

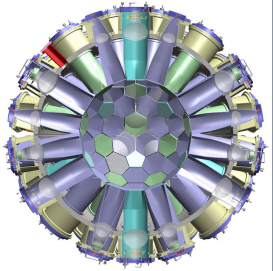
# Geant4 Simulations of Neutron-Argon Interactions

Kimberly J. Palladino  
DEAP/CLEAN Collaboration

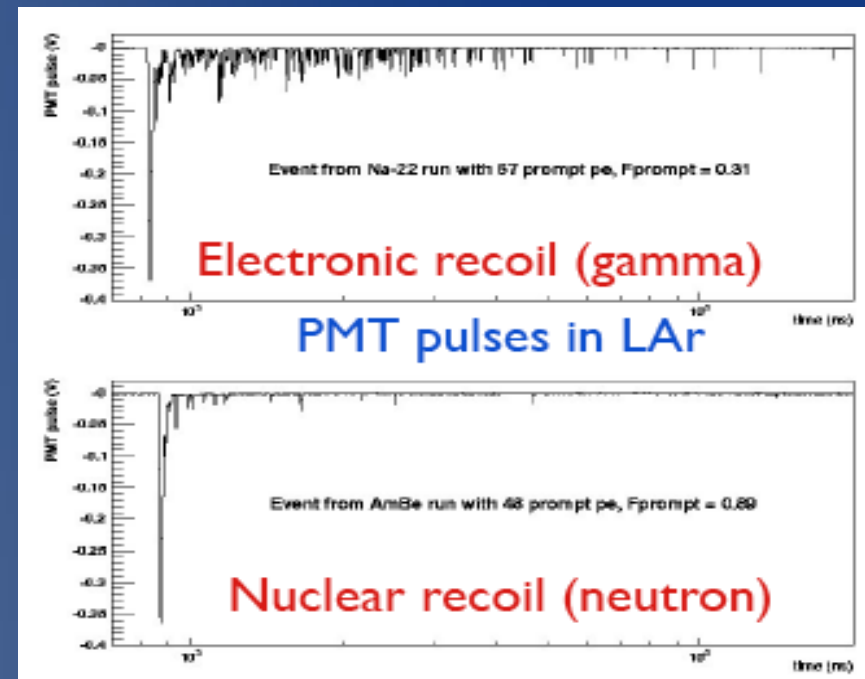
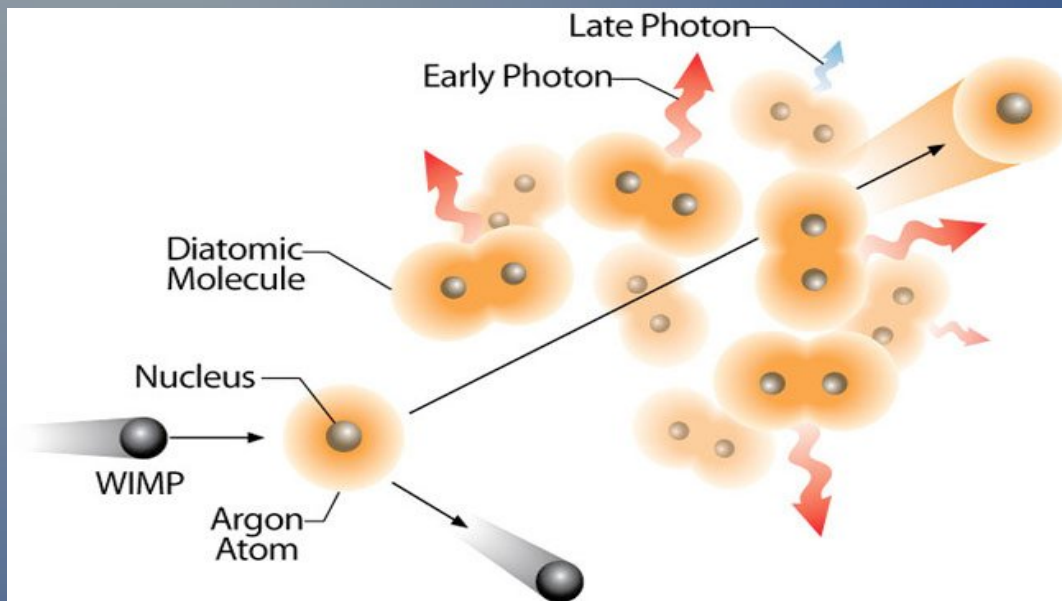
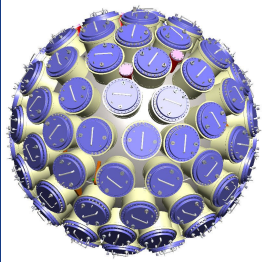
## Outline:

- Motivation from MiniCLEAN
- Pertinent Neutron Physics
- Low Energy Neutrons in Geant4
- Cross Section Studies

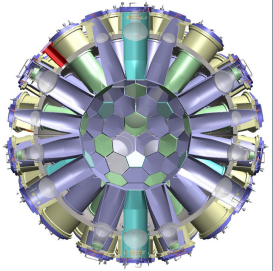




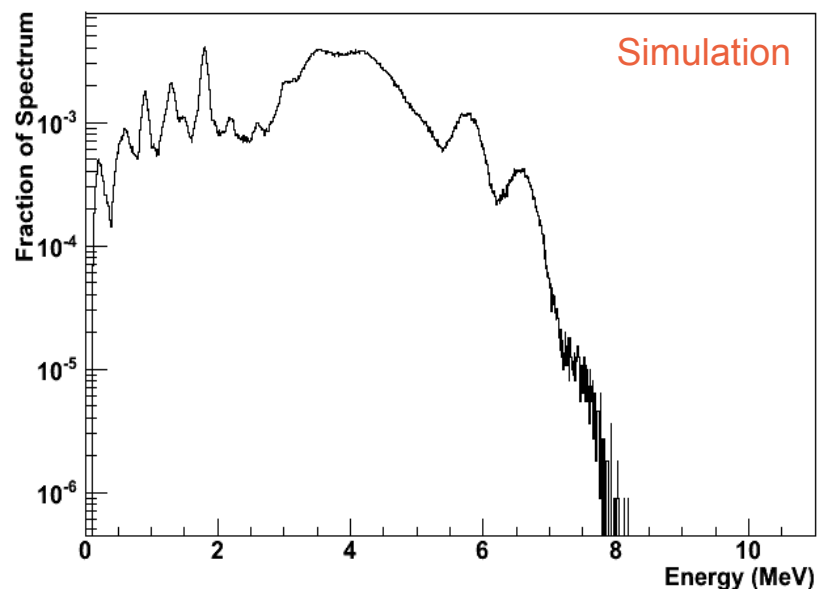
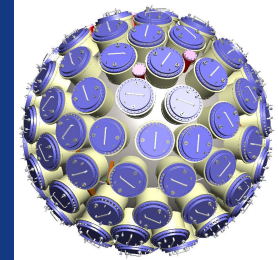
# MiniCLEAN & DM Detection



- MiniCLEAN is a single phase liquid argon direct dark matter detector
- Pulse shape discrimination allows separation of electronic recoils and nuclear recoils  $\rightarrow$  more late light from electron recoils because they are more likely to result in the longer lived state
- For more information on MiniCLEAN, and the DEAP/CLEAN program, see talks by M. Boulay, and D. McKinsey



# Neutron Backgrounds



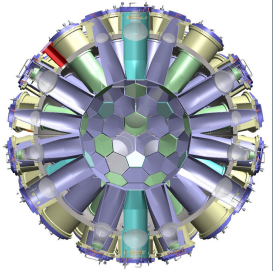
- Nuclear recoils from neutrons are a background for any direct DM search
- Shielding can protect from cosmogenic neutrons and those from the surrounding material.
- We are left with neutrons from within the detector itself

Greatest source of worrisome neutrons for MiniCLEAN are those made in the borosilicate glass of our PMTs.

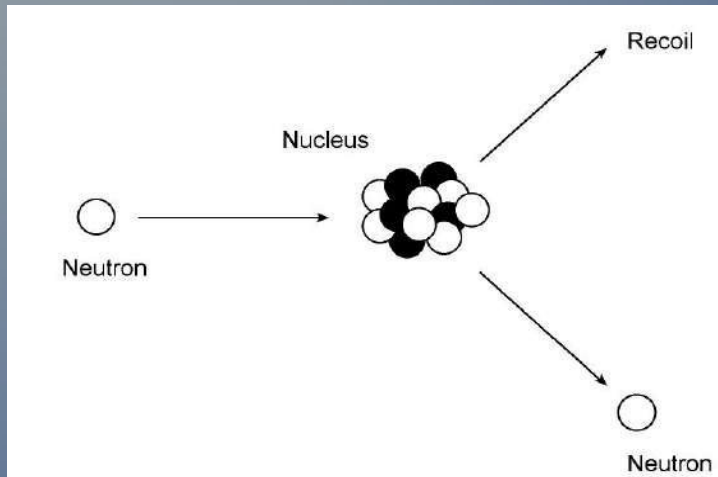
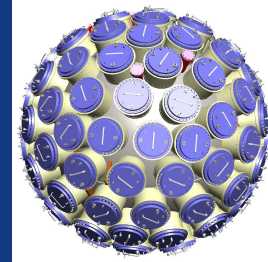
The  $^{238}\text{U}$  and  $^{232}\text{Th}$  alpha chains are followed in the PMT glass composition to generate the neutron spectrum.

Spectrum from [neutronyield.usd.edu](http://neutronyield.usd.edu)

Following the methods of: NIM A 606(2009)651660 (arXiv:0812.4307)  
and doi:10.1016/j.astropartphys.2010.04.003 (arXiv:0912.0211)

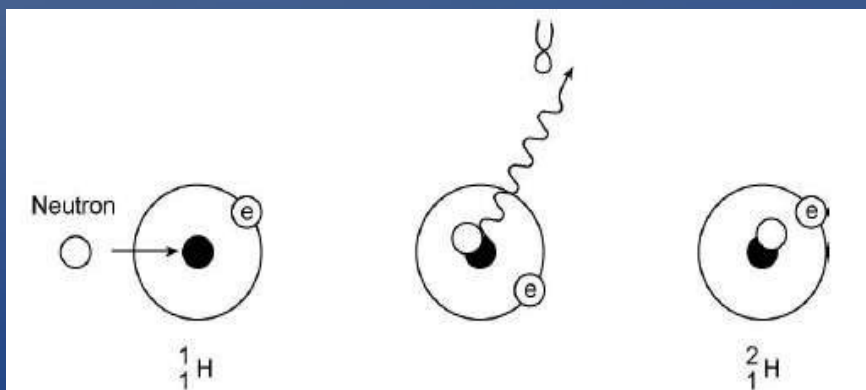
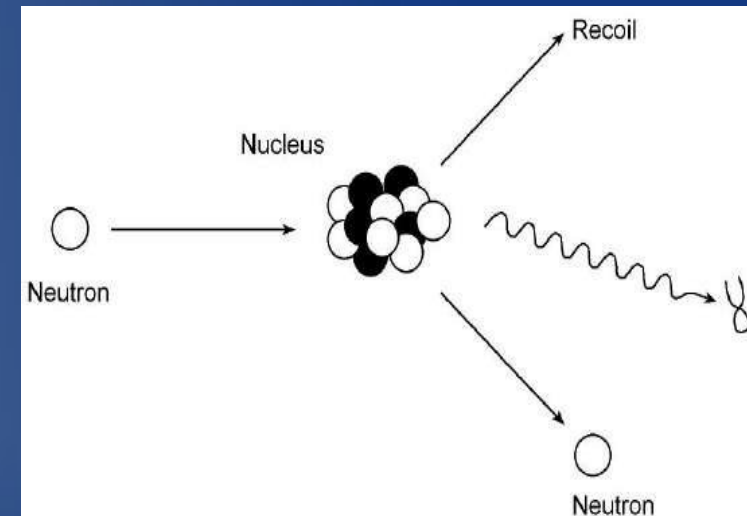


# Neutron Scattering

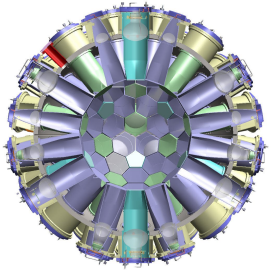


Elastic Scattering: background to a WIMP event  
Maximum energy transfer from neutron to argon of 10%  
For a 50 keVr analysis threshold, the neutron energy threshold is .5 MeV  
Cross section will have resonances

