A Symphony of Scintillation

Noble **E**lement **S**imulation **T**echnique, MC Code for 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

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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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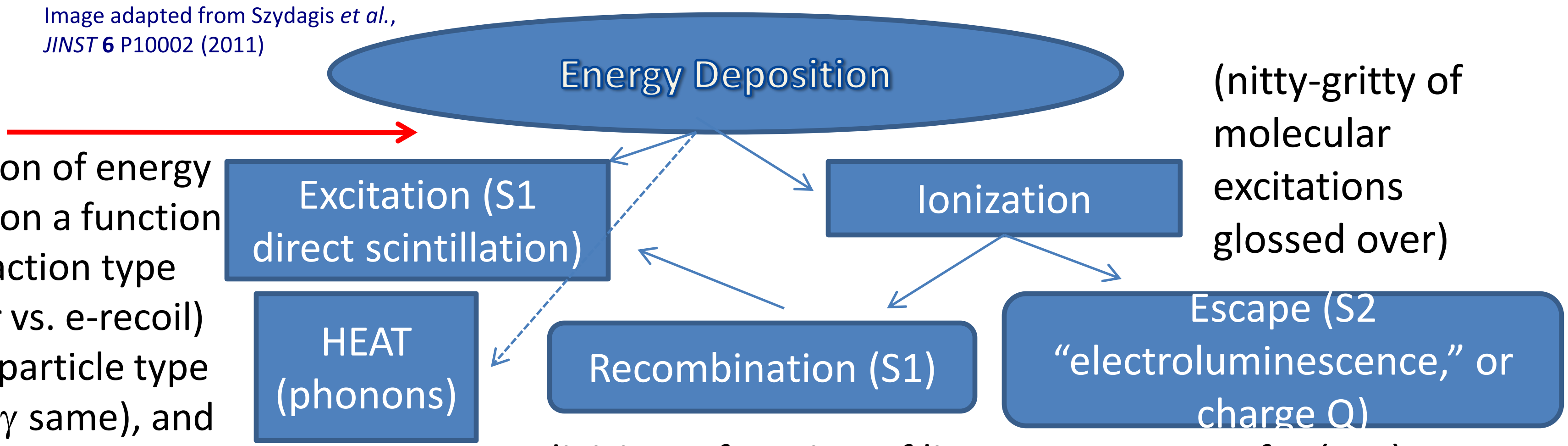
Summer undergraduates (many)

The Purpose and Scope

- 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 neutrino, dark matter, and other experiments which utilize this technology to be on the same page, or at least a comparable page, with simulations
- Bring added realism to the simple model that is present right now in Geant4 for scintillation (G4Scintillation)
- Explore backgrounds at low energy by extending the accuracy of Geant4 physics down to a low energy regime
- Started with LXe (for LUX) and moving on to LAr now

Basic Physics Principles



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

(nitty-gritty of molecular excitations glossed over)

(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!

Definitions

- W: work function (units of energy)
- E: amount of energy deposited in the liquid
- N_{ex} : number of excitons
- N_i : number of ions
- N_{e-} : number of electrons
- N_γ : number of photons (not photo-electrons)
- N_q : total number of quanta produced by an energy deposition. Equals $N_{ex} + N_i = N_\gamma + N_{e-}$
- r: recombination probability for ionization e-'s
- R or Q/Q_0: fractional escape probability

