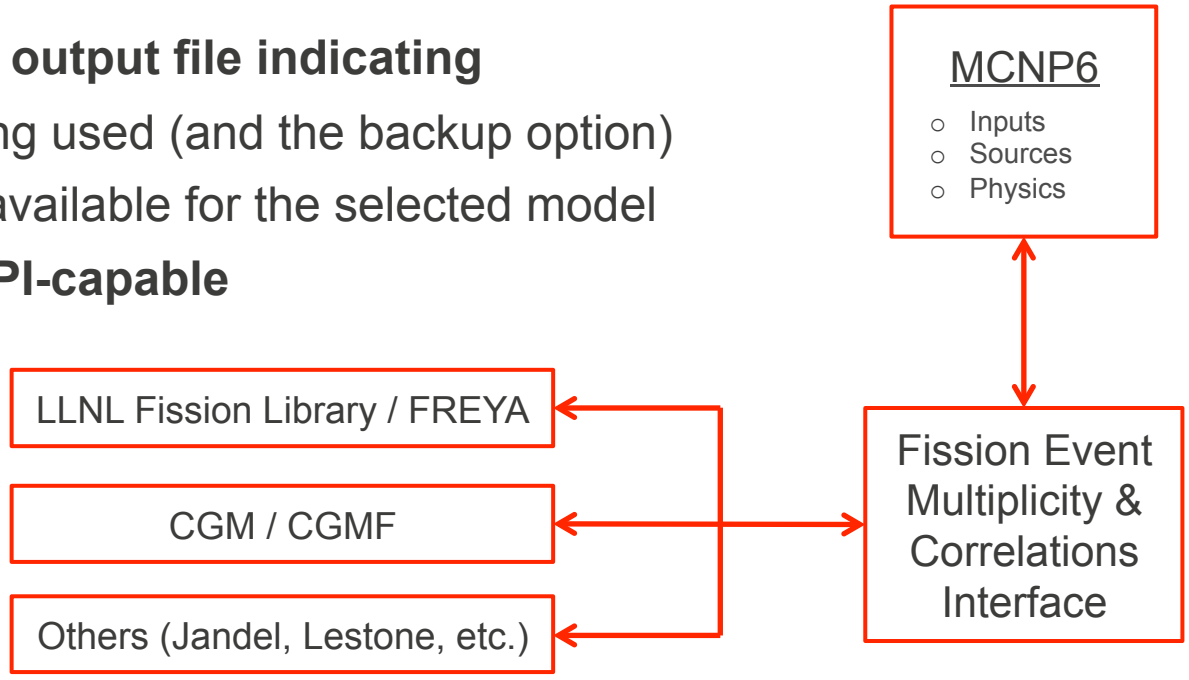
- **LLNL Fission Library 2.0.1**
  - Produces same results from previous version
  - Now includes FREYA 2.0

- **FREYA 2.0**
  - Code and data included
  - Spontaneous fission: ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{244}Cm, and ^{252}Cf
  - Neutron-induced fission: ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu

- **CGMF 1.0.9**
  - Code and data included (also upgraded CGM)
  - Spontaneous fission: ^{240}Pu, ^{242}Pu, and ^{252}Cf
  - Neutron-induced fission: ^{235}U, ^{238}U, and ^{239}Pu

What was done in FY16
New models integrated (2)

- **Standalone versus MCNP-integrated for verification**
- **Completed and cleaned up interface to models**
- **Regressions tests (~30) run and give exact results on Linux, Mac OS/X and Windows systems**
- **Added comments to output file indicating**
  - Which model is being used (and the backup option)
  - What isotopes are available for the selected model
- **Continue-run and MPI-capable**
- **Performance:**
  - CGMF



What was done in FY16 MCNP6.2 user options (1)

- **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).

What was done in FY16
MCNP6.2 user options (2)

- **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.
