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Title: Which nuclear data can be validated with LLNL pulsed-sphere experiments?

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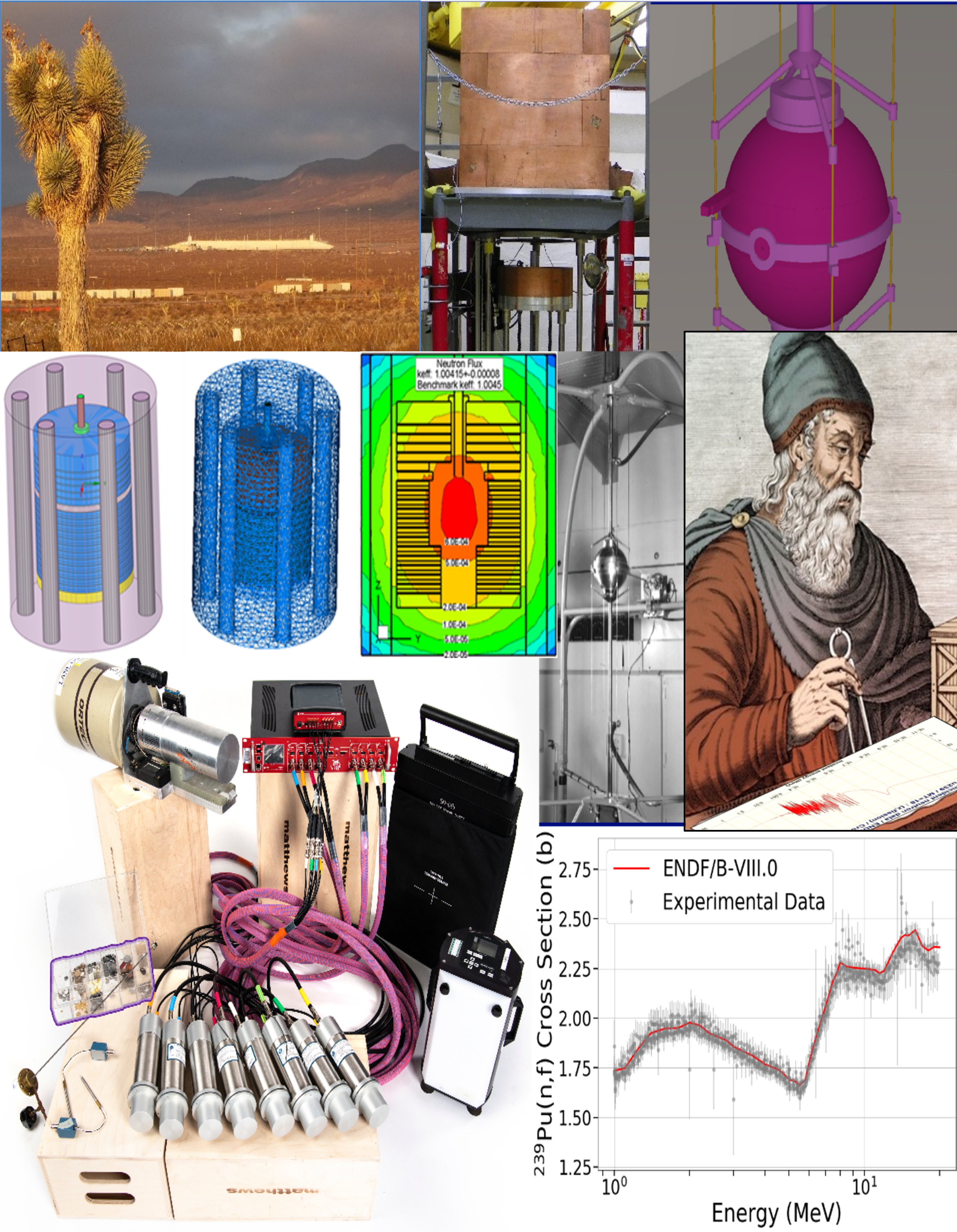

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Which nuclear data can be validated with LLNL pulsed-sphere experiments?

Denise Neudecker

WPEC SG-47, June 16, 21

Based on paper by: D. Neudecker, O. Cabellos, A. Clark, W. Haeck, R. Capote, A. Trkov, M. Rising, Annals of Nuclear Energy 159, 108345 (2021).

Big thanks also go to M. Herman!

Caveat: this talk discusses what nuclear data can be validated with pulsed spheres.

- I am not evaluating a benchmark here!
- I am a nuclear data evaluator who validates nuclear data with respect to these data (partially using ML) and this talk is is from the nuclear-data validation perspective.
- The input deck library was established by S. Frankle.
- I would be excited if these experiments are evaluated as benchmarks for inclusion in SINBAD.

Outline

- Short reminder: What are LLNL pulsed spheres?
- What sphere materials are we using for validation?
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- How do we get sensitivities?
- What nuclear data can we validate?
  - ^{16}O and ^{12}C spheres
  - Fe sphere
  - Pu sphere
- What nuclear data are indicated as problematic for ENDF/B-VIII.0?

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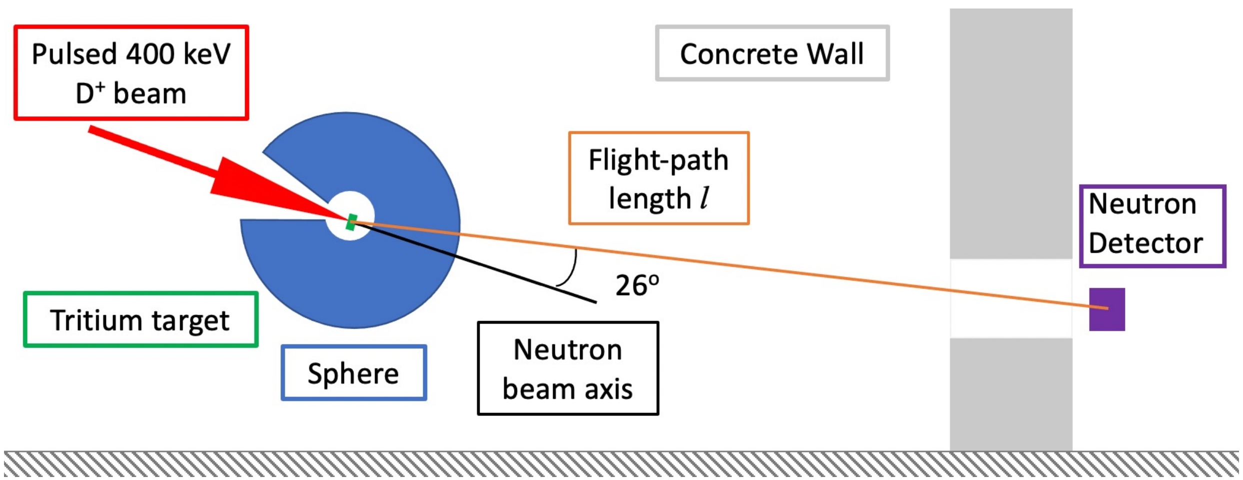
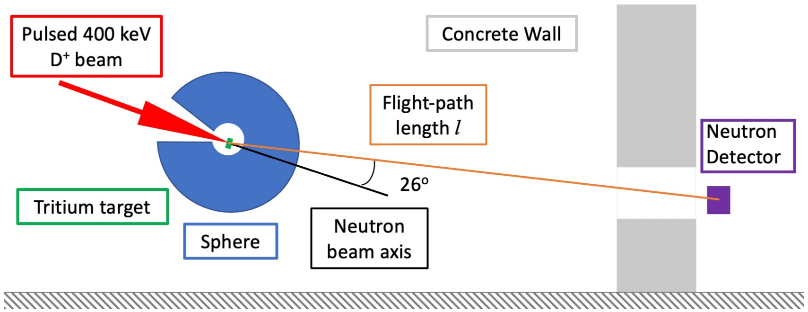
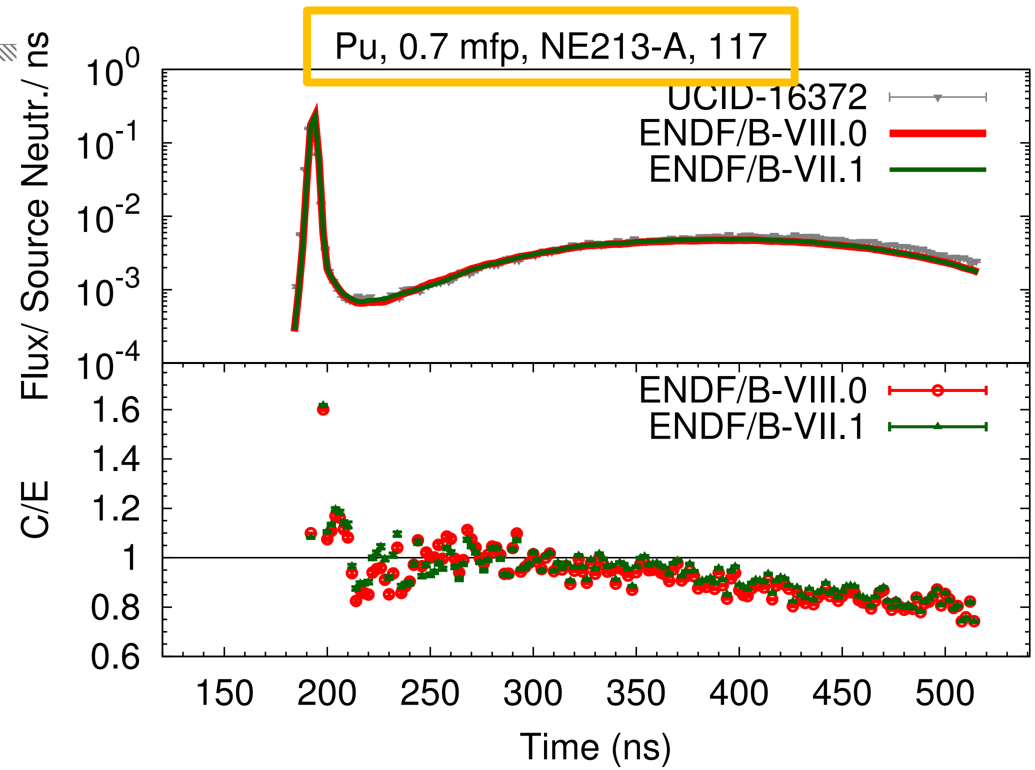
All neutrons leaked from a pulsed sphere are measured at a specific angle.

- LLNL pulsed sphere measurements for materials of H_2O to ^{239}Pu were designed for testing of transport codes and nuclear data, e.g., C. Wong, UCRL-51144, UCRL-ID-91774, Webster, UCID-17332.
- 14-MeV neutron produced via D+T in the center of sphere.



