NEST, The Noble Element Simulation Technique: A Multi-Disciplinary Monte Carlo Tool and Framework for Noble Elements

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Abstract:

The Noble Element Simulation Technique (NEST) allows particle physicists across the community of users of noble elements, especially Xenon and Argon, in different phases, to be able to simulate their detectors as well as the fundamental interactions that comprise their signals and backgrounds. NEST plays a critical role in solving some of the most significant mysteries of modern physics, such as the search for particle dark matter and the quest to understand the neutrino, including the detection of neutrinoless double-beta decay. Moreover, NEST contributes to particle physics in general by improving detector instrumentation and noble liquid detector R&D.

I. INTRODUCTION

The many different fields of physics which employ noble element-based detector technologies for particle detection find themselves at a pivotal point in history. The past decade has been accompanied by an explosion in the use of liquid xenon and argon for particle detection [1–13], and this rise is expected to increase over the coming decades [14–18]. However, for the area of detector simulations, the community remains siloed. Many collaborations build and maintain independent simulation frameworks, inhibiting the broader community from transferring knowledge and from testing or reproducing findings. This affects not only other experimentalists, but also theorists and phenomenologists who reanalyze, reinterpret, and corroborate experimental results.

CERN's GEANT4 (G4) [19–21] commonly provides an initial springboard to collaborations, but while powerful, it also possesses a steep learning curve, and a substantial amount of effort is required to build a complete detector simulation. G4 does not incorporate into its simulations the plethora of calibration data sets available from experiments which measure the scintillation and ionization yields of xenon and argon. Adopting one universal framework for modeling noble liquid microphysics and simulating detected signals will enable future discoveries in the community. Such a global framework already exists: the *Noble Element Simulation Technique*, *i.e.*, NEST [22–26]. While it is not a replacement for GEANT4, which is necessary for *e.g.* determining the precise energy spectrum of one's backgrounds, NEST is specific to noble elements especially as liquids, so it performs noble element-specific tasks with both leading precision and efficiency. Furthermore, NEST exists as both standalone executable codes and a sophisticated G4 interface.

While the xenon (Xe) portion within NEST code is the most mature at present, adding argon (Ar) is crucial for both neutrino and dark matter studies. NEST therefore has recently introduced argon as a detector medium to its framework, including models for its scintillation and ionization response to electronic and nuclear recoils.

II. NEST'S PHYSICS REACH

Utilization of NEST models and code will be critical for existing and future experiments using Xe and Ar for particle detection, at the very least for validating their existing Monte Carlos at first. In the coming decade, Xe will be utilized by experiments such as LUX-ZEPLIN, XENONnT, PANDAX-4T, nEXO, and RED-100. Meanwhile, Ar will be in use for experiments such as DarkSide-20k, DEAP, CENNS-10, the SBN Program, and DUNE. Beyond fundamental physics, Xe/Ar have seen increased applications in medical imaging and nuclear security.

The successes of all of these experiments and physics searches, especially when it comes to any discovery claim of exotic physics including new particles, rely on detailed simulations of the atomic/nuclear processes of energy depositions following an externally or internally-induced interaction. Simulation tools such as NEST are key to various aspects of building and running these experiments. When conducting a measurement or setting a limit, experimenters need to model potential signal(s) and background, often before first light. This later helps in day-to-day operational decisions, informing which combination of detector parameters like field, temperature, and pressure to set, and which calibrations are most important. Finally, a robust plus common Monte Carlo tool helps the particle physics community to decide which future experiments have the greatest potential science reach, by comparing discovery potentials, for example.

One crucial advantage of using NEST for these goals is existing community buy-in. Now the NEST collaboration is composed of physicists from several experimental collaborations: XENON/DARWIN, LUX/LZ, (n)EXO, RED-100, DUNE, MicroBooNE, and SBN. NEST's inter-collaborative nature is allowing knowledge to be shared among a large number of physicists and aids early-career members in making interdisciplinary connections. Given increased community involvement, we will further expand NEST's features, and opportunities for young scientists.

NEST has been cited in a large, diverse set of scientific communications: nearly 200 journal articles and an additional 50+ theses and conference proceedings have cited at least one of the existing four NEST peer-reviewed journal publications [23–26], or the code directly [22]. These include limits on WIMP (the Weakly Interacting Massive

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Particle) interaction through spin-(in)dependent nuclear recoil [1, 3, 4] and other processes [27–29], limits on other forms of dark matter [30–32], searches for other physics signals such as two-neutrino double-electron capture [33] and neutrinoless double-beta decay [6, 34], detector calibrations [35–43], studies of noble-element microphysics [44–47], modelling and projections of future experiments [14–16, 48, 49], and numerous theoretical models [50–52].

