An Introduction of The Noble Element Simulation Technique Version 2.0

Greg Rischbieter,
On Behalf of the NEST Collaboration
CPAD, Brown University, December 2018
https://github.com/NESTCollaboration/nest

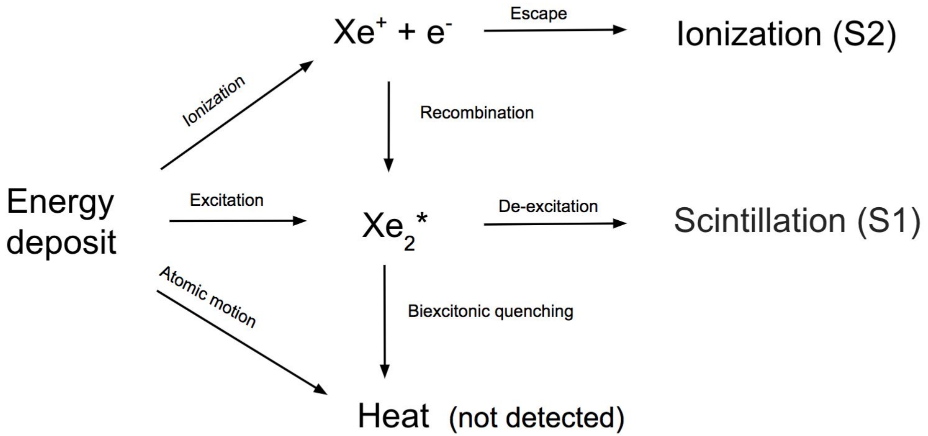
About NEST

- "Inter-collaboration" Collaboration
  - Members from LUX, LZ, XENON, DUNE, and nEXO.
- Fast C++ simulation of more interactions in LXe and GXe than ever before!
  - Important for identifying interactions from actual light and charge yields
  - Temperature, pressure, and density dependencies using NIST
  - LAr models being worked on for future release!
- nest.physics.ucdavis.edu

Website includes link to GitHub download page for full code!
Get it while supplies last!

NEST

Signal production in xenon



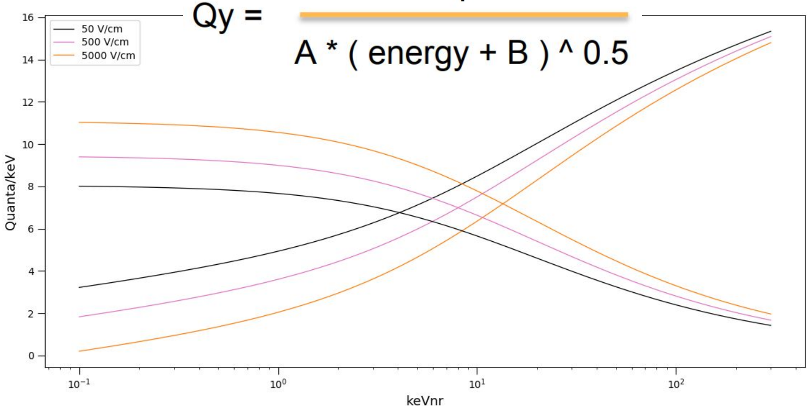
What's New in NESTv2?

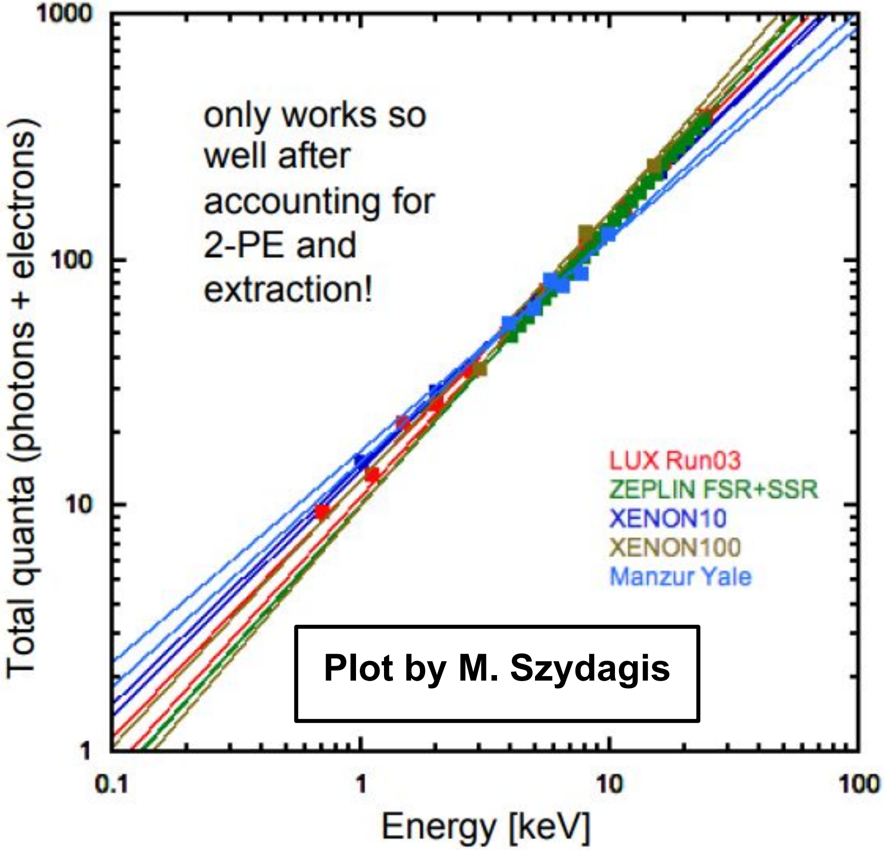
- Comprehensive models for all particle types
- Switched most of the yields equations to simpler functions
    - Older models (TIB and Doke-Birks) weren't fitting the data anymore.
    - e.g. sigmoids, which still closely resemble those older models.
        - Reproduces TIB & Doke-Birks models at low and high energy regimes
- Revisited old data, corrected with new knowledge
    - Includes 2PE effect for VUV photons in PMTs
    - Allowed 'zero-field' to vary
    - Corrected for less-than-perfect extraction efficiency
    - ER: β-model vs. γ-model
- Exciton-Ion ratio is energy-dependent
- For ER & NR, total quanta and charge yields are calculated first
    - Exciton-ion ratio and recombination probabilities are then reverse-engineered.
- Accurately models detector effects for S1-S2 bands (means, widths, leakages)

Nuclear Recoils

- Total quanta is now a power law
  - 12.6 * (Energy)^1.05
    - Elegant → almost linear
  - 12.6 ± 0.9 & 1.05 ± 0.05
  - Consistent with ~1 quanta at 100 eV
- No more Lindhard model
  - Most mean-yields equations replaced with simple functions

$$Qy = \frac{1}{A * (energy + B) ^ 0.5}$$

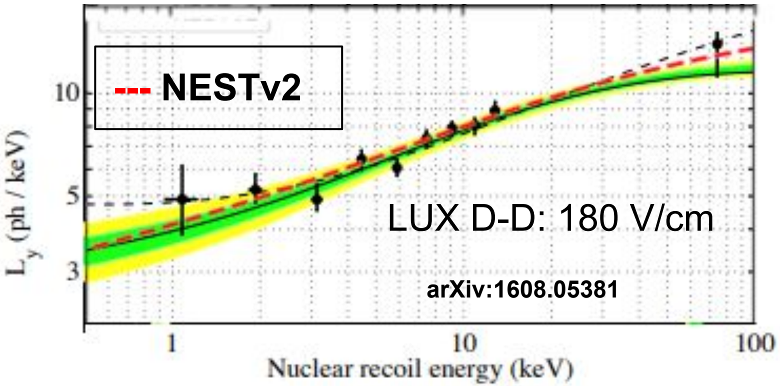


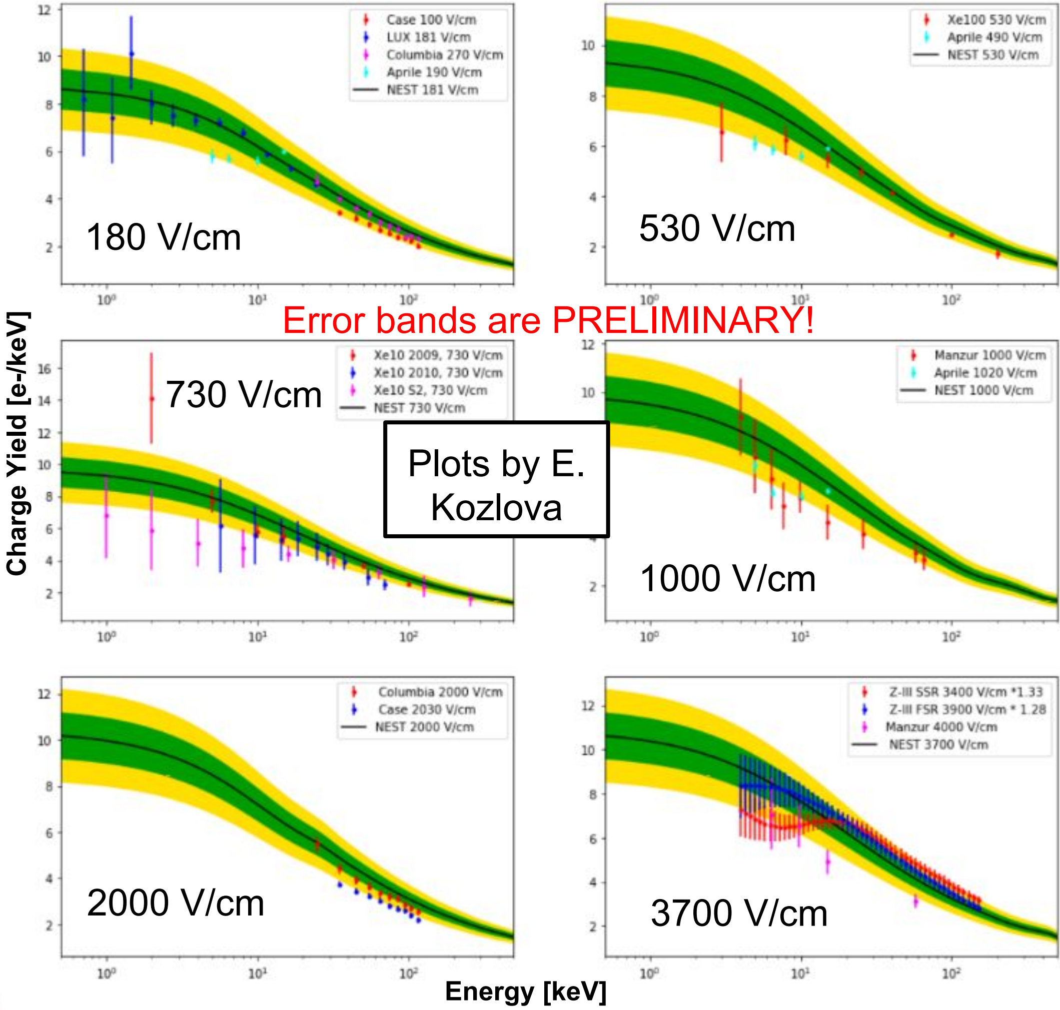


NR Data Comparisons

- Agrees well with many different data sets at a wide variety of energy and field (See Right).
- (See Below) Matches low energy data better than Lindhard (solid) or Bezrukov (dashed) parameterizations

