Geant4 based simulations for novel neutron detector development

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Abstract. A Geant4-based Python/C++ simulation and coding framework, which has been developed and used in order to aid the R&D efforts for thermal neutron detectors at neutron scattering facilities, is described. Built upon configurable geometry and generator modules, it integrates a general purpose object oriented output file format with meta-data, developed in order to facilitate a faster turn-around time when setting up and analysing simulations. Also discussed are the extensions to Geant4 which have been implemented in order to include the effects of low-energy phenomena such as Bragg diffraction in the polycrystalline support materials of the detector. Finally, an example application of the framework is briefly shown.

1. Introduction

The construction of the European Spallation Source[1, 2], which will become the world’s most powerful source of thermal neutrons, is about to begin in Sweden, breaking ground in 2014 and coming online towards the end of the decade. Currently 22 scattering instruments are planned as the baseline suite at the facility, and a crucial part of each such beam-line will be the detector at which neutrons are detected after undergoing scattering in a given sample under study. Detection of neutrons with sub-eV kinetic energies must necessarily proceed through destructive nuclear processes in which energetic secondaries are released. Only a few stable isotopes such as $^3$He, $^{10}$B, $^6$Li, $^{157}$Gd and $^{235}$U have significant relevant cross sections for such interactions, and detector systems must contain such materials as well as incorporate capabilities to detect the resulting secondaries. The dominant detector choice has so far been gaseous $^3$He detectors, based on the high cross section process $n + ^3$He $\rightarrow ^3$H + p. However, due to increased demand and decreased supply, $^3$He will be unavailable in the future for all but the smallest detectors[3, 4]. Thus, an extensive international R&D programme is currently under way[5] in order to develop efficient and cost-effective detectors based on other isotopes.

A promising alternative is gaseous detectors surrounded by solid converters in the form of thin films of $^{10}$B-enriched boron carbide[6, 7]. The basic principle of a successful detection event in the latter is illustrated in figure 1: after conversion one of the released ions travel into the instrumented counting gas where it is detected like any energetic charged particle. Such a detector has an inherent high-rate capability and, due to the high amount of energy released in the reaction and the implied large signals, the possibility for very high suppression of gamma
backgrounds which can otherwise be an issue at neutron instruments. Additionally it is a relatively cheap technology, allowing for large detector coverage when needed. However, high conversion efficiencies requires the neutron to traverse several tens of microns of converter, while the resulting α and Li ions only have a reach in solids of a few microns. Thus, to obtain high detection efficiencies, one must either use many independent layers of gas-facing converters, keep the angle of incidence of the neutron on the converter as low as possible, or a combination of the two. But such configurations inevitably include significant amounts of substrate and support material in the path of the neutron, and although materials with a low scattering cross section such as aluminium are chosen, the scattering herein can still become a concern. All in all, it is highly non-trivial to access the overall performance of a complete detector system, implying the need for accurate full-scale simulations, such as with the framework presented here, built upon Geant4[8, 9]. Whilst this framework has been implemented specifically in order to allow for efficient and flexible investigations of neutron detector designs, it has potential for wider applications in neutron scattering, and in other disciplines, and is intended to make relevant parts of it available to the wider community.

2. General coding framework
All code is developed in a custom multi-user coding framework where software is kept in inter-dependant logical units (“packages”), providing libraries, applications, scripts, (small) data files, and compiled or pure Python modules1.

Supported languages are C++, Python, C and Fortran with Boost C++/Python bindings. The configuration and detection of external dependencies is based on CMake scripts, but most developers will use a single command-line tool to easily and automatically (re-)configure, build and launch unit-tests. In addition, apart from adding a single line to specify the inter-package dependencies (and optionally dependencies on external software), the developer will never have to edit any configuration files when working on a package. Instead, the names of sub-directories in which files are placed inside a package follow certain conventions, interpreted by the build system. As an example, placing one or more files with extensions .hh and .cc inside a subdirectory named app/ will result in them being compiled as C++ into an application named myprog. If the package has a (direct or inherited) dependency on Geant4, the application will be compiled and linked accordingly. Unit testing is an integral part of the framework, and any script or application whose name starts with test will be taken as a unit test.

1 The main code branch is kept in a Mercurial repository at the Data Management and Software Centre at ESS/Copenhagen and supported platforms are currently 32 or 64 bit Linux or OSX with GCC or LLVM/Clang.
An essential feature of the framework, is the ability to gracefully handle missing external dependencies. While **CMake**, **Boost**, **Python** and a C/C++ compiler are always required, other dependencies such as **Geant4** are optional. If missing, packages requiring them will be gracefully disabled, and the rest of the code built as normal. This feature greatly reduces the installation requirements of developers only interested in a sub-set of features, and equally means that developers are not unduly prevented from adding new dependencies.

