NEST

A Symphony of Scintillation

Noble **E**lement **S**imulation **T**echnique, A Model of Both Scintillation and Ionization in Noble Elements

http://nest.physics.ucdavis.edu

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on behalf of the entire NEST development team, of the University of California, Davis, Davis, CA, USA, and Lawrence Livermore National Laboratory, Livermore, CA, USA

Brookhaven National Laboratory, Phone Meeting, Monday 01/14/2013

The People of the NEST Team

UC Davis and LLNL

A small but passionate group of individuals who love their work

<u>Faculty</u>

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<u>Physicists</u>

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Jeremy Mock

Nick Walsh

Mike Woods

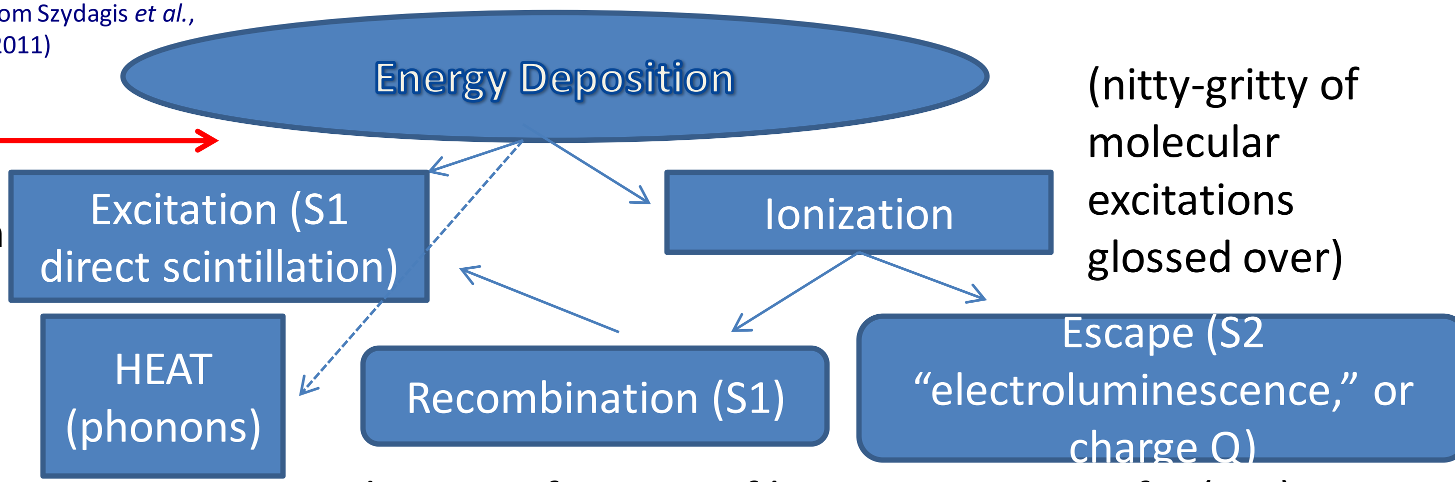
Summer undergraduates (many)

The Purpose and Scope of NEST

- Create a full-fledged sim based on a physical, albeit also heuristic/quasi-empirical approach
- Comb the wealth of data for liquid and gaseous noble elements for different particles, energies, and electric fields, and then combine everything
- Aid the many dark matter, neutrino, and other experiments which utilize this technology to be on the same or a comparable page for simulations
- Bring added realism to the simple model that is present now in Geant4 for scintillation
- Explore backgrounds at low energy by expanding Geant4 physics to be more accurate when you go to a low energy regime: *O*(10 keV) and even lower
- Started with LXe (for LUX) and moving on to LAr now

Basic Physics Principles

Image adapted from Szydagis *et al.*, *JINST* **6** P10002 (2011)



(nitty-gritty of molecular excitations glossed over)

1st division of energy deposition a function of interaction type (nuclear vs. e-recoil) but not particle type (e.g., e-,γ same), and (~) not a function of the parent particle's initial kinetic energy

(infamous "quenching" factor)

division a function of linear energy transfer (LET) or stopping power (dE/dx), because of ionization density considerations, and of the electric field magnitude

- In LAr, the ratio of scintillation from direct excitation (initial S1) to ionization is 21% (across all energies)
- Taking into account recombination, as much as ~50% of the energy goes into scintillation light, NOT charge!

