The Journal of Open Source Software

nrCascadeSim - A simulation tool for nuclear recoil cascades resulting from neutron capture

A. N. Villano[1], **Kitty Harris**[1], **and Staci Brown**[2]

1 Department of Physics, University of Colorado Denver, Denver CO 80217, USA **2** Department of Applied Mathematics & Statistics, University of New Mexico, Albuquerque NM 87131, USA

DOI: 10.21105/joss.03993

Software

- Review
- Repository
- Archive

Editor: Lucy Whalley

Reviewers:

- @matthewfeickert
- @altavir

Submitted: 14 November 2021
Published: 23 February 2022

Summary

Neutron capture-induced nuclear recoils have emerged as an important tool for detector calibrations in direct dark matter detection and coherent elastic neutrino-nucleus scattering (CEνNS).

nrCascadeSim is a C++ command-line tool for generating simulation data for energy deposits resulting from neutron capture on pure materials. Presently, capture events within silicon, germanium, neon, and argon are supported. While the software was developed for solid state detector calibration, it can be used for any application which requires simulated neutron capture-induced nuclear recoil data.

A “cascade” occurs when a neutron becomes part of a nucleus. The neutron can be captured to one of many discrete energy levels, or states; if the energy level is nonzero (not the ground state), then the state will eventually change so that it is zero. This can happen either all at once or in multiple steps — that is, the captured neutron may go from its state to the ground state, or it may go to another state with lower energy that is not the ground state (provided that one exists). The cascade refers to the particular “path” of energy levels that a captured neutron takes to get to the ground state from the neutron separation energy. Currently, the code assumes that the neutrons that enter the nuclear system have zero kinetic energy; this is a good approximation for thermal neutrons because 0.0254 eV (the average kinetic energy of a thermal neutron) is small compared to most nuclear recoil energy scales, making it negligible.

nrCascadeSim models many of these cascades at once and saves the energies along with other useful data to a single file. The output file is a ROOT file (Brun & Rademakers, 1997).

Models Used

When modeling deposits from neutron capture events, we want to look at the recoil of the atom as a result of these cascades. To determine how much energy is deposited, we must track how much the atom slows down between steps of the cascade as well as how each nuclear state change affects the atom’s kinetic energy. nrCascadeSim assumes a constant deceleration that results from the atom colliding with other nearby electrons and nuclei. This means that it must simulate, along with the steps of the cascade, the time between each state — to calculate how much the atom slows down. And it must also simulate the angle between the atom’s momentum before a decay and the momentum boost (gamma ray) resulting from the decay — to calculate the resulting momenta. The time between steps is simulated as an exponential random variable based on the state’s half-life, and the angle is simulated as having an isotropic distribution. Cascade selection is weighted by isotope abundance (Rosman & Taylor, 1998; Sonzogni & Shu, 2020) and cross-section as well as the probability of the energy level. In existing levelfiles, energy levels are derived from (Islam et al., 1991) for germanium and from (Raman et al., 1992) for silicon.

The above process models the recoil energies, and the output gives both the total recoil energy for a cascade as well as the energy per step. For some applications, this may be the desired output, or the user may already have a particular process they will use for converting this energy to what they wish to measure. However, we also include, for convenience, the ionization yield and ionization energy of these recoils. Ionization yield is a fraction that, when multiplied by the energy, gives the ionization energy, and ionization energy is the amount of energy that would be read out if an otherwise equivalent electron recoil were to occur. This calculation is useful because many solid-state detectors read out the ionization energy for nuclear recoils. This ionization yield assumes the Lindhard model (Lindhard et al., 1963).

Figure 1 compares the normalized frequencies of ionization energies from the Lindhard (Lindhard et al., 1963) model with the Sorensen (Sorensen, 2015) yield model, which is applied after the simulation using Python, and applies detector resolution models to both. This figure demonstrates one example of user-applied analysis utilizing the energy deposits at each step instead of the ionization energy.