Exp. neutron-leakage spectra are given for various angles (26, 39, 117), detectors and mfps.





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We have 75 pulsed spheres available for 20 distinc materials, some with varying thickness.

Core	# of exp.	Validates	Core	# of exp.	Validates
Light Water	6	^{1}H, ^{16}O	Teflon	3	^{19}F, ^{12}C
Heavy Water	2	^{2}H,^{16}O	Magnesium	3	$^{24\text{-}26}$Mg
^{6}Li	5	^{6}Li	^{27}Al	2	^{27}Al
^{7}Li	5	^{7}Li	Titanium	2	$^{46\text{-}50}$Ti
^{9}Be	6	^{9}Be	Iron	6	^{12}C, $^{54.56}$Fe
Polyethylene	3	^{1}H, ^{12}C	Lead	2	$^{206\text{-}208}$Pb
Carbon	4	^{12}C	Tungsten	2 (0 ok)	$^{182\text{-}184,186}$W
^{14}Ni	3 (2 ok)	^{14}Ni	^{235}U	7	^{235}U
^{16}O	2 (1 ok)	^{16}O	^{238}U	5	^{238}U
Concrete	4	^{1}H, ^{16}O, ^{28}Si	^{239}Pu	3	^{239}Pu

S. Frankle provided MCNP input decks for these benchmarks, LA-UR-05-5879 (2005).

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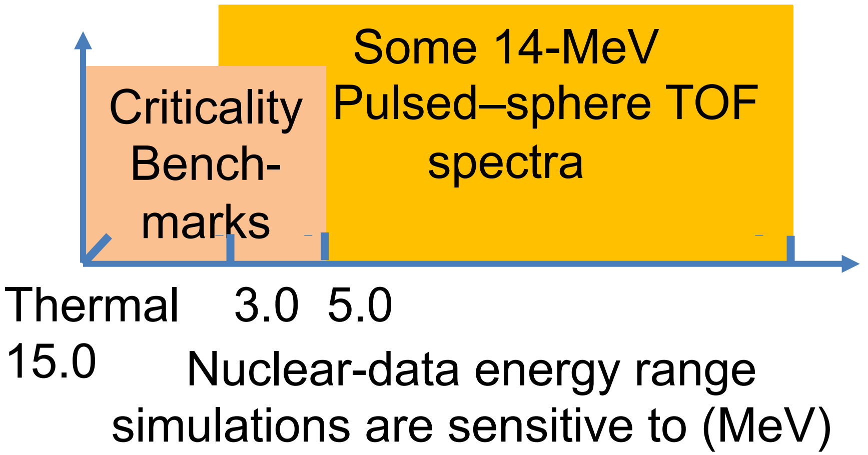
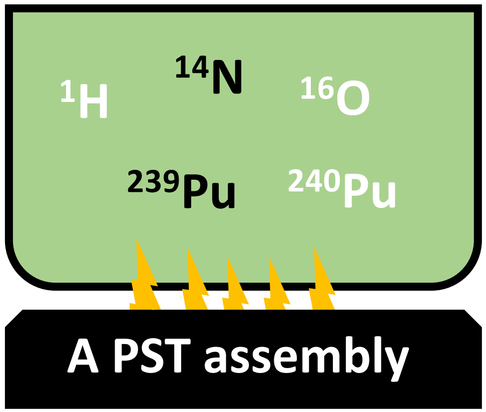
These pulsed spheres provide additional information compared to crits: extended Einc range

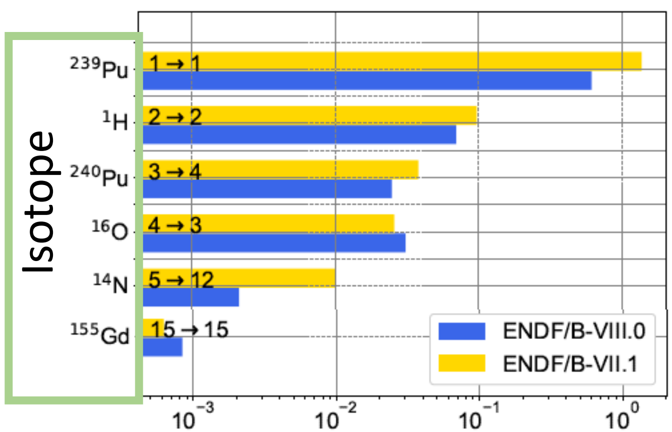
D+T pulsed spheres allow us to validate nuclear data for some materials from 3-15 MeV. Crits allow us to validate nuclear data up to 5 MeV. -> We use them in large-scale validation using ML methods such as described in Neudecker et al., NDS 167, 36 (2020).



Pulsed Sphere TOF spectra allow to validate nuclear data for light elements, structural isotopes, fuels.

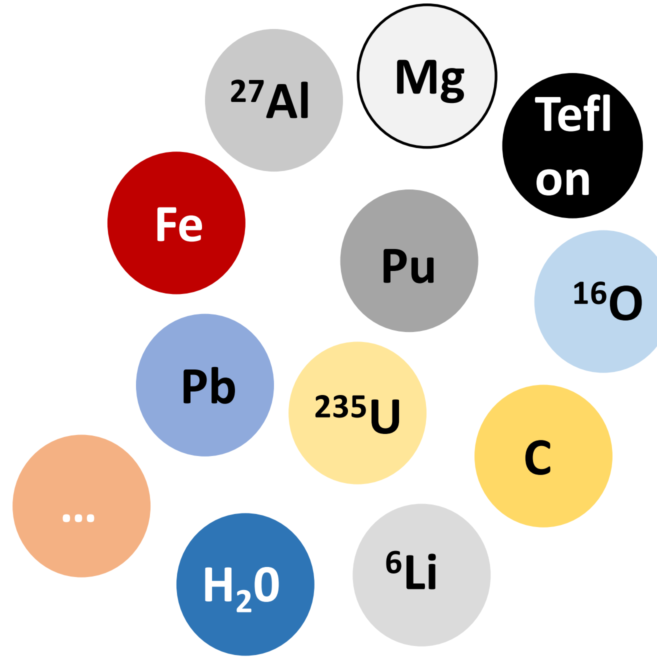
Criticality Benchmarks





Importance of Nuclear Data for Bias

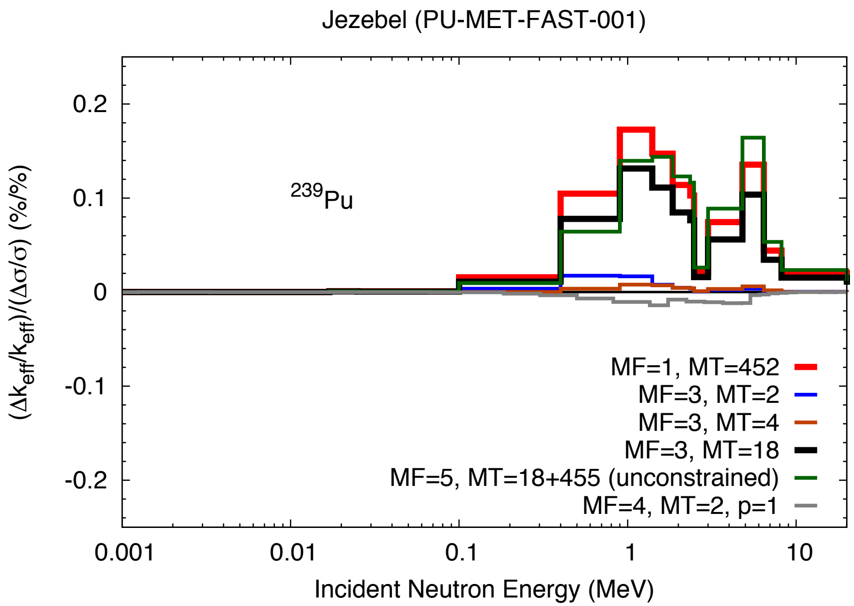
14-MeV LLNL pulsed spheres



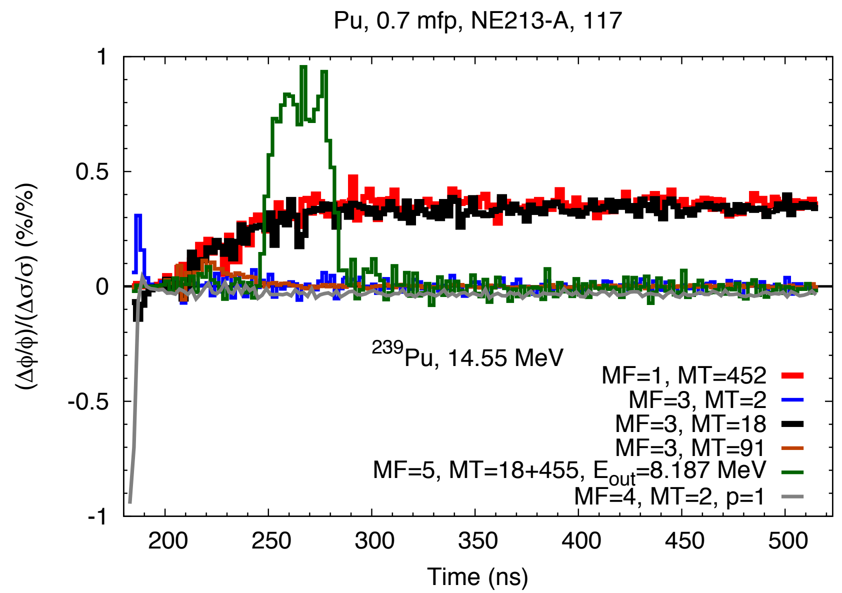
One can pinpoint more explicitly the isotope of particular nuclear data that are problematic.

Pulsed Sphere TOF spectra have different sensitivity to angular distributions and fission-source term.

Criticality Benchmarks



14-MeV LLNL pulsed spheres



Relative sensitivity of average fission neutron multiplicity versus, fission neutron spectrum, fission cross section similar for criticality benchmarks.

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Sensitivities were calculated by O. Cabellos (UPM) and A.R. Clark (LANL) with:

- **Pert card capability in MCNP:** in development, yields sensitivities for: MF={1,2,3,4}
- **MCSEN5 tied to MCNP5.1.30:**
  - R.L. Perel, J.J. Wagschal, Y. Yeivin, NSE 124, 197 (1996).
  - MCSEN yields sensitivities for: MF={1,2,3,4,6}.
- **SANDY and FRENDY codes:**
  - **SANDY (**https://github.com/luca-fiorito-11/sandy**)**
    - SANDY perturbs ENDF/ PENDF files -> NJOY processes into ACE via NJOY.
    - SANDY yields sensitivities for: MF={1,2,3,4,6}.
  - **FRENDY (**https://rpg.jaea.go.jp/main/en/program_frendy/**)**
    - FRENDY perturbs ACE files
    - FRENDY is able to operate on: cross-sections, nubar and CHI

See Oscar Cabellos talk at last WPEC SG-47 meeting.