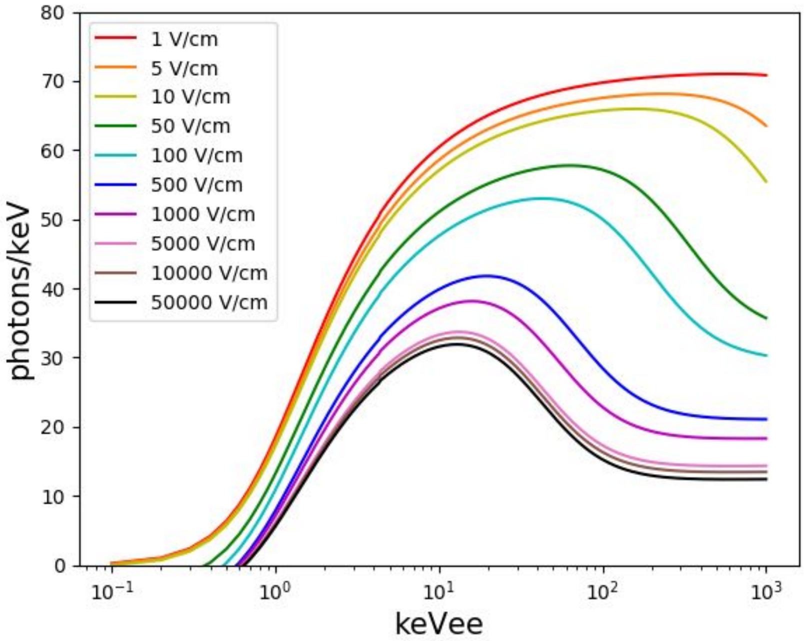
Interplay between scintillation and ionization in liquid xenon Dark Matter searches
Fedor Bezrukov, Felix Kahlhoefer, Manfred Lindner (Heidelberg, Max Planck Inst. & Munich U.), Felix Kahlhoefer (Heidelberg, Max Planck Inst. & Oxford U., Theor. Phys.), Manfred Lindner (Heidelberg, Max Planck Inst.). Nov 2010. 9 pp.
Published in **Astropart.Phys. 35 (2011) 119-127**

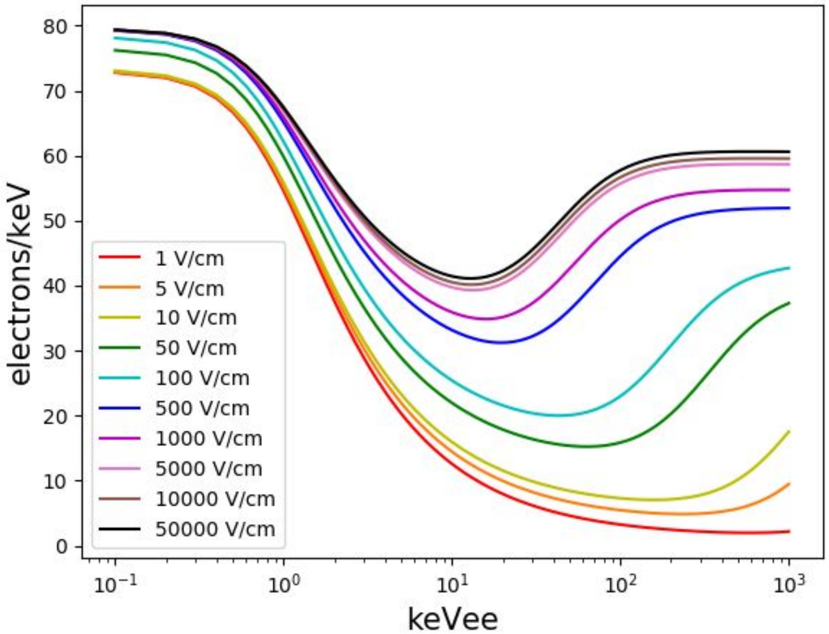




Electronic Recoils -- Sum of Two Sigmoids

- Smooth transition between low and high energies
  - Stitching region hardest to model → Transition between TIB and DB regimes!



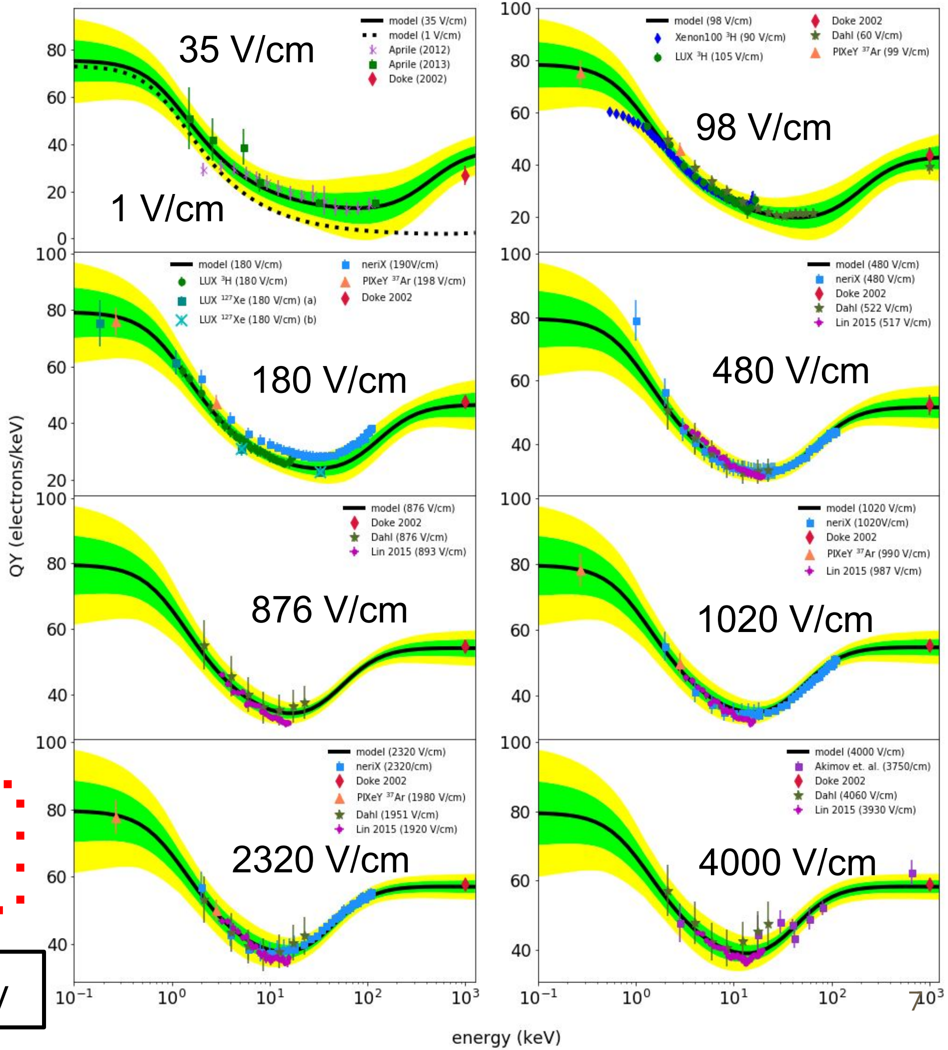


Matches Data for a large range of fields

- QY from β ER and ^{137}Cs Compton Scatters
  - Large field labels correspond to value used in NEST simulation

Error bands are PRELIMINARY!

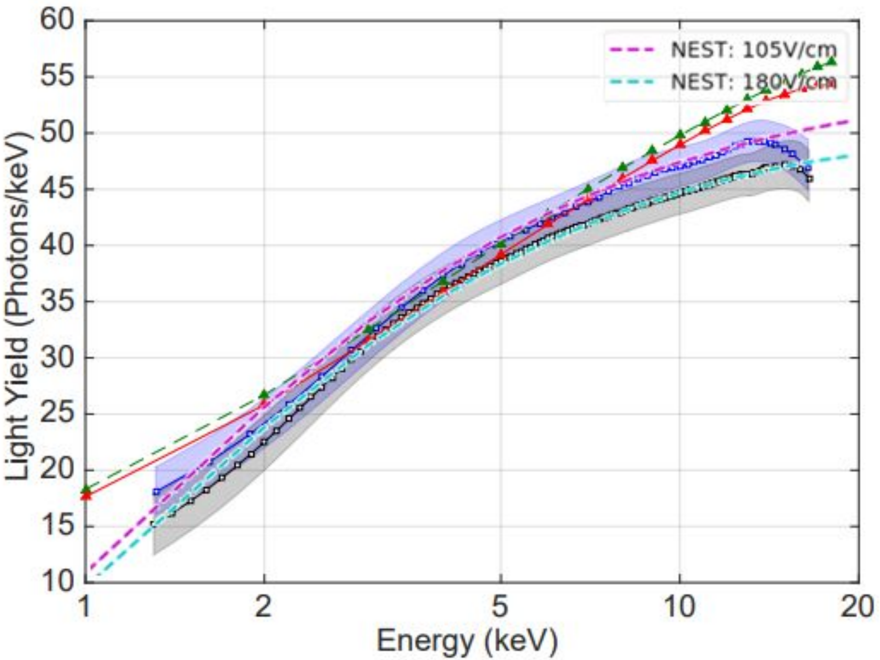
Plot by J. Balajthy

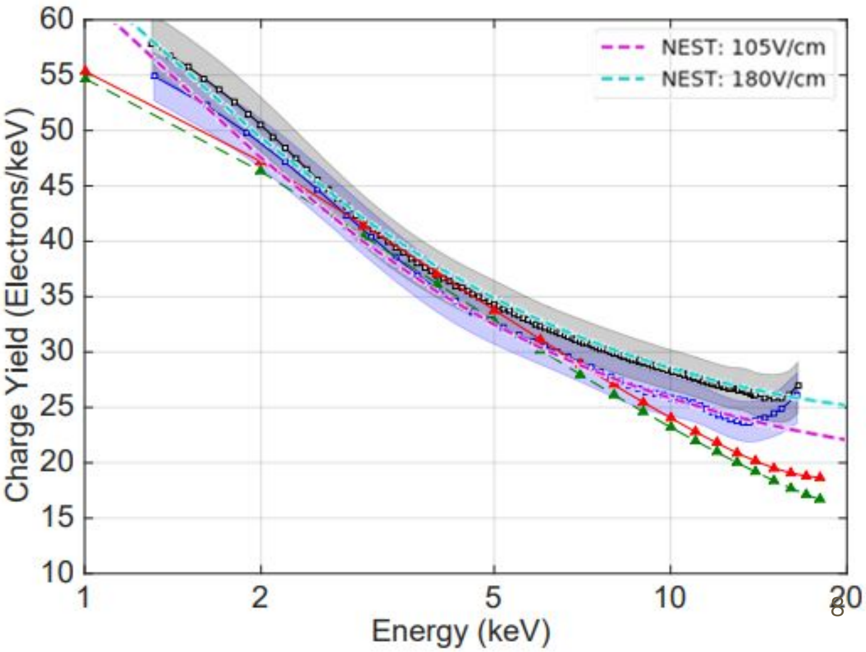


LUX Tritium

Tritium calibration of the LUX dark matter experiment
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Dec 9, 2015. 12 pp.
Published in **Phys.Rev. D93 (2016) no.7, 072009**