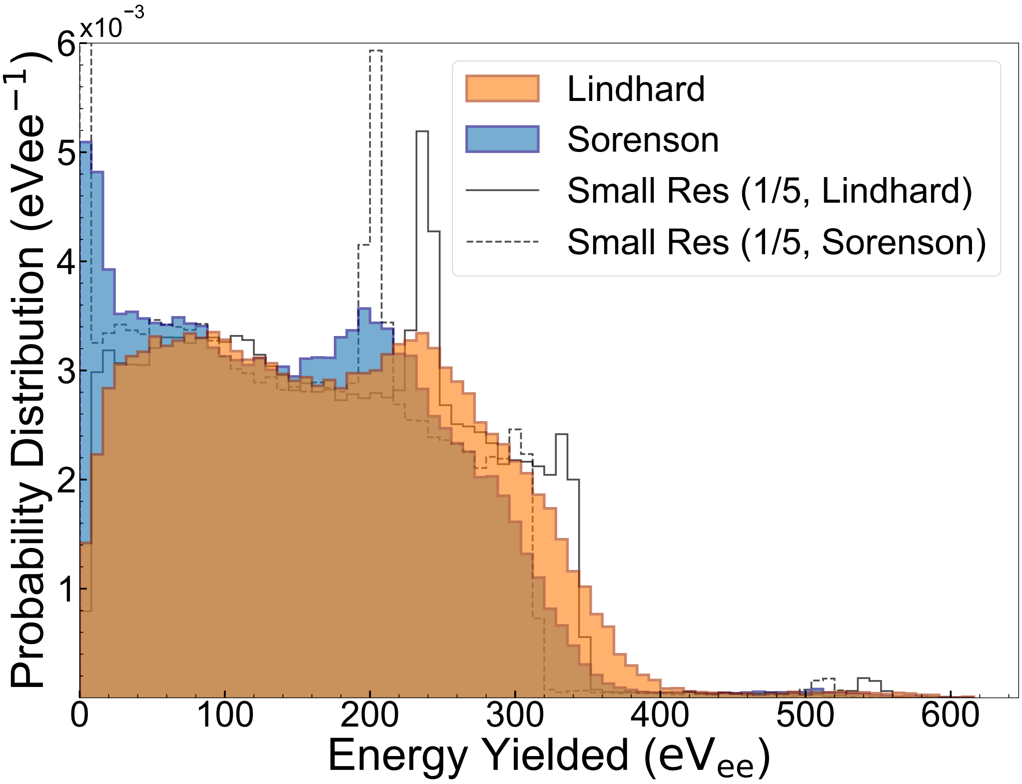

Figure 1: An overlaid histogram showing an example use case in which points are generated and then multiple yield models and resolutions are applied. The "Small Res (1/5)" histograms have Gaussians with 1/5 of the width of their counterparts.

Statement of Need

The goal of this software is to simplify the computation of the nuclear recoil spectrum following neutron capture for a variety of applications. These include nuclear recoil calibrations for dark matter direct detection and coherent neutrino detection (CEνNS). In these cases as the particle detection has become more sensitive (detectors having a lower energy threshold) it is now possible to use the capture-induced nuclear recoil events for detector calibrations. Additionally, thermalized neutrons will provide large backgrounds that have heretofore not been modeled. The key roadblock to studying these scenarios is the complexity of calculating the nuclear recoil spectrum.

nrCascadeSim addresses this need by allowing users to generate nuclear recoil simulations that reflect a variety of single-element detector setups. The energy levels that the recoiling nuclei may pass between and their respective lifetimes are customizable, and multiple isotopes of the same element can be present within the same simulation. Pre-defined energy level files exist for silicon and germanium, which take into account the natural abundance data of each isotope in (Rosman & Taylor, 1998) and (Sonzogni & Shu, 2020). Output values include energy deposits at each step along each individual cascade, total kinetic energy deposits, and ionization energy deposits.

State of the Field

While there are tools, such as the open-source GEANT4 (Agostinelli et al., 2003) framework, that allow users to simulate neutron capture, existing tools are not built specifically for neutron capture-based nuclear recoils as nrCascadeSim is and therefore use some underlying assumptions that nrCascadeSim does not. The main approximation often used in GEANT4 that we avoid in nrCascadeSim is that all recoils decay directly to the ground state. While this works for some applications, it is necessary to be more precise when an accurate spectrum of neutron capture-based recoils is needed for analyses such as calibration or background subtraction. Figure 2 shows a comparison for the energy deposits produced by Geant4 for natural silicon compared with those produced by nrCascadeSim. The figure does not include any instrumentation resolution and shows a highly prominent peak around 1.25 keV recoil energy (coming from capture on ^{29}Si directly to the ground state) whereas the nrCascadeSim shows another direct-to-ground contribution (from capture on ^{28}Si) at around 1.0 keV recoil energy and generally far more "spread out" recoils coming from two- or more step cascades.

