The Noble Element Simulation Technique:

What It Does, and Where It's Going, And What Can We Do Better?

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About NEST

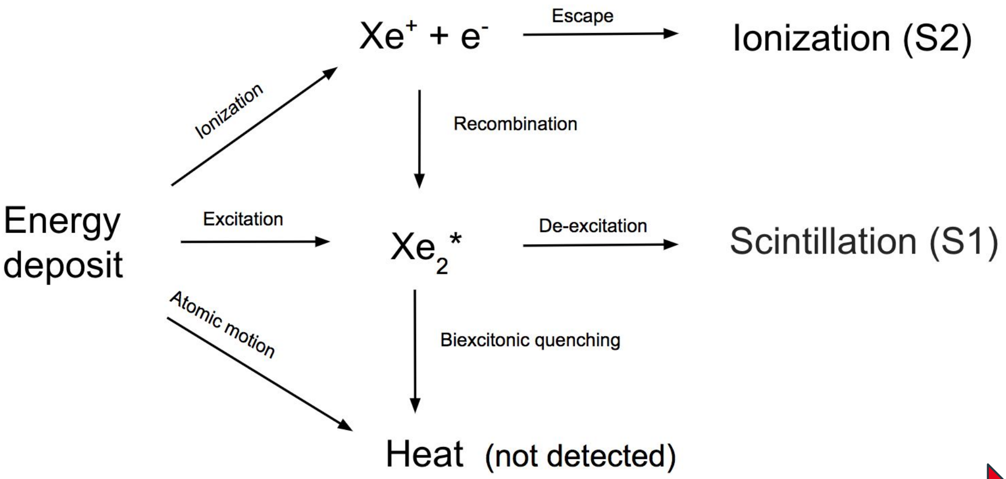
- nest.physics.ucdavis.edu & github.com/NESTCollaboration
- “Inter-collaboration” Collaboration
  - Members from LUX/LZ, XENON, DUNE, nEXO
- Fast, stand-alone C++ code with robust example executable, testNEST
  - Reproduces LXe scintillation and ionization response from most imaginable interaction types
  - Yields as a function of particle type, energy, field, density and target phase
  - Temperature, pressure, and density dependencies from NIST
  - Xenon only? Not for long! LAr models imminent!
- GEANT4 Integration
  - Takes energy depositions and returns light and charge yields
- Plenty of room for growth and upgrades!

The Whole Point:

Providing a Data-Driven Mapping from Observables to Fundamentals

Signal production in xenon

ORIGINAL INTERACTION

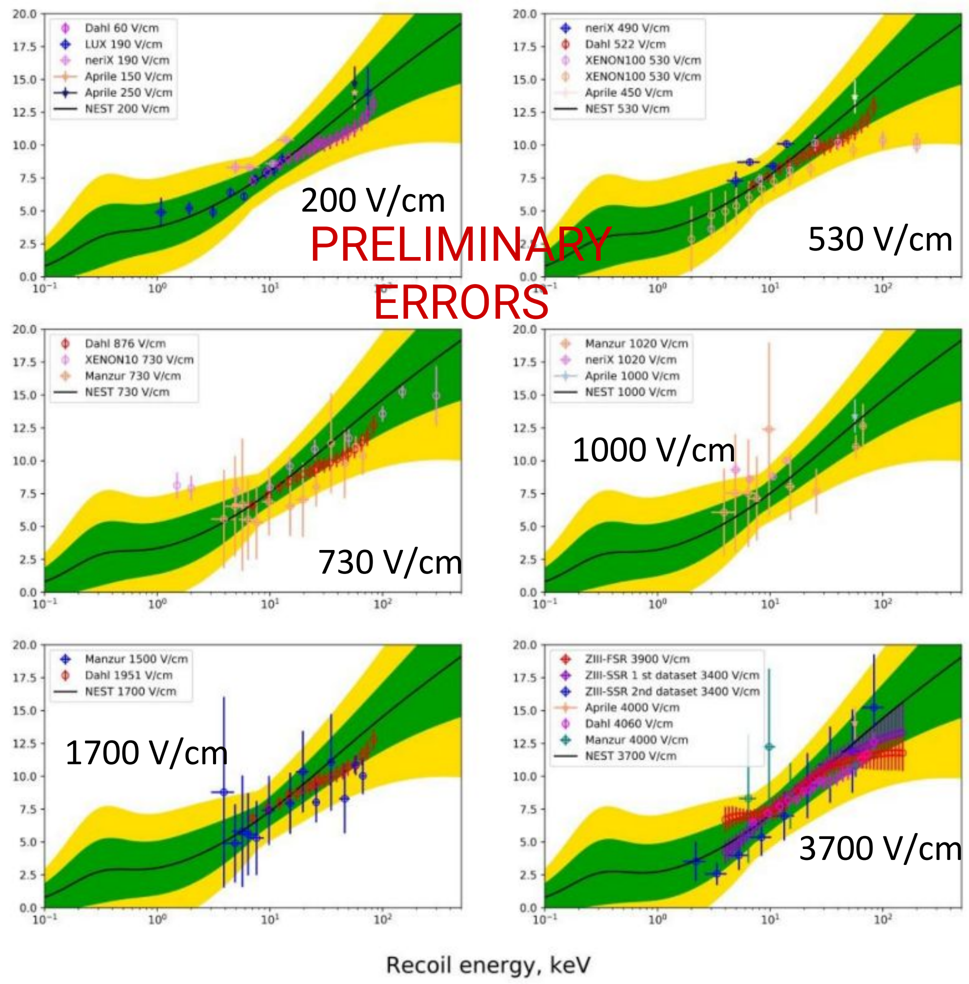


OBSERVABLES

NEST: What to Expect (from calibrations/backgrounds) →

← NEST: Explain what was Observed (Modeling Detector)

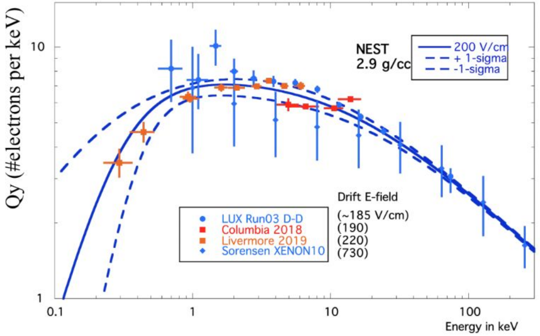
NEST: Where We Are Now



M. Szydagis. (NEST Collaboration) *A Comprehensive, Exhaustive, Complete Analysis of World LXe NR Data With a Final Model.* 2019.