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

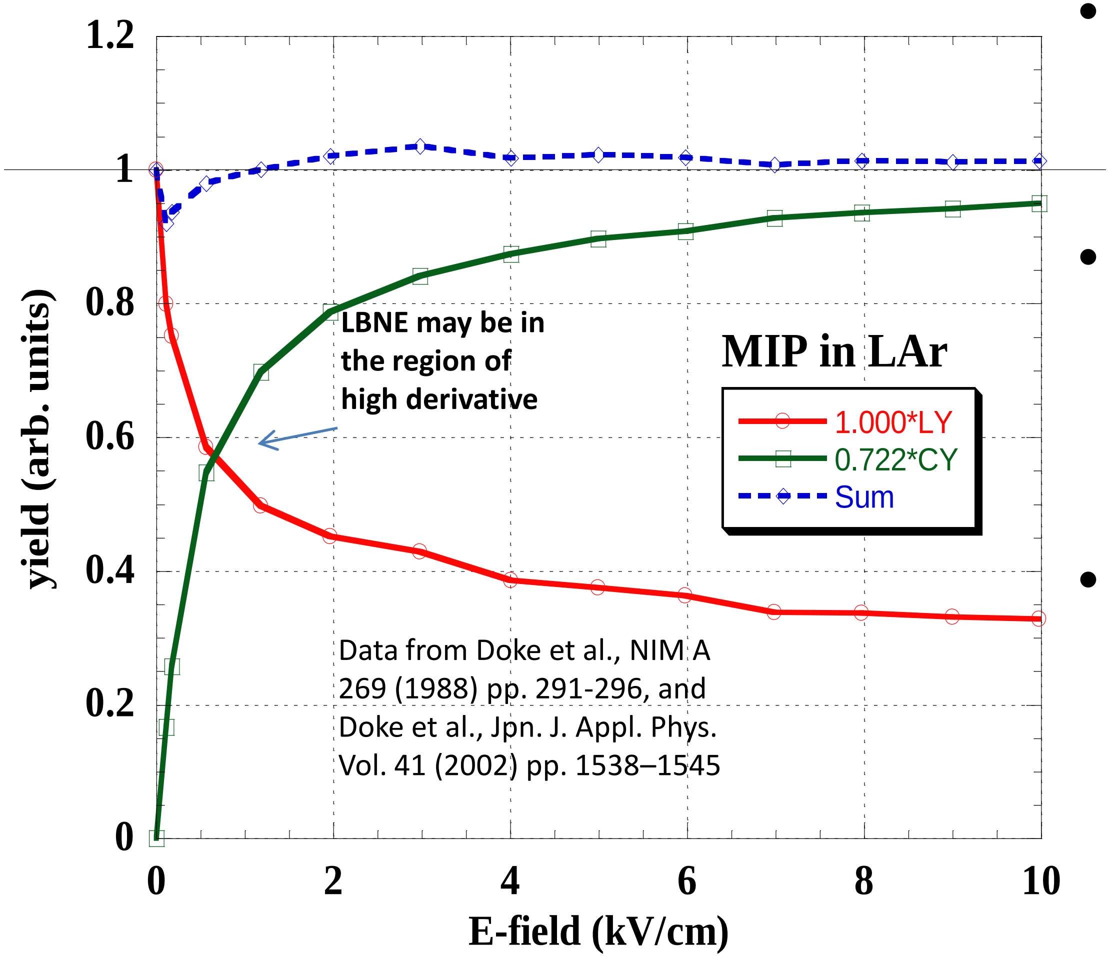
- From C. Thorn's LAr property summary document on docDB: **W = 19.5 eV** for scintillation and **23.6 eV** for ionization

- *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** (no recombination; infinite field)

- This is *not* how G4 treats the scintillation process, and one loses sight of the fundamentals
- dE/dx dependence goes into the recombination probability, not W: at low LET no "quenching"-- less recombination

Confirmed by Re-Analysis

Correct absolute 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, anti-correlation between light yield (LY) and charge (CY) missed
- Combining lets you empirically eliminate non-detector systematics, like recomb. fluctuations
- **In LANL TPC calibrations, we can use mono-energetic sources and sweep the field, a measurement I strongly recommend we make**

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

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Kashirskoe shosse, 31, Moscow, 115409, Russia

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.

