A New Expansion and Realism Addition to the Scintillation Physics in GEANT4

UC Davis and LLNL

Faculty
Mani Tripathi
Bob Svoboda

Postdocs and Research Scientists
Matthew Szydagis
Kareem Kazkaz

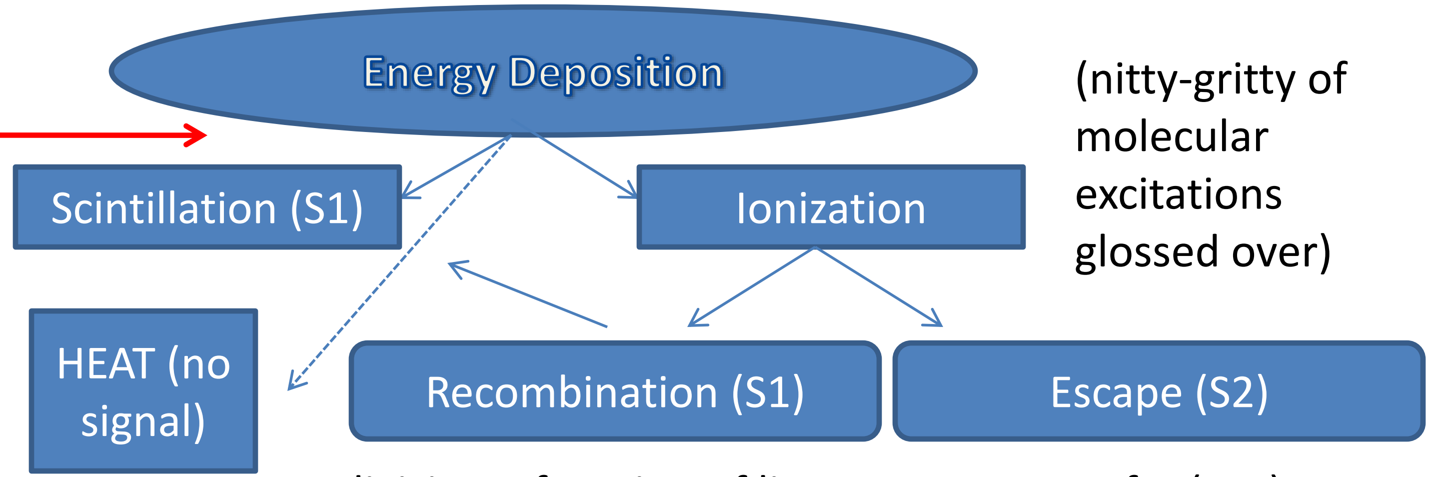
Undergraduates
Nichole Barry
Alex Shei
Dustin Stolp

Graduate Students
Jeremy Mock
Melinda Sweany
Sergey Uvarov
Nick Walsh
Mike Woods

Purpose

- Create a full-fledged simulation based on a heuristic, semi-empirical approach
- Comb the wealth of data for liquid and gaseous noble elements for different particles, energies, electric fields & combine all
- Aid the many dark matter (and $0\nu\mathrm{BB}$ decay) collaborations which utilize this technology to be on the same page w.r.t. to simulation
- Bring realism to the constant-yield model in GEANT4 at present for nobles
- Explore backgrounds at low energy by expanding GEANT4 physics to be more accurate in the energy regime O(1 keV)

Basic Physics Principles



(nitty-gritty of molecular excitations glossed over)

division of deposition energy 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 kinetic energy

(the infamous $\mathcal{L}$ value)

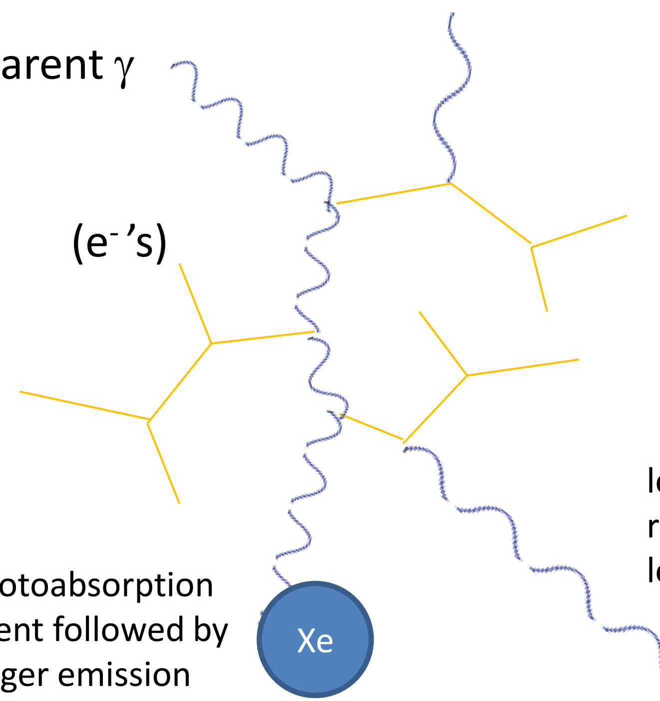
division a function of linear energy transfer (LET) or stopping power (dE/dx) because of ionization density considerations, and of electric field magnitude

- Heat loss for nuclear recoils (Lindhard effect); electron recoils easier to deal with (or are they …?)
- Starting simple: no exotic energy loss mechanisms (like "bi-excitonic" collisions). Explains data?