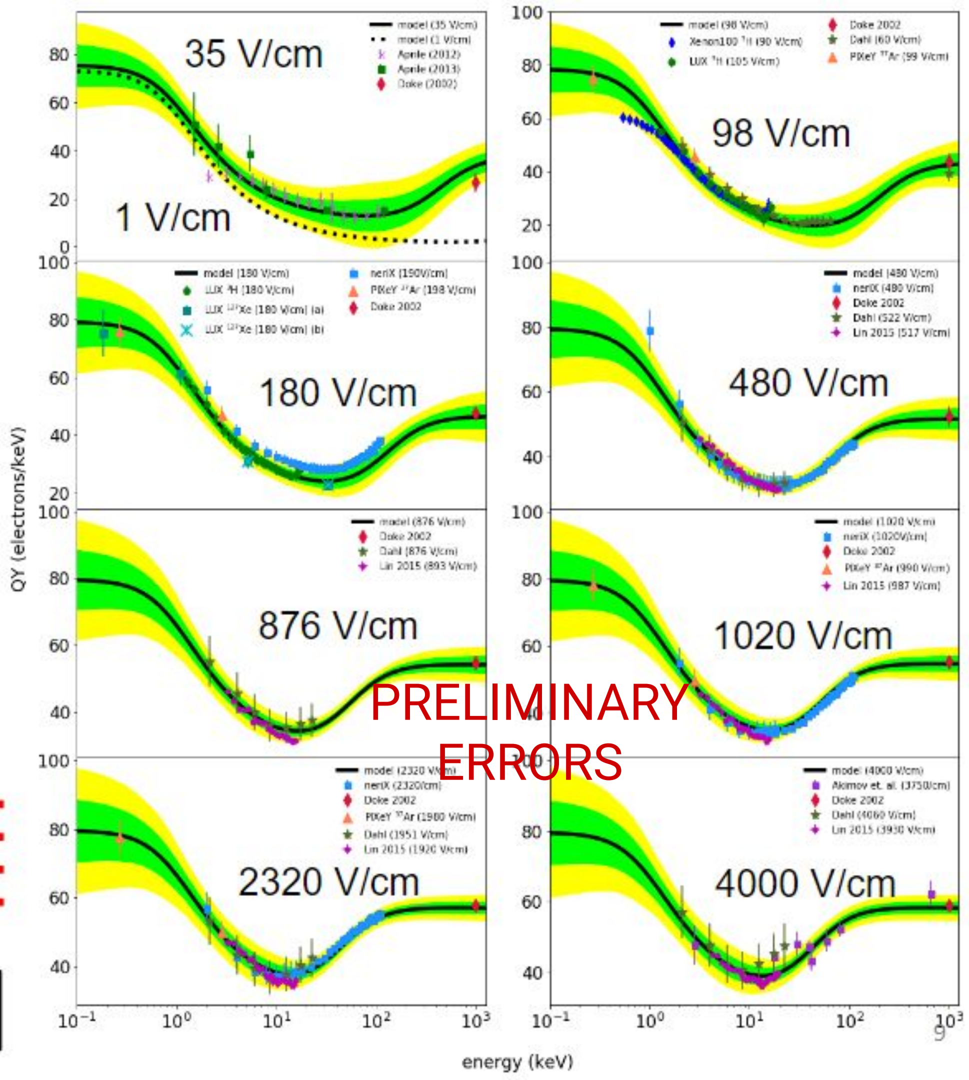
Nuclear Recoils

Recently Updated in NESTv2.0.1 !!



$$N_{e-} + N_\gamma = \frac{\mathcal{L} \cdot E}{W}$$

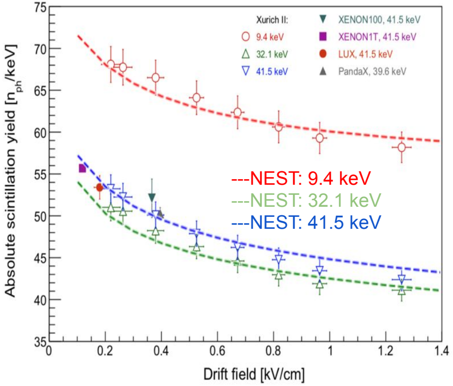
- Procedure:
  - Collect world data; correct for newly understood phenomena; fit functions of field and energy to reproduce data
- Light Yields (photons/keV) shown, similar treatment for Charge Yields
  - Plot by E. Kozlova
- Detailed report available on NEST Website



β Electronic Recoils

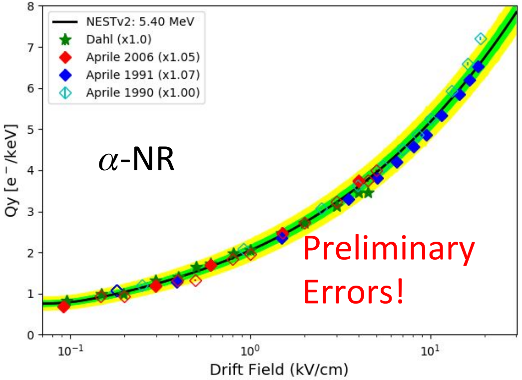
- $$N_{e-} + N_{\gamma} = \frac{E}{W}$$
- Same Procedure as NR, with anti-correlated light and charge yields
- Charge Yields (electrons/keV) shown
  - Plot by J. Balajthy
- Also a good approximation of Compton Scatter data
  - ^{137}Cs Compton Scatters included in fit
- Covers out to MeV range for $0\nu\beta\beta$ decay searches

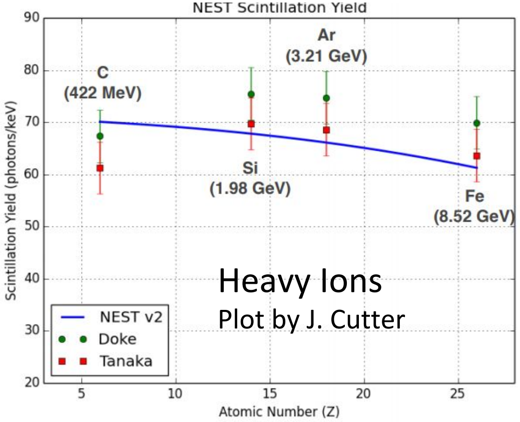
Even More!

