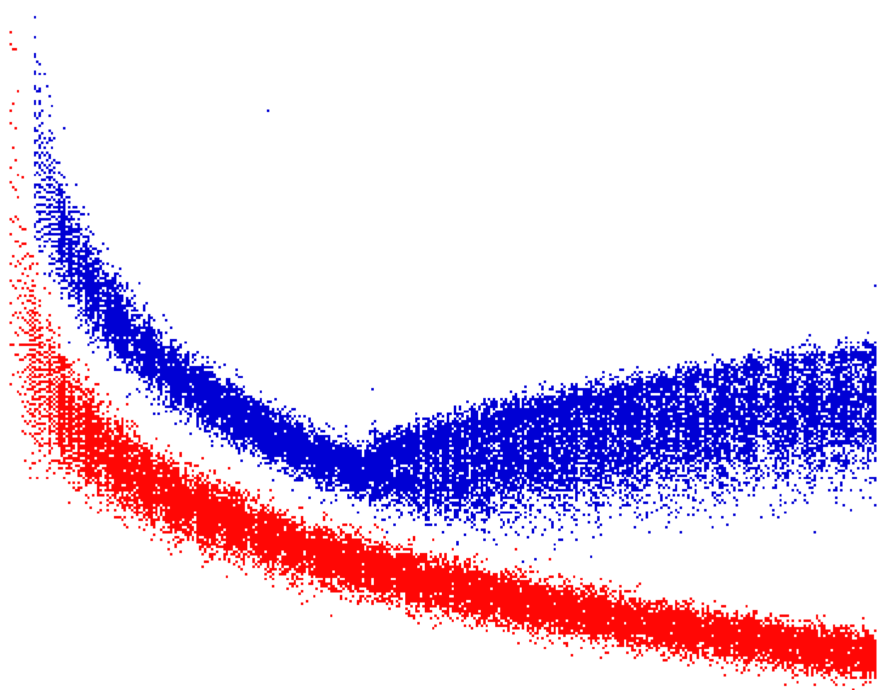
The NEST Companion



I. FAQ Regarding Physics Assumptions

While NEST has been benchmarked against a comprehensive data set, and the best knowledge of scintillation models has been incorporated as much as possible, some things are just unknown, and some things may never be known, or at least always remain controversial. Also, better experiments may force us to change our elegant 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, and is not founded on past experimental data. Whereas the NEST paper (JINST article) covers everything, we reiterate some things here regarding matters of controversial numbers or equations.

Question #1: Why is the excitation ratio kept fixed at 0.06?

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, you should know that we were able to explain a very large amount of data by keeping this number fixed, even for low-energy nuclear recoils (experimental data exists down to a few keV at least). In addition, the effect of changing the ratio can be countered by changing certain Birks' Law parameters, making its exact value a moot point, unless it is not a constant in energy. The Ph.D. Thesis of C.E. Dahl claims it is O(1) for NR, but we were able to explain the same data by changing the one free parameter of the Thomas-Imel model with electric field instead of the excitation ratio. In addition, quoted values of this ratio (for ER) as high as 0.20 exist, but are arguably consistent with 0.06 (see NEST paper).

If you really would like to tinker with this parameter, you can:

a) change the 0.06 line directly in the material properties list, or

b) use the convenient function NEST gives you for this purpose, in your physics list code:
   `theScintProcess->SetScintillationExcitationRatio(0.9);`
   to make the ratio 0.9, for example, overriding the material property default.

However, as explained above, differences in the ratio can be absorbed elsewhere mathematically, and since that is exactly what the NEST development team has already done, it is not recommended that you change this. One exception may be that it is energy-dependent and you wish to tinker with it to obtain better fits to your data, especially at low energies. In that case, please change it in NEST by all means, but just be aware that we've already attempted to absorb the field dependence of NR yield elsewhere.

Question #2: Is perfect anti-correlation of scintillation/ionization maintained at all energies?

The extension of anti-correlation down to low energies for both NR and ER is another assumption that we have made because there really was nothing else we could do other than theorize blindly, due to a paucity of data, especially at the lowest energies possible (sub-keV). NEST generates a number of quanta (sum of excitons plus ions, or, equivalently, final photons and electrons) based on a fixed work function of 13.7 eV for liquid xenon, then assigns excitons and ions binomially. This is followed by assignments of photons and electrons (again, binomially) using a calculated recombination probability. This number of 13.7 eV may be unfamiliar, but all the other ones you know and love are derivatives of this one W, including the oft-quoted but often misunderstood ionization work-function of 15.6 eV (which turns out to really be closer to 14.5 eV). Please read the paper to appreciate this.

It is never possible to observe the full scintillation yield even at zero field because of the escape electron fraction (escape electrons may recombine on ms timescales, longer than most experiments watch, so NEST just lets them go at zero field and does nothing with them), and the non-zero constant in line 373 of G4S1Light.cc tells us that even at infinite field it is not possible to extract all charge, hence past overestimates of the ionization work function (15.6 eV). The best global fit to DokeBirks[0], the volume recombination parameter, unequivocally indicates that this is so. This may be a source of controversy, but many dark matters detectors operate below O(1 kV/cm), below charge yield asymptotes, making the question of what happens at really high field less burning.

<u>Question #3:</u> Isn't Onsager recombination impossible?

Onsager recombination is another matter of great controversy. It is supposed to be impossible, but we get a better fit *at zero field* if we implement it as a significant fraction of recombination (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 perhaps the experimental values for the yield may be too low. Only new experiments can help. However, the 1 MeV electron is not of great importance currently, since even if your experiment deals with O(1 MeV) gammas, the probability of creating electrons that high in energy (as opposed to lower-energy ones) is still very low.

