



#### Neutron-Argon Interactions <20 MeV: Verification of 'Neutron HP' in Geant4

#### Kimberly J. Palladino MiniCLEAN Collaboration







### Outline



- The RAT Simulation Framework
- Motivation for Neutron Studies for MiniCLEAN
- Pertinent Neutron Physics
- Low Energy Neutrons in Geant4
- Cross-Section Studies







- A collaboration pedigree
  - Started by the Braidwood collaboration
  - Extensively uses GLG4sim from KamLAND
  - Inherits conceptually from SNOMAN
  - Gd physics from Double CHOOZ
  - Some use by SNO, SNO+, DEAP collaborations
  - Extensive use by MiniCLEAN collaboration
- Developers:
  - Stan Seibert (sseibert@hep.upenn.edu), Tim Bolton, Dan Gastler, Josh Klein, Hugh Lippincott, Andy Mastbaum, James Nikkel, Gabriel Orebi Gann, Michael Akashi-Ronquest, Stan Seibert, Stephen Sekula, William Seligman, Chris Tunnell, Matthew Worcester
  - Many (most) DEAP/CLEAN collaboration members





## **RAT-** Operational Concept



User Input

- RATDB (.ratdb) constants, settings
- Geant4 geometry (.geo)
- RAT macro (.mac) event generators and processors to run
- HEPEvt or ROOT output

RAT processing:

- Done as an event loop
- Event generators (GLG4sim)
- Event Processors
  - PMT Detection
  - DAQ
  - Trigger
  - Fit
  - Analysis

#### Output

- ROOT files
  - Particle tracking
  - Simulated detector events
  - Analysis values
- Other processor output



# RAT Physics of Interest



#### Scintillation

- Modified version of GLG4sim (not Geant4)
   After each step, determine energy deposited, and using quenching factor determine number of photons produced, drawn from scintillation energy spectrum and time structure, then hands these photons back to Geant4
- No ionization currently
- Re-emission
  - Area of development: currently have surfaces that absorb from one wavelength and draw from re-emission spectra for new photons, but also possible to absorb and re-emit in a bulk material
- PMTs
  - Follow GLG4Sim for PE production and can include Dark Noise



### MiniCLEAN and RAT



# Extensive use at all levels of the experiment

- -Verification of Geant4 physics
- -Engineering design (magnetic compensation, spacing tolerances, etc.)
- -DAQ processing
- -Event reconstruction

#### Simulation and data comparisons for MicroCLEAN and DEAP-1



MicroCLEAN comparison of data and simulation Of <sup>57</sup>Co gamma rays



### 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 (will need discrimination to one in 10<sup>-9</sup> because of <sup>39</sup>Ar)
-> more late light from electron recoils because they are more likely to result in the longer lived (1.6 us) triplet state than the (6 ns) singlet state



### Neutron Backgrounds





•At SNOLab with >6000 m.w.e., instrumented water shielding can protect from neutrons created by muons penetrating to this depth (10 a day in our veto) that 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 <sup>238</sup>U and <sup>232</sup>Th alpha chains are followed in the PMT glass composition to generate the neutron spectrum.

Spectrum from 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% Neutrons below 500 keV cannot produce events above a 50 keVr analysis threshold Cross section has 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 dominates at thermal energies (0.025 eV) also resonances at keV energies Gamma rays and <sup>41</sup>Ar produced <sup>41</sup>Ar decays with a half life of 1.8 hrs to <sup>41</sup>K, producing a keV electron and 1.3 MeV gamma



### Argon Excited States







### 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</li>
- 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

Kimberly J. Palladino AARM Meeting February 2011



### More on Neutron HP



- Using Geant4.9.2 and 4.9.3
  - Cross Sections for <sup>40</sup>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
    - <sup>40</sup>Ar (.996003), <sup>38</sup>Ar(0.000632),
       <sup>36</sup>Ar (0.003365)
- Geant4 Hadronic Physics group adding features, fixing reported bugs



# Reproducing G4NDL





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 ~2 at energies < 45 keV Slight differences at the resonant dip at ~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)

Kimberly J. Palladino AARM Meeting

February 2011



## Comparison with Measurements



Neutron Total Cross Section on <sup>40</sup><sub>18</sub>Ar



Measurements and simulations have really been done with natural argon, at low energies <sup>36</sup>Ar becomes important!

Recall: <sup>40</sup>Ar (.996003), <sup>36</sup>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

Kimberly J. Palladino AARM Meeting February 2011



### 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

Steel





R(world)=1050 mm R<sub>inner</sub>(Outer ss)=1000 mm Thickness:15.679 mm Mass:1575 kg R<sub>inner</sub>(Inner SS)=609.34 mm Thickness: 27.345 mm Mass: 1050 kg R<sub>inner</sub>(PMT glass)=602.385mm Thickness: 7 mm Mass: 72 kg R<sub>inner</sub>(buffer LAr)=402.385mm R<sub>inner</sub>(acrylic)=400.00mm Thickness:2.385 mm Mass:5.5 kg R<400.00 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 The mean number of elastic scatters in Argon for a neutron that scatters at least once is 4.72

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**





Selected Neutron Inelastic Cross Sections on <sup>40</sup><sub>40</sub>Ar Section [barns] G4NDL Inelastic xs ENDF 1n FS xs G4NDL 1n FS Xs's ENDF n'1 gamma xs Simulation Cross Loss 0.8 0.6 0.4 0.2 ٥ 10 12 16 18 14 20 Neutron energy [eV]

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 threshhold of 4 MeV, but is an order of magnitude smaller in cross section Kimberly J. Palladino AARM Meeting February 2011