```

What was done in FY16
MCNP6.2 user options (3)

- **MCNP6.2 ^{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

What was done in FY16
Verification testing (1)

- **Documented in report LA-UR-16-27710 and presented at 2016 ANS ANNTP Conference in Santa Fe, NM**
- **Average multiplicity and energy**

CGMF

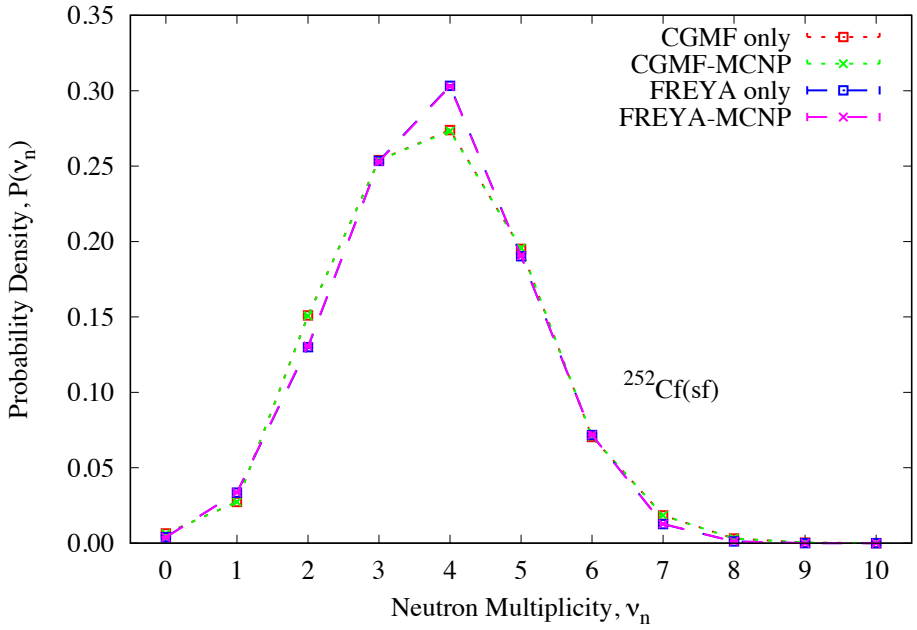
	^{252}Cf(sf)		n(1.0273 MeV)+^{239}Pu		n(thermal)+^{235}U	
Quantity	Standalone	MCNP	Standalone	MCNP	Standalone	MCNP
$\bar{\nu}_N$	3.7415(13)	3.7439(16)	3.0512(11)	3.0481(11)	2.4315(11)	2.4305(11)
$\bar{\chi}_N$	2.0927(8)	2.0920(10)	2.0322(9)	2.0329(9)	1.9726(9)	1.9740(9)
$\bar{\nu}_\gamma$	8.2721(32)	8.2680(37)	7.9039(31)	7.9053(31)	7.4328(30)	7.4425(30)
$\bar{\chi}_\gamma$	0.8561(3)	0.8558(3)	0.9287(3)	0.9293(3)	0.9139(3)	0.9131(3)

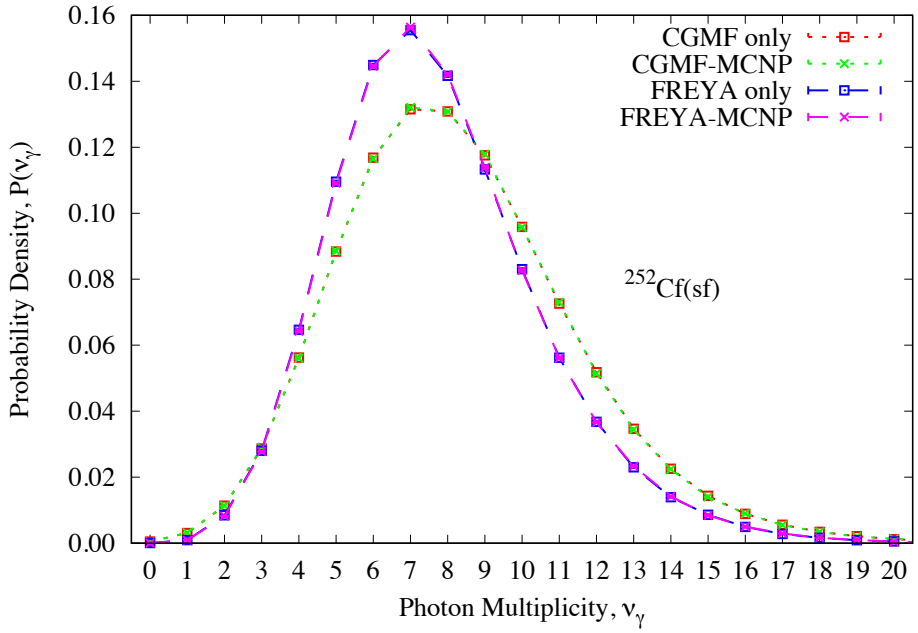
FREYA