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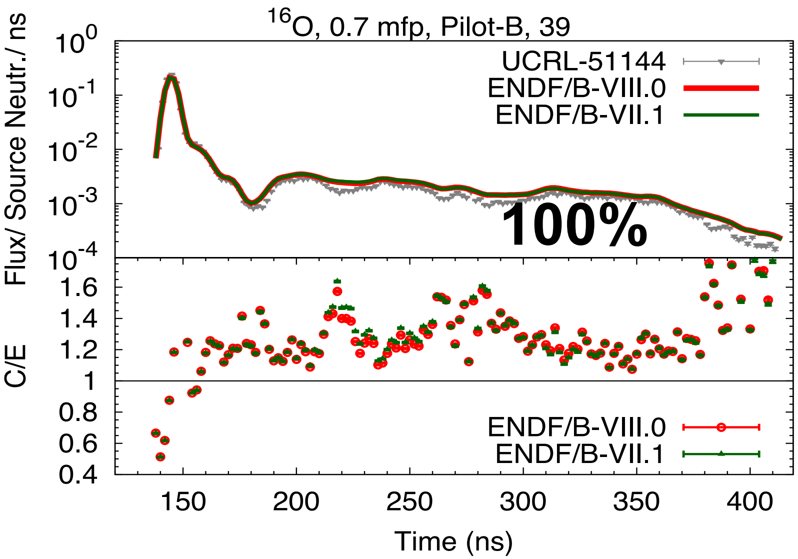
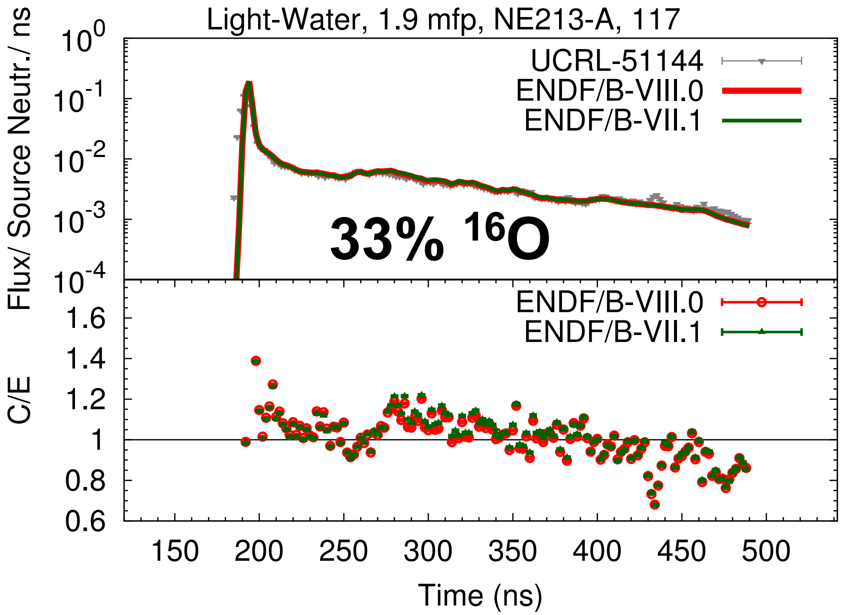
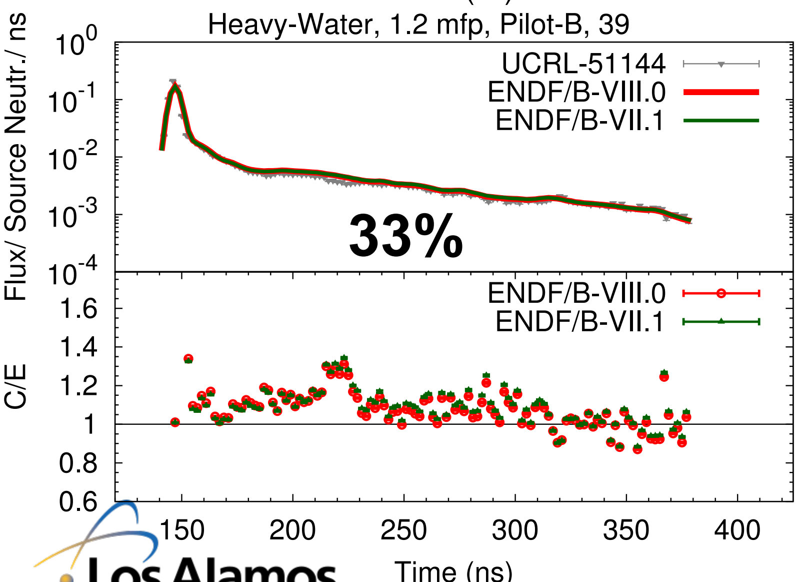
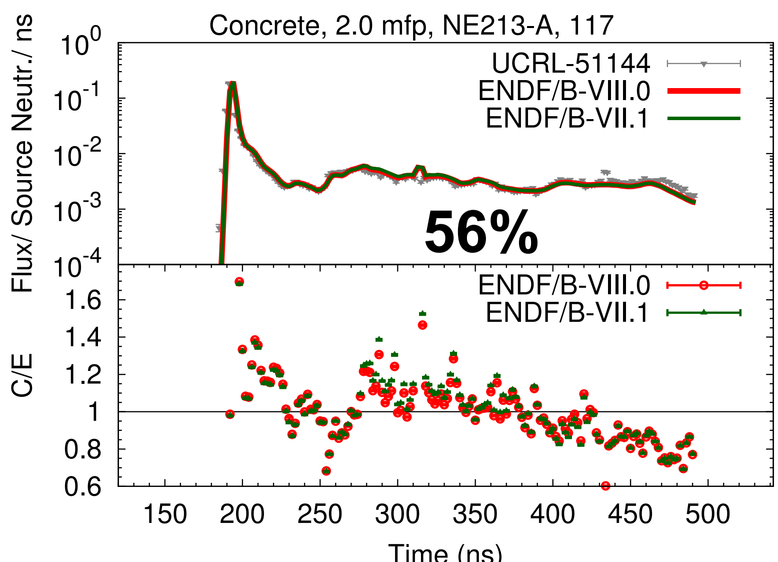
We see issues in neutron spectra containing ^{16}O.

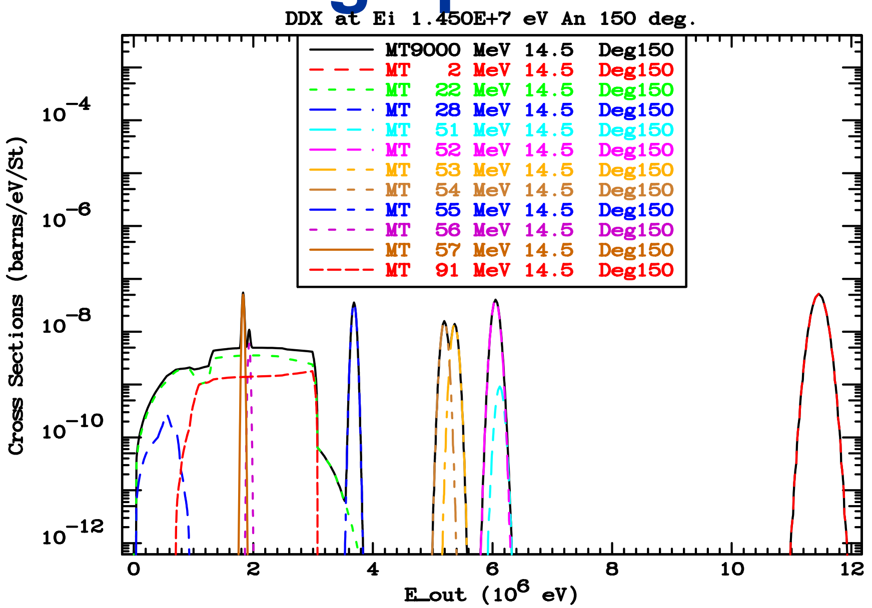


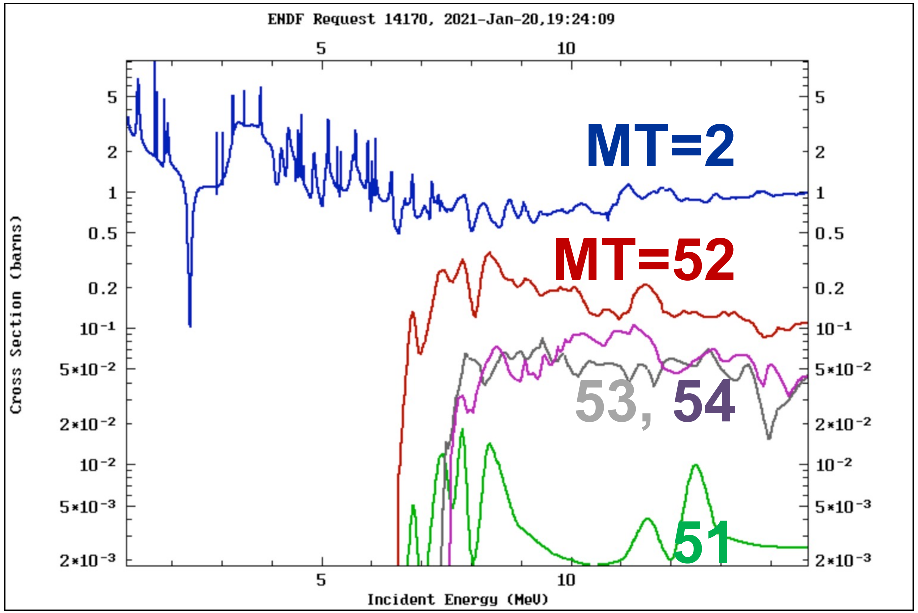






Elastic and inelastic discrete levels matter for simulating spheres containing ^{16}O.