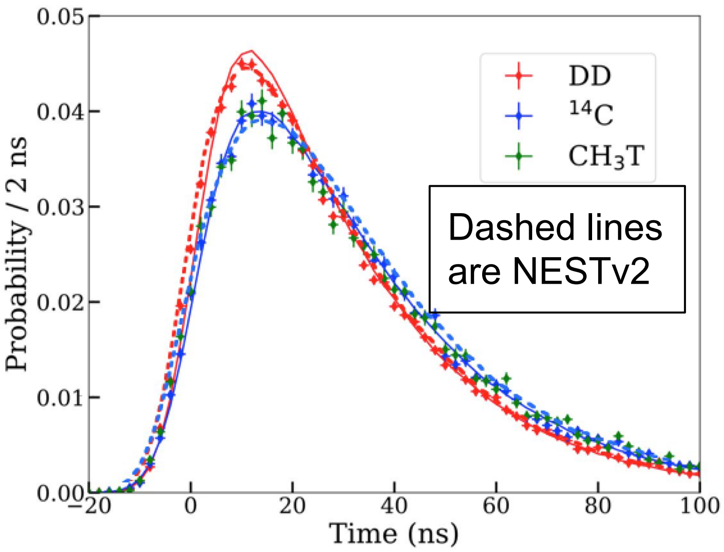
- Great agreement with both light and charge yields
- Note: legend refers to NESTv2; red and green lines are previous NEST
    - Great improvement upon NESTv1's successes

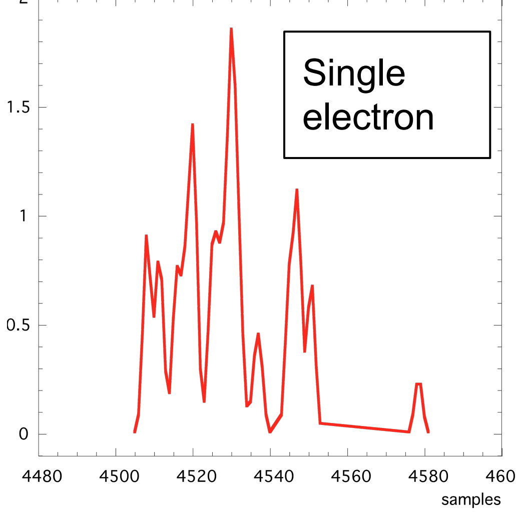




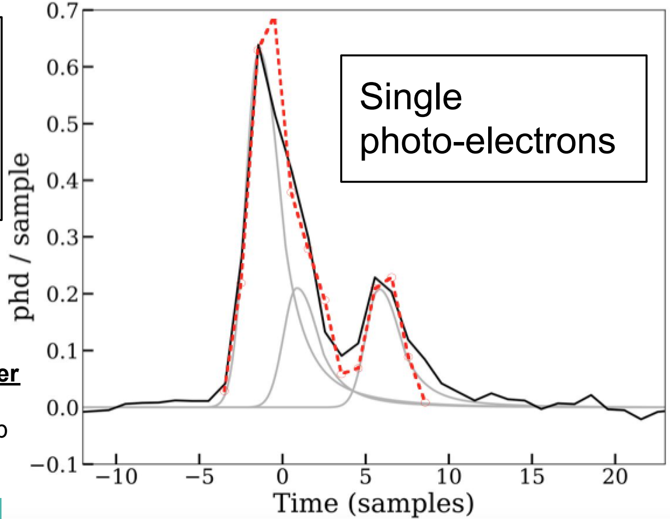
Pulse Shapes

- Uses event position and detector geometry to approximate photon travel time.
- Matches LUX pulse shape discrimination.
- Simulates both components of SE noise in LXe.





ABOVE: Histograms of S1 photon arrival times

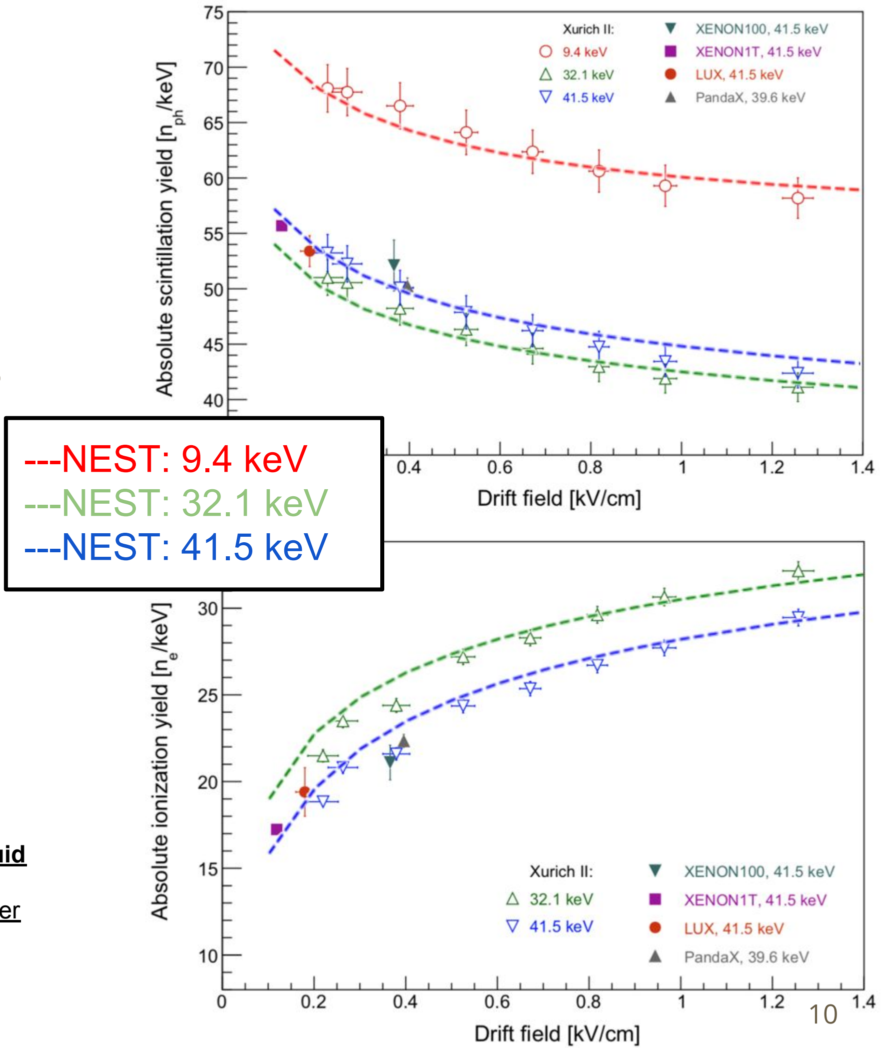


Two distinct components of the delayed single electron noise in liquid xenon emission detectors
P. Sorensen (LBNL, Berkeley), K. Kamdin (LBNL, Berkeley & UC, Berkeley). Nov 19, 2017. 5 pp. Published in **JINST 13 (2018) no.02, P02032**

Liquid xenon scintillation measurements and pulse shape discrimination in the LUX dark matter detector
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Feb 16, 2018. 16 pp.
Published in **Phys.Rev. D97 (2018) no.11, 112002**

^{83m}Kr

- Accurately reproduces both 32.1 keV and 9.4 decays, as well as merged 41.5 keV
- Robust time-dependent model
- Matches individual decays as well as ‘merged’ decay



A Dual-phase Xenon TPC for Scintillation and Ionisation Yield Measurements in Liquid Xenon
Laura Baudis, Yanina Biondi, Chiara Capelli, Michelle Galloway, Shingo Kazama, Alexander Kish, Payam Pakarha, Francesco Piastra, Julien Wulf. Dec 22, 2017. 11 pp

^{83m}Kr

- 1 σ agreement with LUX and XENON100

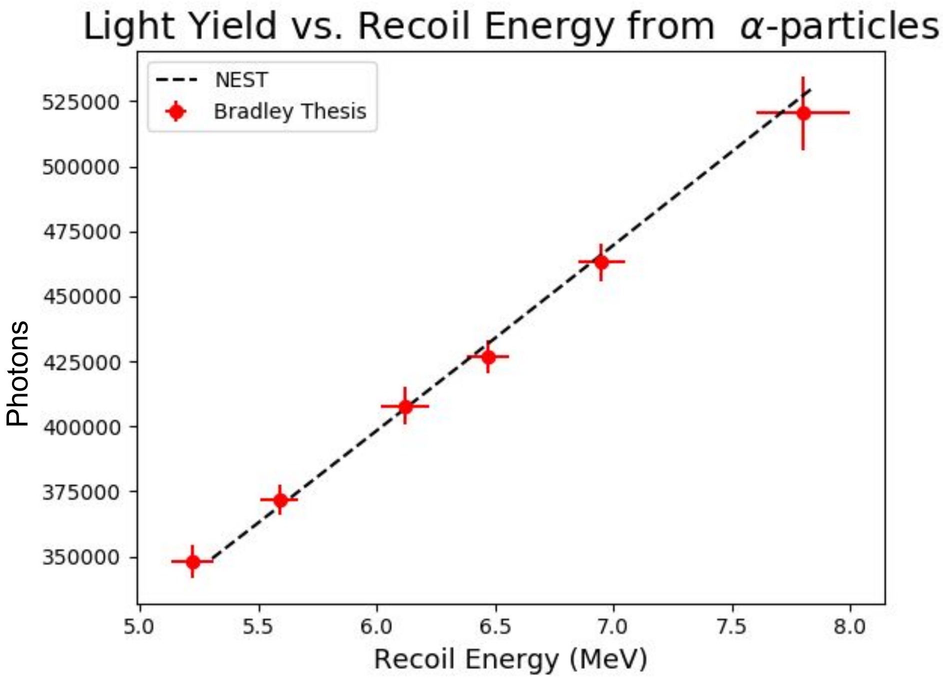
	Drift Field (V/cm)	Quanta/keV	NEST Result
LUX Ly	180	53.4 ± 1.4	53.0
LUX Qy	180	19.4 ± 1.4	20.0
XENON100 Ly	366	52.5 ± 1.8	50.6

Signal yields, energy resolution, and recombination fluctuations in liquid xenon
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Oct 6, 2016. 12 pp.
Published in **Phys.Rev. D95 (2017) no.1, 012008**

Signal Yields of keV Electronic Recoils and Their Discrimination from Nuclear Recoils in Liquid Xenon
XENON Collaboration (E. Aprile (Columbia U.) *et al.*). Sep 28, 2017. 11 pp.
Published in **Phys.Rev. D97 (2018) no.9, 092007**
DOI: 10.1103/PhysRevD.97.092007