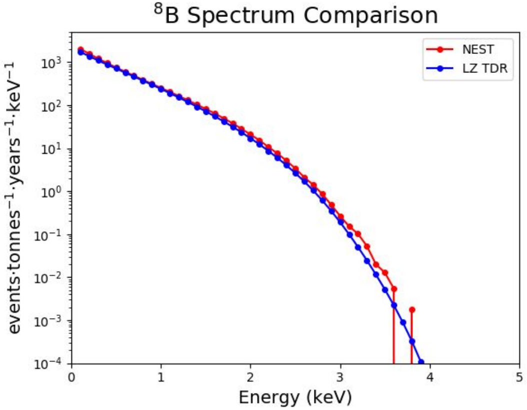


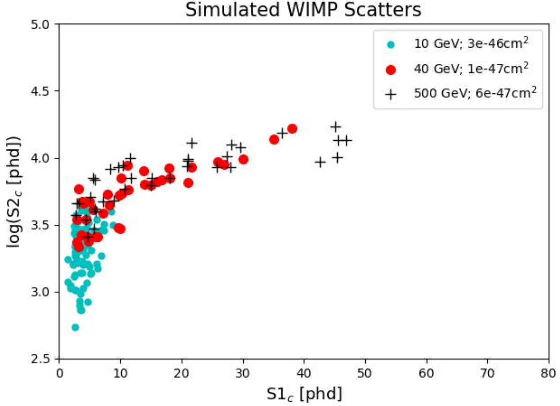
Photoabsorption ER from γ's

Special-case ^{83m}Kr Model with robust time-dependence





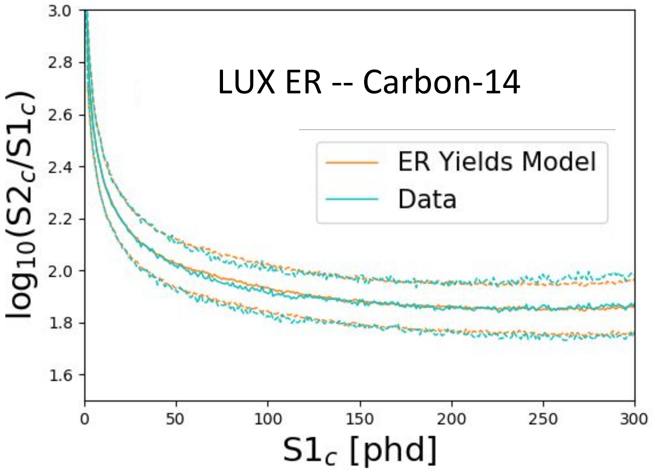


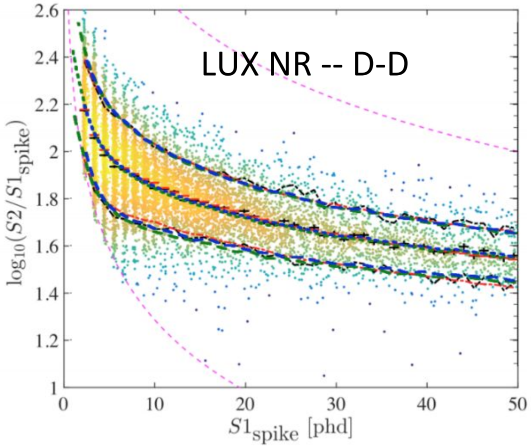


J. Cutter. (NEST Collaboration). *Heavy Ions and Generalized Nuclear Recoils in Xenon with NEST v2.0*. 2019.

Projected WIMP Sensitivity of the LUX-ZEPLIN (LZ) Dark Matter Experiment
LUX-ZEPLIN Collaboration (D.S. Akerib (SLAC & KIPAC, Menlo Park) *et al.*). Feb 16, 2018.

Complete with Detector Modeling

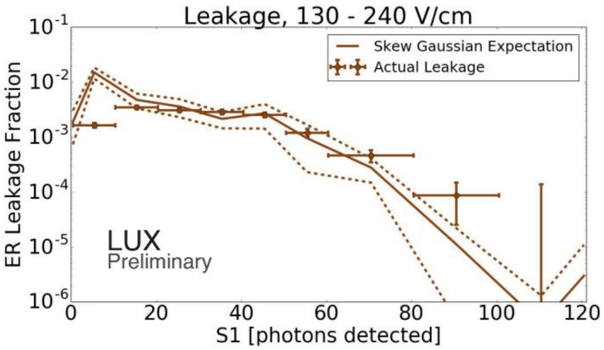




Improved Modeling of β Electronic Recoils in Liquid Xenon Using LUX Calibration Data
LUX Collaboration (D.S. Akerib *et al.*). Oct 9, 2019. 17 pp.
e-Print: **arXiv:1910.04211 [physics.ins-det]**

M. Szydagis. (NEST Collaboration) *A Comprehensive, Exhaustive, Complete Analysis of World LXe NR Data With a Final Model.* 2019.

V. Velan. ***Projected Performance of Future Liquid Xenon Detectors***. Presentation, APS April 14, 2019.



Calculates fluctuations about the mean yields (statistical and recombination fluctuations!)

Accurately simulates ER “leakage” into NR band

Can add in custom detector files to simulate your own detector

nestpy → github.com:NESTCollaboration/nestpy

Not a fan of C++? No Problem!

Thanks to pybind11, you can happily enjoy all of NEST's offerings in your favorite python environment

nestpy

gitter join chat | build passing | DOI 10.5281/zenodo.3360721 | pypi v1.1.3 | repo status Active | python 2.7 | 3.4 | 3.5 | 3.6 | 3.7

These are the Python bindings for the NEST library, which provides a direct wrapping of functionality. The library is not Pythonic at this point but just uses the existing naming conventions from the C++ library.

You do *not* have to have NEST already installed to use this package.

