Noble Element Simulation Technique, MC Code for Both Scintillation and Ionization in Noble Elements.

http://nest.physics.ucdavis.edu

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The People of the NEST Team

UC Davis and LLNL
A small but passionate group of individuals who love their work

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What is NEST?

• That name refers to both a model (or, more accurately, a collection of models) explaining the scintillation and ionization yields of noble elements as a function of particle type (ER, NR, alphas), electric field, and energy or dE/dx

• ... as well as to the C++ code for GEANT4 that implements said model(s), overriding the default

• Goal is to provide a full-fledged MC sim with
  – Mean yields (light AND charge)
  – Energy resolution (and background discrimination)
  – Pulse shapes (S1 AND S2)

• Combed the wealth of data for liquid and gaseous noble elements and combined everything learned

• We cross boundaries: ν’s, DM, HEP, “enemies”
Basic Physics Principles

1st division of energy deposition a function of interaction type (nuclear vs. e-recoil) but not particle type (e.g., $e^-$, $\gamma$ same), and ($\sim$) not a function of the parent particle’s initial kinetic energy but not a function of linear energy transfer (LET) or stopping power ($dE/dx$), because of ionization density considerations, and of the electric field magnitude.

- The ratio of exciton to ion production is $O(0.1)$
- $S1$ is NOT $E$, because energy depositions divide into 2 channels, $S1$ and $S2$, non-linearly: idea from Eric Dahl
- Nuclear recoils also have to deal with Lindhard* but it affects BOTH charge and light production
Basic Physics Principles

• Cornerstone: There is but ONE work function for production of EITHER a scintillation photon or an ionization electron. All others derive from it.

• \( W_{LXe} = 13.7 \pm 0.2 \text{ eV} \quad N_q = (N_{e^-} + N_\gamma) = \frac{E_{dep}}{W} \)


• \( N_\gamma = N_{ex} + r N_i \) and \( N_{e^-} = (1 - r) N_i \) (\( N_{ex} / N_i \) fixed)

• Two recombination models, short and long tracks
  – Thomas-Imel ”box” model (below \( O(10) \) keV)
  – Doke’s modified Birks’ Law

\[
\begin{align*}
    r &= \frac{A \frac{dE}{dx}}{1 + B \frac{dE}{dx}} + C, \\
    B &= \frac{A}{1 - C} \\
    \text{OR} \quad r &= 1 - \frac{\ln(1 + \xi)}{\xi}, \quad \xi = \frac{N_i \alpha'}{4 \alpha^2 v} \\
\end{align*}
\]

• Probability \( r \) makes for a non-linear yield per keV
Comparison With 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 20 minutes ....
- At non-zero field, NEST based primarily on the Dahl thesis
  - His data 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* resolution you can’t avoid
  - Used combined energy, possibly the best energy estimator
- After models built from old data sets, everything else is a prediction of new data, and NOT a fit / spline of data points
- NEST paper (JINST) contains over 70 references (some rare)
- Going against long-standing assumptions from years back: for example, yield NOT flat versus energy, at least for LXe. No such thing as a generic ‘ER’ curve. I dug up old papers long forgotten. The ancient results come back in cycles ....
ER Mean Light Yield in LXe

(See Aaron Manalaysay’s talk)

Zero Field

Non-zero Field (450 V/cm)

As we approach minimally-ionizing, the curve asymptotes
As the energy increases, $dE/dx$ decreases, thus recombination decreases (less light ultimately, at the expense of more charge).

Co-57 $\sim 122$ keV, the reference point for NR light

XENON100 at 530 V/cm field

Aprile, Dark Attack 2012; Melgarejo, IDM 2012

No Co-57 calibration, so NEST was a key part of the WIMP limit calculation.
ER Charge Yield, including Kr-83m

Circles are NEST. Squares and diamonds are the real data.


9.4 keV “anomaly” was identified in the NEST JINST paper ~1 year before Columbia study.

have benefited from technological advancements, leading to more accurate measurements. Recent 9.4 keV data is poorly predicted by the Thomas-Imel model. Curiously, agreements can be achieved by approximating the $^{83m}\text{Kr}$ de-excitation as only a gamma ray and applying the Doke/Birks model despite the low energy. Without such adjustments these data contradict Dahl [11] in this energy.

(NEST curve not shown for $^{57}\text{Co}$ because tautology: basis of model)
NR Light Yield in LXe

(Using very simple assumptions)

We don’t need to reference the 122 keV gamma line anymore. Model gives us absolute numbers.

Only latest, greatest

NEST:
Zero field
500 V/cm

NOT fits to these data
NR Charge Yield in LXe

This curve straight-jacketed: sum of quanta fixed by Lindhard theory, while Dahl gives us the ratio.

Older interpretations of data all over

Line keeps going: predicts 1 e- at ~300 eV on average. Similar to work done by Sorensen not using Dahl data.

P. Sorensen et al., Lowering the low-energy threshold of xenon detectors, PoS (IDM 2010) 017 [arXiv:1011.6439].
ER Energy Resolution: Light


LUX Surface Data
Gaussian Fits
LUXSim + NEST

164 keV
236 keV (=39.6 + 196.6 keV)
662 keV (Cs-137)

Backscatter peak ~200 keV
Peak: 30 keV x-ray

May be the first time that Monte Carlo peak width is not informed by the data!