3. Geant4 Simulation framework

Embedded in the coding framework is a **Geant4**-based simulation framework in which geometry and generator implementations are encapsulated as configurable modules, normally instantiated and attached to the framework in a short **Python** script. Despite typically being just a handful of lines long, such a script is immediately a fully-featured application which one can use to query, control and launch all relevant aspects of the chosen simulation setup from either the command line or by adding additional calls in the script itself. Notably, the configurability relating to geometry extends to materials as well, which makes investigations into the role of different materials as easy as changing a parameter at the command line (this can also be used to enable the custom materials with crystal diffraction discussed in section 3.2). In addition to sheer convenience, the complete configurability from either **Python** or the command line facilitates easy scanning of parameter space when optimising proposed detector layouts.

By default, the framework is set up to write out results in the **GRIFF** format presented in section 3.1. It furthermore enables multiprocessing, handles random number streams, **Geant4** physics lists and thresholds, and allows for the launch of a graphical viewer to inspect the geometry and simulation results (either using the one shipped with **Geant4** or a custom **OpenSceneGraph** based one which is currently being developed). Finally, the framework provides a number of other useful features, such as providing a simple switch to enable cross sections for all active physics processes to be dumped to a separate file.

3.1. **GRIFF** file format and analysis framework

A general purpose object oriented output file format, **GRIFF**, with meta-data has been implemented, in order to facilitate a faster turn-around time when setting up and analysing simulations, as well as allowing more complex and detailed whole-event analyses. It is optimised for easy, fast and reliable analyses from either C++ or **Python** of low-multiplicity physics, but supports filtering for scenarios involving higher multiplicities or statistics.

Installed through the **Geant4** stepping action hook, the entire event will by default be written to the file, including information normally available to traditional **Geant4** in-job analyses such as information about volumes and particle data. The file can thus be opened and read without a **Geant4** installation, and provides the user with an object oriented access to information from the entire event as illustrated in figure 3. Easy navigation between objects (e.g. from a track to its daughter tracks or constituent steps) is naturally included. As illustrated in the figure, one additional layer is interspersed between the track and step layers: series of consecutive steps of a track within a given volume are grouped together in *segments*. Not only does this facilitate a more efficient data layout, it also is a highly useful concept at the analysis level.

If necessary, **GRIFF** supports two means of filtering output. Due to the contained coordinates, step data requires the most disk space, and the primary global filtering method is therefore to reduce the amount of steps written out. Either by completely omitting step data, or by combining all steps on a segment into one meta-step. Alternatively, users can register custom step-filters, thereby gaining complete control of the stored output.

Hidden from the user, the actual on-disk layout of **GRIFF** files is illustrated in figure 2: After a short file header, one event block is appended for each event. Data inside the block is kept in three sections containing shared, brief and full data respectively. Data unique to individual
tracks, segments and steps is kept in the two latter, while as the name implies, common data relevant across events is kept in the shared data section. This includes any strings and metadata relating to volumes, particles and job configuration, which can then be referenced economically through simple indices in the other sections (in current and following events). This means that in order to load the \( N \)th event, the shared data sections of events 1 through \( N \) must have been loaded. Such a layout was chosen to enable direct streaming to disk without the need for additional post-processing, but typically only the first few events in a file will contain shared data.

The actual loading of an event is a highly efficient operation: The brief data section is loaded into memory and wrapped with pre-allocated thin track and segment classes. Data deserialisation is granular and happens only on demand when a particular property of an object is queried, and step objects are only created for a particular segment if needed.

3.2. Extending Geant4 with NXSLib

For neutron wavelengths of \( O(1\text{\AA}) \), coherent scattering in the form of Bragg diffraction dominates in polycrystalline materials such as aluminium. This important effect is, however, not present in Geant4 out of the box, and has been included through integration with the polycrystal library NXSLib\[10–12\]. Figures 4 and 5 show the important effect of this correction on the relevant neutron scattering cross sections in aluminium\(^2\). The NXSLib–Geant4 integration augments the existing rich capabilities of Geant4 to become a complete tool for investigations of a multitude of phenomena at neutron scattering facilities, and will be described in more detail in a dedicated future publication.

4. Example application: novel SANS detector geometry

An illustrative application of the framework is in the development of a novel new detector geometry for a small angle neutron scattering instrument\[14\], visualised in figure 6. Diffractive scattering in support materials will be a major challenge and simulations are essential to develop the final design of such a detector. An example performance plot resulting from such studies is shown in figure 7.

\(^2\) Where relevant figures were created using Geant4.9.6.p02 and the QGSP_BIC_HP physics list.
Figure 4. Original and NXSLib-corrected cross sections for neutron interactions in Geant4 compared to data[13].

Figure 5. Scattering angles in aluminium provided through NXSLib. A similar plot based on uncorrected Geant4 is featureless.

Figure 6. Proposed neutron detector with the sample located at the entrance of the vacuum vessel (red), with pointing absorbers to limit background scattering (blue/purple) and actual detector boxes (green).

Figure 7. Difference between measured and actual neutron direction for different wavelengths.

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