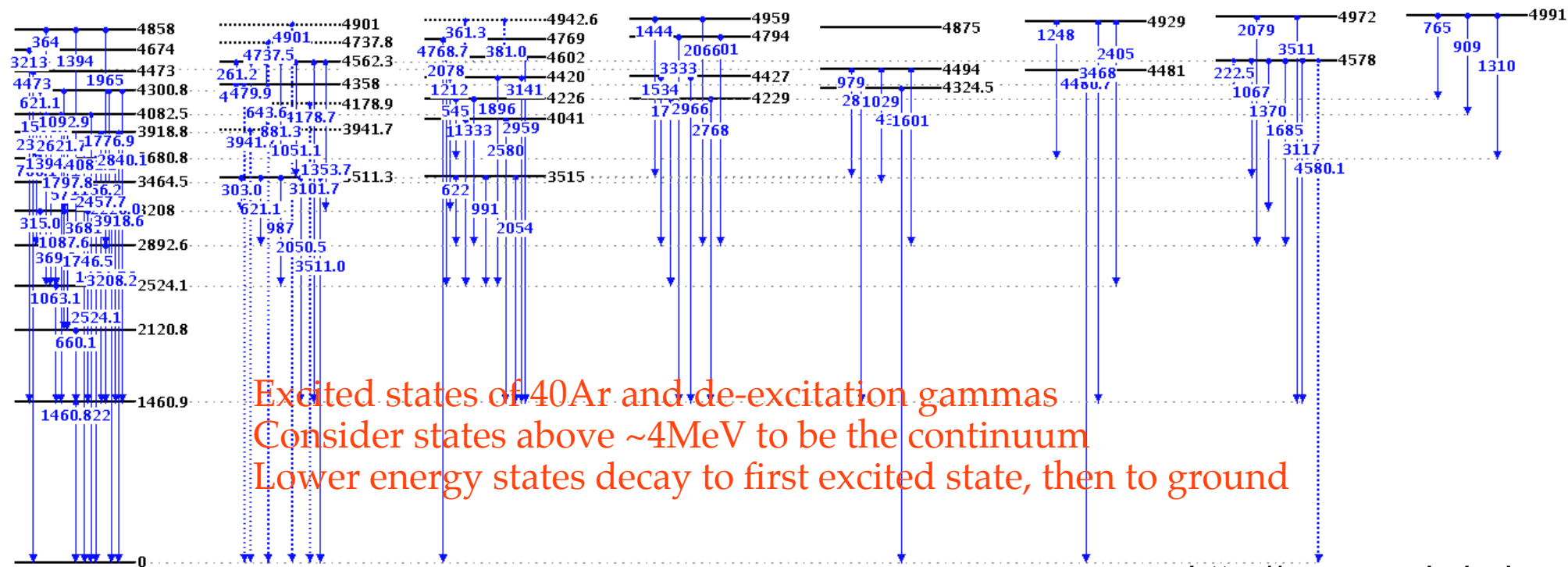
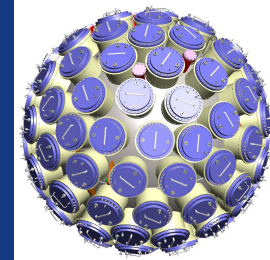
Inelastic Scattering: for our energy region of interest, primarily 1n, gamma in the final state  
Thresholds and energy loss set by argon nuclear excited states



Neutron Capture: Cross section at thermal energies (0.025 eV) also resonances at keV energies  
Gamma rays and  $^{41}\text{Ar}$  produced  
 $^{41}\text{Ar}$  decays with a half life of 1.8 hrs to  $^{41}\text{K}$ , producing a keV electron and 1.3 MeV gamma



# Argon Excited States

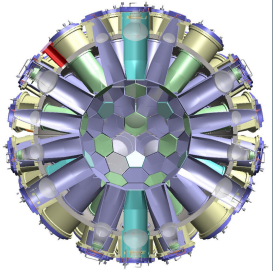


Excited states of  $^{40}\text{Ar}$  and de-excitation gammas  
 Consider states above ~4MeV to be the continuum  
 Lower energy states decay to first excited state, then to ground

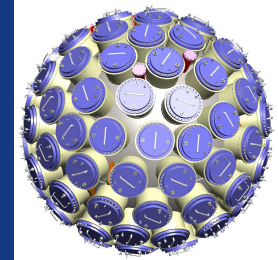
<http://www.nndc.bnl.gov>

$^{40}_{18}\text{Ar}_{22}$

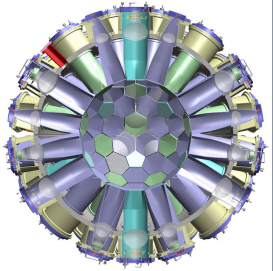




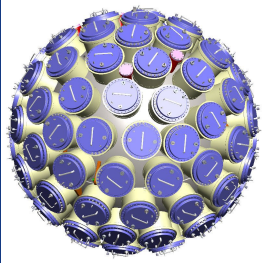
# Geant4 and Neutrons



- Look at Geant4's neutron physics
  - Cross-section implementation
- Compare these cross sections to:
  - ENDF/B-VII
  - Measurements
  - Other evaluated databases/simulation packages
- Look individually at Elastic, Inelastic and Capture Processes
- Impact of these processes from the view of a dark matter search



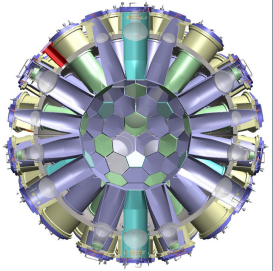
# Neutron HP



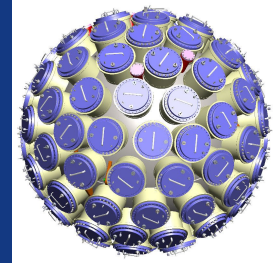
- Geant4 uses the high precision neutron processes  $<20$  MeV
- Uses energy-dependent cross section and final state data from G4NDL3.13 (G4NDL) for Elastic, Inelastic, Capture and Fission (not applicable in Argon)
  - Elastic scatters have cross section information, and final state distribution's Legendre polynomials
  - Inelastic scatters are more complicated
    - Total inelastic cross section
    - Final state cross sections (1n, alpha, proton, 2n, etc.)
    - Cross sections for the different argon nuclear excited states, isotropic emission
    - De-excitation gammas
  - Captures have cross section information



Jimmy Neutron



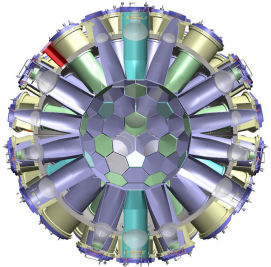
# More on Neutron HP



- Using Geant4.9.2 and 4.9.3
  - Cross Sections for  $^{40}\text{Ar}$  same back to G4NDL3.9
  - Cross sections come from ENDF/B-VI resonances
- Able to use natural abundances or user-specified
- Are there cross sections for your isotopes in G4NDL?
  - They aren't for Neon!
  - Main argon isotopes are all present
    - $^{40}\text{Ar}$  (.996003),  $^{38}\text{Ar}$ (0.000632),  
 $^{36}\text{Ar}$  (0.003365)
- Geant4 Hadronic Physics group adding features, fixing reported bugs



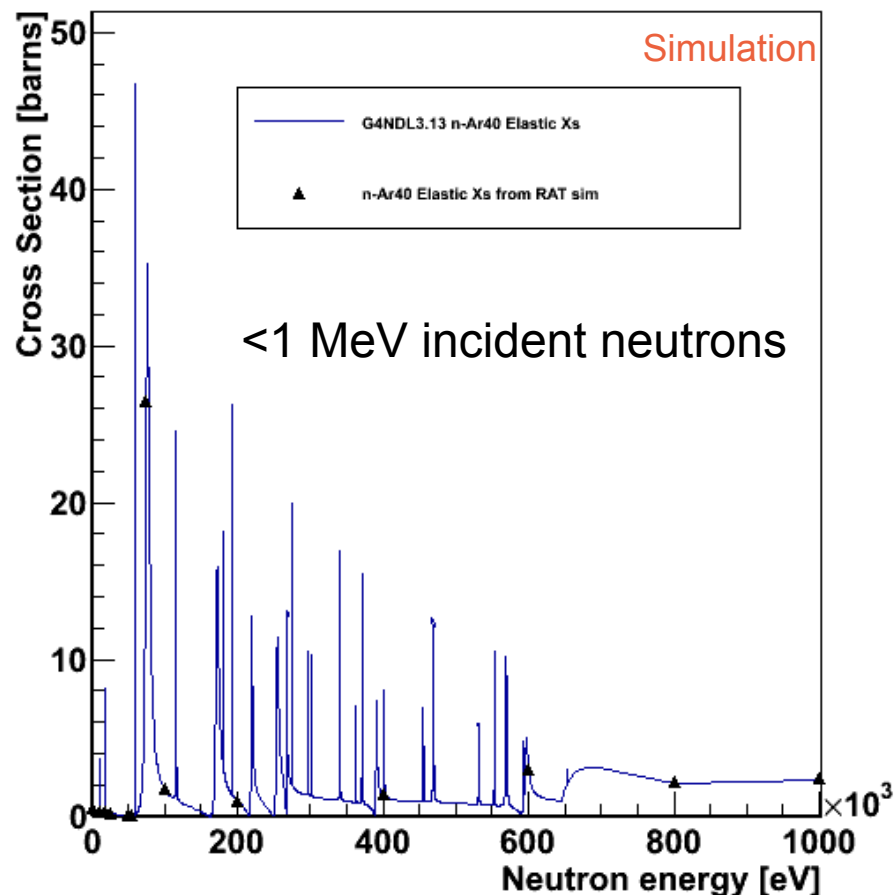




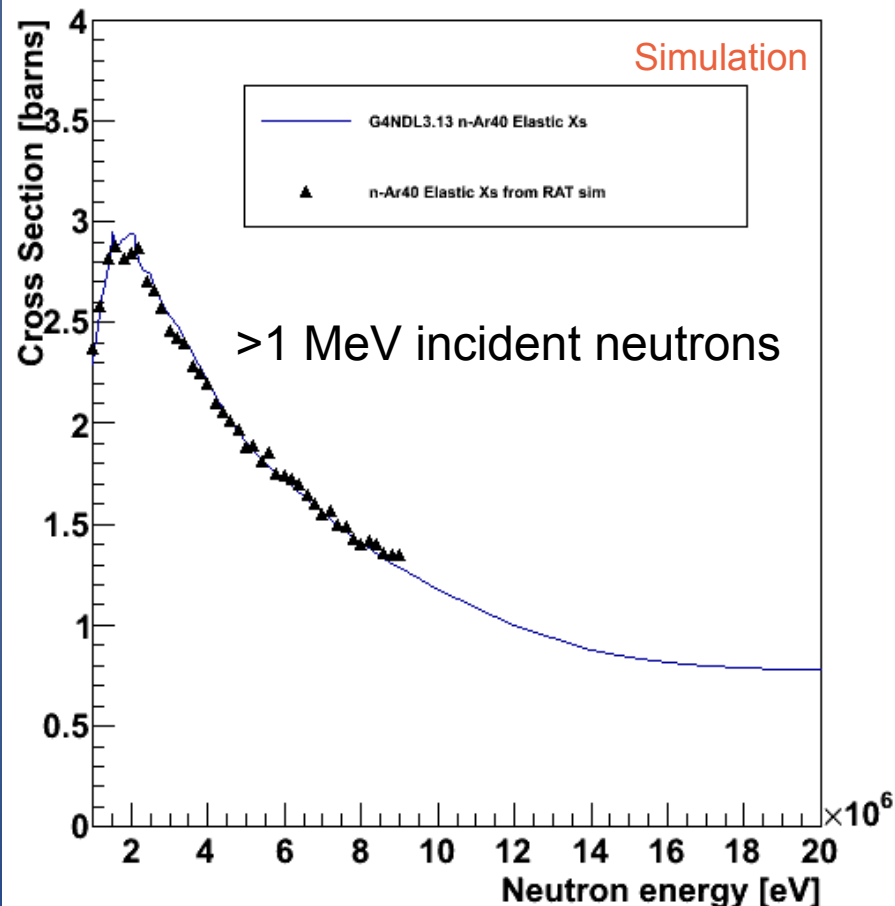
# Reproducing G4NDL



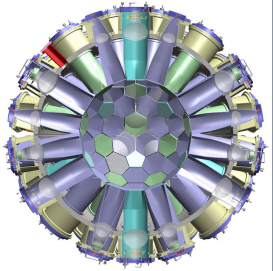
Neutron Elastic Cross Section on  $^{40}_{18}\text{Ar}$



