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Simulation Tools for Detector and Instrument Design

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on behalf of the ESS Detector Group

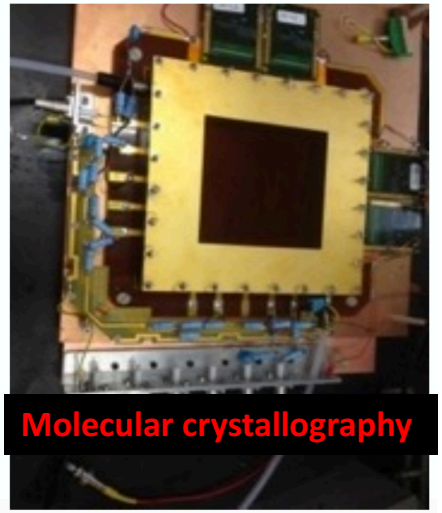
European Spallation Source ERIC

ICNS conference, Daejeon, July 2017

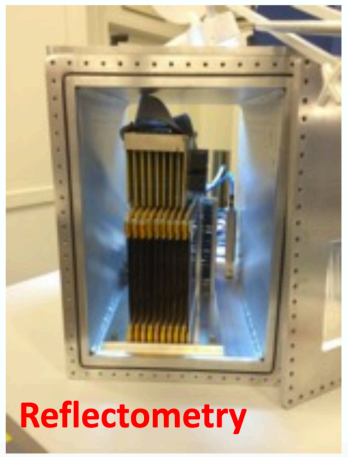
Introduction

- Numerous advances in neutron detector technologies for upcoming ESS instruments
- New simulation tools are available to the community.
- Possible to tailor the detector design to the application
- Speed up the development period

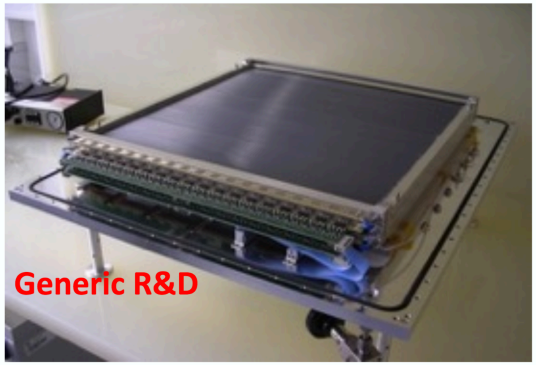
Gd-GEM (ESS/CERN/LiU)



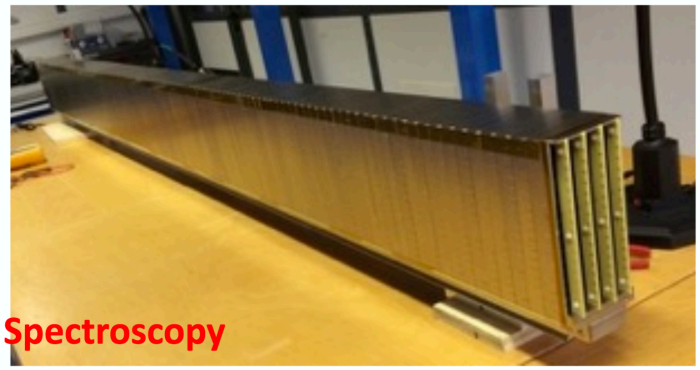
MultiBlade (ESS/Wigner/LU/LiU)



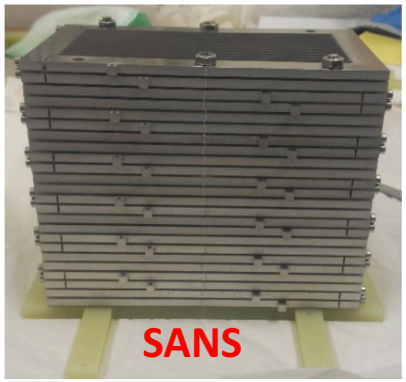
B-MWPC/ Macrostructures (ESS/FRM2)



MultiGrid (ILL/ESS/LiU)

