Noble Element Simulation Technique
for Geant4

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

Shanghai Jiao Tong University, Shanghai, China, Tues., Sept. 20, 2011 @2pm
The People of the NEST Team

UC Davis and LLNL, California
A very small but passionate group of individuals who love this work

Faculty
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Undergraduate Students
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Why simulate scintillating noble elements well?

• Direct dark matter detection or calibration for it (past, present, future experiments)
  – LUX, XENON, ZEPLIN, LZ, WArP, DarkSide, ArDM, XMASS, DARWIN, MAX, Xürich, Xed, XeCube, PANDA-X, PIXeY, DEAP, CLEAN, …… 1- and 2-phase

• Double beta decay ($2\nu\beta\beta$, $0\nu\beta\beta$) projects too
  – EXO, NEXT (both $^{136}\text{Xe}$-enriched)

• Positron Emission Tomography (PET) scans for medical applications: detect 511 keV $\gamma$’s

• Other particle detection applications, e.g., collider experiments (MEG, Olive, et al.)
The Purpose and Scope of **NEST**

- Create a full-fledged simulation based on 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, double beta decay, and other experiments which utilize this technology to be on the same or comparable page for simulations
- Bring added realism to the simple model that is present now in Geant4.9.4 for scintillation
- Explore backgrounds at low energy by expanding Geant4 physics to be more accurate when you go to a low energy regime: $O(1) \text{ keV}$ and even lower
- Have to start somewhere: LXe, for sake of LUX
Basic Physics Principles

- Heat loss for nuclear recoils (Lindhard effect); electron recoils easier to deal with (or are they...?)
- Start simple: no exotic energy loss mechanisms (like “bi-excitonic” collisions). Explains the data?
Model Framework: Start with Electron Recoils

- Look at the Geant4 tracking verbosity: different energy depositions from the secondary electrons and gammas in an EM cascade.
- Allow for the recombination% to fluctuate stochastically by treating every electron recoil individually.

```
* 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     0.00078  0.484       0.484       LiquidXenon initStep
1     -1.07  -3.87  -141     0.0269     0.000678 0.484       0.484       LiquidXenon compt0
2     -1.14  -4.18  -140     0.00542    0.565      1.05       LiquidXenon phot0

* 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     0.00795  0.00306    0.00306    LiquidXenon eIoni0
1     -1.14  -4.18  -140     0.00877    0.00795  0.00306    0.00306    LiquidXenon eIoni0
```

- Compton and other scattering, electron ionization or Brem.
- More and more e-recoils increasingly lower in energy.

Parent γ

Shower of secondary electrons and gammas, tertiary, etc.

Electron recoils

Photo-absorption event (followed by Auger emission)
The Recombination Probability

1 – (overall recombination frac), or, the escape frac

- Needed for predicting the light yield correctly (at least for LXe, LAr): most of the scintillation comes from recombined electrons (not excited)
- Many theories, models exist; we combine two physically motivated ones that fit majority of xenon data and fit best
- Curve adapted/splined continuously for electric fields: more field implies more low-energy ionization e’s (from the higher-energy recoils) escape (and drift)

Not clear a priori what curve to use (at upper right) as a basis for entire model. Birks’ Law of scintillation? Jaffé?

arXiv:1106.1613
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 $\gamma$ scintillates less than 10?
  – Makes electron recoils look more like nuclear recoils
• Not understood until recently -- an $L_{\text{eff}}$ clue...?
A Solution at Long Last?

• Lower energy particles have shorter ranges (generally)
• In terms of physics we define “short range” as being smaller than the electron-ion thermalization distance: about 4-5 μm (Mozumder, 1995)
• More electrons get away without recombining and going on to make scintillation (original concept from the Ph.D. Thesis of C.E. Dahl, 2009)
• A marriage of two models: Thomas-Imel model to explain short-range particles, and Doke (modified form of Birks’) for long-range: box vs. column geometries
• Same physics, but in different limits; in Thomas-Imel limit, recombination is independent of dE/dx
Putting it All Together to Predict the Yield

First: Let’s look at zero-field scintillation yield from gamma rays

Szydagis et al. 2011

- best reproduction based on model
- Doke/Birks’ Law only
- Thomas-Imel box model only

- rich features understood
- diving fast at low energy
- here is Obodovskii data from an earlier slide (red)

(outliers typically explained)

models merged

- flat yield at higher energies

not all authors use error bars

arXiv:1106.1613

Doke (2001) Calculation
(Not to be confused with Doke/Birks’ Law)