Installing from PyPI

For 64-bit Linux or Mac systems, instally 'nestpy' should just require running:

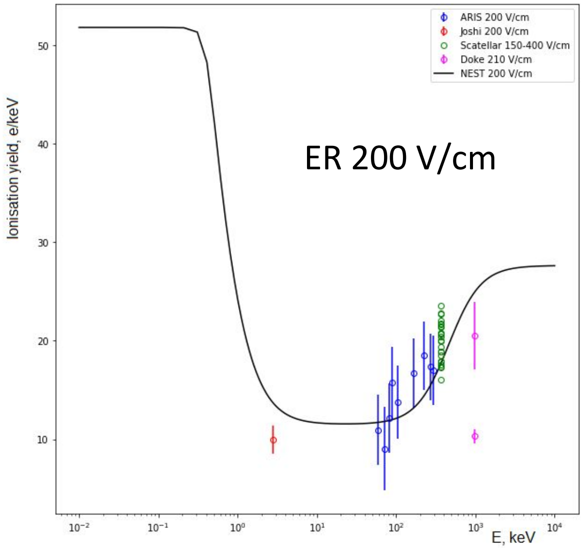
```
pip install nestpy
```

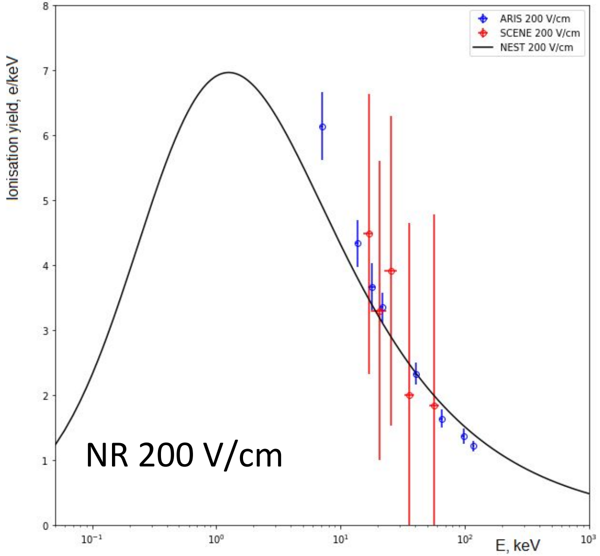
Where NEST is Headed...

Plans for the Future

Updated LAr Models Under Development

Plots by J. Mueller and E. Kozlova





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 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**

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**

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**

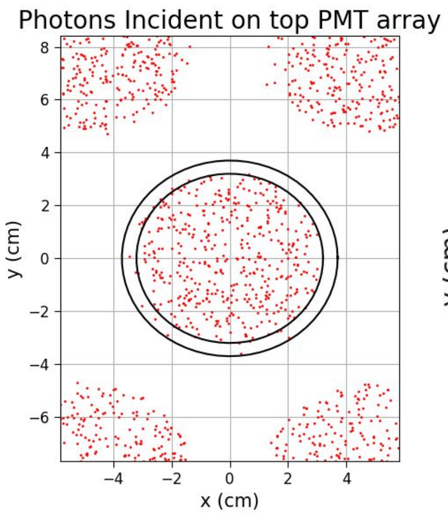
Critical test of geminate recombination in liquid argon R. T. Scaltettar, P. J. Doe, H. -J. Mahler, and H. H. Chen.
Phys. Rev. A 25, 2419(R) – Published 1 April 1982

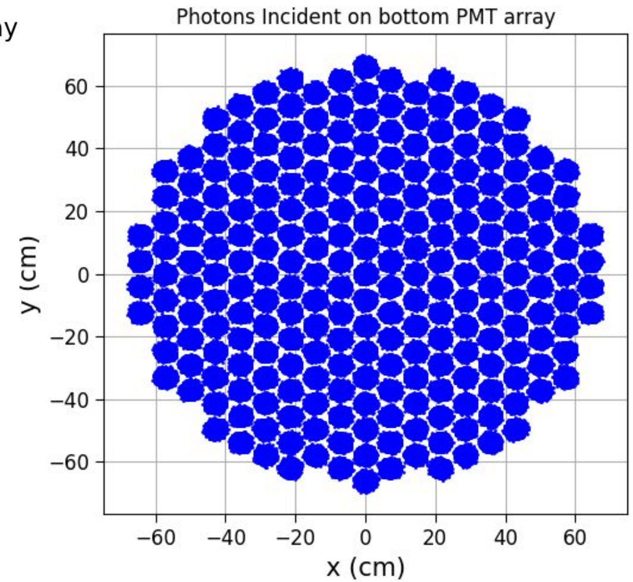
X-ray ionization yields and energy spectra in liquid argon
A. Bondar, A. Buzulutskov, A. Dolgov, L. Shekhtman, A. Sokolov.
May 9, 2015. 6 pp.
Published in **Nucl.Instrum.Meth. A816 (2016) 119-124**

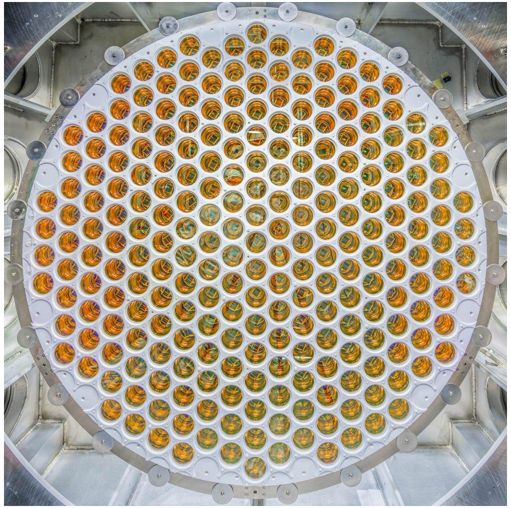
Surface-based Ray-tracing with *NEST-light*

Fast and efficient optical simulations!

Attempting to accurately reproduce S1 and S2 hit patterns by properly modeling reflection, absorption, and refraction using detailed detector geometry for cylindrical two-phased TPCs





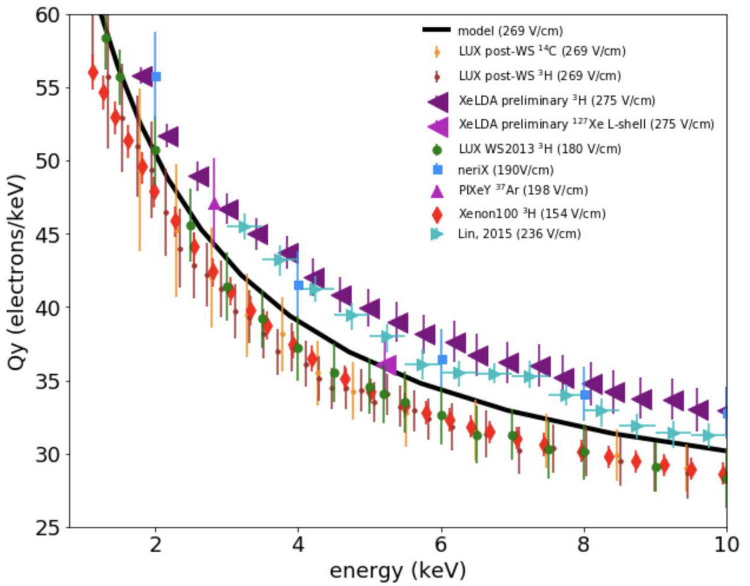


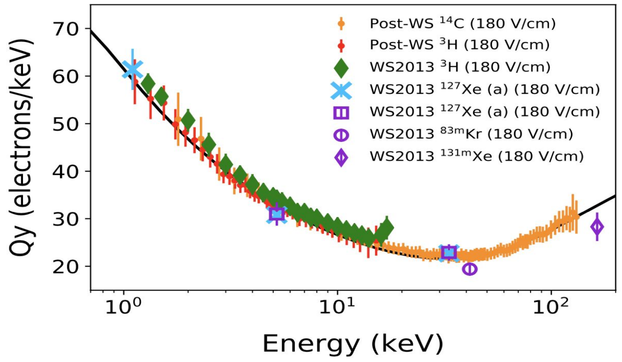
State of the ER Union:

Can Yields from β, Compton Scatters, and Electron Capture Remain Unified in a Single Model?