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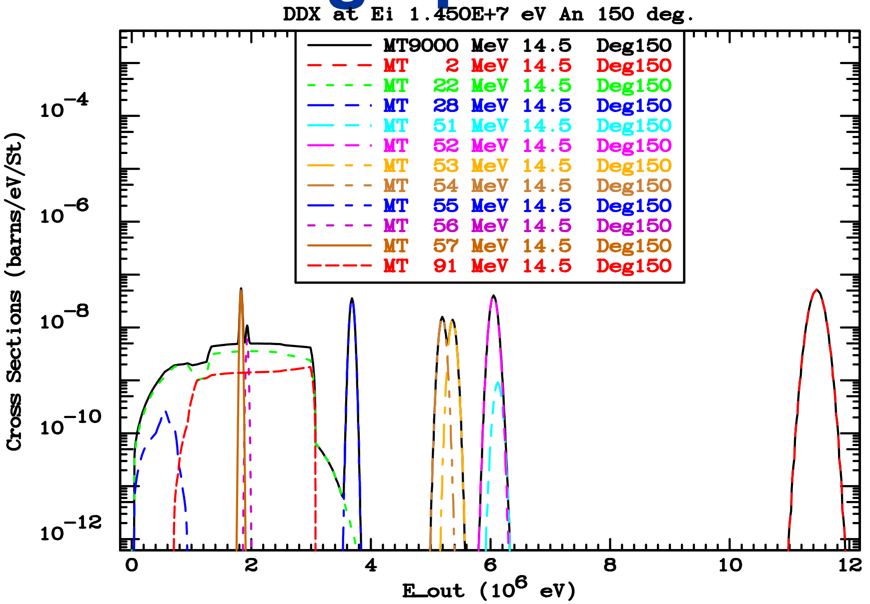
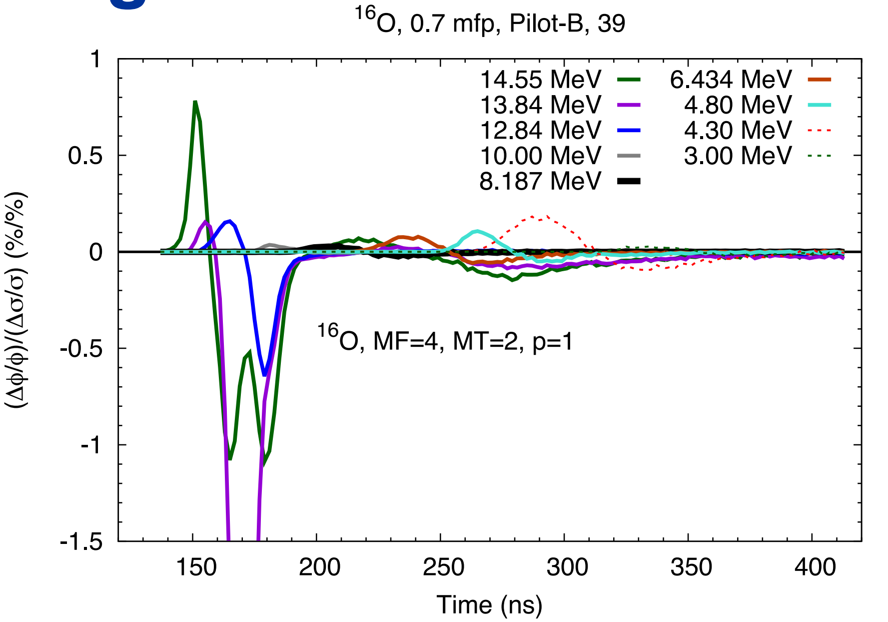
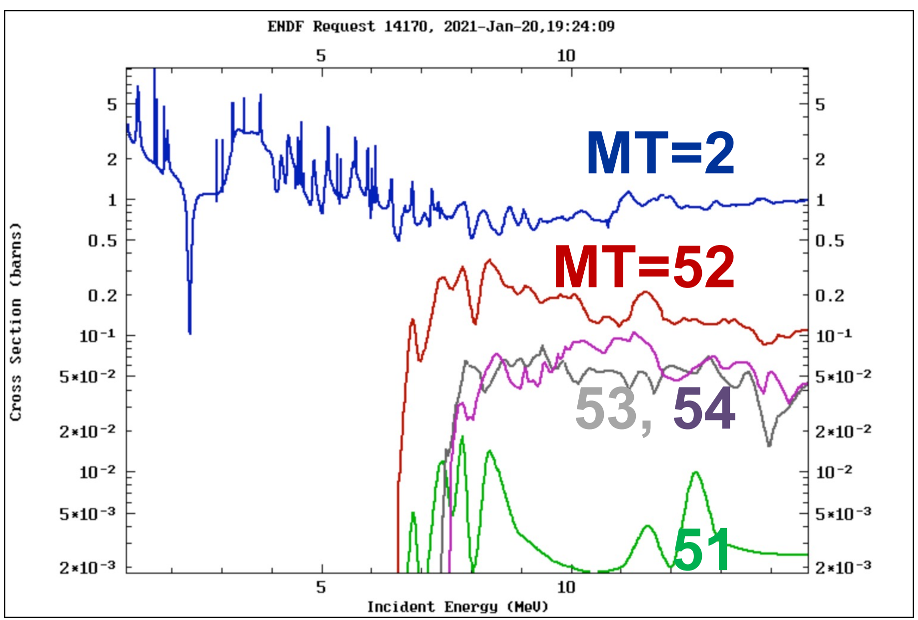
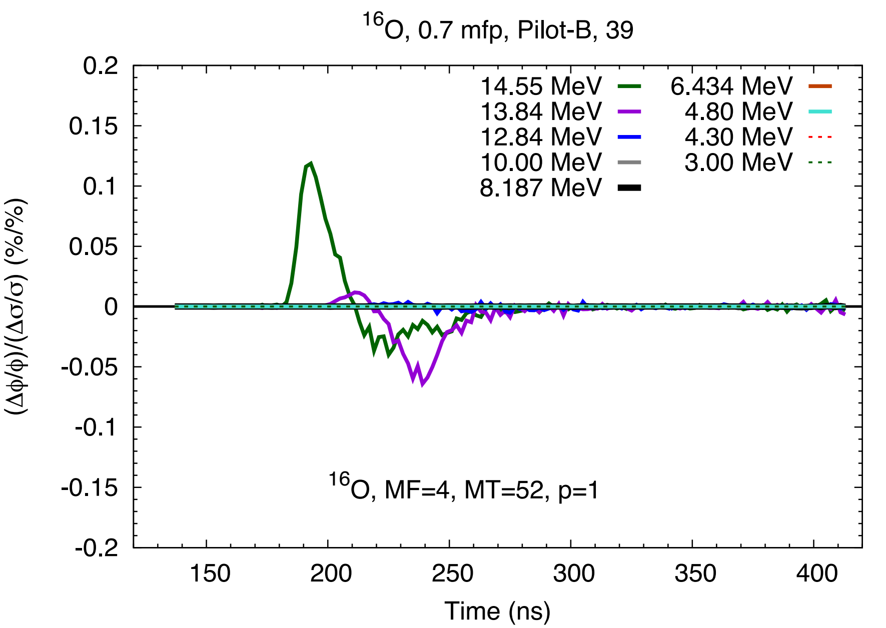
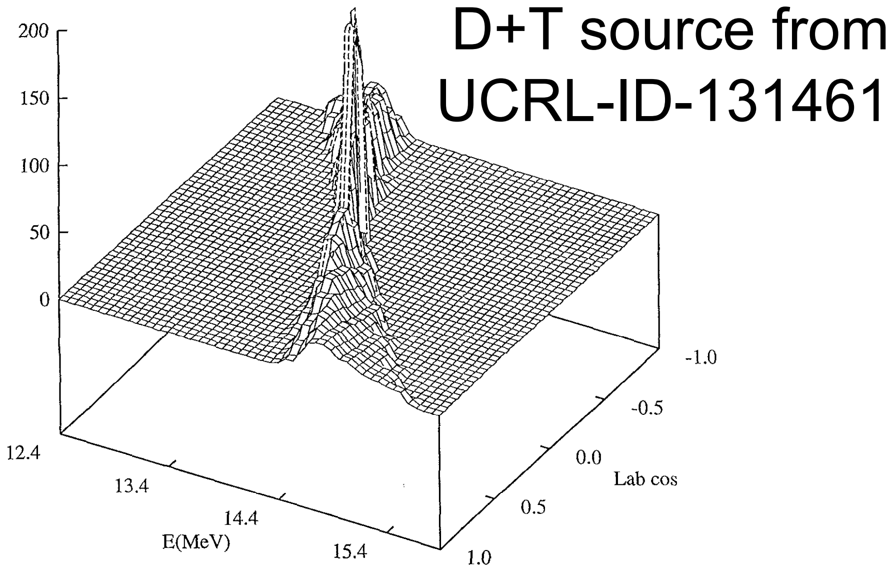


