

Get the full code here, from GitHub: <https://github.com/NESTCollaboration/nest>

NEST, or, the Noble Element Simulation Technique

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HSF Detector Simulation WG Meeting March 8, 2021

Outline

1. What is NEST?

- a. What can it simulate?
- b. Institutions

2. Microphysics Basis

- a. Equation Examples: Mean Yields
- b. Example of Widths

3. Mean Yields

- a. Liquid Xe NR (Nuclear Recoil) total
- b. Liquid Ar NR
- c. Breakdown into Light and Charge Yields, first for LXe, then LAr
- d. Comparison of NR to ER (Electron Recoil)

4. Pulse Shapes

5. Timing

6. Software Tools

7. Applications

8. More Comparisons with Actual Data

- a. Energy Resolution versus Energy
- b. Low-Energy ER peaks in LXe, LAr
- c. Efficiency and Threshold
- d. Leakage of background into signal region

9. Future Work

10. Conclusions

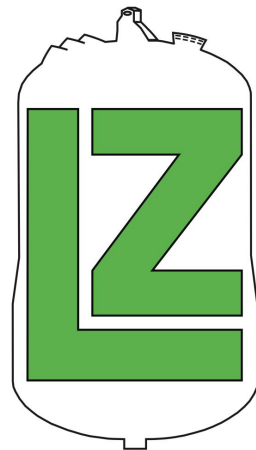
11. References

What is NEST? Benefits

- Noble Element Simulation Technique: it's neutral / impartial, open source
- A non-partisan, inter-collaboration collaboration (similar to G4 collab)
- Name also of software, which does LXe, GXe, SXe; LAr (preliminary testing)
- Primary parameters: particle or interaction type, E-fields, density or phase, and energy or dE/dx (latter more critical for MeV to GeV scale energies: ER)
- Using it means reducing your systematics by relying not only on your own calibration data, but upon all of those who came before you. One can stop reinventing the wheel, with “NEST-like” but private / secret software
- Integrated into Geant4 and Garfield++. Other languages: ROOT, Python

Who is on NEST; Also, Who Uses It?

- Has reps from XENON1T/nT/DARWIN, LUX/LZ, (n)EXO, RED, DUNE, SBN, MicroBooNE, COHERENT, and CENNS!



- Users from PandaX and DEAP as well to a degree



- Hoping to get more on board, like: NEXT for GXe, Darkside for LAr



And, What Can It Simulate? Outputs

- MC capabilities: growing all the time, with multiple options like G4 (processes)
- Mean scintillation light and ionization (charge) yields versus parameters earlier
- Energy resolution: the width in those yields, and their skewness
- BG discrimination: leakage of events into signal region, *e.g.* in a WIMP search
- Pulse timing profiles, including widths and general shapes: both primary and secondary scintillation. Based on G4Scintillation class, except does ionization
- Built-in calculation of the efficiency or threshold, and the $\log(S2)$ or $S2/S1$ band means & widths
- Basic spin-independent and spin-dependent WIMP limit calculator (Feldman-Cousins)
- Detector effects like photon detection $< 100\%$, on top of detector-independent aspects like yields
- Noise: correlated, anti-correlated, and uncorrelated sources all simulated now

The Institutions Represented Right Now on



nest.physics.ucdavis.edu



UNIVERSITY AT ALBANY
State University of New York (me!)

UC DAVIS



Rensselaer

Berkeley
UNIVERSITY OF CALIFORNIA



ITEP



RICE



Lawrence Livermore
National Laboratory

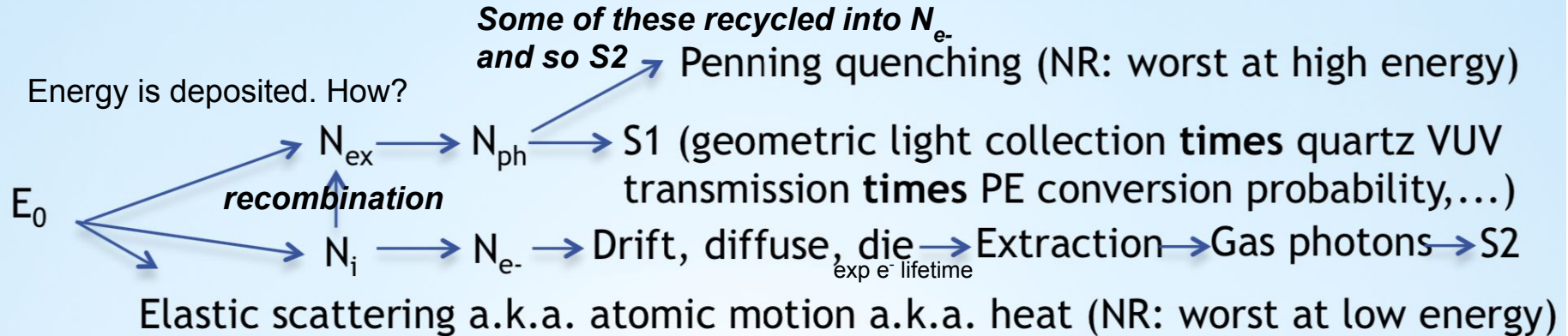
Unfunded, but still
REAL collaboration!

UC San Diego

Colorado
State
University



The Microphysics of Energy Partitioning: It is Not Trivial!



- Chain reaction set off by 1 NR (nuclear recoil) or 1 ER (electron recoil) leads to many NRs and ERs, with 3 primary processes occurring
 - Elastic (“billiard-ball”) scattering or inelastic: electron excitation and ionization
- Almost every arrow above is energy dependent and many electric field dependent
- NEST also comes with all the trimmings: for instance, e^- drift speed & diffusion
 - Singlet/triplet t 's considered, not ignored as in above simplified diagram. Also, extraction efficiency

Example Equations: for Low-Energy NR Light/Charge Yields

- Threading the needle - between fully theoretical and fully empirical

$$N_q = \alpha E^\beta, \alpha = 11_{-0.5}^{+2.0} \text{ and } \beta = 1.1 \pm 0.05; \quad L \equiv \frac{N_q}{E} W, \quad W \sim 13.7 \text{ eV}$$

- Advantages of the NEST approach

[A Comprehensive, Exhaustive, Complete Analysis of World LXe NR Data With a Final Model](#)

- “Follow the data” fails by itself: systematic errors, like uncorrected Eddington biases in past results. Also, can only interpolate
- “Follow the theories” fails because which one? Everything breaks down at low enough energies like the famous Lindhard model for example. But can extrapolate

$$TIB = \gamma \mathcal{E}^\delta \left(\frac{\rho}{\rho_0} \right)^{0.3}, \gamma = 0.0480 \pm 0.0021 \text{ and } \delta = -0.0533 \pm 0.0068$$

$$N_{e^-} = \frac{E}{TIB \sqrt{E + \epsilon}} \left(1 - \frac{1}{1 + \left(\frac{E}{\zeta} \right)^\eta} \right)$$

- Provide end users good defaults, but also great flexibility. NEST is not just the Gospel-Truth answers any longer

$$\epsilon = 12.6_{-2.9}^{+3.4} \text{ keV and } \zeta = 0.3 \pm 0.1 \text{ keV and } \eta = 2 \pm 1$$

