Physics Assumptions

NEST is based on the latest, greatest, and best knowledge, as much as possible, but some things are unknown, and some things may never be known, or at least always remain controversial. Also, better experiments may force us to change our pretty mathematical models. We hope that you, the user of NEST, will run experiments with your detectors, and pleasantly find that NEST already perfectly predicts your data. Wouldn't that be nice? But, of course, that may not always be the case as experiments venture into virgin territory, where NEST only has predictions or extrapolations, but is not founded on previous/past experimental data. The NEST paper covers almost all of the following already, but we reiterate some things here regarding matters of controversial numbers or equations.

First, there is no reason to believe the excitation ratio (the initial ratio of excitons to ions produced in the medium) remains fixed at 0.06 in liquid xenon for all particles, all energies, and all electric fields. However, we were able to explain a massive amount of data keeping this number fixed and instead introducing a dE/dx-dependent fraction of electrons which will not recombine even at infinite field. In effect, this is equivalent to having an energy-dependent excitation ratio, making the "correctness" of the oft-quoted value of 0.06 a philosophical point. But sticking the correction to it into Birks' law, thus making it non-constant, enables reconciliation of disparate results ranging up to 0.20. The Ph.D. Thesis of C.E. Dahl claims it is O(1) for NR, and we have updated our model to reflect this, setting it exactly equal to 1.0 at zero field as an ansatz solution, and using a power-law spline to Dahl's data at field. This makes NEST agree extremely well now with XENON100 and ZEPLIN-III L_eff data at zero-field, and agree with at least some charge yield at field (though much of those data are contradictory).

Despite needing to change the one free parameter of the Thomas-Imel model at zero field to match the Columbia Compton data, to 0.05, we leave the original 0.19 for NR since it fits the data better.

We assume that the number of excitons and ions produced by NR are equal or roughly equal as a result of the following compelling evidence this is the case:
(1) the light and charge yields of NR change extremely slowly with the electric field magnitude,
(2) the recombination fluctuations are curiously much smaller than for ER,
(3) when fitting non-zero field data, allowing this ratio to be a free parameter one finds best fits for ratios that are approximately unity (Dahl thesis),
(4) values near 1 permit usage of nearly the same recombination probability as for ER, for any field, and
(5) ion-ion and atom-atom scattering data show that this ratio is 1 at least for argon.

To make changes to the excitation ratio for electron recoil, go to line 298 of G4S1Light.cc, where it has the density dependence, for all phases of xenon. For NR, go to line 530, where it is field-dependent.

The extension of anti-correlation down to low energies for all particles is another assumption we have made because there really was nothing else we could do, due to a paucity of non-zero-field data, especially at keV and sub-keV energies. NEST generates a number of undifferentiated quanta based on a fixed LXe W=13.7 eV, then assigns excitons and ions binomially, then assigns photons and electrons binomially (with a non-binomial fudge factor added to explain the poor resolution of real data). This less-familiar number of 13.7 may not be the one you are used to, but all other ones you know and love are derivatives of this one W (read the paper to understand), including the oft-quoted but often misunderstood 15.6 eV (which turns out is really closer to 14.5 eV – please read the paper to see).

Onsager recombination is another matter of great controversy. It is supposed to be impossible, but we get a best fit at zero field with a significant amount of it (though none at non-zero field). In G4S1Light.cc, it is represented by the variable DokeBirks[2], if you wish to investigate it further. We have opted not to have a special case for high-energy electrons as laid out in the NEST paper, so the yield of 1 MeV electrons may be a bit high in NEST, or experimental values for the yield may be too low perhaps. Only new experiments can help, but the 1 MeV electron is not of great importance currently, since even if your experiment deals with O(1 MeV) gammas, for calibration, the probability of creating electrons that high in energy as opposed to lower-energy ones is still low.

Nuclear recoil will of course likely never cease to be controversial due to its extreme importance in the setting of dark matter limits. NEST makes incredibly simple assumptions, the least easy to defend however being that NEST simply changes the 'k' value of Lindhard theory to the Hitachi-corrected, lower one based NOT on his model of bi-excitonic quenching, but upon a first-principles recalculation of the nuclear and electronic stopping powers of nuclear recoils in liquid xenon. See line 516:

```
G4double kappa = 0.133*pow(z1,(2./3.))*pow(a2,(-1./2.))*(2./3.);
```

Without the (2/3), this is just standard Lindhard theory. We recommend leaving this as is, since it agrees with the latest and greatest L_eff data (Horn and Plante). Please note that since the Hitachi L- factor reduces both electron and photon yields roughly equally, the light yield and charge yields by themselves are reduced, but an S2 over S1 plot is not affected, so that your discrimination power predictions based on NEST will be the same regardless of these modifications made to the Lindhard factor.

Known Potential Bugs

Multiple Scattering

The way that NEST is laid out, as a discrete physics process and not a user "end-of-event" action, energy must be handled in a special fashion to ensure that an entire event is properly taken into account. If particles traverse the liquid multiple times, the goal energy for dumping all quanta may need to ebb and flow. We have performed many tests and, so far, it appears that even multiply-scattering gammas will be correctly tracked and generate the right amounts of scintillation and ionization, but it is perhaps possible for an ultra-high-energy gamma that scatters again and again to break NEST. If so, let so know.