	^{252}Cf(sf)		n(1.0273 MeV)+^{239}Pu		n(thermal)+^{235}U	
Quantity	Standalone	MCNP	Standalone	MCNP	Standalone	MCNP
$\bar{\nu}_N$	3.7464(13)	3.7463(13)	3.0101(12)	3.0124(12)	2.4180(11)	2.4187(11)
$\bar{\chi}_N$	2.2840(10)	2.2815(10)	2.1534(10)	2.1530(10)	1.9641(11)	1.9642(10)
$\bar{\nu}_\gamma$	7.7291(28)	7.7364(28)	6.8770(24)	6.8764(24)	6.4665(24)	6.4701(24)
$\bar{\chi}_\gamma$	0.9052(3)	0.9051(3)	1.0097(4)	1.0098(4)	0.9898(4)	0.9889(3)

What was done in FY16
Verification testing (2)

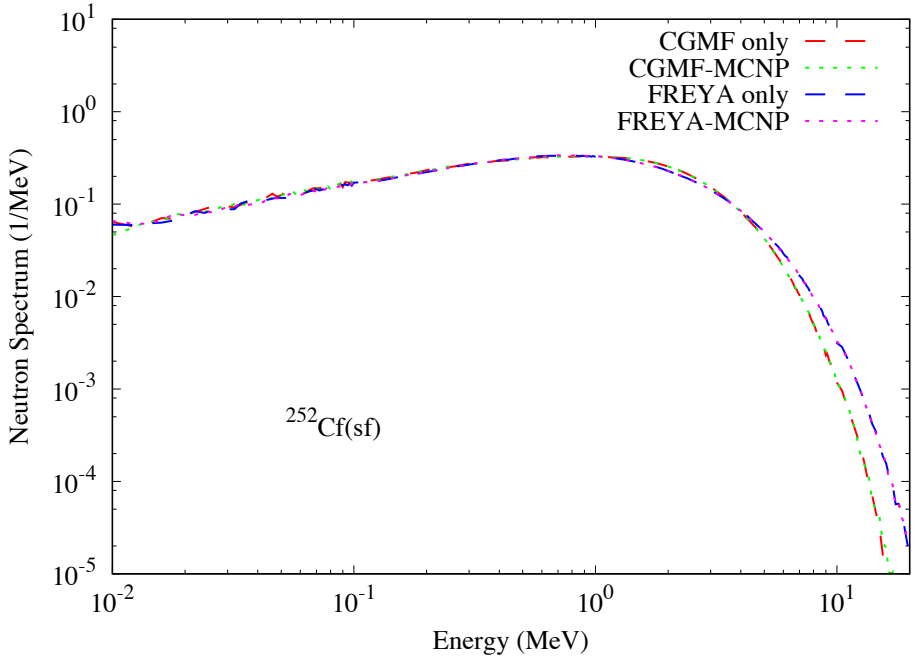
- **Neutron and Gamma-ray Multiplicity**
- **^{252}Cf spontaneous fission**

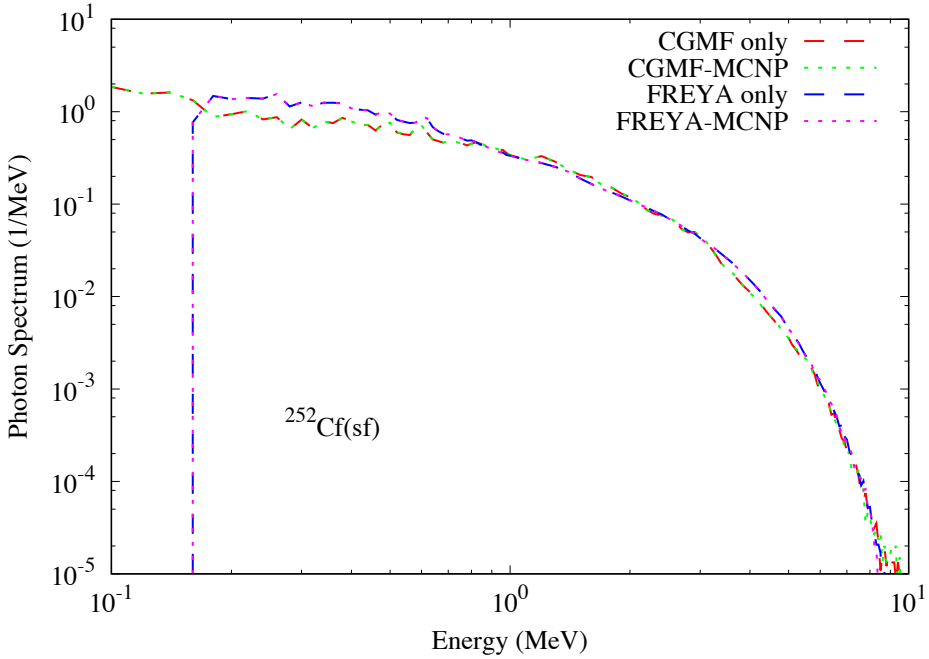




What was done in FY16
Verification testing (3)

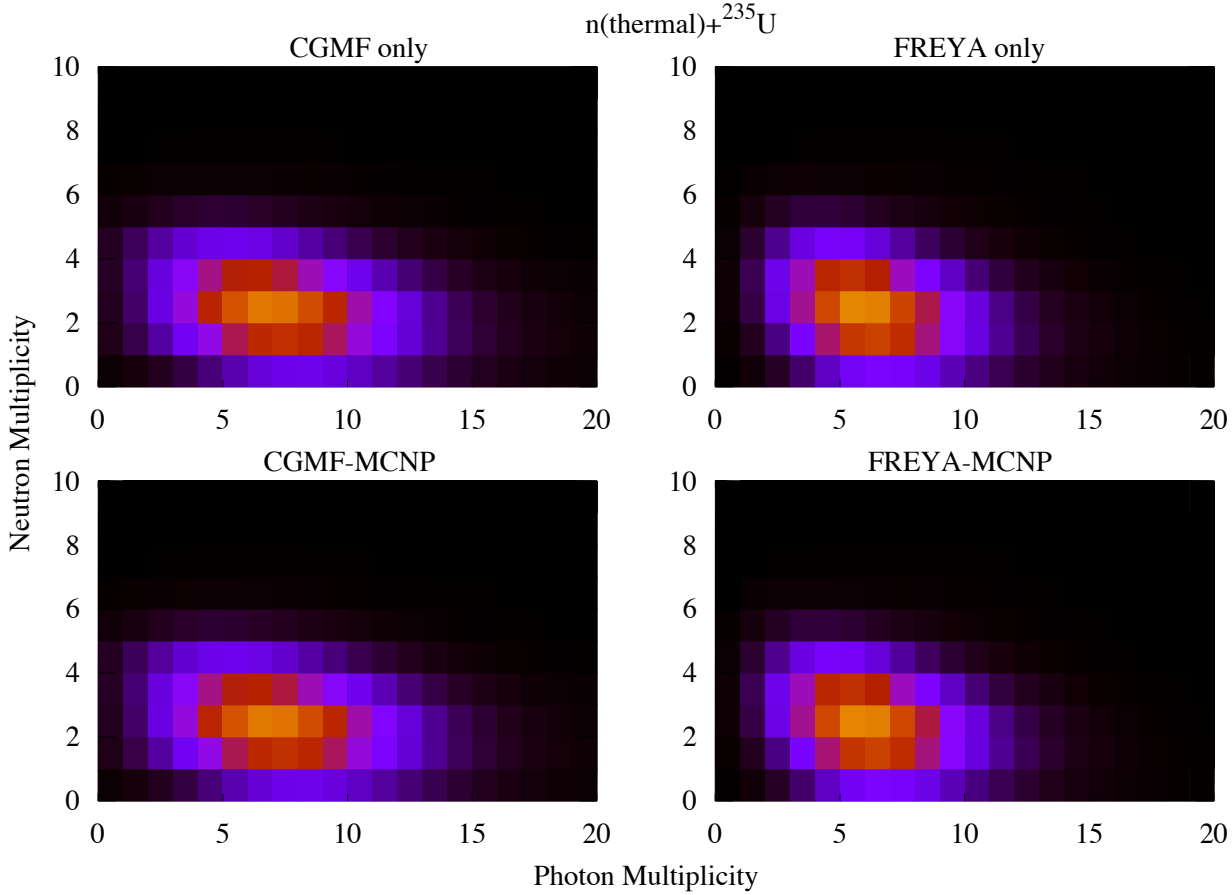
- **Neutron and Gamma-ray Energy Spectra**
- **^{252}Cf spontaneous fission**