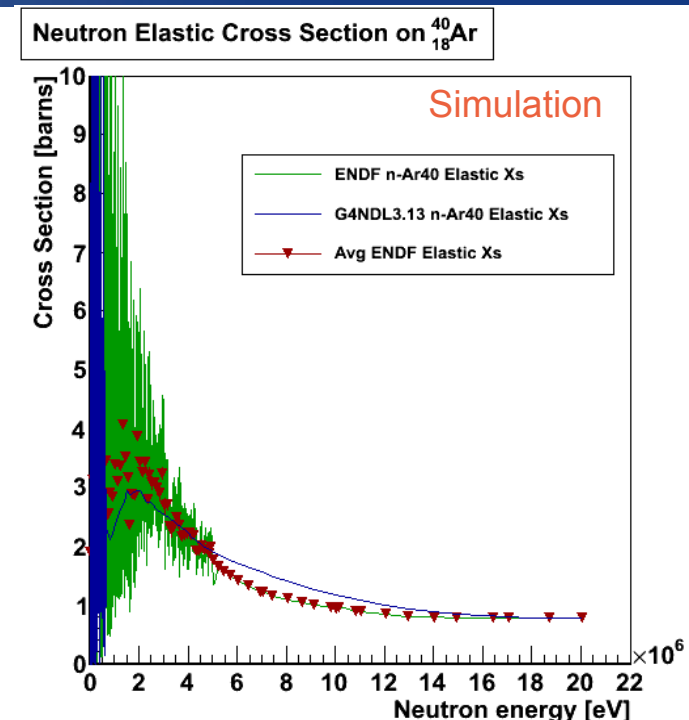
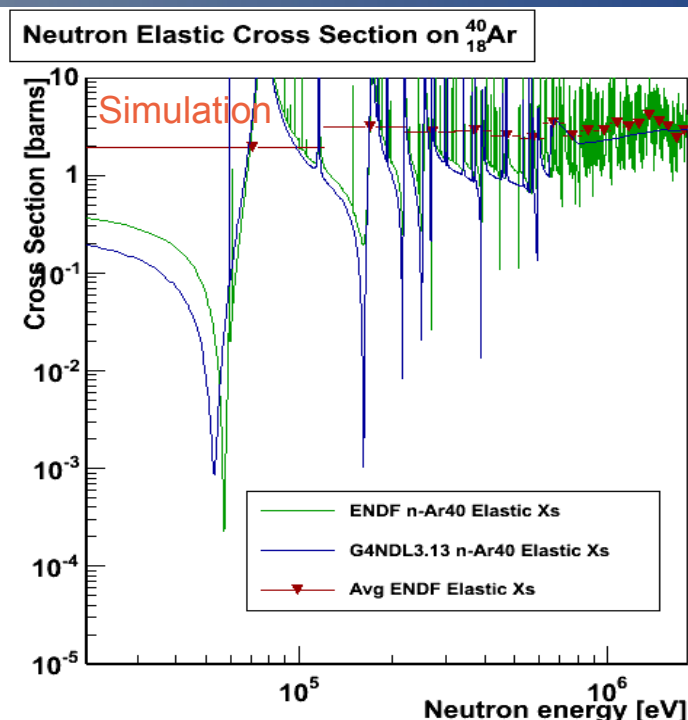
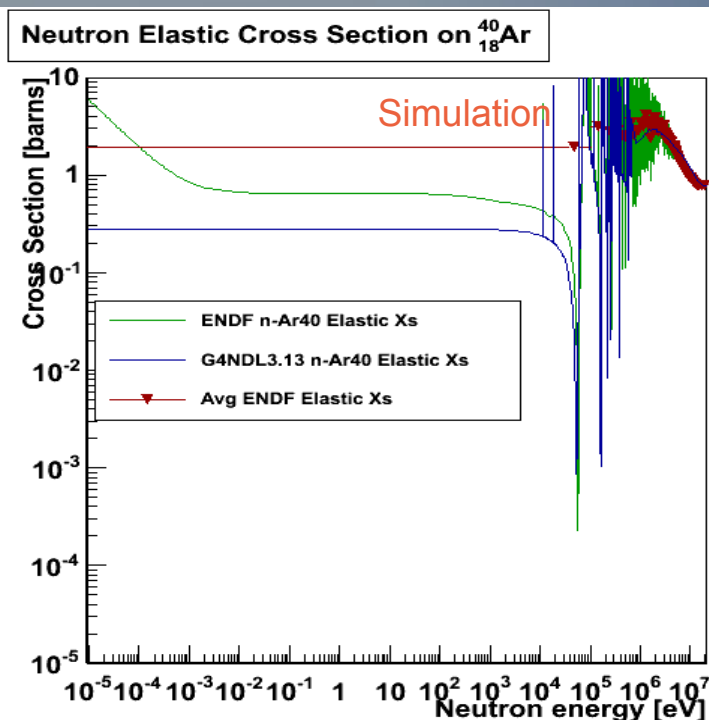
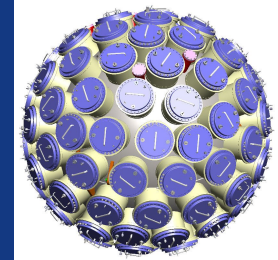
Neutron Elastic Cross Section on  $^{40}_{18}\text{Ar}$



Monoenergetic neutrons shot into liquid natural argon, Inelastic processes turned off  
Input cross sections are reproduced.



# Comparison with ENDF/B-VII



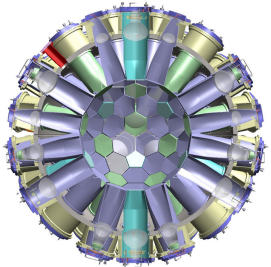
ENDF/B-VII provides cross sections, more resonances than G4NDL

Differences of  $\sim 2$  at energies  $< 45$  keV

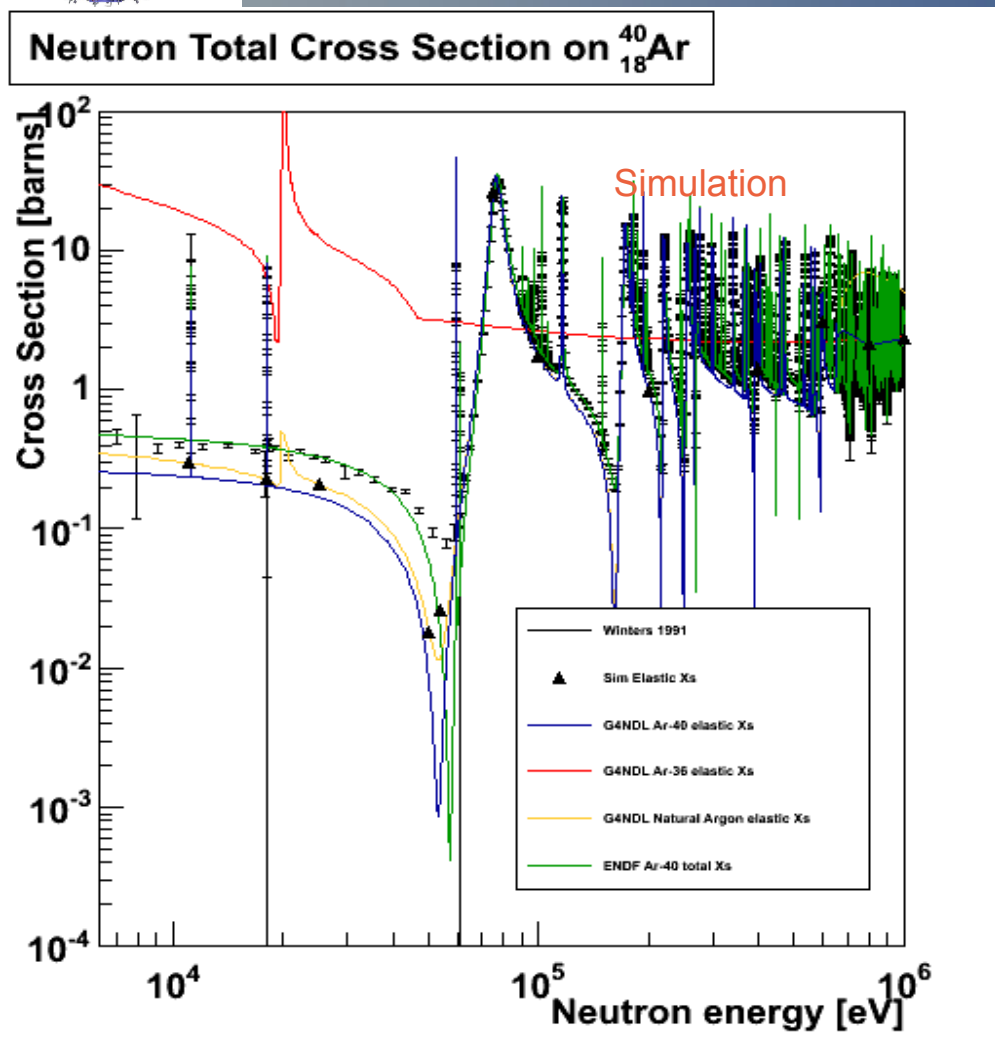
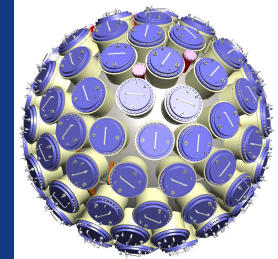
Slight differences at the resonant dip at  $\sim 50$  keV

Above 1 MeV, 30% effects at peak and on the tail

ENDF/B-VII is in agreement with other datasets: ROSFOND (Russian), JENDL3.3 (Japanese), JENDL4.0, JEFF3.1 (European)



# Comparison with Measurements



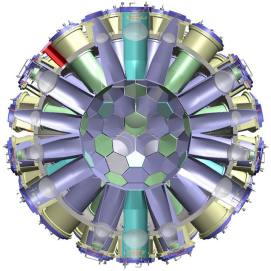
Measurements and simulations have really been done with natural argon, at low energies  $^{36}\text{Ar}$  becomes important!

Recall:  $^{40}\text{Ar}$  (.996003),  $^{36}\text{Ar}$  (0.003365)

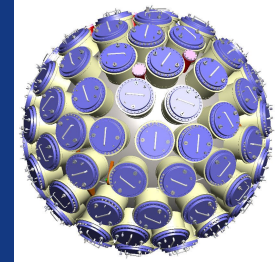
Measurements from Winters et al PRC, 43, 492, 1991

From 7 keV to 50 MeV

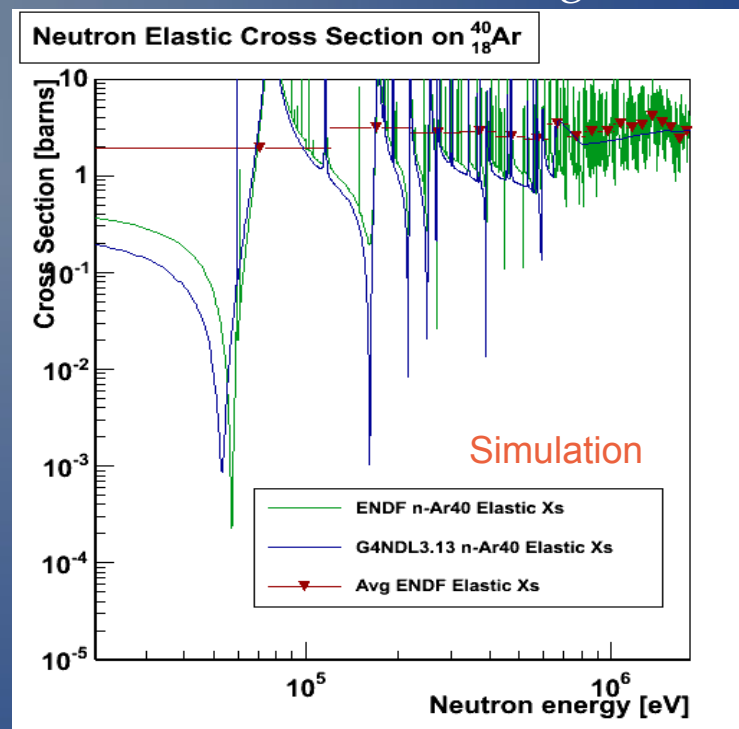
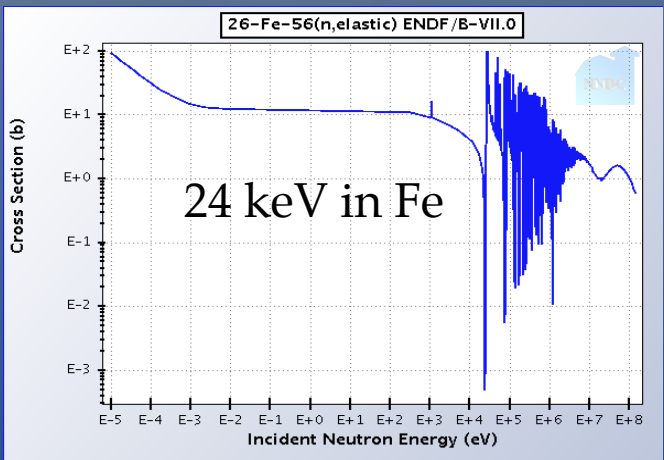
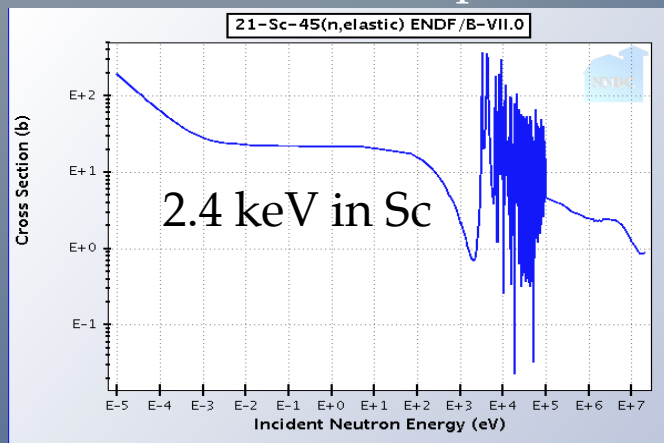
ENDF normalized to their data, which is on the NNDC website