α-Model

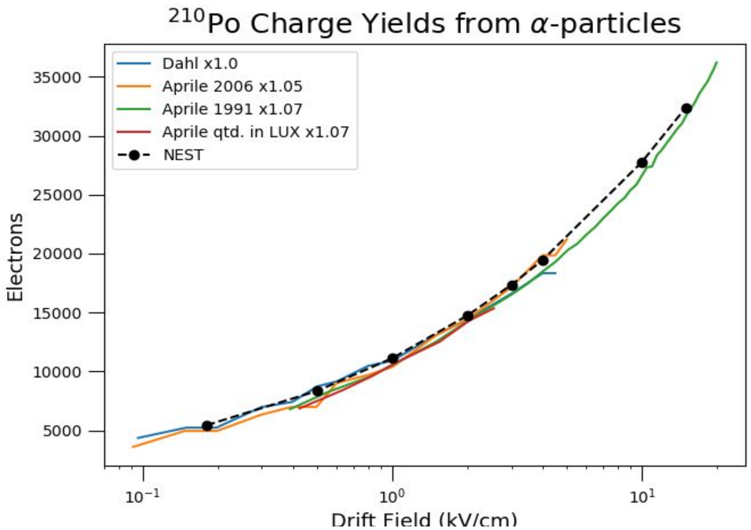
- L-factor fixed by fitting to Adam Bradley's thesis data
  - (LUX: 180V/cm)
- Uses a modified TIB model here
  - Energy-independent for simplicity

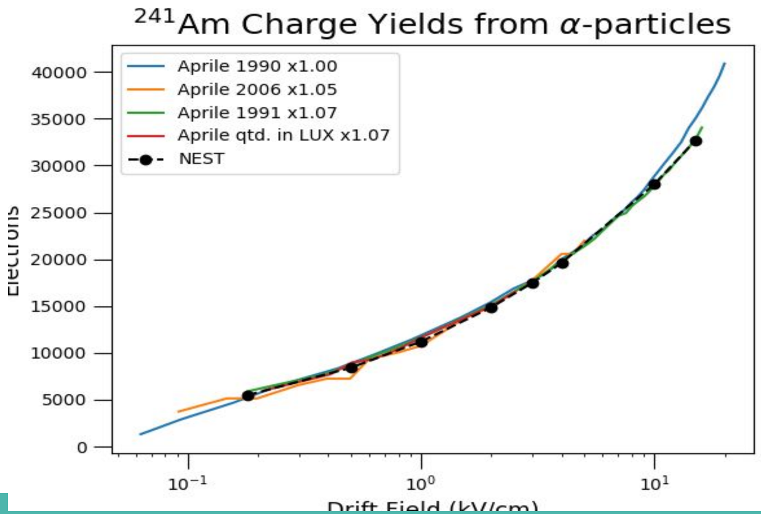


A.W. Bradley. **LUX THERMOSYPHON CRYOGENICS AND RADON-RELATED BACKGROUNDS FOR THE FIRST WIMP RESULT.** Doctoral Dissertation. Case Western Reserve University. May 2014.

α-Model

- Again, only worked by correcting data for extraction efficiency, as on slide 4 (NR).
- Good agreement for strong fields





Simultaneous measurement of ionization and scintillation from nuclear recoils in liquid xenon as target for a dark matter experiment
E. Aprile, C.E. Dahl, L. DeViveiros, R. Gaitskell, K.L. Giboni, J. Kwong, P. Majewski, Kaixuan Ni, T. Shutt, M. Yamashita. Jan 2006.
Published in **Phys.Rev.Lett. 97 (2006) 081302**

E. Aprile, et.al. **Ionization of liquid xenon by 241Am and 210Po alpha particles.** Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 307, Issue 1,1991.

E. Aprile et. al "A study of the scintillation light induced in liquid xenon by electrons and alpha particles," in *IEEE Transactions on Nuclear Science*, vol. 37, no. 2, pp. 553-558, Apr 1990.

Energy Resolution

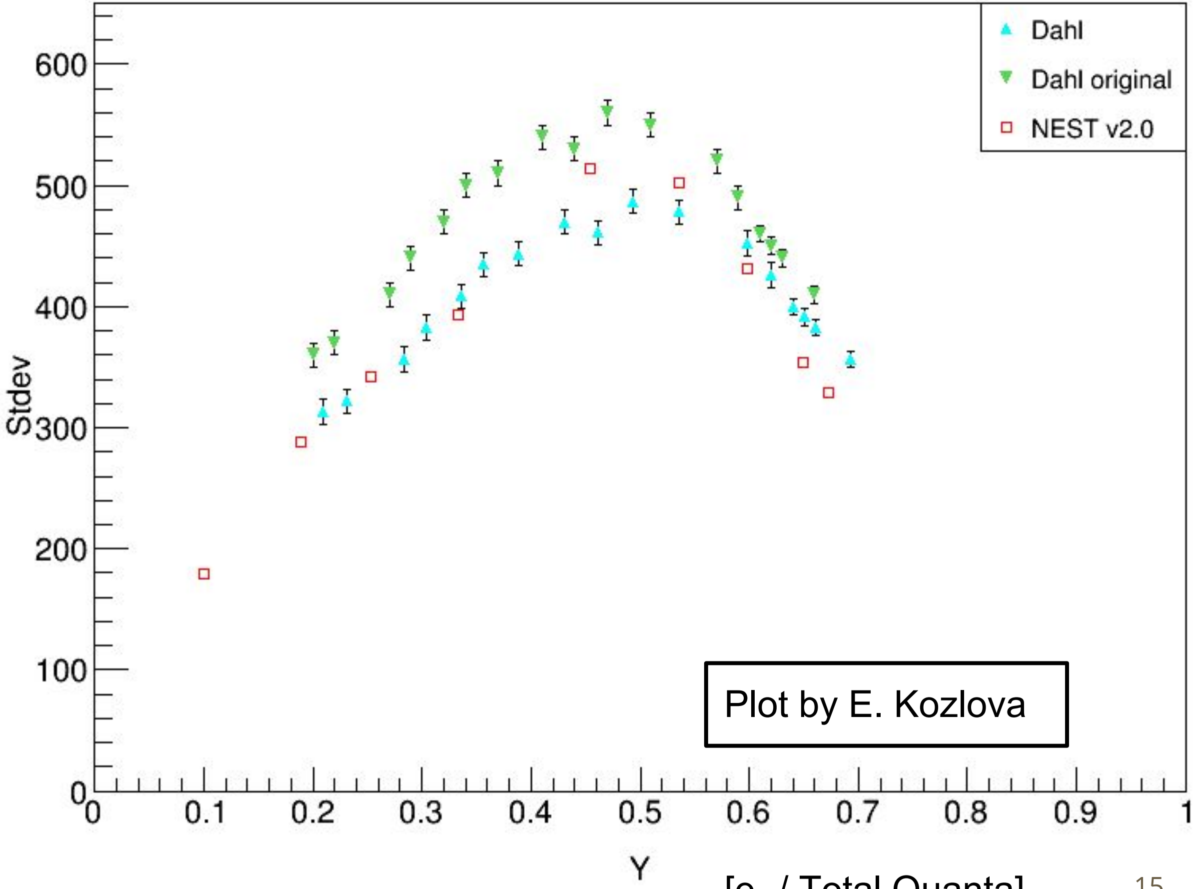
- Quantum Fluctuations
  - First estimates of fluctuations in energy resolution and fluctuations in quanta produced were by Ugo Fano in the 1940's. **On the Theory of Ionization Yield of Radiations in Different Substances.** U.Fano. Phys. Rev. **70**, 44 – Published 1 July 1946
  - There is energy "lost" when photons are produced in LXe from electron recoils!
  - $E = W*(n_\gamma + n_e)$ → Work Function: W = 13.7 eV
  - Fluctuations modeled using an empirical "Fano-like" factor proportional to sqrt(energy)*sqrt(field)
- Recombination Fluctuations
  - Binomial recombination has never matched data well.
  - Same equation as cited in LUX Signal Yields Publication: $\sigma_T{}^2=(1-p)*n_i*p + (\sigma_p n_i)^2$
    - σ_p in NEST is both field-dependent and energy-dependent

Signal yields, energy resolution, and recombination fluctuations in liquid xenon
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Oct 6, 2016. 12 pp.
Published in **Phys.Rev. D95 (2017) no.1, 012008**
DOI: 10.1103/PhysRevD.95.012008

Recombination Fluctuations

- Comparing to Eric Dahl's PhD thesis data.
- x-axis is the electron fraction.
- Corrected Dahl data for overestimation
    - Corrected 15% downward for 2PE effect and extraction eff.

The Physics of Background Discrimination in Liquid Xenon, and the First Results from XENON10 in the Hunt for WIMP Dark Matter. C.E. Dahl. Doctoral Dissertation. Princeton University. September 2009

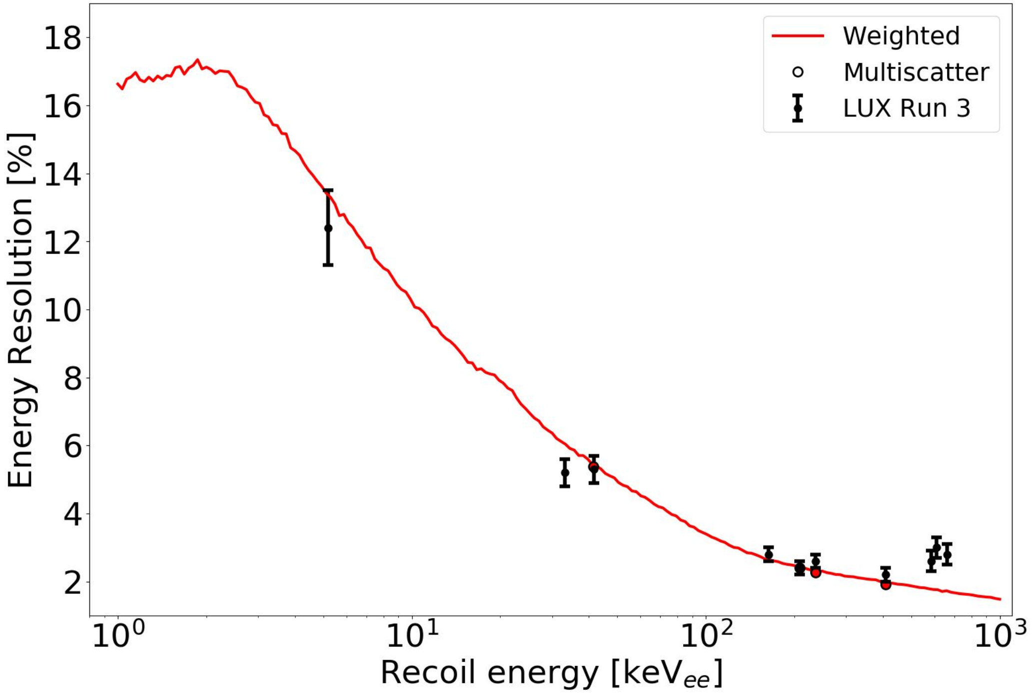


[e- / Total Quanta]

Energy Resolution: LUX

- Good Fit to LUX Run 3.
- β-model better at lower energies. Fit here uses a weighted combination of NEST's β and γ models.