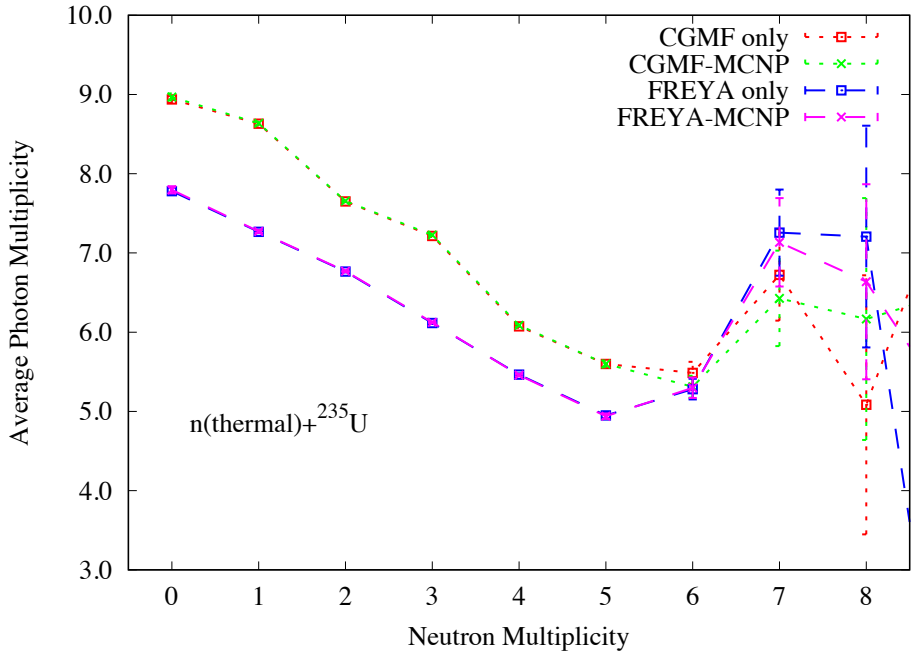
What was done in FY16
Verification testing (4)

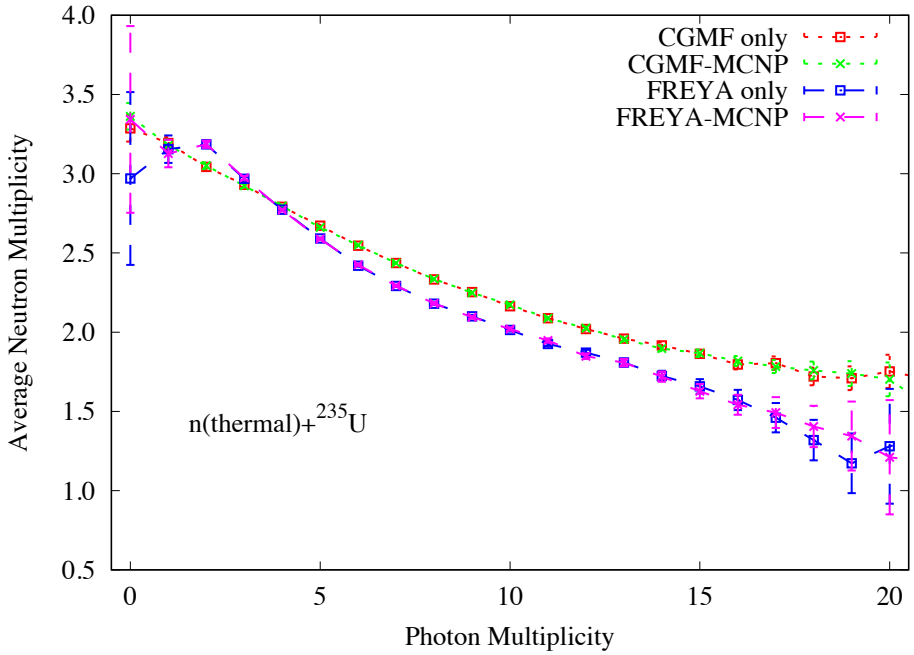
- **Neutron and Gamma-ray Multiplicity Correlations**
- **n(thermal)+^{235}U neutron-induced fission**



What was done in FY16
Verification testing (5)

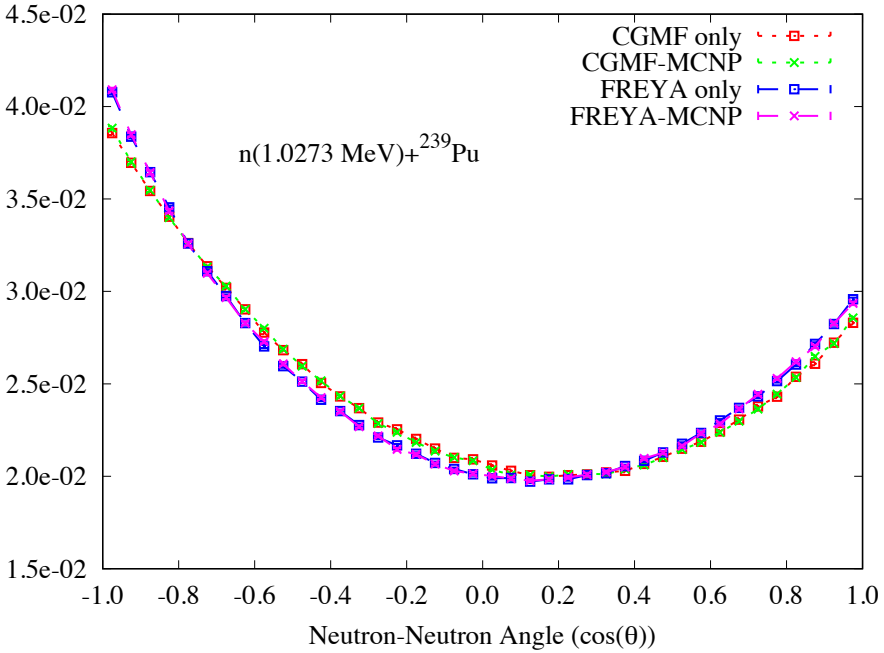
- **Neutron and Gamma-ray Multiplicity Correlations**
- **n(thermal)+^{235}U neutron-induced fission**

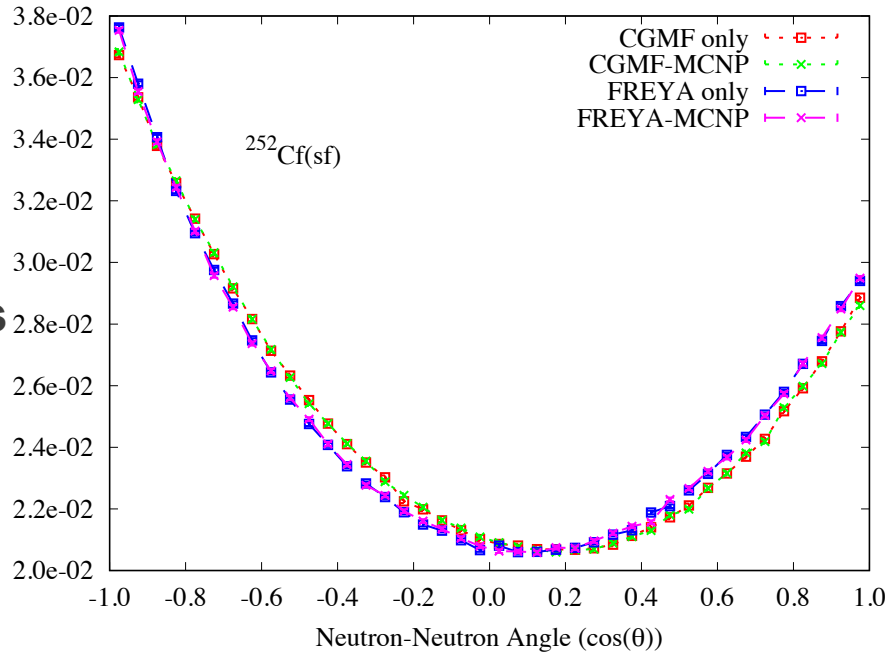


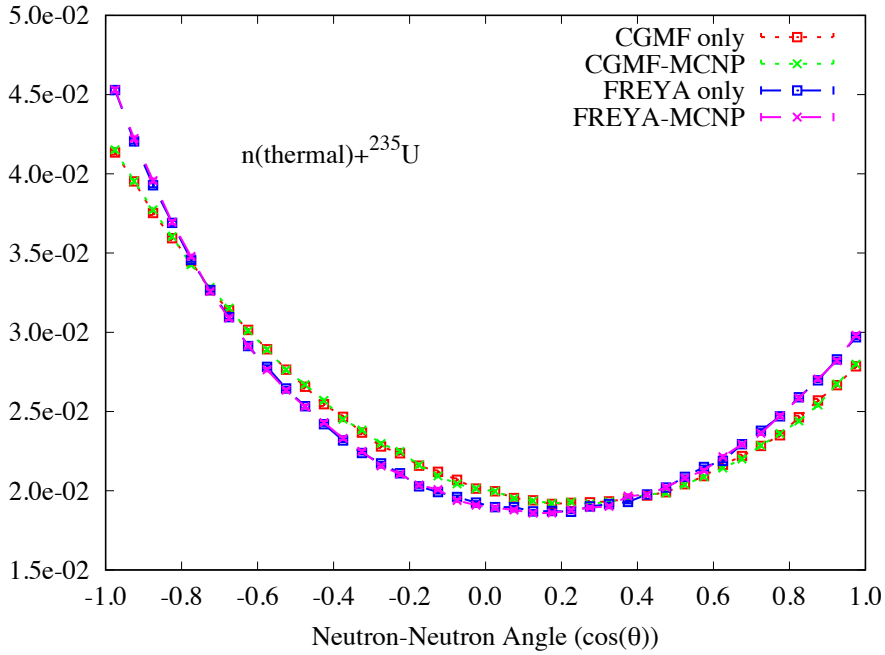


What was done in FY16
Verification testing (6)

- **Neutron-Neutron Angular Correlations**
  - n(1.0273 MeV)+^{239}Pu fission
  - n(thermal)+^{235}U fission
  - ^{252}Cf spontaneous fission







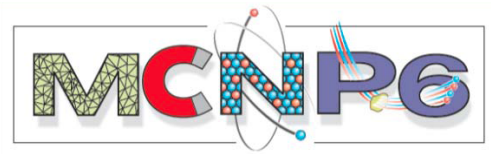
What was done in FY16
Verification testing (7)

- **Why is this so important?**
