EXTENDING CRYSTAL STRUCTURE CAPABILITIES

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CURRENT STATUS

- Geant4 crystal structures implemented and working:
  - Very flexible structure thanks to the G4ExtendedMaterial class, updates can be done without any change to existing G4 classes.
  - Store the lattice parameters (unit cell) and elasticity tensors (used by phonon)
  - Capability of compute structur factor and other properties (can be updated with more function depending on the future needs)

- Currently used by the G4Channeling process:
  - The process get the crystal lattice orientation from the G4LogicalCrystalVolume and the evaluated data from the G4ChannelingData (subclass of G4MaterialExtension)

PROCESSES

- Future updates are related to the needs of the processes:
  - Migration of "Phonon" example
    - Use the version in the G4 code repository or the complete package from Kelsey and Agnese (https://github.com/kelseymh/G4CMP)?
    - Do we want to add support for charge carriers ?
  - Channeling process
    - The process needs update to take into account spin precession (not related to the crystal structures)
    - Calculation of the data for channeling can be moved into G4, but libraries for FTT need to be added (is it possible?)

PROCESSES

- Future updates are related to the needs of the processes:
  - Implementation of "Coherent X-ray scattering":
    - G. Paternò has developed a process for "Coherent scattering" in Geant4 (https://www.ncbi.nlm.nih.gov/pubmed/29724659)
    - We are working on the integration into G4
  - Implementation of "Diffraction"
    - Neutron diffraction library (https://github.com/mctools/ncrystal/releases/tag/v0.9.11) is released outside G4
    - The development of a X-ray diffraction in crystal process is under study by G. Paternò and me.

FUTURE UPDATES

- Desiderata:
  - Support for powders/polycrystals:
    - Is it a "crystal" property?, i.e. we will add this parameter to the crystal structure file?
  - Automatic crystal structure details from CIF files
    - The database is huge, parsing a CIF file would help to automatically retrieve all the parameters for a single cell.
    - FTEs and skills are missing for this specific task
  - Documentation to help developer use the crystal packages
    - Developers seem to be not able/do not want to use the crystal package. May the presence of documentation help?