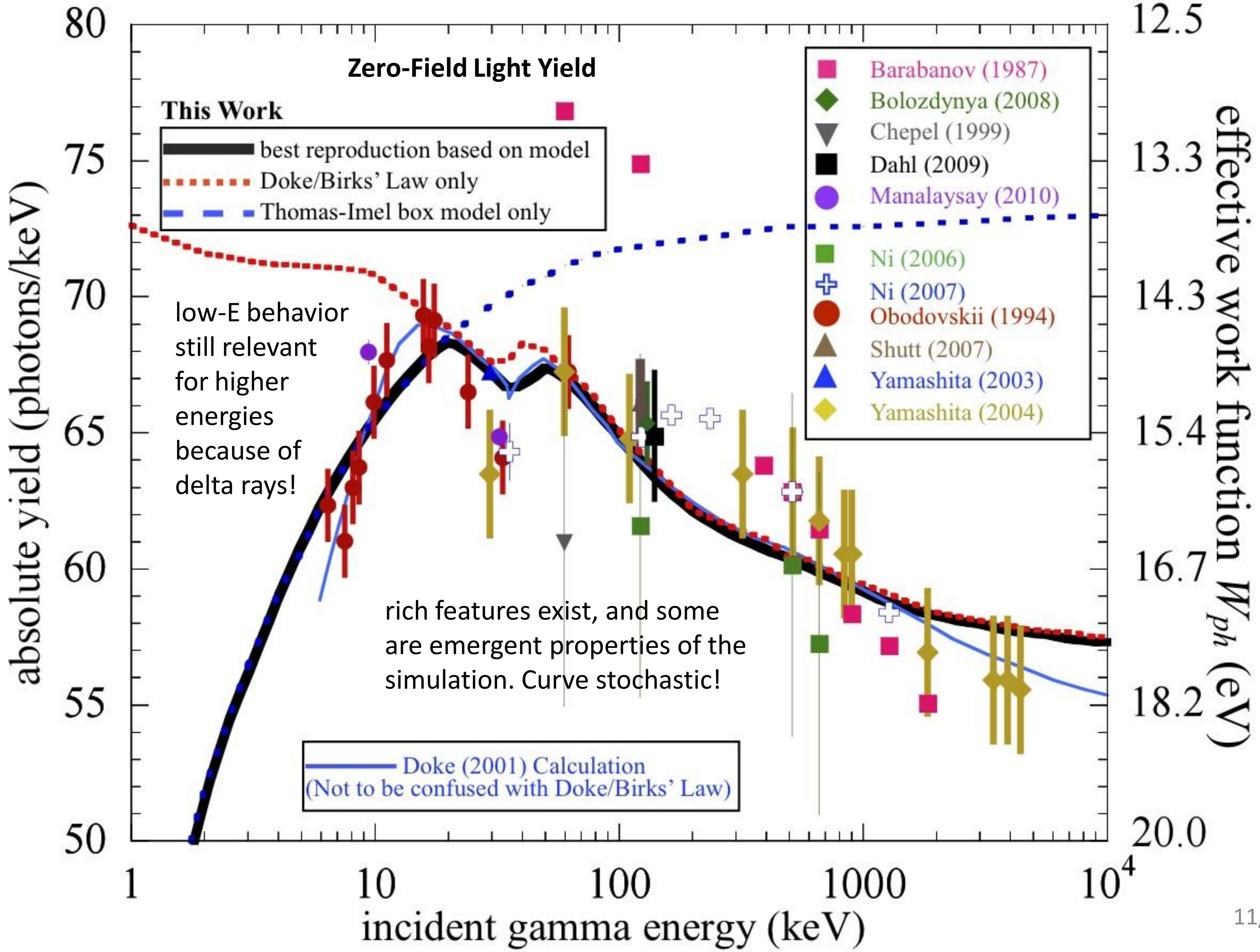
JAFFE SATURATION CURVES

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

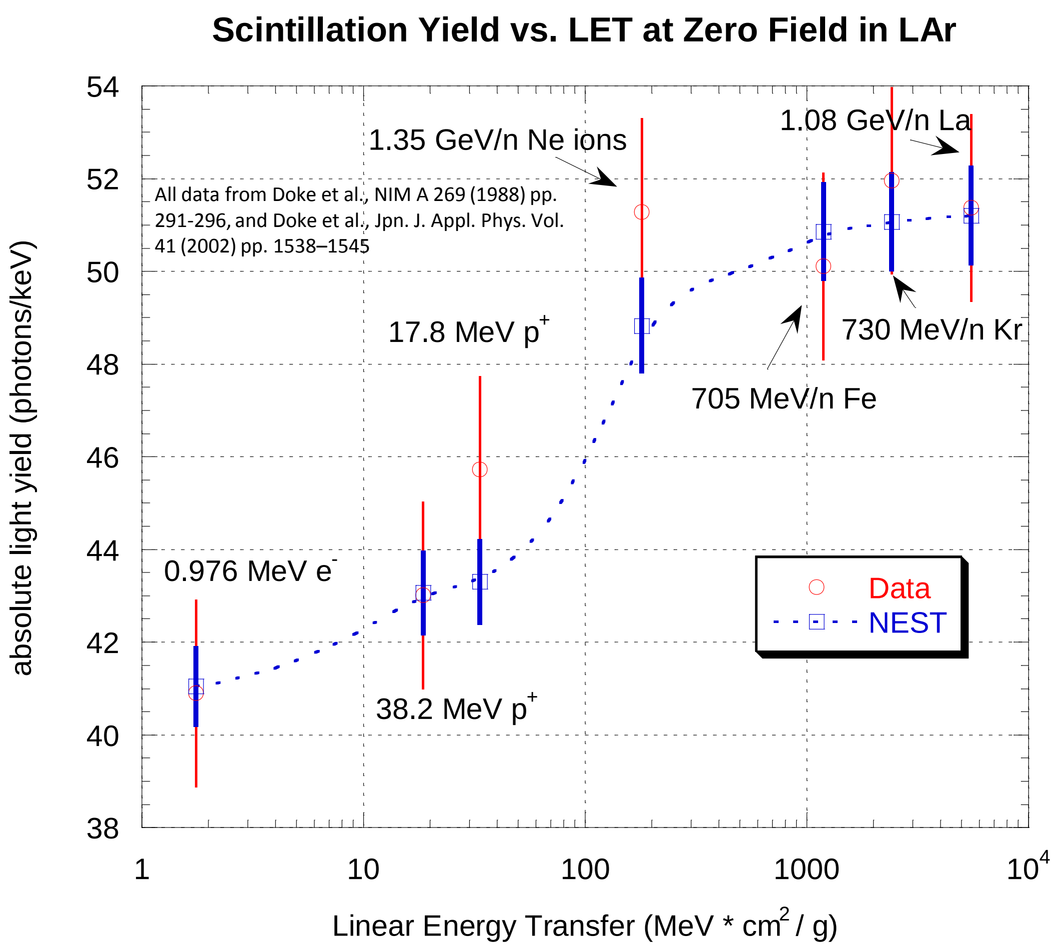
$$kB = 0.05F^{-0.85}$$

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]