  - With the size of MCNP at ~500K source code lines, integration of these kinds of features is complicated and prone to mistakes
  - Previously, when zero neutrons were emitted in neutron-induced fission, zero gamma rays were also emitted
  - This bug has been fixed for MCNP6.2

- **New MCNPTools available with MCNP6.2 release**
  - Used the PTRAC (sources, collisions, terminations, etc.) feature
    - Tabulated all averages, distributions and correlations from the MCNP simulations
    - How the MCNP zero neutron/gamma-ray bug was discovered

- **Integrated fission event generator models appear to be implemented correctly!**

What is being done now
Release of MCNP6.2



- **Soon! (April/May 2017)**
- **Finalizing documentation and references**
- **Testing on all supported platforms**

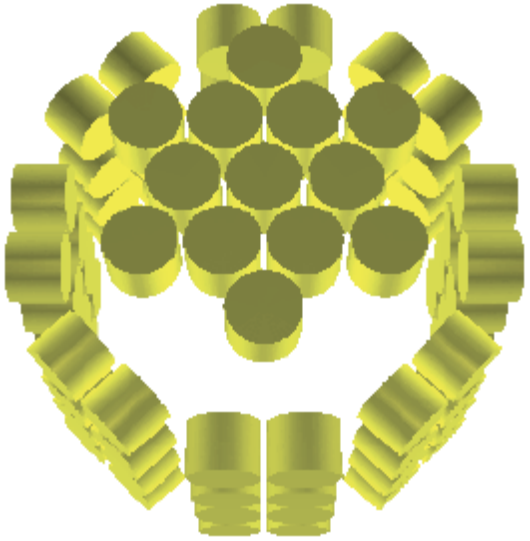
- **What's new in MCNP6.2?**