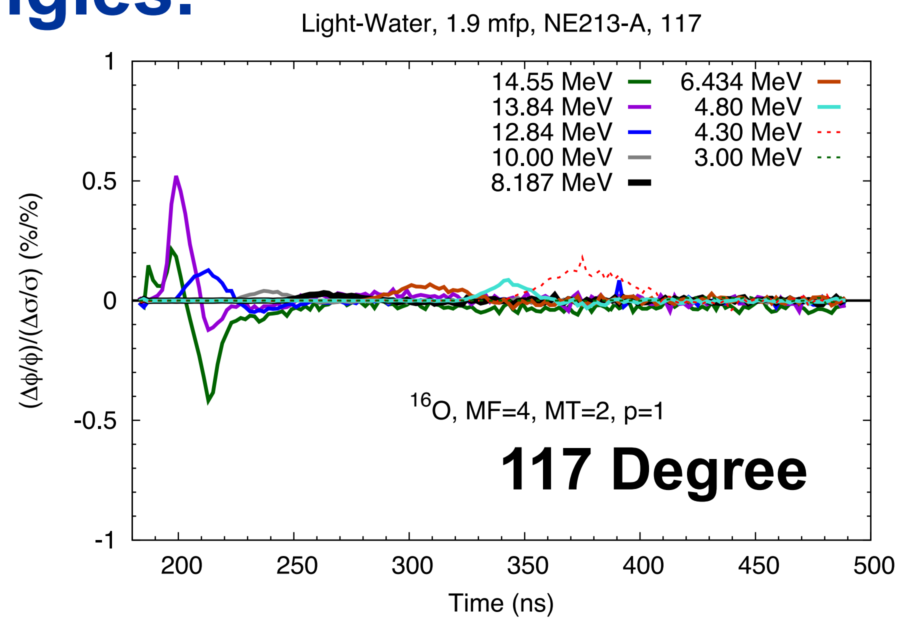


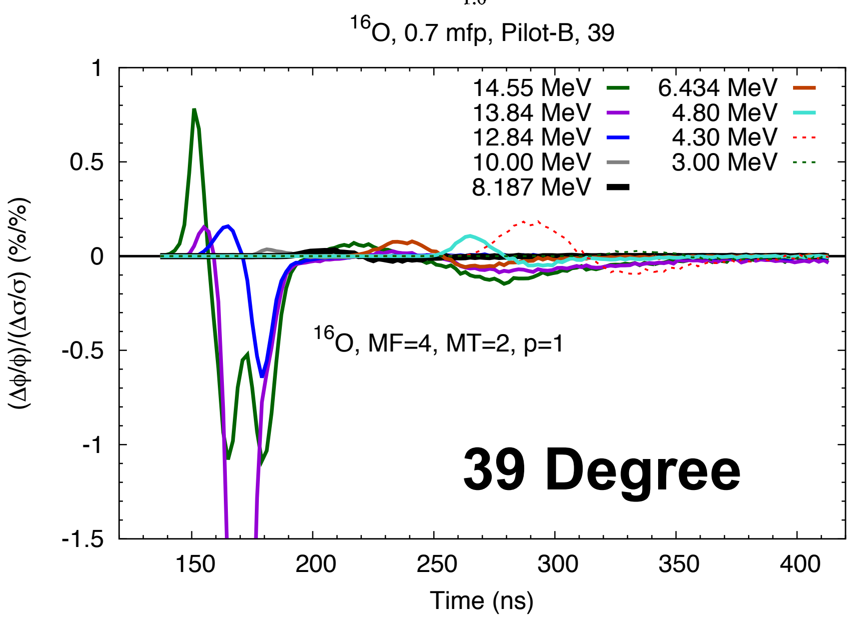


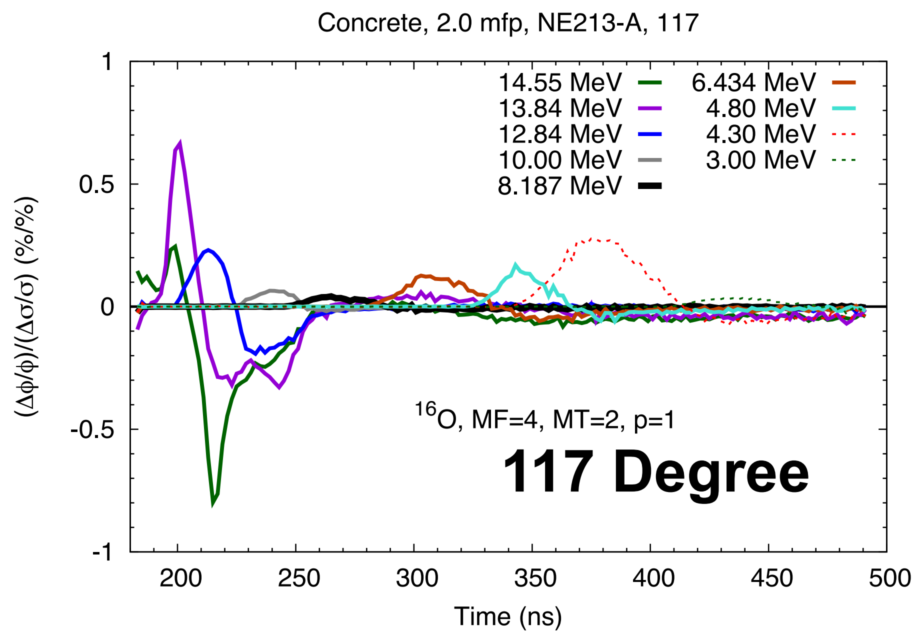


We query slightly different incident-energy ranges when looking at different angles.

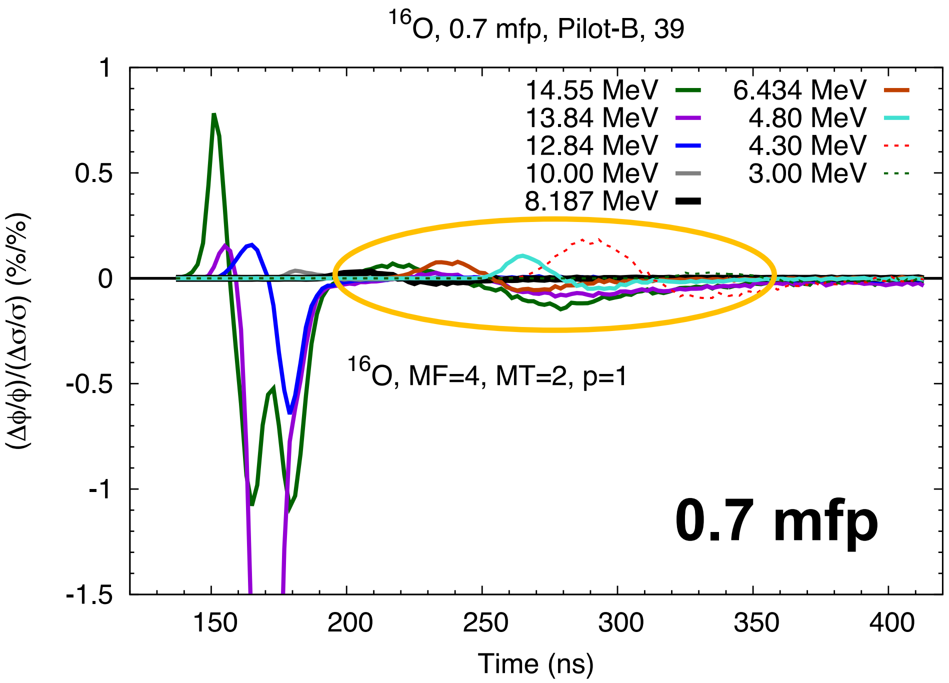


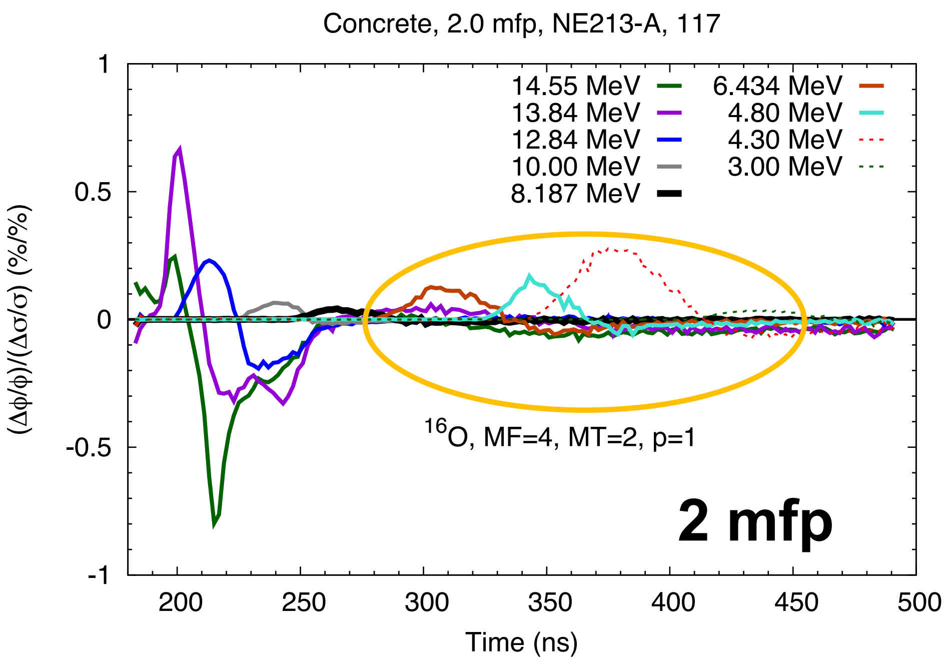






The probability of inelastic scatters and multiple scatters depends on mfp … AND





Elastic scattering after inelastic scattering.
Enhanced for larger mfp.

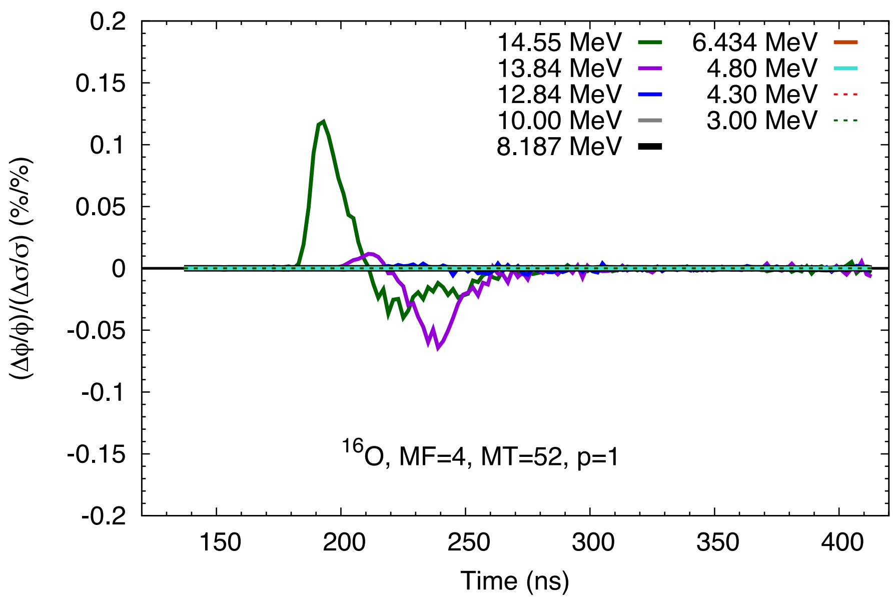
The probability of inelastic scatters and multiple scatters depends on mfp AND LEVEL SCHEME!

Discrete Levels of ^{16}O from RIPL-3.0

```
--------------------------------------------------------------------------------------------------
NL    EL[MeV]      S/P   F      T1/2[s] Ng s unc               s-info   nd m          p      mode
                                            Nf     Eg[MeV]      Pg           Pe              Icc
--------------------------------------------------------------------------------------------------
 1    0.000000     0.0   1 -1.000E+00   0 u                      0+    0
 2    6.049400     0.0   1  6.700E-11   1 u                      0+    0
                                              1     6.0482  1.000E+00  1.000E+00  0.000E+00
 3    6.129890     3.0  -1  1.840E-11   1 u                      3-    0
                                              1     6.1286  1.000E+00  1.000E+00  0.000E+00
 4    6.917100     2.0   1  4.700E-15   3 u                      2+    0
                                              3     0.7872  7.997E-05  7.997E-05  0.000E+00
                                              2     0.8677  2.699E-04  2.699E-04  0.000E+00
                                              1     6.9155  9.997E-01  9.997E-01  0.000E+00
```

Only inelastic scatters induced by D+T source because scattering from MT=52 leaves not enough energy.