# Dip in Elastic Cross Section



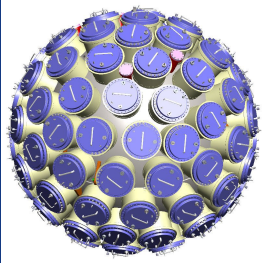
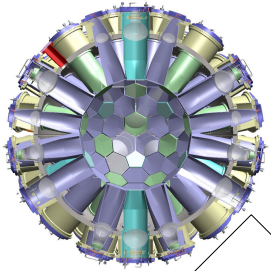
Interference between s-wave and hard-sphere scattering  
gives deep, broad resonant dips in the cross section  
Exploited elsewhere to make monoenergetic neutron beams



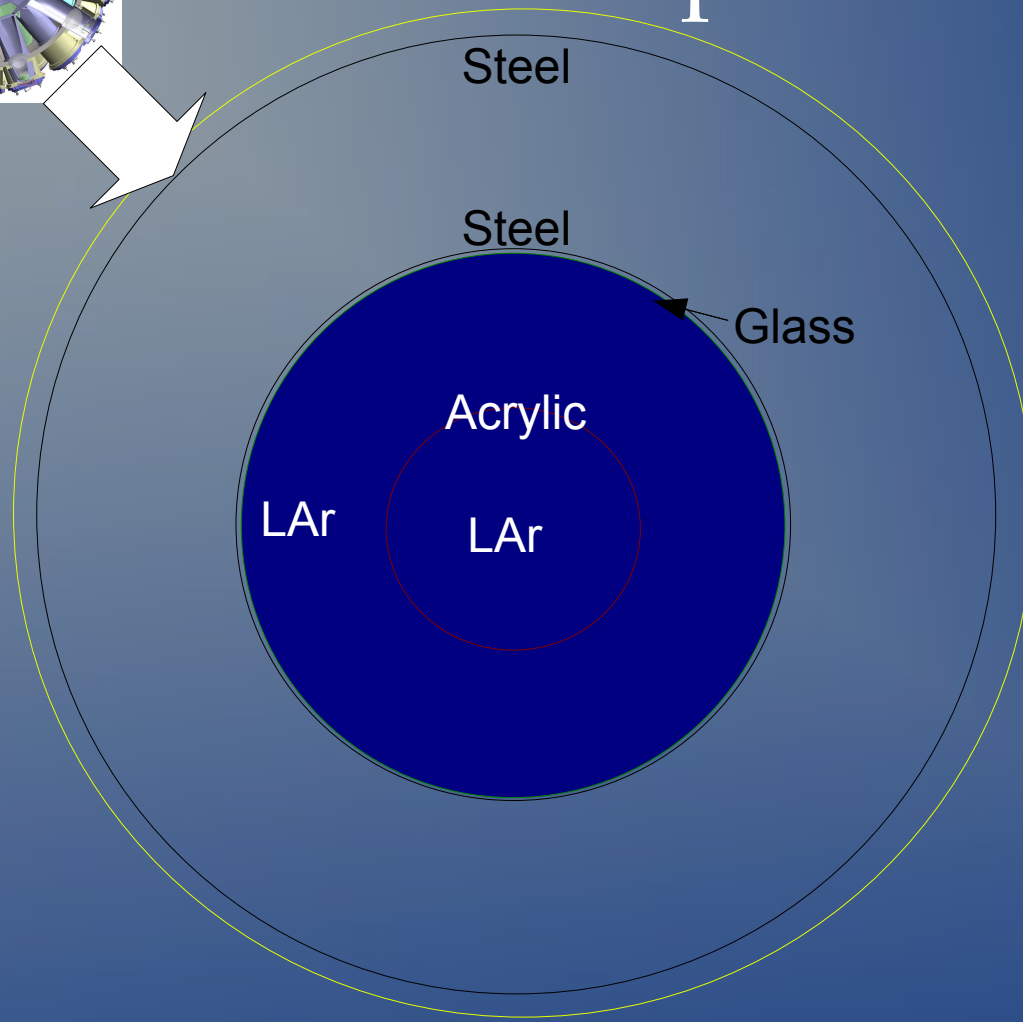
Some uncertainty in depth and position, but Said Mughabghab of BNL, editor of the Atlas of Neutron Resonances, communicates that it is:

- between 46 and 51 keV
- a minima of 4 mb
- at this energy, an equivalent mean free path of 118 m

Neutrons will not thermalize quickly in liquid Argon



# Simple Geometry



$R(\text{world})=1050 \text{ mm}$

$R_{\text{inner}}(\text{Outer ss})=1000 \text{ mm}$

Thickness: 15.679 mm

Mass: 1575 kg

$R_{\text{inner}}(\text{Inner SS})=609.34 \text{ mm}$

Thickness: 27.345 mm

Mass: 1050 kg

$R_{\text{inner}}(\text{PMT glass})=602.385 \text{ mm}$

Thickness: 7 mm

Mass: 72 kg

$R_{\text{inner}}(\text{buffer LAr})=402.385 \text{ mm}$

$R_{\text{inner}}(\text{acrylic})=400.00 \text{ mm}$

Thickness: 2.385 mm

Mass: 5.5 kg

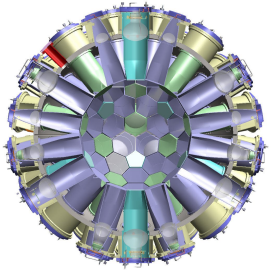
$R < 400.00 \text{ mm}$  LAr target

Spherical Model, just used for neutron physics studies

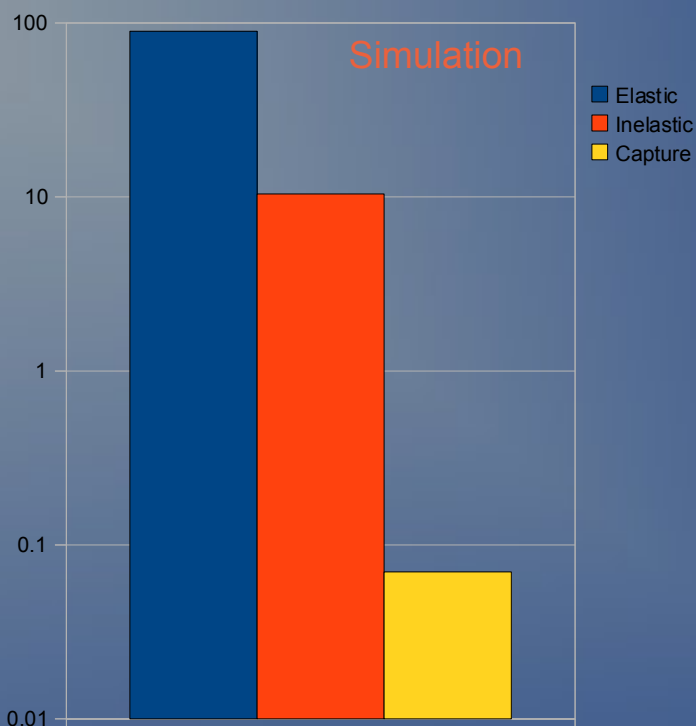
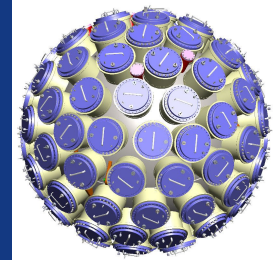
60 cm radius of LAr

Neutrons initialized in sphere of glass just outside the argon and are emitted isotropically





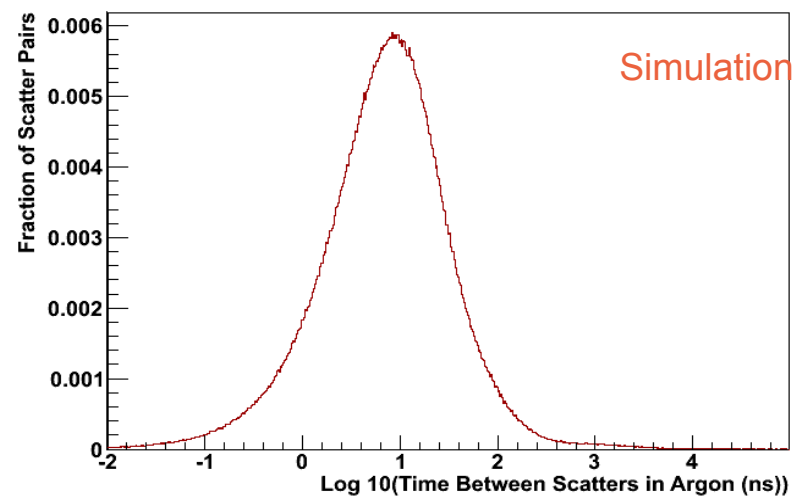
# Elastic Scatters: Multiple Scatters



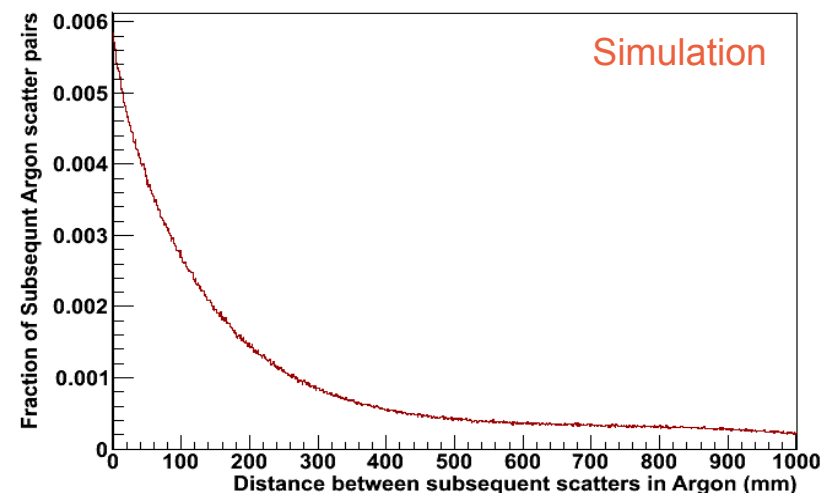
Relative Frequency of Neutron-Argon Interactions

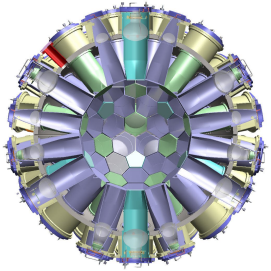
~90% of all neutron scatters in argon are elastic  
 Mean of ~2.5 elastic scatters per neutron simulated  
 (and that includes all neutrons that never scatter in the argon because they never entered it)