Electric Field

Going either too low or too high in field may yield unexpected results. For NR, this is less of an issue: all nuclear recoils lie in only one regime, the Thomas-Imel model, so that there are no messy transition points which can move with field. However, NR data has not been verified below 60 V/cm, and the model currently has a sudden jump from 0 to non-0 field. Above 4,060 V/cm there is no data either, but the yields have experimentally been seen to asymptote very hard, and so our extrapolatory splines (see lines 728-729 of G4S1Light.cc) take this into account. Thus, in theory, you can go out to "infinite" field with NR in NEST. In the case of ER, because of the need for two models, Thomas-Imel and Doke, and the need to mix two different kinds of recombination, volume and Onsager/geminate, things get a little bit messy at low field, especially since several quantities go to infinity as field goes to zero. Between 0 and 50 V/cm it is not guaranteed that the S1 yield will be lower than at 0 field and higher than at 50 V/cm, which is of course unphysical, so such fields should be avoided. A paucity of data at these fields made it difficult to build a model of the physics here. Lastly, above O(10 kV/cm) multiple peaks begin to appear in yield for 10-20 keVee even at single energies because the yield is a sharper function of dE/dx.

Too High of an Accuracy
Increasing the accuracy of the simulation by severely decreasing the minimum step sizes taken by the ionization physics processes for various particles in your electromagnetic physics list is not recommended. NEST is robust against slight perturbations, but increasing the accuracy to be <<1 um will results in a severe underestimate in both light and charge yields. This is because charged particles like electrons will be forced to undergo many more steps in the simulation, and at every step the number of quanta to be created (a double) gets turned into an integer since you can't generate a floating-point number of particles (in either the simulation or real life!) Thus a round-down occurs. Though 0.5 is added before the conversion (line 542 G4S1Light.cc), this becomes insufficient as the number of finite steps taken in a simulation goes to infinity for a particle that in real life continuously deposits energy.

Bonus Features

There are several features in the released version which were never described in the current one and only publication, but are rather subjects of (very near-) future NEST publications:

-Good predictions for proton, alpha, and heavier-ion zero-field yields, assuming 100% electron recoil
- S1 pulse shape, with accurate singlet/triplet ratio, as a function of LET, electric field, and particle type
-S2 pulse shape as a function of anode electric field strength and liquid depth and gas density
-Nuclear recoil charge and light yields as functions of electric field (current paper only does zero field)
-Reasonably accurate 1st-order energy resolution, though without detector effects (up to end user)
    - Fano factor included (a very small effect, except for the LXe weirdness)
    - recombination fluctuations (mentioned)
    - exciton/ion fluctuations (strictly binomial assumed)
    - particle history and stochastic dE/dx variation (GEANT)

We provide these features so that both S1 and S2 yields and pulse shapes form a complete picture for you in the code, which is well beyond the work included in the published papers. We did not wish to have a piece-meal release, with S1-only code. You are free to capitalize upon all of the features which come with NEST V0.98 and cite the one existing paper, but as more and more NEST papers come out, we ask that you cite the paper or papers appropriate for the work you are doing.

Benchmarks

Computer System
NEST was checked against Geant4 versions 4.9.2, 4.9.3, and 4.9.4 up to and including patch 4. It should work in theory with 4.9.5, but we have not personally tested it with that version as of yet.

You can find benchmark plots on the website. If you're wondering how long it takes to run simulations, take the initial kinetic energy of the type of energy-depositing particle you want to study, and then divide by the work function of 13.7 eV. This gives you a number of quanta. Now multiply by the number of events you want to run (parent particles) to get a total, total number of quanta for a simulation (this is counting both photons and electrons together). On a machine with the following specs:

ADM Phenom II 3.0 GHz Quad Core
1.5 TB HDD
4 GB Memory

OR, the following:

Intel Xeon 2.53 GHz Quad Core
NAS
32 GB Memeory

It should take about 0.5 ms per quantum. So, for example, a set of 100 gamma rays 122 keV in energy will generate ~8900 electrons and scintillation photons, and thus take ~7 min. to run. Note, however, that this is only if you kill and count optical photons in your liquid xenon volume, letting it be your sensitive volume, without allowing them to propagate to your virtual light detectors in your simulated geometry. Depending on the size of your detector and the number of bounces an optical photon can undergo on average before reaching a photo-sensitive device, the simulation can run for longer, and with S2 photons now enabled in NEST it will take a great deal longer, especially if you want to run a lot of parent particles to get good event statistics. So, lesson is, get a fast computer! (You will also need a lot of hard disk storage and/or need to do a lot of compressing. Doing O(1e6) events in a O(100 kg) Xe detector will take up ~5 TB already without S1 light propagation or any S2 light at all.)

Particles, Energies, Fields

NEST was tested with a wide range of particles and energies, sometimes without experimental backing, so NEST is making a whole host of predictions. We have looked at

- Soft/hard x-rays and Gamma rays (200 eV – 20 MeV)
- Electrons (20 eV – 50 MeV)
- Alphas (1 – 10 MeV, with electric field dependence now correct) and Protons (40 MeV)
- Nuclear Recoil (25 eV – 500 keV)
- Miscellaneous heavy ions out to GeV scales

We've gone as low as possible where there is a finite if small chance of scintillation (W=13.7 eV) and as high as possible without breaking our computer –usually from a lack of RAM, or hard disk space! We generated anywhere between 10 parent particles in Geant4, for the GeV-scale energies, to 10,000,000 for the lower-energy nuclear recoil events, in order to get good statistics.

We've also looked at electric fields between 0 and ~20 kV/cm, where there is experimental data. We hope that you will use and enjoy NEST, and don't hesitate to write mmszydagis@ucdavis.edu with questions, comments, problems, or concerns, and the NEST development team will do its best to aid you. Happy hunting for dark matter, beta decay, neutrinos, or whatever it is that you are searching for!

Matthew Szydagis 01/25/13