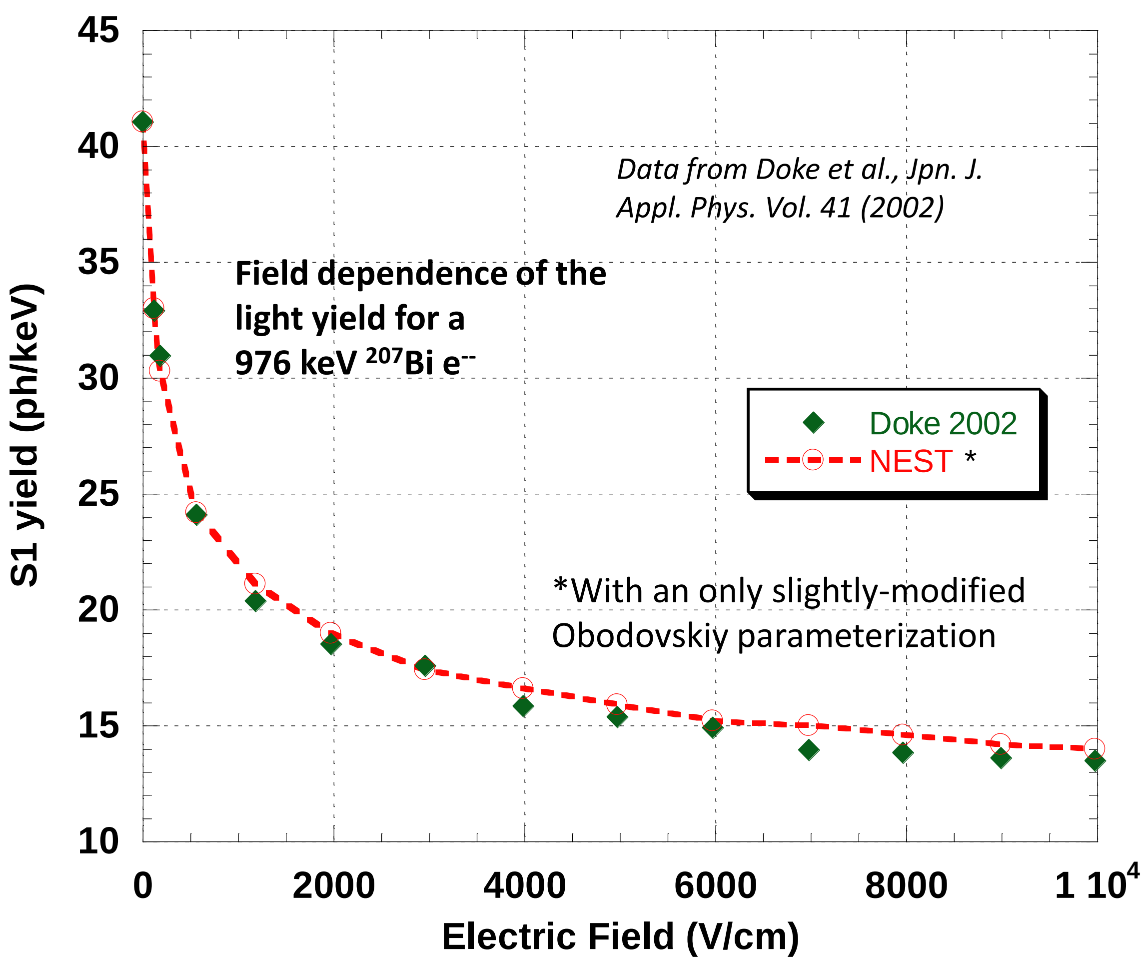


Zero Field Liquid Argon



- 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: excitons plus recombination, both geminate (fast) and volume