Mean distance between neutron-Argon scatters is 24 cm

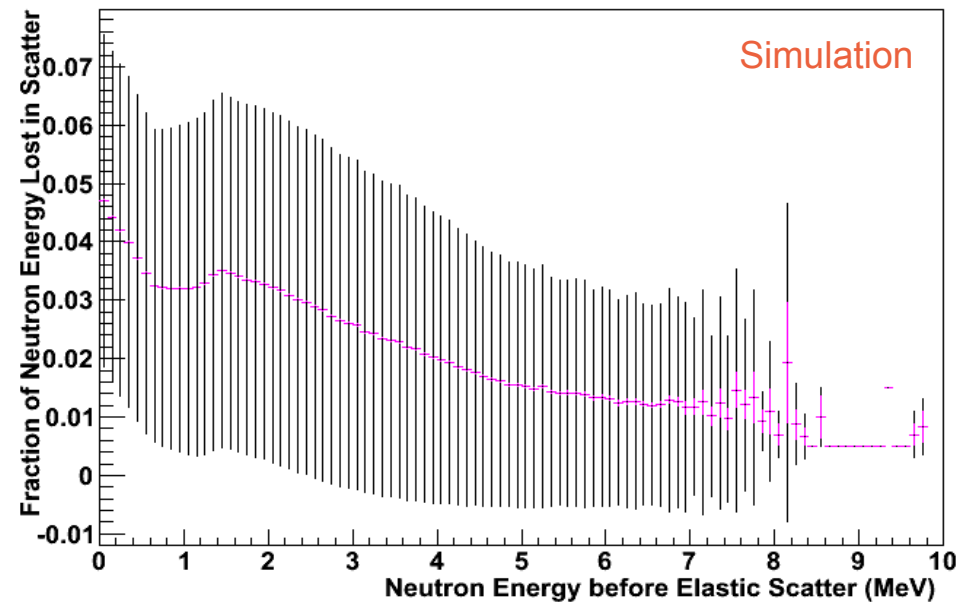
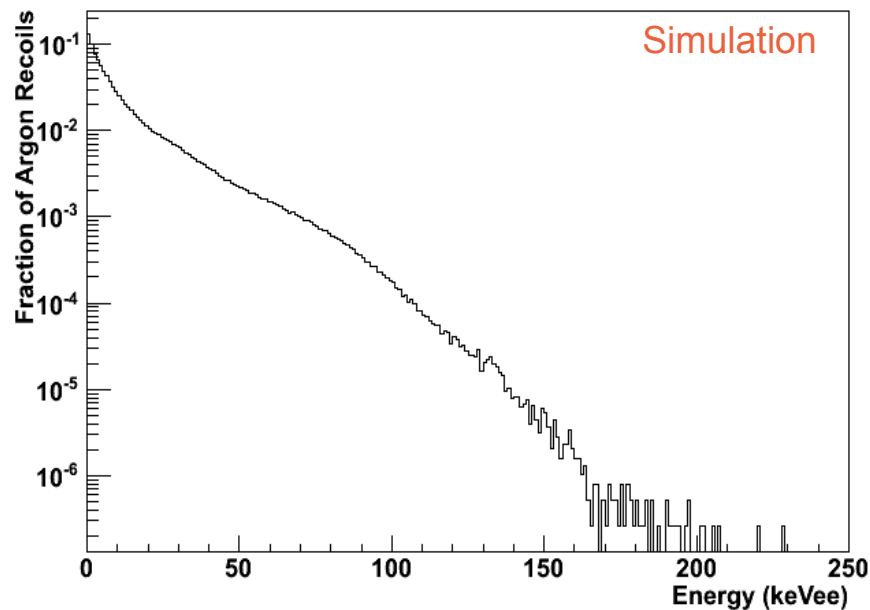
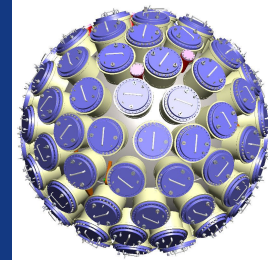


With a mean time of 7 ns between subsequent scatters in argon



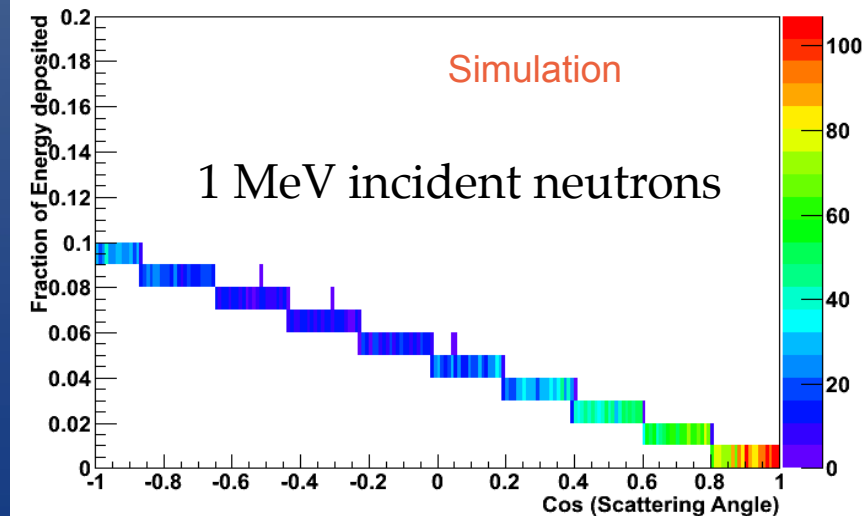


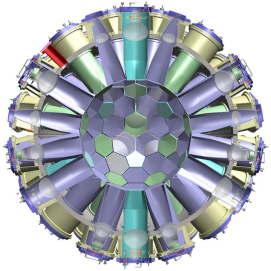
# Elastic Scatters: Energy Loss



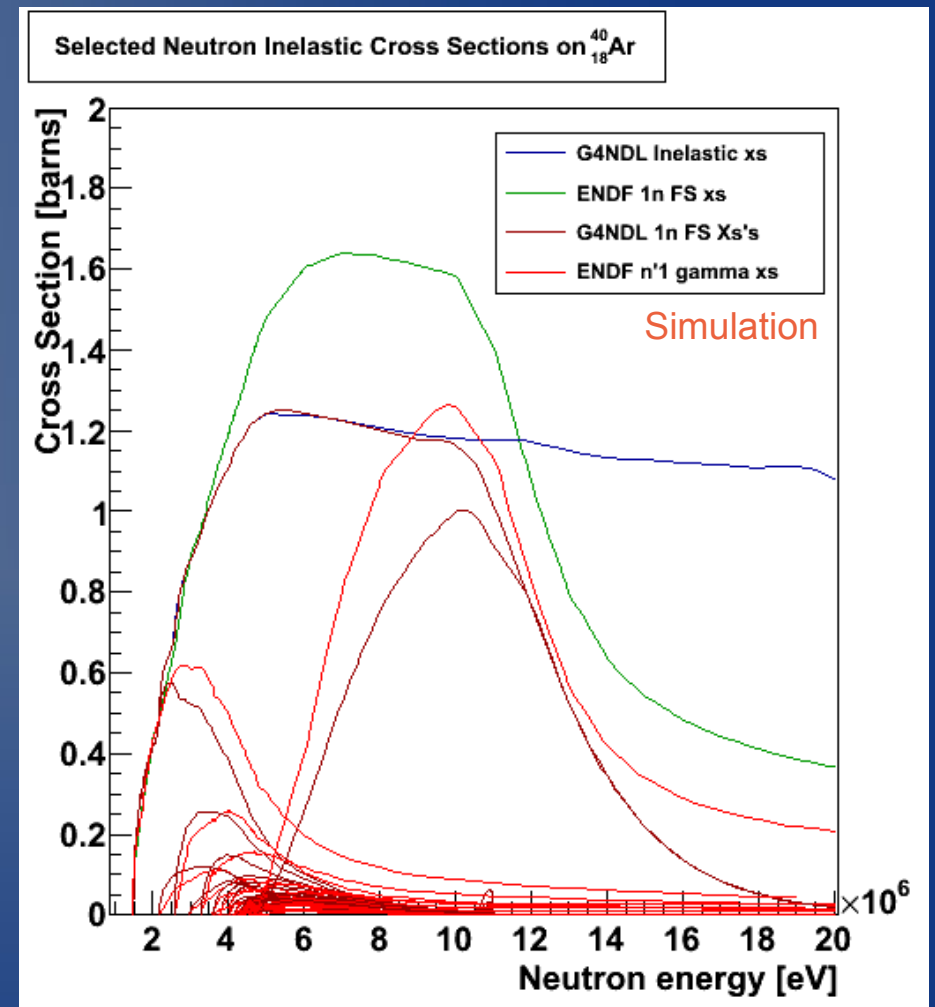
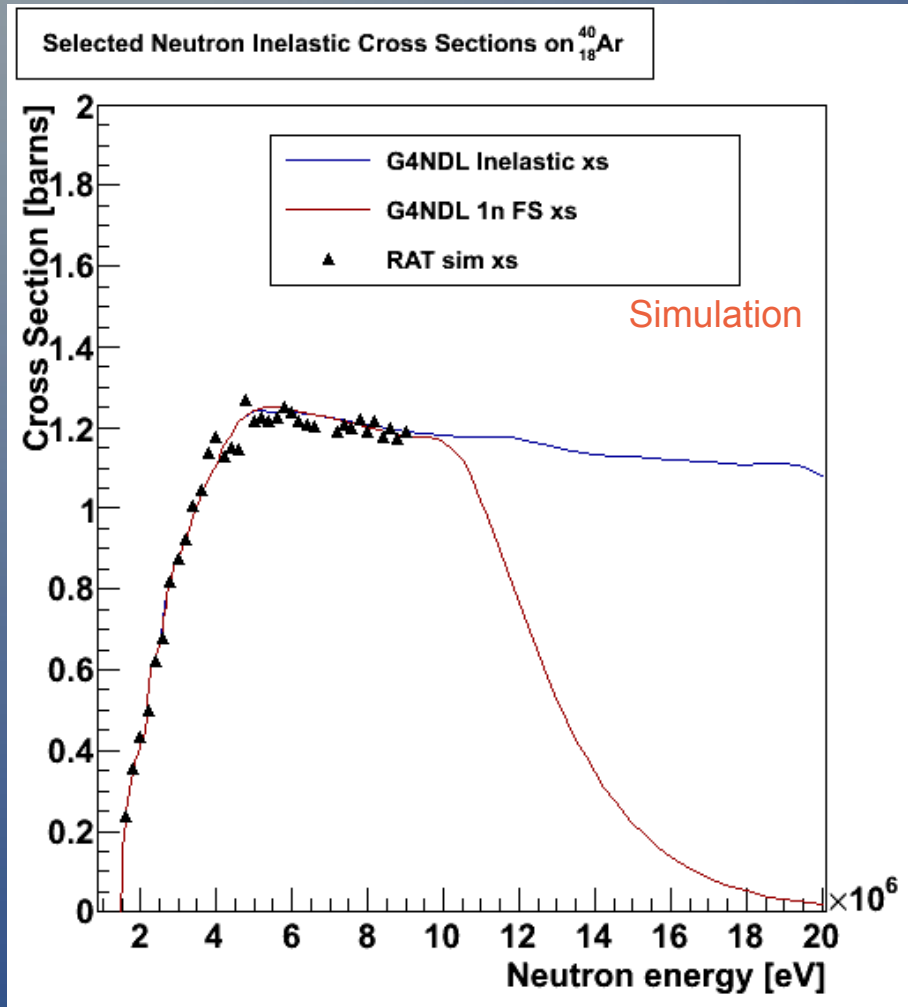
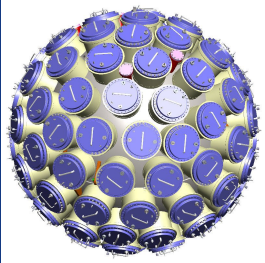
Argon recoils, no radial cuts,  
PMT Alpha-n spectrum in Simple Geometry  
Quenching factor of 0.25 from  
Gastler et. al. arXiv:1004.0373

Neutrons may only lose up to 10%  
of their energy to the argon nuclei,  
Average much less: 3.1% at 1 MeV





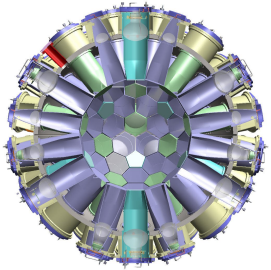
# Inelastic Cross Sections



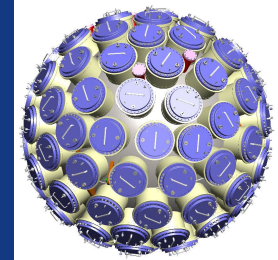
Total Inelastic Cross Section is reproduced

But values are 25% lower than ENDF/B-VII

Fewer independent excited states in G4NDL, missing 1 alpha final state which has a threshold of 4 MeV, but is an order of magnitude smaller in cross section



# Inelastic Gammas

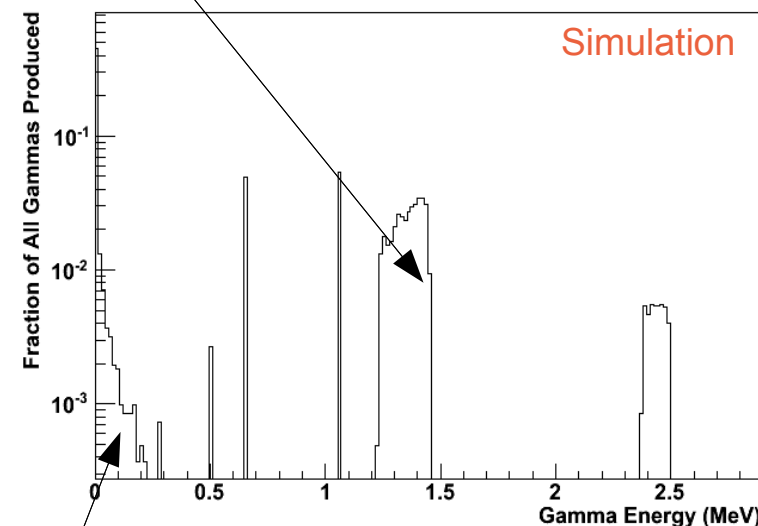


Peculiar energies of gammas from first excited state:  
Not monoenergetic at 1.46 MeV, as expected

```
*****
* G4Track Information: Particle = neutron, Track ID = 4, Parent ID = 1
*****

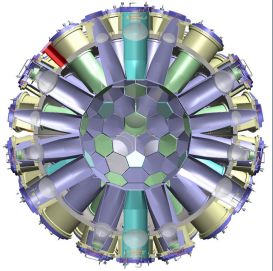
Step#  X    Y    Z    KineE  dStep  StepLeng  TrakLeng  Volume  Process
0   12 cm -21.9 cm -50.2 cm 3.41 MeV 0 eV  0 fm  0 fm  InnerVacuum  initStep
1   37.8 cm -18.1 cm -35.6 cm 0 eV  0 eV  29.9 cm  29.9 cm  InnerVacuum  NeutronInelastic

:---- List of 2ndaries - #SpawnInStep= 5(Rest= 0,Along= 0,Post= 5), #SpawnTotal= 5 -----
: 37.8 cm -18.1 cm -35.6 cm 1.29 MeV  neutron
: 37.8 cm -18.1 cm -35.6 cm 29.9 keV  Ar40[0.0]
: 37.8 cm -18.1 cm -35.6 cm 1.44 MeV  gamma
: 37.8 cm -18.1 cm -35.6 cm 660 keV  gamma
: 37.8 cm -18.1 cm -35.6 cm 129 keV  gamma
:----- EndOf2ndaries Info -----
```