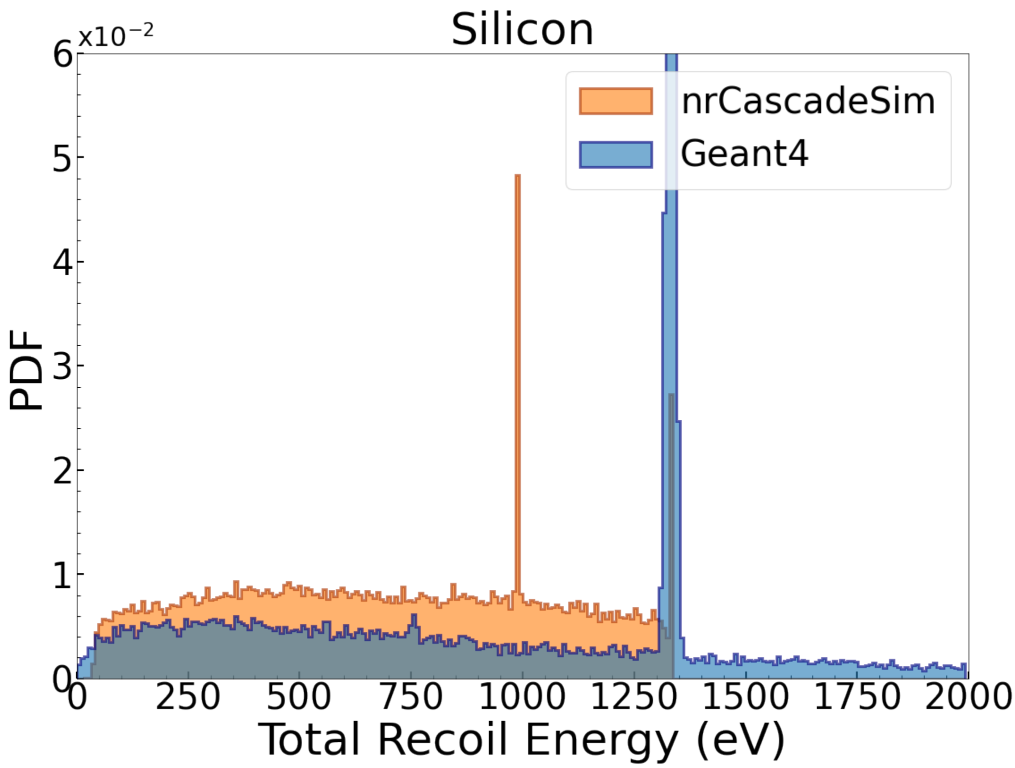

Figure 2: An overlaid histogram showing how the Geant4 v10.7.3 energy deposits compare with those from nrCascadeSim for natural silicon.

Recently, the power of the neutron capture-induced events has been acknowledged in the CEνNS field (Thulliez et al., 2021). That initial study, however, used the FIFRELIN code (Litaize & Serot, 2010), which was originally developed for modeling fission fragments and has been updated to use statistical models of gamma emission for the purpose of modeling fission-fragment deexcitation (Litaize et al., 2014). `nrCascadeSim` takes the complementary approach of beginning with small to medium-sized nuclei and modeling the cascades in more exact detail. The goal is for the code to be extended to heavier nuclei but still using this detailed approach.

Acknowledgments

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of High Energy Physics (HEP) under Award Number DE-SC0021364.

References

Agostinelli, S., Allison, J., Amako, K., Apostolakis, J., Araujo, H., Arce, P., Asai, M., Axen, D., Banerjee, S., Barrand, G., Behner, F., Bellagamba, L., Boudreau, J., Broglia, L., Brunengo, A., Burkhardt, H., Chauvie, S., Chuma, J., Chytracek, R., & Cooperman, G. (2003). GEANT4 - a simulation toolkit. *Nuclear Instruments and Methods in Physics Research A*, *506*, 250–303. https://doi.org/10.1016/S0168-9002(03)01368-8

Brun, R., & Rademakers, F. (1997). ROOT - an object oriented data analysis framework. *Nucl. Inst. & Meth. In Phys. Res. A*, *389*, 81–86. See also "ROOT" [software], Release v6.22/00, 02/07/2020, (No DOI available for this version, closest version linked). https://doi.org/10.5281/zenodo.3895852

Islam, M. A., Kennett, T. J., & Prestwich, W. V. (1991). Radiative strength functions of germanium from thermal neutron capture. *Physical Review C*, *43*, 1086–1098. https://doi.org/10.1103/physrevc.43.1086

Lindhard, J., Nielsen, V., & Scharff, M. (1963). Integral equations governing radiation effects. *Mat. Fys. Medd. Dan. Vid. Selsk.*, *33*, 1–41.

Litaize, O., & Serot, O. (2010). Investigation of phenomenological models for the monte carlo simulation of the prompt fission neutron and \ensuremath{\gamma} emission. *Phys. Rev. C*, *82*, 054616. https://doi.org/10.1103/PhysRevC.82.054616

Litaize, O., Serot, O., & Berge, L. (2014). https://www.oecd-nea.org/science/meetings/pnd22/presentations/1-LITAIZE.pdf

Raman, S., Jurney, E. T., & Lynn, J. E. (1992). Thermal-neutron capture by silicon isotopes. *Physical Review C*, *46*, 972–983. https://doi.org/10.1103/PhysRevC.46.972

Rosman, K. J. R., & Taylor, P. D. P. (1998). Isotopic compositions of the elements 1997. In *Pure & Appl. Chem.* (Vol. 70, pp. 217–235). International Union of Pure; Applied Chemistry. https://doi.org/10.1515/iupac.70.0026

Sonzogni, A., & Shu, B. (2020). *Nudat 2*. Brookhaven National Laboratory. https://www.nndc.bnl.gov/nudat2/

Sorensen, P. (2015). Atomic limits in the search for galactic dark matter. *Phys. Rev. D*, *91*. https://doi.org/10.1103/PhysRevD.91.083509

Thulliez, L.others. (2021). *Calibration of nuclear recoils at the 100 eV scale using neutron capture*. *16*(07), P07032. https://doi.org/10.1088/1748-0221/16/07/p07032