  - New/upgraded fission multiplicity models
    - LLNL Fission Library / FREYA
    - CGMF
  - ISC : Intrinsic Source Constructor
    - Used to generate radiation sources for transport code input (SDEF)
  - MCNPTools
    - Library that provides object-oriented access to MCNP outputs
      - MCTAL files
      - MESHTAL B (MCNP5/FMESH) files
      - PTRAC files

What is being done now
Validation testing (1)

- **Presented at 2016 ANS ANNTP Conference in Santa Fe, NM (J. Verbeke)**
- **Used MCNPTools to convert PTRAC to format for post-processing**
- **Re-run these simulations with CGMF and FREYA in MCNP6.2**

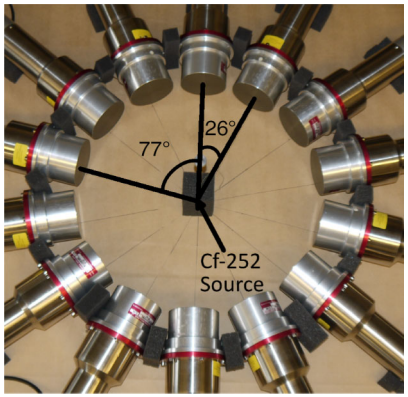
```
Cf source Birthday-cake liquid scintillator array
c
c CELLS
 17    13    -.874    -17    imp:n,p,h=1    $ scintillator 17
 18    13    -.874    -18    imp:n,p,h=1    $ scintillator 18
...