Basic Physics Principles

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

C.E. Dahl, Ph.D. Thesis, Princeton University, 2009

- W_{LAr} = 19.5 +/- ~0.1 eV $N_q = (N_{e-} + N_\gamma) = E_{dep} / W$

Doke et al., Jpn. J. Appl. Phys. Vol. 41 (2002) pp. 1538–1545

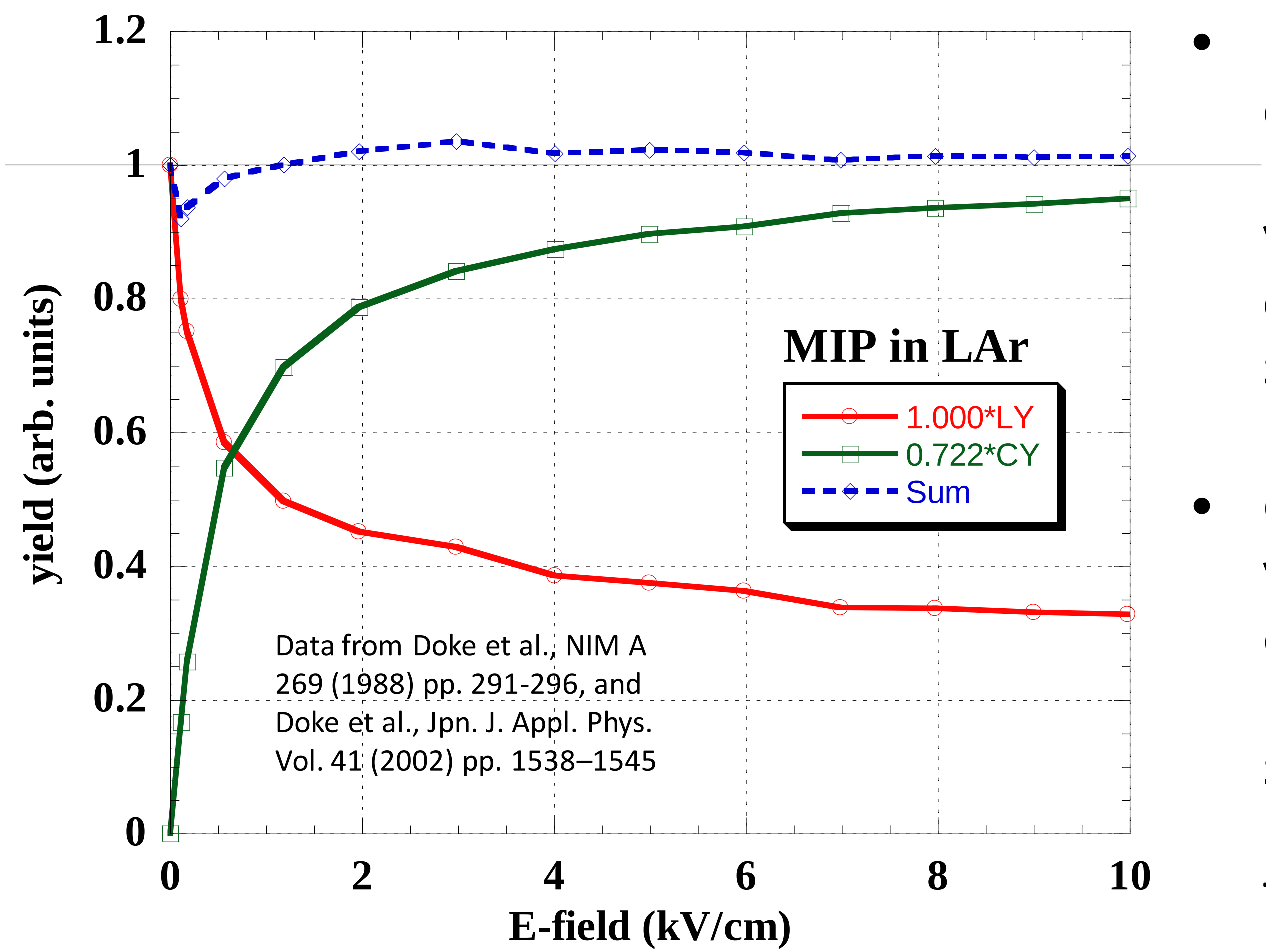
- $N_\gamma = N_{ex} + r\, N_i$ and $N_{e-} = (1 - r)\, N_i$ (N_{ex} / N_i fixed)
- Two recombination models
  - Thomas-Imel "box" model (below $O(10)$ keV)
  - Doke's modified Birks' Law from 1988
- *Recombination probability* makes for non-linear yield: 2x energy does not mean 2x light + charge
- Excellent vetting against much past data (LXe)

The Work Function

- From Craig's LAr property summary document: **W = 19.5 eV** for scintillation and **23.6 eV** for ionization
- NEST unifies these two processes into just one work function
- $W\_scint = E / (N_{ex} + N_i)$ = 19.5 eV (complete recombination)
- $W\_ion = E / Ni = (E/N_i)*(N_{ex} + N_i)/(N_{ex} + N_i) = (N_{ex} + N_i)/N_i * E/(N_{ex}+N_i) = (N_{ex}/N_i + 1) * E/(N_{ex}+N_i)$ = 1.21***19.5** = **23.6 eV** (complete non-recombination, at infinite field)
- This is not how Geant4 treats the scintillation process, and one loses sight of the fundamental physics as a result
- This is not just numerology: it works, and it's not my own idea: See the Ph.D. Thesis of Eric Dahl (Princeton, 2009). I'm sure that others have thought of this as well…
- dE/dx dependence goes into the recombination probability, and not the work function: at low LET there is no "quenching," just a different amount of recombination

Re-Analysis of Old Data

Correct Energy = a * LY + b * CY
(we fix a field, and the yield is pretty flat in the GeV regime, so a, b "fixed")



- In LAr, the anti-correlation between light yield (LY) and charge yield (CY) simply got missed before
- Combining lets you empirically eliminate certain non-detector systematics, like recombination fluctuations

