The NEST Simulation Framework for Low Energy Response in Liquid Xenon

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Outline

- Liquid xenon as a detection medium
  - Applications to rare event searches
- What is NEST?
  - Simulation package
  - Physics models / parameterization
- Nuclear recoils
- Recombination fluctuations
- Electronic recoils
- Summary

Liquid xenon TPCs

Measure low energy particle interactions by combining two signals:

- Prompt scintillation **light** (S1)
  - Transparent to Xe scintillation
- Drifted ionization **charge** (S2)

Applications in many low-background searches:

- Dark matter
- Coherent neutrino-nucleus scattering
- Neutrinoless $\beta\beta$ decay

Advantages:

- 3-D position reconstruction
- Self-shielding
- Highly scalable
- No long-lived radioactive isotopes

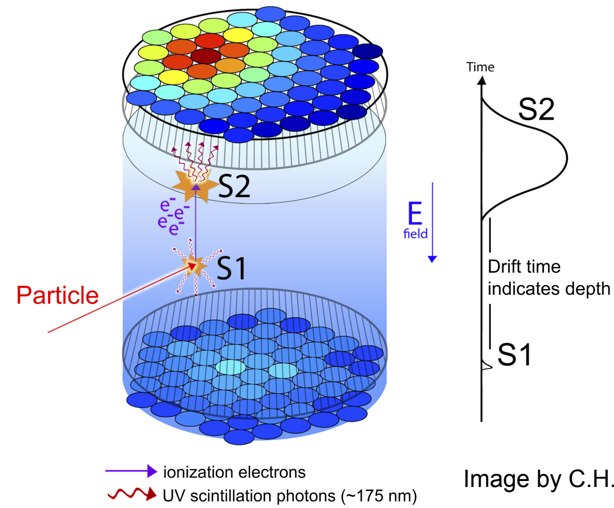
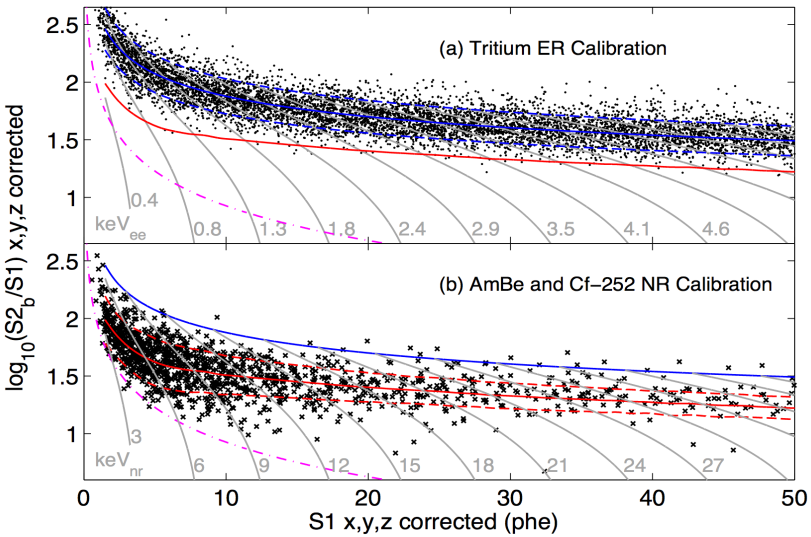


Image by C.H. Faham (LBL)

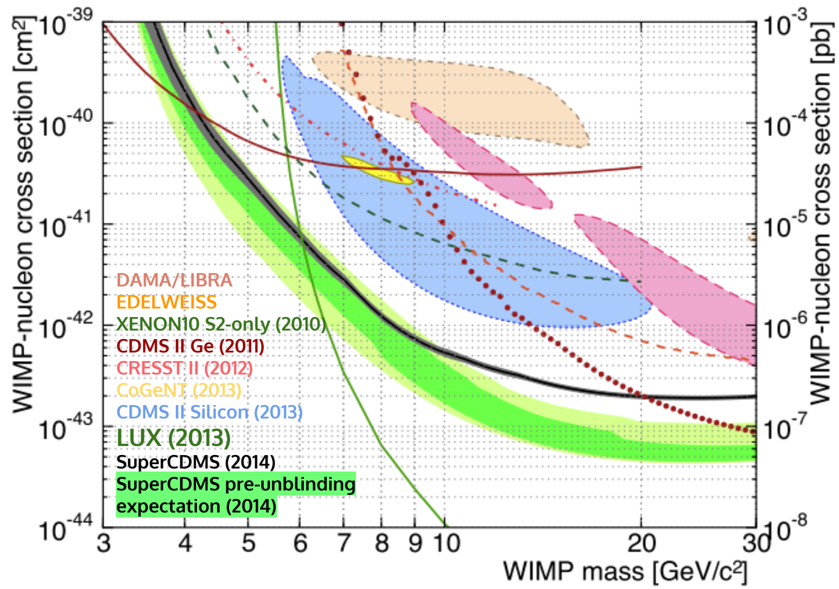
The low-energy regime (dark matter, CNS)

Discrimination between electronic recoil (ER) backgrounds and nuclear recoil (NR) signals is critical

D. Akerib *et al.*, *Phys. Rev. Lett.* 112 (2014) 091303.



R. Agnese *et al. Phys. Rev. Lett.* 112, 241302



Understanding experimental thresholds is difficult due to large uncertainties in calibrations. This affects controversial regions in dark matter searches

We need to understand the physics of nuclear and electronic recoils to understand low-energy response and discrimination

NEST:
The **N**oble **E**lement **S**imulation **T**echnique

NEST is a(n):