Plot by V. Velan

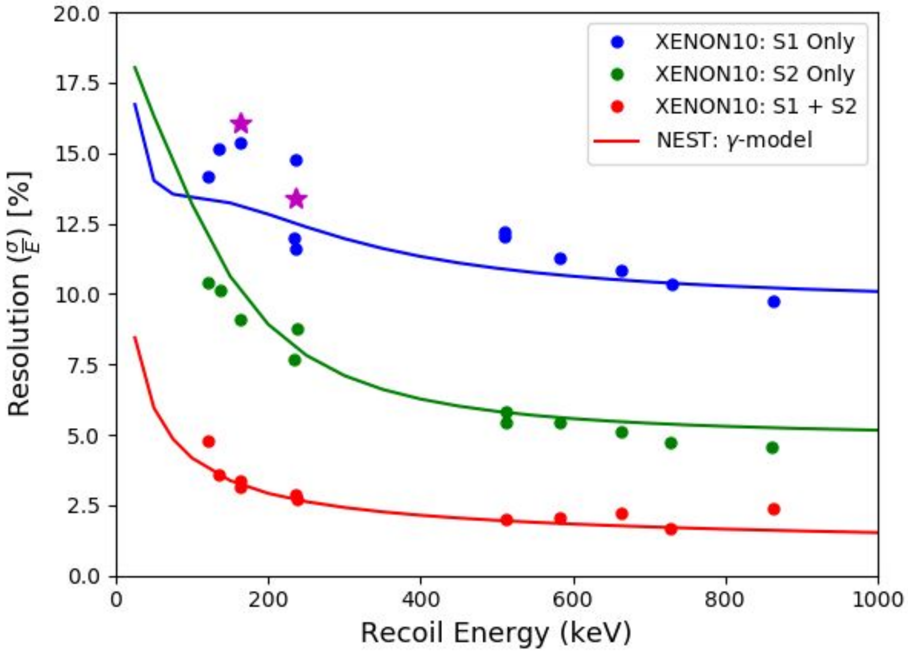


Signal yields, energy resolution, and recombination fluctuations in liquid xenon
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Oct 6, 2016. 12 pp.
Published in **Phys.Rev. D95 (2017) no.1, 012008**
DOI: 10.1103/PhysRevD.95.012008

Energy Resolution: XENON10

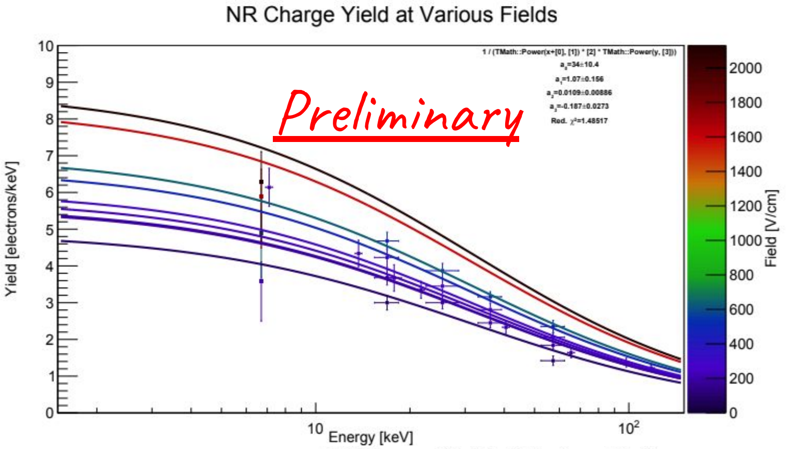
arXiv.org/pdf/1001.2834.pdf

- Good agreement with XENON10 energy resolution
  - Optimized a Fano-like factor for best agreement → Data suggested field & energy dependence
  - Data suggests that the Fano factor is both energy-dependent and field-dependent
- Magenta stars are ^{129m}Xe & ^{131m}Xe
  - Decay in many steps (γ and X rays), used NEST to combine the yields from each decay and added them together
  - ^{83m}Kr model suggests that multi-step decays have subtle time-dependence



ArgNEST-- Fitting to NR and ER Charge Yields

- LAr Models Coming Soon!



Plots by E. Kozlova

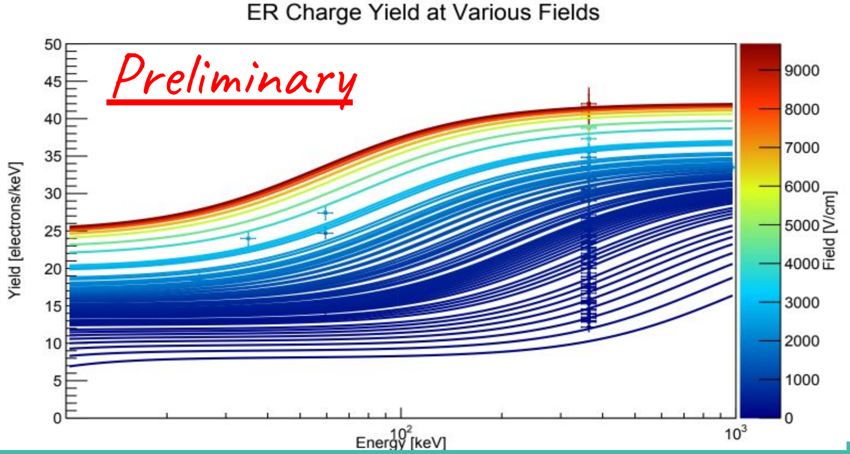
First demonstration of a sub-keV electron recoil energy threshold in a liquid argon ionization chamber
S. Sangiorgio (LLNL, Livermore) *et al.*. Jan 2013. 4 pp.
Published in **Nucl.Instrum.Meth. A728 (2013) 69-72**

X-ray ionization yields and energy spectra in liquid argon
A. Bondar, A. Buzulutskov, A. Dolgov, L. Shekhtman, A. Sokolov. May 9, 2015. 6 pp.
Published in **Nucl.Instrum.Meth. A816 (2016) 119-124**

Measurement of Scintillation and Ionization Yield and Scintillation Pulse Shape from Nuclear Recoils in Liquid Argon
SCENE Collaboration (H. Cao (Princeton U.) *et al.*). Jun 18, 2014. 29 pp.
Published in **Phys.Rev. D91 (2015) 092007**

First measurement of the ionization yield of nuclear recoils in liquid argon
T.H. Joshi *et al.*. Feb 10, 2014. 5 pp.
Published in **Phys.Rev.Lett. 112 (2014) 171303**

Measurement of the liquid argon energy response to nuclear and electronic recoils
P. Agnes (Houston U. & APC, Paris) *et al.*. Jan 20, 2018. 14 pp.
Published in **Phys.Rev. D97 (2018) no.11, 112005**



Measurement of the ionization yield of nuclear recoils in liquid argon at 80 and 233 keV
A. Bondar, et. al. Jul 28, 2014. 6 pp.
Published in **EPL 108 (2014) no.1, 12001**

Critical test of geminate recombination in liquid argon R. T. Scalettar, P. J. Doe, H. -J. Mahler, and H. H. Chen. Phys. Rev. A 25, 2419(R) – Published 1 April 1982

Conclusion

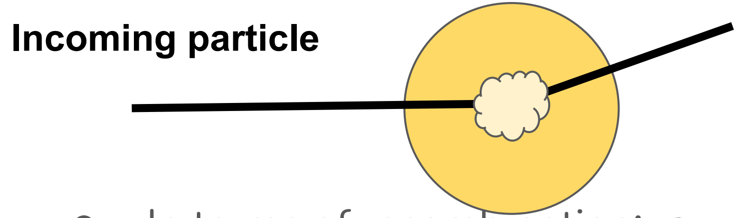
- NESTv2 is a powerful simulation tool free to use, and it takes seconds to run!
- Accurately simulates many different interactions in LXe and GXe, while Argon models are being worked on as we speak.
  - User-friendly code so you can add any other interactions that you might find useful.
- You can build your own detector model and begin calculating light and charge yields!
- Future work:
  - NEST *Lite* → Simulation of optical processes in Noble Element Detectors
  - Molecular dynamics modeling based on first principles
- Get yourself a copy!
  - **https://github.com/NESTCollaboration/nest**
  - **nest.physics.ucdavis.edu**

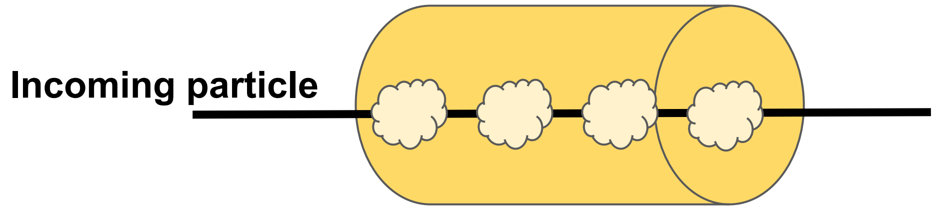
Thank You!!

Backup Slides

Besides the many many in the previous slide’s attachment!

