Optimization of detector design for instruments with simulations: Tools and applications

Kalliopi Kanaki (ESS)

Xiao Xiao Cai (ESS/DTU)

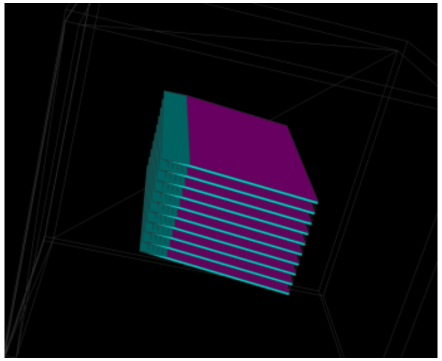
Eszter Dian (Hungarian Academy of Sciences, Centre for Energy Research/ESS)

Simulation efforts in DG (Detector Group)

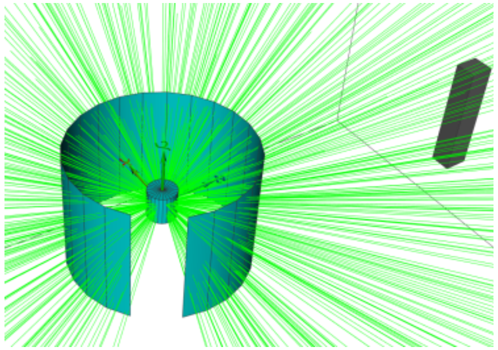
PROJECTS (G. Albani, X. X. Cai, E. Dian, G. Galgóczi, K. Kanaki, T. Kittelmann, M. Klausz, D. Lucsányi, V. Maulerova, D. Pfeiffer, J. Scherzinger, I. Stefanescu, C. Søgaard)

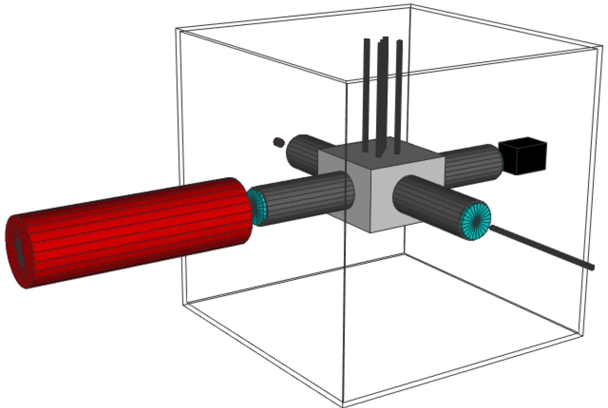
- The majority of detector demonstrators have been modeled (MultiGrid, MultiBlade, He3, BAND-GEM, B/Gd-GEM, Jalousie, Si sensors, boron-coated straws, macro-structured MWPC, flat MWPC, plastic scintillators, Source Testing Facility@LU)
- Geant4 is the main working horse.

Multi-Blade

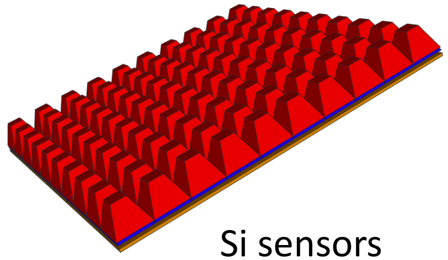


Multi-Grid



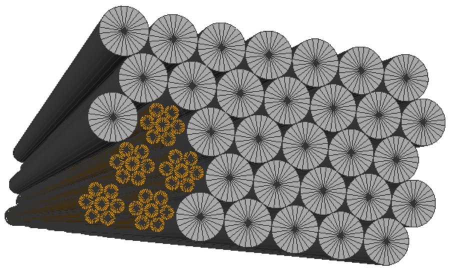


Source Testing Facility

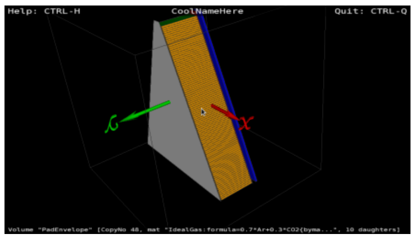


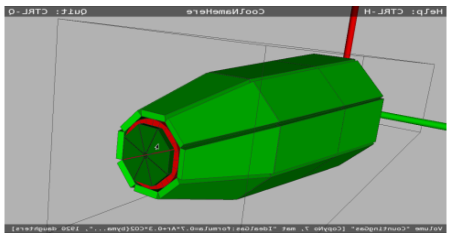
Si sensors

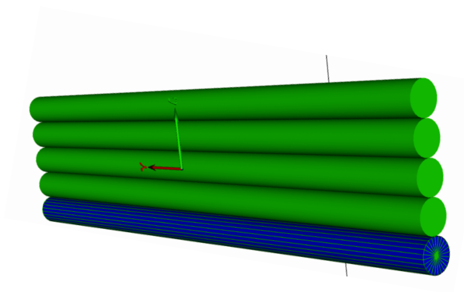
Boron-coated straws



BAND-GEM







He3

Simulation efforts in DG (Detector Group)

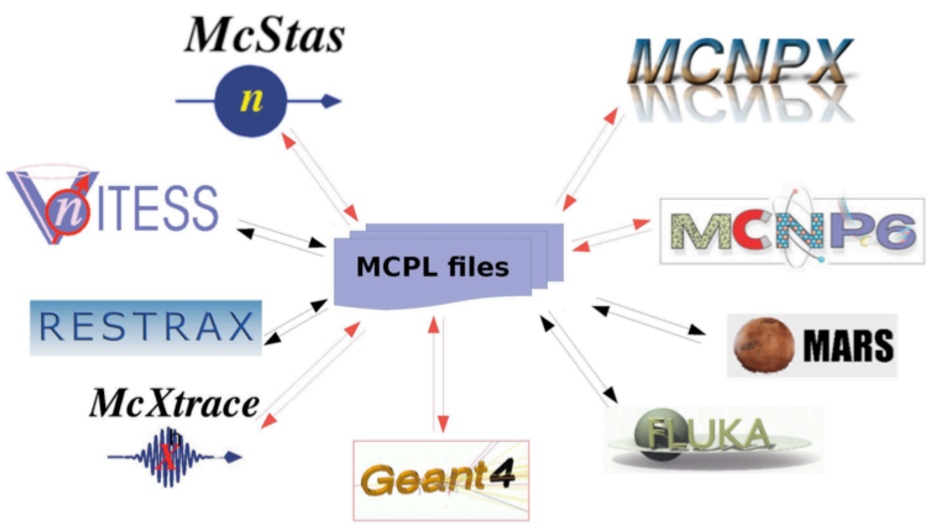
TOOLS & UTILITIES (T. Kittelmann, X.X. Cai)

- MCPL – Monte Carlo Particle Lists: glues the IO between Geant4, McStas, MCNP and more
- ESS Detector Group Coding Framework for detector modelling with Geant4
- NXSG4: extension library for description of neutron interactions in 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**: neutron interactions with poly- and single-crystals, and background processes (see Xiao Xiao's presentation)

Overview of simulation tools summarized at https://arxiv.org/abs/1708.02135, submitted to Physica B Condensed Matter

Monte Carlo Particle Lists: MCPL

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



Red: already implemented, MCNP5 added recently

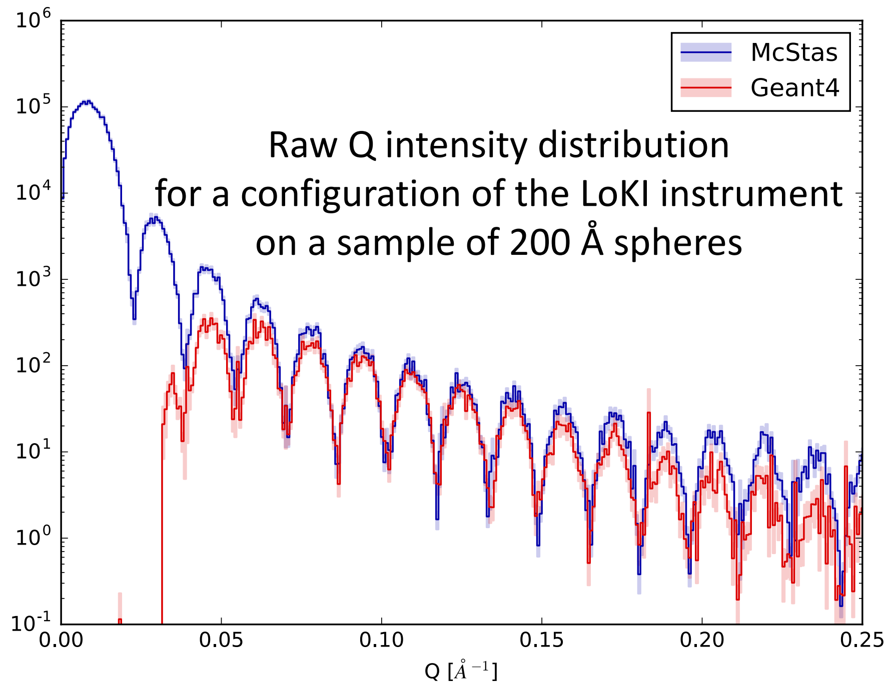
Contact:
mcpl-developers@cern.ch

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
- Available “instrument generators” in mcpl format
  - LoKI
  - SKADI
  - ESTIA
  - BIFROST (in progress)
  - Official repository of models?????

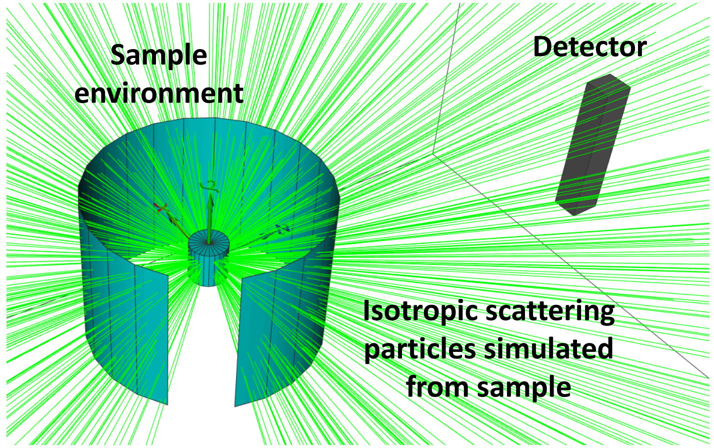


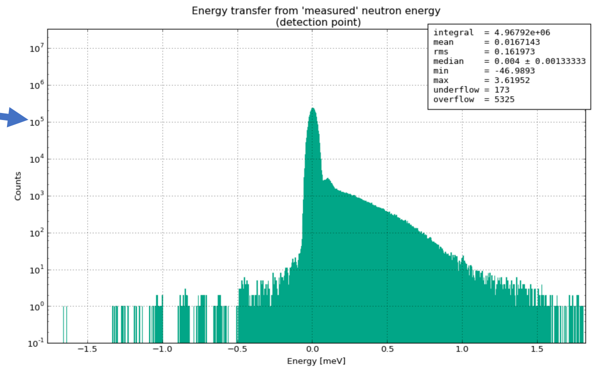
T. Kittelmann et al., “Monte Carlo Particle Lists: MCPL”, Computer Physics Communications, Volume 218, September 2017, Pages 17-42, ISSN 0010-4655

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





T. Kittelmann, et. al, J. Phys. Conf. Ser., 513 (2014) 022017

Available, just send an e-mail!

