What's New in Version 0.98 of NEST?

- No more teleportation inward of thermal electrons that are generated outside of R_MAX
- Electrons generated outside R_MAX now produce zero S2, a new source of gamma-X events
- Diffusion along the drift axis is now handled using legitimate position instead of time variables
- To avoid negative time errors, a check is placed on particle birth times, enforcing times >= 0
- To mimic/approximate real-life diffusion of electrons around grid wires, electrons are no longer stopped by them, but now pass uninhibited through grid wire material and make S2
- To avoid S2 photon creation in the liquid or in the anode, photon positions are squeezed in
- The "no motion" check in the S2 code has been reduced to 1e-7 nm to avoid genuine small pre- and post-step difference for photons generated as a result of small mean free path
- The conversion efficiency for electrical energy into electroluminescence for LXe has been raised to 101% to offset a 1% underproduction in yield caused by how G4 does mean free paths
- In the course of diffusion, drift electrons can no longer be born below one's PMT bank or above one's liquid-gas border, if the locations of both are set correctly. They are forced back. For a two-phase detector, an exception is granted for genuine gas events
- Gas Xe physics model greatly improved: now has longitudinal diffusion (approximation for transverse), alpha light and charge yields as functions of density and field, electron recoil (gamma-ray) light and charge yields as a function of these plus energy, NR yield predictions
- By default, primary electrons generated near a volume border are allowed to scintillate. They were previously not permitted, because of errors in recombination calculation
- Bug where NEST turned off but particle entered noble element and crashed sim fixed
- Special case of counter-intuitive low diffusion in low-field LXe handled now
- Different electron trapping time at a liquid-gas interface, depending on the strength of the electroluminescence field, and no trapping time if it is an all-gas detector
- Zero-field recombination fluctuation model toned down at low energies to match what is done for non-zero-field and to better match real-life energy resolution
- Modifications to the Thomas-Imel recombination parameter and the T-I/Birks cross-over distance for the zero-field LXe model to better match the Columbia Compton scattering data and make the transition to non-zero field more realistically smooth for both numbers
- Fixed timing bug where events generated at times greater than 999 sec. cycled back to zero
- Complete revision of the metastable Kr-83m physics so that the light and charge yields are matches for both of its lines, for zero and non-zero field, and the resolution/shape works
- Liquid argon modeling improved: new Birks' constant field dependence, flatter yield per unit energy at zero field, to better match data, more accurate wavelength distribution, revision of Thomas-Imel parameter at all fields, singlet-to-triplet ratio dE/dx-dependent for alphas, ER, NR, correct alpha light yield with bi-excitonic quenching of the scintillation; diffusion, drift speed
- Ability to easily simply run with a global electric field and no liquid-gas border definition, for simpler detectors or for not wanting to define the different field regions between grid planes
- Muon tracks now handled properly: were previously treated as electron tracks
- Removed low-temperature warning from Miller drift model (good down to ~160 K at least)
- Fixed bug where in high-yield events some quanta were being generated at strange times caused by subtraction of very large doubles, corresponding to high-time events

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- Removed "track stuck" error for thermal electrons trapped on liquid/gas surface at zero field
- Added more functionality for changing to different elements (other than xenon) in the S2 code
- *Updated S2 yield formula to conform to latest work by Monteiro and Fonseca at Coimbra*
- Non-zero component for the singlet state in the S2 pulse, default of 10% for xenon and argon
- Default electron purity of 2m in the S2 code to represent a modern pure detector
- Energy deposited per interaction site now recorded so that LET can be calculated per site
- *A mathematical mistake in the singlet-triplet ratio repaired for ER, NR, and alphas for LXe, LAr*
- New LET dependence of the recombination time at zero field based on latest XMASS work
- Re-did the LXe electron diffusion coefficients so that both D_T and D_L are now simple power laws with respect to the electric field, and XENON10 and XENON100 data are now reproduced
- Combined variables BORDER, QE_EFF, and GASGAP into one header file (G4S1Light.hh) which is #included by both G4S2Light.cc and G4S1Light.cc
- New bool variable "InaAndOuts" handles the entry and exit of particles traveling between the liquid and gas phases of a two-phase detector multiple times making S1 all along the way
- A negative energy as the goal energy for scintillation dumping is not permitted. To force a dump (e.g. for NR) the goal energy is now set to the current total energy recorded, and if a particle that has not dumped any energy leaves the active volume, the goal energy is set to zero
- *Fixed "atan2" quadrant problem (2 places: particle generation and radial squeezing to avoid boundaries) that was creating thermal electrons only in half of the possible quadrants*
- Eliminated 3 causes of dreaded "NAN": No longer allowing exactly (0,0) as a coordinate (2 places), no electron diffusion at zero field (power law going to infinity), negative square root in diffusion equation prevented for electrons too close to the surface (with a fabs command)
- Can turn thermal electrons off completely at zero field with the SinglePhase command
- *Gas xenon yield and energy resolution models complete for use in high-pressure gas Xe TPCs*
- *Energy resolution modeling finalized for LXe at all fields and energies for both ER and NR, leading to an accurate post-diction of the discrimination power of past detectors (XENON10, XENONO100, Case Xed detector, ZEPLIN-III), including the discrimination increase in the WIMP search regime, modeled as the non-Poissonian recombination fluctuations going to zero*
- *Better LAr support in G4S1Light, plus other elements (Ne, He, Kr): very preliminary numbers (LXe FULL and complete now with this new version of NEST)*
- Slight density dependence for both the Thomas-Imel and Doke recombination parameters
- Added "floor" commands everyone for double to integer conversions for numbers of physical particles, and ensured rounding is done properly everywhere with a "+0.5"
- Added messenger class functionality for user-defined variables (LUXSim code base only)
- *New "gain" variables in G4S1Light.hh allow for "quick and dirty" simulation of both S1 and S2 without full propagation of photons all the way to phe*
- *Updated L_eff model setting the exciton-ion ratio to 1.00 instead of 0.06 for NR, which when used in conjunction with the Hitachi electronic LET, fits the Plante (XENON100) and Horn (ZEPLIN-III) data the very best (while still remaining only 1-sigma above Manzur from Yale)*
- *Field sign now matters for setting e- drift direction (speed set only by magnitude), by region!*
- *Miller electron drift speed now the default for LXe instead of Gushchin (with T dependence)*
- 5 MeV is now the border where the Doke model is used exclusively instead of TIB