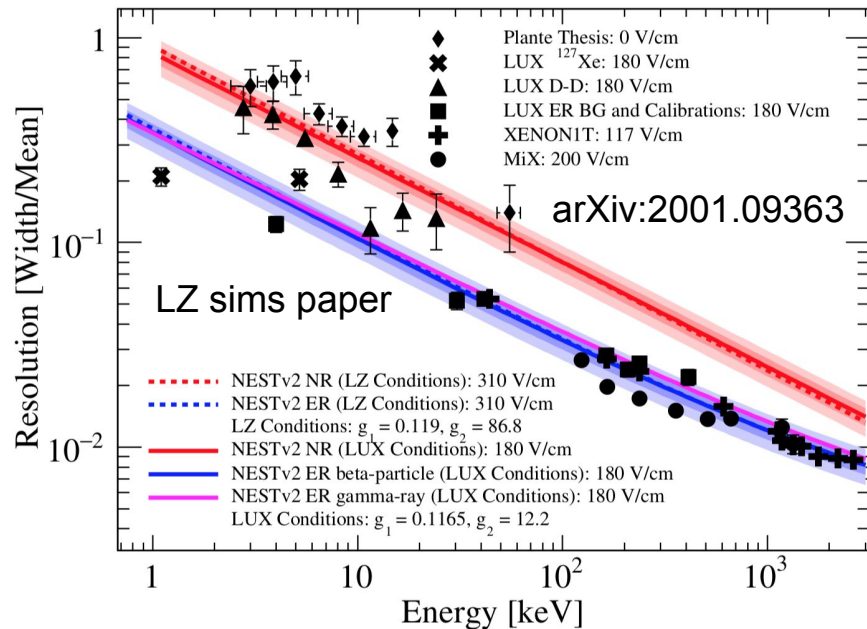
- It is also a framework, kind of like G4
- ADAPTABLE: Lindhard, Hitachi, Sarkis

- Electron recoils, alphas, etc. different

$$Q_y = N_e / \text{keV}, \quad L_y = N_q / \text{keV} - Q_y \text{ (temporary)}, \quad N_{ph} = L_y * \text{keV} * \left(1 - \frac{1}{1 + \left(\frac{\text{keV}}{\theta} \right)^\iota} \right), \quad L_y = N_{ph} / \text{keV} \text{ (final)}.$$

theta = 0.3 +/- 0.05 keV, iota = 2 +/- 0.5, Nq = Nph + Ne- (re-done)

Photons and electrons fit, then excitons and ions backed out: unlike earlier NEST versions



The end result on resolution vs. energy is very detector specific, and not always simple power law

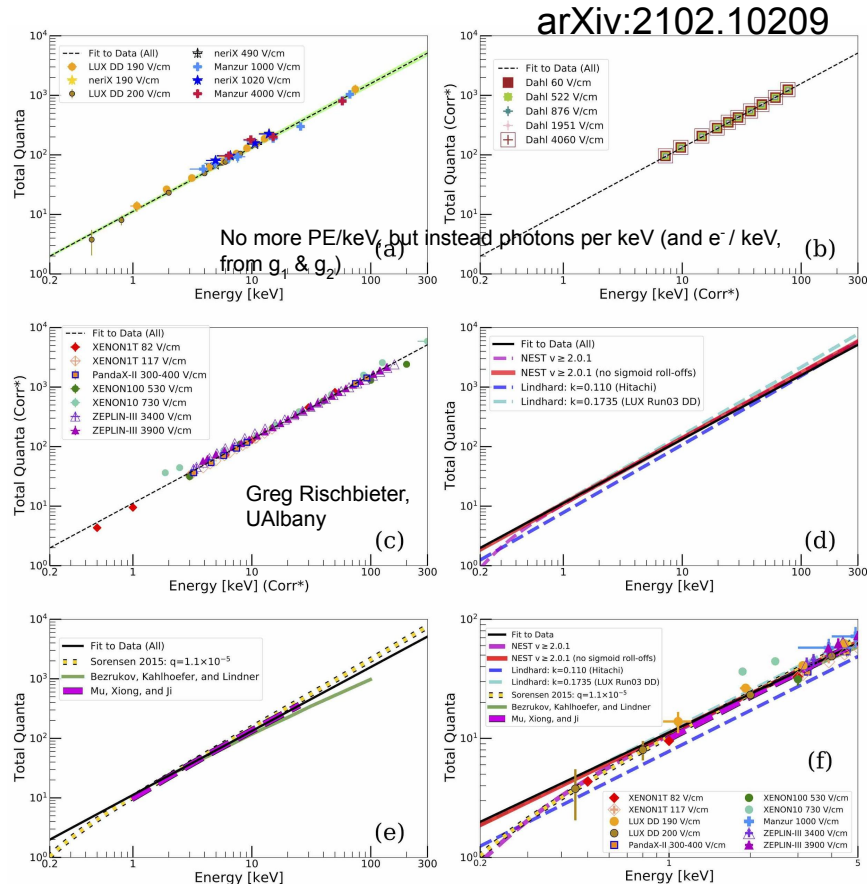
Plot by my PhD student Greg Rischbieter.
 Nominally sub-threshold events can “pop up”

Real-Life Fluctuations: A Multi-Faceted Approach

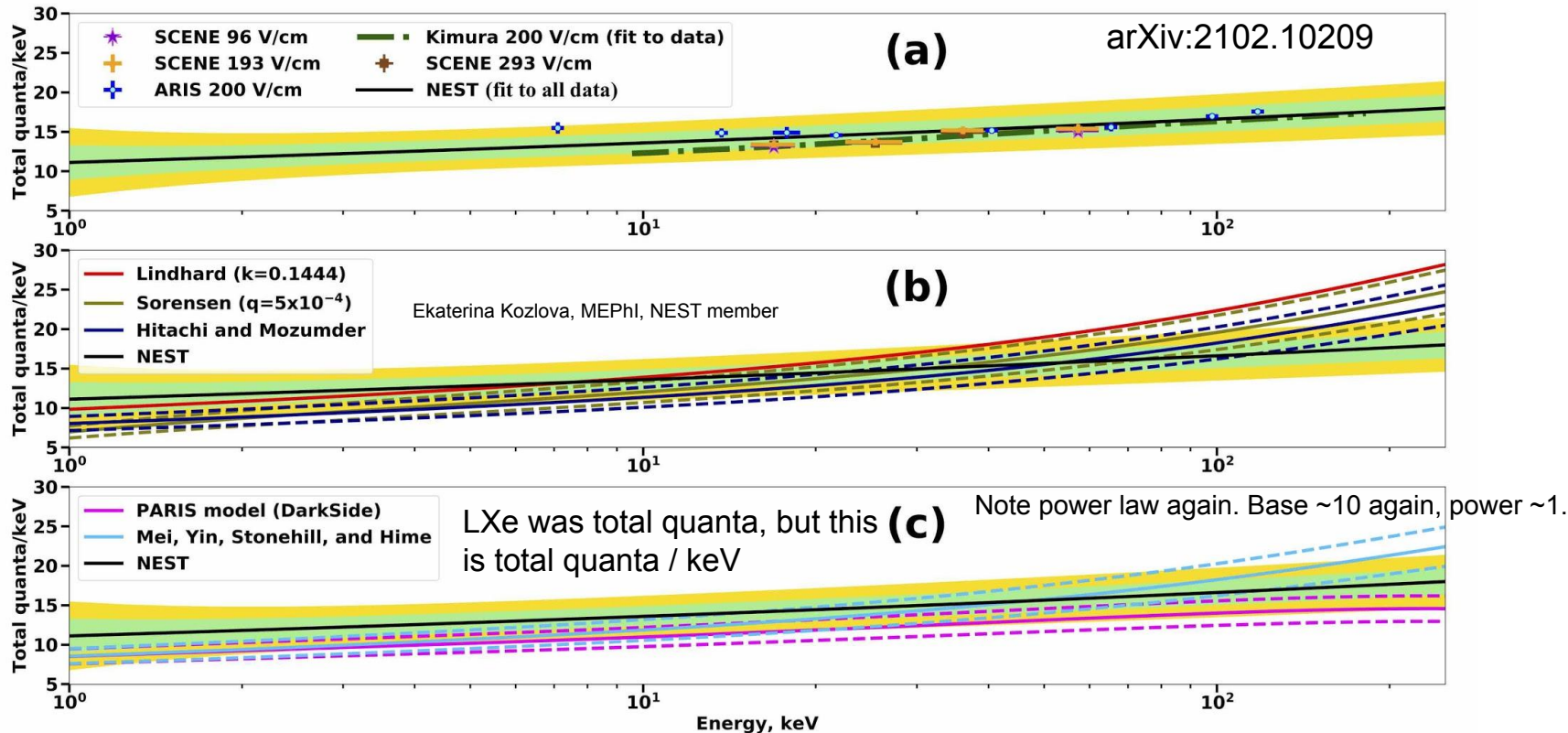
- Fano factors on excitation and ionization, affecting the total number of quanta: Correlated “noise”
- Recombination fluctuations: anti-correlation
- Detector effects like binominal light collection, from one’s calibrations
 - g_1 and g_2 ($\text{SE} * e^- \text{EE}$) most important
- Additional, uncorrelated noise: linear by default, proportional to the primary and secondary light’s pulse areas