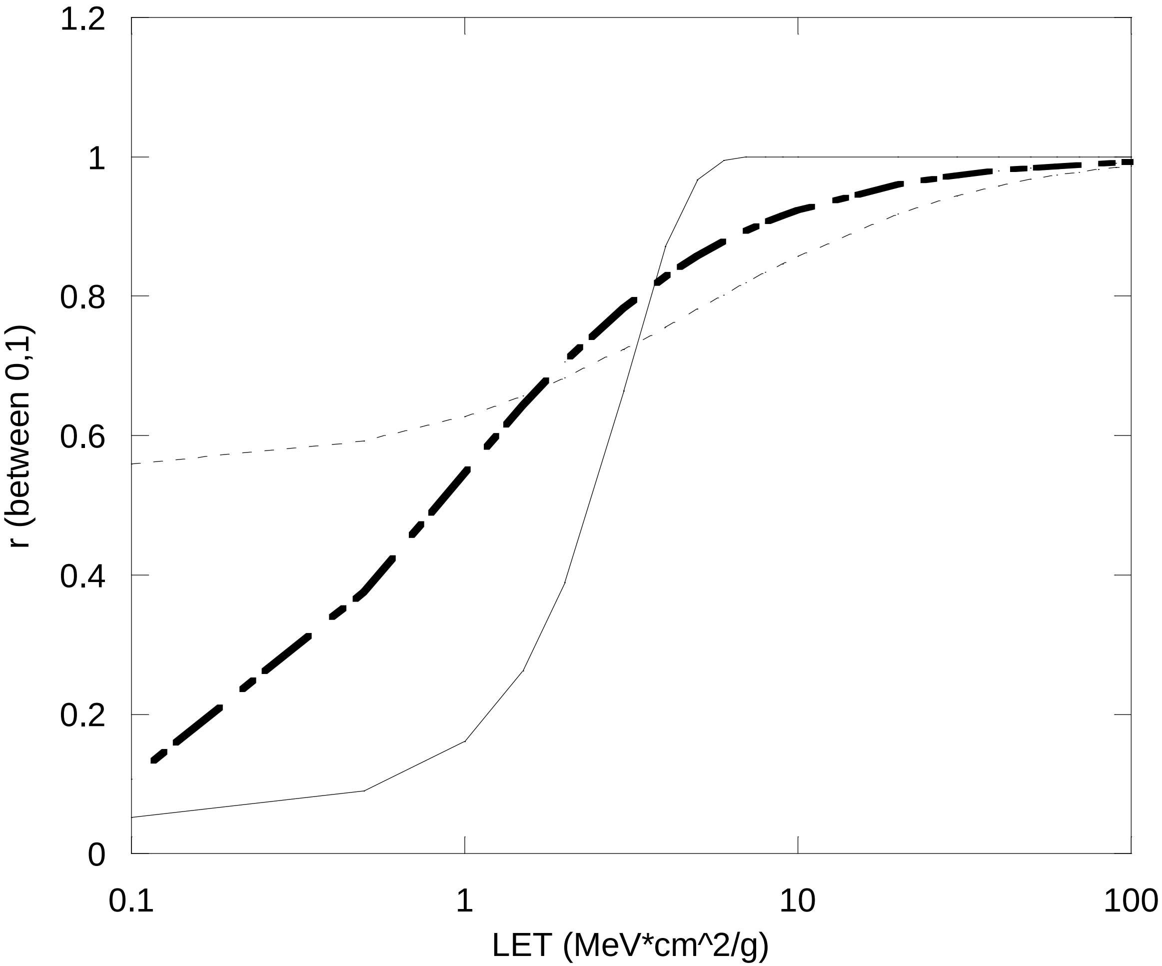
Model Framework: Electron Recoils

- Looking at the GEANT tracking verbosity: different energy depositions from the secondary electrons and gammas in an EM-cascade
- Let's allow the recombination to fluctuate stochastically by treating every electron recoil on its own

```
* G4Track Information:   Particle = gamma,   Track ID = 3,   Parent ID = 1
*******************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0   -0.717    -4.18     -141    0.0298        0        0         0 LiquidXenon initStep
    1    -1.07    -3.87     -141    0.0269 0.000678    0.484     0.484 LiquidXenon compt
    2    -1.14    -4.18     -140         0  0.00542    0.565      1.05 LiquidXenon phot

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

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0    -1.14    -4.18     -140    0.0215        0        0         0 LiquidXenon initStep
    1    -1.14    -4.18     -140   0.00877  0.00795  0.00306   0.00306 LiquidXenon eIoni
```