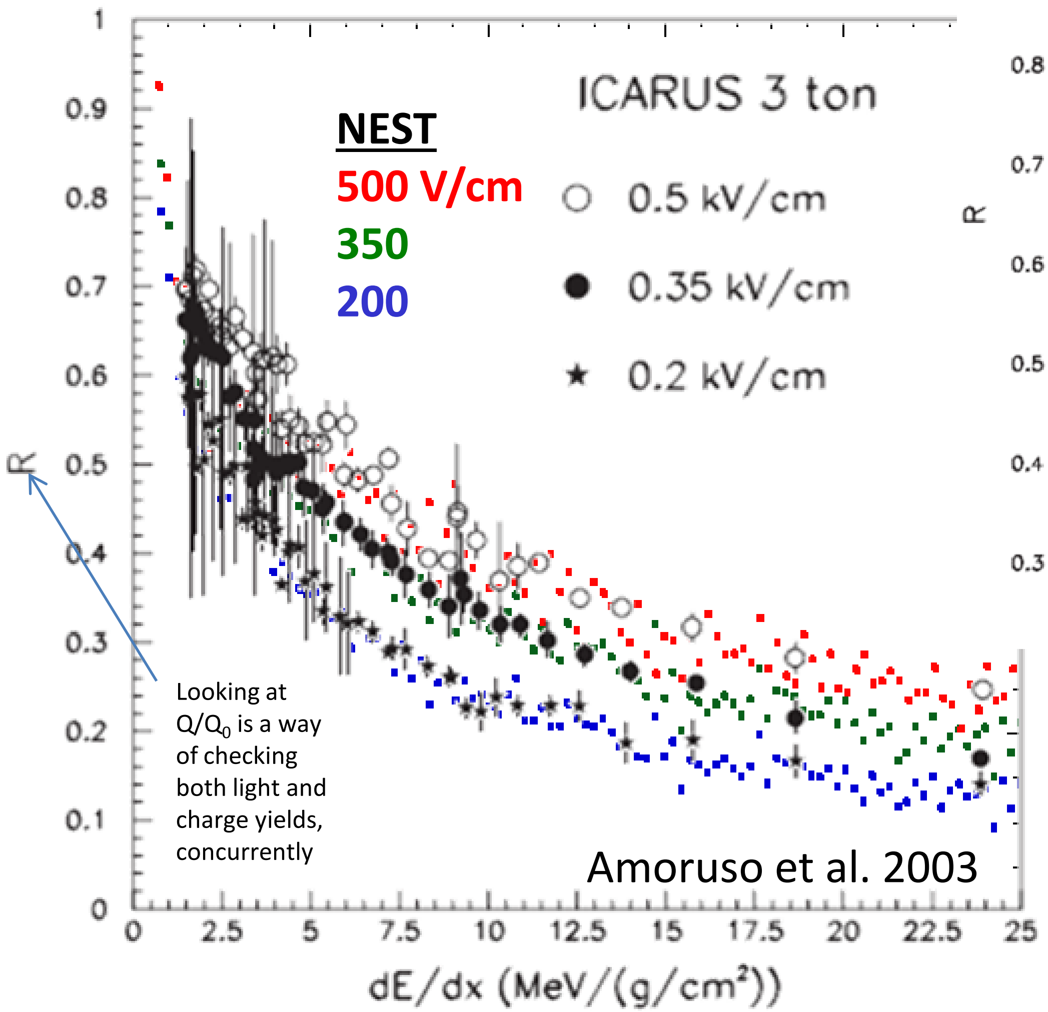
MIPs at Any Field

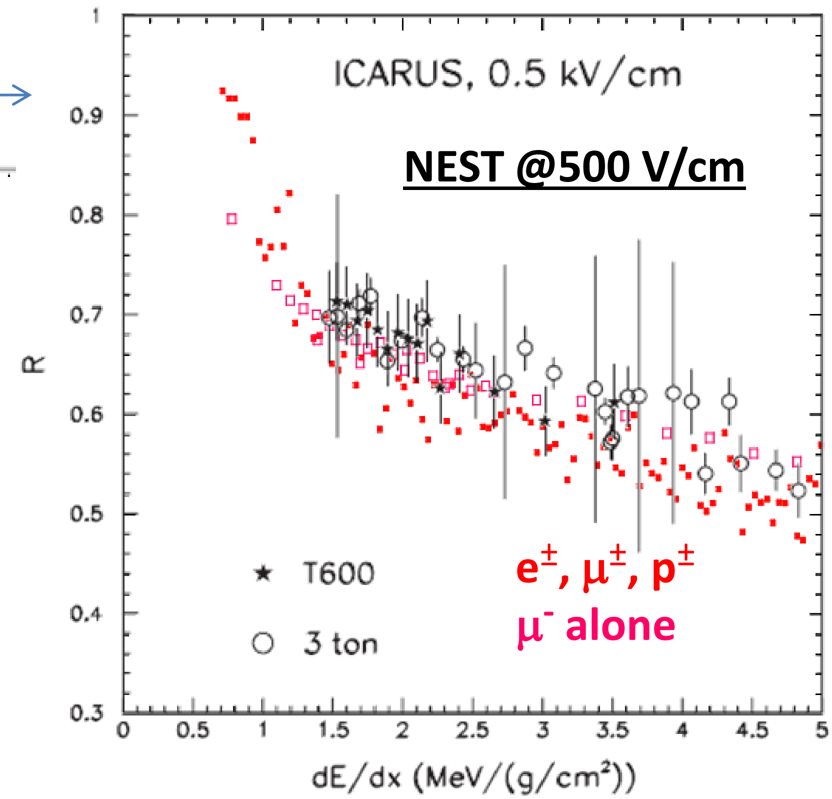


- Generalization for any field possible, not just the common low fields such as 500 V/cm field
- Makes it simple to use NEST to optimize the field for a detector: energy resolution and energy (LY) threshold considerations

More Comparison to Data

Particle type does matter!