What's New in Version 0.95 of NEST?

- G4S1Light (and G4S2Light) is now a RestDiscrete (instead of Discrete) process, making it possible for the physics processes to detect stopped (0 kinetic energy) nuclei that have come from originally excited nuclei, thus making it so NEST can find the endpoint of the event, and allowing the physics process names ("S1" and "S2") to appear properly in tracking verbosity
- Better backwards compatibility with Geant 4.9.3 by use of slightly different functions & units
- Density is now read from the material properties instead of set artificially with #define
- Minimum and maximum energies can be set at the top of G4S1Light.cc with #define
- The high-energy limit for which ER is only Doke to make sim run faster is now 1 MeV (was 10)
- Radial tolerance of 0.2 mm to prevent scintillation quanta for edge events from appearing outside of the active volume of your detector
- Implementation of a maximum radius so that diffusing ionization electrons are not placed outside the active volume by the G4S1Light physics process. (Their originally polar angle is maintained; their radius is simply re-calculated.)
- New particle type (thermalelectron) for the ionization electrons, and ability to turn electron diffusion in the liquid on and off for debugging purposes
- Implementation of a Boolean (ThomasImelTail) for correcting strange electrons produced by Geant4 which travel the "incorrect" distance given their initial kinetic energy
- Implementation of a Boolean (OutElectrons) which leads to no scintillation for e- that leave the active volume (usually skirting boundary), as well as Bremsstrahlung gammas which leave, as they may produce inaccurate results (and should be fiducialized away anyway)
- Correct electron drift speed now implemented as a function of electric field and a function of temperature (liquid) or density (gas). You MUST specify the density and temperature of your liquid, and the density, temperature, and pressure of your gas now when you set up your sim. At zero field, the electrons are given a nominal thermal energy
- Electron LET calculation split off into separate function, with protection against zero-energy depositions causing infinities, and electron mass in kg is defined at top of G4S1Light.cc
- Bi-excitonic quenching for alphas to better reproduce their real-life yield
- Ability to do an approximate quantum efficiency right at photon birth, to save simulation time
- Binomial fluctuations, such as for recombination, have been split off and consolidated into one function, which using the Gaussian approximation for large numbers of particles in order to make the simulation run even faster
- Improved initialization and reset of certain Boolean variables by waiting for Parent ID = 0 and its first step as well as after scintillation has been dumped
- Support for high-energy neutrons where if energy is recorded as deposited instead of a nuclear recoil being created, then NEST assumes that there was a nuclear recoil and gives it the average A of xenon for Lindhard calculations
- Checks the atomic number Z and density and state of the current material. (NEST currently supports only mono-atomic, noble scintillators.)
- Removal of vestigial variables (FASTCOMPONENT, SLOWCOMPONENT, liquidXeScint)
- No longer counts artifact energy depositions recorded by Geant4 at a volume boundary towards scintillation (ignores them)

