

Geant4 Based Simulations for Novel Neutron Detector Development



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The European Spallation Source

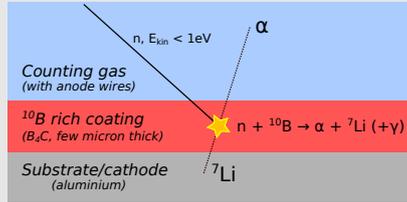
- Will commence operations in Lund, Sweden in 2019 with an initial instrument suite of 7 instruments, growing to 22 in 2025
- Through spallation induced by the worlds most powerful proton beam (5MW), it will become the worlds most intense source of thermal neutrons
- Will facilitate a versatile scientific and technological programme in areas encompassing material science, chemistry and biology



Principles of detection

- Detection of $E_{kin} < 1\text{eV}$ neutrons must necessarily proceed through destructive nuclear processes in which energetic secondaries are created
- Only a few stable isotopes such as ^3He , ^{10}B , ^6Li , ^{157}Gd , ^{235}U ... have significant cross-sections
- High X-section (and dominant detector choice so far): $n + ^3\text{He} \rightarrow ^3\text{H} + p$
- But ^3He now unavailable for all but smallest detectors \Rightarrow Intensive R&D needed for replacements!

Solid state Boron-10 detector: converter plus wire chamber



- Cheap, high rate capability
- Good suppression of gamma backgrounds
- Reaction products travel only few μm in solids \Rightarrow Converter must be $\sim 1 \mu\text{m}$ thick
- Low per-surface efficiency at 90°
- Good efficiency requires many surfaces and/or low angles of incidence
- Scattering in substrate & support a concern
- All in all, complex to access performance \Rightarrow high need of realistic simulations

Custom multi-user coding framework

- Primary languages C++/python (with boost-python bindings)
- SW kept in interdependant logical units ("packages"), providing libraries, applications, scripts, python modules, etc.
- Configuration based on CMake
- Optionally use one single command to (re)configure and build on demand
- No need to "install everything and the kitchen sink" in order to access a few specific features: Gracefully and automatically disable relevant packages in case of missing external dependencies such as ROOT, Geant4, OpenSceneGraph, HDF5, etc.
- Integrated unit testing
- Supported platforms: Linux, OSX, GCC, LLVM/Clang, 32bit, 64bit
- Main branch kept in Mercurial repository at ESS/DMSC

Geant4 framework

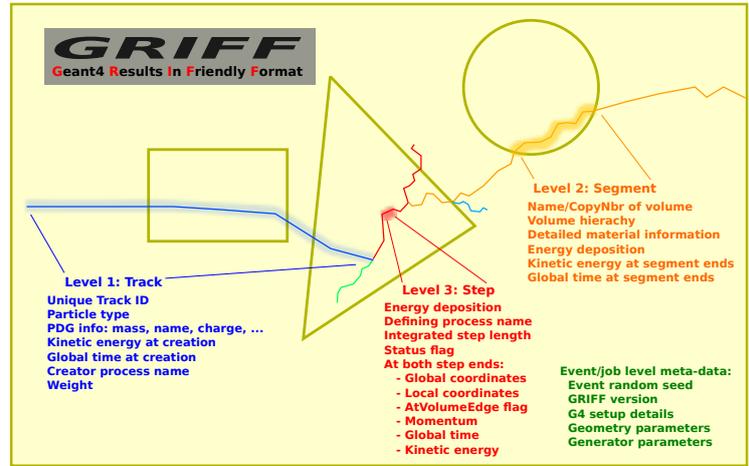
- Users supply geometry and generator modules, written in C++, loaded via python
- Parameters (including for materials) can be set and queried in python or from the command-line, facilitating easy scanning of parameter space
- Easy dumping of x-sections and choice of physics list
- Custom 3D OpenSceneGraph viewer
- Multiprocessing support
- Intend to make relevant parts available for external users
- Integrated GRIFF output and neutron diffraction capabilities

GRIFF

- Optimized for easy, fast and reliable analyses of low-multiplicity physics, but supports several options for output filtering for scenarios involving higher multiplicities or statistics
- Format heavily optimised for on-disk size and reading speed. Readable without G4
- Allows efficient object-oriented analysis of whole event from python or C++ (see box for contained event data)
- Contains metadata such as geometry and generator parameters

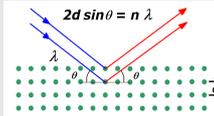
Neutron diffraction in polycrystals

- For neutrons with $\lambda = O(1\text{\AA})$, diffractive scattering becomes important
- Physics not included in Geant4 out of the box
- Functionality achieved by integration with polycrystal library NXSLib (see box)
- This augments the existing rich capabilities of Geant4 to become a complete tool for investigations of a multitude of phenomena at neutron scattering facilities

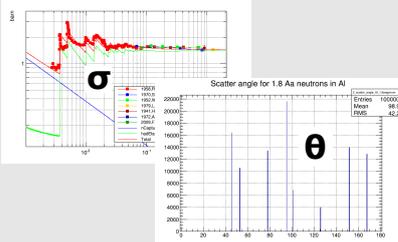


Neutron diffraction in polycrystals (Al, Cu, ...)

- Neutrons with $\lambda \approx 1\text{\AA}$ scatters coherently on crystal planes at angles given by Bragg condition:
- NXSLib by M. Boin provides first principle calculation of relevant quantities, based on crystal unit cell definition:

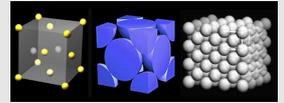


- Affects X-section and angular distribution:



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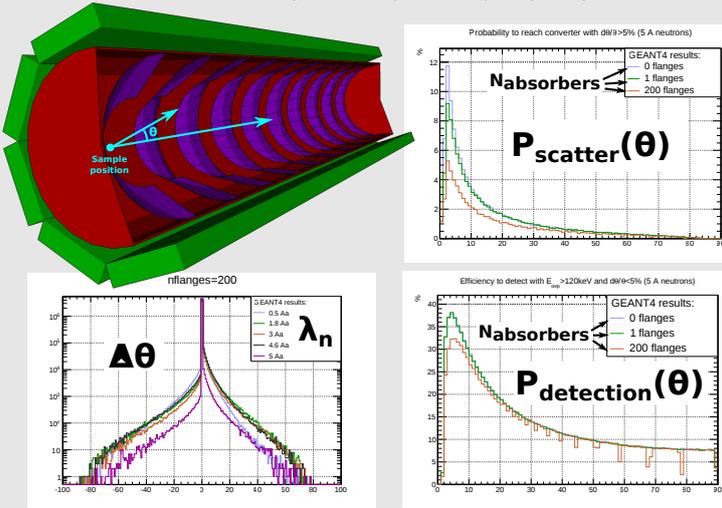
[shell:root@dm3] data> cat Al.nxs
lattice group = 225
lattice a = 4.049
lattice b = 4.049
lattice c = 4.049
lattice alpha = 98
lattice beta = 98
lattice gamma = 98
[atoms]
old atom = Al 3.449 0.088 0.23 26.98 429 0 0 0 0 0 0 0
    
```



- Unit cell must be associated to G4Material during geometry construction
- Details of Geant4/NXSLib integration to be described in separate paper

Example: Novel Small Angle Scattering Instrument

- Completely new detector concept
- Diffractive scattering in support materials a major challenge
- Simulations essential to investigate and improve competing designs



Example: Tests with small prototype

- Collect test-beam data from radioactive sources or existing facilities
- Simulations necessary to fully understand data and for proper planning
- Test data essential for tuning of simulation