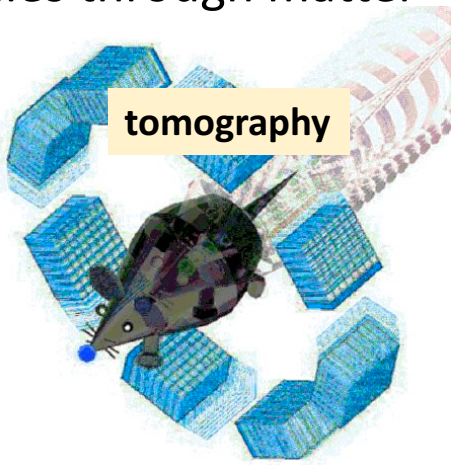


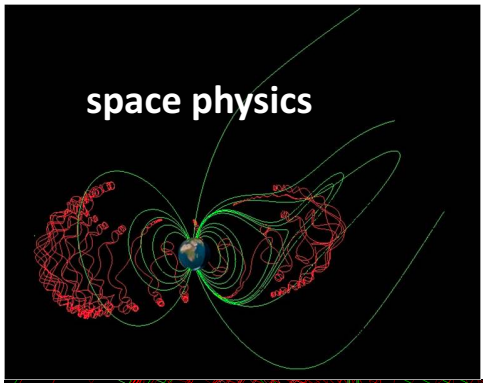
BandGEM (Milan/CNR/INFN/CERN/ESS)

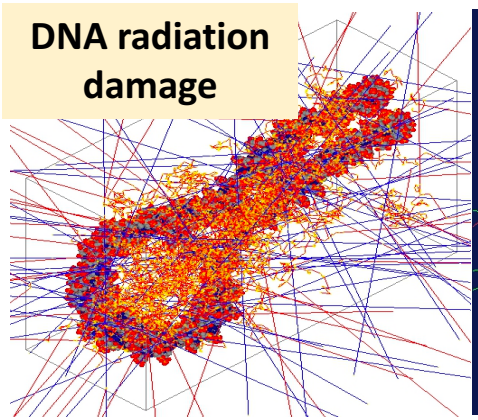


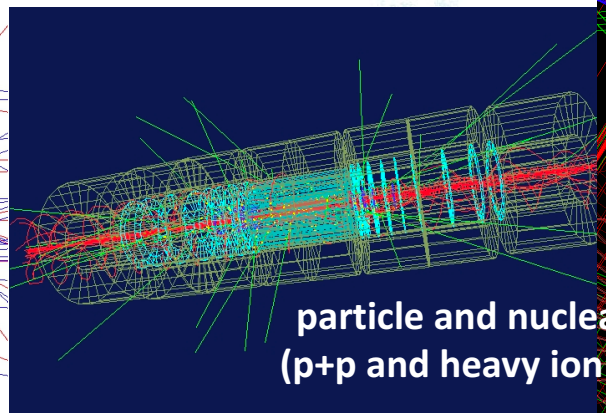
Geant4: GEometry ANd Tracking

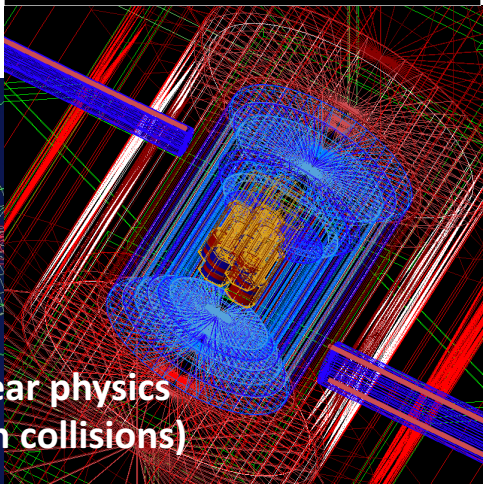
- Monte Carlo toolkit for simulating passage of particles through matter
- Contains facilities to handle geometry, detector response, visualization and analysis
- Created at CERN by high energy physics community
- Other applications include:
  - Space physics
  - Radiation
  - Medical physics
- Expanding to neutron scattering