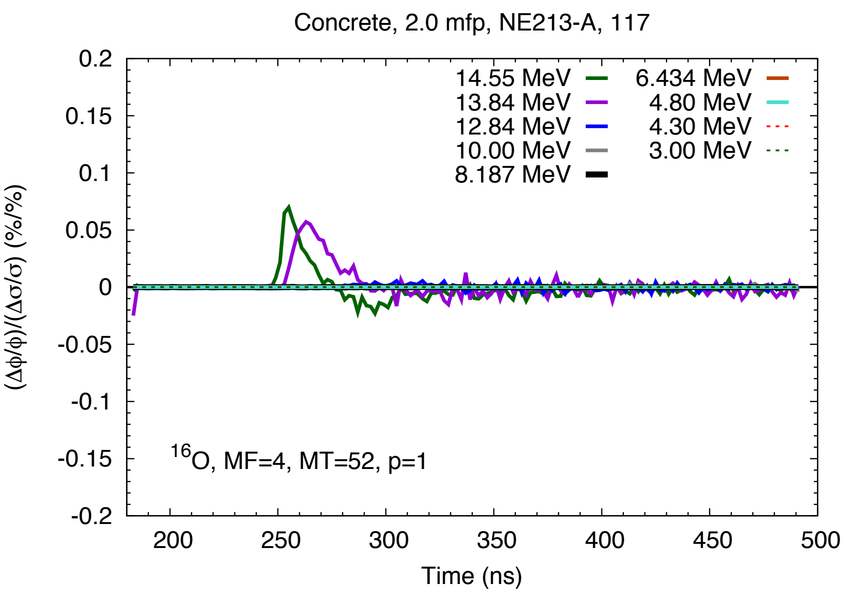
^{16}O, 0.7 mfp, Pilot-B, 39

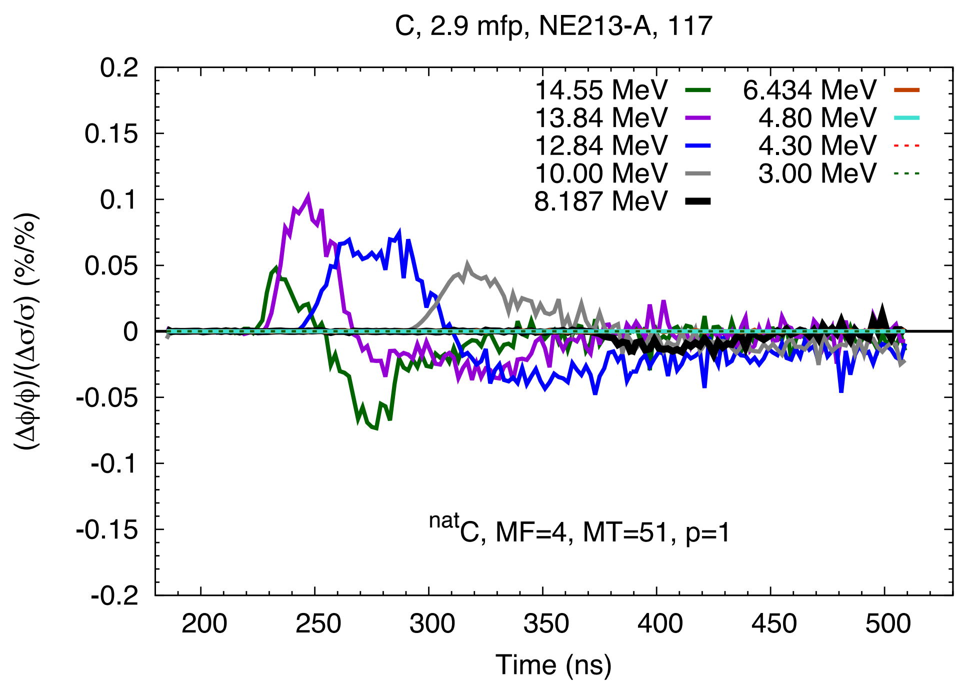


… level scheme! Different level scheme of ^{12}C leads to more multiple scatters.

Discrete Levels of ^{12}C from RIPL-3.0

```
---------------------------------------------------------------------------------------------
NL    EL[MeV]      S/P   F      T1/2[s]  Ng  s  unc                  s-info   nd  m        p       mode
                                              Nf      Eg[MeV]       Pg           Pe              Icc
---------------------------------------------------------------------------------------------
 1    0.000000     0.0   1  -1.000E+00   0  u                          0+    0
 2    4.439820     2.0   1   4.224E-14   1  u                          2+    1  =   1.0000E+02 %IT
                                              1        4.4389   9.987E-01   1.000E+00   1.322E-03
 3    7.654070     0.0   1   4.906E-17   1  u                          0+    2  =   1.0000E+02 %A
                                              2        3.2138   4.156E-04   4.160E-04   8.760E-04
 4    9.641000     3.0  -1   9.918E-21   1  u                          3-    2  =   1.0000E+02 %A
                                              1        9.6370   4.100E-07   4.100E-07   0.000E+00
```





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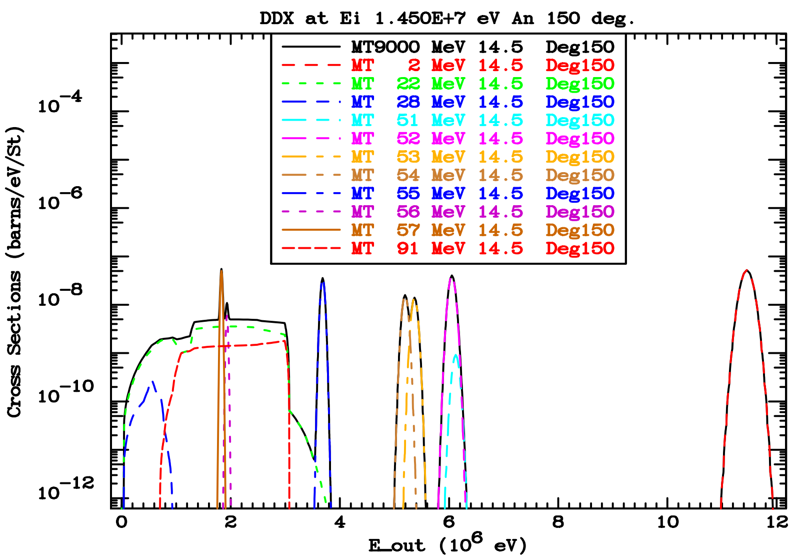
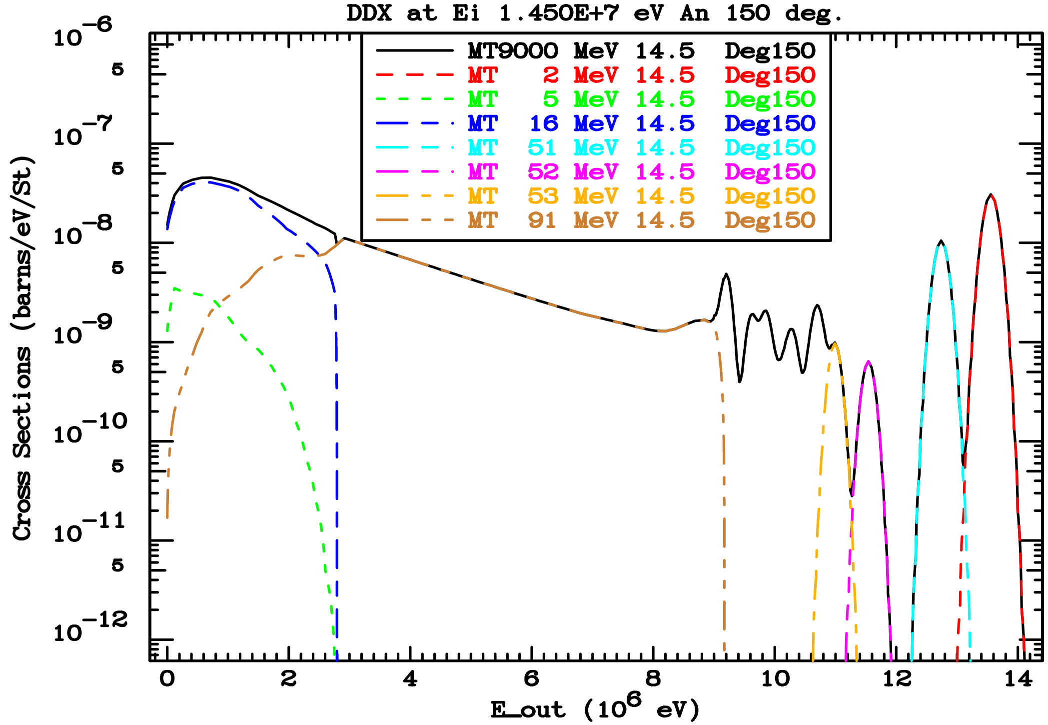
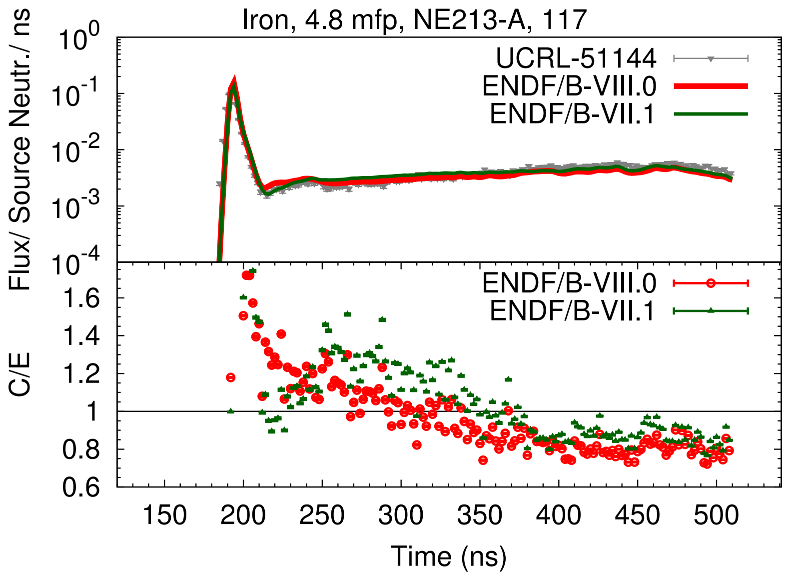
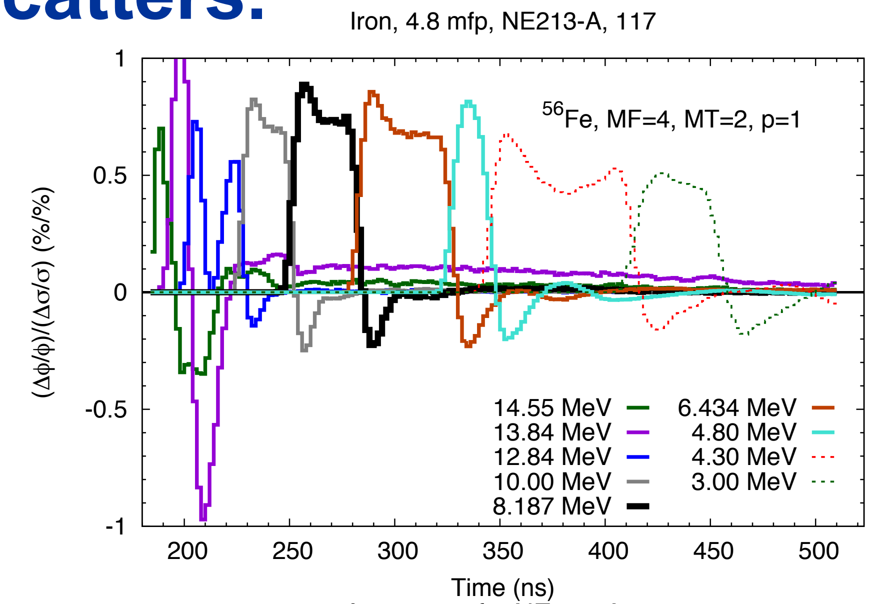
Iron sphere allow us to study in detail MF={3,6}, MT=91. This is typical for heavier elements.