As more data become available, it will become clear if the different ER-producing mechanisms require separate yield models

Compton/β likely to remain unified, but perhaps inner-shell electron captures require a unique model





Plots by J. Balajthy

Preliminary XeLDA data from D. Temples. *Understanding neutrino background implications in LXe-TPC dark matter searches using 127Xe electron captures.* Oral Presentation. TAUP 2019.

Plans for Moving Towards v3?

- First-principles model
  - Can Molecular Dynamics be used to properly and efficiently model the scintillation and ionization response of Noble targets?
  - Incorporate Van der Waals forces and Lennard-Jones Potentials
  - 1st principles approach provides signal and background information where calibrations cannot
- Machine Learning
  - Optimized position and energy reconstruction of energy depositions using neural networks
  - NEST allows training where calibrations cannot -- homogenous NR (more signal-like) as opposed to calibrations that are near detector edge, and more BG-like ER

Where Do We Need To Improve?

1. Increased Usability
    a. More documentation, helping to flush out the full capabilities of the simulation package
    b. Dividing the code into more step-by-step calculations, showing the user where/how NEST calculates certain quantities and allowing for easier user-manipulation
2. How Do We Optimize Model Fitting?
    a. Currently, model fitting is a very manual process
    b. Higher-dimensional optimization ⟶ Application to use machine learning methods
    c. This would provide an easier way of defining the likelihood of model parameters
3. These things are limited by funding and human-power

But what does the community want from NEST? How do those from differing collaborations use NEST?

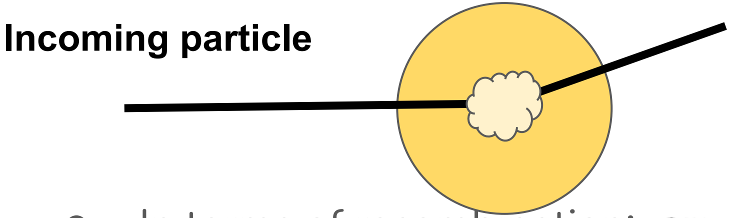
Conclusion

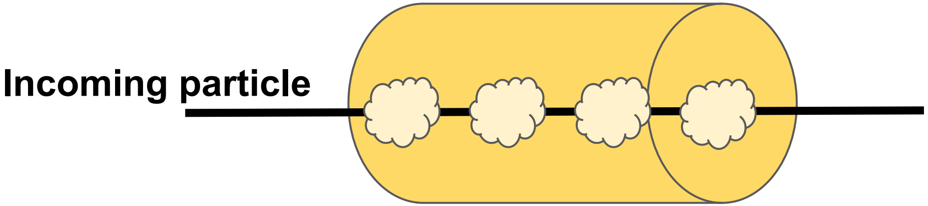
- NEST v2 is an efficient and robust calculation that is ready to use for your xenon detector (And argon detectors soon)
- NEST has a very large potential for growth
  - Amount of available data will only increase, making NEST more accurate as time goes on, and will include more features
- For growth to be successful, NEST needs:
  - Support! Whether that means funding or just more collaborators, time and money are always the largest limiting factors
  - Community Input! NEST is designed for the entire community, not just a single experiment. Understanding the most pressing simulation/modeling needs in other collaborations will help make NEST even more applicable

Thank You!

LEAVING: Main Presentation
ENTERING: Backup Slides

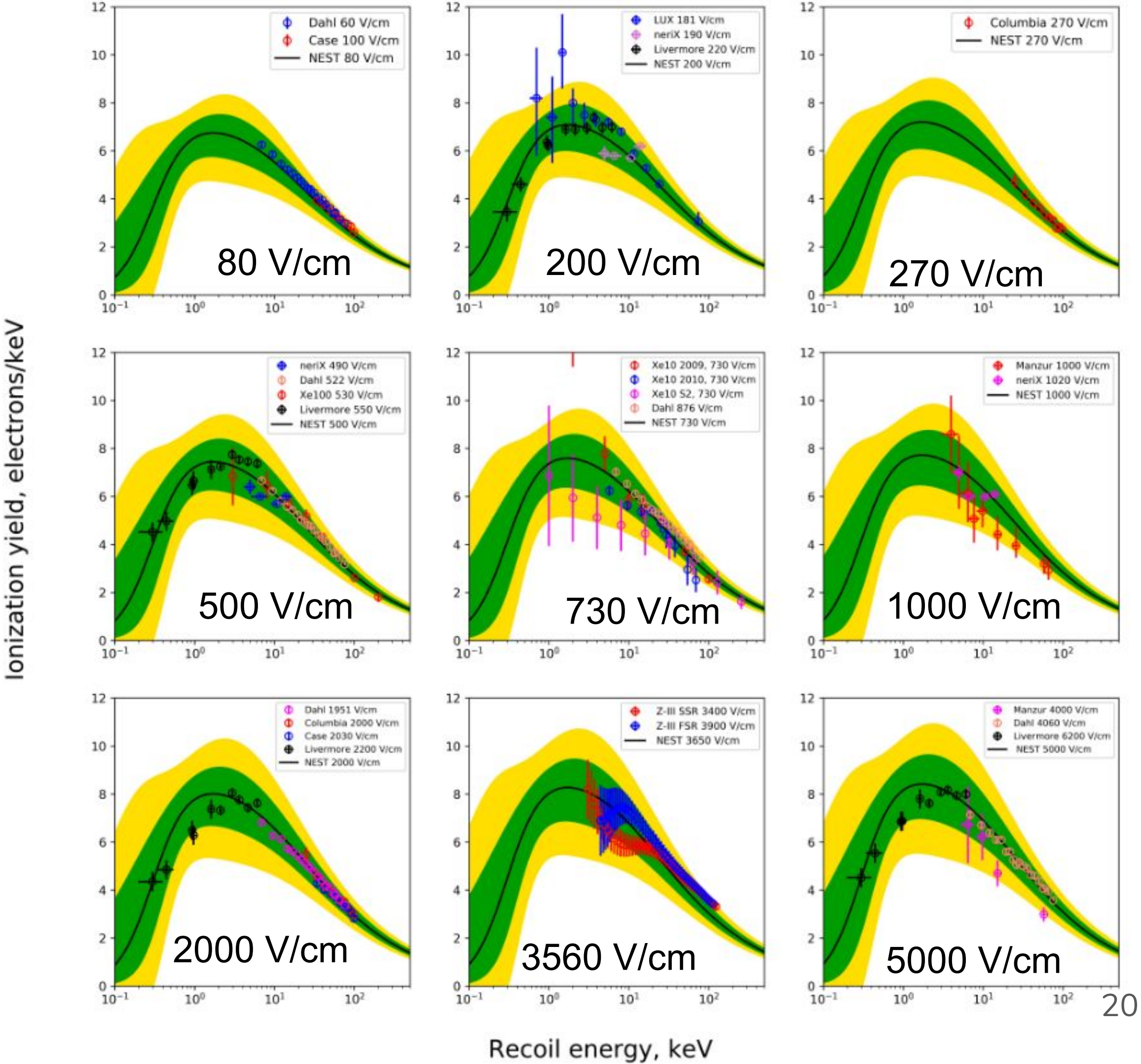
Previous Yield Models: Thomas-Imel vs. Doke-Birks