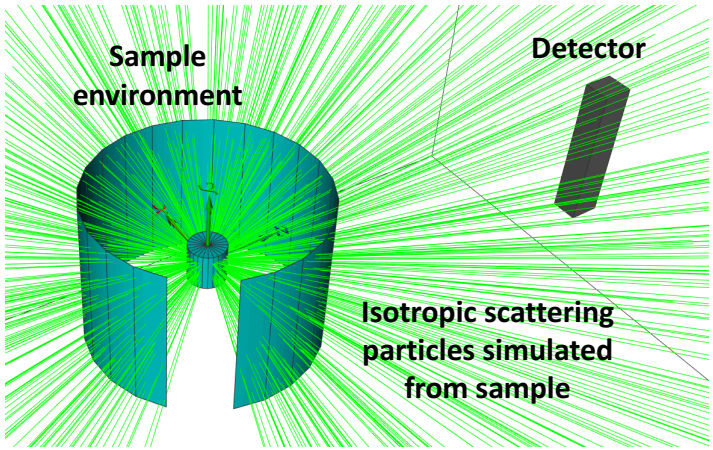


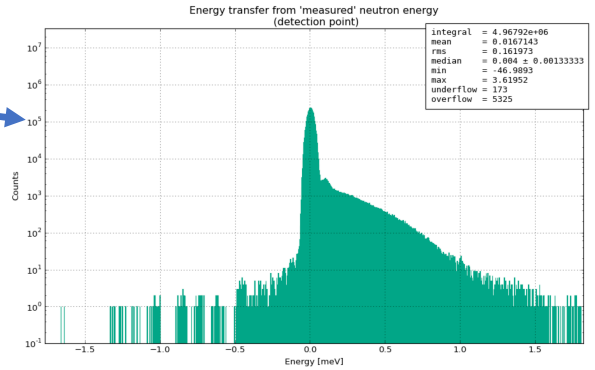
Nuclear Instruments and Methods in Physics Research A **506** (2003) 250-303
IEEE Transactions on Nuclear Science **53** No. 1 (2006) 270-278
Nuclear Instruments and Methods in Physics Research A **835** (2016) 186-225

ESS Detector Group Simulation Framework

(T. Kittelmann, X. X. Cai, K. Kanaki)

- **Geant4 simulation framework**
  - **Developed by ESS Detector Group**
  - Used by other ESS groups e.g. Accelerator Division, Target Division, Neutron Optics and Shielding Group, in-kind collaborators
- Includes:
  - User-friendly build system
  - Python interface
  - 3D visualisation (via Open Scene Graph)
  - Easy-to-handle histograms for analysis
  - Griff: an user-friendly binary format for saving results
  - Powerful parameter scanning without source code recompilation
- Intuitive & well documented
- Fast development of new simulations
- A subset of its tools is presented in this talk





T. Kittelmann et al., "Geant4 based simulations for novel neutron detector development", arXiv:1311.1009v1

Available, just send an e-mail!

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Kalliopi Kanaki: kalliopi.kanaki@esss.se

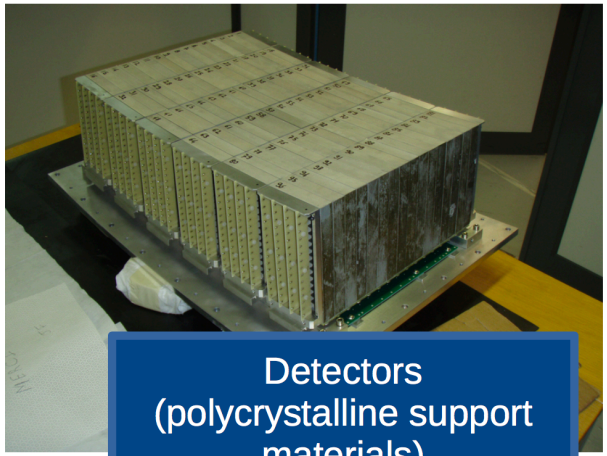
The NCrystal project

(X. X. Cai, T. Kittelmann)

Monochromator (single crystals)

User sample (anything, like crystals)

Filter (single- or poly-crystals)