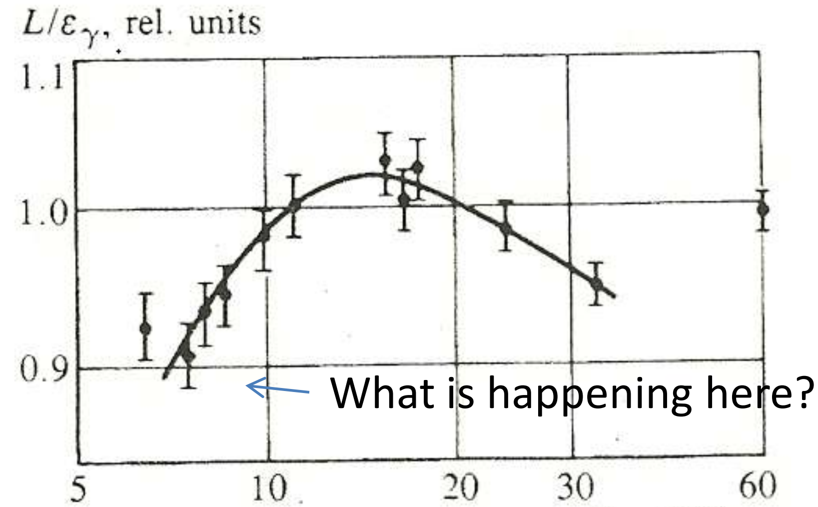
The Recombination Probability



- Important for predicting the light yield correctly (at least for Xe, Ar): most primary scintillation comes from recombined electrons (not direct)
- Many theoretical models tried; we picked one theoretically motivated that fits majority of xenon data + fits best
- Curve adapted continuously for electric fields: more field -> more low-energy ionization e's (from the higher-energy recoils) escape (and drift)

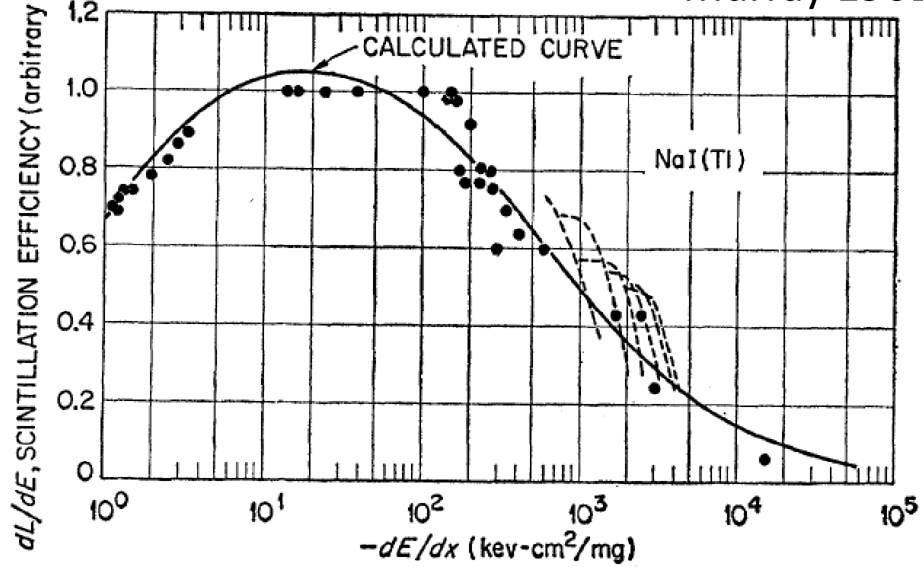
Anomalous Low-Energy Behavior

- Seen also in NaI[Tl] crystal
- Important region we must understand: what happens to electron/nuclear recoil discrimination here? What backgrounds are relevant?
- Unnatural for noble, and cannot be explained by a simple turn-over in the recombination probability
  - How to explain why a 5 keV γ scintillates less than 10?
  - Makes electron recoils look more like nuclear recoils
- Not understood for years in xenon; is it an $\mathscr{L}_{eff}$ clue…?



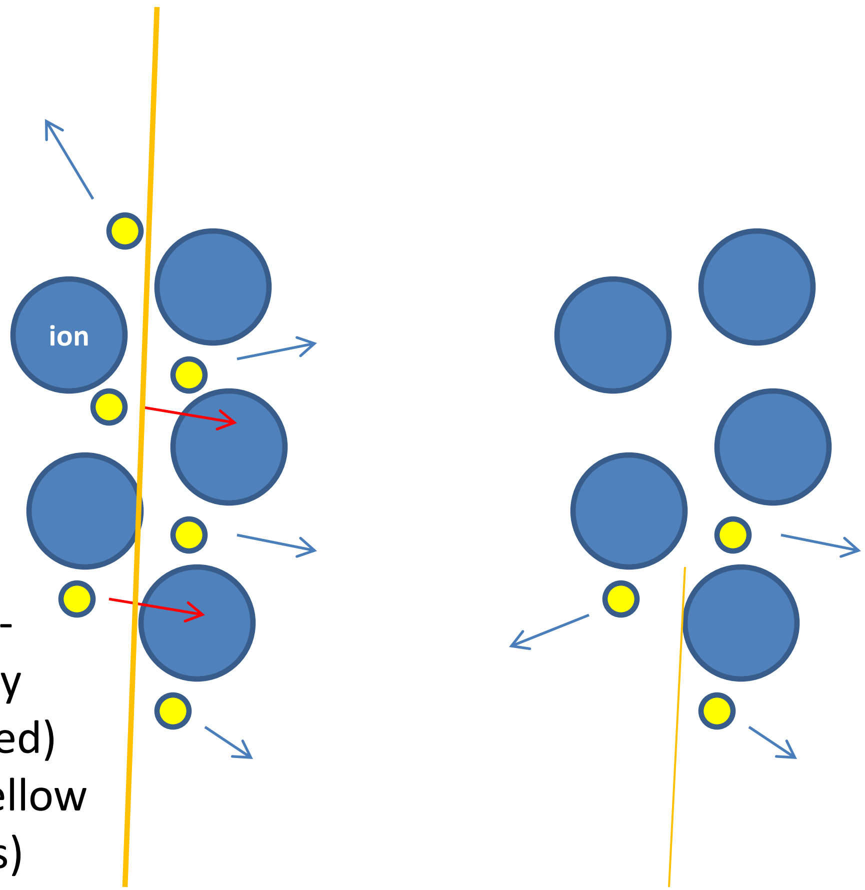
Obodovsky 1994

Murray 1961



A Solution at Last?