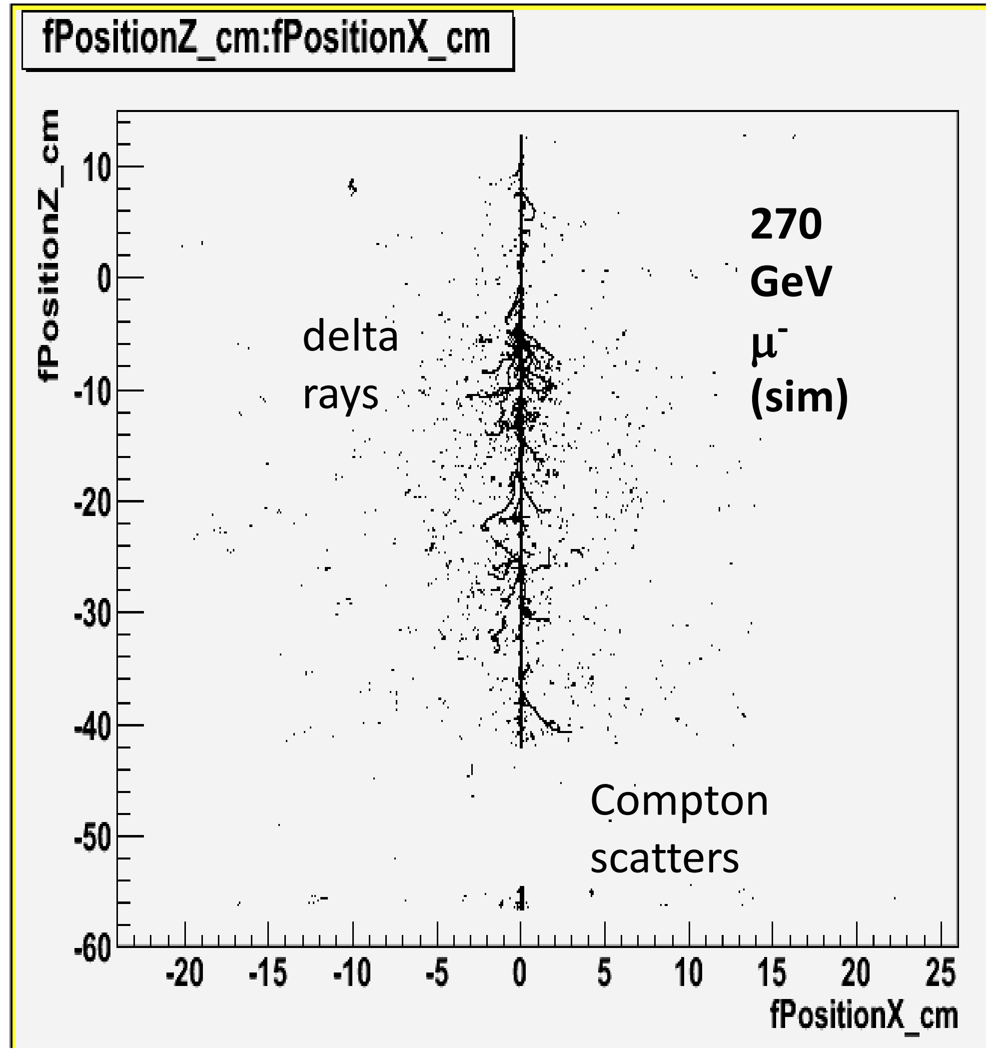




- Demonstration that a -0.85 instead of a -1 power law for the Birks field dependence OK

Secret to Success

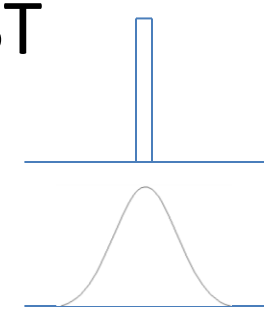
- See Christmas-tree structure of secondary tracks. Many are low enough in energy to be governed by the Thomas-Imel box model of recombination.
- Using T-I box in concert with Birks eliminates the need for artificial re-normalization, and other MC correction factors*