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
```

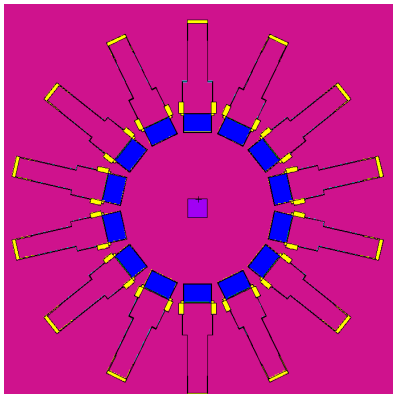
MCNPX Model Depiction of Liquid Scintillator Detector Array at LLNL

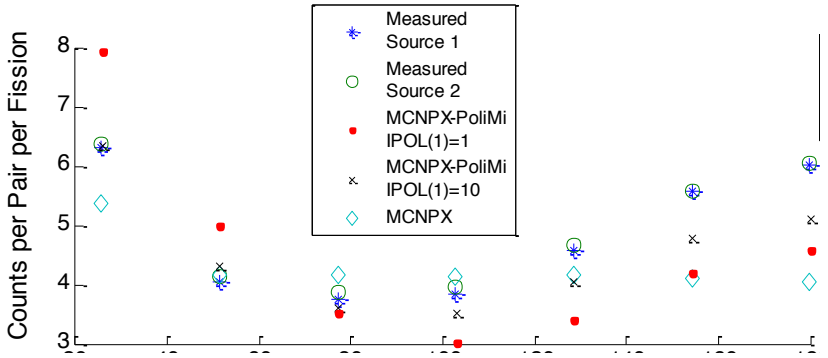


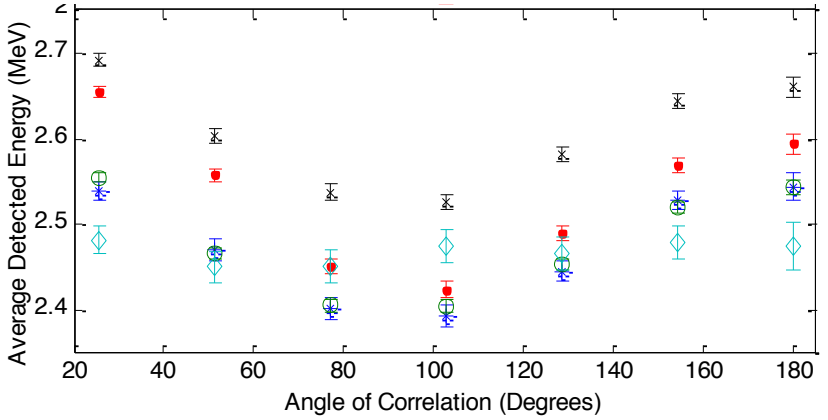
What is being done now
Validation testing (2)

- **University of Michigan differential measurements of angular correlations**
- **Priority is to compare against experimental measurements**
- **Follow-up of 2014 NSE paper by S.A. Pozzi *et al*.**
- **Submitted an abstract to IRRMA X meeting in Chicago, IL, July 9-13**
- **Transport and post-processing code comparisons**
  - MCNP6 / DRiFT
  - MCNP6 / MPPost
  - MCNPX-PoliMi / MPPost
  - MCNPX-PoliMi / DRiFT



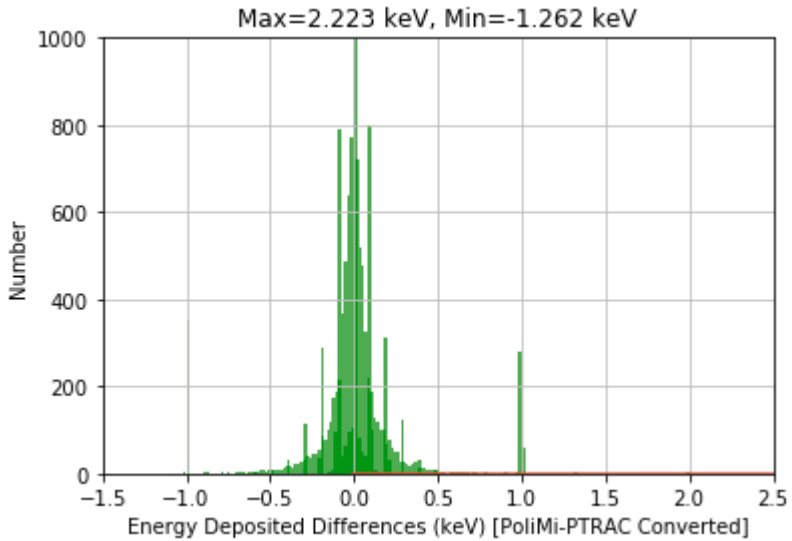


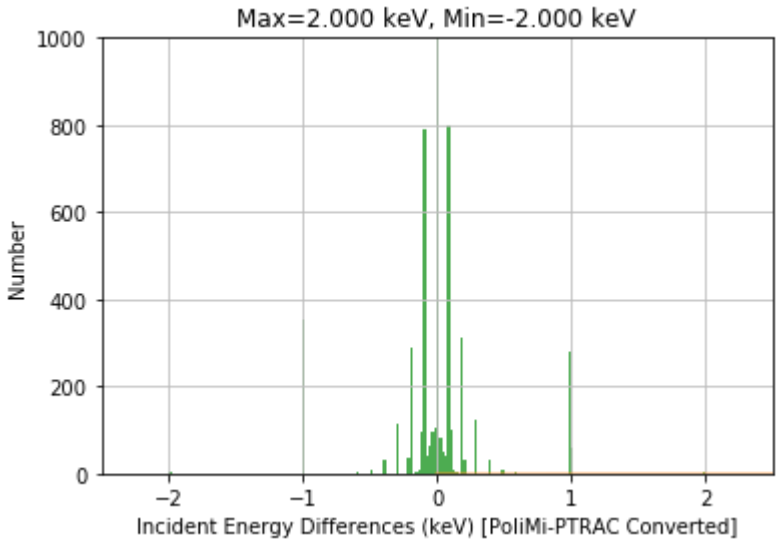




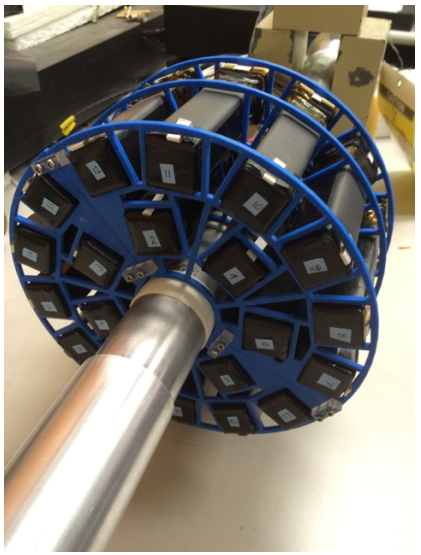
What is being done now
Validation testing (3)

- **To perform MCNP6 / MPPost and MCNPX-PoliMi / DRiFT calculations, the outputs may need to be converted**
- **Tested PTRAC to MCNPX-PoliMi collision output file conversion script**
  - Again, used MCNPTools for PTRAC reading
  - Agreement is very reasonable with small discrepancies
    - Deposited energy differences – inelastic scatter on Carbon (<0.009% source with > 1keV diff)
    - Incident energy differences – elastic scatter on Hydrogen (<0.004% source with > 1keV diff)



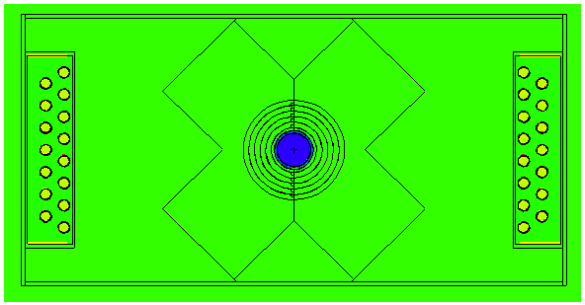


What is being done now
Validation testing (4)



- **Starting last summer, alpha testing new models began**
  - Students from CNEC and CVT are participating
  - Testing list-mode output through PTRAC
  - Collaboration with Univ. of Michigan (UMich), LLNL & LBNL

- **In progress validation models include**
  - NISC experiments (K. Meierbachtol, M. Andrews)
  - UMich scintillator array (M. Marcath, M. Rising)
  - LLNL scintillator array (J. Verbeke, M. Rising)
  - LANL detector arrays at LANSCE, DANCE & NEUANCE (C. Walker – LANL, M. Pinilla – KSU)
  - Subcritical BeRP ball experiments (J. Arthur – UMich)
  - Criticality validation (D. Timmons - UNM)
  - Others…



What will be done in FY17
New MCNP6.2 tools released

- **In MCNP6.2 release:**
  - (M)ISC : MCNP / general intrinsic source constructor
  - MCNPTools : MCNP outputs