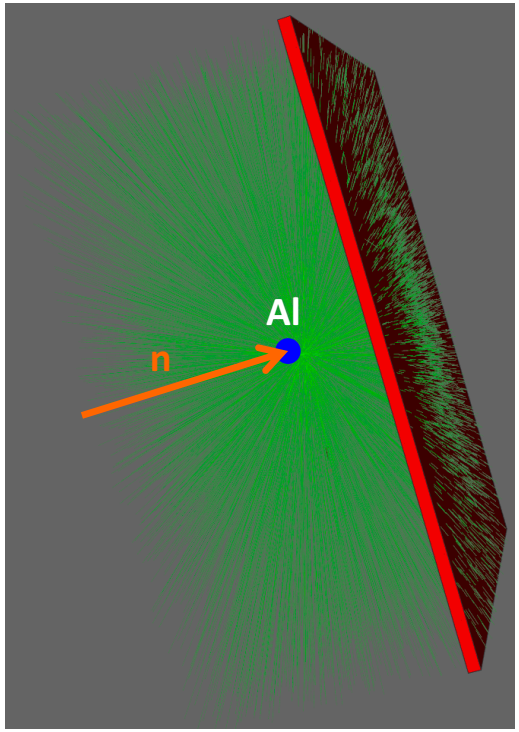


Detectors (polycrystalline support materials)

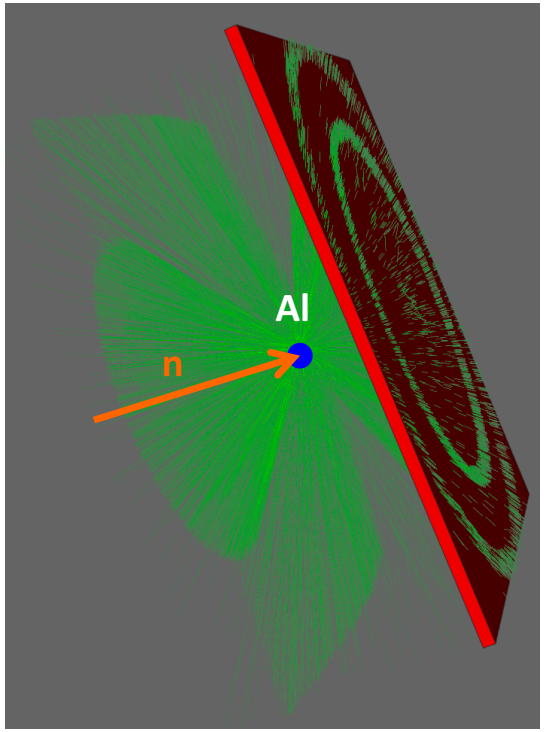
- Several crystalline components in a neutron instrument → correct modelling of interaction with poly- and single-crystal materials is essential.
- NXSG4 library created to handle Bragg scattering on poly-crystalline materials (T. Kittelmann, M. Boin. "Polycrystalline neutron scattering for Geant4: NXSG4", Computer Physics Communications 189, 114-118 (2015), doi:10.1016/j.cpc.2014.11.009)
- NCrystal advances this effort
- Validated cross section curves available to Geant4, McStas or any other application via a well-defined interface
- NCrystal 1.0 prerelease is already available within the ESS simulation framework.
  - Includes single- and poly-crystal Bragg scattering
  - Simple (empirical or first principle) parameterization of background contributions
- NCrystal 2.0 is on its way
  - Improved treatment of inelastic scattering with sampling of 2D scattering kernels or 1D phonon spectra
- Will appear at: https://github.com/mctools (mid-July)

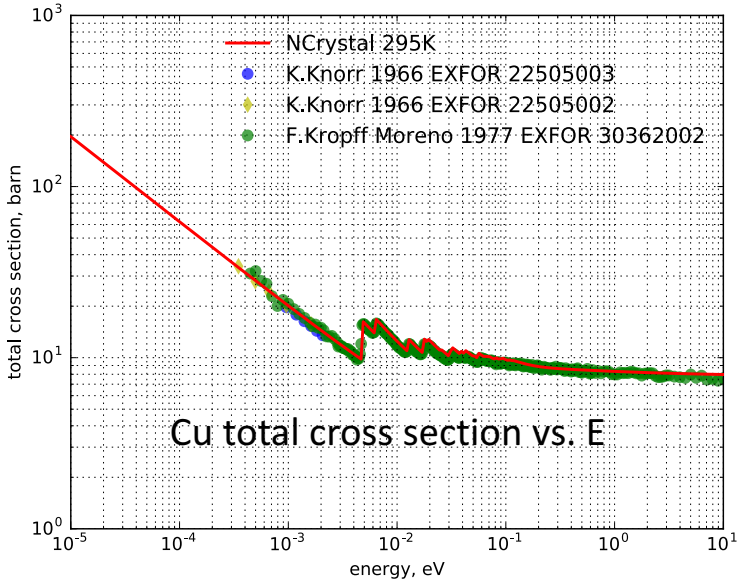
Scattering in Geant4 without and with NCrystal