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Thomas Kittelmann: thomas.kittelmann@esss.se
Xiao Xiao Cai: xcai@dtu.dk
Kalliopi Kanaki: kalliopi.kanaki@esss.se

Structure of today’s NSS seminar

- Focus on utilities: “Monte Carlo simulation of thermal neutron scattering processes in condensed matter “ by Xiao Xiao Cai

- Focus on an application: “An application – the Multi-Grid Detector Model” by Eszter Dian

Monte Carlo simulation of thermal neutron scattering processes in condensed matter

Complete detector and experiment simulation

Xiao Xiao Cai, DTU & ESS
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Thomas Kittelmann, ESS
(thomas.kittelmann@esss.dk)

EUROPEAN SPALLATION SOURCE

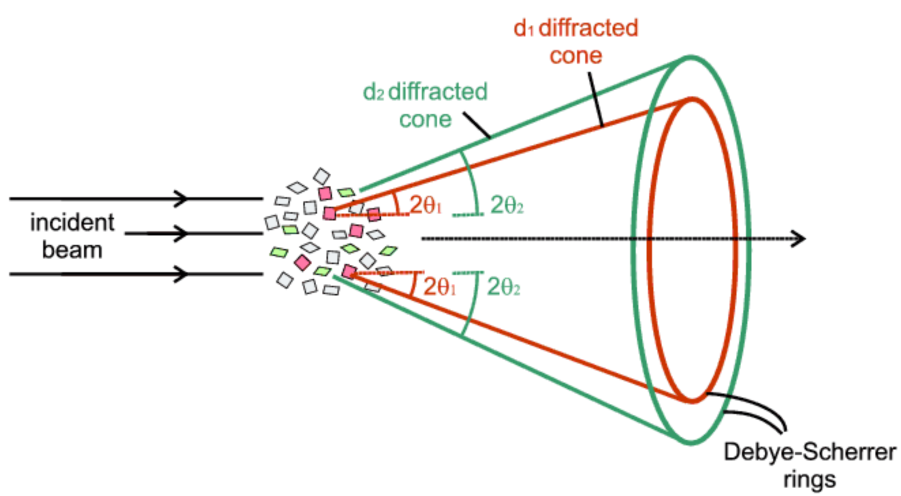
DTU Nutech
Center for Nuclear Technologies

brightness

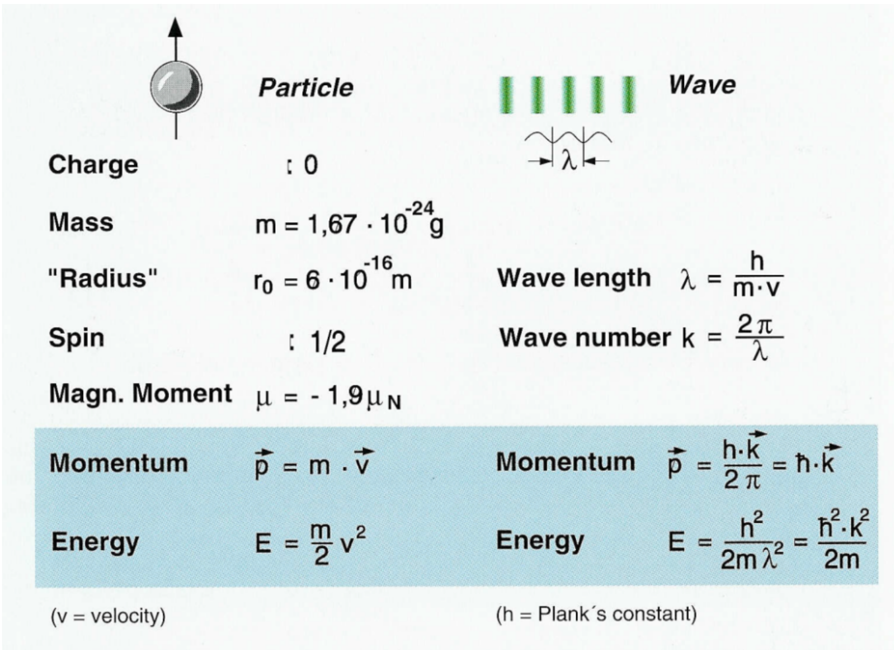
grant agreement 676548

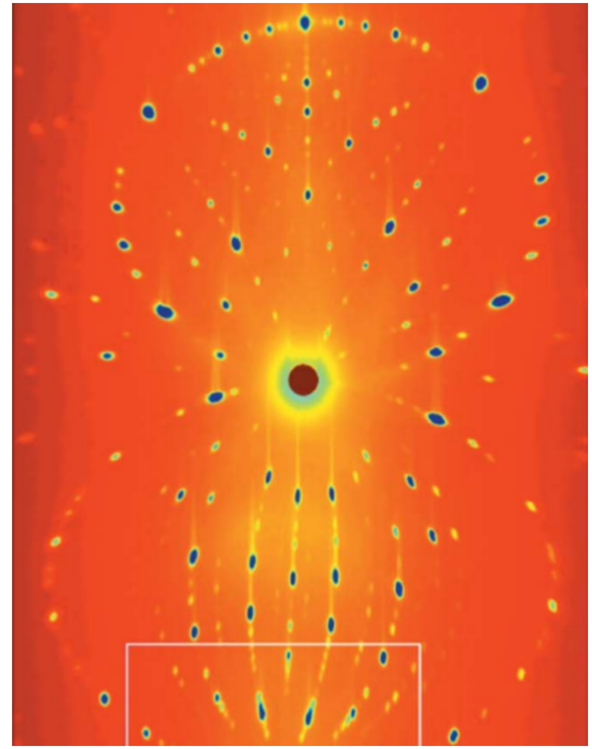
Crystalline materials

- Arguably, the most important material type for detectors.
- Nuclear scattering in these materials is described as neutron-phonon scattering, where a phonon is a quantum state of collective excitation.
- Often used in their powder and polycrystalline forms.



Wave–particle duality





A measured neutron laue transmission pattern of a crystal.
Taken from Zerdane et al., Acta Cryst. (2015). B71, 293–299.

Wave–particle duality implies different behaviours of neutron interactions with matter. Transmission pattern of neutron is generally discrete when the wavelength is comparable with the target structure (i.e. coupling distances of atomic motions in the case of thermal neutrons).

Neutron nuclear scattering

- Classical: free gas approximation
  - Neutron scatters with a freely moving target nucleus, elastically in the centre-of-mass frame.
- Quantum: space time correlation
  - G, known as the time-dependent pair-correlation function.
  - I, known as the intermediate scattering function, is measurable in neutron spin echo spectroscopy.
  - S, known as the dynamic structure factor or scattering kernel, is measurable in inelastic neutron scattering.

The work of modelling the quantum thermal scattering boils down to two parts:

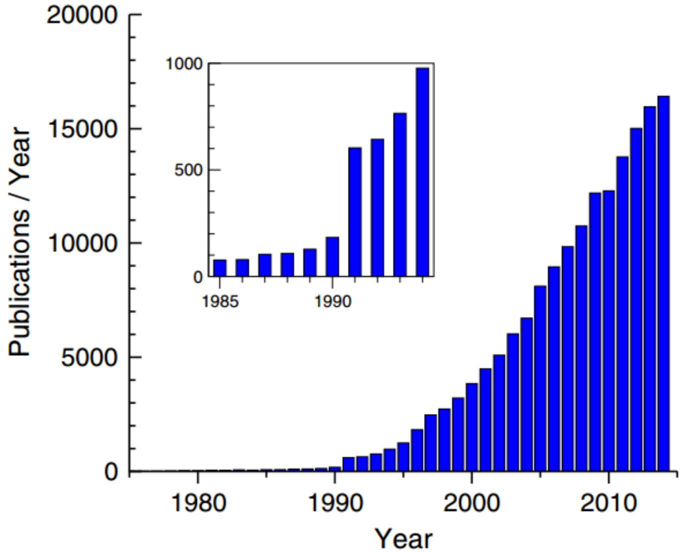
- generating a numerical representation of the physical properties (e.g. S)
- sampling the numerical data.

$$\frac{\partial^2\sigma}{\partial E'\partial\Omega} = b^2\sqrt{\frac{E'}{E}}\int\int G(r,t)\exp(i\kappa r)\exp(i\omega t)\mathrm{d}r\mathrm{d}t$$
$$= b^2\sqrt{\frac{E'}{E}}\int I(\boldsymbol{\kappa},t)\exp(i\omega t)\mathrm{d}t$$
$$= b^2\sqrt{\frac{E'}{E}}S(\boldsymbol{\kappa},\omega)$$

Getting numerical representations of physical properties (e.g. S)

The DFT (density functional theory) community is flourishing

- Ab initio methods are promising techniques for predicting material properties.
- In many cases, the disagreement between the calculated and measured total scattering cross sections is approaching the intrinsic uncertainty of employed theoretical approximations and the uncertainty in the experiments.



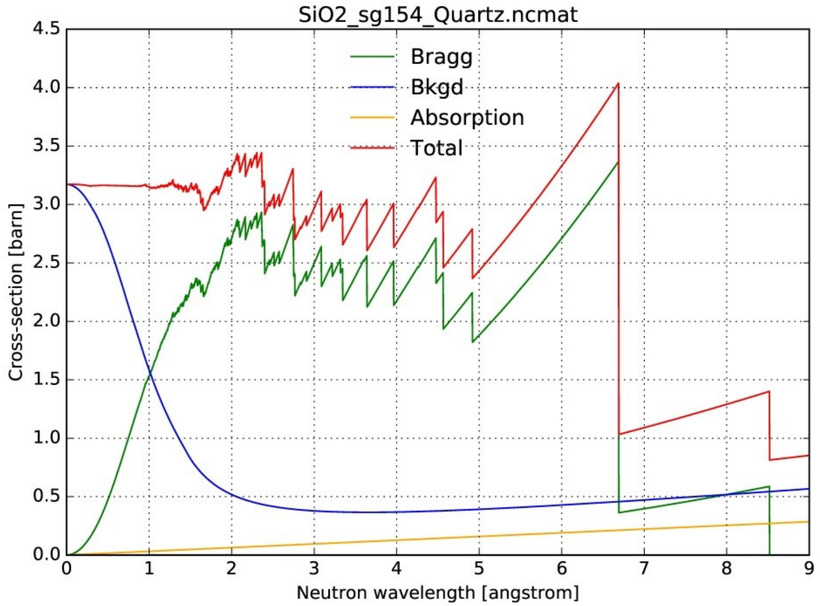
R.O Jones, Rev. Mod. Phys., vol 87, 2015

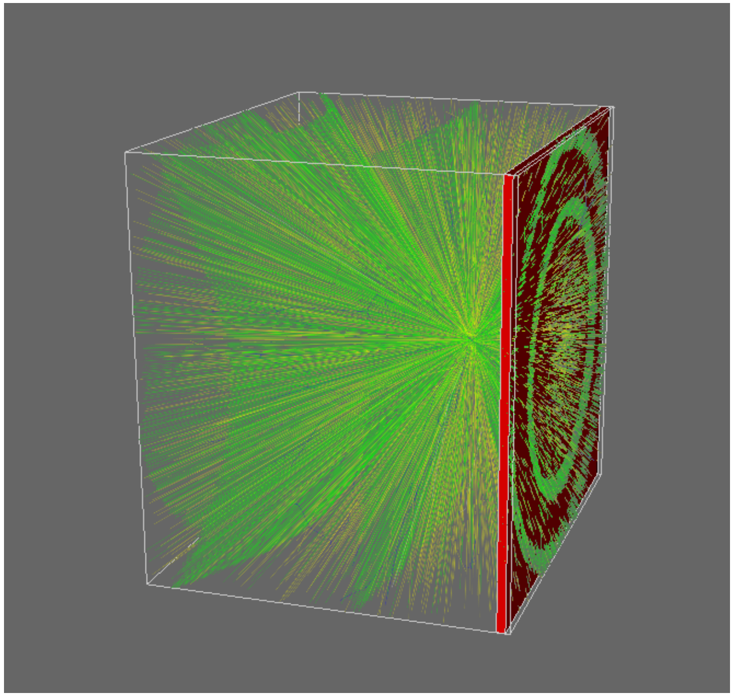
NCrystal: a library for thermal neutron transport in crystals (http://mctools.github.io/ncrystal/)

- Objectives:
  - Create open source library which is capable of providing crystallographic information and in particular facilitates simulation of thermal neutron interactions with crystals in new or existing frameworks.
  - In particular we wanted to use it to make the Geant4 simulation toolkit capable of including such detailed neutron+crystal physics.
  - Should be relatively simple to add new materials and get reasonable results (simply providing unit cell parameters of the crystal should be enough), and possible to provide more detailed data (e.g. scattering kernels from DFT calculations) for increased realism.
  - Code should be robust, fast and maintainable with many interfaces (C++, C, Python, Geant4, McStas, ...)
- Functionalities:
  - Load crystal information from variety of crystallographic file formats
  - Provide relevant derived quantities (like lists of hkl reflection planes and associated structure factors).
  - Large number of physics models available, representing both different physics processes and different models for a given physics process:
    - Provides cross sections and ability to sample scattering distributions (using application specific RNG if desired)
    - Justify the selection of models numerically.
  - Unified configuration interface (a simple string) across all interfaces. The same string defines the the identical physics model, regardless the programming languages or platforms.

Cross section in absolute scale.
Thoroughly validated.
Examples provided for Geant4 and McStas.

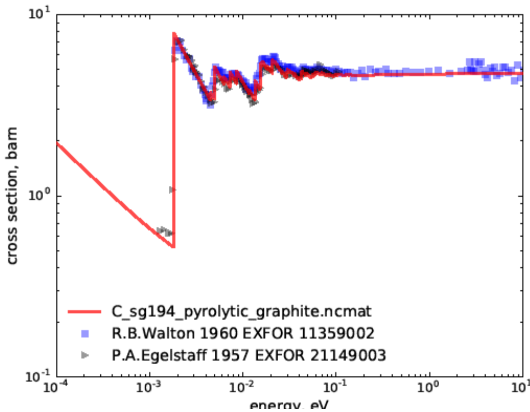
NCrystal polycrystal/powder

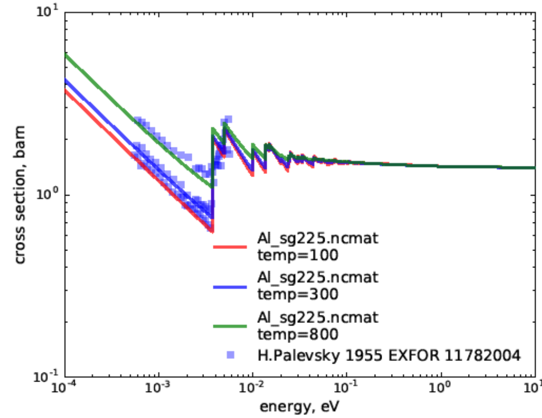


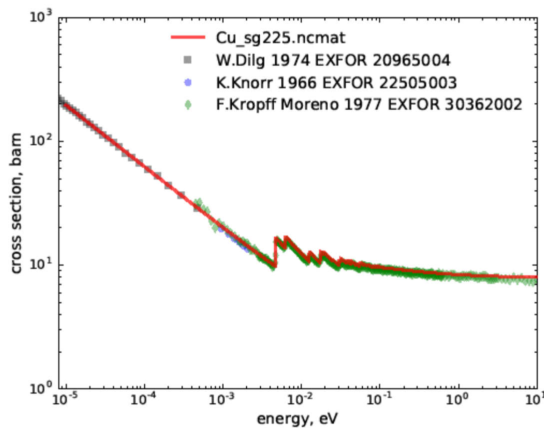


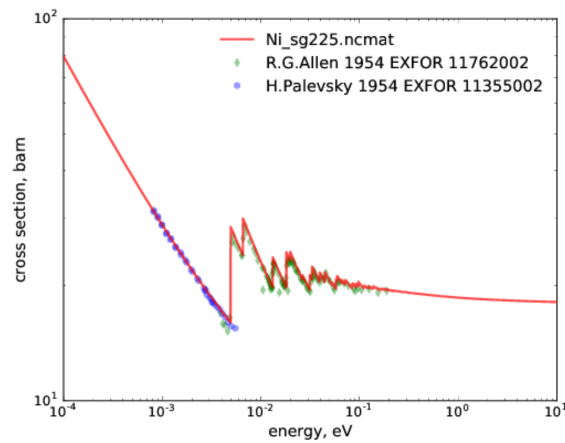
- On the left, contributions from different processes to the total cross section in quartz.
- On the right, neutron (in green) and secondary gamma (in yellow) trajectories generated by neutron scattering with Al powder at the centre of the box. Generated in NCrystal-enabled Geant4.