e^- recoiling from the parent gamma



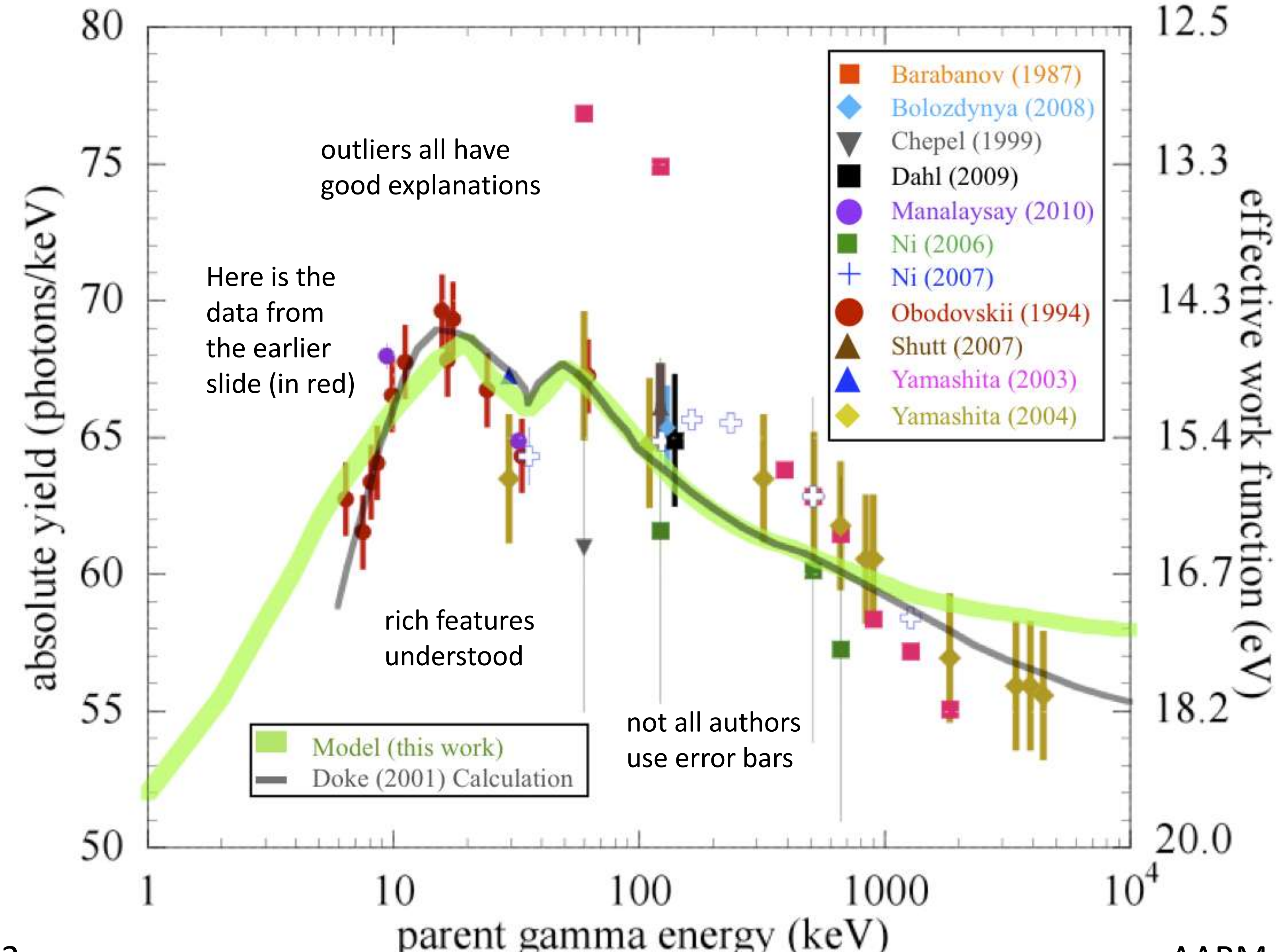
lower-energy (ionized) e^- (yellow circles)

LONG TRACK (HIGH-ENERGY)
-Many ionizations
-Freed electrons have many opportunities to recombine with ions all along the track