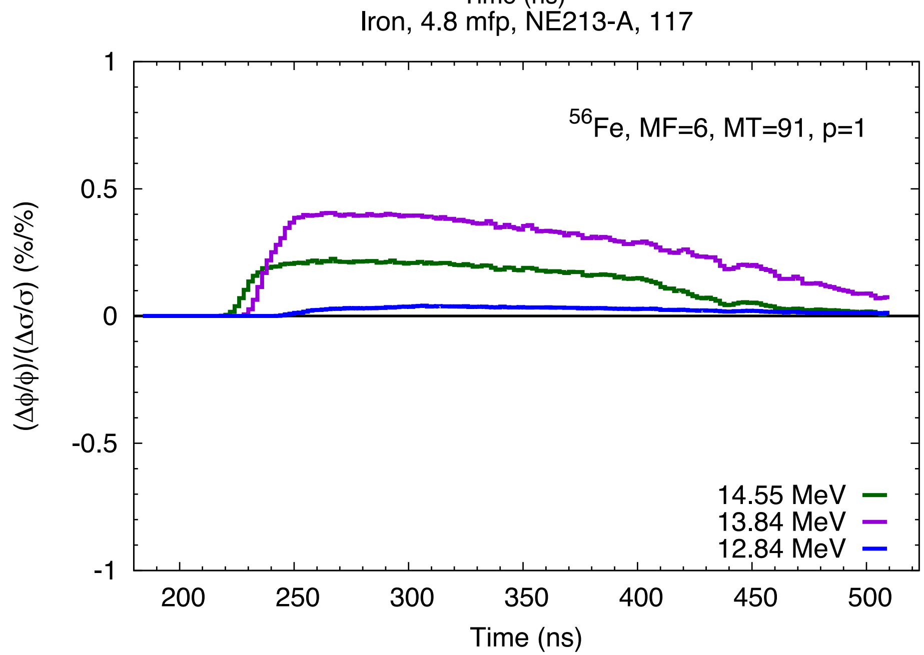




As iron sphere are more sensitive to MF={3,6}, MT=91 -> more multiple scatters.







Q-value MT=91: 2.33 MeV

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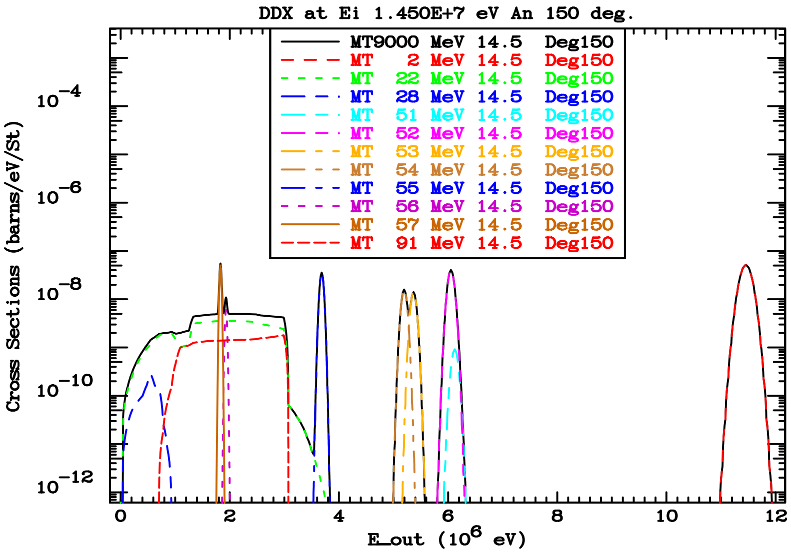
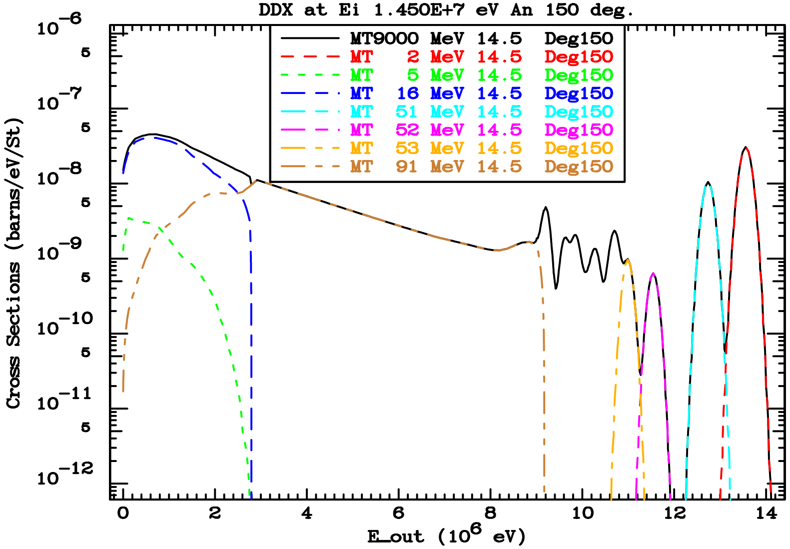
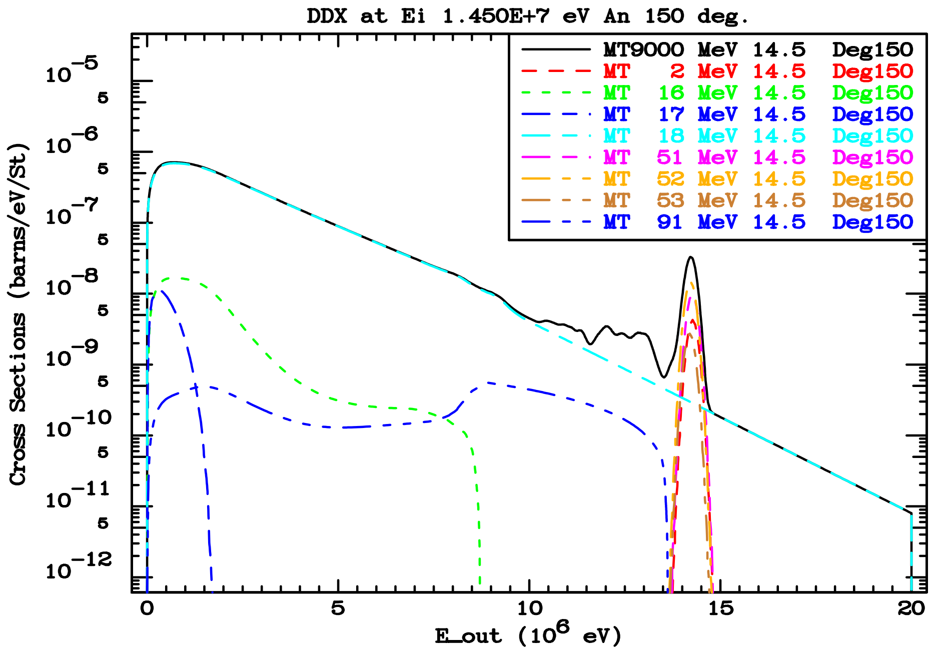
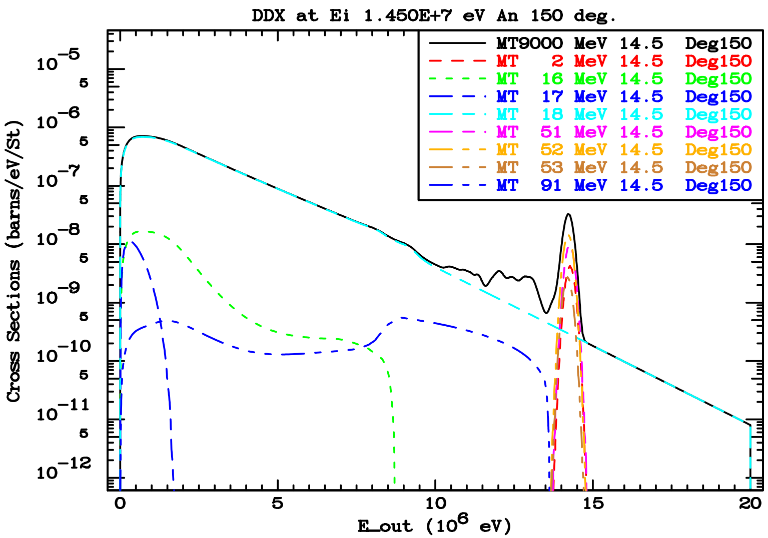
Pu sphere allow us to study in detail fission source term and MT=91.