Total cross section calculated by NCrystal (v0.9.1) in powders



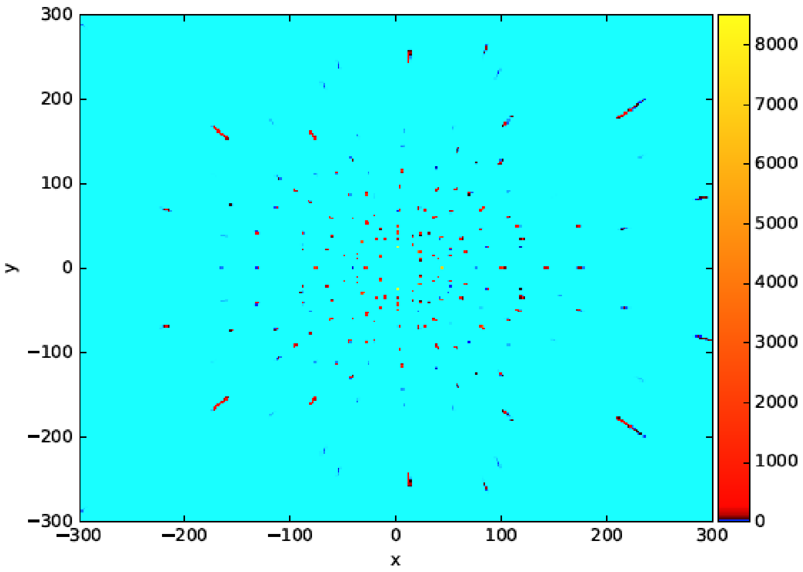


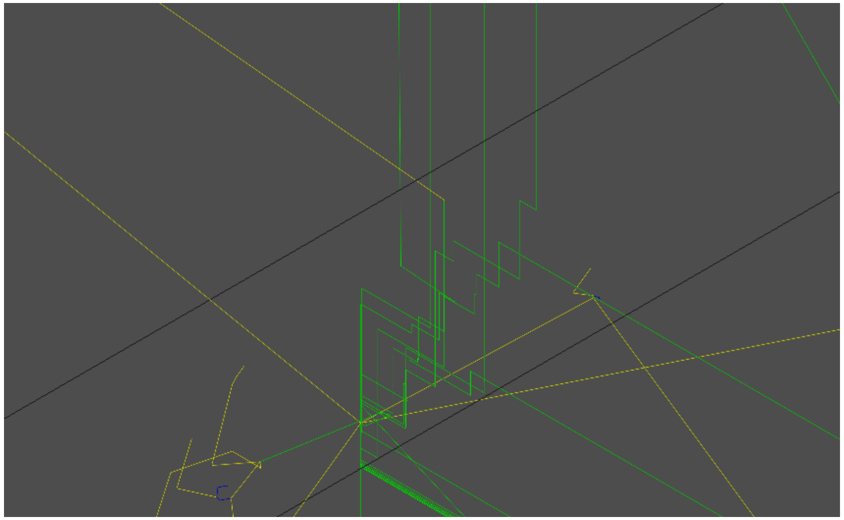




Additional 30 validation figures are available at https://github.com/mctools/ncrystal/wiki/Data-library

NCrystal single-crystal

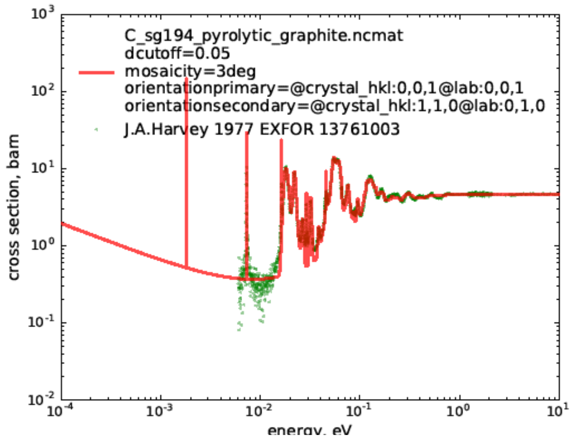


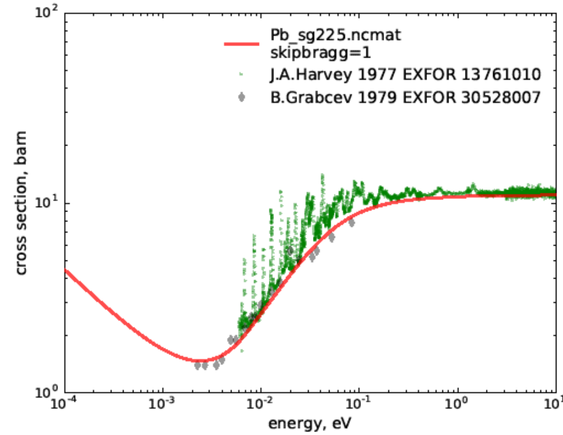


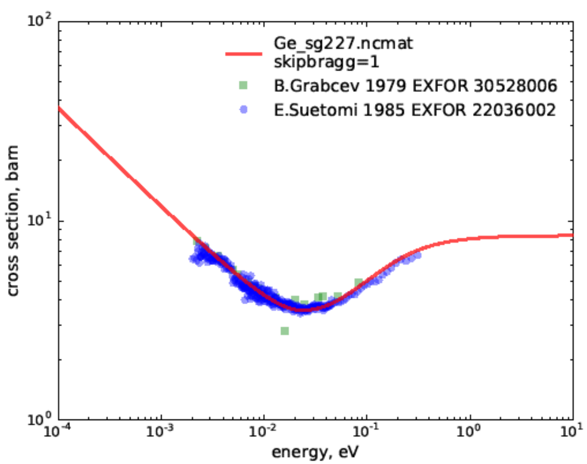
The single-crystal model is a high accuracy Darwin equation solver for ideal mosaic crystals in arbitrary geometry. Energy resolution and divergent of the reflected beams are in excellent agreement with analytical models.

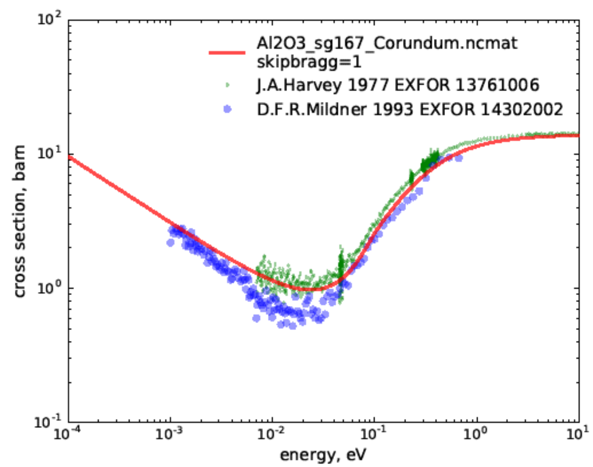
- On the left, simulated neutron transmission pattern of Leiteite ($ZnAs_2O_4$) on a 2D position sensitive detector.
- The zig-zag walk of thermal neutrons in a Ge single crystal, as a result of ping-ponging by the reflection planes with opposite normals. Generated by NCrystal-enabled Geant4.

Total cross section calculated by NCrystal (v0.9.1) in single crystals









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Status of NCrystal

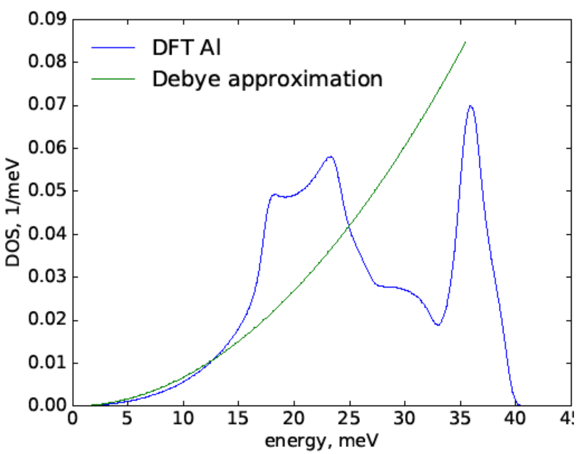
- Initial release(v0.9.1 released Aug 2017)
  - Detailed treatment for the coherent elastic scattering (i.e. Bragg diffraction) in single- and poly-crystals.
  - Reliable for estimating the total inelastic scattering cross section (based on the Debye approximation with high order phonon expansion).
  - Data files for 35 materials are available in this release.
  - Additional data files can be made available by request.
  - X. X. Cai and T. Kittelmann, NCrystal, https://doi.org/10.5281/zenodo.853186, available at http://mctools.github.io/ncrystal/.
- Next major release spring 2018 (in preparation)
  - Detailed treatment for the inelastic scatterings

Physics model in the next release

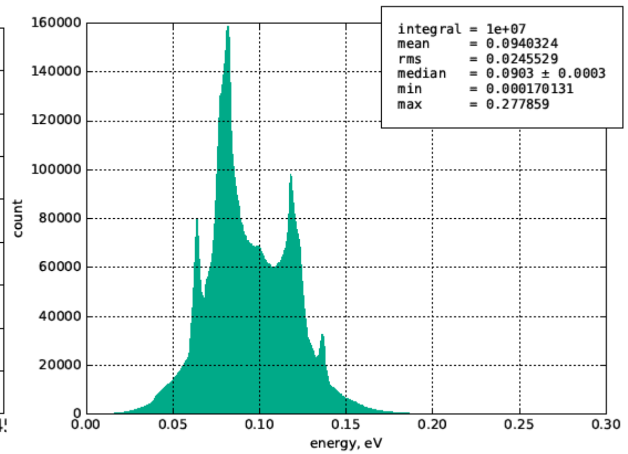
- The main objective of the next release is to improve the inelastic scattering model, which is currently under a few layers of approximations.
  (1) harmonic approximation
  (2) incoherent approximation
  (3) Debye approximation
- Theory is ready. A prototype is validated. In the quality assurance phase of generating data files.
- Users can provide their own physics (e.g. for liquids) that are compiled in the form of S(Q,w) in a .ncmat file.

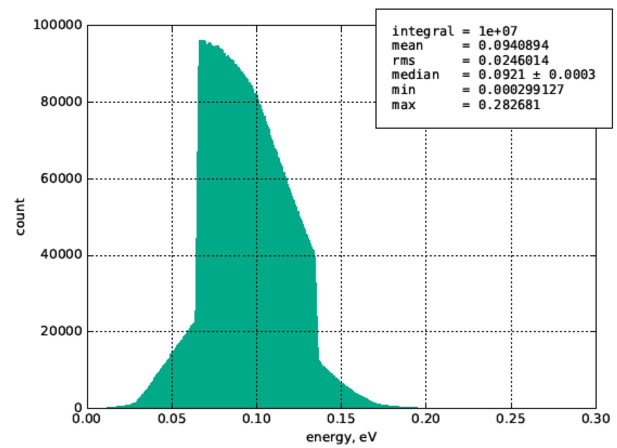
Debye approximation

- An optional add-on for the incoherent approximates. Describe the vDOS (vibrational density of states) by a power law curve.
- Effective for total cross section estimation.
- Valid if the scattering media is large.