free-gas model



polycrystalline material



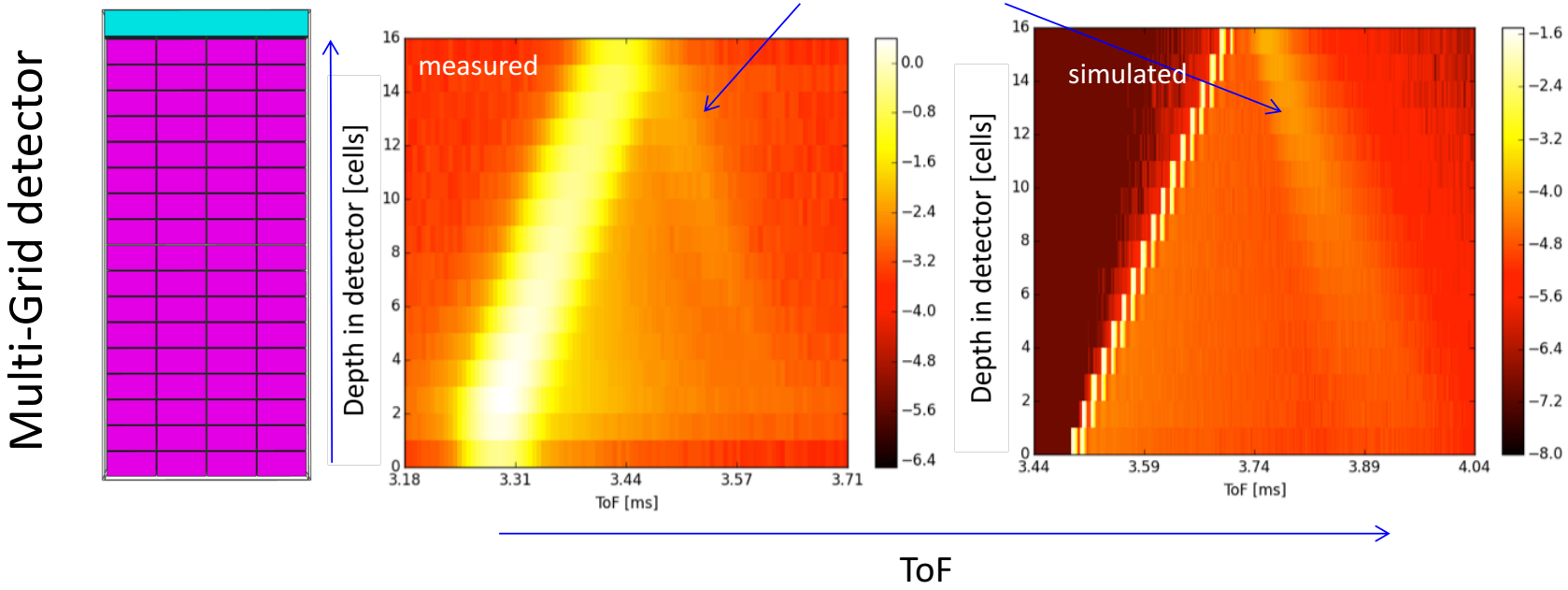


Agreement between NCrystal cross sections and published data

Reproduction of Bragg scattering in Geant4

(E. Dian, see A. Khaplanov's talk in ThuB1-1, 13.07, 10:00)