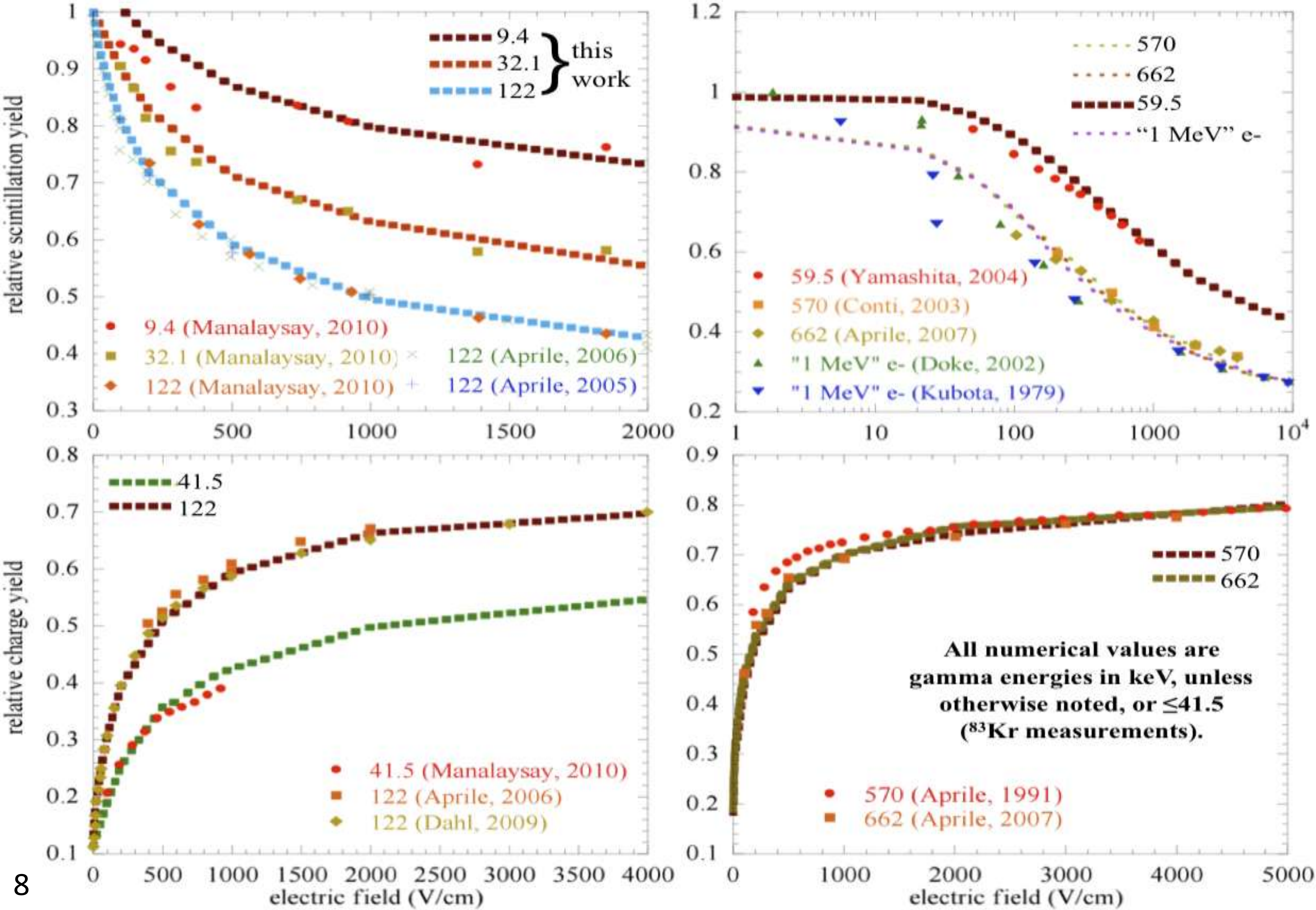
SHORT TRACK (LOW-ENERGY)
-Fewer ionizations
-Freed electrons are now attracted by fewer ions, so can escape more easily

- Low-energy particles have short ranges
- Liberated electrons see fewer opportunities to get recaptured by the ionized atoms, so more get away without recombining and going on to make scintillation
- GEANT4 does not simulate the lowest-energy ionization electrons, but we can approximate
  - Define minimum track length
  - Force dE/dx to decrease