<u>Question #4:</u> How does NEST address the Leff controversy?

Nuclear recoil will, of course, likely never cease to be controversial due to its extreme importance in dark matter search experiments. The NEST model is built upon incredibly simple assumptions, except in its use of the Hitachi-corrected NR model, which has lower (than Lindhard) values of Leff based on his model of bi-excitonic quenching. Please feel free to restore the 'k' value to that of regular Lindhard theory (which just by itself surprisingly does a great job), by commenting out line 305 of G4S1Light.cc:

```
kappa = 0.110; //Hitachi correction, comment out for Lindhard
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Future versions will either use more recent experimental data to once and for all to decide between models, or, if data frustratingly remain ambiguous, allow for a run-time, command-line option. Please note that since the Hitachi quenching factor reduces both electron and photon yields roughly equally, light yield and charge yield by themselves are reduced, but an S2 over S1 plot is not affected. Hence, your discrimination power predictions based on NEST will be the <u>same</u> regardless.

<u>Question #5:</u> How is variation in scintillation wavelength handled?

If you comment out line 605 in G4S1Light.cc and let line 606 stand instead, then you will get a realistic Gaussian spread in scintillation wavelength instead of just getting all optical photons being emitted with exactly 7 eV energy. But make sure your sim can handle it without a G4Exception complaining about a material property out of range. This is usually caused by your refractive index not being defined for a sufficiently wide range of the possible photon wavelengths.

II. Known Potential Bugs

1. 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.

2. Electric Field

Going either too low or too high in electric field may yield unexpected results. For NR, this is a non-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. NR data below 60 V/cm do not exist, but since the yields vary so weakly with field for NR, you are practically at zero at that field even. Above 4,060 V/cm there are no data either, but the yields have experimentally been seen to asymptote very quickly at high fields, hence our extrapolated spline fits (see lines 515-530 of G4S1Light.cc) take this into account. Thus, in theory, you can go out to infinite field with NR in NEST.

As for 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 complicated at extremely low field, especially since several quantities, like the model cross-over distance and the Thomas-Imel parameter (ThomasImel), go to infinity, then sharply snap back down to finite values at zero field. Between 0 and 10 V/cm it is not guaranteed that the S1 yield will be lower than at 0 field and higher than at 10 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 histograms for 10-20 keVee. A cause has not yet been traced.

3. Too High An Accuracy

Increasing the accuracy of the simulation by severely decreasing the minimum step sizes taken during 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 (most defaults, such as Livermore's, are 100 um) will results in a severe underestimate in both light and charge yields. This is because charged particles such as electrons will be forced to undergo many more steps in the simulation. Consequently, at every step, the number of quanta to be created (a double precision variable) 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 322 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.

4. Metastable Kr-83

This wonderful real-life calibration tool has partially vexed us. You may find the accuracy of the electric field dependence of its yields slowly fading at 500+ V/cm. The NEST team is actively investigating.

III. Bonus Features

There are several features in the beta version which were never described in the current publication, but are rather subjects of imminent NEST publications:

- Good predictions for proton, alpha, and heavier-ion zero-field yields, assuming 100% ER.
- S1 pulse shape, with accurate excimer timing, as function of LET, electric field, and particle type.
- NR charge and light yields as functions of electric field (current paper only does zero field).
- Reasonably accurate 0th-order energy resolution, though without detector effects
    - Fano factor
    - recombination fluctuations
    - exciton/ion fluctuations
    - particle history

We include these features so that a complete picture of S1 is provided, in preparation for the next big thing: S2 pulse shape! We did not wish to have a piece-meal release of S1 code. You are free to capitalize upon all features in NEST V0.9 beta and cite the one existing paper, but if during the review process of your work more NEST papers come out, we ask that you update your citation(s).

Despite the fact that S2 is not yet included, you can already generate great plots of log (S2/S1), since the correct number of ionization electrons are generated - the number of S2 photons is of course proportional to the number of the “escape” electrons. If your detector is zero field and one-phase, then of course this does not matter, of if you have a non-zero-field detector with a charge amp as a substitute for S2 light production then you’re also golden already.

IV. Benchmarks

1. Computer System

NEST has been used with Geant 4.9.4 up to and including patch 2. Earlier versions are not supported.

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 Memory

It should take about 0.2 ms per quantum if you have tracking verbosity, or 0.5 ms if you leave it on (not recommended when you're running big sims). So, for example, a set of 100 gamma rays 122 keV in energy will generate ~8900 electrons and scintillation photons, and thus take 2-3 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 once we add S2 photons to NEST it will take a lot longer, especially if you want to run a lot of parent particles to get good event statistics. So, use a very fast computer. You will also need a lot of hard disk storage and/or need to do a good deal of compressing. Doing O(1e6) events in a O(100 kg) Xe detector will take up O(1) TB already without S1 light propagation, nor any recorded S2 light.

2. Particles, Energies, Fields

NEST was tested with a wide variety of particles and energies, sometimes without experimental backing, so that 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, but electric field dependence not yet correct) and Protons (40 MeV)
- Nuclear Recoil Xe-131 test case (25 eV – 500 keV)
- Miscellaneous heavy ions up to GeV scales

We've gone as low as possible where there is a finite albeit tiny chance of scintillation (W = 13.7 eV) and as high as possible given our RAM and hard disk space considerations. We generated anywhere between 10 parent particles in Geant4, for the GeV-scale energies, to 10,000,000 for the low energy nuclear recoils, in order to get good statistics. We've also looked at electric fields between 0 and 20 kV/cm (basically, everywhere 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, or whatever it is you are searching for!