Back-scatter from the unshielded rear wall of the detector at 4.6 Å

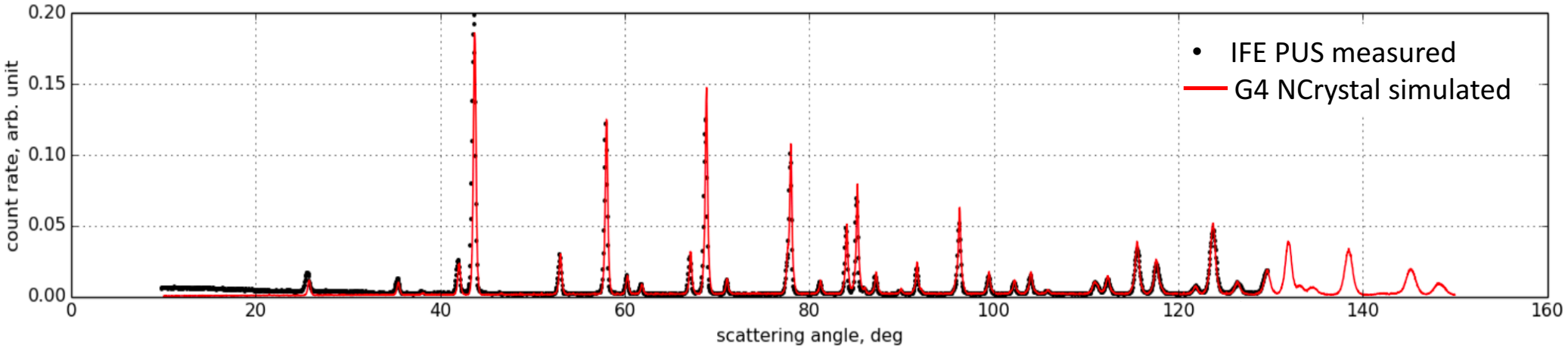


Measured ToF-depth characteristic and backscatter phenomena reproduced with simulation at 4.1 and 4.6 Å

A. Khaplanov et al. "In-beam test of the Boron-10 Multi-Grid neutron detector at the IN6 time-of-flight spectrometer at the ILL", Journal of Physics: Conference Series 528 (2014); doi:10.1088/1742-6596/528/1/012040

Simulation of the PUS@IFE diffractometer

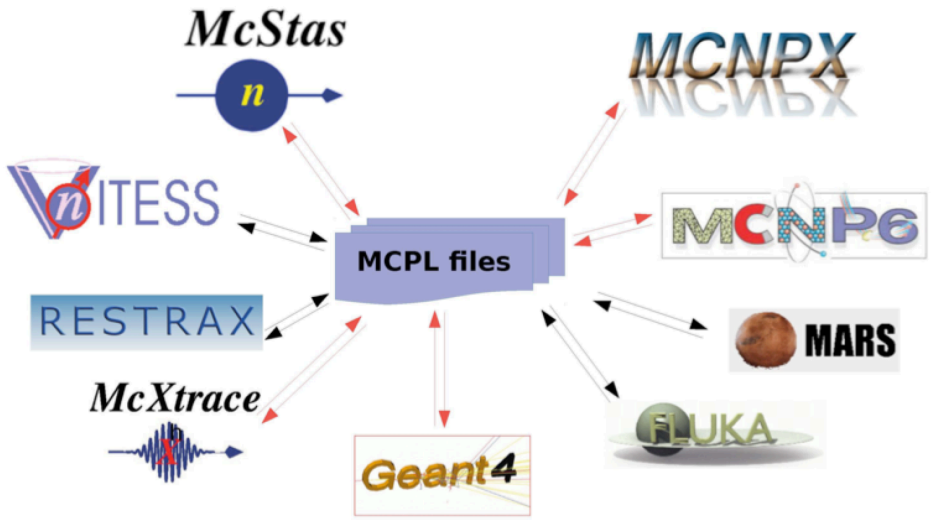
(X. X. Cai)



- Simulation includes collimator, Ge monochromator, Al_2O_3 sample, shielding between sample and monochromator
  - Very good agreement with the measured diffraction pattern at intensities, peak positions and widths
  - Discrepancy at low angles understood and will improve with NCrystal 2.0
- Long list of materials are validated and available (~50 materials validated, simple and compound)
- NCrystal currently being integrated with Geant4 and McStas
- NCrystal is a crucial component to a complete simulation of a neutron instrument.