The vDOS from DFT and its Debye approximation

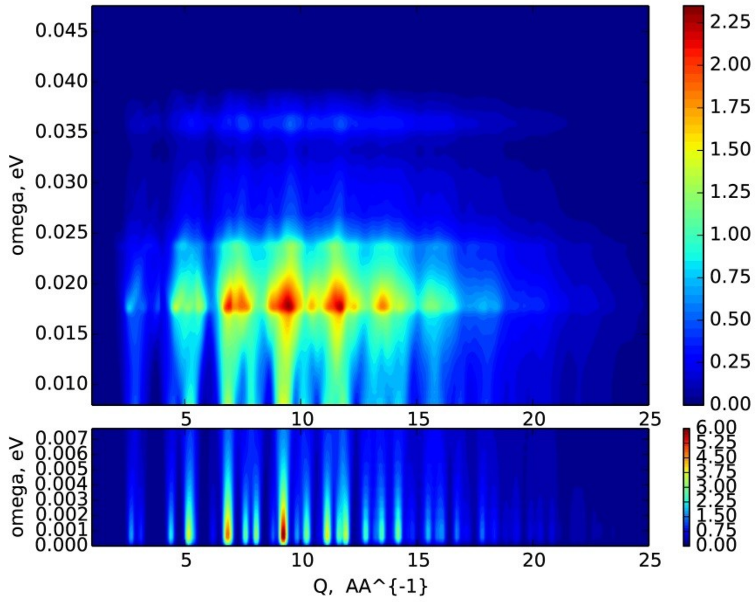


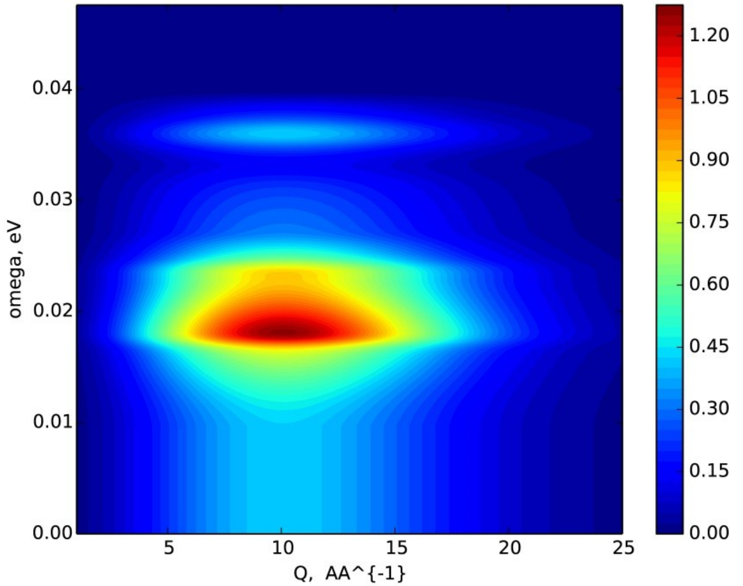


Energy distributions of 1e7 inelastically scattered neutrons (0.1eV initial kinetic energy). Left, based on the vDOS; right, based on the Debye curve. Statistically equivalent mean.

Incoherent approximation

- It approximates G(r,t) by G(0,t). Considering only the correlation of an atom with itself at different time. Unable to reproduce the structure peaks originated from the coherent interference.
- The vDOS is only dynamical perperty considered. Used for the inelastic scattering.
- OK for
  - hydrogen rich and other strong incoherent materials, where the incoherent scattering is dominant.
  - coherent material with large size (a few time of the free mean path), so the structure peaks smear out after a few scatterings.
- Bad for thin Coherent scatterers

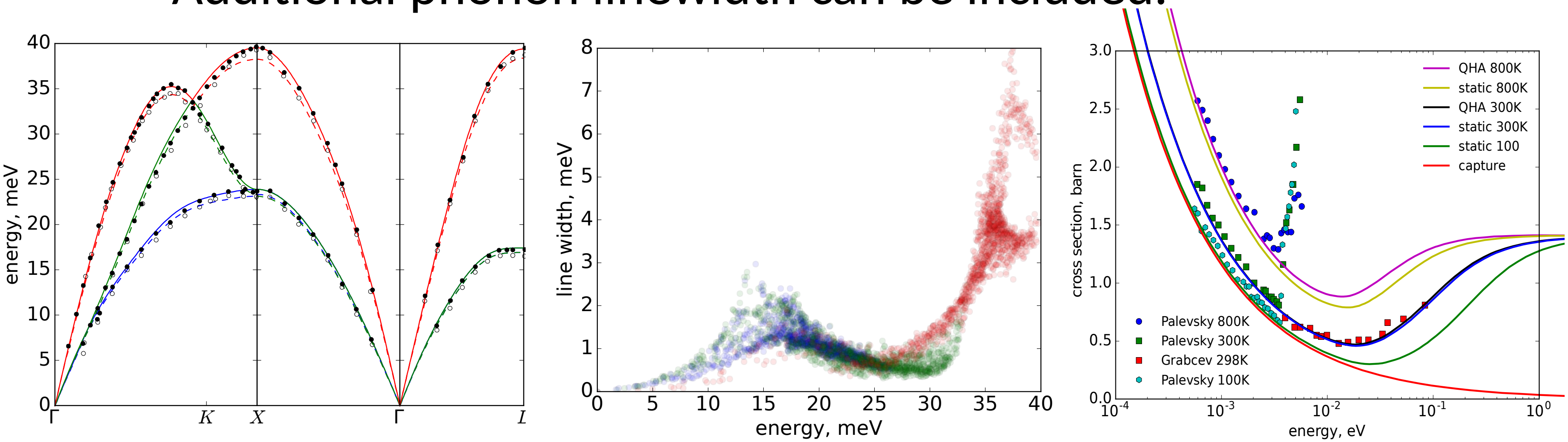




On the left, the coherent S(Q,ω) for Al powder. On the right, the corresponding approximation.

Harmonic approximation

- It assumes the atomic displacement is small comparing to atomic distances; phonon is not interacting with the media.
  - Good for materials at low temperatures
  - Bad for materials at high temperatures
- Quasi-harmonic approximation will be applied in its place. Additional phonon linewidth can be included.



Left, phonon dispersion of Al at 80K and 300K. Middle, phonon linewidth of Al at 800K. Al cross section at 100K, 300K and 800K.

Summary

- NCrystal is enabled by default in the detector group coding framework. Examples are also provided for stand alone Geant4 and McStas simulations.
- NCrystal is easy to use. It requires only a few lines of modification on existing Geant4 or McStas simulations.
- Geant4 can simulate a large variety of particles in a wide energy range. Along with NCrystal, it is feasible to simulate neutron instruments in full scale to understand the intrinsic radiation background.
- NCrystal is available at http://mctools.github.io/ncrystal/.

676548

Optimization of detector design for instruments with simulations: Tools and applications

K. Kanaki, X. X. Cai, R, E. Dian

European Spallation Source ESS ERIC
HAS Centre for Energy Research

19 September 2017,NSS seminar, Lund

An application –
The Multi-Grid Detector Model

Eszter Dian[1,2]
PhD student
[1]Hungarian Academy of Sciences, Centre for Energy Research
[2]European Spallation Source ESS ERIC

Detector background study with Monte Carlo codes

- Sources of neutron detector background
  - Neutron induced gamma background (MCNP6)
    - Prompt gamma radiation from neutron capture
    - Decay gammas from neutron activation

↓

^{41}Ar activity saturates at **128 mBq/cm³** ⟶ low

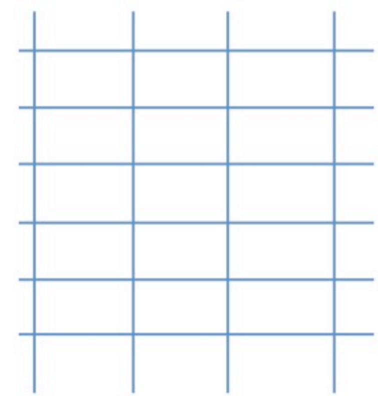
Negligible signal from self-activation

  - Scattered neutrons (Geant4)
    - Elastic, inelastic
    - Coherent, incoherent

Great impact of Coding Framework!

General neutron activation study prepared with MCNP6 for ESS operation conditions
- Ar/CO_2 counting gas
- Aluminum-frame

E. Dian et al.
[10.1016/j.apradiso.2017.06.003](https://doi.org/10.1016/j.apradiso.2017.06.003)



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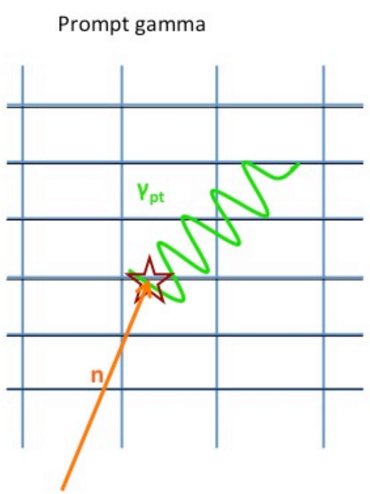

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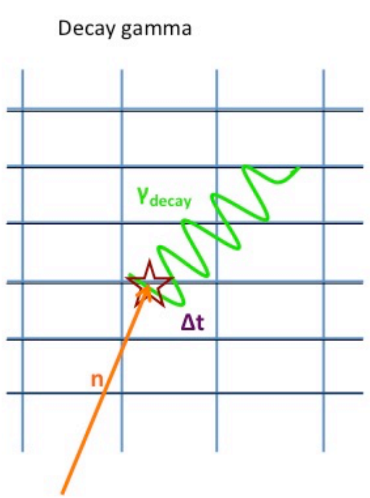

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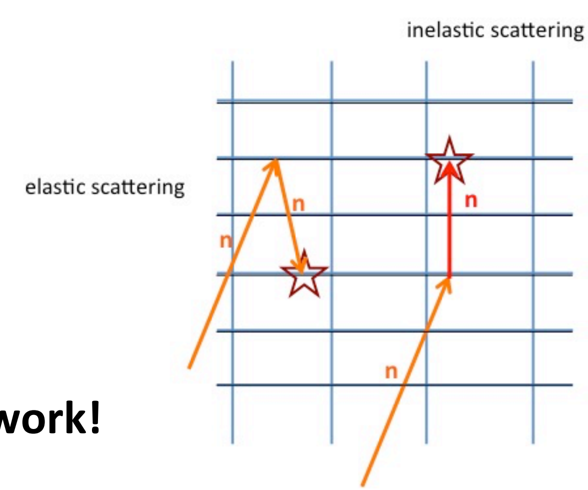
- Aluminum-frame

E. Dian et al.
[10.1016/j.apradiso.2017.06.003](https://doi.org/10.1016/j.apradiso.2017.06.003)

Negligible signal from self-activation

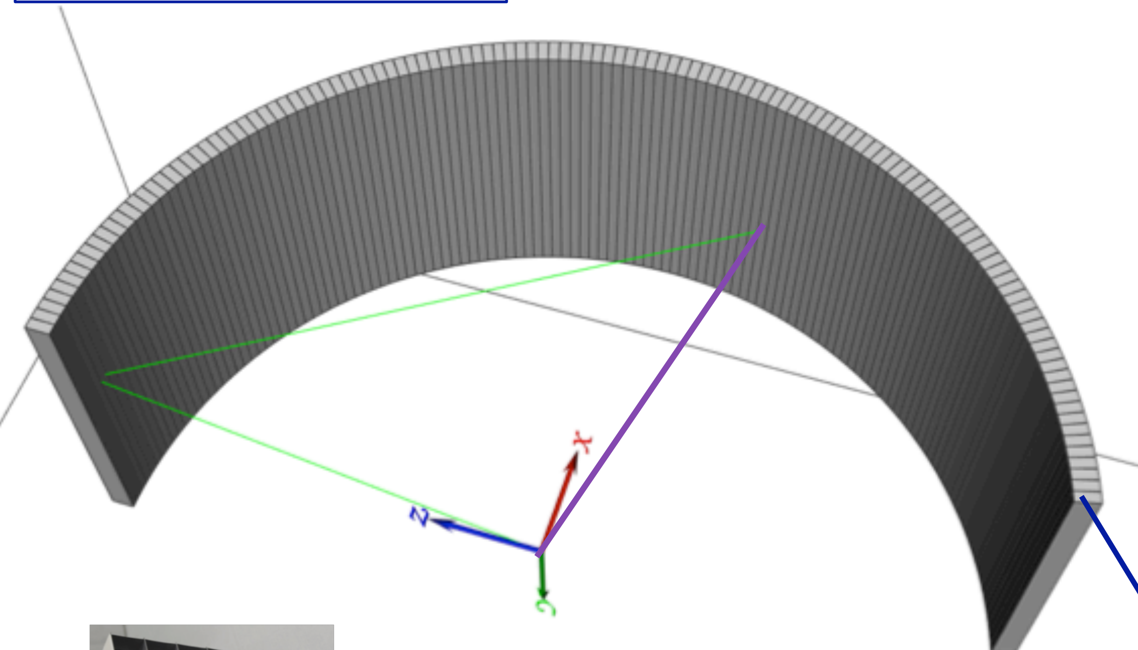
  - Scattered neutrons (Geant4)
    - Elastic, inelastic
    - Coherent, incoherent



Great impact of Coding Framework!