The dE/dx Dependence

- NEST takes the Birks' Law for scintillation yield and converts it into a recombination probability instead
- $dL/dE = A\,(dE/dx) / (1+B\,dE/dx)$ becomes
- $r = A\,(dE/dx) / (1+B\,dE/dx)$, which goes from 0 to 1 (if $A = B$)
- (NEST adds a '$+C$' for geminate recombination at zero field)
- dQ/dE can be thought of as escape probability, or, one minus the recombination probability. Let's derive the ICARUS formula used by default in LArSoft. $\mathscr{R} = Q/Q_0 = 1 - r =$

$$1 - \frac{k_B \frac{dE}{dx}}{1 + k_B \frac{dE}{dx}} = \frac{1 + k_B \frac{dE}{dx}}{1 + k_B \frac{dE}{dx}} - \frac{k_B \frac{dE}{dx}}{1 + k_B \frac{dE}{dx}} = \frac{1}{1 + k_B \frac{dE}{dx}}$$

0.8 in Amoruso

- ICARUS adds a normalization factor, but that breaks the (anti-) correlation between LY, CY. Non-unity normalization can not be easily justified if looking at a dimensionless recombination factor (as opposed to raw charge yield).

Field Dependence

- $k_B = k$/field (ICARUS, and other past works)
- Simple formula, but does it have to correct?
- Can “repair” the normalization constant (make it 1.0) if we generalize this equation to a power law, and do not rely solely on Birks (recall the Thomas-Imel recombination model)

Saturation curves and energy resolution of LRG ionization spectrometers

I. Obodovskiy

Moscow Engineering and Physical Institute
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Abstract: **Energy resolution of LRG ionization spectrometers is up to now very important and not fully understandable parameter. It is no doubt that at least part of contributions into overall energy resolution determines by the free-ion yield non-linearity. Two opportunities of free-ion yield definition are discussed – Jaffe approach and Birks’ law. Experimental results known up to now are analyzed to receive parameters that can be used for energy resolution calculations.**

INTRODUCTION

The considerable part of energy resolution of LRG ionization spectrometers is determined by free-ion yield nonlinearity, i.e. by the dependence of free-ion yield on electron energy.

One way is to choose some function that gives the best fit of the dependence of free-ion yield on electric field strength, the so called saturation curve. Then one needs to consider the dependence of the parameter of this function on electron energy or energy transfer and dopant concentration in mixtures.

The other way to parameterize the saturation effect is to take a function which describe the dependence of free-ion yield on electron energy or energy transfer. Then one needs to consider the dependence of the parameter of this function on electric field strength and dopant concentration in mixtures.