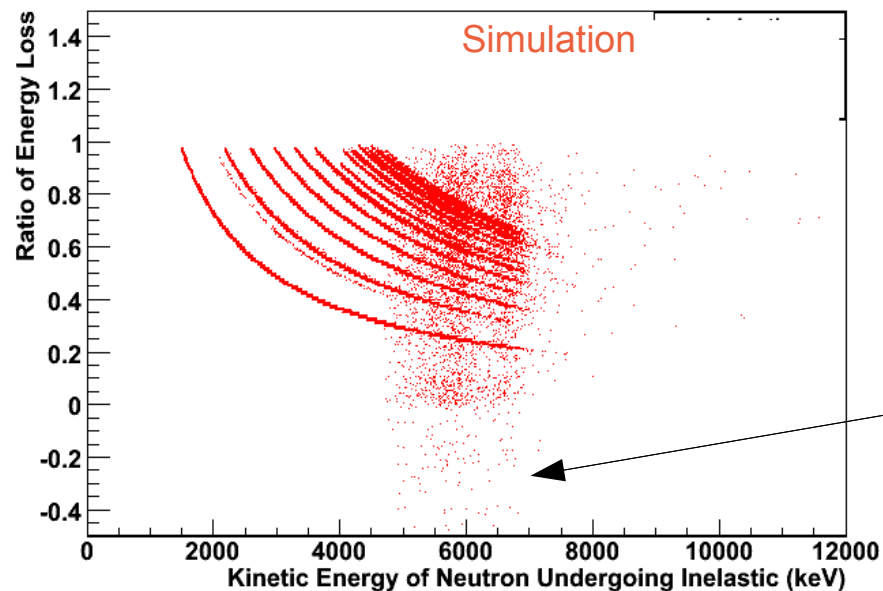
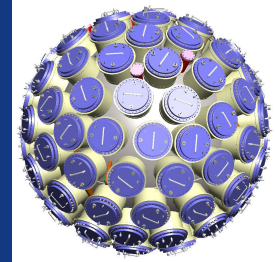


Large numbers of keV gammas, seem to be unphysical  
Although we have also considered them to be from electron  
Capture: right energy scale, not the right values

Gamma energies produced  
by 3 MeV neutrons  
inelastically scattering  
in liquid argon: first 4  
excited states are accessible



# Importance of Inelastic Scatters



C. Zhang

My colleague Chao Zhang has submitted a bug report on this issue:

G4 bug report #1054

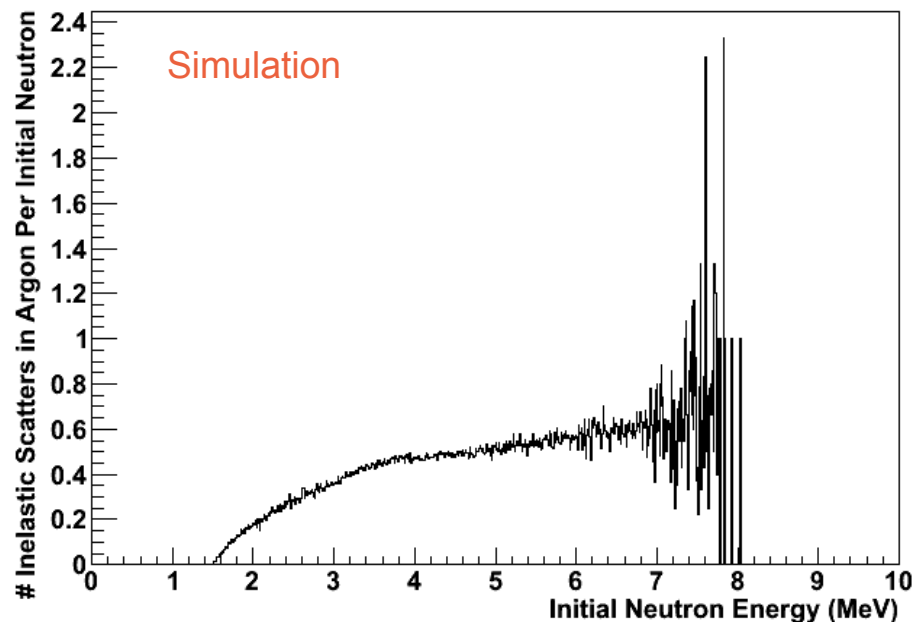
[http://bugzilla-geant4.kek.jp/show\\_bug.cgi?id=1054](http://bugzilla-geant4.kek.jp/show_bug.cgi?id=1054)

Neutrons starting with 4-7 MeV are likely to inelastically scatter in the liquid argon

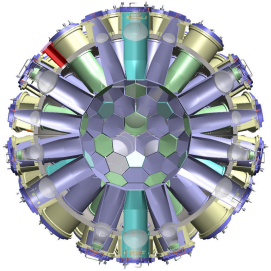
Simulations with a PMT Alpha-N neutron spectrum in a simplified, spherical MiniCLEAN geometry

Clear lines when excited states are accessed  
Broad when accessing the continuum states

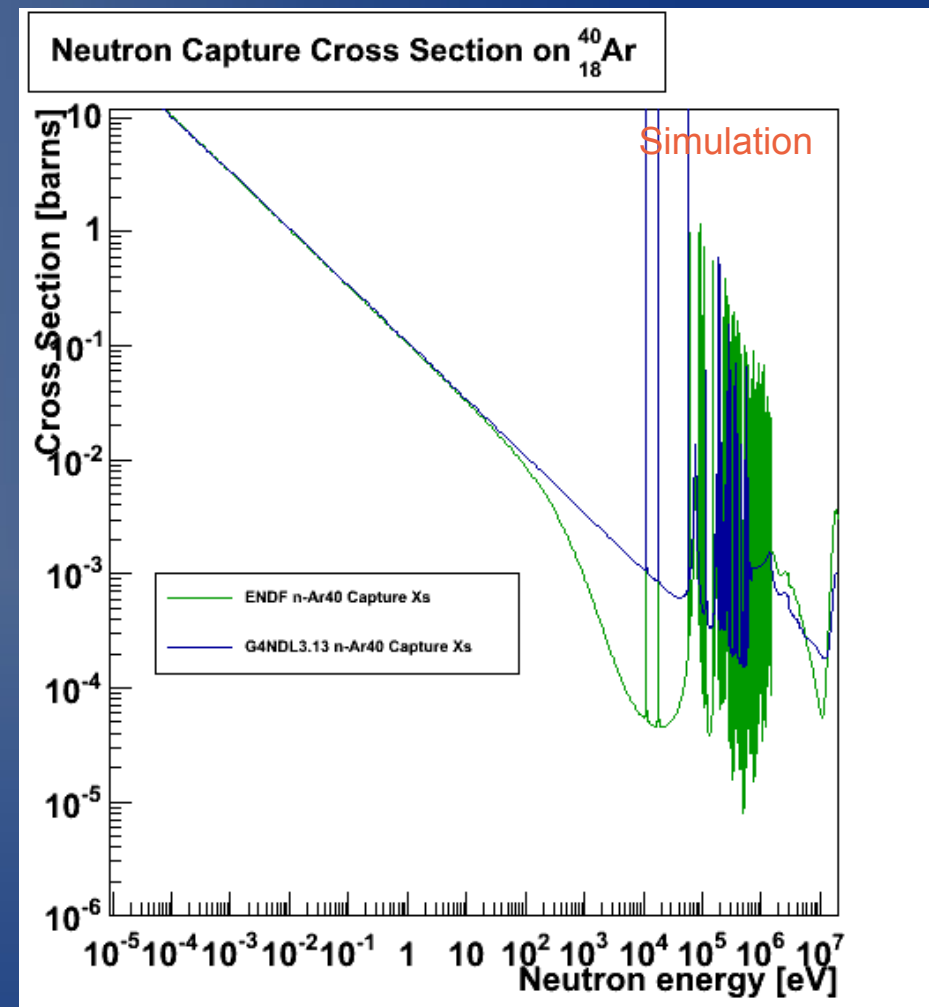
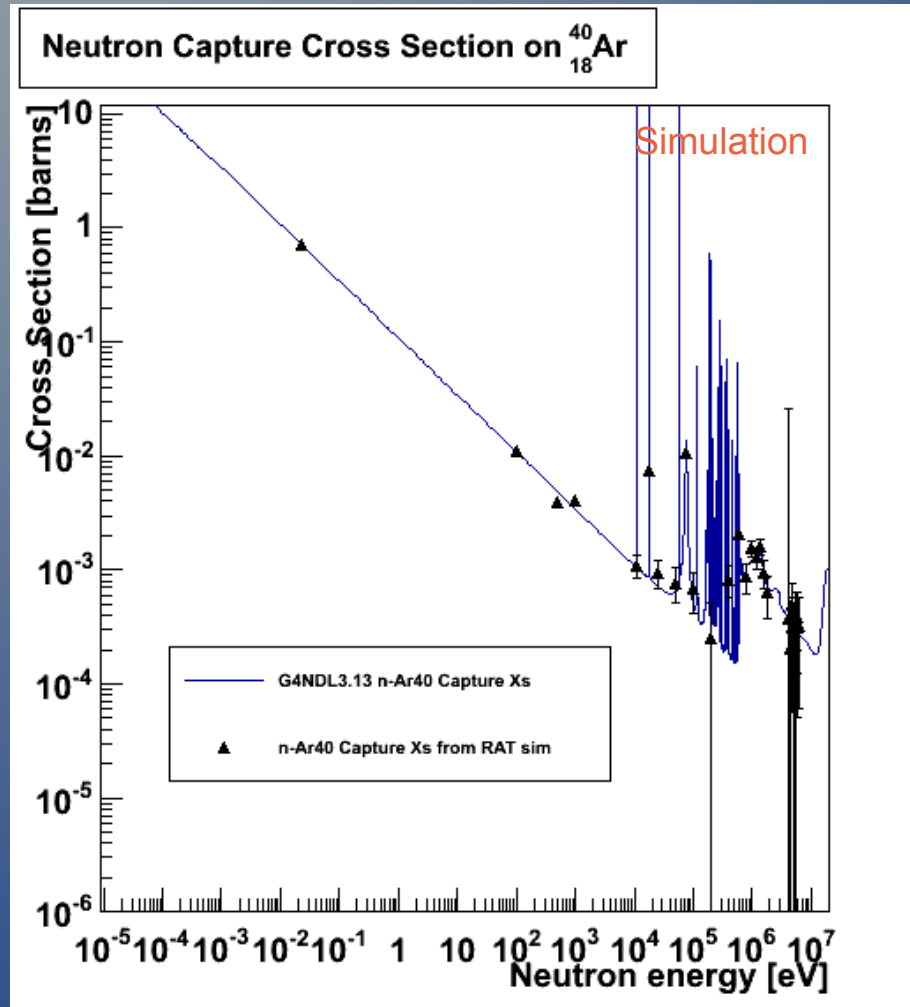
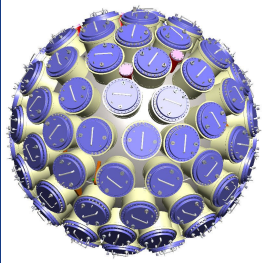
But, energy non-conservation!

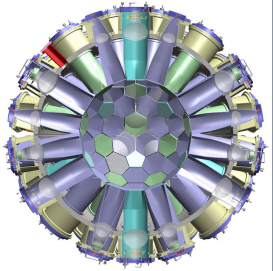




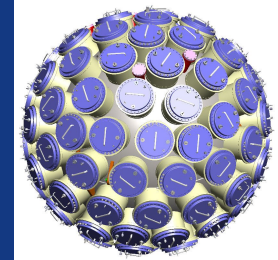


# Capture Cross Section





# Summary



- There are small cross section differences between G4NDL and ENDF/B-VII and a few unexpected features to neutron-Argon interactions in Geant4.
- Although fairly small effects, these introduce uncertainties in the neutron simulations in Geant4 that may affect numbers of expected backgrounds.
- Important features of neutron interactions in argon
  - Inelastic processes are important for neutron energy loss
  - Neutrons will most likely scatter multiple times elastically in the detector
  - $^{40}\text{Ar}$  has a substantial dip in the elastic cross section at  $\sim 50$  keV, where neutrons have a mean free path of 118 m
- Geant4 neutron physics should be verified for every material!