- Main function in G4S1Light.cc returns, not wasting any time running for zero particles, if there's insufficient energy for scintillation
- To avoid placement of scintillation quanta where they should not be, they are no longer placed stochastically in a small sphere, but only at the point of energy deposition
- Again to avoid bad placement in the wrong volume, the pre-step point is used if a particle is leaving the volume with the scintillator
- The distance used to determine multiple scattering is now fixed at 0.4 mm (the mean distance traveled by the ~30 keV K-edge X-ray in LXe) instead of being a variable determined by the electron-ion thermalization distance and the electric field
- This distance is made infinite for alphas, whose data is best matched by a Thomas-Imel treatment treating all alpha interactions as single whole interaction sites
- 0-energy interaction sites, such as boundary crossings, are no longer stored in the library of possible scintillation sites by G4S1Light.cc (in terms of positions and times)
- The header file G4S1Light.hh explicitly forbids certain particle types from scintillating: (anti-) neutrinos, optical photons, and thermal electrons (used to forbid neutrons, but those may sometimes be said by Geant4 to deposit energy instead of explicitly producing a nuclear recoil)
- Fixed problem where scintillation not dumped properly at end of event and carries over to next after next, and eventually leads to RAM overload and core dump
- The energy "goal" for dumping scintillation is now set to the current total energy deposit in order to force a dump for nuclear recoil instead of to -1, which could wreak havoc
- Do not require a track to be killed or have 0 kinetic energy for scintillation to be dumped, to allow for the case where it leaves the active volume (for good).
- Force alpha particles to always be in Thomas-Imel regime (because of their high dE/dx). Alphas also granted unique field dependence in Thomas-Imel model to better match data
- Fixed glitch where Hitachi-Lindhard energy conversion resulted in negative energy at sub-keV energies. Function now linear without offset.
- Removed mistake where integer divided by integer instead of float by float in calculation of Thomas-Imel parameter. (This correction mostly affects only sub-keV energies.)
- Scintillation energy now 6.97 eV instead of 7.00, and has Gaussian 1-sigma of 0.23 eV. MAKE SURE you define the index of refraction low enough in wavelength (out to 8.5 eV) to handle
- Thermal electrons are delayed at the liquid-gas boundary (delayed electron emission)
- Electron diffusion is field- and depth-dependent (parameterized based on empirical data)
- Removed unnecessary variables from particle creation, such as forcing of a particular parent ID, or so-called touchable handle (no effect on results)
- *Density-dependent Fano factor and exciton-to-ion ratios now implemented, for xenon. Applicability is high: the functions span gas and liquid from 0 to ~3.2+ g/cm^3.*
- *Simpler installation with transparent flexibility for using elements other than xenon and phases other than liquid engineered by moving definitions of scintillation-related material properties out from the materials list and instead embedding them into G4S1Light.cc*
- *Implementation of electroluminescence in gas xenon (S2)*
- *Preliminary numbers for liquid argon yield (S1)*
- *Preliminary numbers for gaseous xenon yield and energy resolution (S1). Note, however, that for gas Xe S1 and liquid Ar S1, the singlet/triplet ratios/times are not yet implemented correctly. They are there still only for liquid Xe (and gas Xe S2).*

Advanced Configuration (Below updated for V0.98)

- Ensure that you specify a temperature, density, pressure, and state/phase for each noble element in your simulation or you will get errors!
- Ensure that you define the index of refraction of xenon in your materials list out to at least 8.58 eV / 144.5 nm in order to handle the new Gaussian scint. wavelength
- Read over the top part of G4S1Light.cc where all the #define's are
    - Set MIN_ENE and MAX_ENE as desired if only studying scintillation in certain energy ranges, so that you can save on simulation time
    - Set R_MAX to the inner or outer circular radius of the inner volume of your detector, if you wish (addresses edge event bugs and makes edge gamma-X)
    - Turn electron diffusion to "true" or "false," as desired. Leave true for realistic S2 shape driven by electron diffusion in liquid, but diffusion may lead electrons to bleeding into unexpected areas of geometry, if far outside of the fiducial volume
    - Set MillerDriftSpeed to true, or to false to get Gushchin, depending on whose electron drift velocity you believe, and who agrees better with your own data
    - Set SinglePhase to true if desired (kills all ionization electrons before birth in order to make the simulation run faster)
    - ThomasImelTail set to true allows Geant4 to generate electrons of high energies but strange short track lengths, which thus produce strange amounts of scintillation (being in the high-energy regime according to energy but according to length being low). Setting this to false corrects these electrons.
    - Remove those rare electrons (rare because track lengths so short, compared to gammas) which exit the detector with OutElectrons=false. This is to prevent electrons from partially depositing energy acting strange (low-dE/dx, low energy)
- Read over the top part of G4S1Light.hh where all the #define's are
    - Use GASGAP to set the size of your electro-luminescence gap (the distance from the top of your liquid, or top of gas S1 region for gas-only detector, to anode)
    - If running a two-phase detector, set BORDER to the z-coordinate (with a unit) of the liquid gas boundary (future release will do this on its own perhaps)
    - Set your quantum efficiency to a nominal value using QE_EFF. This saves simulation time by some killing photons at birth. If you make your active volume the sensitive detector instead of your PMTs, you can use this number as the product of QE and light collection, and run fast sims with no photon propagation
    - For running fast sims without full S2 photon propagation, you can kill the thermal electrons in the active volume and re-adjust their number manually with "phe_per_e," representing the number of S2 phe per electron extracted
    - Set the coordinates (syntax: number*unit) of your different E-field regions, for a two-phase detector, for gamma-X studies, or leave all numbers non-positive to force NEST to default to just one overall field in the liquid and one field in the gas
- Adjust the electron purity at the top of G4S2Light.cc (in terms of distance, not time!)
- If you want S2 electrons to pass through grids, set GRID_DENSITY depending on material
- For the S2 model to work properly, set "gainField" in kV/cm at line 962 of G4S1Light.cc