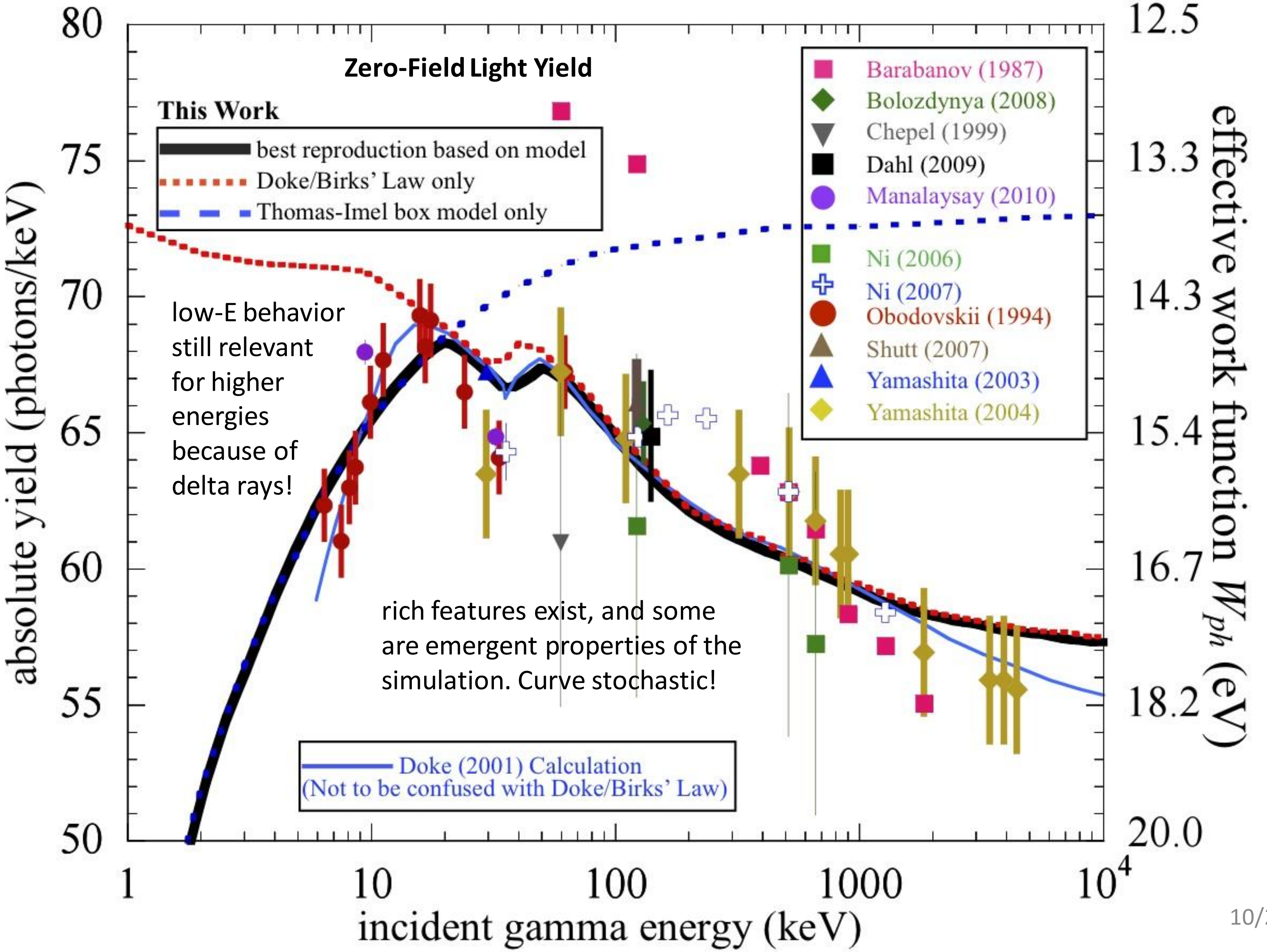
JAFFE SATURATION CURVES

<= Obodovskiy collected ALL available LAr scintillation and ionization data, and he got a different answer than ICARUS (though he included their data in his parameter fitting…)

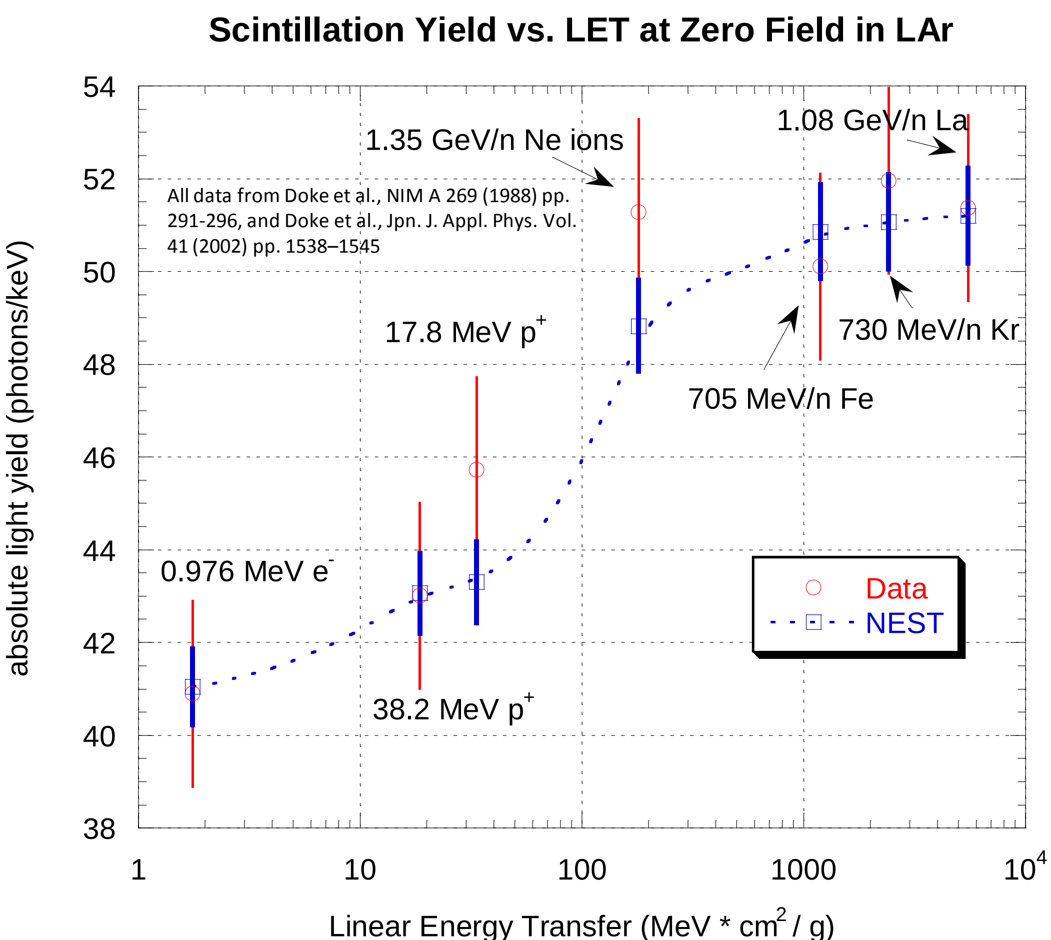
$$kB = 0.05F^{-0.85}$$

Example From Liquid Xenon

Szydagis et al., **NEST: A Comprehensive Model for Scintillation Yield in Liquid Xenon**, [2011 JINST 6 P10002]; e-Print: [arxiv:1106.1613 [physics.ins-det]]