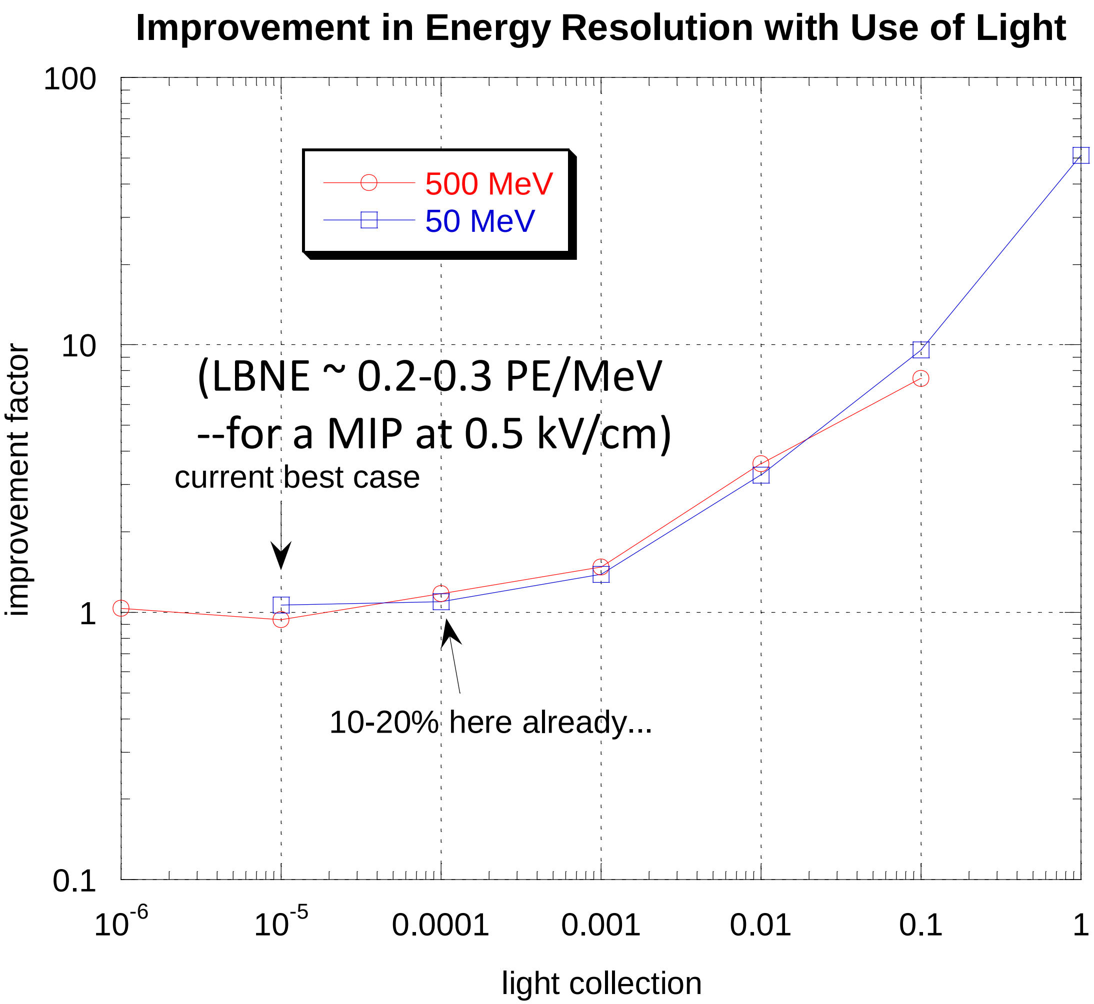
* You also need a short G4 track-length cut-off

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 the electric field vector not yet included