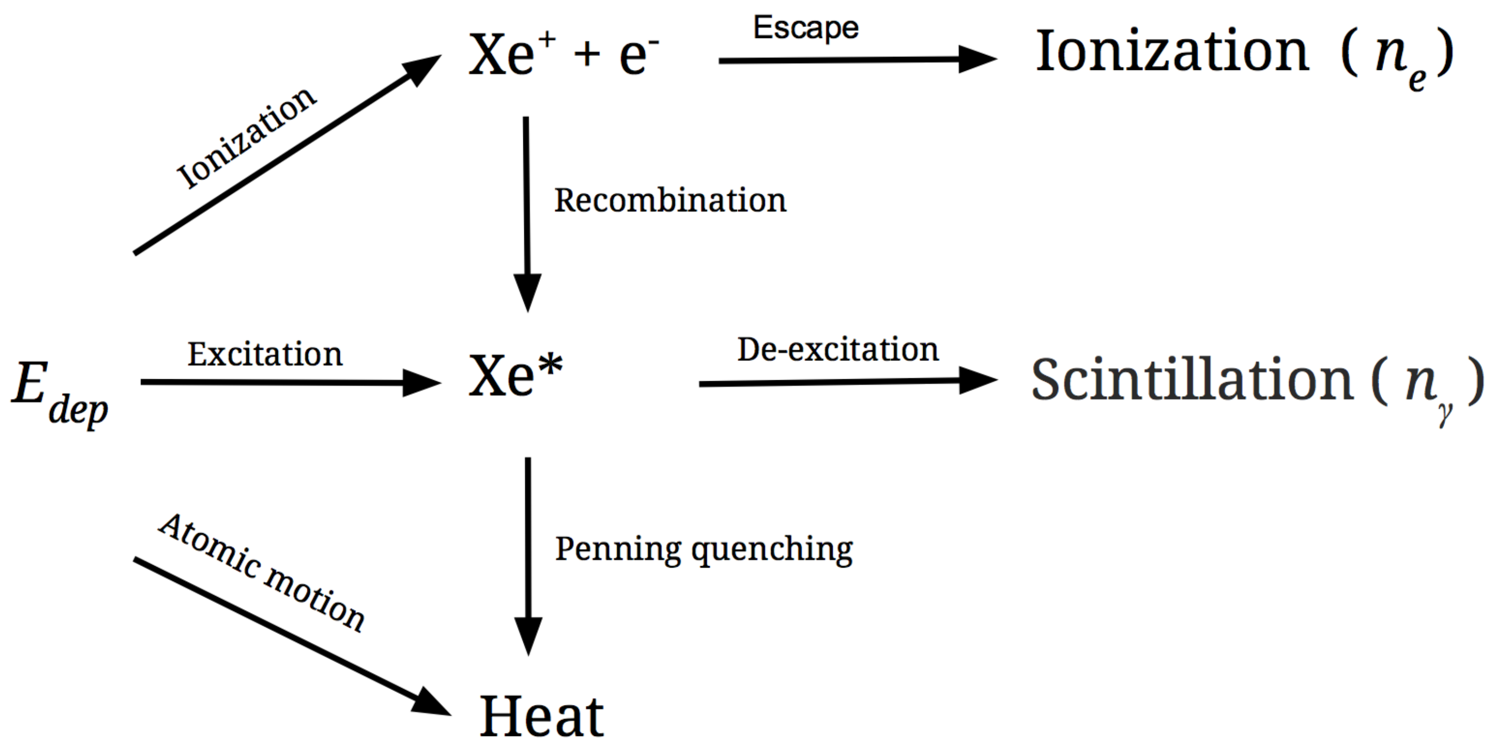
- Detector-independent simulation framework
- Comprehensive physical model of interactions in liquid xenon
- External package compatible with Geant4, for easy integration into full simulations
- Stand-alone code for fast calculations of yields and rates in simplified simulations (available soon)

NEST is free and publicly available:

http://www.albany.edu/physics/NEST.shtml

http://nest.physics.ucdavis.edu

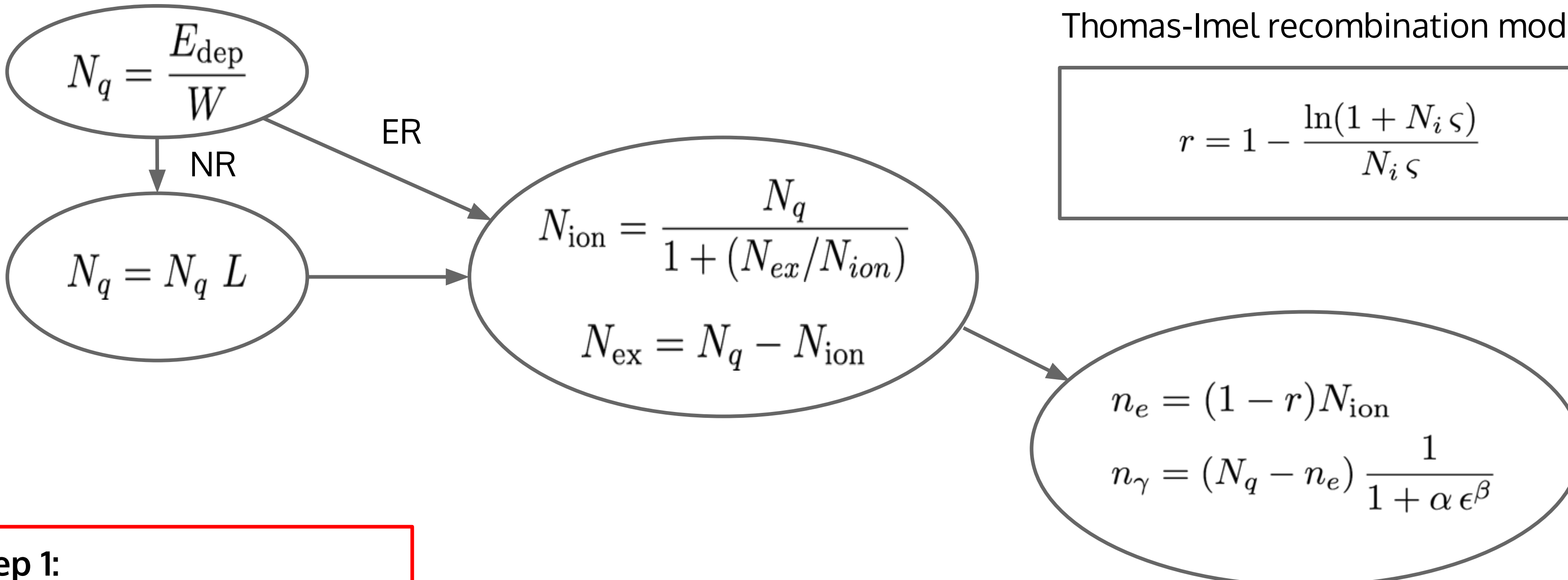
A picture of interactions in LXe



NEST algorithm

Thomas-Imel recombination model

$$r = 1 - \frac{\ln(1 + N_i\,\varsigma)}{N_i\,\varsigma}$$



Step 1:
Quanta are generated. If it's a nuclear recoil, the Lindhard effect is applied.

$$L = \frac{k\,g}{1 + k\,g}$$

Step 2:
Quanta are split initially into ions and excitons. The exciton-to-ion ratio differs between ER and NR.