- 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 → 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 → 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: $QY \approx 26.7 + 0.12\Delta E - 0.0005\Delta E^2 + \mathcal{O}(\Delta E^3)$

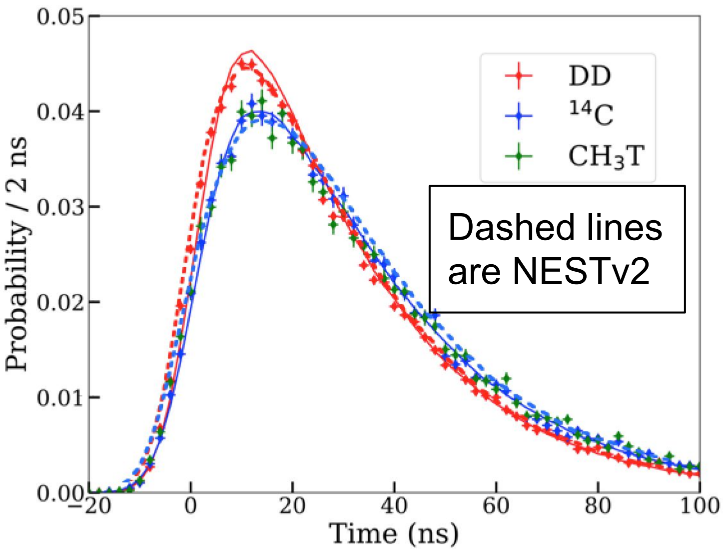
NR Charge Yields Fit to World Data

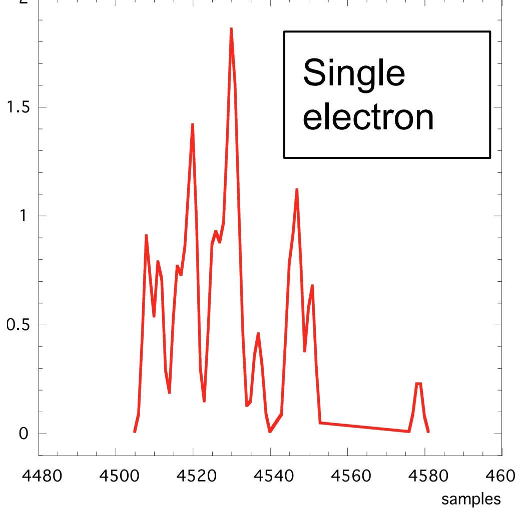


M. Szydagis. (NEST Collaboration) *A Comprehensive, Exhaustive, Complete Analysis of World LXe NR Data With a Final Model.* 2019.