# DEAP/CLEAN Collaborators



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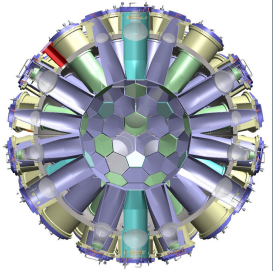
M.S. Kos, R.W. Schnee, B. Wang

## TRIUMF

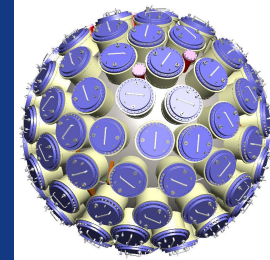
P.-A. Amaudruz, A. Muir, F. Retiere

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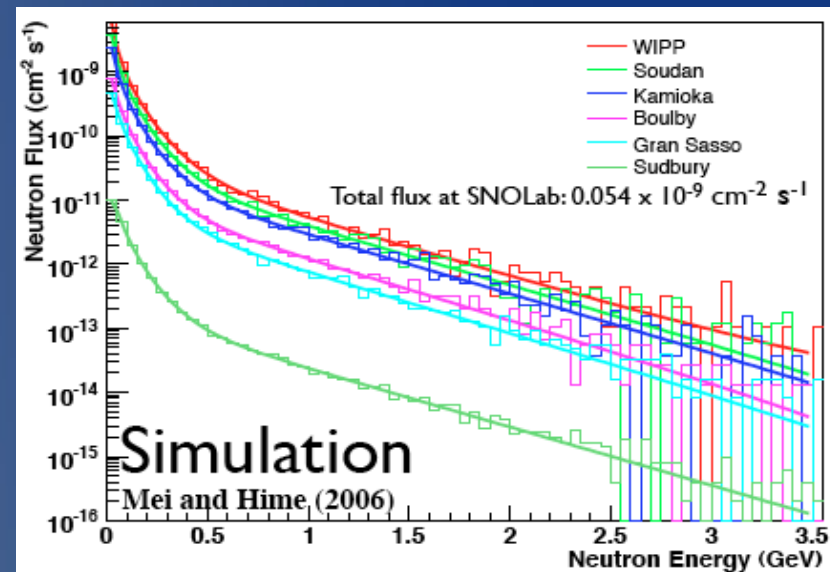
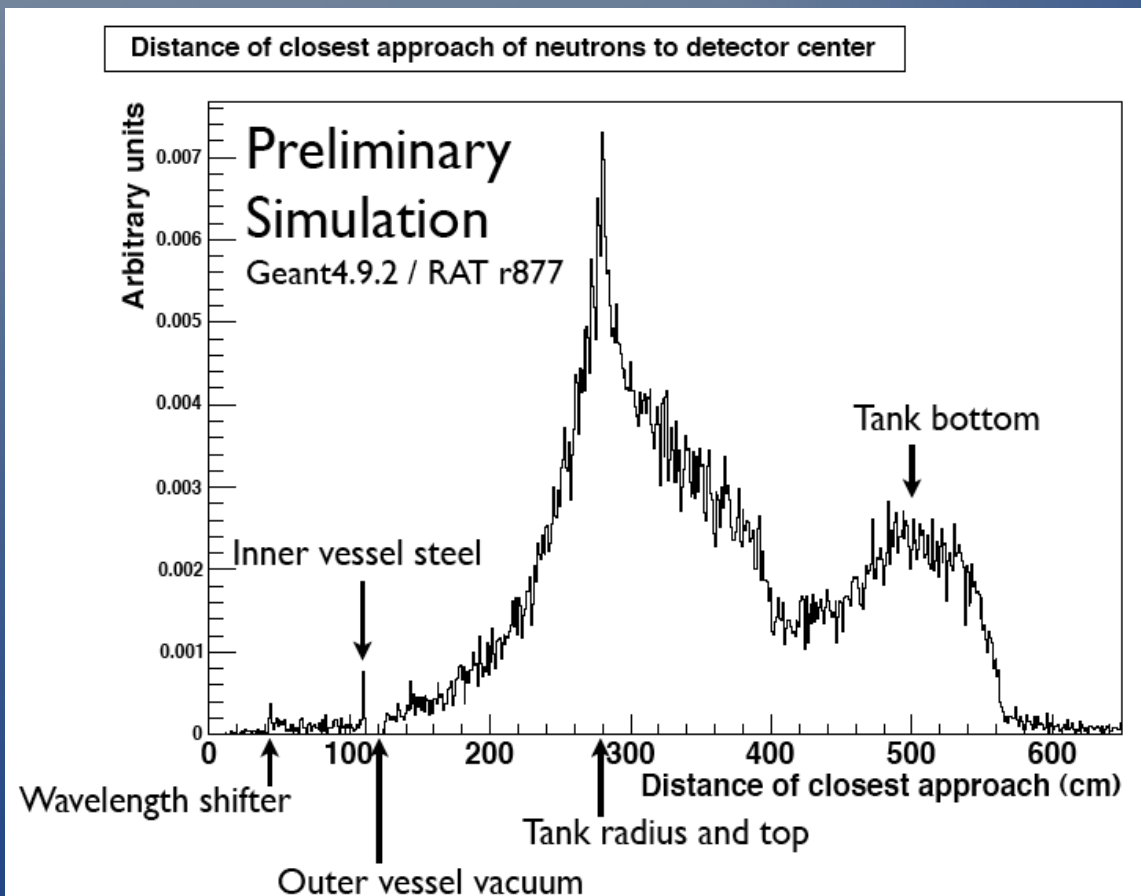
W.H. Lippincott, D.N. McKinsey, J.A. Nikkel, Y. Shin



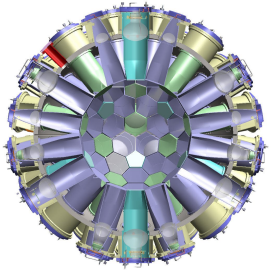
# Cosmogenic Neutrons



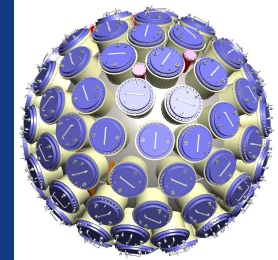
Water tank of 2.8 m radius, 7.9 m height  
Shield gammas and neutrons from cavern walls  
Tag through-going muons



A conservative estimate of muon induced neutrons that originate in the cavern walls with no tagged muon and then create a background signal in the ROI is  $<0.1$  / year



# PMT Neutrons



U238

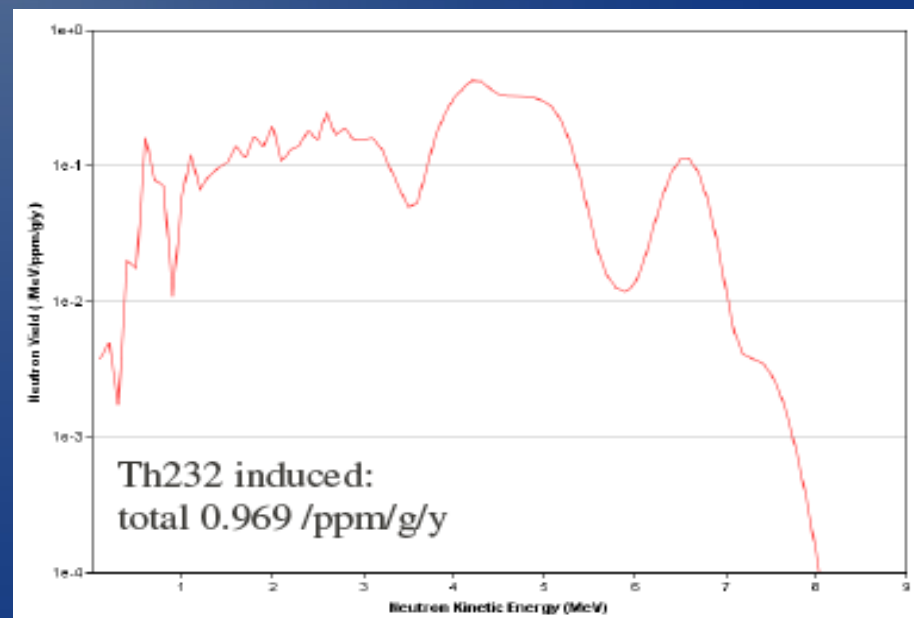
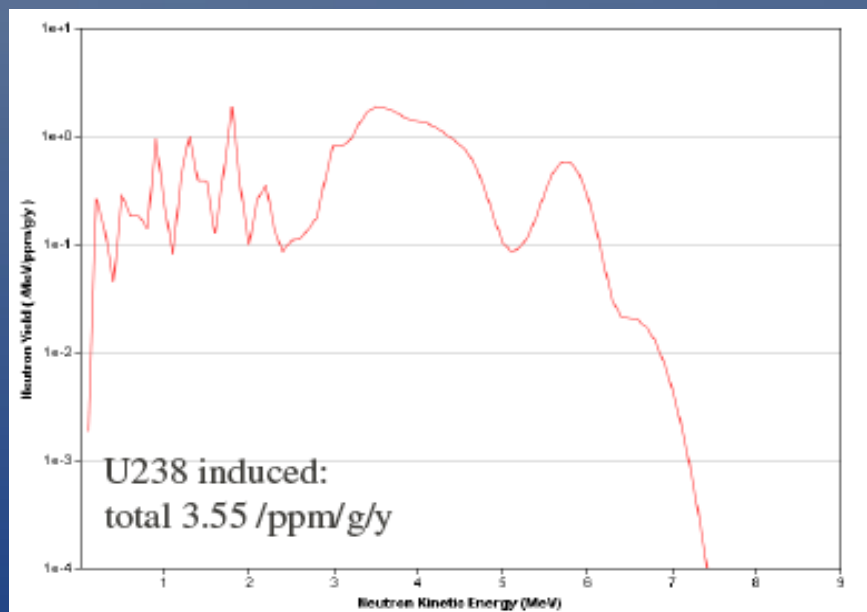
Th232

Energy(keV)	Branch Ratio(%)
4198	79
4151	21
4775	71.4
4722	28.6
4688	76.3
4621	23.7
4784	94.4
4602	5.6
5490	100
6002	100
6902	0.01
7687	99.99
5304	100

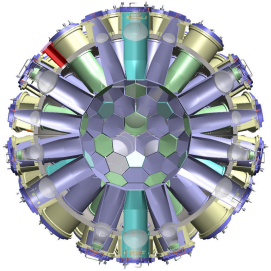
Energy(keV)	Branch Ratio(%)
4013	77.9
3954	22.1
5423	71.5
5340	28.5
5685	94.9
5449	5.1
6288	100
6778	100
8784	64
6090	9.8
6050	26.2