Step 3:
Electron/ion pairs recombine to produce photons. The Thomas Imel box model is implemented at this stage, as well as Penning quenching.

NEST algorithm

$$N_q = \frac{E_{\mathrm{dep}}}{\ldots}$$

$$N_q = \ldots$$

NEST predicts absolute number of electrons AND number of photons.

- Conserves energy
- Assumes anti-correlation

Energy scale uses combined information to improve resolution

$$E_{ER} = (n_\gamma + n_e)\, W$$

$$E_{NR} = \frac{(n_\gamma + n_e)\, W}{L}$$

Thomas-Imel recombination model

$$r = 1 - \frac{\ln(1 + N_i\, \varsigma)}{N_i\, \varsigma}$$

$$n_e = (1 - r) N_{\mathrm{ion}}$$

$$n_\gamma = (N_q - n_e)\, \frac{1}{1 + \alpha\, \epsilon^{\beta}}$$

Step 1:
Quanta are ge… a nuclear reco… effect is applie…

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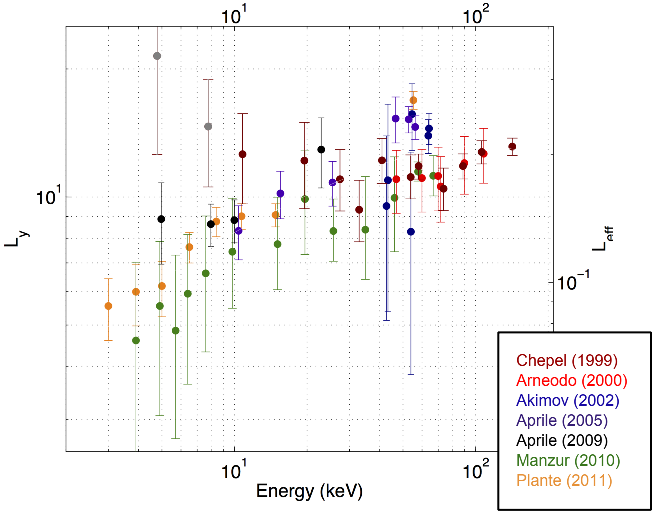
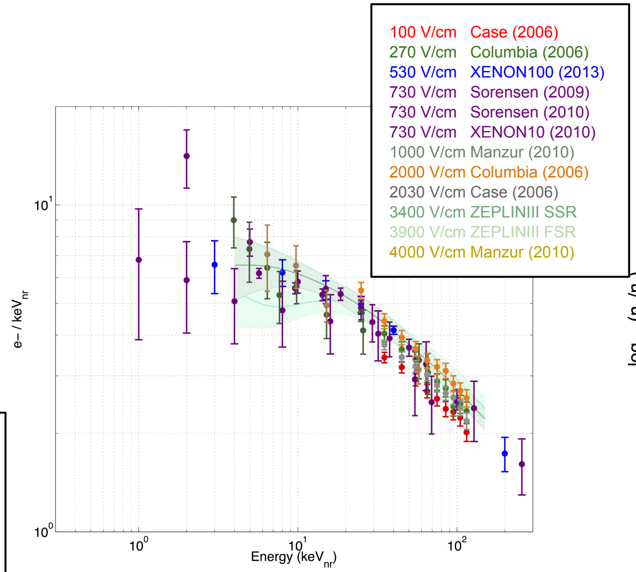
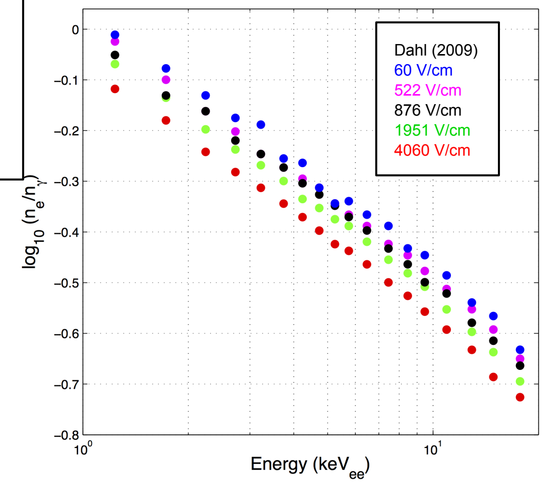
The nuclear recoil model



L_{eff} - scintillation yield



Q_y - ionization yield



Electron / photon ratio

To fit to all of these data, we construct a global likelihood function and optimize.

$$\mathcal{L} = \prod \frac{1}{\sqrt{2\pi}\,\sigma_{exp}} \exp\left(\frac{-(x_{exp}-\mu)^2}{2\,\sigma_{exp}^2}\right) \qquad \mu \in \left\{ \mathcal{L}_{eff},\ \mathcal{Q}_y,\ \frac{N_e}{N_{ph}} \right\}$$

Parameterization and best fits

Four quantities that are fit:

$\frac{N_{ex}}{N_i}$	Initial ionization
ς	Recombination
k	Nuclear recoil efficiency
$\frac{1}{1+\alpha\,\epsilon^{\beta}}$	Biexcitonic quenching

Nine free parameters - a, b, c, d, f, k, alpha, beta, "zero field"

$$\frac{N_{ex}}{N_i} = \mathrm{c}\ (\mathrm{E}_{field})^{\mathrm{d}}\ (1 - e^{-\mathrm{f}\ E})$$