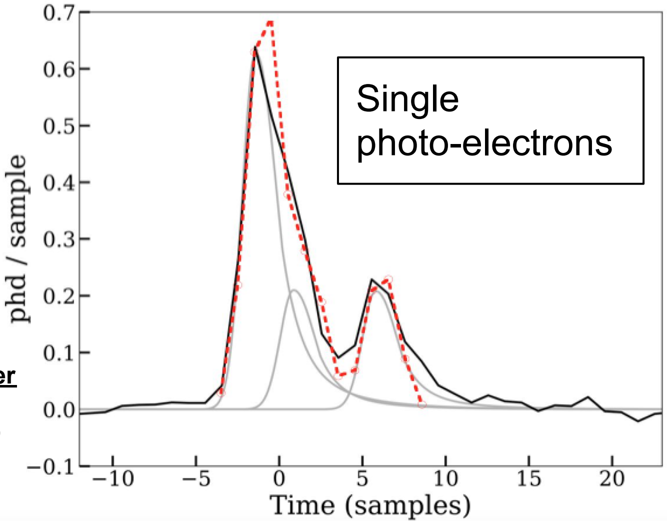
Pulse Shapes

- 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**

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

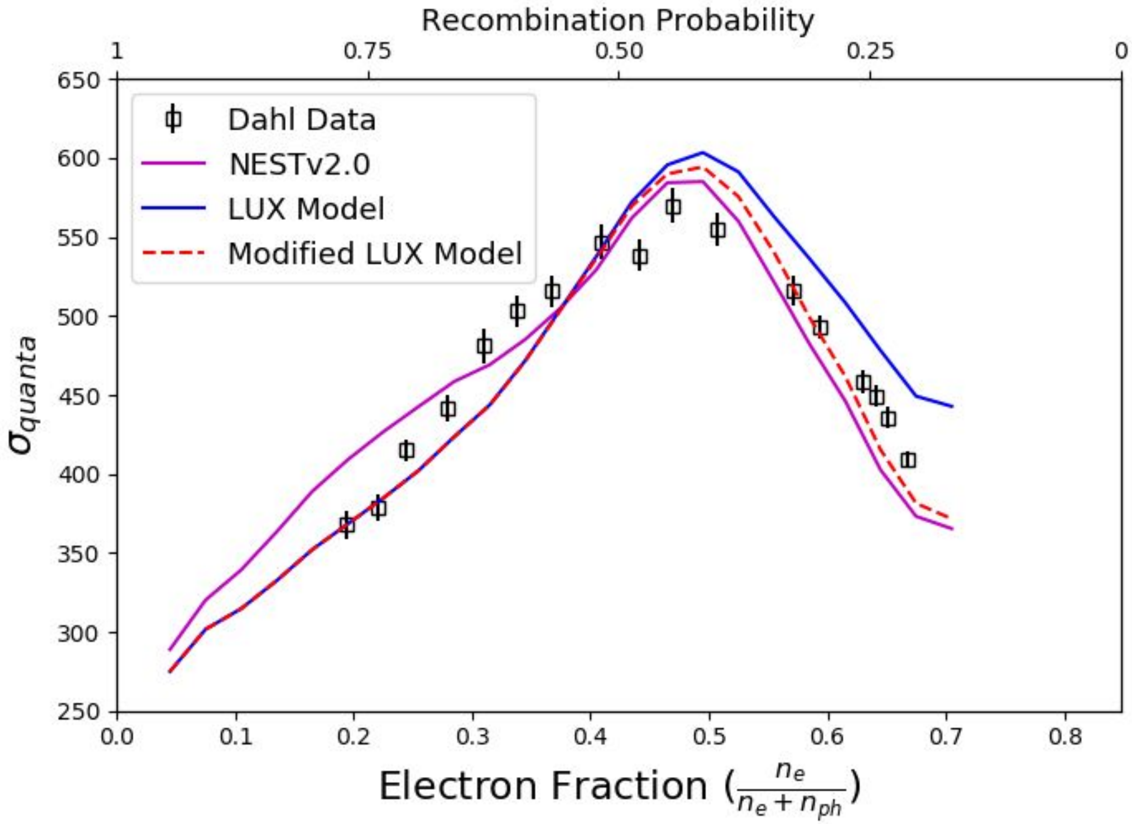
Signal yields, energy resolution, and recombination fluctuations in liquid xenon
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Oct 6, 2016. 12 pp.
Published in **Phys.Rev. D95 (2017) no.1, 012008**
DOI: 10.1103/PhysRevD.95.012008

Recombination Fluctuations

- Comparing to Eric Dahl's PhD thesis data

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

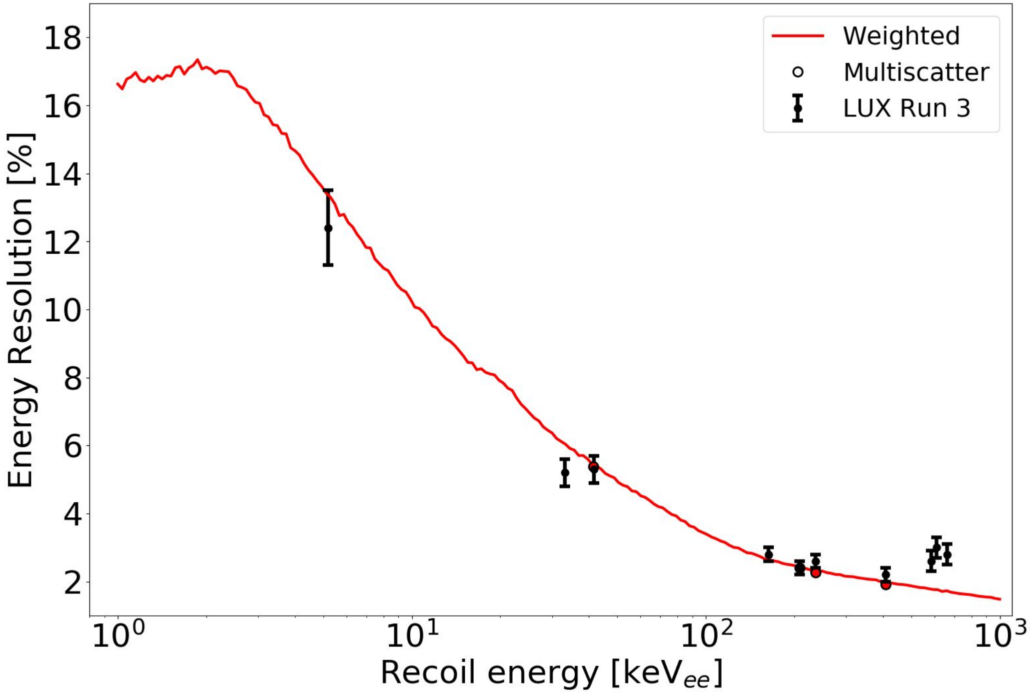
Improved Modeling of β Electronic Recoils in Liquid Xenon Using LUX Calibration Data
LUX Collaboration (D.S. Akerib *et al.*). Oct 9, 2019. 17 pp.
e-Print: **arXiv:1910.04211 [physics.ins-det]**



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

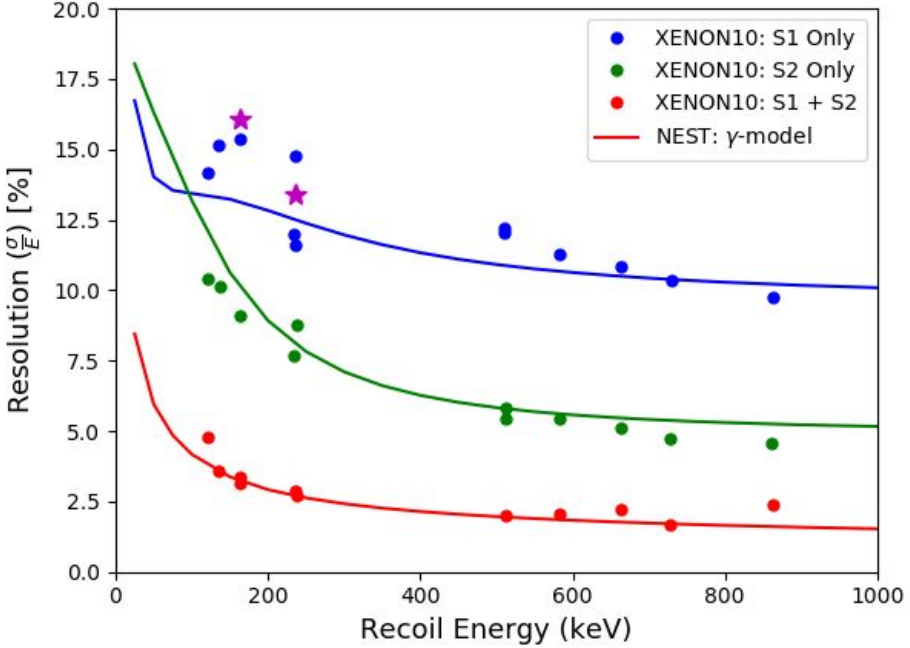


Signal yields, energy resolution, and recombination fluctuations in liquid xenon
LUX Collaboration (D.S. Akerib (Case Western Reserve U. & SLAC & KIPAC, Menlo Park) *et al.*). Oct 6, 2016. 12 pp.
Published in **Phys.Rev. D95 (2017) no.1, 012008**
DOI: 10.1103/PhysRevD.95.012008