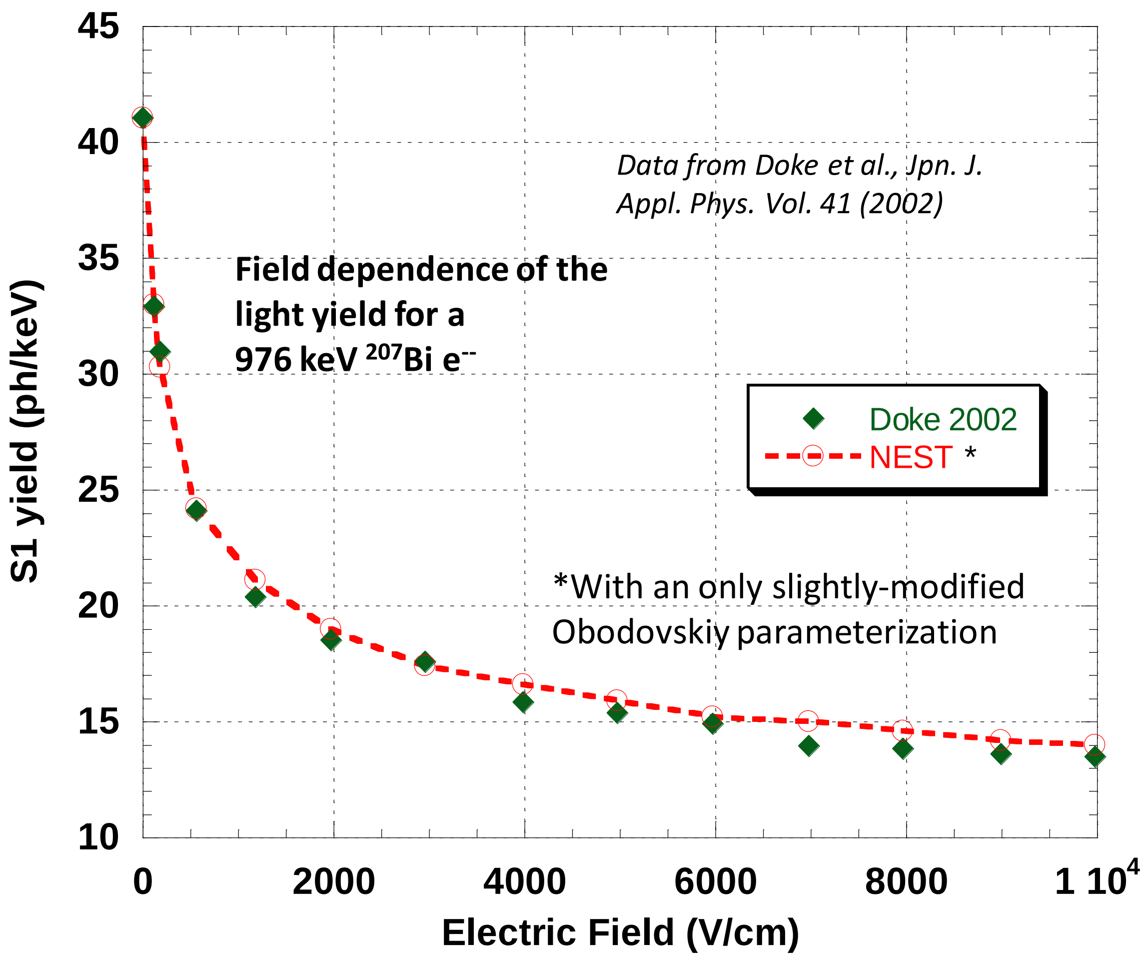
Zero-Field Liquid Argon



- NEST does not have HIPs (highly-ionizing particles) yet, but eventually
- NEST grew out of lower energies (for DM searches in Xe), graduating to the multi-MeV to GeV regime successfully
- Summing all sources of LY

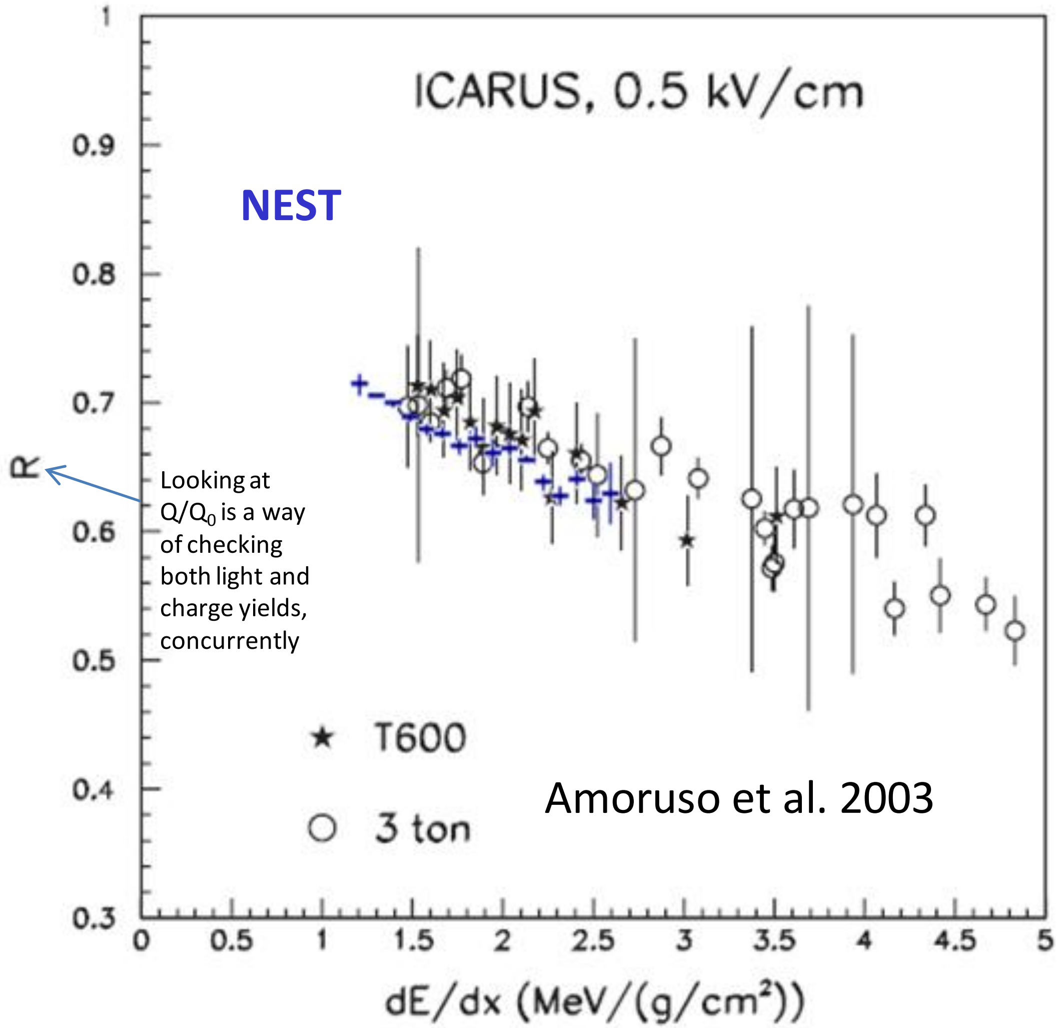
$$\mathrm{d}L/\mathrm{d}E = (\mathrm{d}L/\mathrm{d}E)_{\mathrm{v}} + (\mathrm{d}L/\mathrm{d}E)_{\mathrm{g}} + (\mathrm{d}L/\mathrm{d}E)_{\mathrm{ex}} = \frac{SKC(\mathrm{d}E/\mathrm{d}x)}{1 + C(\mathrm{d}E/\mathrm{d}x)} + \eta_0 .$$