<http://neutronyield.usd.edu>

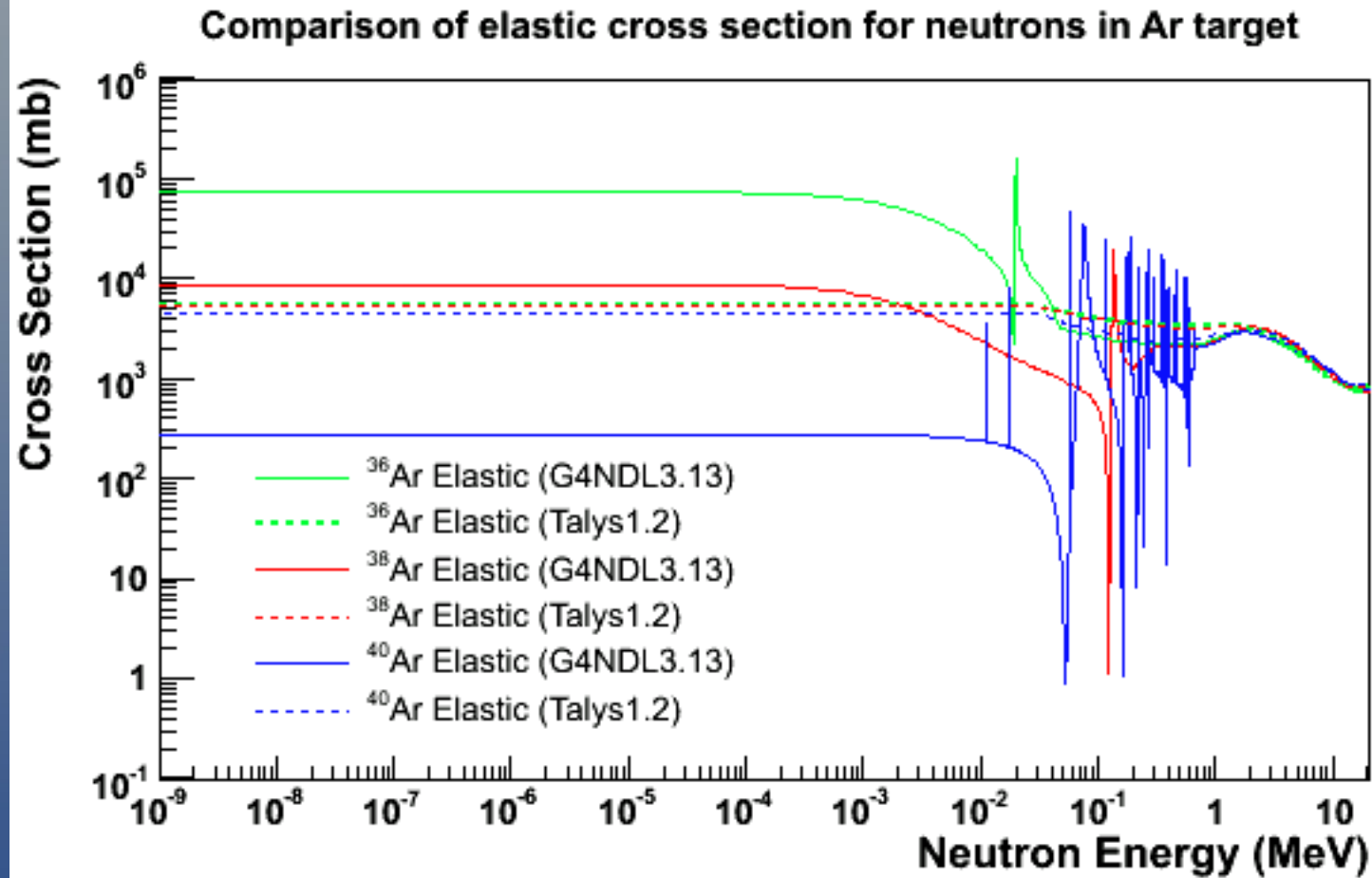
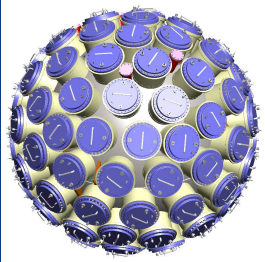
- Decay in secular equilibrium, follow 8 and 6 alphas from  $^{238}\text{U}$  and  $^{232}\text{Th}$  respectively
- Input glass composition
- Primary contribution to neutrons comes from Boron
- Assay of PMT for radio isotope content:
  - $^{238}\text{U}$ : 0.10287 ppm
  - $^{232}\text{Th}$ : 0.16974 ppm





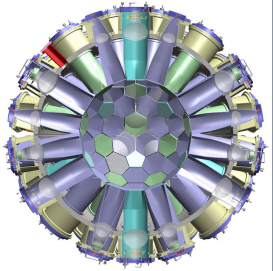


# TALYS

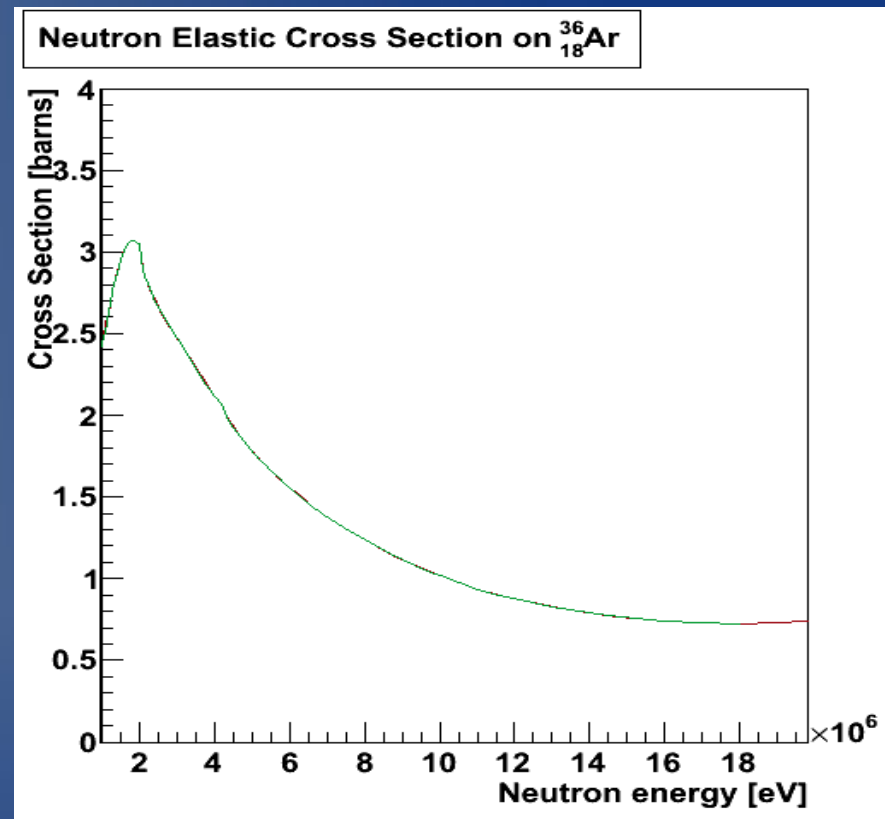
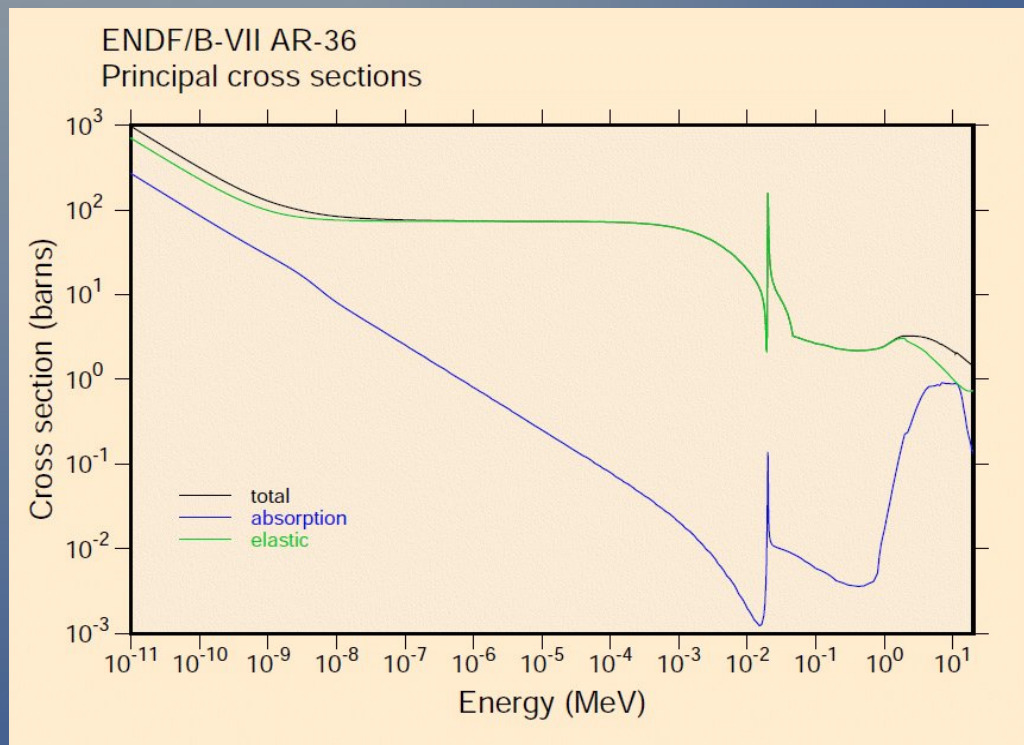
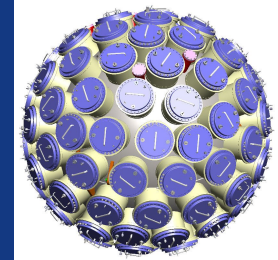


C. Zhang

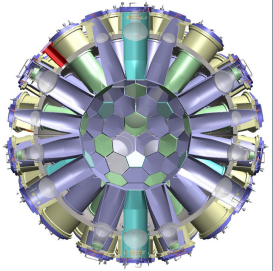
TALYS has no resonances input



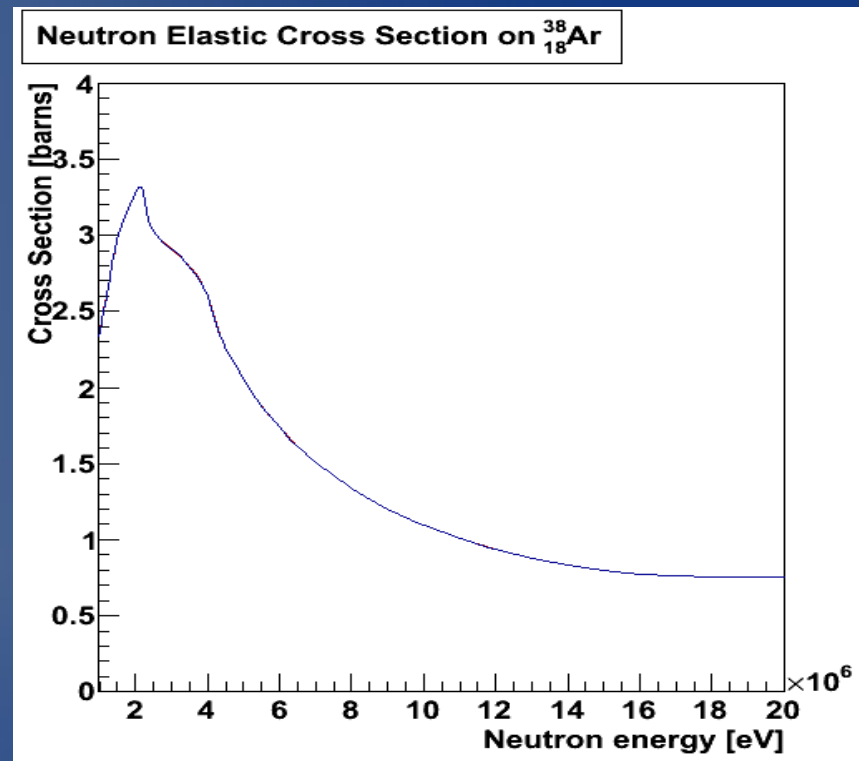
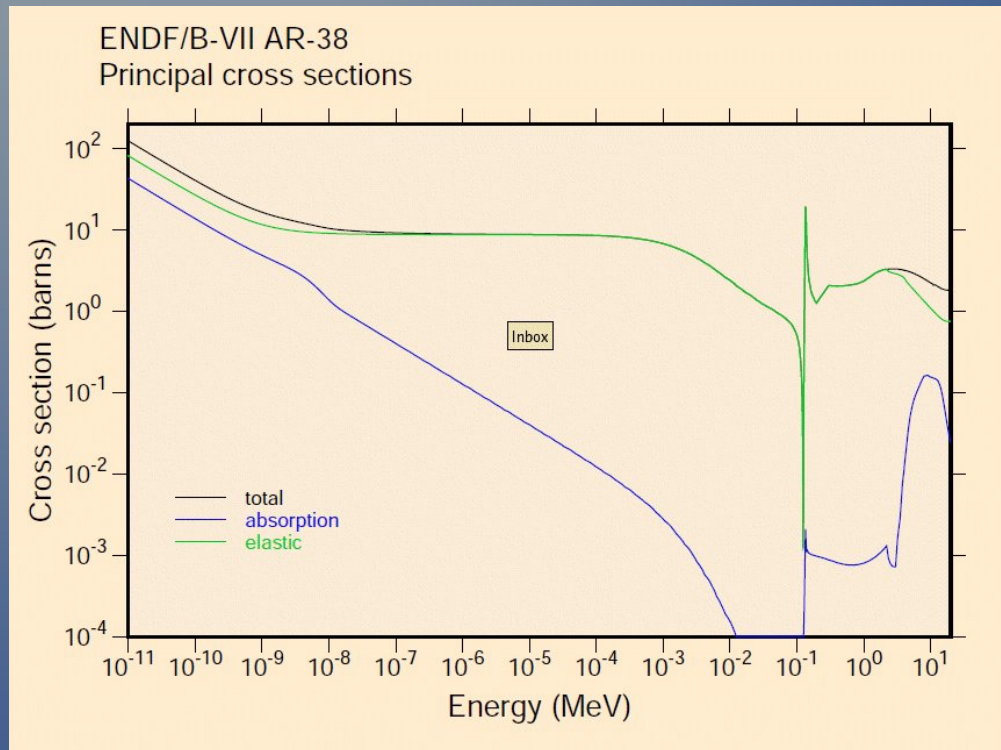
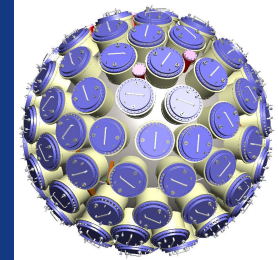
# Argon 36



ENDF and G4NDL values are in agreement,  
Can't see the other line!



# Argon 38



ENDF and G4NDL values are in agreement,  
Can't see the other line!