$$\varsigma = \mathrm{a}(\mathrm{E}_{field})^{\mathrm{b}}$$

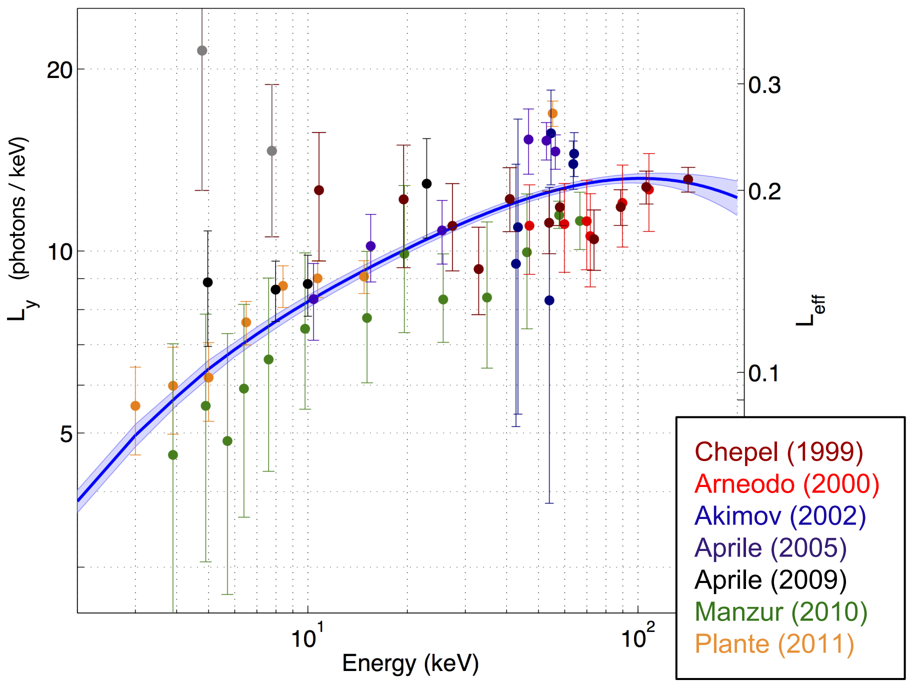
$$k$$

$\alpha\ ,\beta$ (biexcitonic quenching)

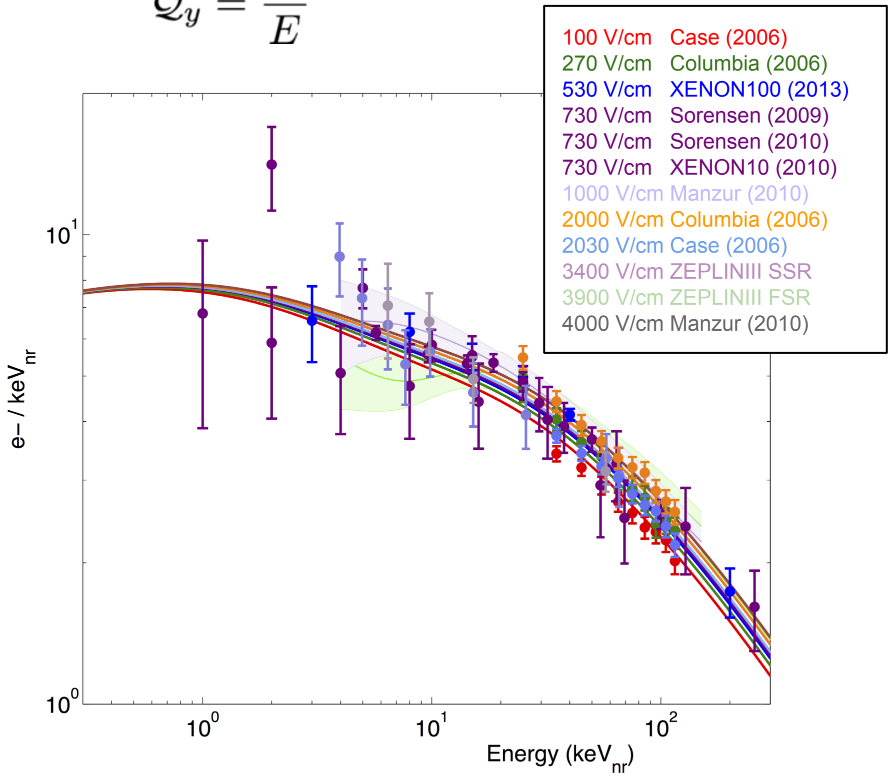
Variable	*a*	*b*	*c*	*d*	*f*	*k*	α	β	F_0
Best fit	0.0554	-0.0620	1.240	-0.0472	-239	0.1394	3.12	1.141	1.03
68% CL -	-0.0029	-0.0056	-0.079	-0.0088	-27.7	-0.0026	-0.38	-0.086	-1.03
68% CL +	+0.0023	+0.0065	+0.07	+0.0073	+9.0	+0.0032	+5.50	+0.453	+14

L_{eff} and Q_y - from best fit model

$$\mathcal{L}_{eff} = \frac{n_\gamma}{E} \times \frac{1}{n_\gamma(^{60}\text{Co})}$$



$$Q_y = \frac{n_e}{E}$$



Modeling recombination fluctuations

In LXe, recombination fluctuations are very different than the expected due to a binomial process (Dobi 2014):

$$\sigma^2_{bin} = r\,(1-r)\,N_i \qquad \sigma^2_{obs} = \frac{1}{185} \times N_i^2$$

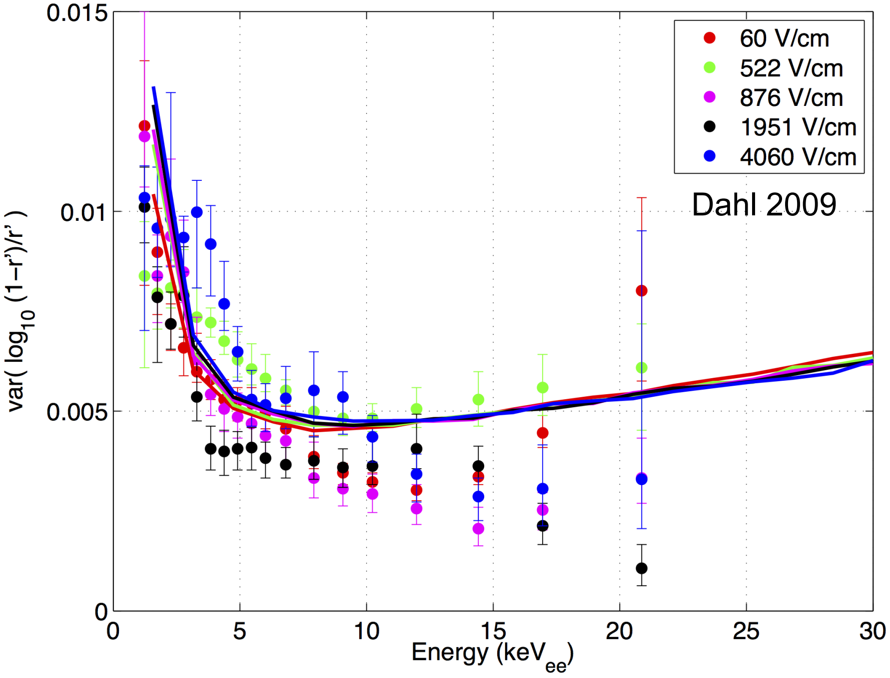
In NEST v1.0, we use a Fano-like factor proportional to N_i to fit to existing data:

$$\mathcal{F}_r = \mathcal{C}\,N_i$$

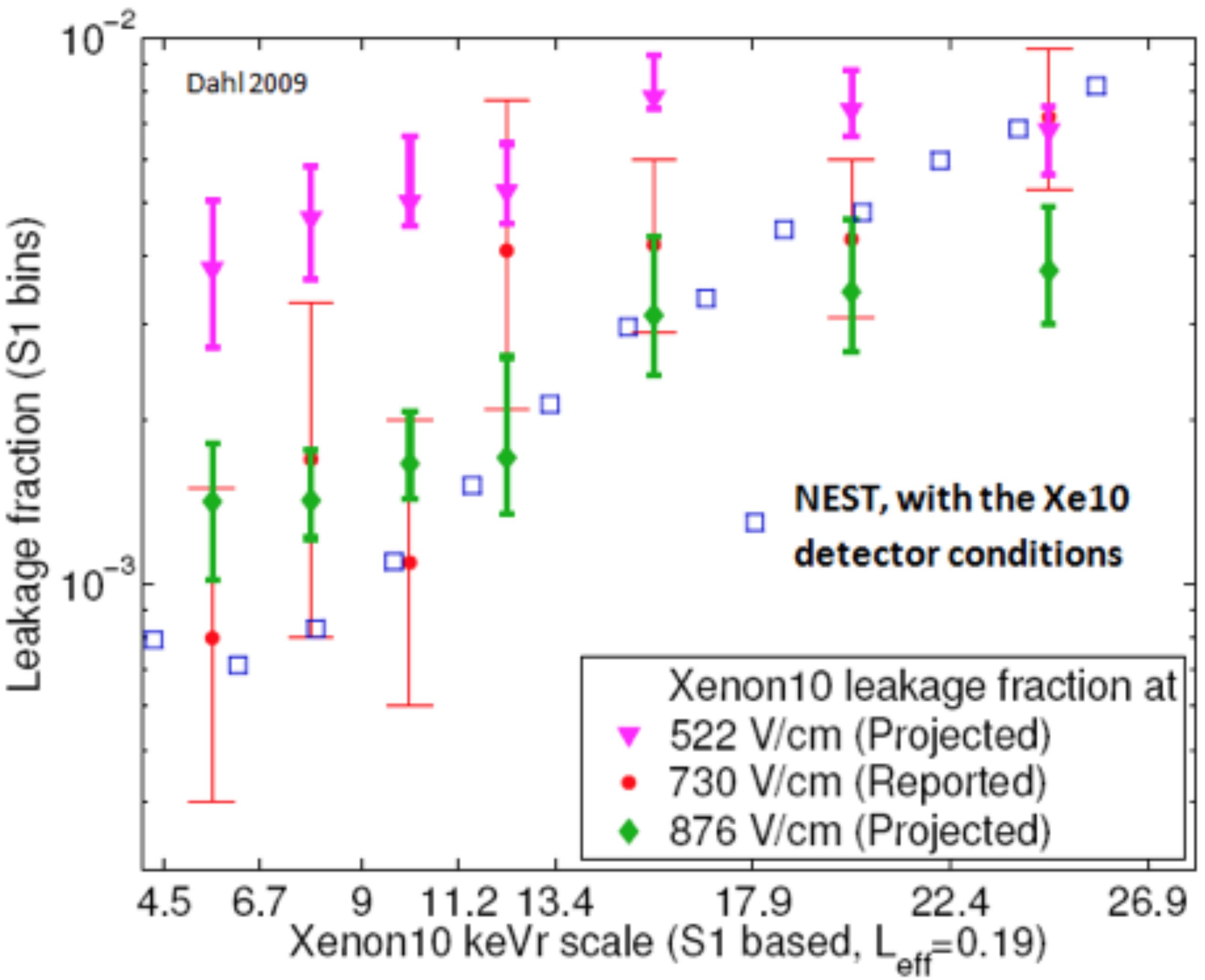
Then, the variance is treated as follows:

$$\sigma^2_R = \mathcal{F}_r\,N_i$$

and fit to data from Dahl (2009) shown to the right.



NR vs. ER Discrimination



Culmination plot. ER and NR band means and widths match very well. Trend counter-intuitive: worse result *away* from threshold

This is very close to the LZ design voltage.

The electronic (ER) recoil model

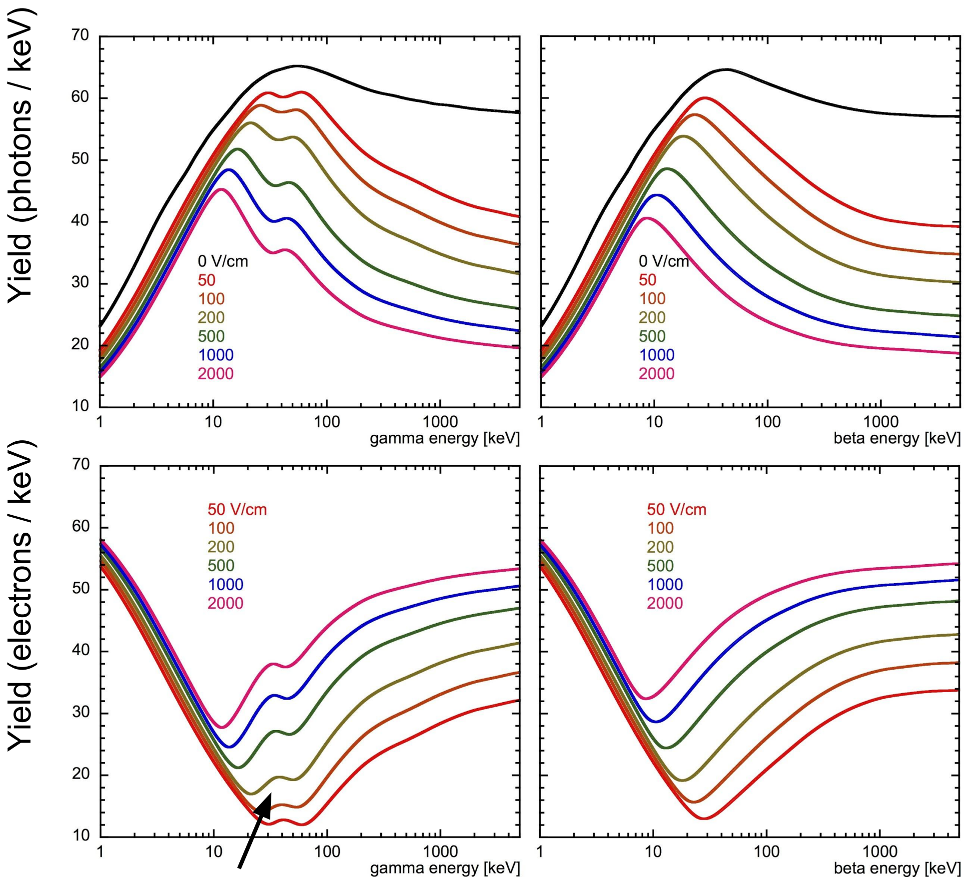
Constructed with the same underlying framework as the NR model, resulting in a consistent picture of low energy interactions.