Energy Resolution

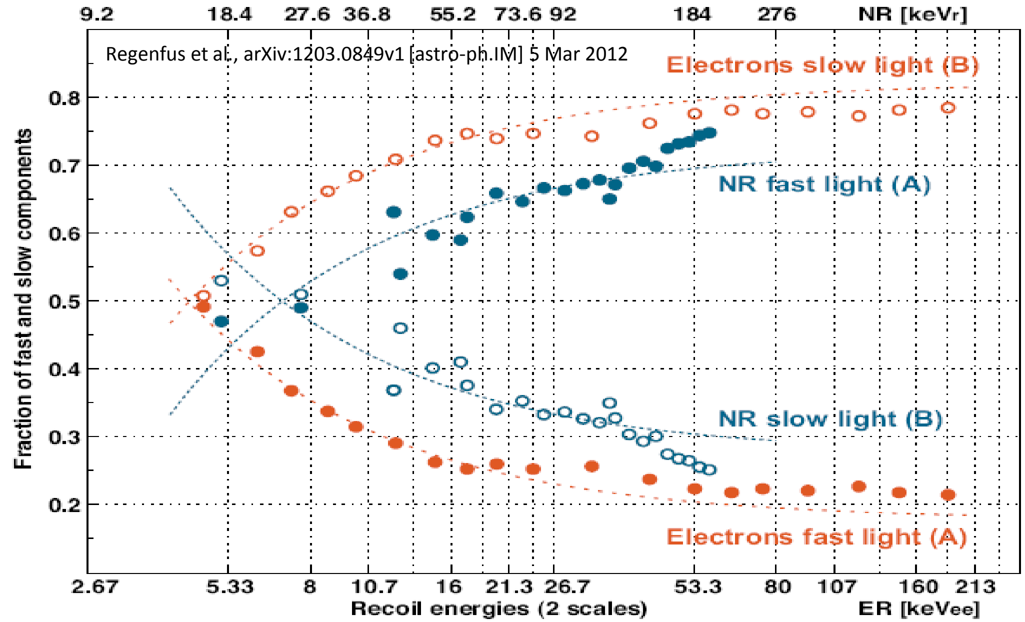


	LC (frac)	CY [%]	LY [%]	comb [%]	opt [%]	<-- with	improv
500 MeV	1.00E-06	0.33	79.32	0	0.32	0.001	1.0313
	1.00E-05	0.31	9.07	3.28	0.33	0.1	0.93939
	1.00E-04	0.34	3.96	1.19	0.29	900	1.1724
	0.001	0.34	1.2	0.33	0.23	300	1.4783
	0.01	0.36	0.72	0.12	0.1	90	3.6
	0.1	0.27	0.48	0.037	0.036	11	7.5
50 MeV	1.00E-06	0.98	100				
	1.00E-05	1.21	29.01	10.96	1.14	0	1.0614
	1.00E-04	1.01	9.95	3.51	0.92	900	1.0978
	0.001	0.93	3.8	1.11	0.67	300	1.3881
	0.01	1.11	2.39	0.37	0.34	90	3.2647
	0.1	1.05	2.18	0.11	0.11	10	9.5455
	1	0.97	1.91	0.019	0.019	1	51.053

- **We have some ways to go before seeing an enhancement, but this result tells us that we should NOT neglect optimization of LY**
- Proven in LXe: see "Correlated fluctuations between luminescence and ionization in liquid xenon", E. Conti et al., Phys. Rev. B 68, 054201 (2003) . Real in LAr too (p. 7)

Understanding Pulse Shape

- The latest version of NEST 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, non-constant ratio of triplet to singlet



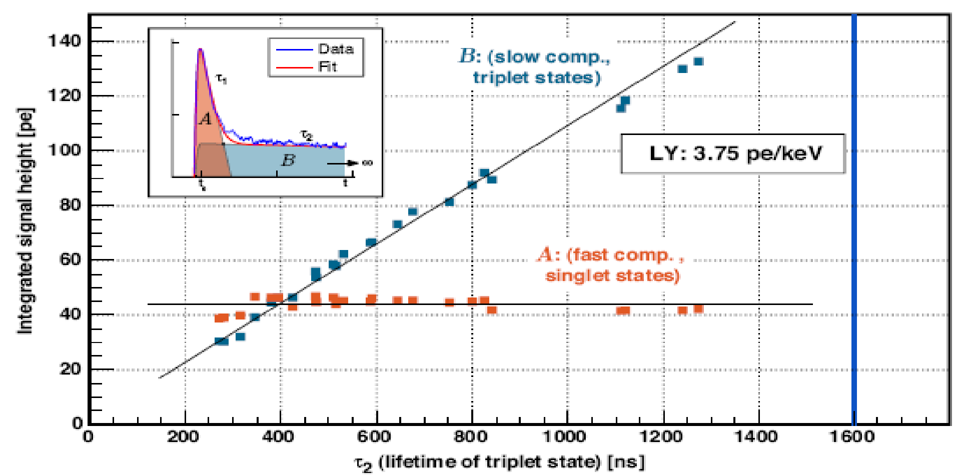
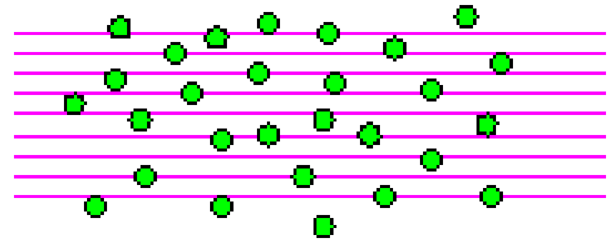


Figure 3. *Yield of the fast and slow scintillation components under different purity conditions.*

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 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
*******************************************************************************

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

Conclusions

- Simulation package NEST has a firm grasp of microphysics
- **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**
- Extensive empirical verification against past data underway 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

- **LANL TPC running will help to improve our understanding of the microphysics if the light collection is great and it gets combined with charge, to verify the anti-correlation between scintillation and charge and hopefully augment our energy resolution successfully**

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....)