All these references attest to NEST's relevance spanning many frontiers: Cosmic, Neutrino, Instrumentation, and Computation (including multiple topical groups in each). In the near term, NEST should see both increased first-principles sophistication of current models, as well as an expansion to other elements, namely helium, which has been proposed as a target for lower-mass dark matter [53, 54]. Current limitations on determining the latent variables that govern the atomic microphysics of the detector are an outstanding obstacle to increasing detector sensitivity. Overcoming this would involve exploration of new statistical and machine learning methods. NEST is uniquely suited to the training of machine learning techniques due in part to its ability to rapidly generate high-statistic, high-fidelity simulated data sets. Therefore, the future of NEST may bring both increased discovery potential to detection experiments, as well as the possibility of determining the basics of noble element atomic microphysics, understood primarily empirically at present.

III. A SUMMARY OF NEST FEATURES

The NEST package is a collection of analytical models and detector parameterizations, in addition to C++, Python, and ROOT codes that anyone can use to simulate particle interactions in Xe or Ar. It is maintained by $O(10)$ scientists, *i.e.* the NEST Collaboration, which spans multiple leading (and often competing) dark matter, neutrino, and R&D experiments, enumerated earlier.

NEST offers a variety of utilities. Pooling all of world data, the collaboration has developed models for the light yields (the primary scintillation, or S1) and charge yields (also the secondary scintillation, or S2) from various interactions: electronic recoils produced by gamma-/x-rays (Compton scattering as well as via photo-absorption) and betas, nuclear recoils from neutrons, from coherent neutrino scattering, from dark matter itself, energy deposits by alphas or heavier non-noble nuclei, and lastly exotic decays such the the double internal conversion of $^{83\mathrm{m}}$Kr, a critical calibration source. In using NEST, one single experiment can utilize global data to reduce systematic uncertainties, as these yields (functions of field, particle, and energy) should be detector-agnostic, with detector-specific effects simulated "on top" of these. Also, NEST can reproduce the S1 and S2 pulse shapes (time profiles).

NEST outputs include energy resolution, efficiency, threshold, and the "band" means or medians and widths for $\log_{10}$(S2), $\log_{10}$(S2/S1), S2, or S2/S1 versus S1, S2, or (combined) energy. "Raw" averages, Gaussian centroids, and skew-normal peak fits are all customizable options. NEST's recent version includes improved response functions for similarly-appearing though fundamentally different interactions: for example, betas and gamma-rays, notoriously difficult to separate by their signatures in the detector, have unique models in NEST depending on detector configuration settings. For a WIMP signal, NEST is fine-tuned and based on neutron calibrations but will not include effects WIMPs would not exhibit, like multiple scattering and inherent position non-uniformity.

The NEST semi-empirical models have been demonstrated to exhibit extraordinary postdictive and predictive matches to data in the liquid and gas phases [26], as well as preliminarily to xenon data in the solid phase. For dual-phase time projection chambers (TPCs) specifically, sample templates are available for an end-user to define their own detector configuration. The current examples are XENON10, Xed, ZEPLIN-III [55], and LUX's initial science run. The configuration settings include parameters like TPC size, photomultiplier tube response, scintillation light collection efficiency, and the electric fields (including possible non-uniformities) in liquid and gas.

NEST, while presently semi-empirical, relies in part on several first-principles approaches: the Thomas-Imel box model of electron recombination [56], the Doke / Birks' Law for scintillation [57], and the Lindhard equation [58]. However, NEST remains dependent upon quality experimental data. To augment NEST's extrapolative abilities, additional resources are necessary to implement molecular dynamics or similar first-principle techniques.

Beyond its wide-ranging accuracy, NEST has been optimized for performance speed by relying on simple analytical models; *e.g.*, on a single-core system, one user can simulate 10^6 β-induced electronic recoils in less than one minute, with energies up to and including the MeV scale even. Furthermore, its availability in multiple programming languages and as various library function calls enables NEST to be relatively easily integrated into existing C++ and Python codes, as well as G4 simulations. The code is free and open-source, and changes are documented on both GitHub and Zenodo [22]. The NEST collaboration hosts analysis notes and links to posters and talks on their website `nest.physics.ucdavis.edu/`.

IV. CONCLUSIONS

NEST enables Xe/Ar experimentalists to develop high-fidelity MC simulations, aids early-career scientists in establishing themselves among peers and senior scientists, and at its heart helps physicists to understand the reach of noble targets for a variety of novel physics searches. It challenges progressive siloing in the community, attesting that when data and knowledge are combined, we benefit from statistical robustness and efficiency of detector response MCs. Lastly, NEST's global fits allow uniquely sensitive constraints on rare physics processes which are still sought only at the individual-experiment level. We look forward to NEST's future in physics as we expand on its use for a diverse set of science objectives.

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