Snowmass2021 - Letter of Interest

Simulations of Low-Energy Crystal Physics for Dark Matter Detectors

Thematic Area: CompF2: Theoretical Calculations and Simulation
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SuperCDMS Collaboration

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Abstract: Increasingly accurate and fast detector simulations are crucial to maximizing the discovery potential of the upcoming generation of dark matter searches employing cryogenic crystals. An efficient model for the development and maintenance of the necessary software tools would consist of a specifically funded initiative across multiple experiments. Expert person-power is of the utmost importance, while another key ingredient is access to the necessary computational power on well-supported, reliably-maintained, accessible platforms.

Introduction: Experiments employing cryogenic crystal detectors play a key role in the global dark matter (DM) search program. The upcoming generation of these experiments, including SuperCDMS SNOLAB [1], will achieve lower backgrounds and energy thresholds than their successors, through a variety of improvements in detector technologies and shielding. In order to take full advantage of these increased capabilities, and maximize the experiments' new discovery reach at lower DM masses and lower interaction cross-sections, faster and more accurate detector simulations are crucial. Some of the simulation challenges are shared with other DM and neutrino experiments, while others are much more specialized. Addressing these challenges requires support for the construction of specialized software tools that build upon existing HEP frameworks. Success depends upon the availability of high-power scientific computing resources accessible to all members of international collaborations, and of expert person-power.

GEANT4 and G4CMP: A prime example of the above paradigm is the Geant4 Condensed Matter Physics (G4CMP) package [2, 3, 4], an application library that provides a collection of particle types, physics processes, and supporting utilities to simulate a limited set of solid-state physics processes in Geant4. Developed for the low-temperature community, G4CMP supports production and propagation of acoustic phonons and electron-hole pairs through solid crystals, as well as boundary processes (interactions at the surfaces of crystal volumes). The boundary processes are modelled on Geant4's optical physics process, and support reflection, transmission, and absorption with configurable probabilities. Since phonon sensors typically involve a superconducting film to couple the substrate to a sensor (SQUID, TES, etc.), G4CMP also includes a class that implements a parametric model for that coupling, modelling energy exchanges between phonons and quasiparticles from broken Cooper pairs.

Individual "user" applications, such as the MC for SuperCDMS detectors in particular, are linked against G4CMP. The user application defines a collection of dynamical parameters for each crystal detector material; skin surfaces (for bare crystal substrates) and border surfaces (having sensor/device volumes attached) with different property parameters; and active sensors (for phonons and/or charges) on the surfaces. G4CMP can thus be used for various crystal materials – such as silicon, germanium, and diamond – and for various detector geometries. The package is currently used extensively in the SuperCDMS detector Monte Carlo software, as well as by the LiteBIRD experiment [5], the CALDER project [6], and by small groups involved in quantum information science (QIS). The CRESST and EDELWEISS experiments, by way of the EURECA collaboration [7], have a particular interest in the MC for SuperCDMS detectors.

G4CMP was first developed at Stanford / SLAC National Accelerator Lab. Since then, Bowdoin College, Ferrara University, and Texas A&M University have become important contributors. Improvements to G4CMP are ongoing, with the goal of ensuring usefulness to multiple experiments in the community going forward.

Upcoming Challenges: There are a number of areas where simulations of DM detectors are limited by the available software. Some development work in these areas may be possible within individual collaborations, but the majority requires support across the DM community, and even across nuclear and particle physics. These include:

- Charge transport in semiconductor crystals at high voltage
- Low-energy processes, including transition radiation and secondary electron emission
- Optical diffractive transport in Geant4 (for thermal modeling of realistic geometries)
- Validation and comparison of Geant4 to MCNP (a general-purpose Monte Carlo N-Particle code [8, 9], developed as Los Alamos National Laboratory, that can be used for neutron, photon, and electron transport)

- Nuclear recoil yield models at the microscopic level

Computing Resources: Cryogenic crystal detectors share with other DM and neutrino experiments the resource challenges associated with the need for higher statistics and more accurate simulated event properties, especially as analyses delve into the use of raw detector-level information and/or Machine Learning techniques. In the case of cryogenic crystals, the proliferation of huge numbers of low-energy phonons can lead to dozens of CPU-hours and gigabytes of memory being consumed in the simulation of a single event. Techniques such as re-weighting and "down-sampling" (e.g. only simulating a fraction of the phonons at certain energies) can help reduce the resource usage. Nonetheless, access to the necessary computational power on well-supported, reliably-maintained platforms is still crucial for experiments such as SuperCDMS. While some collaborations include universities that can provide use of their own clusters, computing resources at American national laboratories have traditionally played an important role. This role is increasingly being taken over by internationally-available Grid computing platforms. Going forward, national lab computing resources will be of limited value to international collaborations unless they are accessible to all collaborators, regardless of country of origin.

Expert Person-Power: The development and maintenance of tools such as G4CMP critically depends upon the availability of expert person-power. Expecting experimental collaborations that employ the tools to each find support for a significant fraction of even one full-time-equivalent researcher from their operations funding is not an optimal model. For example, the entire G4CMP package is currently being maintained by just a few part-time developers, which creates high potential for single-point-of-failures, under-resourcing, inability to train new developers, and long-term unsustainability. A far more efficient model involves a specifically funded initiative across multiple experiments. Historically, American national laboratories had as part of their explicit mission the provision of community-wide software tools which neither individual university groups nor even collaboration of multiple groups could develop or maintain. Geant3 and Geant4, TopDraw(er) at SLAC and FNAL, MCNP at LANL, and a number of packages at LLNL were all developed as part of the labs' mission to serve the whole particle physics community. Restored DOE support and approval for these efforts at national labs, particularly for Geant, would be greatly beneficial.

References

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