#### 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	l ceq	Simulation
***************************************	*** 04	
Step# X Y Z KineE dEStep StepLeng TrakLeng Volume Process		
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	action acti	
: 37.8 cm -18.1 cm -35.6 cm 20.9 keV Ar40[0.0]		
: 37.8 cm -18.1 cm -35.6 cm 1.44 MeV gamma	10 <sup>-3</sup> = 4	
: 37.8 cm -18.1 cm -35.6 cm 660 keV gamma		
: 37.8 cm -18.1 cm -35.6 cm 1 29 keV gamma	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2 2.5
: EndOf2ndaries Info		Gamma Energy (MeV)

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

> 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



- RAT is an easy to use and versatile simulation framework
  - Contact Stan Seibert at sseibert@hep.upenn.edu
- For Neutron-Argon interactions <20 MeV, Neutron HP broadly gives results in agreement with the cross-sectional information from ENDF/B-VII

#### – But bugs and some differences introduce uncertainties

• Similar checks, including looking at data, nuclear crosssection models, and full simulations in Geant4 are probably necessary at all energy ranges for all important materials

# DEAP/CLEAN Collaborators

#### University of Alberta

B. Beltran, P. Gorel, A. Hallin, S. Liu, C. Ng, K.S. Olsen, J. Soukup

#### Boston University

D. Gastler, E. Kearns

#### Carleton University

M. Bowcock, K. Graham, P. Gravelle, C. Oullet

#### Harvard University

#### J. Doyle

#### Los Alamos National Laboratory

R. Bourque, V.M. Gehman, J. Griego, R. Henning-Yeomans, A. Hime, F. Lopez, J. Oertel, K. Rielage, L. Rodriguez, S. Seibert, D. Steele

#### Massachusetts Institute of Technology

L. Feng, J.A. Formaggio, S. Jaditz, J. Kelsey, J. Monroe, K. Palladino

#### National Institute Standards and Technology

K. Coakley

#### University of New Mexico

M. Bodmer, F. Giuliani, M. Gold, D. Loomba, J. Matthews, P. Palni

#### University of North Carolina/TUNL

M.Akashi-Ronquest, R. Henning

#### University of Pennsylvania

T. Caldwell, J.R. Klein, A. Mastbaum, G.D. Orebi Gann

#### Queen's University

M. Boulay, B. Cai, M. Chen, S. Florian, R. Gagnon, V. Golovko, P. Harvey, M. Kuzniak, J. Lidgard, A. McDonald, T. Noble, P. Pasuthip, C. Pollman, W. Rau, P. Skensved, T. Sonley, M. Ward

#### SNOLAB Institute

M. Batygov, F.A. Duncan, I. Lawson, O. Li, P. Liimatainen, K. McFarlane, T. O'Malley, E. Vazquez-Jauregi

#### University of South Dakota

V. Guiseppe, D.-M. Mei, G. Perumpilly, C. Zhang

Syracuse University

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

#### TRIUMF

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

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





#### **Backup Slides**

Kimberly J. Palladino AARM Meeting February 2011



# Elastic Angular Distribution



From Chao Zhang





Geant4 simulations of monoenergetic neutrons elastically scattering in Argon Uniform distribution for low energy neutrons

**ENDF** Differential Cross Section



### **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



U.	238	Th2	232	
Energy (keV) 4198 4151 4775 4722 4688 4621 4784 4602 5490 6002 6902 7697	Branch Ratio(%) 79 21 71.4 28.6 76.3 23.7 94.4 5.6 100 100 0.01 99.99	Energy (keV) 4013 3954 5423 5340 5685 5449 6288 6778 8784 6090 6050	Branch Ratio(%) 77.9 22.1 71.5 28.5 94.9 5.1 100 100 64 9.8 26.2	
5304	100			



#### http://neutronyield.usd.edu

- •Decay in secular equilibrium, follow 8 and 6 alphas from <sup>238</sup>U and <sup>232</sup>Th respectively
- Input glass composition
- Primary contribution to neutrons comes from Boron
  Assay of PMT for radio isotope content:
- - <sup>238</sup>U: 0.10287 ppm
  - <sup>232</sup>Th: 0.16974 ppm











C. Zhang

TALYS has no resonances input



Can't see the other line!

















10<sup>1</sup>

 $10^{-1}$   $10^{0}$ 

Argon 38



Can't see the other line!



Inbox

Energy (MeV)

 $10^{-3}$ 

 $10^{-8}$   $10^{-7}$   $10^{-6}$   $10^{-5}$   $10^{-4}$ 



ENDF and G4NDL values are in agreement,





 $10^{2}$ 

10<sup>1</sup>

Cross section (barns) 00100 Cross section (barns)

10<sup>-1</sup>

10-2 -

10-3

10-4 10-11

otal absorption

10-10 10-9



## **Pulse Shape Discrimination**





Boulay et al. arXiv:0904.2930

In LAr,  $\tau_{\text{triplet}} = 1.6 \text{ us}, \tau_{\text{singlet}} = 6 \text{ ns}$ F<sub>prompt</sub> ~ .3 for electron recoils, .8 for nuclear



Boulay and Hime, Astropart. Phys. 25, 179 (2006)

How well can discrimination work? DEAP-1 has demonstrated (stat. Limited) <  $6 \times 10^{-8} 43 < E < 86 \text{ keV}_{ee}$ Necessary in LAr because of <sup>39</sup>Ar

Also seen <10<sup>-3</sup> in LNe Nikkel et al., Astropart. Phys., 29,161 (2008)

Kimberly J. Palladino AARM Meeting February 2011



## Neutron HP 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
  - 40Ar has a substantial dip in the elastic cross section
     at ~50 keV, where neutrons have a mean free path of 118 m
- Geant4 neutron physics should be verified for every material!