MIPs at Any Field



- Generalization to any electric field possible, not just the common low fields such as 500 V/cm field
- Makes it simple to use NEST to optimize the field for a detector: energy resolution and energy (LY) threshold considerations

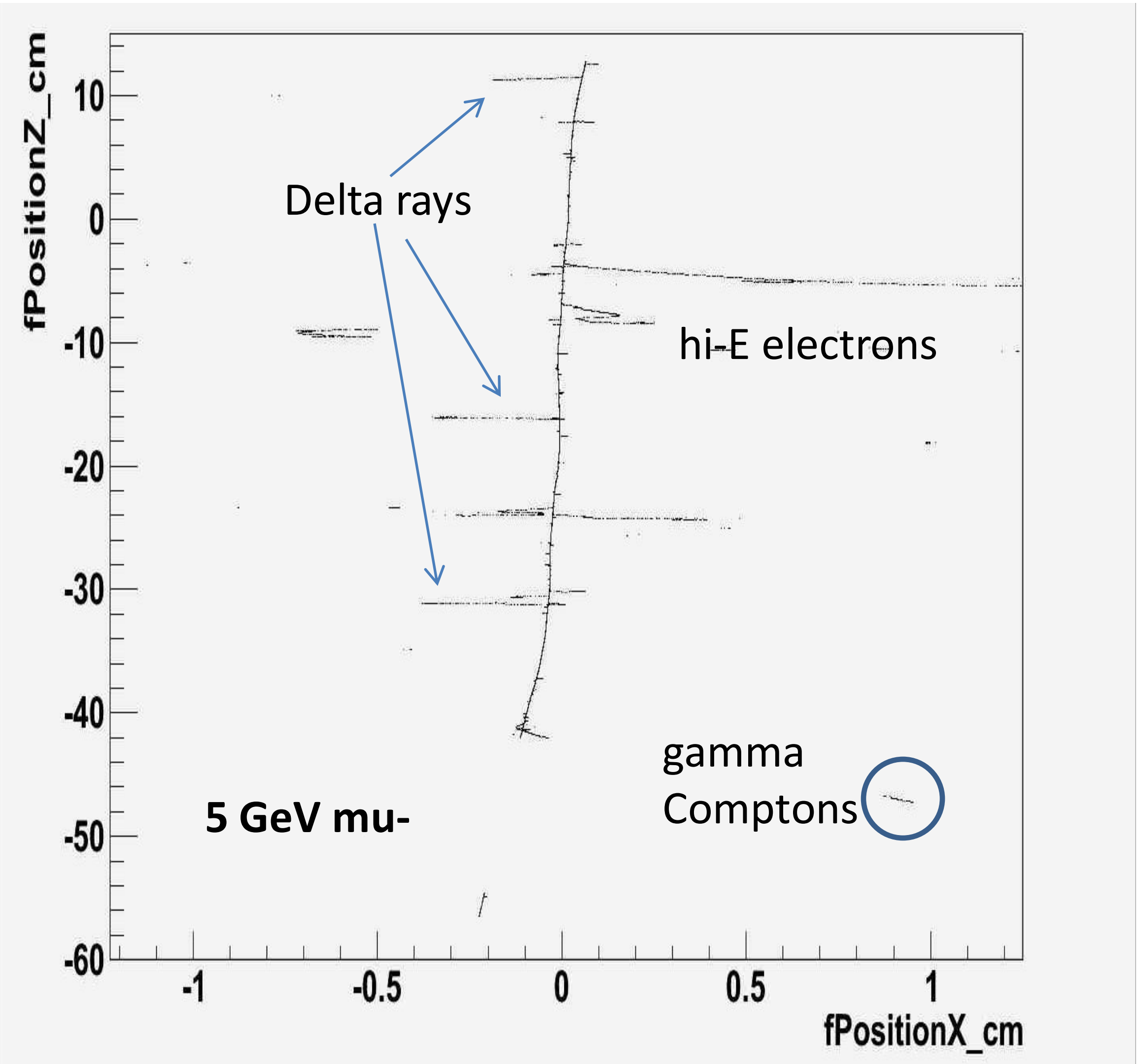
More Comparison to Data



- Progressing through simulations out to higher LET's
- Needed to tweak the power law amplitude for the Birks' constant's field dependence from 0.05 to 0.07
- Following through on other fields (200 and 350 V/cm)
- Particle type matters