Monte Carlo Particle Lists: MCPL

(T. Kittelmann, E. Klinkby, E. B. Knudsen, P. Willendrup)



Red: already implemented, MCNP5 added recently

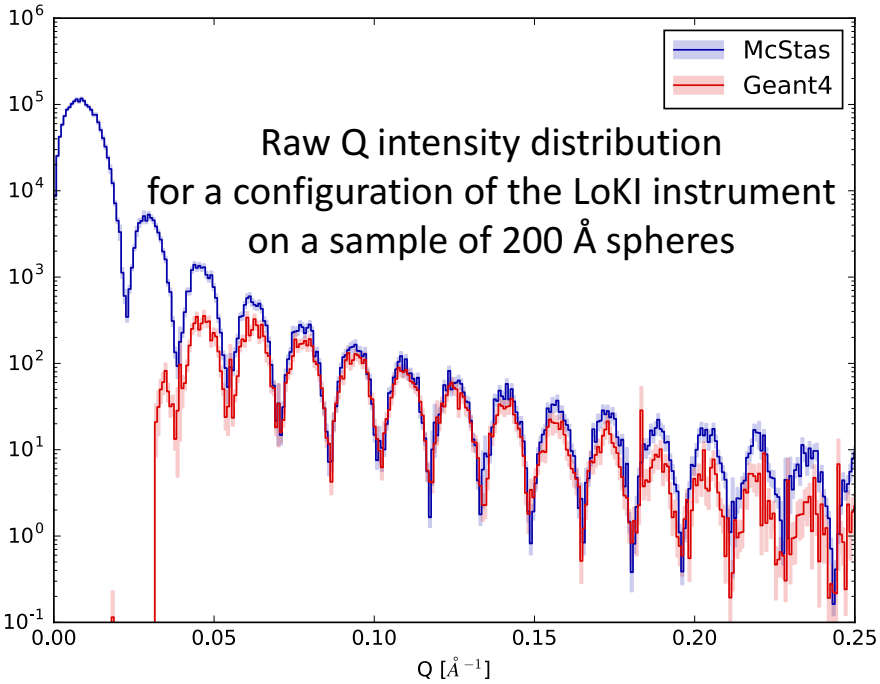
Contact:
mcpl-developers@cern.ch

T. Kittelmann et al., "Monte Carlo Particle Lists: MCPL", Computer Physics Communications, Volume 218, September 2017, Pages 17-42, ISSN 0010-4655
https://doi.org/10.1016/j.cpc.2017.04.012
http://sine2020.eu/news-and-media/mcpl-a-new-format-that-simplifies-data-interchange-between-applications.html

- Well-defined and flexible binary file format containing full information of particle properties
- Facilitates communication among software packages (e.g. McStas, Geant4, MCNP)
  - Can be easily implemented for other simulation packages
  - C/C++/python hooks available
- Can be used within a single software application
- MCPL files can be modified, merged, filtered and histogrammed
  - With a single terminal command
  - Enhanced facilities within the ESS simulation framework
- https://mctools.github.io/mcpl/
- Open source tool, available to everyone

MCPL use-case for detector optimization

- Detector design can benefit from optimization against ‘realistic’ input (not only monochromatic or pencil beams)
- Simulate the McStas instrument output at the sample position
- Use the MCPL output file as input for Geant4 detector simulations
- Study detector rates, efficiency, scattering, resolution effects
- Look at scientific quantities from detector simulation



T. Kittelmann et al., “Monte Carlo Particle Lists: MCPL”, Computer Physics Communications, Volume 218, September 2017, Pages 17-42, ISSN 0010-4655

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Summary

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- Advances and improvements in simulation tools for the neutron scattering community are presented.
- **NCrystal** allows a detailed evaluation of instrument and detector performance.
  - Bragg scattering on polycrystalline materials
  - Bragg scattering on single crystals
  - Accurate treatment of inelastic scattering component
  - Includes library of validated materials
- **MCPL**, an efficient exchange file format, improves communication between simulation tools
- Tools publicly available for everyone to use (and expand)
  - Already available in the **ESS simulation framework**

Thank you for your attention!