Large area detector for chopper spectroscopy – Multi-Grid

Geant4 @Coding Framework



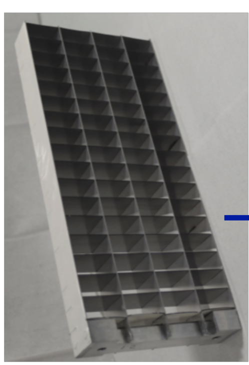
Multi-Grid

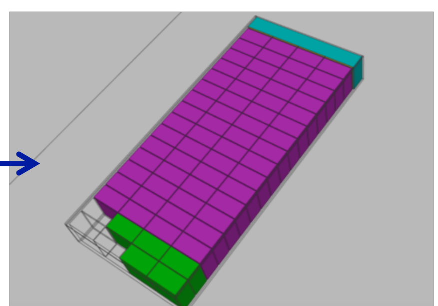
- Large area detector
- Inelastic instrument, chopper spectroscopy

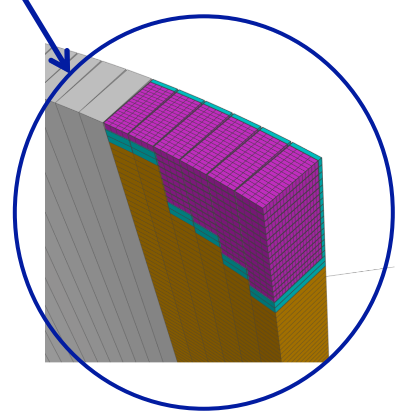
Low background is essential

- Solid B_4C converter + Ar/CO_2
- Aluminium frame – **crystalline Al**

Scattered neutron background induced in detector







A. Khaplanov et al.

http://dx.doi.org/10.1016/j.nima.2012.12.021

Scattered neutron background

- Neutron scattering on detector and environment
- Study and distinguish background effects

↓

- Guidelines for detector design

Prototype

↓

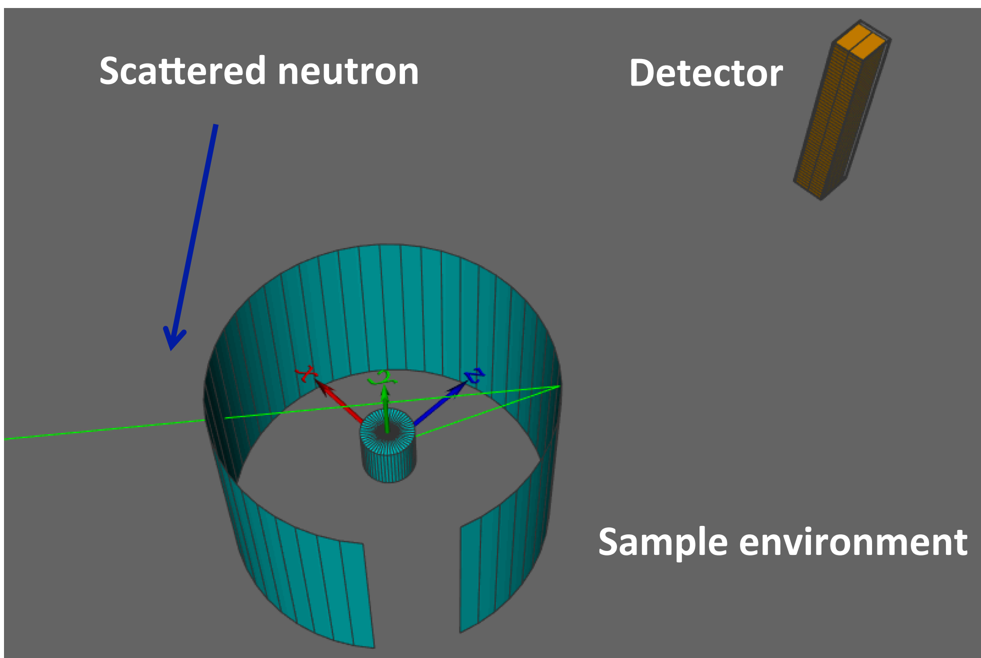
Full-scale detector model

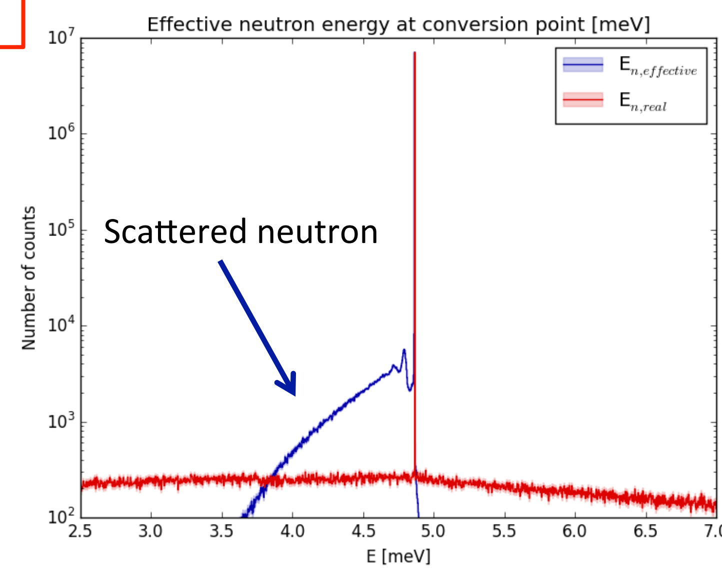
Validation

↓

Optimization

Realistic simulation





Real and measurable neutron energy

Geant4 @Coding Framework

Multi-Grid detector test at ILL

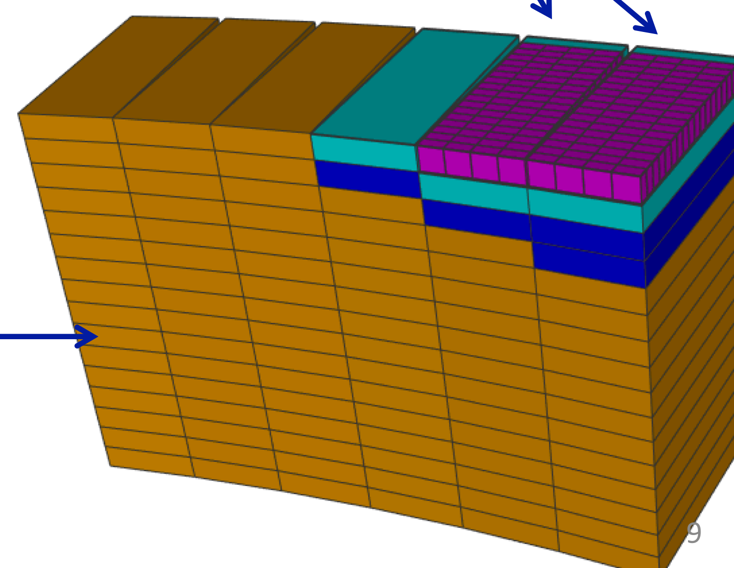
Geant4 @Coding Framework

S. Agostinelli et al
doi:10.1016/S0168-9002(03)01368-8
T. Kittelmann et al
doi:10.1088/1742-6596/513/2/022017

In-beam test of the Boron-10 Multi-Grid neutron detector at the IN6 time-of-flight spectrometer at the ILL

A. Khaplanov et al.
http://iopscience.iop.org/article/10.1088/1742-6596/528/1/012040/pdf

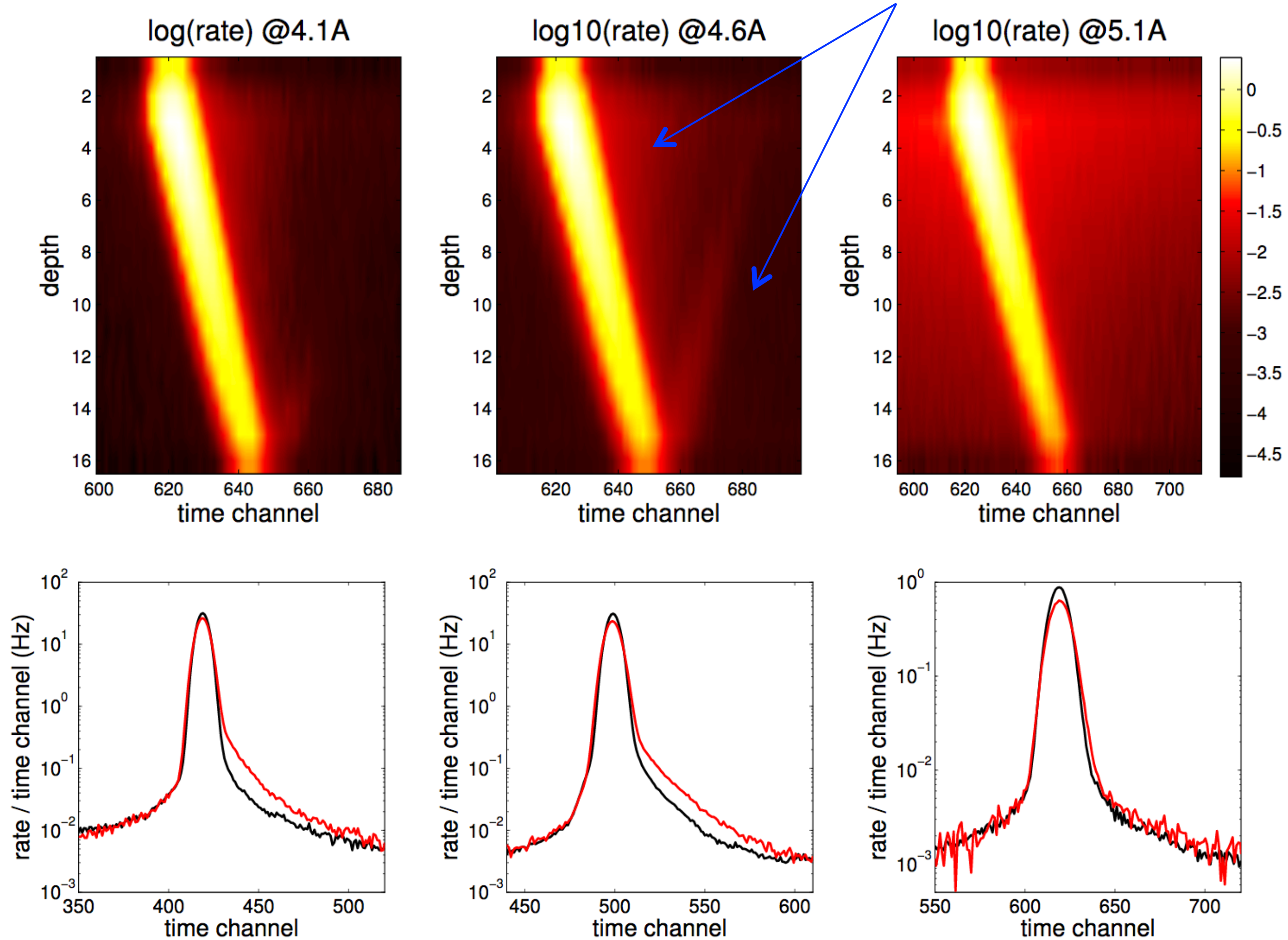
No shielding on the rear wall of grids



Multi-Grid detector test at ILL

Measured data (ToF, depth of detection)

Measured scattering phenomena can be studied with simulation inside the detector



MultiGrid detector test at ILL

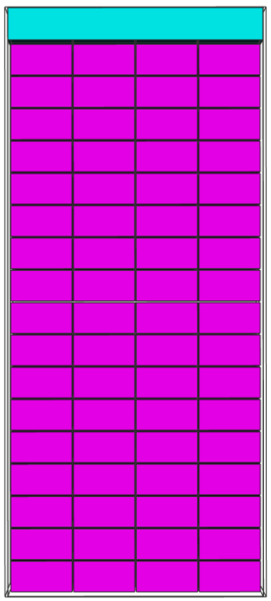
Measured and simulated ToF-depth of detection