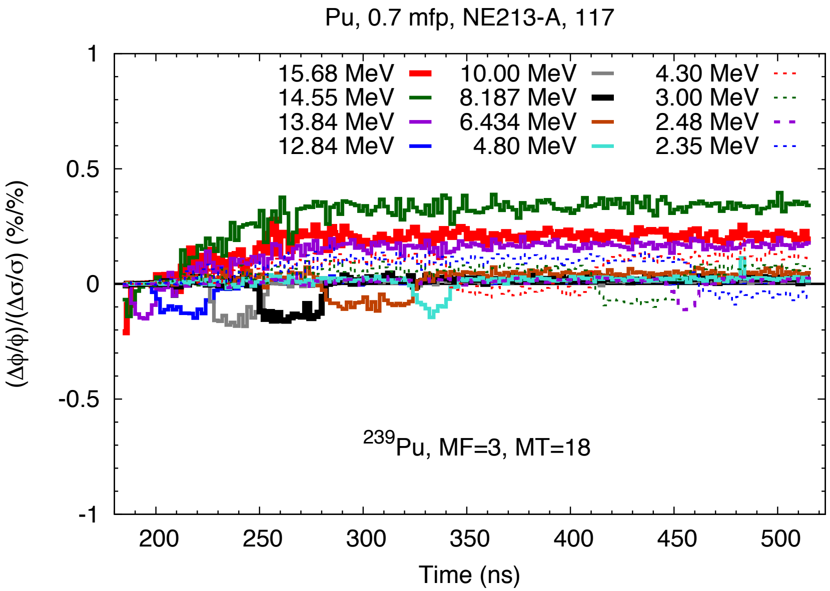


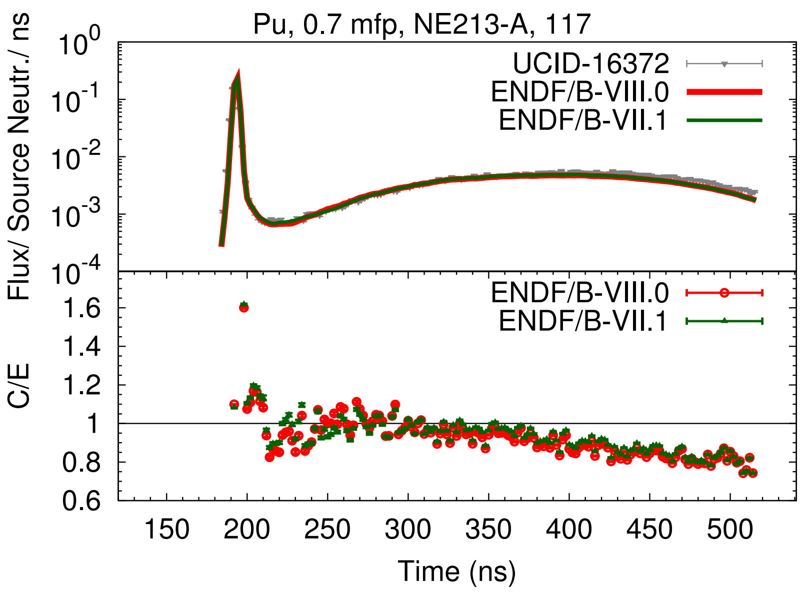


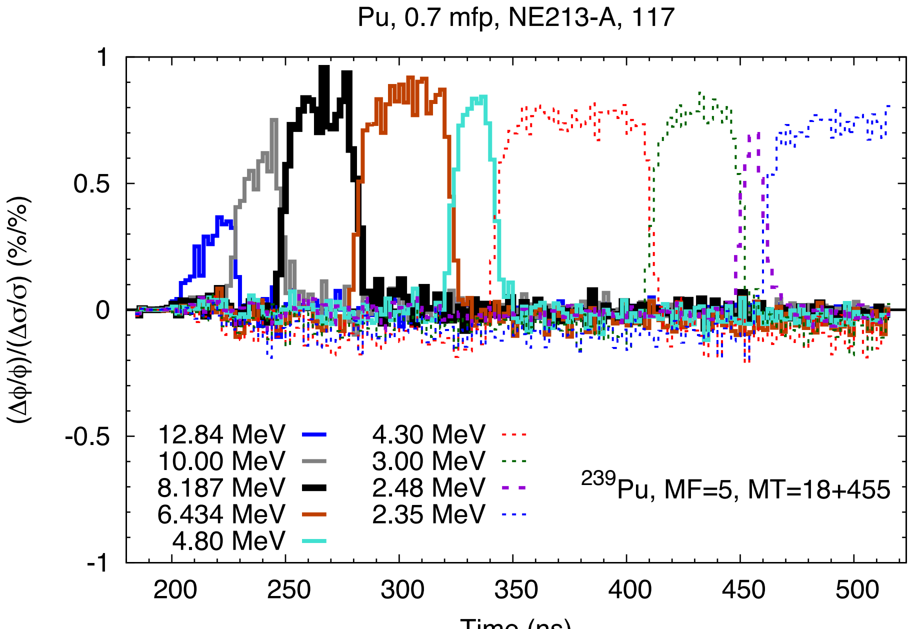


Pu 0.7 mpf sphere allow us to study in detail fission source term and MT=91 from 13-15 MeV.

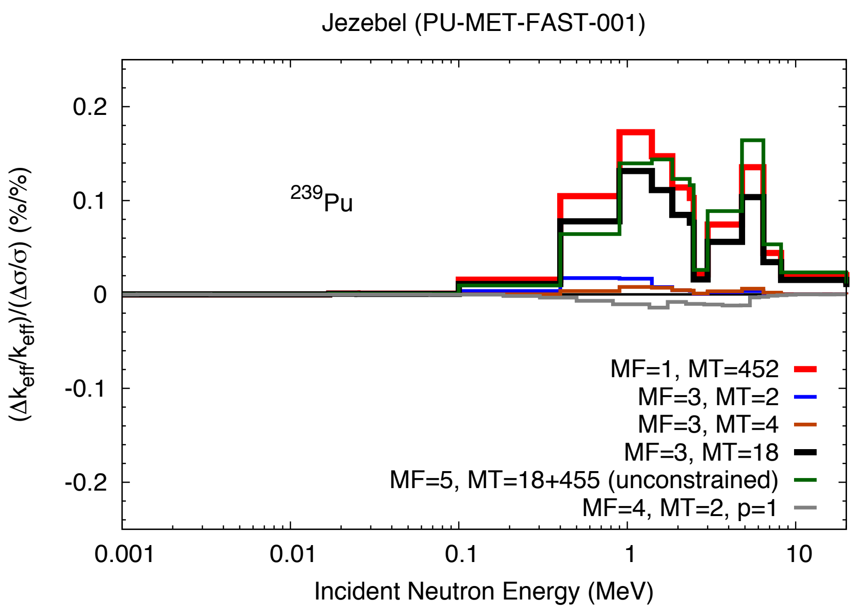


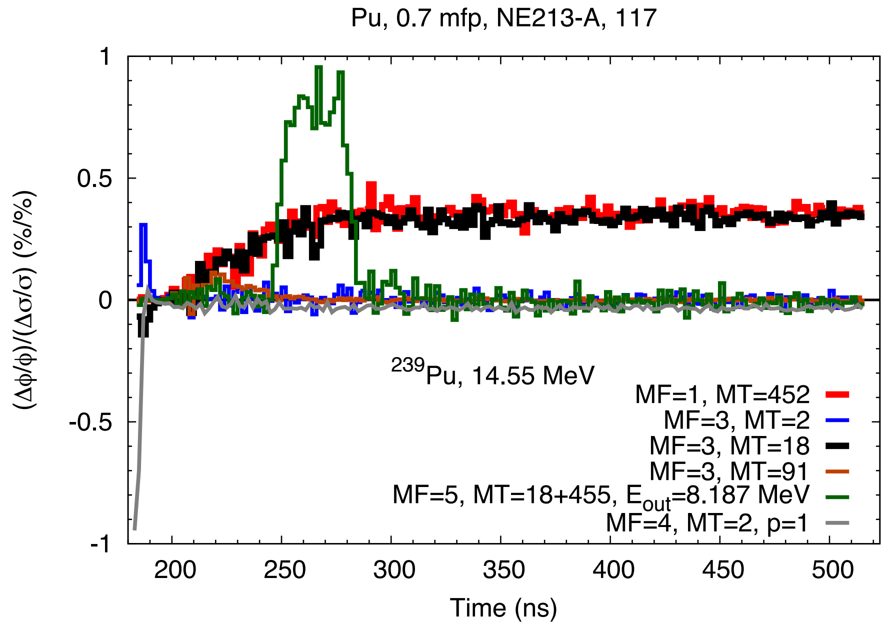






Pu sphere allow us to study in detail fission source term and MT=91.





Relative sensitivity of average fission neutron multiplicity versus, fission neutron spectrum, fission cross section similar for criticality benchmarks.

Impact of angular distributions and fission-neutron spectrum for TOF spectra different from criticality benchmarks.

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These experiments allow us to find potential issues in nuclear data!

Table 6: Those nuclear data in ENDF/B-VIII.0 that are recommended to be further investigated are identified by their MF and MT numbers.

Isotope	MF, MT of data recommended to be further investigated
^{6}Li	MF=3, MT=$\{4, 51-90\}$;MF=4, MT=$\{2, 51\}$;
^{7}Li	MF=4, MT=2;
^{12}C	MF=3, MT=$\{4, >50\}$; MF=4, MT=$\{2, 51\}$; MF=6, MT=91;
^{16}O	MF=3, MT=$\{2, 4\}$; MF=4, MT=$\{2, 51\}$; MF=6, MT=91;
^{19}F	MF=3, MT=$\{2, 4\}$;
^{24}Mg	MF=3, MT=2; MF=4, MT=2; MF=6, MT=91;
^{25}Mg	MF=3, MT=91; MF=6, MT=91;
^{26}Mg	MF=3, MT=2; MF=4, MT=2; MF=6, MT=91;
^{27}Al	MF=3, MT=4; MF=4, MT=2; MF=6, MT=91;
^{48}Ti	MF=3, MT=91; MF=4, MT=2; MF=6, MT=91;
^{56}Fe	MF=3, MT=$\{2, 4, 91\}$; MF=4, MT=2; MF=6, MT=91;
^{208}Pb	MF=3, MT=$\{4, 91\}$; MF=6, MT=$\{16, 91\}$;
^{235}U	MF=1, MT=452; MF=3, MT=$\{2, 4, 91\}$; MF=4, MT=2; MF=5, MT=18; MF=6, MT=91;
^{238}U	MF=3, MT=$\{4, 91\}$; MF=4, MT=2; MF=5, MT=18; MF=6, MT=91;
^{239}Pu	MF=1, MT=452; MF=3, MT=$\{18, 91\}$; MF=5, MT=18; MF=6, MT=91

Caveat: D+T pulsed spheres are NOT benchmarks yet -> evaluating them as benchmarks for possible inclusion in SINBAD would be great!

Conclusions

- LLNL pulsed sphere are a very valuable experiment series to validate scattering and fission nuclear data.
- **It would be great if they could be evaluated as benchmarks and make it into SINBAD!**
- We see potential issues in ENDF/B-VIII.0 ^{6}Li, ^{12}C, ^{16}O, $^{24-26}$Mg, ^{27}Al, ^{48}Ti, ^{56}Fe, and ^{208}Pb nuclear data. Good agreement is found with ^{1,2}H, ^{7}Li, ^{9}Be, ^{14}N, ^{235,238}U, and ^{239}Pu nuclear data.

Thank you for your attention!

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