Secret to Success

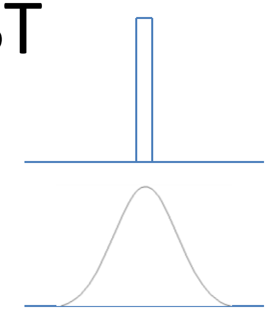
- See Christmas-tree structure of secondary tracks. Many are low enough in energy to be governed by the Thomas-Imel box model of recombination.
- Using T-I in concert with Birks eliminates the need for artificial re-normalization, and other MC “fudge factors”*



* You also need a short G4 track-length cut-off

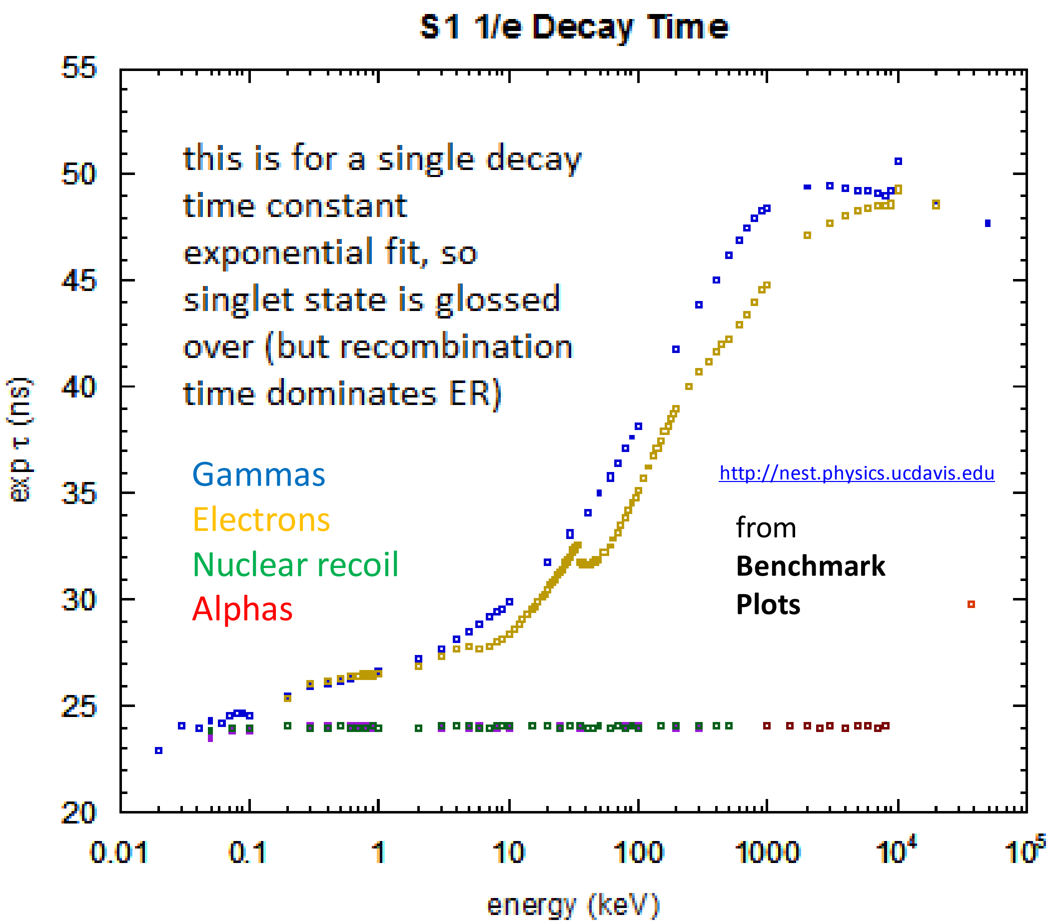
Energy Resolution

- Long list of effects now included in NEST
  - Fano factor (a very small effect)
  - N_{ex} vs. N_i (binomial fluctuation)
  - Recombination fluctuations
    - Binomial (to recombine, or not to recombine)
    - Non-binomial for LXe (no fudge factor for LAr)
  - Geant4 stochastic dE/dx variation
  - Particle track history (also Geant4)
  - Finite quantum efficiency (end-user)
  - Imperfect light collection (Geant4)
- Angle of particle track with respect to electric field vector not yet included