Previous Yield Models: Thomas-Imel vs. Doke-Birks

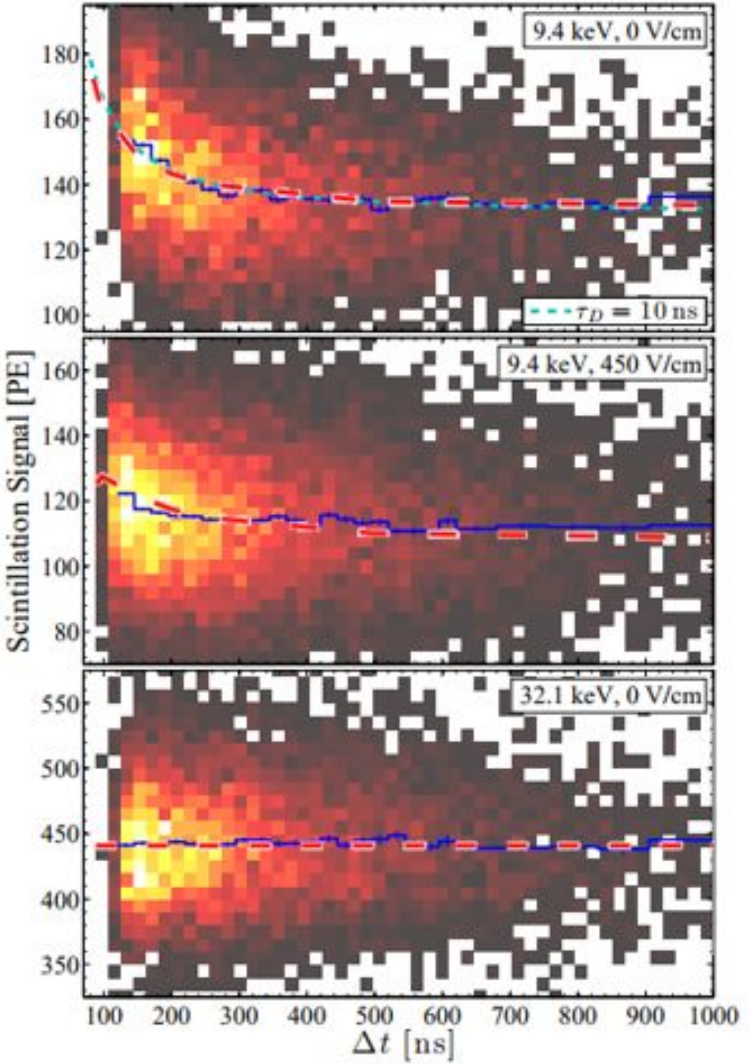




- In terms of recombination: $QY = n_{e^-}/E = \frac{(1-r)}{E} * N_{ions}$
  - N_{ions} is approximately energy divided by the work function: E/W
- Thomas-Imel Box Model $\rightarrow$ Low energy approximation (no particle track)
  - Quanta are spherically distributed
  - $(1-r) = \frac{1}{\xi}\ln(1+\xi)$ where $\xi \equiv A \cdot N_{ions}$ for some constant, A
  - So $QY = \frac{1}{A \cdot E} \cdot \ln\left(1 + A \cdot \frac{E}{W}\right)$
  - At 180 V/cm, A = 0.03 and expanding about E=2 keV, $QY \approx 25.6 - 6.85\Delta E + 2.18\Delta E^2 + \mathcal{O}(\Delta E^3)$
    - NEST Model at 180V/cm about 2 keV: $QY \approx 34.67 - 12.67\Delta E + 4.7\Delta E^2 + \mathcal{O}(\Delta E^3)$
- Doke-Birks $\rightarrow$ High energy approximation (particle create tracks)
  - Quanta are cylindrically distributed (superposition of many spheres)
  - $QY = \frac{N_{ions}/E}{1 + k_B \cdot dE/dx}$, and $\frac{dE}{dx} \sim E^{-3/4}$ for xenon at keV-range energies (k_B is Birk's constant)
  - So now, $QY = \frac{1/W}{1 + k_B^* \cdot E^{-3/4}}$ (11)
  - At 180 V/cm, $k_B^* \approx 42$ and expanding about E=100 keV, $QY \approx 26.6 + 0.11\Delta E - 0.0005\Delta E^2 + \mathcal{O}(\Delta E^3)$
    - NEST Model at 180V/cm about 100 keV: $QY \approx 26.7 + 0.12\Delta E - 0.0005\Delta E^2 + \mathcal{O}(\Delta E^3)$

Scintillation Signal v. Time

Kr83m data suggests that the total light yield from the 9.4 keV decay has a slight time dependence



Response of liquid xenon to Compton electrons down to 1.5 keV
Laura Baudis, Hrvoje Dujmovic (Zurich U.), Christopher Geis (Zurich U. & Unlisted, DE), Andreas James, Alexander Kish, Aaron Manalaysay, Teresa Marrodan Undagoitia, Marc Schumann (Zurich U.). Mar 27, 2013. 14 pp.
Published in **Phys.Rev. D87 (2013) no.11, 115015**

ER in GXe

density (g/cc)	keVee	W_sc (eV)	NEST W_sc (eV)
0.08	622	61 +/- 18 [1]	66 **
0.0057	5.9	111 +/- 16 [2]	97.8
0.0899	60	75 +/- 11 [3]	69.4

** Gamma Model found 83.8 eV for 662 keVee

[1] **Ionization and scintillation of nuclear recoils in gaseous xenon**
NEXT Collaboration (J. Renner (LBL, Berkeley & UC, Berkeley) *et al.*). Sep 9, 2014. 13 pp.
Published in **Nucl.Instrum.Meth. A793 (2015) 62-74**

[2] **Absolute primary scintillation yield of gaseous xenon under low drift electric fields for 5.9 keV X-rays**
Carmo, S.J.C. et. al. 2008.
Published in **Journal of Instrumentation**, **Volume 3**.July 16, 2008

[3] A. Parsons *et al*., "High pressure gas scintillation drift chambers with wave-shifter fiber readout," in *IEEE Transactions on Nuclear Science*, vol. 37, no. 2, pp. 541-546, Apr 1990.
doi: 10.1109/23.106674

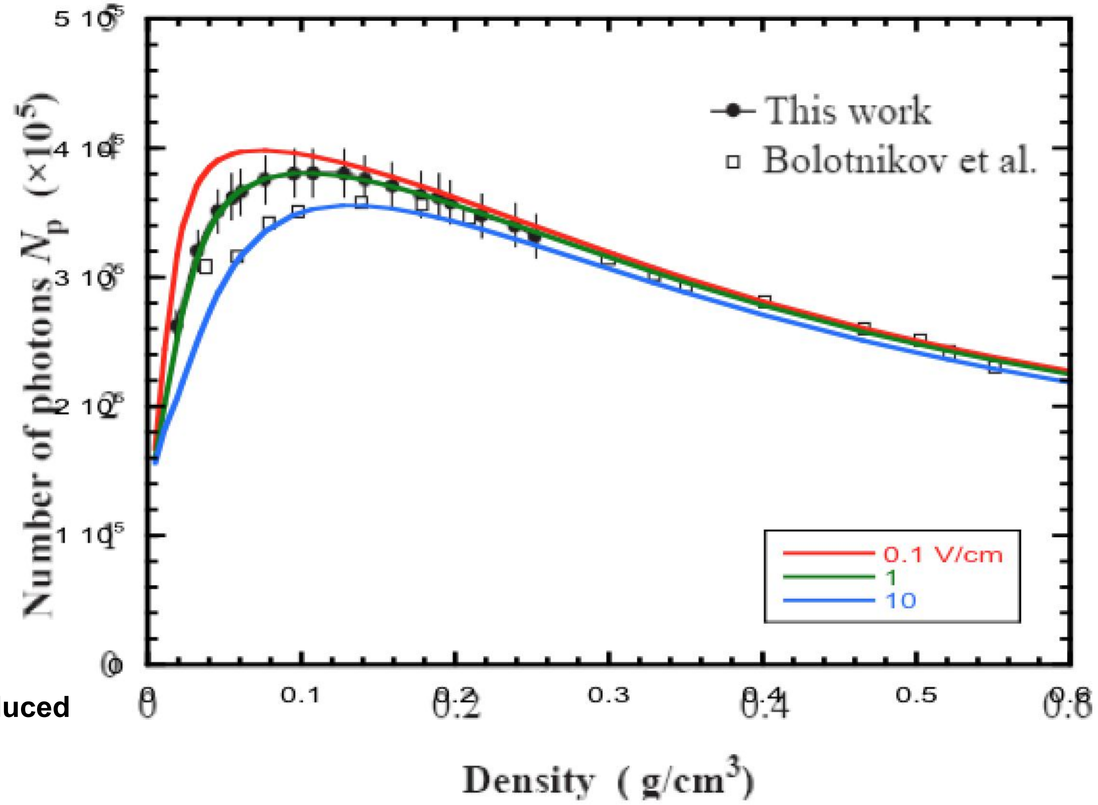
*Light yields (1000 / W) were nearly constant for field ranges ~200-25000 V/cm

[1] states W_i = 24.7 eV -- NEST result is 30.2 eV

Gamma Model: 27.5 eV

α-Model for GXe

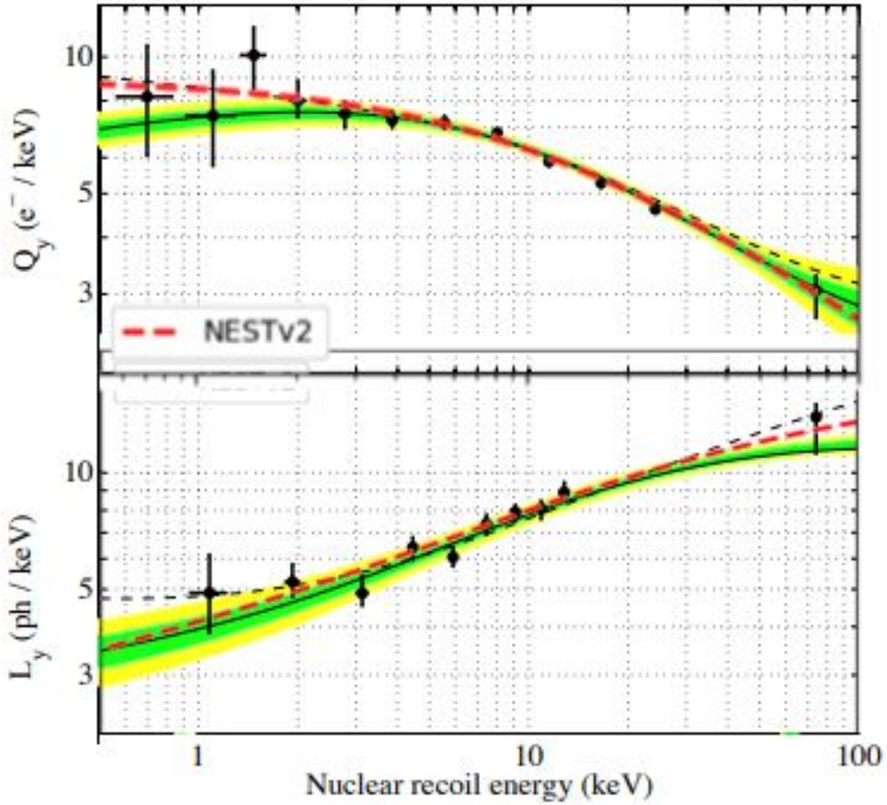
- Most GXe α data is contradictory (data shown is 0 V/cm).
- NESTv2 splits many of the differences between contradictions.
  - Floating "zero-field" was critical here!



M. Miyajima et. al. **Absolute number of photons produced by alpha-particles in liquid and gaseous xenon**. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, Volume 63, Issue 3, 1992, Pages 297-308,ISSN 0168-583X

LUX D-D Comparisons

- Cleaner match to light and charge yields than before!
- Solid and dashed black lines are the Lindhard and Bezrukov parameterizations, respectively.