- **To be released at a future date:**
  - DRiFT : Detector Response Function Toolkit

- **Presented at workshop at 2016 ANS ANNTP Conference in Santa Fe, NM (look on website under technical references and workshops)**
  - LA-UR-16-27559 : MCNP6 basics
  - LA-UR-16-27301 : fission multiplicity models
  - LA-UR-16-27265 : ISC and MCNPTools info
  - LA-UR-16-27166 : DRiFT

What will be done in FY17
Code upgrades and modernization

- **In general, MCNP will see major infrastructure and coding changes in the upcoming years**
  - Modernization
    - Common software engineering practices
    - Utilize software engineering tools (git, cmake, etc.)
  - Minimize impact on users

- **Improve parallel capabilities**
  - OMP threading for models
  - PTRAC / event logger improvements
    - MPI capable
    - Thread safe
  - Physics algorithm improvements
    - Closer to analog
    - ENDF/B-VIII – separate photon production channels

What else…
Where has this been presented

- **Meetings and workshops in FY14-FY16**
  - 2014 ANS Winter Meeting – M. Rising *et al*. in NNP Division
  - 2015 ANS M&C + SNA + MC – MCNP workshop
  - 2015 UNM Seminar – M. Rising
  - 2016 ANS PHYSOR & NCSP TPR – UNM student work
  - 2016 ANS ANNTP Conference – MCNP workshop
  - 2016 NECDC – same as PHYSOR/NCSP work above

- **Upcoming meetings and workshops in FY17**
  - 2017 Nuclear Engineering Capability Review – LANL
  - 2017 ANS Summer Meeting – M. Rising & A. Sood in RPS Division
  - 2017 IRRMA X Conference – M. Andrews, M. Rising & M. Marcath
  - 2017 ANS NCSD Topical Meeting – MCNP workshop
  - Others…

What else…
Conclusions

- **Needs to have validation tests documented and included**
  - Would have been nice to have more results prior to MCNP6.2 release
  - All of the ongoing work is extremely promising
- **Should be continue-run, MPI-capable and thread-safe**
  - Need performance improvements (for CGMF especially)
  - Other MCNP features like PTRAC need work too

- **MCNP tasks for this LCP should be attainable**
  - Physics algorithm improvements ➔ priority after MCNP6.2 release
  - Parallel code capabilities ➔ priority after MCNP6.2 release
  - List-mode analyzer utilities ➔ some already made available
  - Perform MCNP6 simulations of NISC experiments ➔ ongoing

THANK YOU!

Questions?