Office of Defense Nuclear Nonproliferation
Research and Development

University and Industry Technical Interchange
(UITI2013) Review Meeting

The Noble Element Simulation Technique

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Introduction

◆ Project title: **NEST, The Noble Element Simulation Technique**

◆ Lead organization: **University of California Davis**. Participating organizations, including associated national laboratories: **Lawrence Livermore National Laboratory (LLNL)**. Principal Investigators: **Matthew Szydagis, Mani Tripathi**

◆ The NEST model is pertinent to the mission of nonproliferation because noble element detectors are applicable to reactor monitoring.

◆ The primary objective of the NEST model/code is providing high-quality, high-fidelity computer simulation of the microphysics of the excitation, ionization, and recombination processes arising as a result of energy depositions caused by gamma rays, neutrons, or neutrinos, in noble gasses and liquids.

◆ NEST can help eliminate the use of poor approximations of the real physics occurring used in the past and predict the non-linear response as a function of energy, dE/dx, electric field magnitude, and particle type.
Technical Challenges and Progress

- We can already reproduce the vast majority of nuclear and electron recoil data on scintillation light and ionization yields in liquid xenon (LXe).

- Gaseous xenon, gaseous argon, and liquid argon (LAr) are also viable target media for noble element based detectors, so their scintillation microphysics needs to be modeled as well.

- One technical challenge for both xenon and argon is getting accurate data on ultra-low-energy nuclear recoils, which would be induced by coherent scattering of nuclear reactor anti-neutrinos. These are needed for accurate computer modeling.

- The overarching long-term goal of NEST is applicability to all noble elements in all phases, with a demonstration of postdictive power for older data, and predictive power for new data.
Basic Physics Principles

- Excitation and ionization are **anti-correlated**, and the ratio of exciton to ion production is $O(0.1 - 1)$, depending on element, energy, recoil type.

- Due to the **Lindhard effect**, nuclear recoils are more efficient at producing more nuclear recoils than producing electron recoils, and as a result they produce a reduced amount of light and charge.

- Lower ionization density or higher drift field leads to less **recombination**

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M. Szydagis et al., *JINST* 6 P10002 (2011)
Foundational Equations

• Cornerstone: There is but ONE work function for production of a scintillation photon OR ionization electron. Others derive from it.

• $W_{LXe} = 13.7 \pm 0.2$ eV (E. Dahl, 2009) $N_q = (N_{e-} + N_\gamma) = \frac{E_{dep}}{W}$

• Photons $N_\gamma = N_{ex} + r N_i$ and electrons $N_{e-} = (1 - r) N_i$

• Two models of the recombination probability as a function of $E$ or $dE/dx$, and field, chosen based upon the interaction’s track length
  – Thomas-Imel Box (< O(10) keV electron recoils, and all nuclear ones)
  – Birks’ Law of scintillators, with its parameters functions of field

\[ r = 1 - \frac{\ln(1 + \xi)}{\xi}, \quad \xi \equiv \frac{N_i \alpha'}{4a^2v} \quad \text{OR} \quad r = \frac{A \frac{dE}{dx}}{1 + B \frac{dE}{dx}} + C, \quad B = A/(1 - C) \]

• Recombination causes noble light and charge yields per unit energy to be non-linear versus energy: twice the energy does not necessarily imply twice the signal, in either channel
Comparison to Data

- Reviewing only NEST’s “greatest hits” here, demonstrating not only its postdictions but also its predictive power for new data, but only scratching the surface in 15 minutes.

- At non-zero field, NEST is based primarily on the Ph.D. thesis of Eric Dahl (Princeton University, 2009). Why?
  - His data is extensive in field (.06 to 4 kV/cm) and energy (> ~2 keV)
  - Dahl attempted to reconstruct the original, absolute number of quanta and estimate the *intrinsic* energy resolution
  - He used the “combined” energy, possibly the best energy estimator

- After models were built from old data sets, everything else is a prediction of new data, and NOT a fit or spline of the data points

- NEST paper (JINST) contains over 70 references (some rare)

- Going against long-standing assumptions from years back: for instance, yield is NOT constant vs. energy, at least for LXe.
• As the energy increases, dE/dx decreases, thus recombination decreases (less light ultimately, at the expense of more charge)

XENON100 dark matter experiment at 530 V/cm

Aprile, Dark Attack 2012 Conference
LXe Nuclear Recoil Charge Yield

- Low-energy xenon recoil most critical for detection of nuclear recoil from neutrinos, for the purposes of reactor monitoring
- Data all over, but the NEST curve is largely conservative
- Nuclear recoil events will produce an increasing amount of charge per unit energy as the amount of light decreases as $E \rightarrow 0$ and is undetectable

P. Sorensen et al., Lowering the low-energy threshold of xenon detectors, PoS (IDM 2010) 017
LAr Nuclear Recoil Charge Yield

- Real data will be able to disambiguate these different models.
- The “Mei-like model” assumes that the sum of the light and charge yields continues to decrease smoothly as energy goes to zero.
- The “Bezrukov style” model assumes that there is a slight increase instead at low energy (idea supported by some data).

Prediction performed here done to support the work reported on in Sangiorgio et al., arXiv:1301.4290

\[
\frac{\alpha}{(a^2v)} = 0.07 \quad \frac{N_{ex}}{N_i} = 1.000
\]

\( O(1) \) electron at \( O(100) \) eV
Energy Resolution

LUX Surface Data
Gaussian Fit
LUXSim with NEST

D.S. Akerib et al. (LUX, the Large Underground Xenon Collaboration) Astropart. Phys. 45 (2013) pp. 34.

- To the best of my knowledge, this is the first time that a Monte Carlo peak width is not circularly informed by the data!

- Recombination fluctuations modeled

662 keV $\gamma$ ($^{137}$Cs)
Pulse Shape

• Both the S1 and S2 pulse shapes have been modeled in NEST

• Long list of effects
  – Single time
  – Triplet time
  – Singlet/triplet ratio
  – Recombination time
  – $e^-$ drift speed
  – Diffusion
  – $e^-$ trapping time

• Important for simulating a detector fully and realistically: making sim look like actual data

Mock et al., 2013, in preparation
Conclusions and Future Work

• NEST can predict the response of a generic noble liquid (or noble gas) detector to either ionizing or non-ionizing radiation.

• Public code available for download to the entire physics community

• Liquid xenon is essentially finished, but there is still work being done for liquid argon, although it is progressing rapidly to the same level

• NEST applies to many fields of physics research, including dark matter, neutrinos, high-energy physics, and medical physics, so that working on it can provide good cross-disciplinary training for new students, toward a career in any one of a number of different fields