Energy Resolution: XENON10

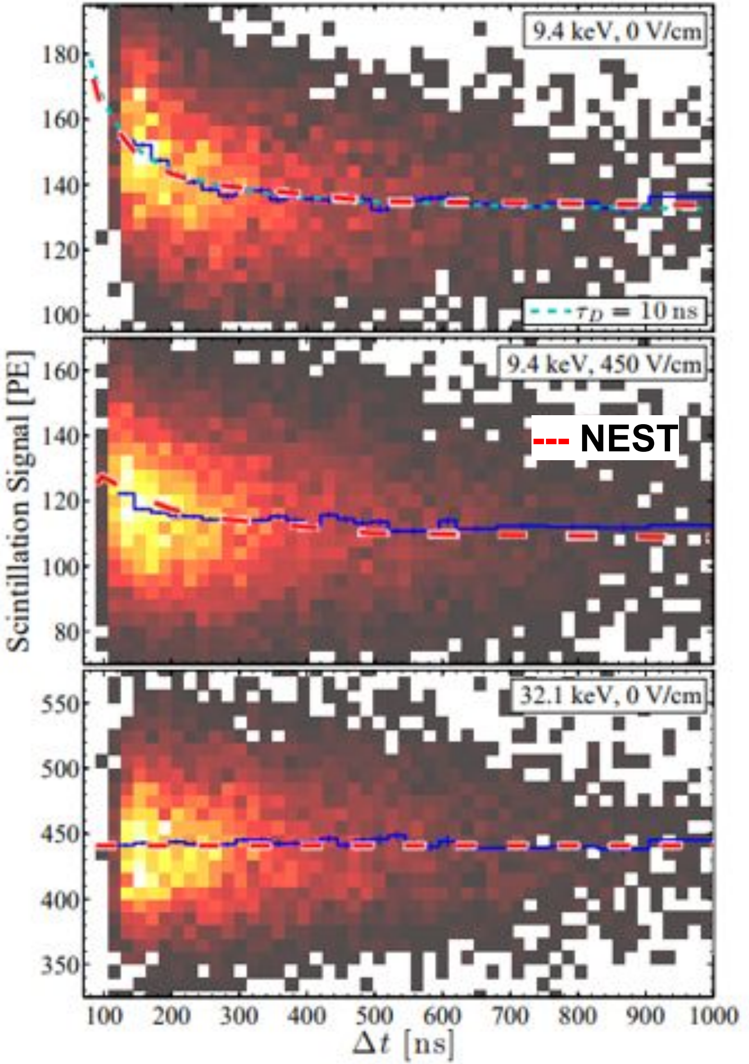
arXiv.org:1001.2834

- 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



Scintillation Signal v. Time

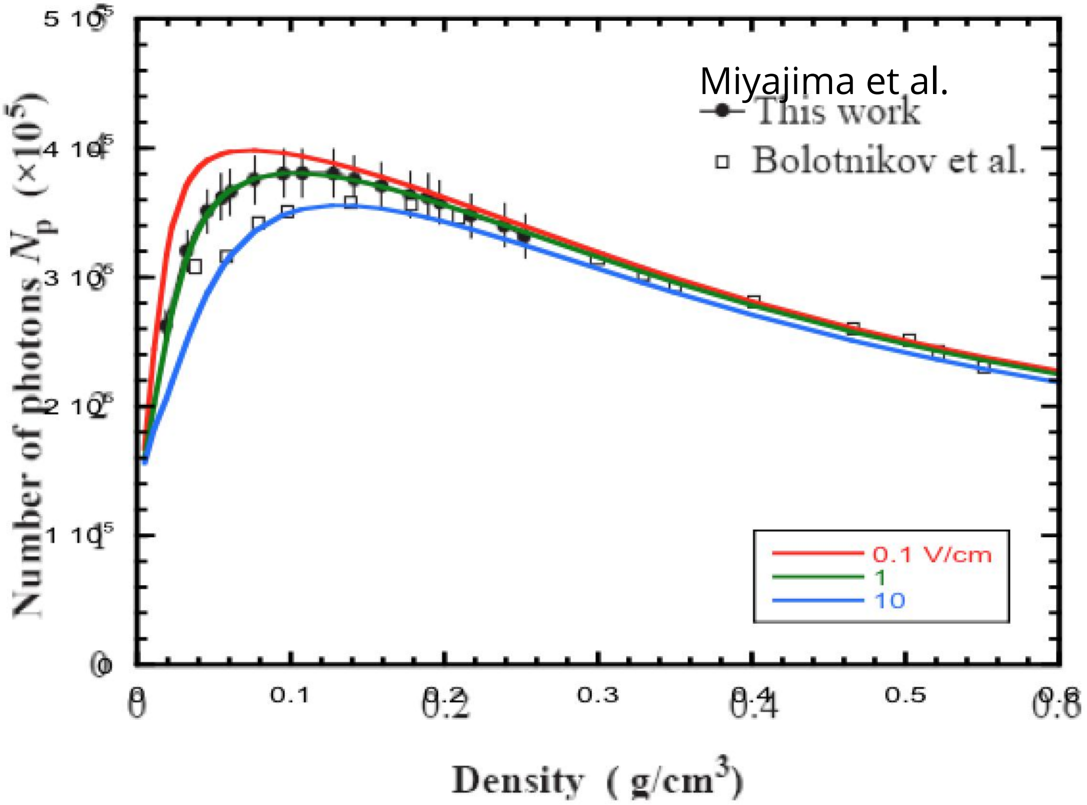
Kr83m data suggests that the total light yield from the 9.4 keV decay has a slight time dependence



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**

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

ER in GXe

density (g/cc)	keVee	W_sc (eV)	NEST W_sc (eV)
0.08	662	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

ER from γ-rays

- γ ER different from β ER

Error Bands are PRELIMINARY!