Recombination model uses a piecewise concatenation of Thomas-Imel Box model and Doke-Birks' model:

$$r = 1 - \frac{\ln(1 + N_i\,\varsigma)}{N_i\,\varsigma} \qquad \text{if track} < 4.6\ \mu\text{m}$$

$$r = \frac{A \cdot \text{LET}}{1 + B \cdot \text{LET}} + C \qquad \text{if track} > 4.6\ \mu\text{m}$$

A global fit is planned when new data becomes available

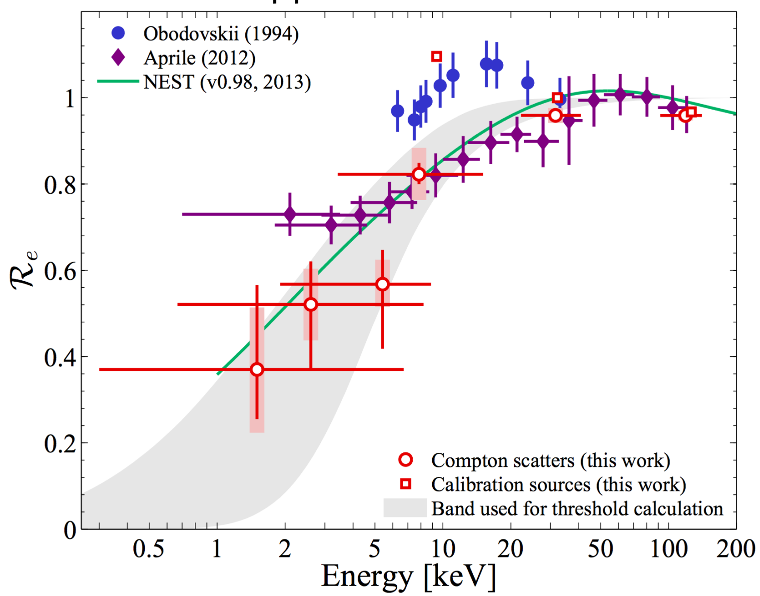


Resonance at Xe K-edge for Auger e⁻ production

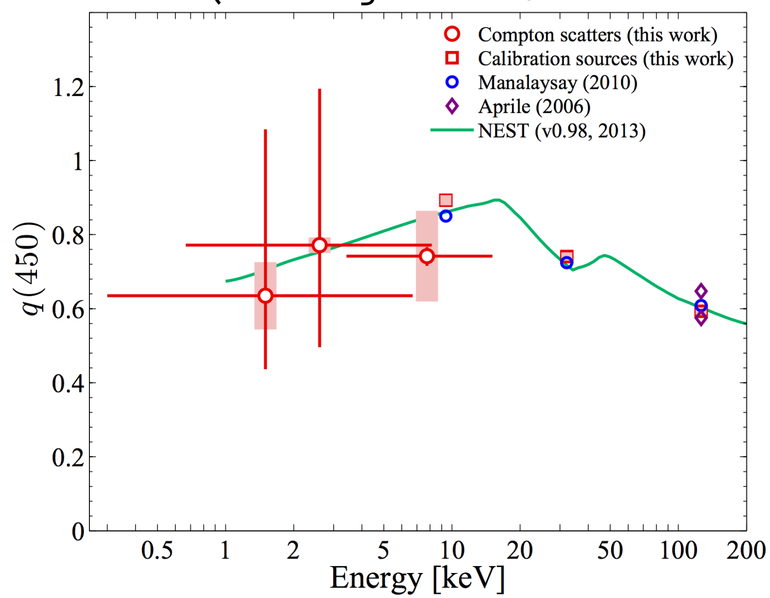
The ER model in the literature

NEST has been used by others to predict the results of measurements:

No applied electric field



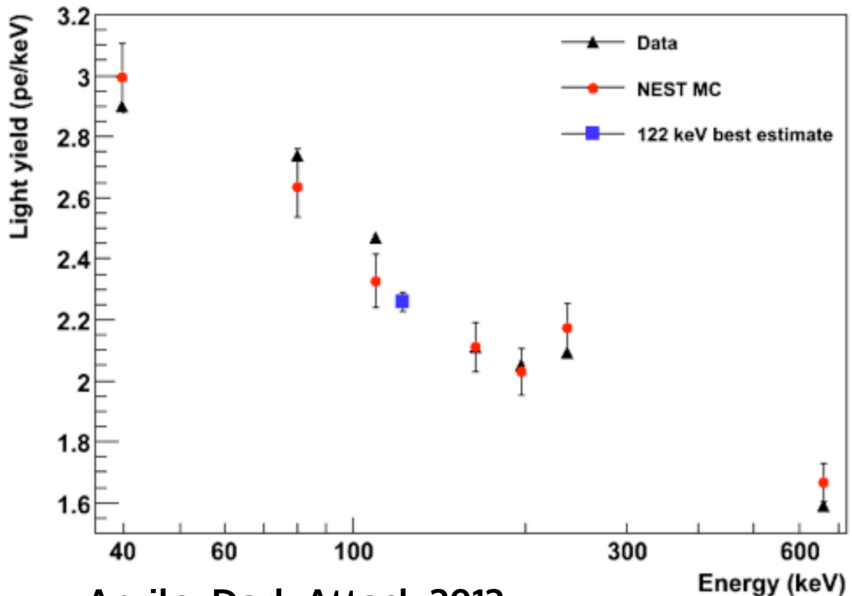
Quenching at 450 V/cm



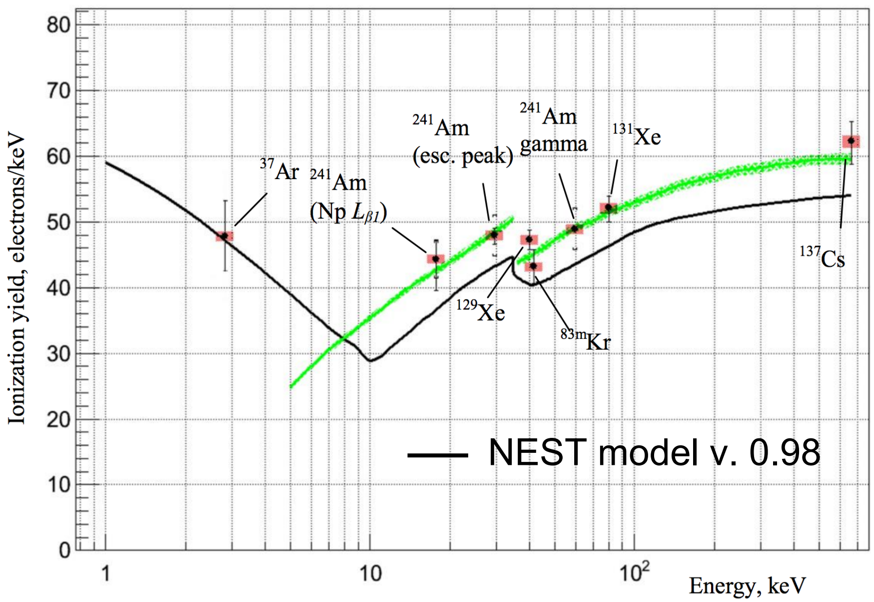
Baudis et al., Phys. Rev. D 87 (2013) 115015

ER model in the literature (cont.)

Data from XENON100 detector, 530 V/cm



Aprile, Dark Attack 2012



Akimov et al., JINST 9 (2014) P11014

The NEST collaboration

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Summary

- The NEST model is a successful picture of low energy yields in liquid xenon
  - Incorporates multiple physics models
  - Predicts both light and charge yield given energy and applied field
- Recent improvements to NR and fluctuations are highly relevant for current and future experiments
- Code is easily implemented in simulations, and has been used by many groups to compare to data
- For more details, visit:
  - **http://www.albany.edu/physics/NEST.shtml**
  - **http://nest.physics.ucdavis.edu/site/**

Backup slides

Free parameters in NEST (NR)

Four quantities that are allowed to vary

- $\frac{N_{ex}}{N_i}$ Initial ionization
- $\frac{\alpha}{a^2\, v}$ Recombination
- k Nuclear recoil efficiency
- $\frac{1}{1+\alpha\,\epsilon^{\beta}}$ Biexcitonic quenching

→

Nine free parameters - a, b, c, d, f, k, alpha, beta, “zero field”

$$\frac{N_{ex}}{N_i} = \mathrm{c}\ (\mathrm{E}_{field})^{\mathrm{d}}\left(1 - e^{-\mathrm{f}\ E}\right)$$

$$\frac{\alpha}{a^2 v} = \mathrm{a}\ (\mathrm{E}_{field})^{\mathrm{b}}$$

k

$\alpha\,,\beta$ (biexcitonic quenching)

We also introduce as a free parameter an “effective zero field”. The scintillation efficiency is typically measured at zero field, but our model blows up.

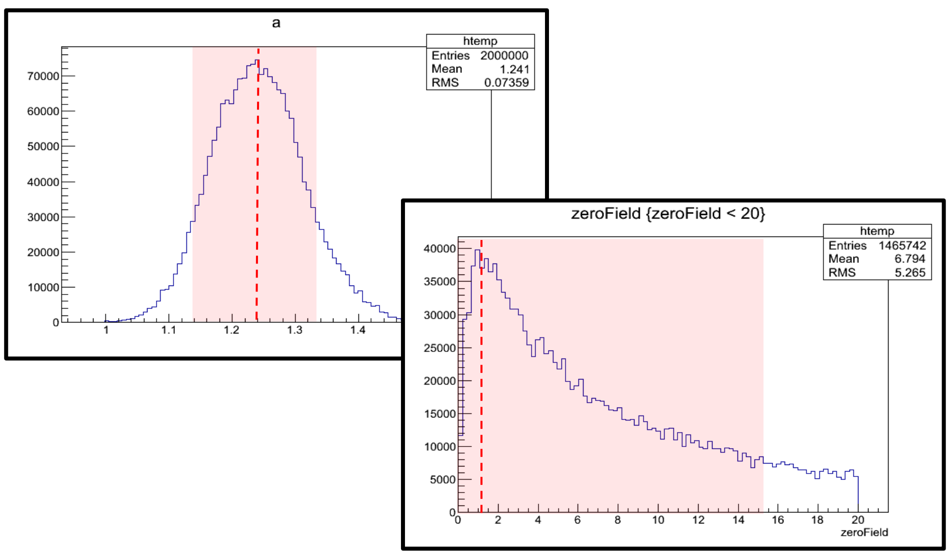
MCMC estimation of parameters

We assume that the likelihood function we've constructed is proportional to the probability of our model given this set of data:

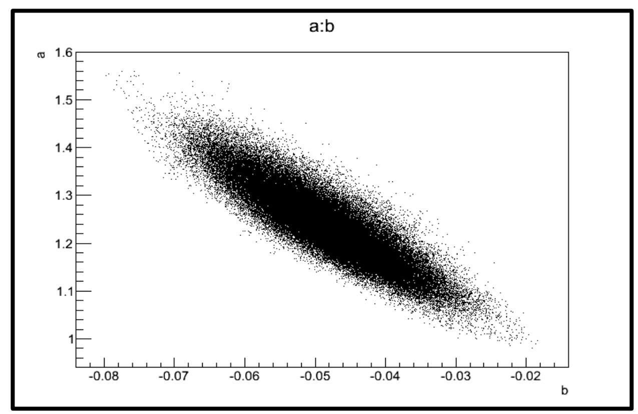
$$\mathcal{L}(\theta \,|\, x) \propto P(\theta \,|\, x)$$

Then, sampling gives us the underlying PDF, without solving analytically.

Best fits and errors can be found by histogramming the samples and reading off the maximum:



It's also easy to get covariances by histogramming samples in 2D. Helpful for error analysis.