Putting it All Together to Predict Yield

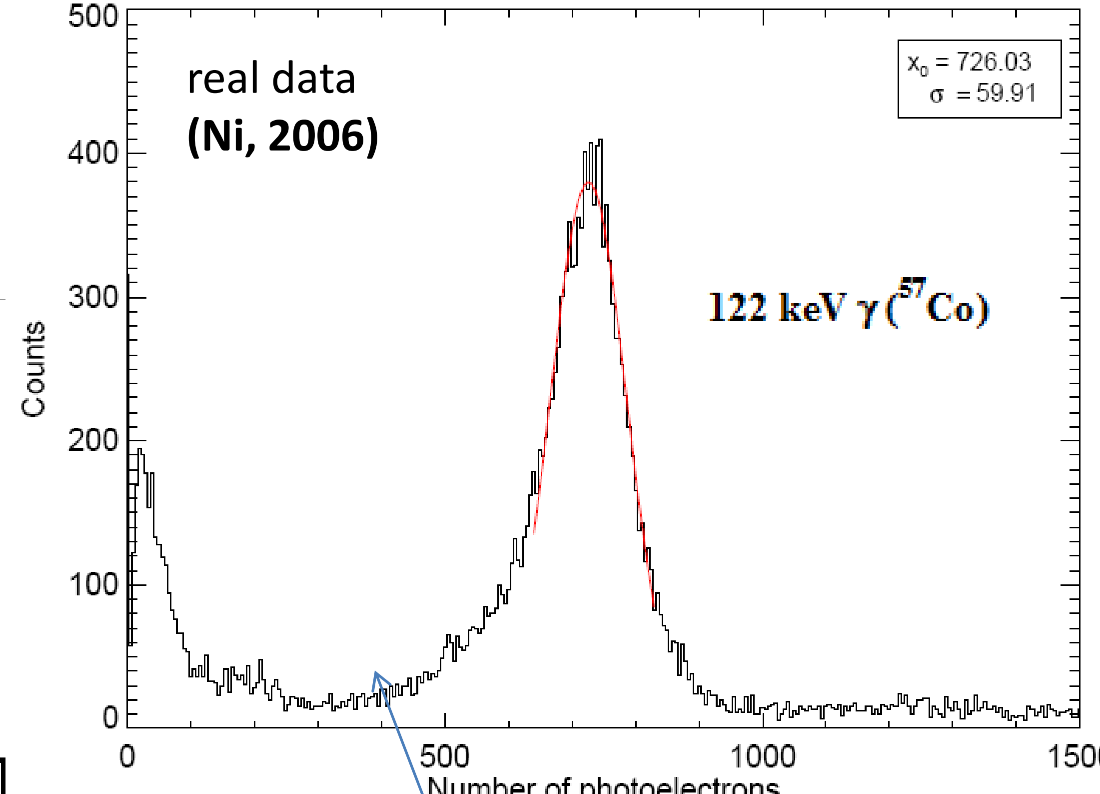


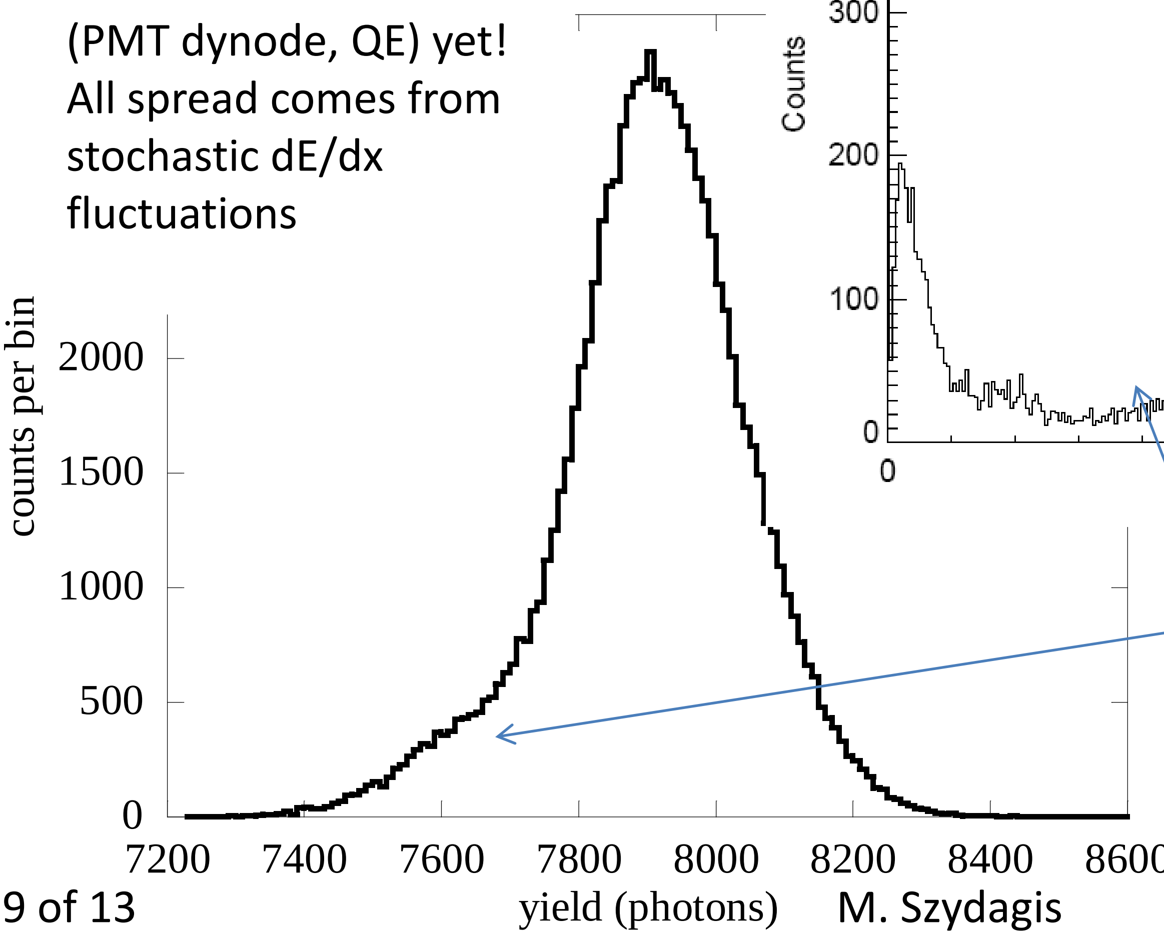
The Electric Field Dependence of Scintillation and Charge Yields