What is total (NR) yield like? (LXe). Detector Independent

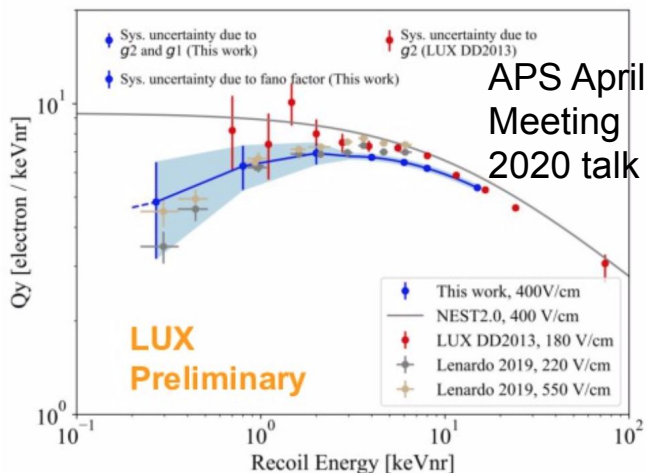
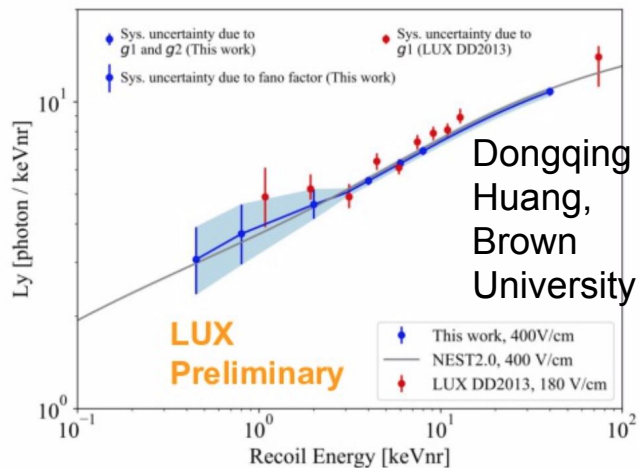
- Remarkably consistency over >20 experiments across the decades
 - Simple power law fits >400 points well
- Shockingly, there is no statistically significant evidence of deviation from the Lindhard model at keV scales!
 - The claims of its death have been greatly exaggerated (Xe not like other elements)
- In the past one channel was picked and then disagreement with Lindhard claimed, typically scintillation
 - L often confused with “L_eff”
- These are the **absolute** yields
 - NEST has done away with relative yields



Liquid Argon Example: Also NR (Neutron Calibrations)

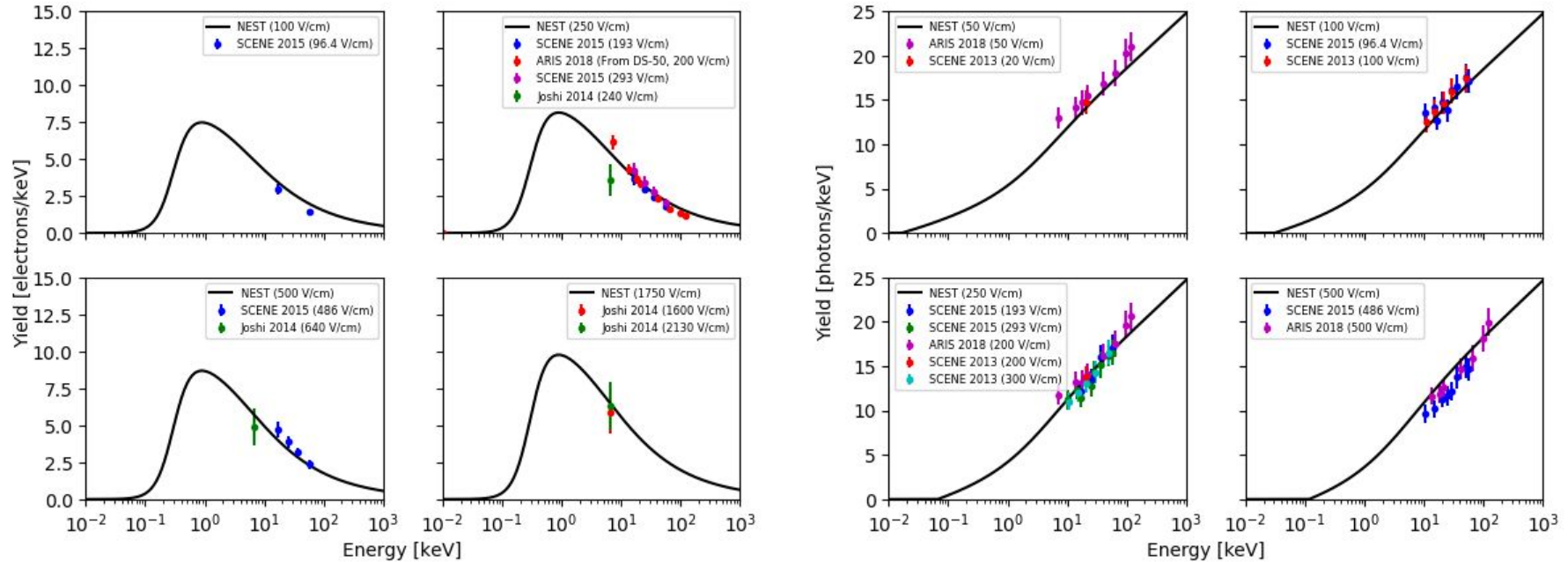


LXe Breakdown into the L_y and Q_y



- Light has been measured sub-keV now
- Charge even lower in energy than light
 - Example of what happens when you follow data too closely instead of model: turnover “predicted” in 2013 by NEST with Lindhard + Thomas-Imler box (first principles) but abandoned to follow data more closely later
- What causes Q_y shape with turn-over?
 - L-factor is going down, but escape prob going up (recomb prob down) as energy \Rightarrow 0
- What ultimately happens at the lowest energies? Quantum-mechanical hard cut-off?
 - NEST simulates a sudden drop to 0 quanta (no light nor charge) at ~ 200 eV (field-dep)
- Pendulum has swung back and forth between NEST versions over the years
 - But it is enormously beneficial to be “semi-empirical”