Cosmo-genically activated Xenon

M. Woods
The recombination fluctuations have been modeled as worse than binomial, with a field-dependent Fano-like factor $O(10)-O(100)$ which disappears at low energies. Based on

Aprile et al., NIM A 302, p. 177 (1991)
ER Resolution: $\log(S2/S1)$ Band

Analogue for $\log_{10}(S2/S1)$

NEST (876 V/cm)

NR (solid)

ER (hollow)

Dahl 2009

Not pictured -- NR width also handled by NEST: Fano $\sim 1$
NR vs. ER Discrimination

The trend is counter-intuitive: worse result *away* from threshold.

No time to discuss: tails, non-Gaussian leakages...

Culmination plot. ER and NR band means and widths must all be correct.
Gaseous Xenon
(The mystery of liquid’s worse energy resolution)

$E_\gamma = 662$ keV
Field = 7 kV/cm

Binomial-only level: no monkey business there

Nygren 2009
Bolotnikov et al. 1997
Liquid Argon NR and ER

Note: RAT, codebase pre-dating NEST, already does zero-field LAr very well (talk with S. Seibert)

R = 1 – r is a way of checking on both light and charge yields, concurrently.

Regenfus et al., arXiv:1203.0849


Pulse shape: LXe examples

+ S1 effects included: a singlet time, triplet time, ratio (function of particle type), non-exponential recombination time (function of dE/dx and field)
+ S2 effects: drift speed, singlet, triplet, diffusion, and electron trapping prior to extraction.
Conclusions

• Simulation package NEST has a firm grasp of microphysics.
• Though NEST does not track individual atoms or excimers, it is closer to first principles, considering the excitation, ionization, and recombination physics, resorting to empirical interpolations as indirect fits or not at all.
• Extensive empirical verification against past data undertaken using multiple papers instead of only one experiment.
• Liquid xenon is essentially finished, but there is still work being done for liquid argon, although it is progressing rapidly.
• User-editable code for the entire community.
• Our understanding of the microphysics is only as good as the best data. Models are beautiful but nature is ugly. NEST is constantly improving. Always on look-out for more physical motivations. Currently, all parameters justifiable except for the size of the recombination fluctuations (in liquid xenon).
Anti-correlation in Argon

Correct absolute energy scale = $a \times LY + b \times CY$

(see the IDM 2012 talk)

- In LAr, anti-correlation between light yield (LY) and charge (CY) missed
- Combining lets you empirically eliminate the effect of recombination fluctuations and energy loss into scintillation
- In high-light-yield prototype TPCs, we can use mono-energetic sources and sweep the field to test this .....
LAr Pulse Shape

- The latest version of NEST (98) has incorporated some of these results.
- The upper plot has been converted into a function of LET instead of E (soon impurity concentration too).
- This should be a significant step forward in LAr modeling, giving us the correct ratio of triplet to singlet light (it’s not flat).

Figure 3. Yield of the fast and slow scintillation components under different purity conditions.
Understanding Charge Collection

• New G4Particle for drift e-’s
• Analogous to optical photons versus gamma rays
• Normal electrons, if born with tiny energies, are absorbed immediately in GEANT
• Full sims take much longer than parameterized ones, but this new particle (the “thermalelectron”) allows tracking of individual ionization sites, and simulated 3-D electric field, purity, and diffusion mapping
• To decrease simulation time, NEST has a built-in feature for charge yield reduction

* G4Track Information: Particle = e-, Track ID = 5, Parent ID = 3

<table>
<thead>
<tr>
<th>Step#</th>
<th>X(mm)</th>
<th>Y(mm)</th>
<th>Z(mm)</th>
<th>KinE(MeV)</th>
<th>dE(MeV)</th>
<th>StepLeng</th>
<th>TrackLeng</th>
</tr>
</thead>
</table>

**Field Dependence of Light, Charge Yields in LXe**

*This Work*

- 9.4 keV ($^{83m}$Kr)
- 32.1 keV ($^{83m}$Kr)
- 29.8 keV γ
- 59.5 keV γ
- 122 keV γ

- 9.4 (Manalaysay, 2010)
- 29.8 (Yamashita, 2004)
- 32.1 (Manalaysay, 2010)
- 59.5 (Yamashita, 2004)
- 122 (Aprile, 2005)
- 122 (Aprile, 2006)
- 122 (Manalaysay, 2010)

*77% photon detection efficiency (unspecified in source) assumed in order to set absolute scale for data and match simulation.*

**Field Dependence of Light, Charge Yields in LXe**

*This Work*

- 368 keV e⁻ ($^{113}$Sn)*
- 122 keV γ
- 41.5 keV ($^{83m}$Kr)

- 368 (Thomas & Imel, 1987)
- 122 (Aprile, 2006)
- 122 (Dahl, 2009)
- 41.5 (Manalaysay, 2010)

*This IC electron dominates, but other higher-energy products exist. The simulation accounts for this.*

**This Work**

- 976 keV e⁻
- 662 keV γ
- 511 keV γ

- 976 keV e⁻
- 662 keV γ
- 511 or 570 keV γ

- “1 MeV” e⁻ (Doke, 2002)
- 570 (Conti, 2003)
- 570 (Aprile, 1991)
- 570 (Aprile, 2007)
- 511 (Amaudruz, 2009)
Recombination Fluctuations Model

- Regular Fano factor left alone
- Recombination fluctuations have been modeled as worse than binomial, with a 1-sigma of $\sqrt{F_e \cdot N_e}$, per interaction site
- Field-dependent but energy-independent (except at low E)