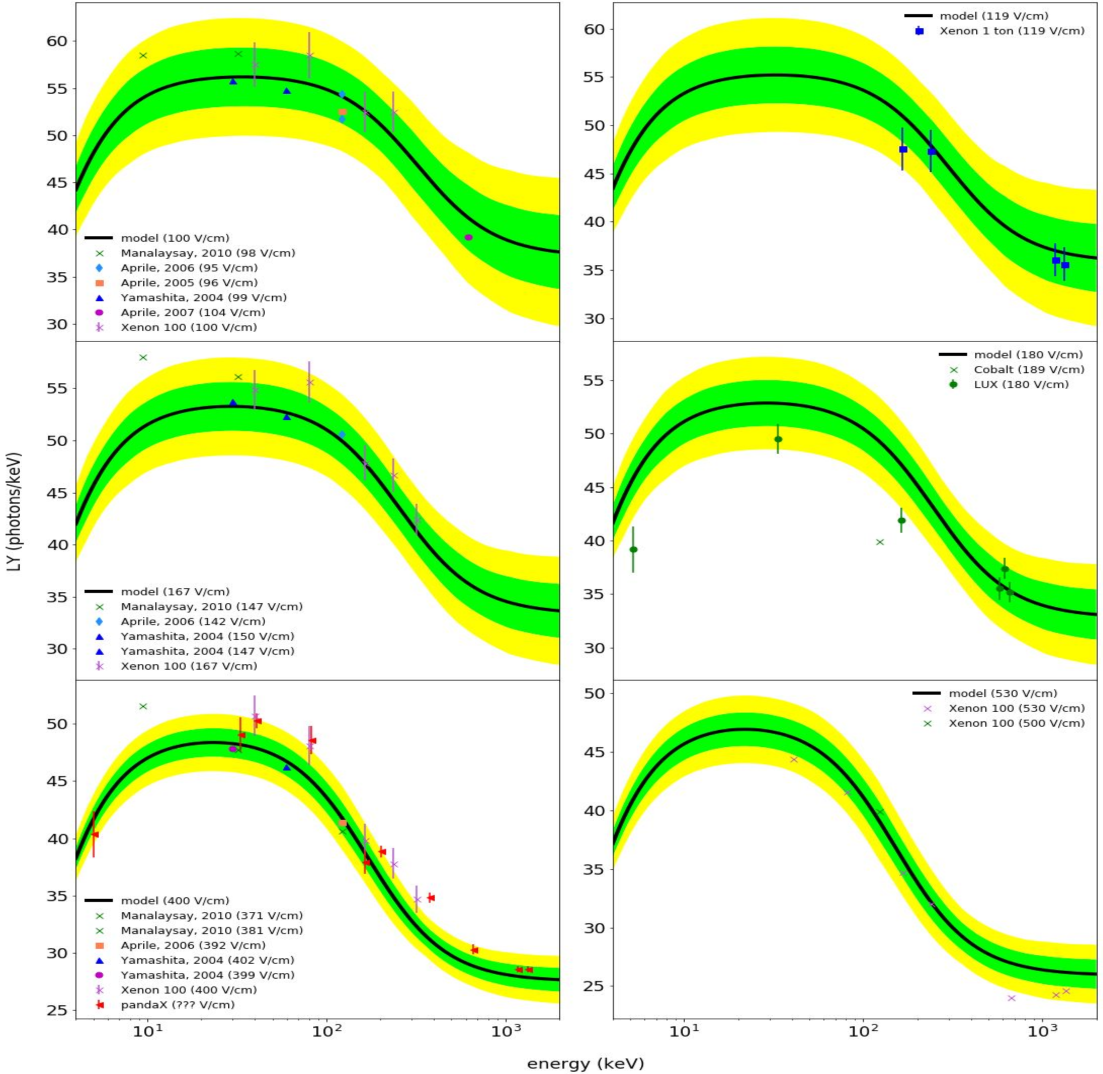


Improved Limits on Scattering of Weakly Interacting Massive Particles from Reanalysis of 2013 LUX Data
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Dec 10, 2015. 7 pp.
Published in **Phys.Rev.Lett. 116 (2016) no.16, 161301**

ER from γ-rays

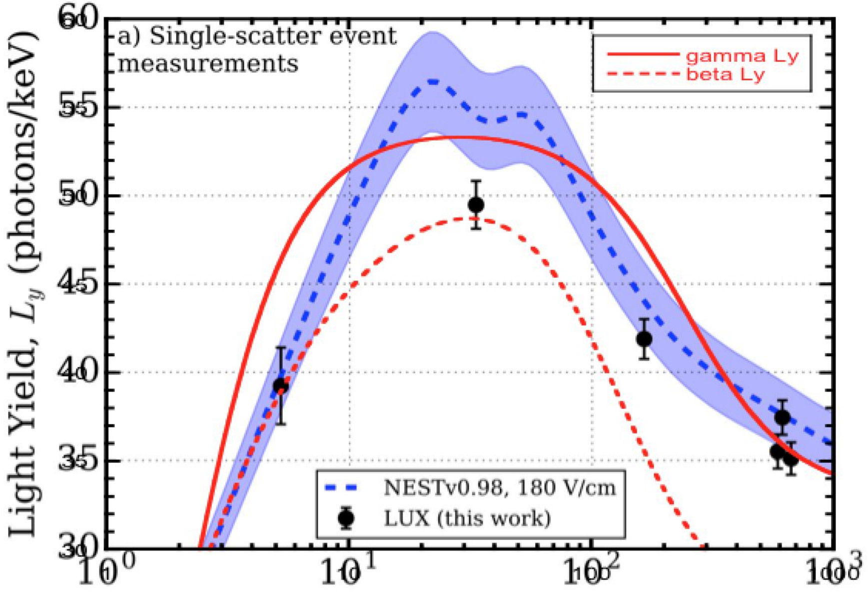
- γ ER different from β ER

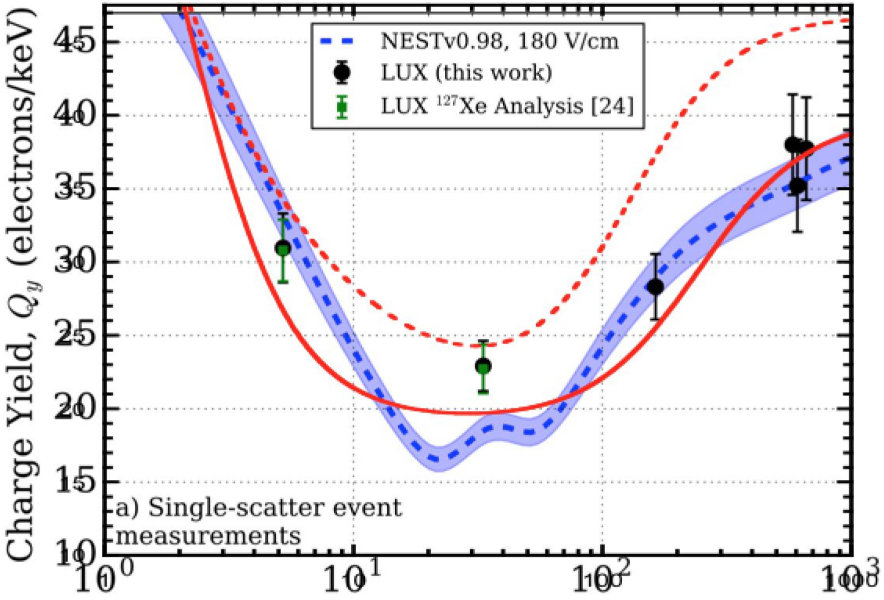
Error Bands are PRELIMINARY!



ER from γ-rays

- LUXRun3 (180V/cm), NEST in RED
- β-model does better at lower energies, γ-model matches high energies



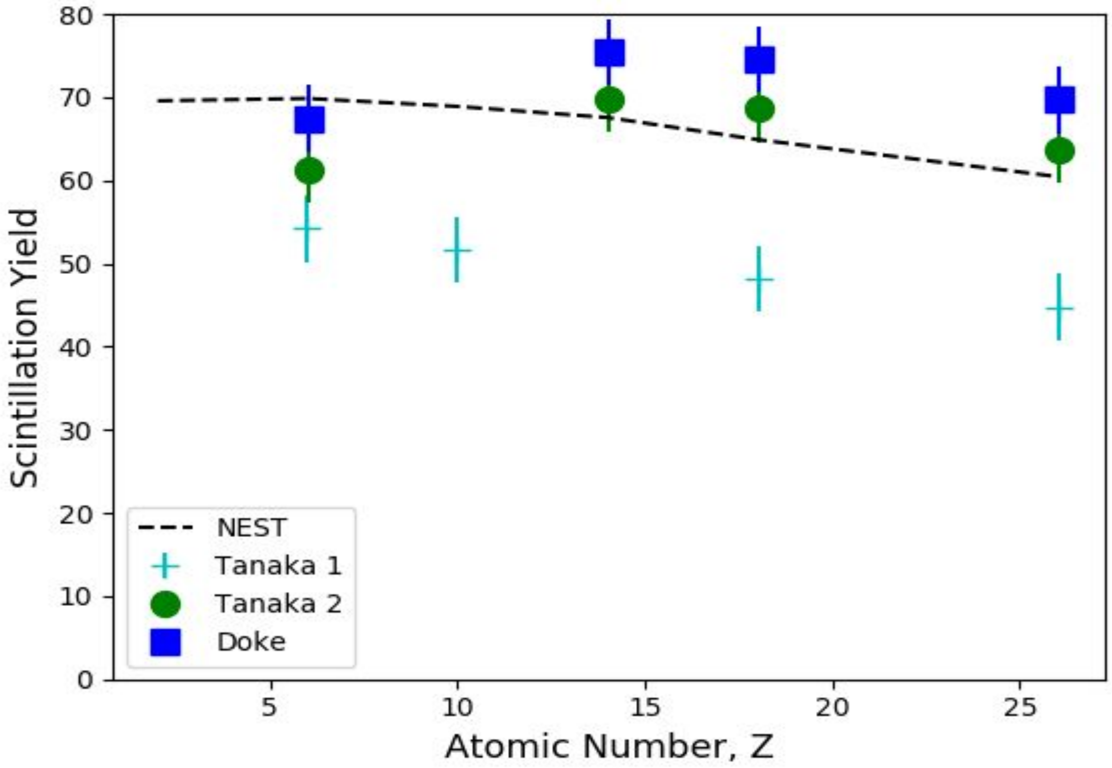


Heavy Nuclei

- Expanded the α-model to include scattering events with heavy ions
- Again, contradictory data sets, splits the difference

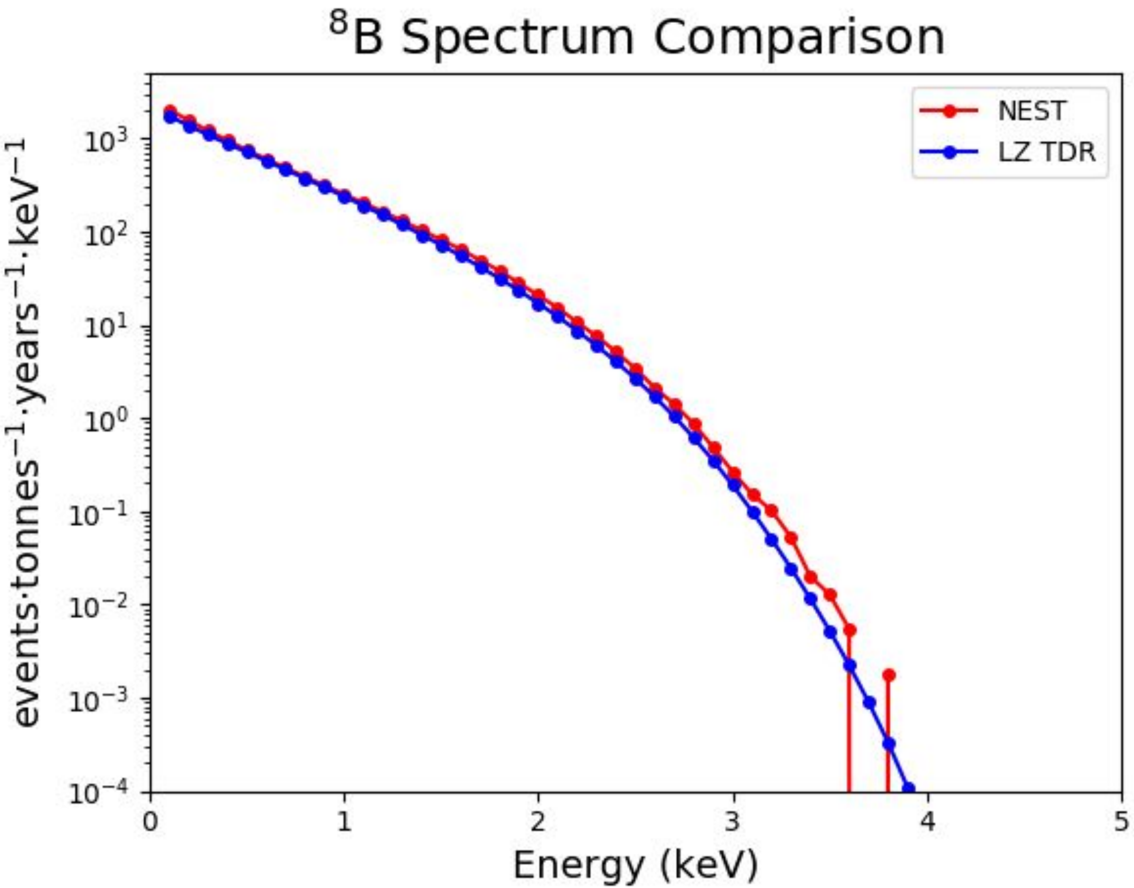
Absolute Scintillation Yields in Liquid Argon and Xenon for Various Particles
T. Doke, et. al. 2002.
Japanese Journal of Applied Physics, Volume 41, Part 1, Number 3A

LET dependence of scintillation yields in liquid xenon
M. Tanaka, et. al. 2001



Boron-8

- Great agreement with LZ TDR ^8B spectrum.
- Not a look-up table!