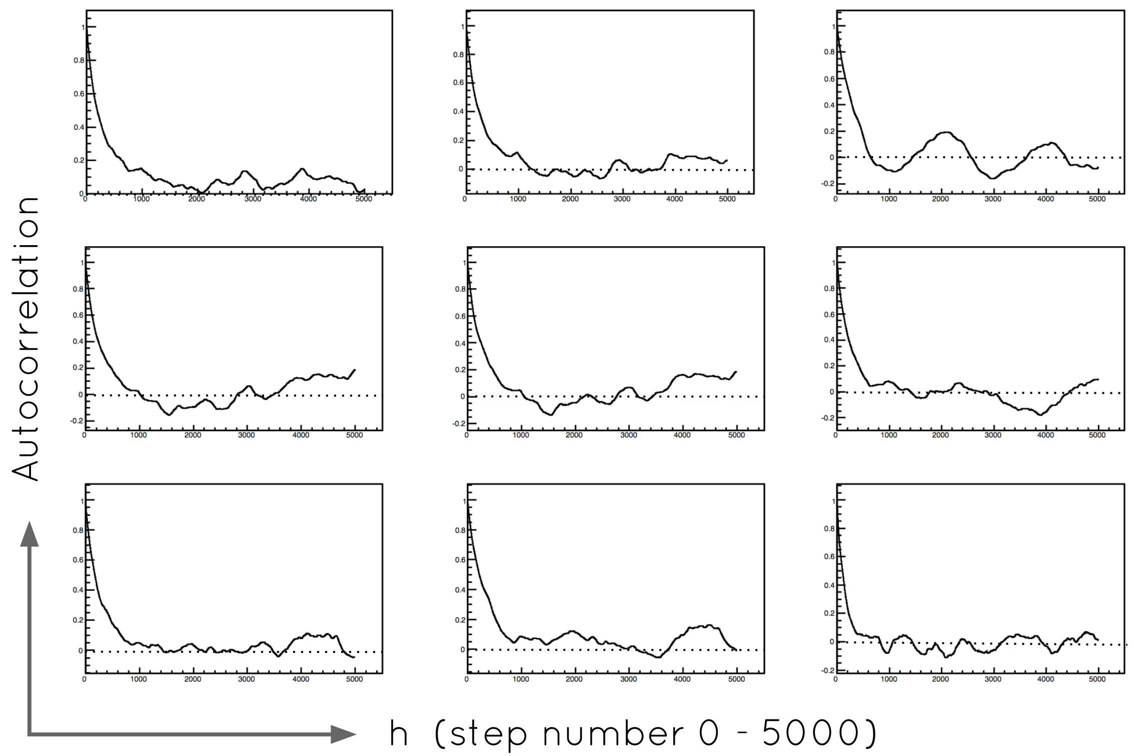
Ensuring a fair sample

We study the autocorrelation of each variable:

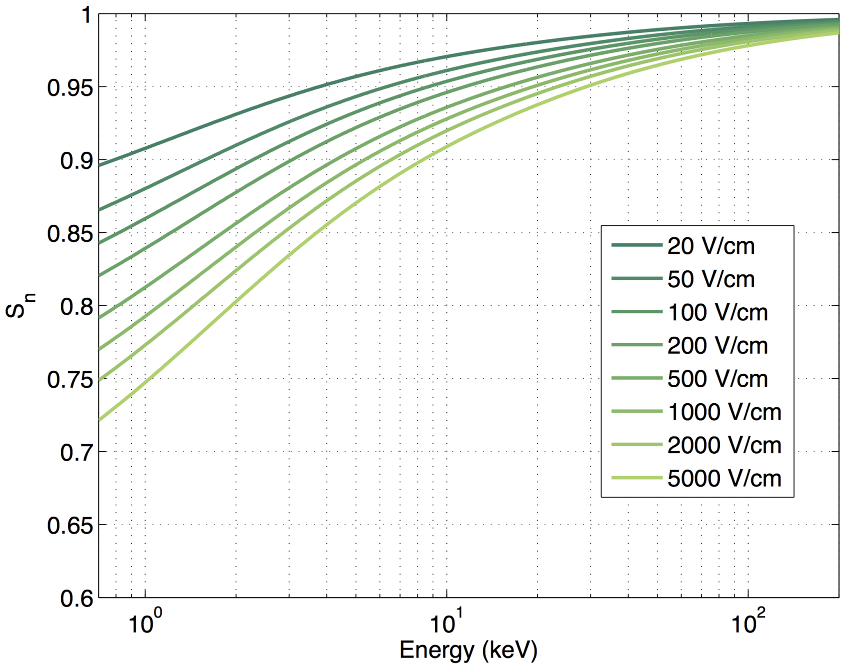
$$R(i, i+h) = \frac{\mathrm{E}\left[(X_i - \mu_i)\left(X_{(i+h)} - \mu_{(i+h)}\right)\right]}{\sigma_i \, \sigma_{(i+h)}}$$

To ensure a fair sample, must be sure that $N_{samples} >> Length_R$

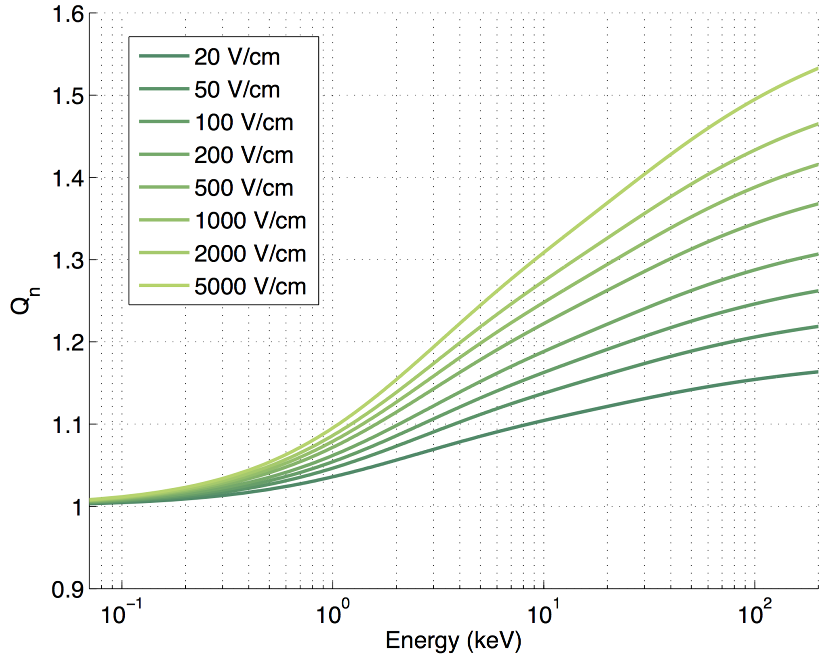
- In our case, we use 3,000,000 samples



Field dependence of scintillation / ionization



Light yield relative to 0 V/cm



Charge yield relative to 0 V/cm

Larger version of comparison to Mu et al.