That Same Breakdown, but now for liquid Argon NR



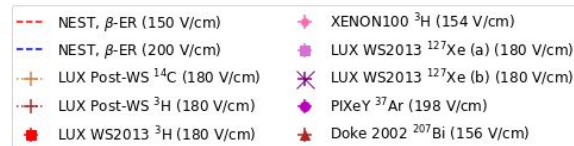
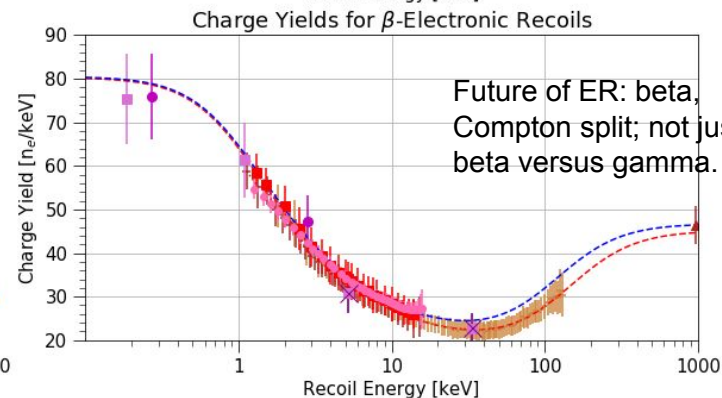
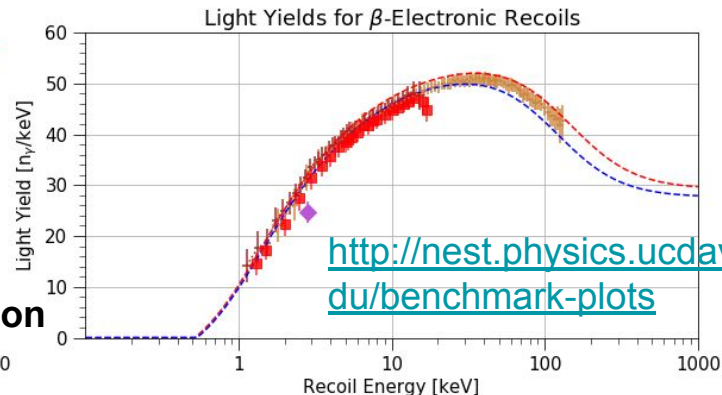
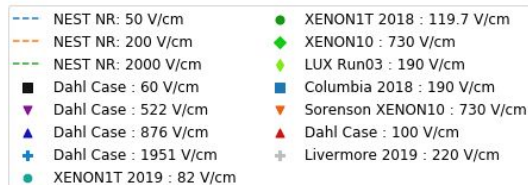
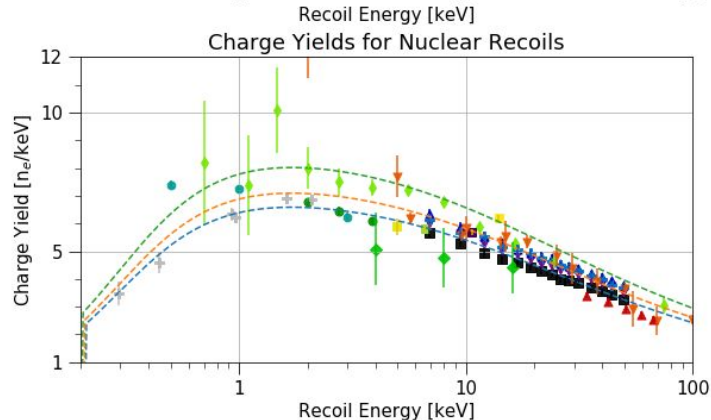
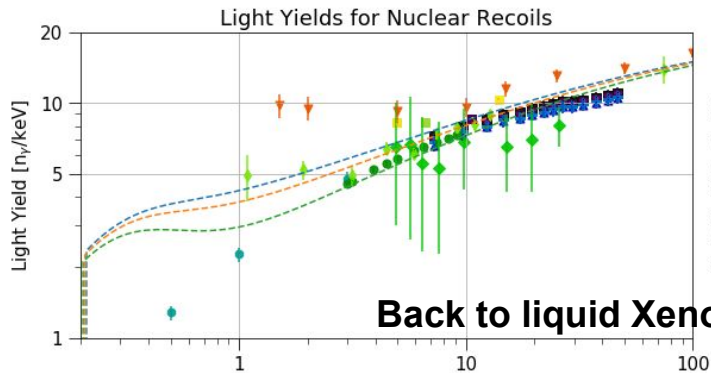
Analyses / plots by Justin Mueller, Colorado State/DUNE for the NEST collaboration. PI: Michael Mooney.

Plots by Sophia Andalaro, Rice University, of NEST (PI: Chris Tunnell)

NEST splits differences, or is conservative

And for sources we hunt everywhere, including PhD theses and talks.

NEST can help predict future detector performance not just “post-dict”