Reproducing Spread in Yield

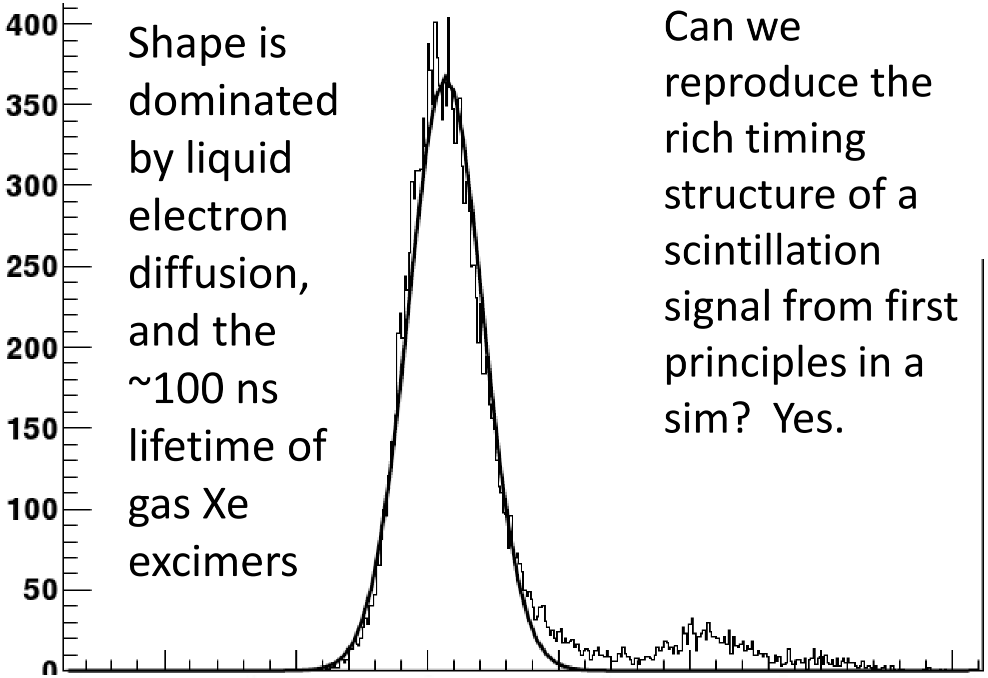
fake data (GEANT4 toy xenon model simulation) at lower left.
No Fano factor, no other sources of variation (PMT dynode, QE) yet!
All spread comes from stochastic dE/dx fluctuations





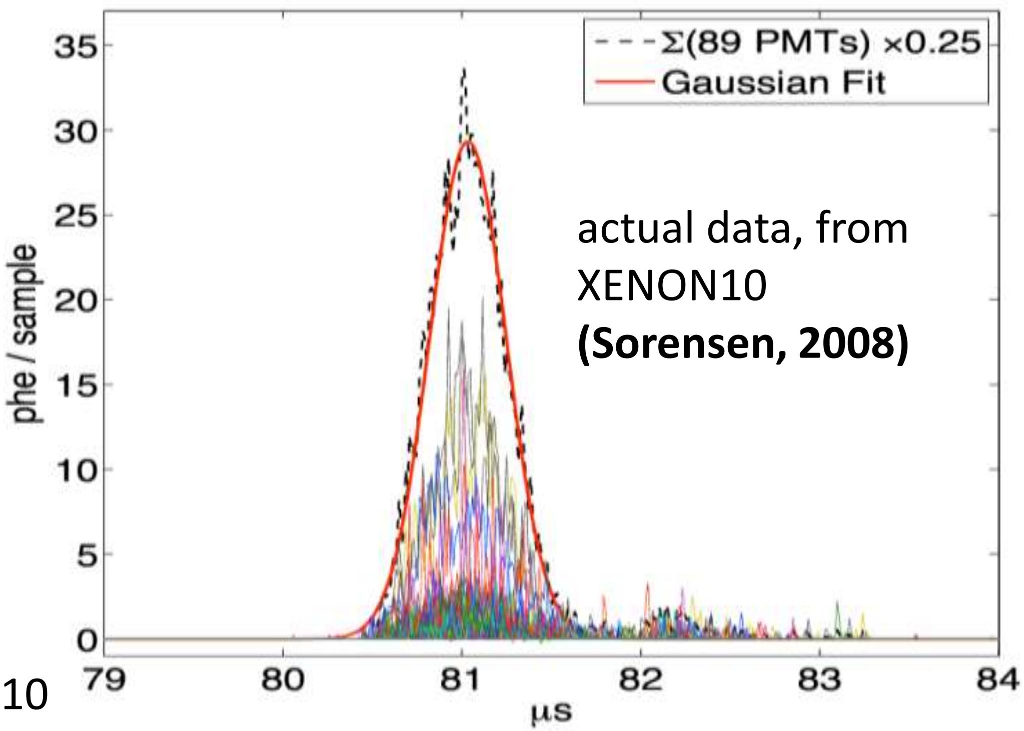
The asymmetrical shape is reproduced with Monte Carlo! Is caused by characteristic x-rays indirectly produced by one parent gamma

Understanding the Raw Pulse Shapes (S1, S2)