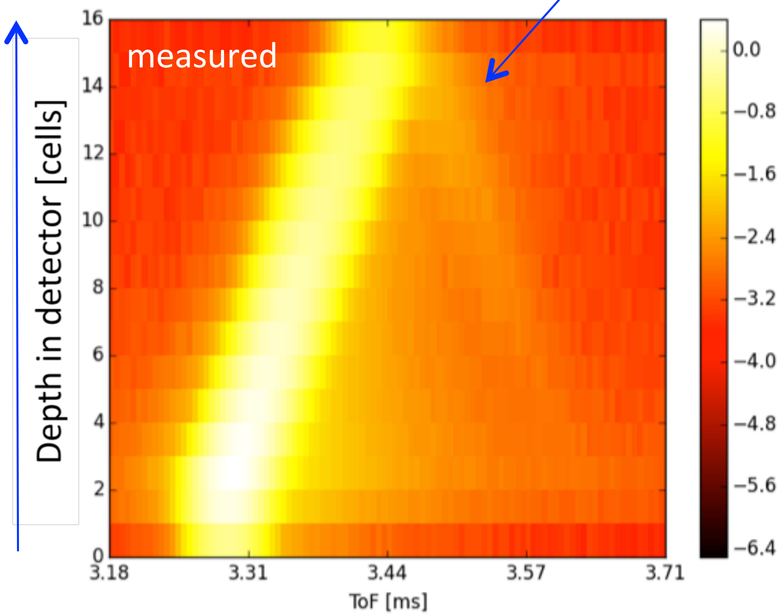
Geant4 @Coding Framework

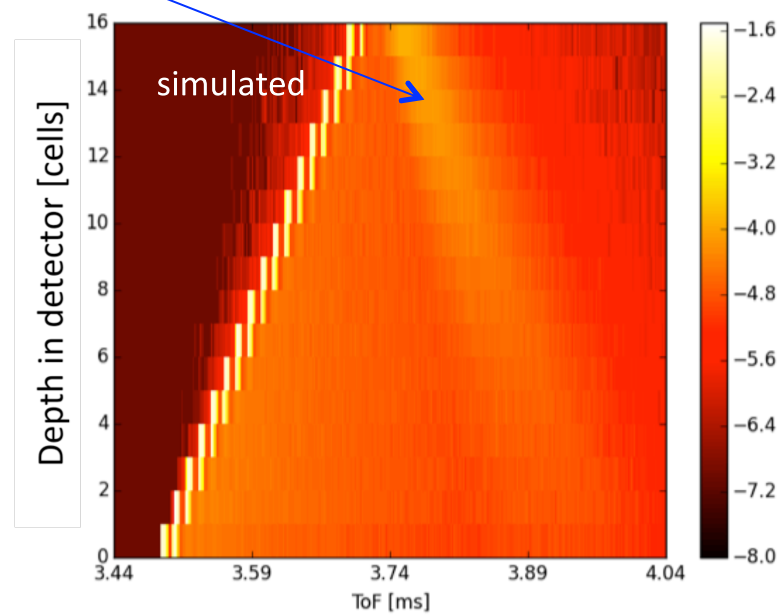
NXSG4

http://nxsg4.web.cern.ch/nxsg4/

Backscatter from the unshielded rear wall of the detector at 4.6 Å







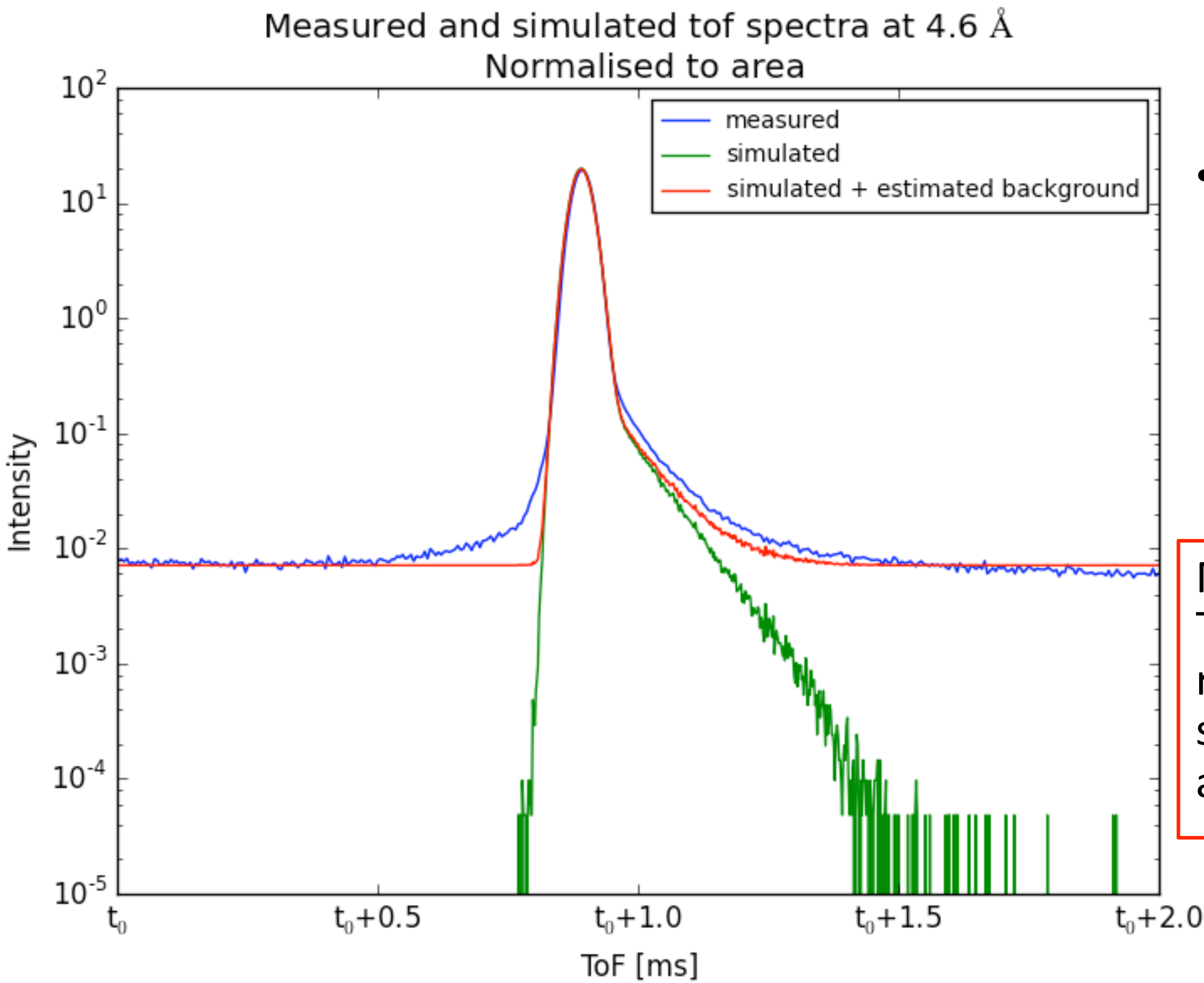
ToF

Validation

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

MultiGrid detector test at ILL
Measured and simulated ToF spectra

NXSG4



- Estimated flat alpha-background added (red), unique for this prototype

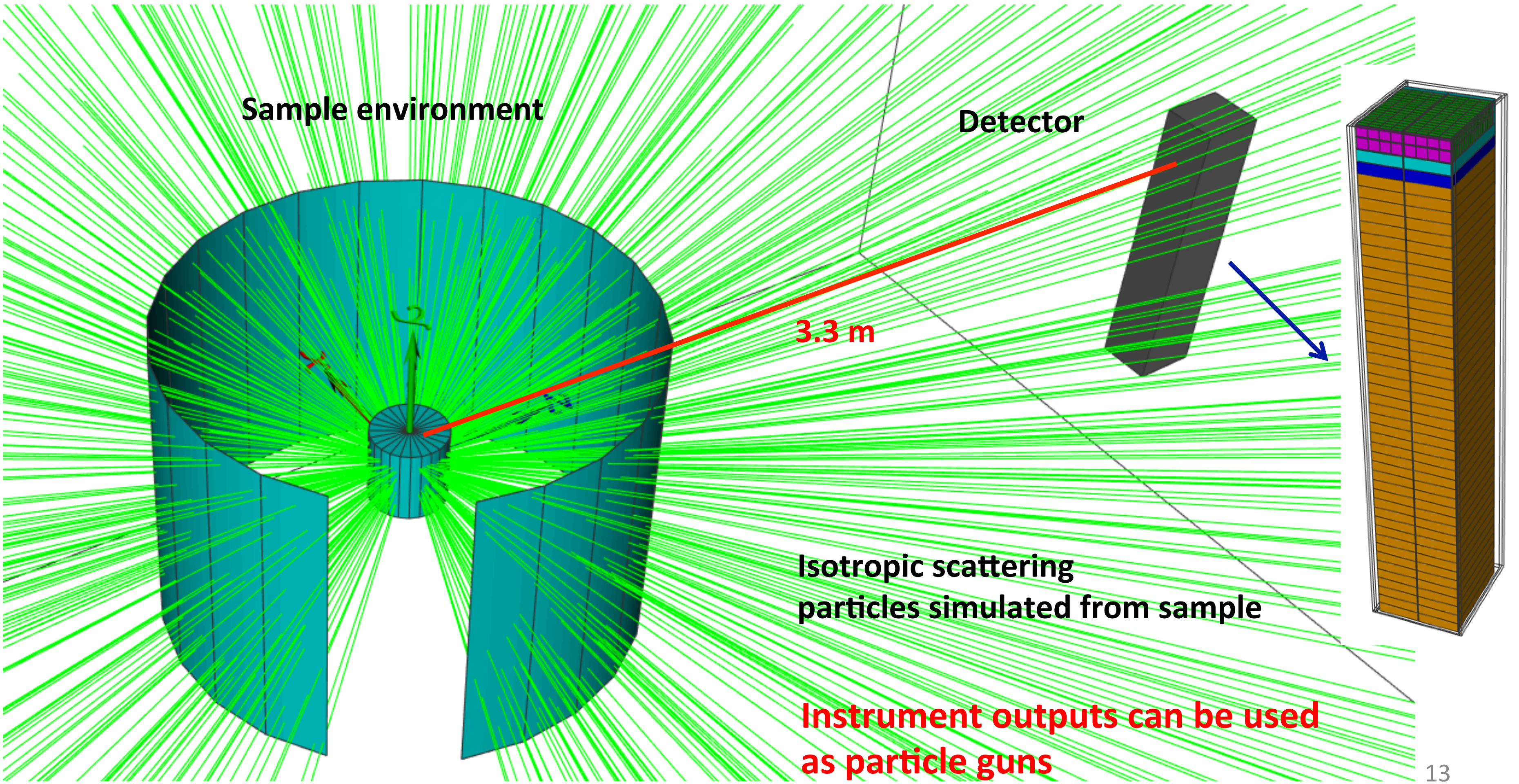
Measured ToF-spectrum reproduced with simulation at 4.1 and 4.6 Å

Validation

Multi-Grid detector test at CNCS, SNS

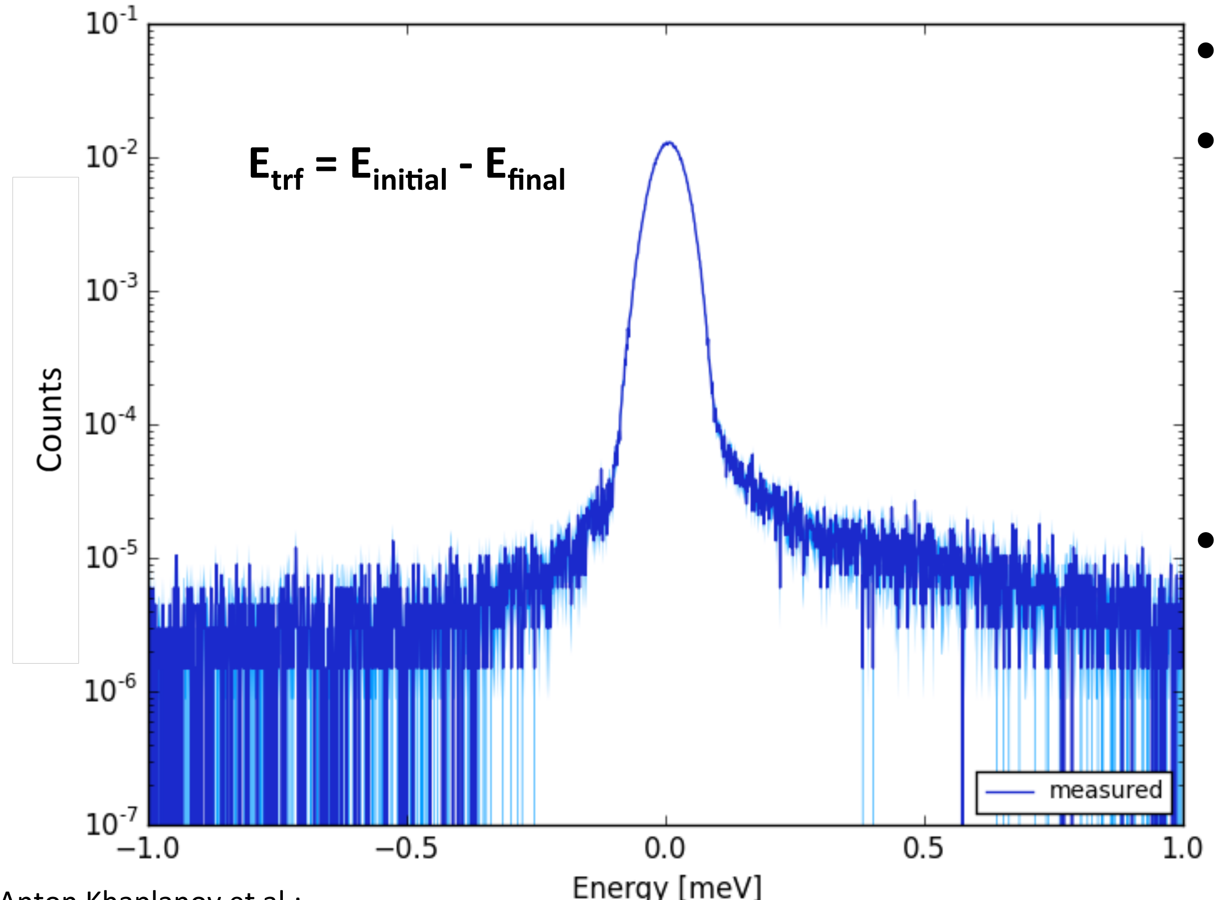
Geant4 @Coding Framework

NXSG4



MultiGrid detector test at CNCS, SNS

Derived energy transfer at 3.678 meV from measurement



- Chopper spectroscopy
- Measured quantities:
  - ToF
  - detection-coordinates

↓

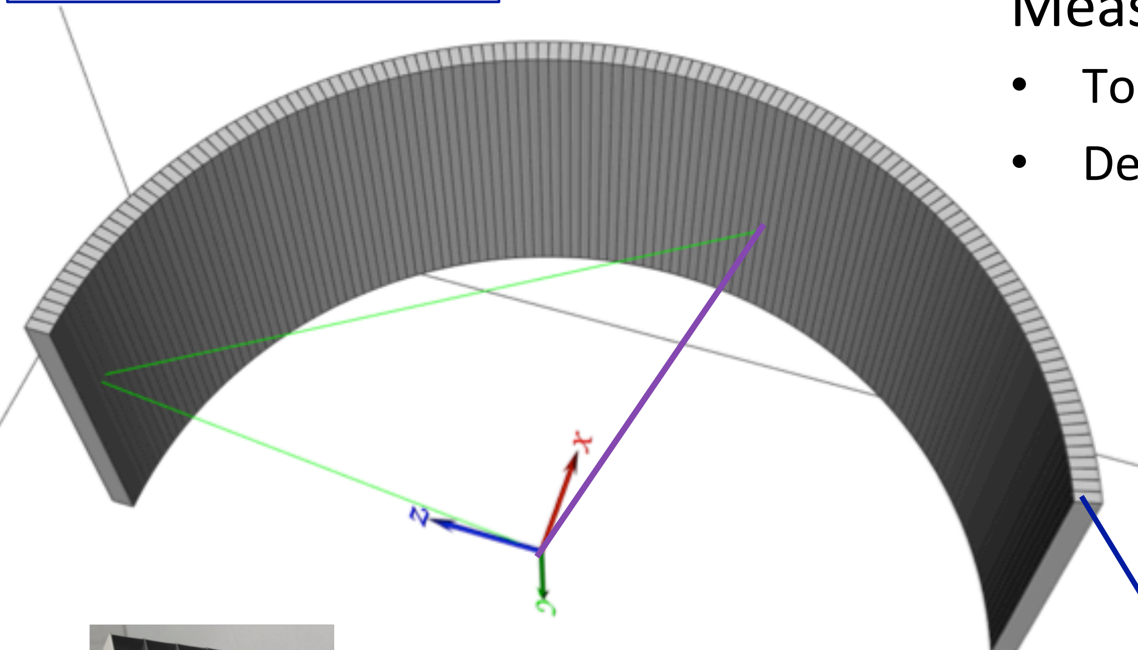
- Energy transfer:

$E_{trf} = E_{initial} – E_{final}$

Anton Khaplanov et al.:
Multi-Grid Detector for Neutron Spectroscopy: Results Obtained on Time-of-Flight Spectrometer CNCS
doi:10.1088/1748-0221/12/04/P04030, https://arxiv.org/abs/1703.03626

Large area detector for chopper spectroscopy – Multi-Grid

Geant4 @Coding Framework



Measured data:

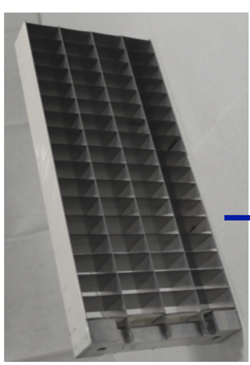
- ToF
- Detection point coordinates

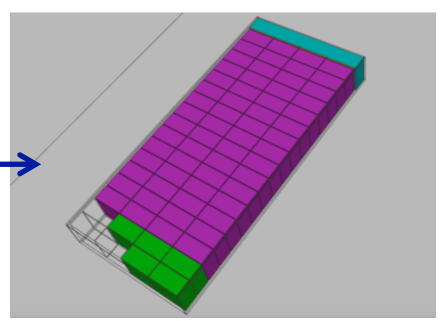
} Energy

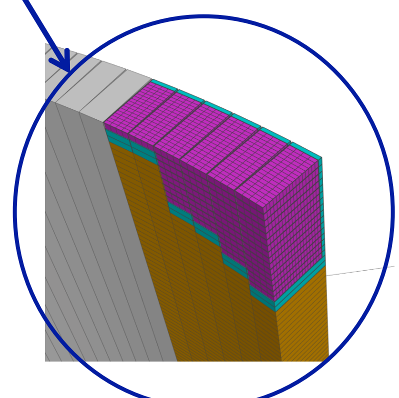
Sample – detection point distance

≠

Real neutron path







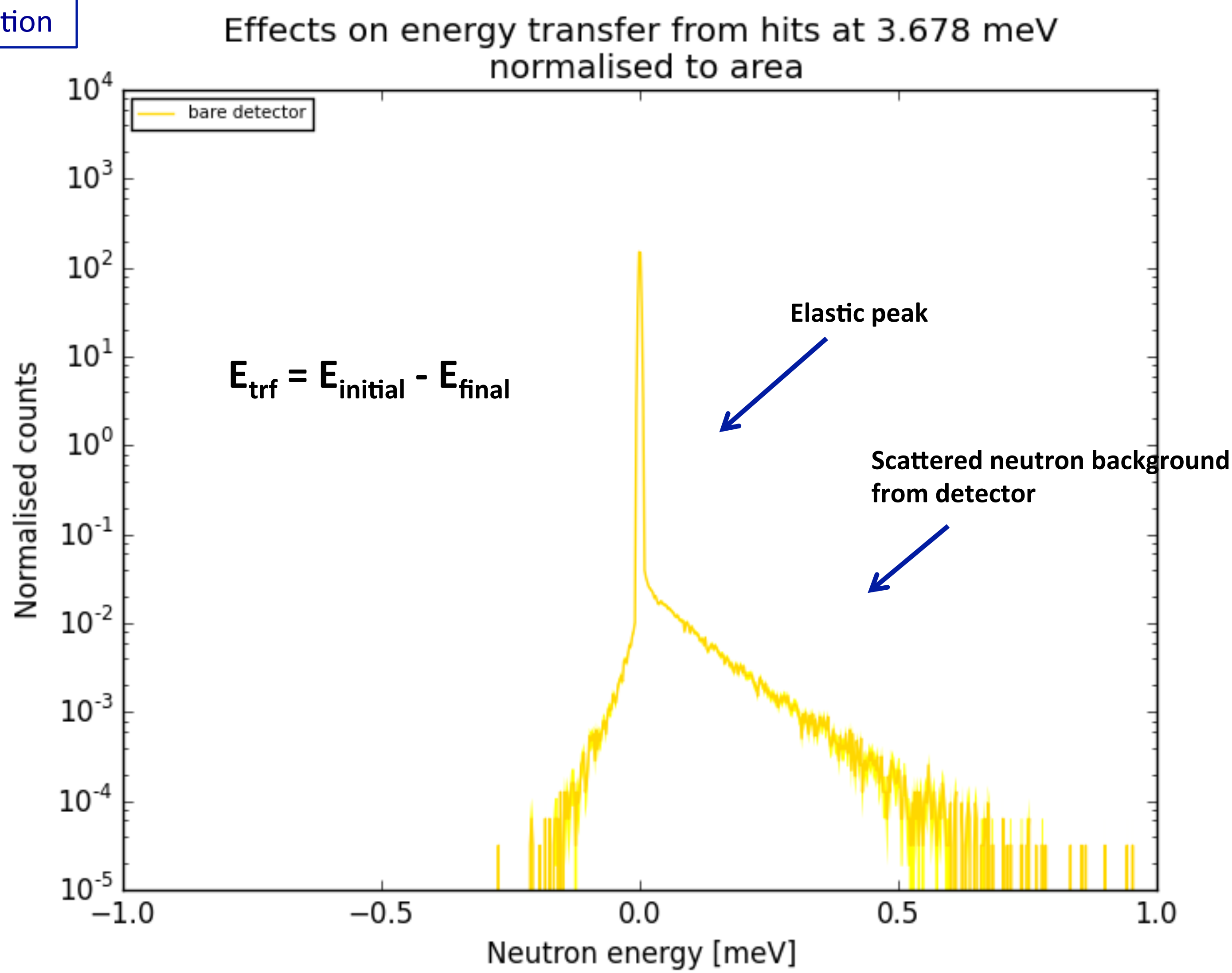
A. Khaplanov et al.