Low-E Pulse Shape Examples

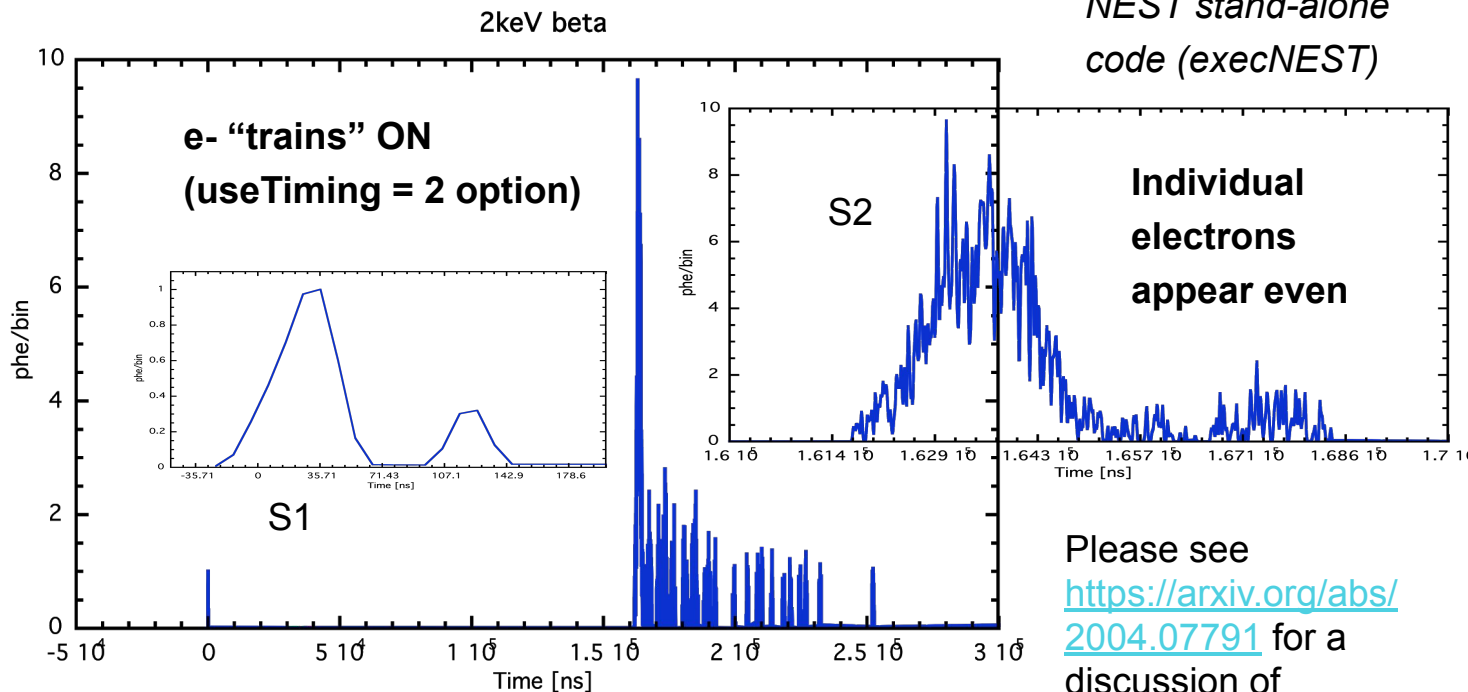
*This is NOT LUX or
LZ proprietary
software: this is
NEST stand-alone
code (execNEST)*

The NEST MC can
approximate your
DAQ and analysis
chain. Use it for
training pulse
finders/classifiers

One of its “best kept
secrets.” Few people
capitalize

Even does photon
arrival times,
analytically (no
ray-tracing) following
Phys. Rev. D97,
112002 (2018)

Note our EXO and
DUNE teams
working on non-light
S2 (wire readout)



ER in this example, but just like NR: treat as generic

Please see
<https://arxiv.org/abs/2004.07791> for a
discussion of
post-S2 phenomena

Timing: How Long Does the NEST Code Take to Run?

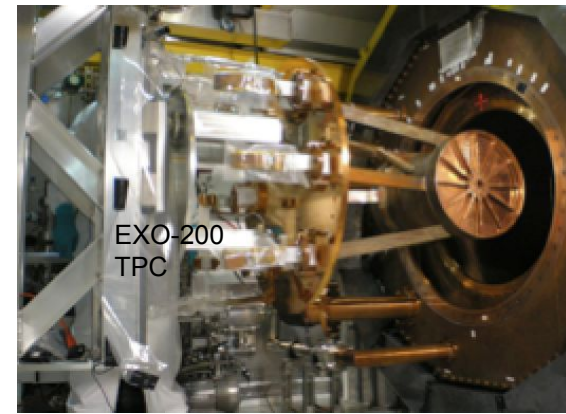
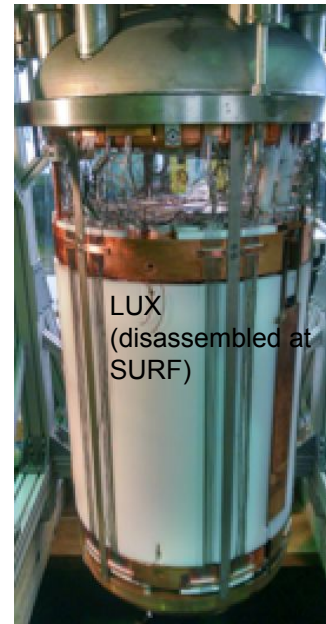
- Pulse shapes (S1, but specially TPC S2s) slow the NEST code down by x100
- Without them, however, NEST is $O(10,000)$ x faster than G4's scintillation class
 - This depends on operating system and machine of course, so this is just crude approximation
- This is also not an entirely fair comparison, however, as Geant4 does more
 - NEST is NOT a simulation of the backgrounds of all your components, their mean free paths,...
 - In addition, NEST uses an analytical model for photon propagation (or none if pulse shapes off)
- But, you can do 10^6 1 MeV beta events in <1h on your laptop (no parallelization)
 - keV-scale (NR, WIMP-like) events takes only seconds, from true energy all the way to S1 & S2
 - Reducing precision in the single photon detection at MeV scale can cut this down by order mag
- NEST and Geant4 are complementary: we have best of both worlds
 - You can run NEST as standalone code or as fully integrated from within Geant4: makes quanta

Breakdown into the Distinct Tools in the Software Package

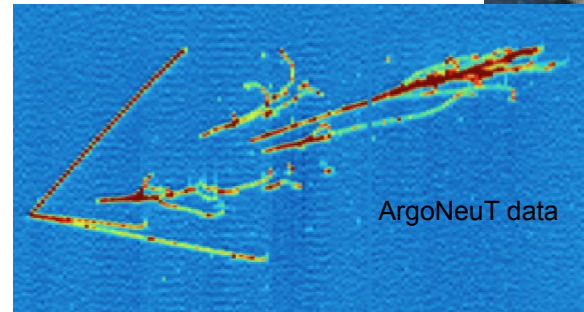
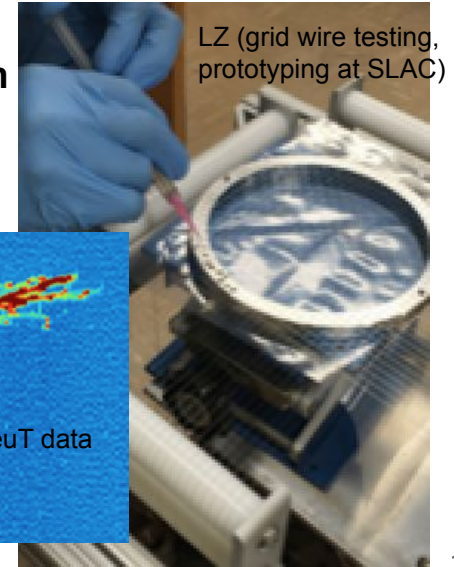
- execNEST: C++. Extreme swiss-army knife tool that does all the basics
 - rootNEST: runs on execNEST output and does Gaussian fits, skew, limits, etc.
 - Right now only old-school cut-and-count sensitivity projections: not PLR, ML, Yellin (yet)
 - nestpy: features of execNEST and rootNEST, but for the python language
 - “loop” NEST: C++, python versions for fitting to new data, if need be
 - Helps you understand yield uncertainties. Nothing fancy yet, but code is expanding
-
- G4Integration folder contains the C++ interface to Geant4, with instructions. By Jason Brodsky of Lawrence Livermore National Laboratory / nEXO
 - Garfield interface contributed by Ryan Linehan of Stanford Univ. / LZ