And what about non-zero field...?
This Work
- 9.4 keV $^{83m}$Kr
- 32.1 keV $^{83m}$Kr
- 29.8 keV $^{83m}$Kr
- 59.5 keV $^{83m}$Kr
- 122 keV $^{83m}$Kr

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

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

This Work
- 511 keV $^{83m}$Kr
- 570 keV $^{83m}$Kr
- 662 keV $^{83m}$Kr
- 976 keV $^{83m}$Kr

This Work
- 368 keV e$^{-}$ ($^{113}$Sn)
- 122 keV $^{83m}$Kr
- 41.5 keV $^{83m}$Kr

This Work
- 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 $^{83m}$Kr
- 511 or 570 keV $^{83m}$Kr

arXiv:1106.1613
Reproducing the Spread of the Yield

Geant4 toy xenon model simulation at the lower left, with the spread dominated by stochastic, individual $dE/dx$ fluctuations along tracks.

Similar asymmetrical shapes, caused a bit by characteristic x-rays indirectly produced by one parent gamma, and by detector effects.

Real data (Ni, 2006)
Energy Resolution

Preliminary NEST Predictions for Zero Electric Field

*The sources of INTRINSIC non-perfect resolution, at all electric fields*

- Fano factor (extremely small effect until lower energies)
- Binomial fluctuations in the recombination probability
- Binomial fluctuations in the numbers of excitons versus ions (small)
- Particle track history, including stochastic dE/dx effects

same color code as earlier for particles
Switching Gears: Nuclear Recoil

This is likely the strongest prediction, with the simplest assumptions, ever devised!
Simulated ER and NR bands in S2/S1

0.45 kV/cm electric field

NO artificial smearing, Gaussian or otherwise, was added to NEST to yield the result depicted.

Now it has become possible, with NEST, to study/predict the discrimination power of your experiment before you even built it or calibrate, with a reliable simulation.
understanding the raw pulse shapes (S1, S2)

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

actual data, from XENON10 (Sorensen, 2008)

Very Gaussian-like

differences between ER, NR disappear with field

diffusion, and the ~100 ns lifetime of gas Xe excimers need new particles as well as processes in Geant4 to see this happen

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

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

very Gaussian-like

brief introductory

benchmark plots

http://nest.physics.ucdavis.edu

from Benchmark Plots

this is for a single decay time constant exponential fit, so singlet state is glossed over (but recombination time dominates ER)

D. Stolp

understanding the raw pulse shapes (S1, S2)
LXe Properties: The Finer Points

- We compiled all available (Xe) experimental data in the literature and performed a meta-analysis of it.
- NEST scintillation wavelength is 178 nm (6.97 eV) with 14 nm FWHM, consistent with past results.
- Compiled lifetimes, ratios for singlet, triplet states (unique for the different interaction types!)
- Studied physics of electron drift, so we can soon more fully simulate 2-phase detectors with NEST in Geant4.

<table>
<thead>
<tr>
<th>Particle</th>
<th>(\tau_1)</th>
<th>(\tau_3)</th>
<th>(A_1/A_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>e</td>
<td>2.2 ± 0.3</td>
<td>27 ± 1</td>
<td>0.6 ± 0.2</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>3.77 ± 0.31*</td>
<td>23.7 ± 2.4*</td>
<td>11.6 ± 9.71*</td>
</tr>
<tr>
<td>(n+{^{252}}\text{Cf})</td>
<td>5.1 ± 0.45</td>
<td>23.2 ± 1.5</td>
<td>7.8 ± 1.5</td>
</tr>
</tbody>
</table>

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

Will tell you your drift time.

Electrons will drift through liquid in NEST and then make S2 in the gas stage.

Rich physics here too like everywhere else.
Status and Future

- Upgrade to **G4Scintillation** physics process, called **G4S1Light**, available for download on-line; speaking with GEANT about inclusion in upcoming version.
- Fully simulating DAQ chain (pulse shaping, etc.).
- Another new G4 physics process: **G4S2Light** soon!
- Representatives of many collaborations already members of the NEST mailing list, and downloading.
- No more rules of thumb, nor extrapolations from past detectors: build your geometry and go.
- Dial in a particle type and energy, set your electric field, and watch your sims give reliable results.
- Next: **GXe, L/GAr, Ne, He, Kr, solids** – complete?
References

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

THANK YOU
Bonus Slides
simulation and real data exhibit similar width, with no artificial smearing
nuclear recoil energy (keV)
electrons per keV

definitions:
- max Gn
- Horn 2011
- min 3400
- max Blue
- Horn 2011
- min 3400