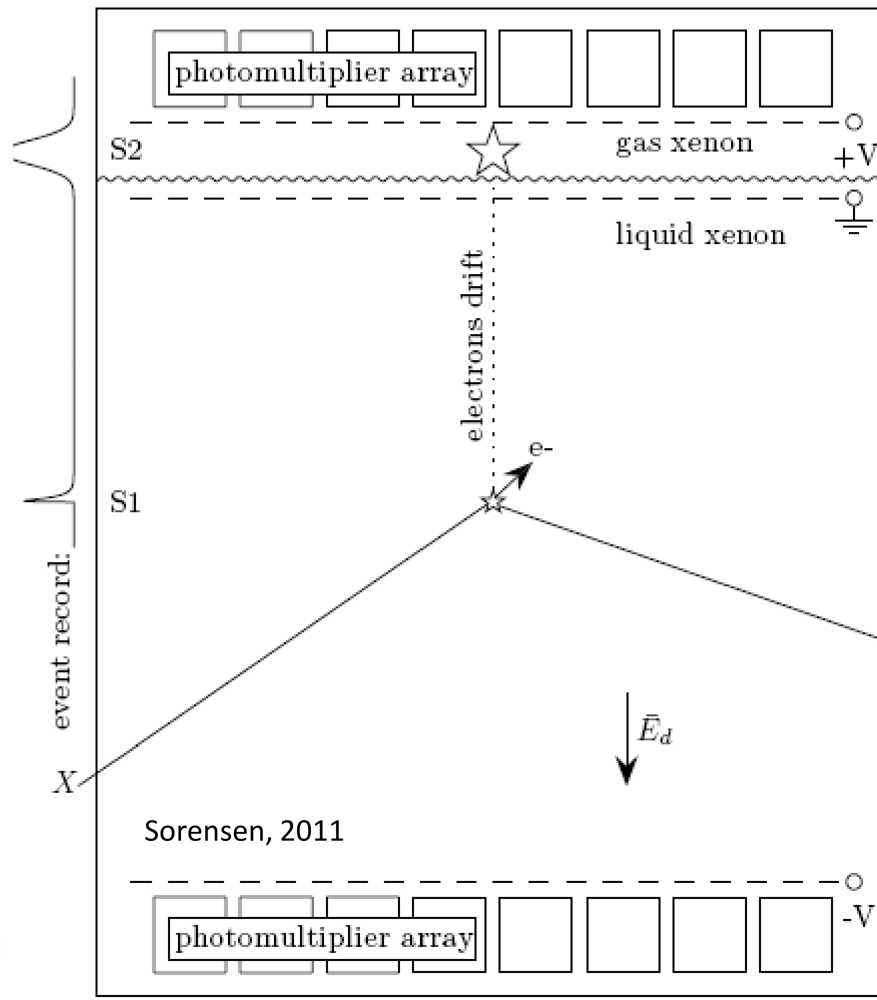


Shape is dominated by liquid electron diffusion, and the ~100 ns lifetime of gas Xe excimers

Can we reproduce the rich timing structure of a scintillation signal from first principles in a sim? Yes.



actual data, from XENON10 **(Sorensen, 2008)**



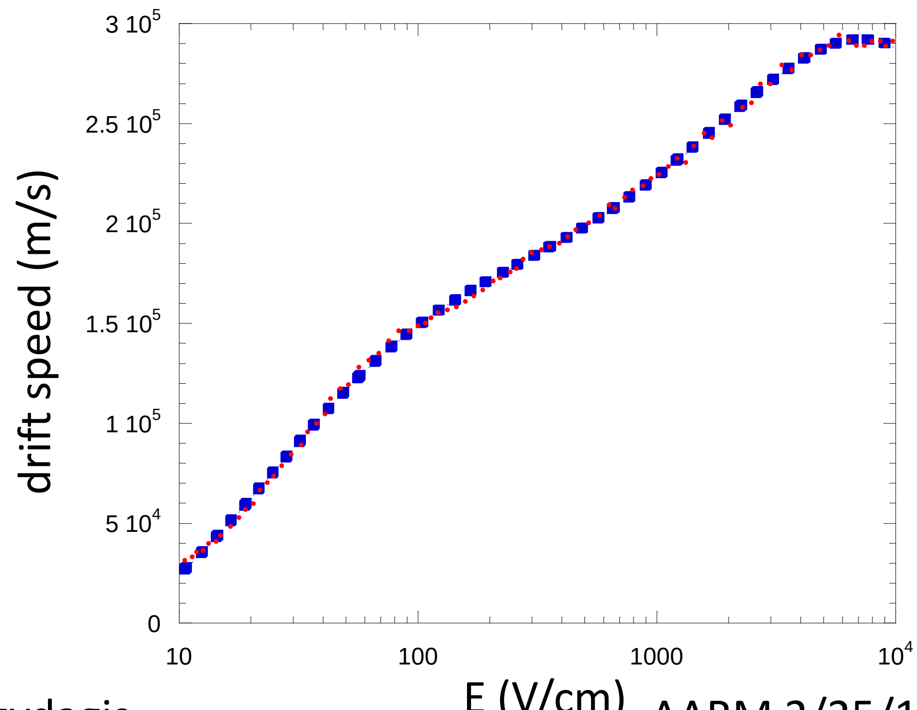
Sorensen, 2011

LXe Properties: The Finer Points

- We compiled all available (Xe) experimental data in the literature and performed a meta-analysis of it
- Scintillation wavelength is 174 nm (7.1 eV) with 11.5 nm FWHM, averaged over all results
- Compiled lifetimes, ratios for singlet, triplet states (unique for different interactions!)
- Studied the physics of electron drift so we can now simulate 2-phase detectors w/field well

Particle	τ_1	τ_3	A_1/A_3
e	2.2 ± 0.3	27 ± 1	0.6 ± 0.2
α	$3.77 \pm 0.31^{\star}$	$23.7 \pm 2.4^{\star}$	$11.6 \pm 9.71^{\star}$
$n+^{252}$Cf	5.1 ± 0.45	23.2 ± 1.5	7.8 ± 1.5

Liquid xenon thermal electron drift velocity versus electric field (data in red, fit in blue)



Status and Future

- Preparing upgrade for **G4Scintillation.cc** , speaking with GEANT about inclusion in next version
- Fully simulating a DAQ chain (pulse shaping, etc.)
- Adding Fano factor, checking energy resolution
- LUXSim will eventually become the first application of the work presented here to a real detector
- No more heuristics, no more rules of thumb and extrapolations from past detectors
- Dial in a particle type and energy, set your electric fields, and watch it go and give reliable results
- Repeat: argon, neon – complete picture