The Applications of NEST

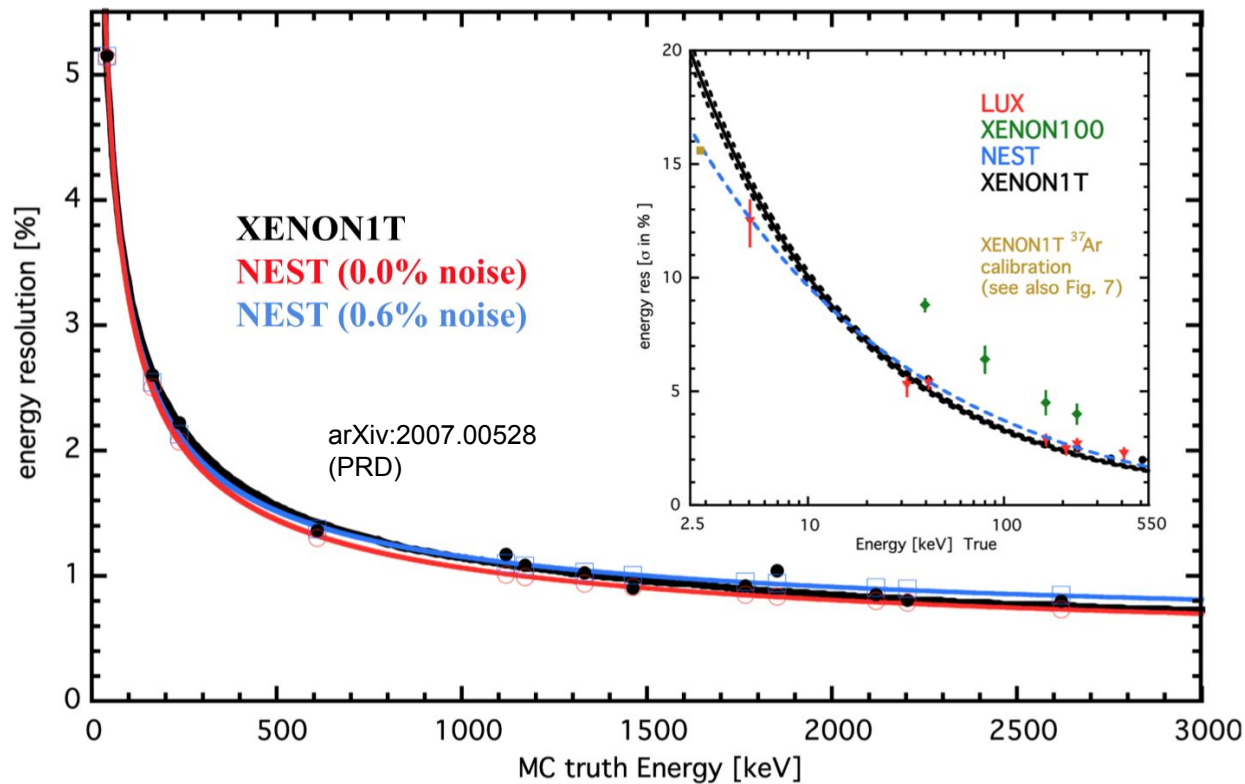
- Direct detection of dark matter
 - Not just WIMPs. ALPs too for example
- Non-dark-matter new physics but related, like keV solar axions
- Neutrinoless double-beta decay
 - Related: double-electron capture, e^+ 's
- PET scans: liquid Xe better?
- General gamma-ray, n detection
 - Noble elements for national security?
- Long and short baselines of nu physics: large-scale LAr TPCs, GAr
- Potential interest in ATLAS?
 - Since it has a liquid Ar calorimeter
- Coherent nu scattering (CEvNS)
 - Including solar and supernova



**exam
ples**

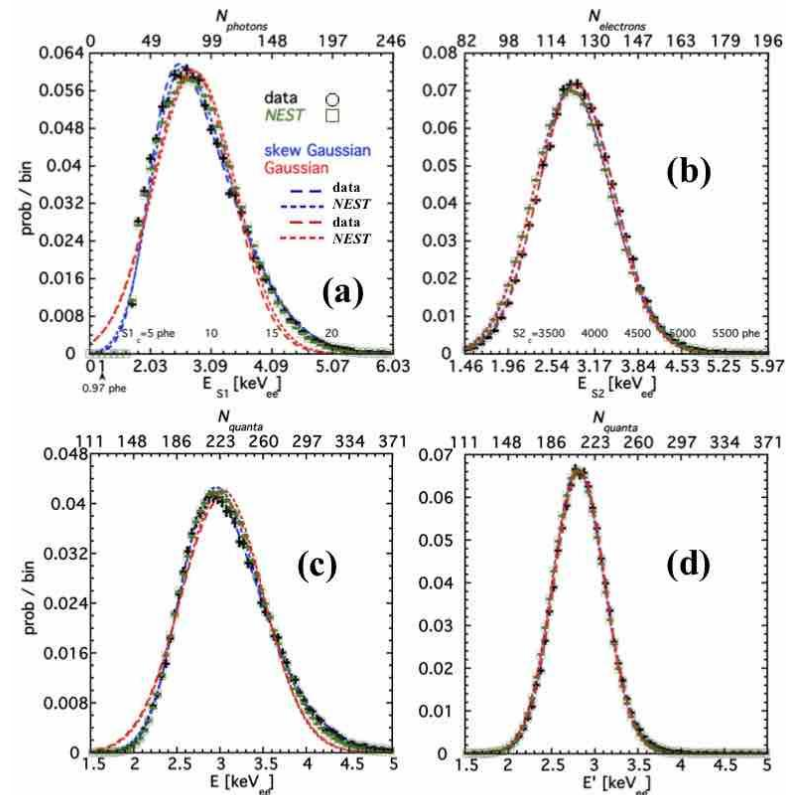


Examples of NEST Output Reproducing Real Last-Stage Data



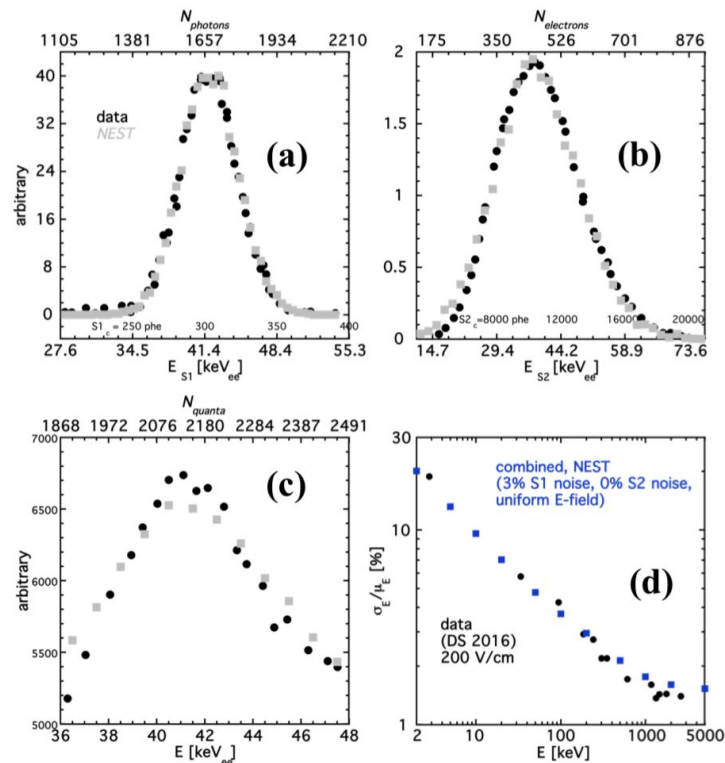
- Combined energy resolution in the XENON1T detector
 - S1 and S2 combined
- NEST matched even with a version that came out before XENON1T paper!
 - Despite detector idiosyncrasies
- This is NOT detector agnostic however