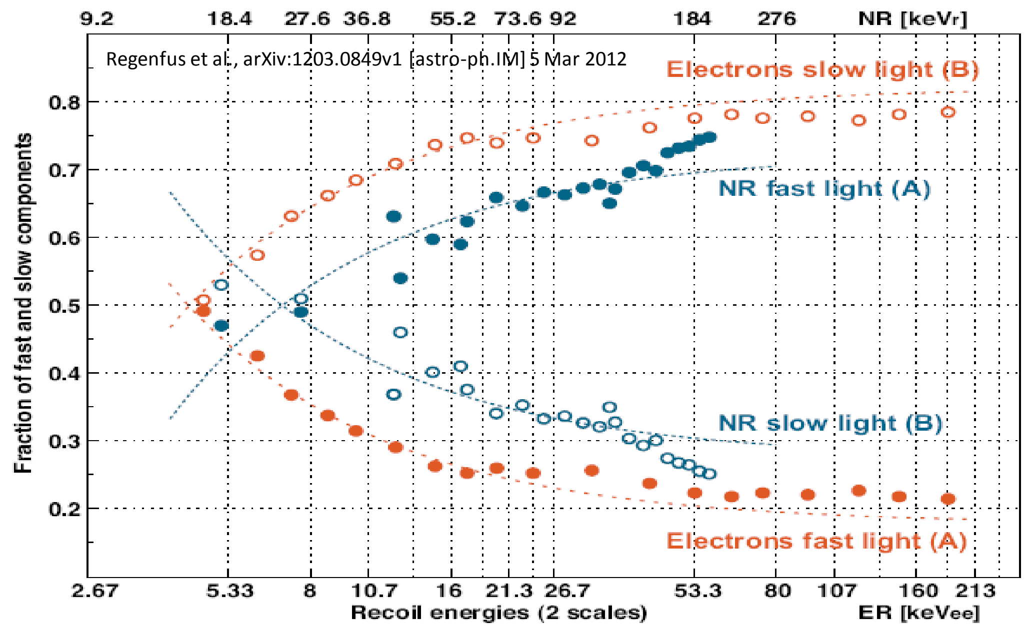
Understanding Pulse Shape (Xe)

- Two exponential time constants corresponding with the triplet and singlet Xe dimer states, but the triplet dominates
- Recombination goes as 1 / time, but time constant not fixed (related to the LET). Constant is < 1 ns in LAr even at zero field (Kubota, 1979)



Understanding Pulse Shape (Ar)

- The next version of NEST will incorporate these results at right
- We will convert this into a function of LET instead of energy, and impurity concentration
- This will be a big step forward in LAr modeling, giving us the correct, non-constant ratio of triplet to singlet



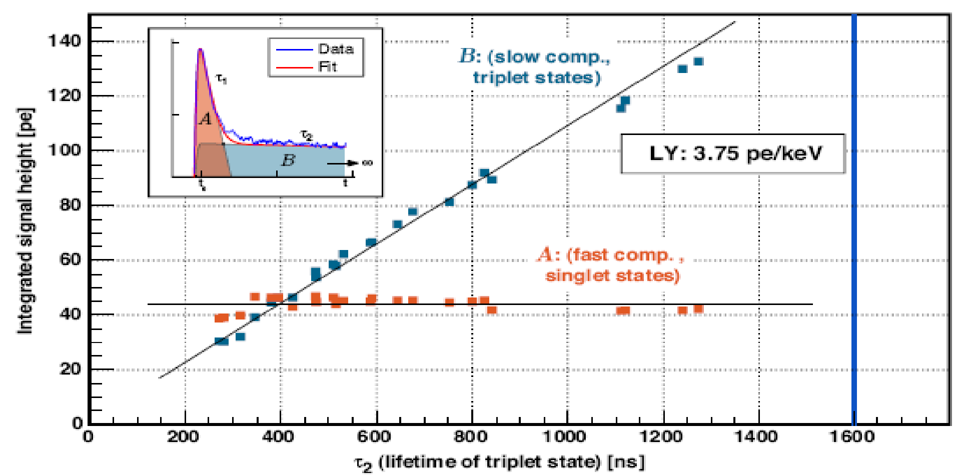
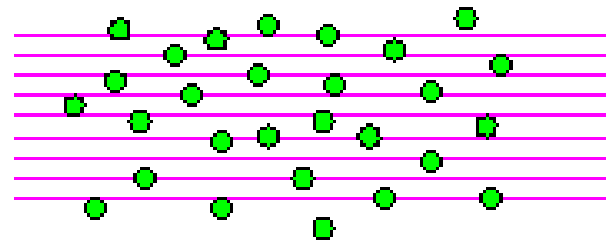


Figure 3. *Yield of the fast and slow scintillation components under different purity conditions.*

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 run 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 speed simulation time, NEST has a built-in feature for charge yield reduction

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

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng
```

Conclusions

- NEST has a firmer grasp of the microphysics than other approaches. It is not “faith-based” or just connect-the-dots
- **It is closer to first principles, considering the excitation, ionization, and recombination physics, resorting to empirical fits/splines/extrapolations as indirect fits or not at all**
- Anti-correlation between scintillation and charge falls out naturally without a need for unphysical correction factors
- Easy to install: no other software dependencies than Geant4. Just ~1 day of work to override the G4Scintillation process
- Extensive empirical verification against past data underway using multiple sources instead of only one experiment
- Liquid xenon is essentially finished, but there is still work being done for liquid argon, though it is progressing rapidly

References

- For all of the references used in this talk, please consult the full bibliography of

  M. Szydagis et al., NEST: A Comprehensive Model For Scintillation Yield in Liquid Xenon 2011 **JINST** 6 P10002. arxiv:1106.1613

  (Our paper does not have everything covered in this talk or already available in the code, but more papers are on the way....)