LUX-ZEPLIN (LZ) Technical Design Report
B.J. Mount (Black Hills State U.) *et al.*. Mar 27, 2017. 392 pp.
LBNL-1007256, FERMILAB-TM-2653-AE-E-PPD
e-Print: **arXiv:1703.09144 [physics.ins-det]**

Dark Matter in NESTv2

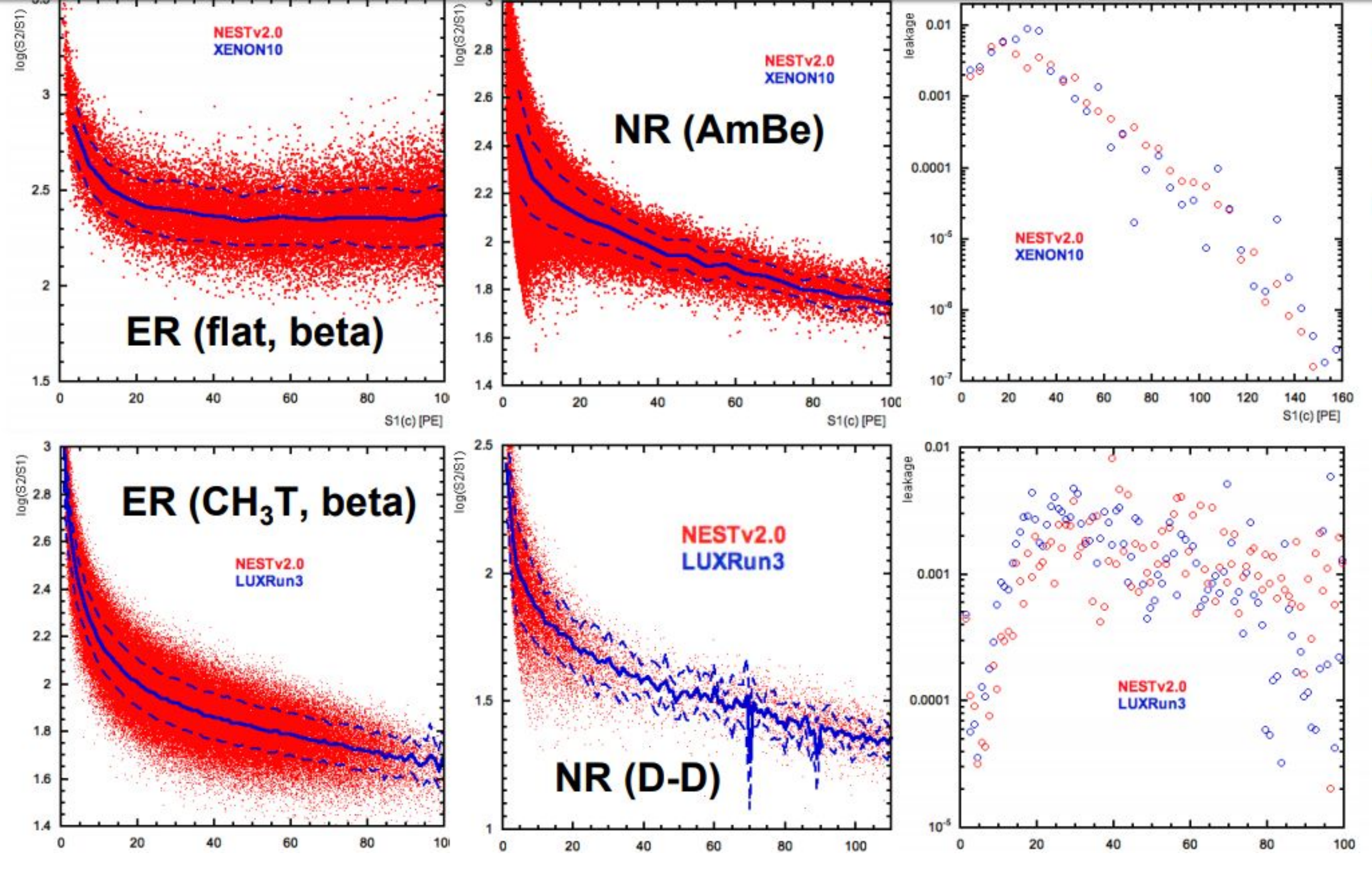
- Uses WIMP spectrum equations following methods described in 2010 publication by McCabe.

Astrophysical uncertainties of dark matter direct detection experiments. Christopher McCabe. Phys. Rev. D **82**, 023530 – Published 29 July 2010

- Trivial to add other species of DM to NEST thanks to modular setup in the code.

- I have plans to incorporate Nuclear Dark Matter spectra using equations starting from a 2016 paper from the Royal Holloway University of London.

Can Tonne-Scale Direct Detection Experiments Discover Nuclear Dark Matter?
A. Butcher, R. Kirk, J. Monroe, S.M. West (Royal Holloway, U. of London). Oct 6, 2016. 23 pp.
Published in **JCAP 1710 (2017) no.10, 035**



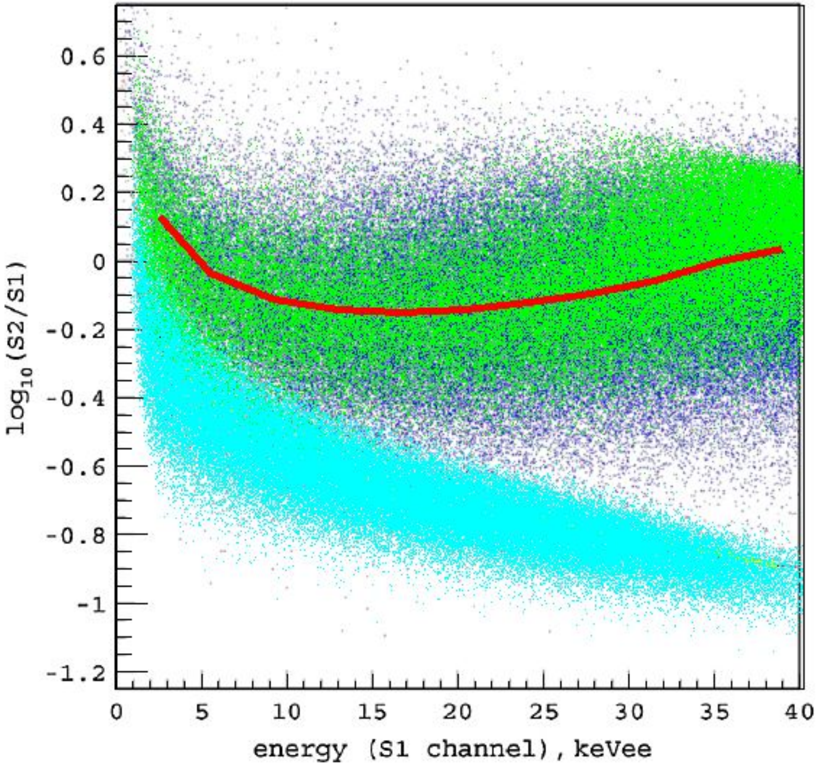
Going Full-Scale with Detector Effects

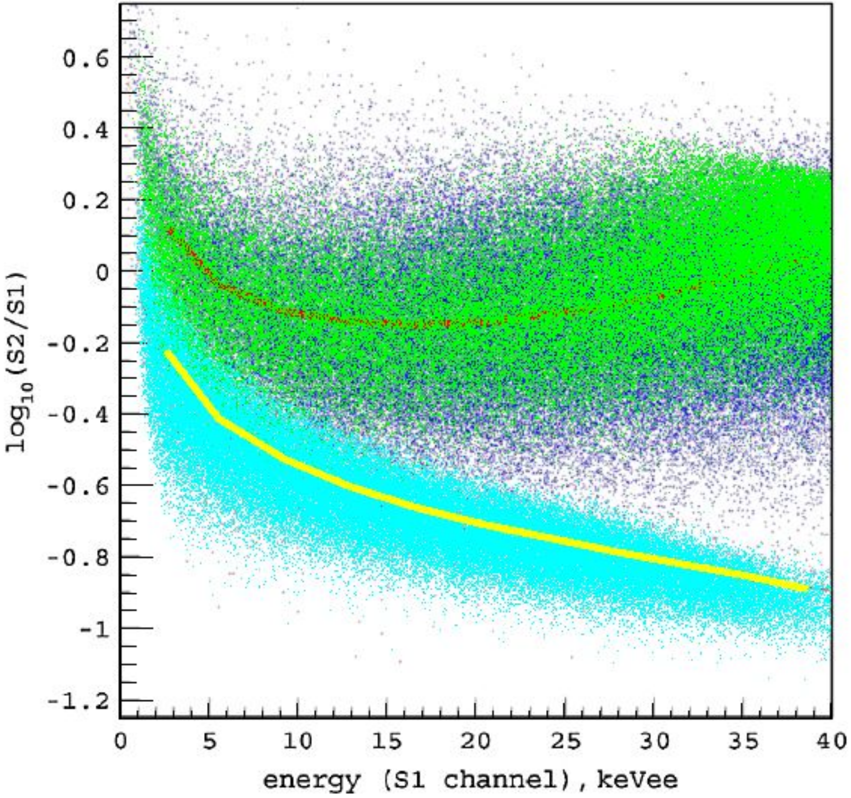
NESTv2 accurately reproduces NR and ER bands.

X10 detector file example provided with NESTv2. Easy to change and add your own detector!

ZEPLIN-III Resolution comparison

Light blue & yellow → AmBe data
Green, dark blue, and red → β data





Limits on the spin-dependent WIMP-nucleon cross-sections from the first science run of the ZEPLIN-III experiment

ZEPLIN-III Collaboration (V.N. Lebedenko (Imperial Coll., London) *et al.*). Jan 2009.

4 pp.

Published in **Phys.Rev.Lett. 103 (2009) 151302**