Focusing on a Low-Energy Peak, and Breaking it Apart

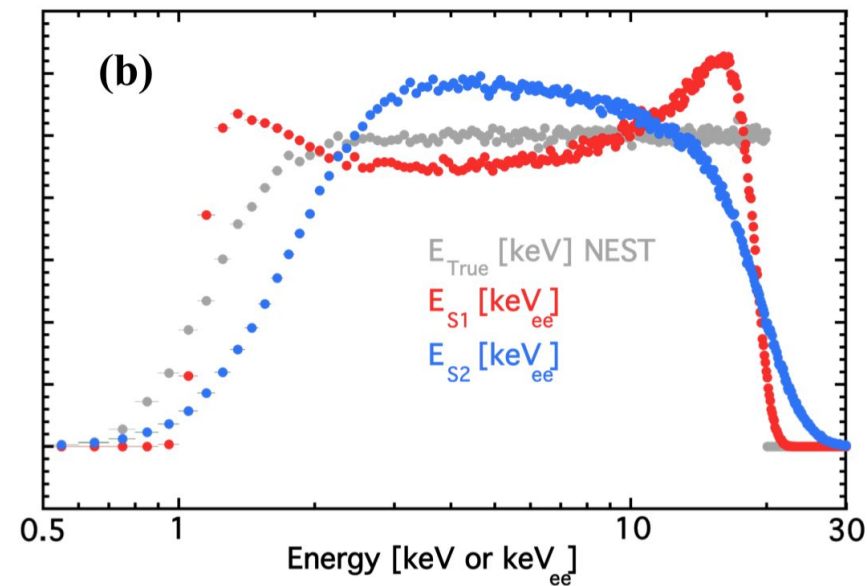
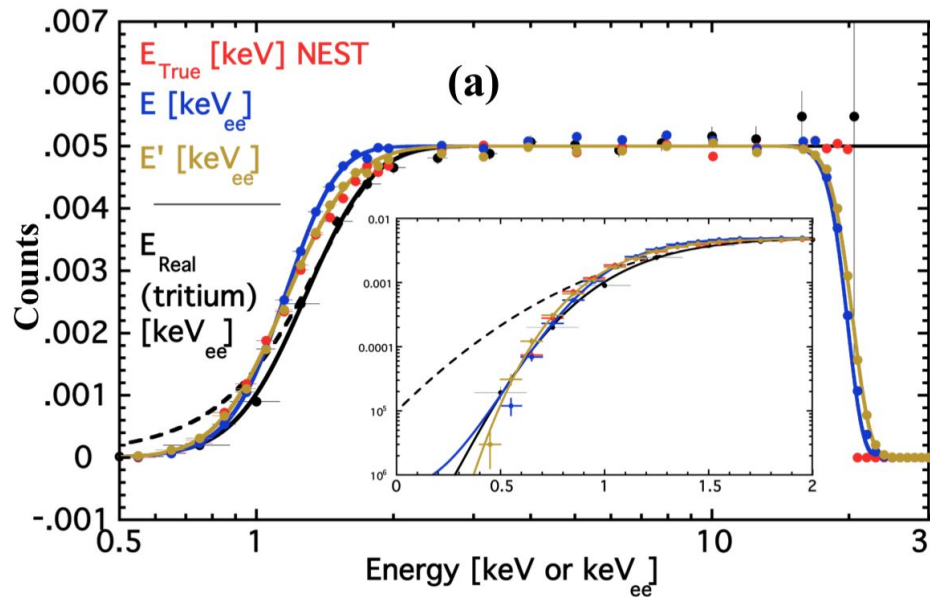


arXiv:2102.10209. Liquid Xenon

- 2.82 keV ^{37}Ar peak (e^- capture process) at left, 41.5 keV ^{83m}Kr at right
- Outstanding low-energy (keV scale) ER calibration peaks for e.g. dark matter searches
- S1-only, S2-only, combined, and optimal combination or E_{res} (a, b, c, d)
- Switching gears here from XENON to PIXeY and DarkSide: adjusting detector parameters
- NEST just works out of the box, with minimal tuning, to none

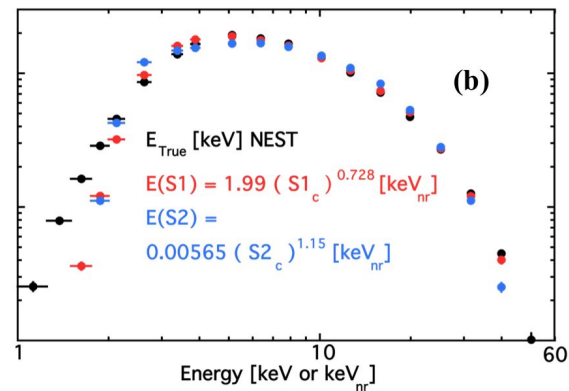
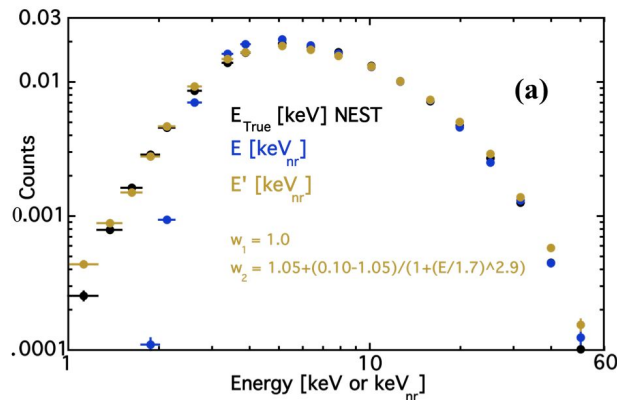


Liquid Argon



Efficiency vs. Energy

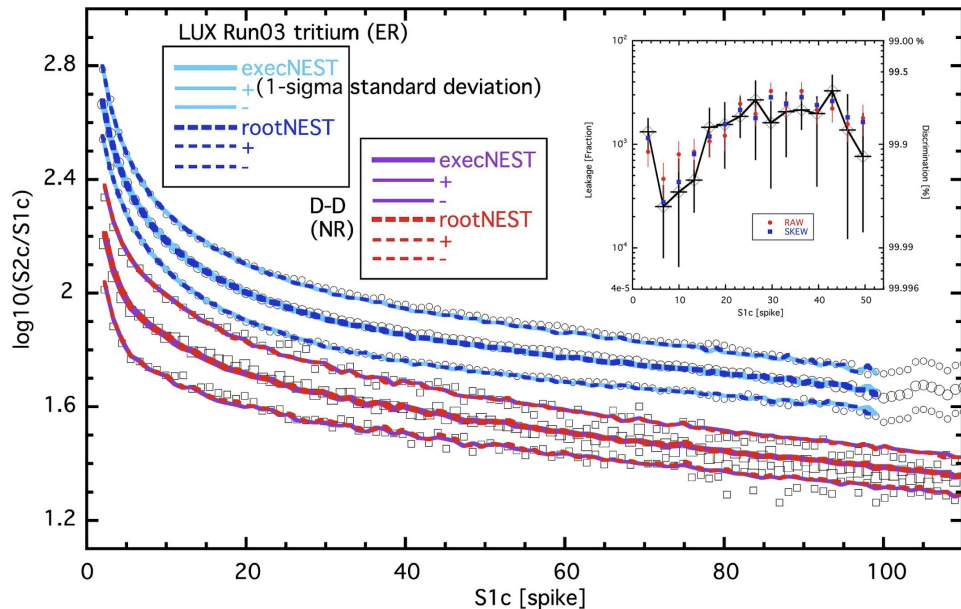
- electron recoil above
- Below, nuclear recoil



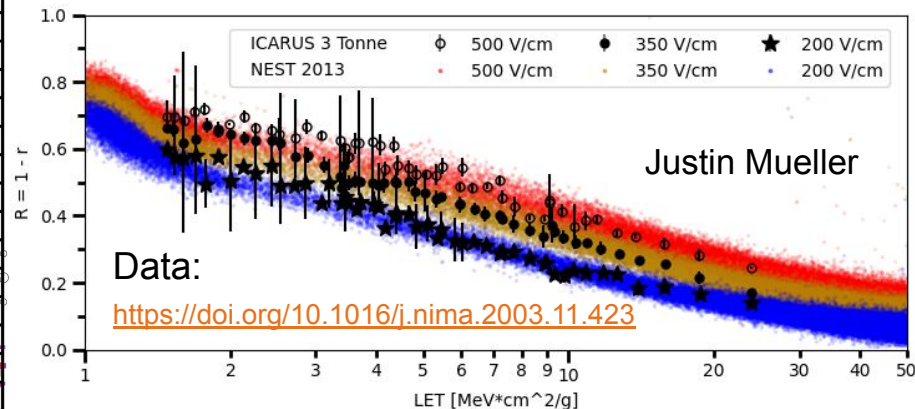
Background Discrimination: S2/S1 in LXe, but dE/dx in LAr

Note there was a 2013 model back in the day written by me for LBNE at time (in G4). **Birks' Law**

Delta rays, not in LArSoft (DUNE) by default, key.
Affect both means and widths. GEANT4 is **needed!**

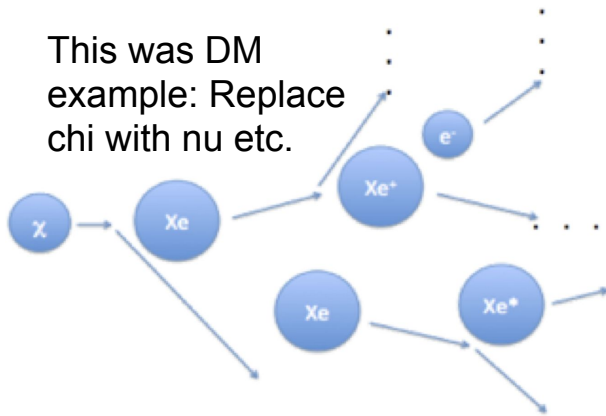


- Note: NOT wearing my LZ/LUX hat today. Speaking for NEST today. This is merely one example

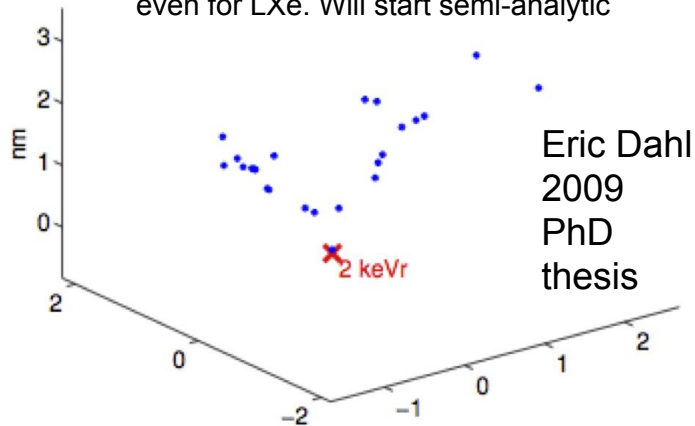


- Charge above essentially, but only ~half the story for energy: anti-correlation a real effect as in Xe
- Particles types at same dE/dx differ

This was DM
example: Replace
chi with nu etc.



Baby steps: E basis into dE/dx basis
even for LXe. Will start semi-analytic



What is the Future of NEST?

- For extrapolation where no data, go fully “theoretical”: molecular dynamics simulations?
 - Simulate van der Waals forces between the Xe and Ar atoms in liquid, with e.g. 12-6 Lennard-Jones potential from chemistry and atomic physics.
 - Do (cylindrical TPC-specific?) optical photon tracking, instead of relying on Geant4, which is volume instead of surface-based, so slow. Faster than Opticks, Chroma?
- Need to interest funding agencies. In the U.S. that would be DOE and NSF.
 - No success in half a decade in securing funds for this
 - Interdisciplinary in full sense of word: beyond HEP. We require AMO expertise.
- Massive supercomputing resources will be needed to simulate many picosec-sized steps
 - Ironically, though, lower energies easier: few atoms

- Knowing me, I'll be very much running out of time before I reach this slide!

Summary and Outlook

- NEST is quite robust, balancing not just theory and experiment, but also speed (at MeV scale can still simulate millions of event/minute) and precision
 - Allows you to extrapolate not just interpolate, and predict not just postdict data
 - Splits general phenomena from detector idiosyncrasies, but does not ignore the latter
- Constantly being updated, but also being careful to avoid ambulance chasing
 - Minor releases ~monthly, major ~bi-annual. Continuous integration with Travis
- Most important conclusion: NEST works for both Xenon (liquid & gas) and Argon, using similar often identical equations/formulae/functions
 - Has in 10 yr. reduced MC errors from ~100% to 10% incorporating always the world-leading calibrations from ANY experiment. Not restricted to LUX and LZ, where NEST started
 - High speed allows you to train machine learning very fast for detectors using these elements
- Allows you to extract efficiency from PE/keV -> photons, electrons / keV!
 - Excellent for comparing between experiments. Good for theorists and phenomenologists



More References

- Cite us using Zenodo: <https://zenodo.org/record/4569211#.YELizS2ZPVo>
 - Version 2.2.1 has just been tagged, with many bug fixes and a good deal of new features!
 - You can get a fully citable DOI for your publications. Reproducibility, history
- NEST papers (4 so far) listed here: <http://nest.physics.ucdavis.edu>
 - All old talks listed here as well for download, and various pre-publication analysis reports
 - Validation plots, an online calculator (means only, outdated: better to just download code)
- See numerous relevant XENON, LZ, LUX papers, cited throughout this talk
- Multiple new NEST papers coming as well, really big ones! Be on lookout!

Questions?