http://dx.doi.org/10.1016/j.nima.2012.12.021

MultiGrid detector test at CNCS, SNS

Geant4 simulation

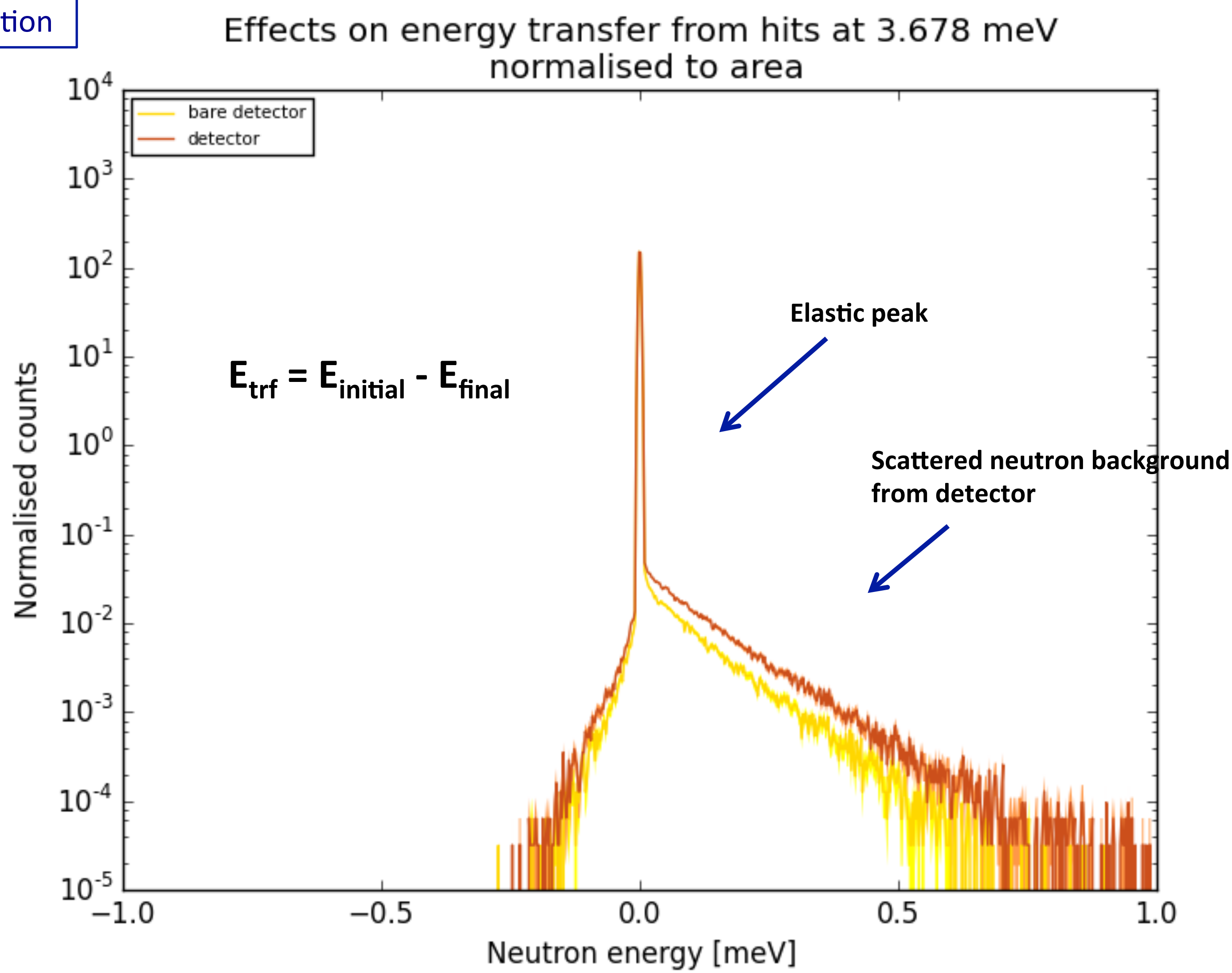
NXSG4



MultiGrid detector test at CNCS, SNS

Geant4 simulation

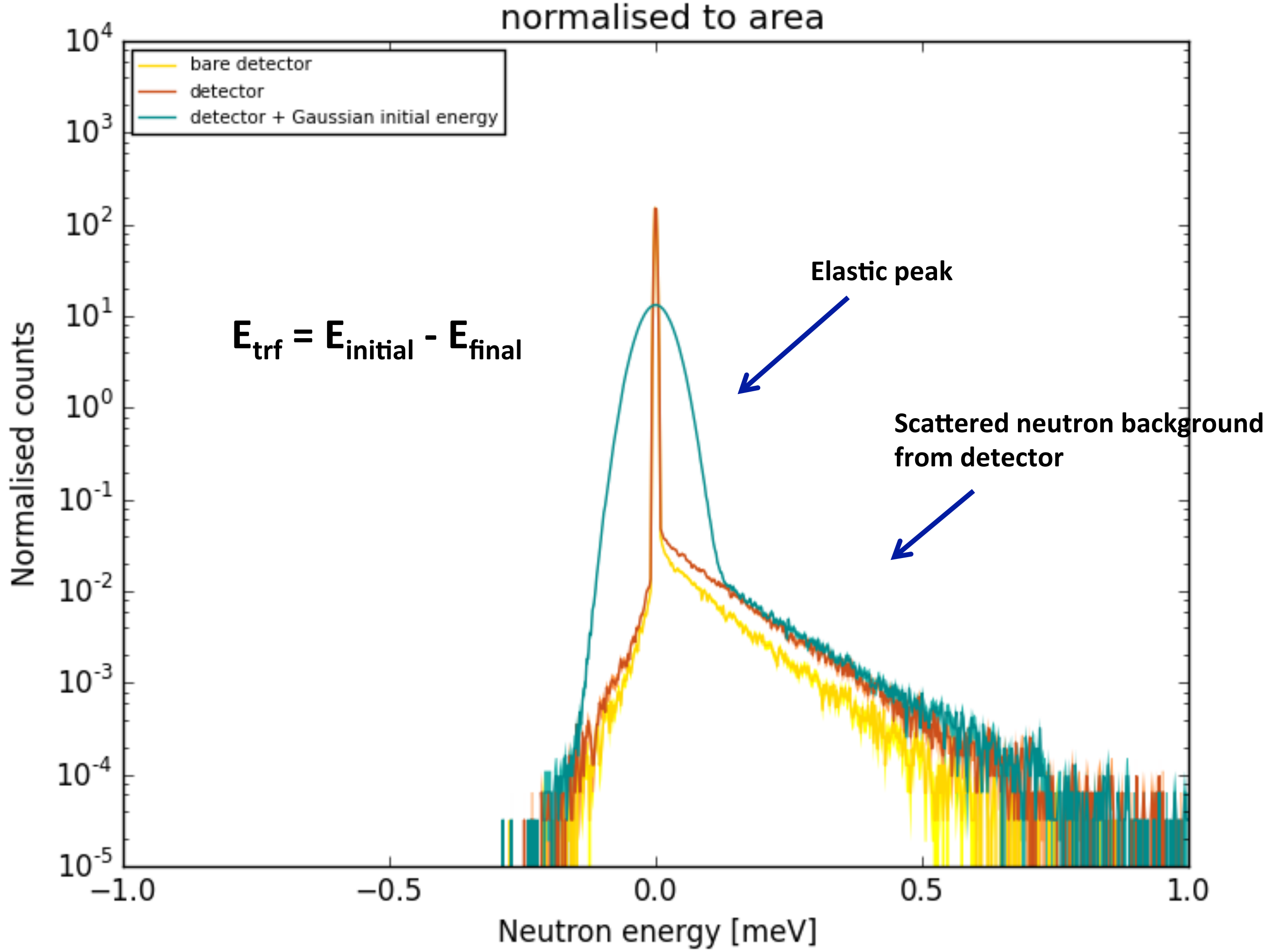
NXSG4



MultiGrid detector test at CNCS, SNS

Geant4 simulation

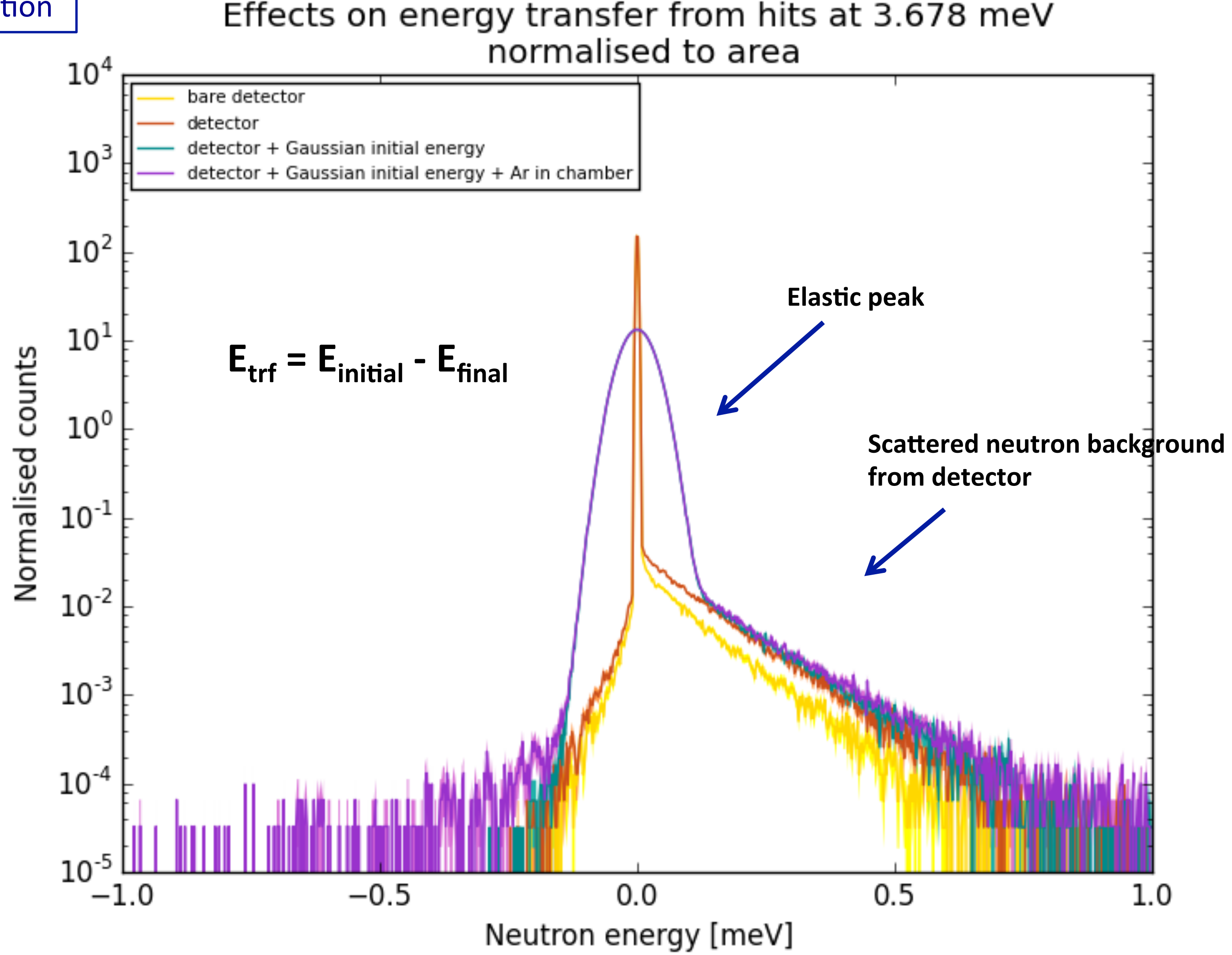
NXSG4



MultiGrid detector test at CNCS, SNS

Geant4 simulation

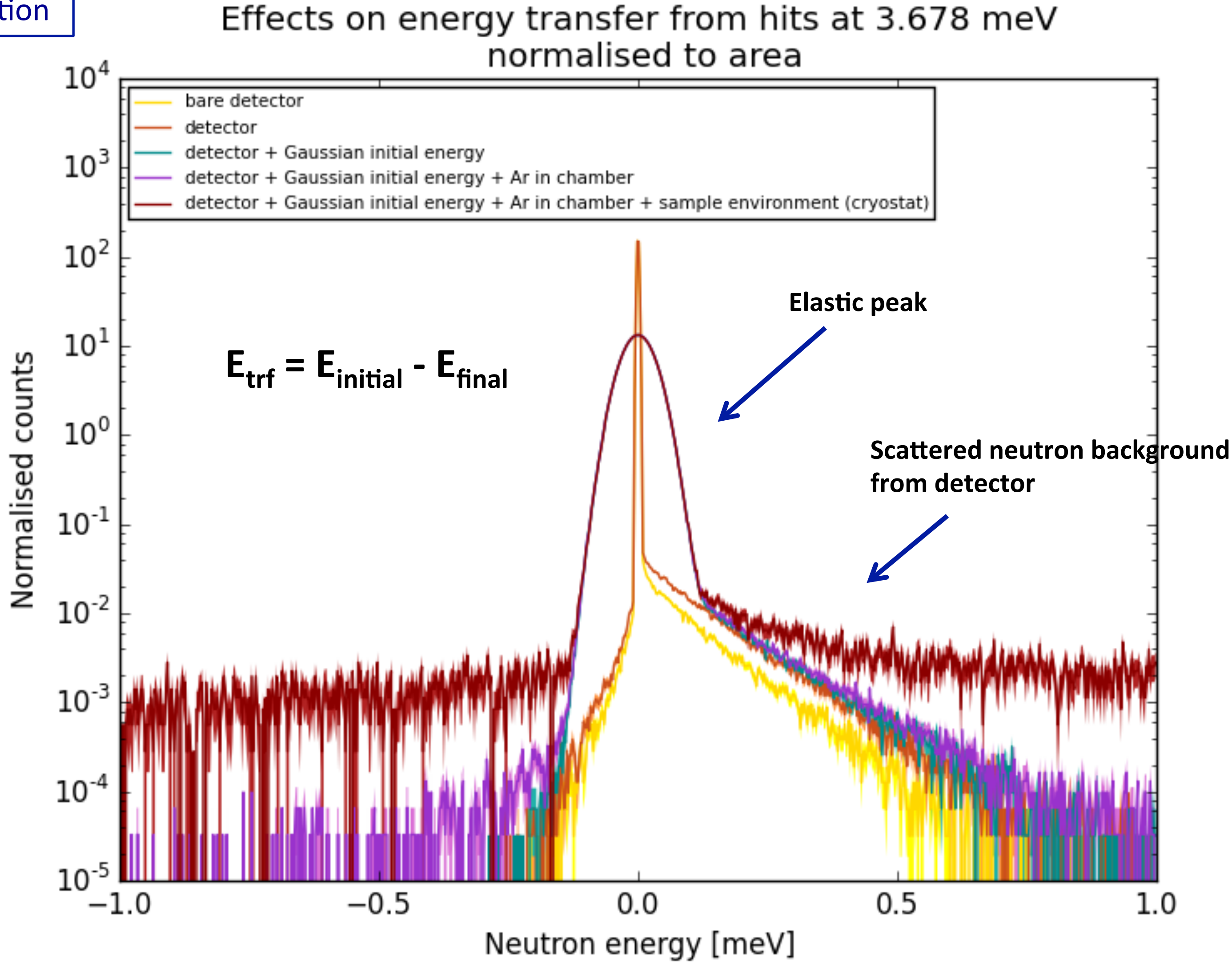
NXSG4



MultiGrid detector test at CNCS, SNS

Geant4 simulation

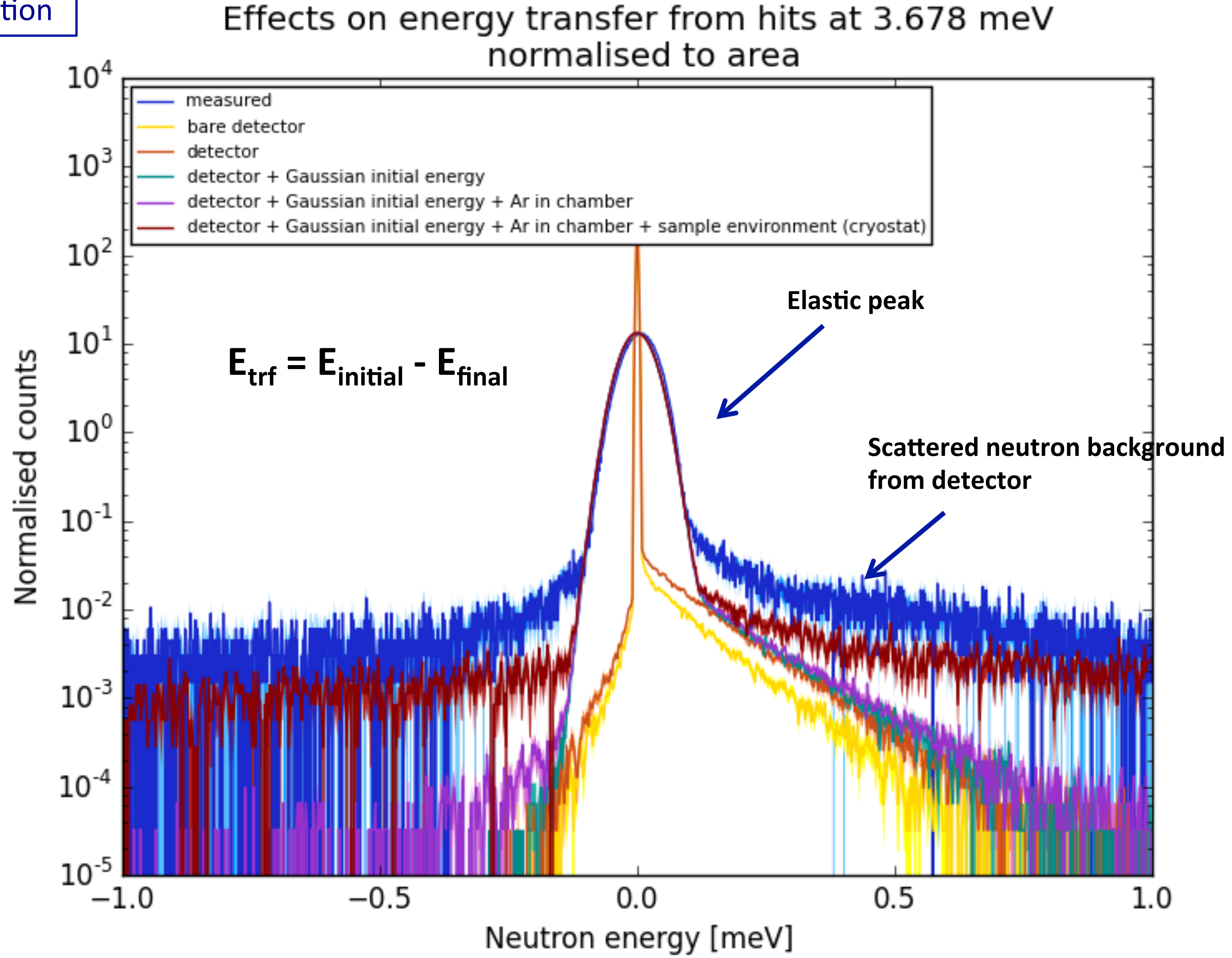
NXSG4



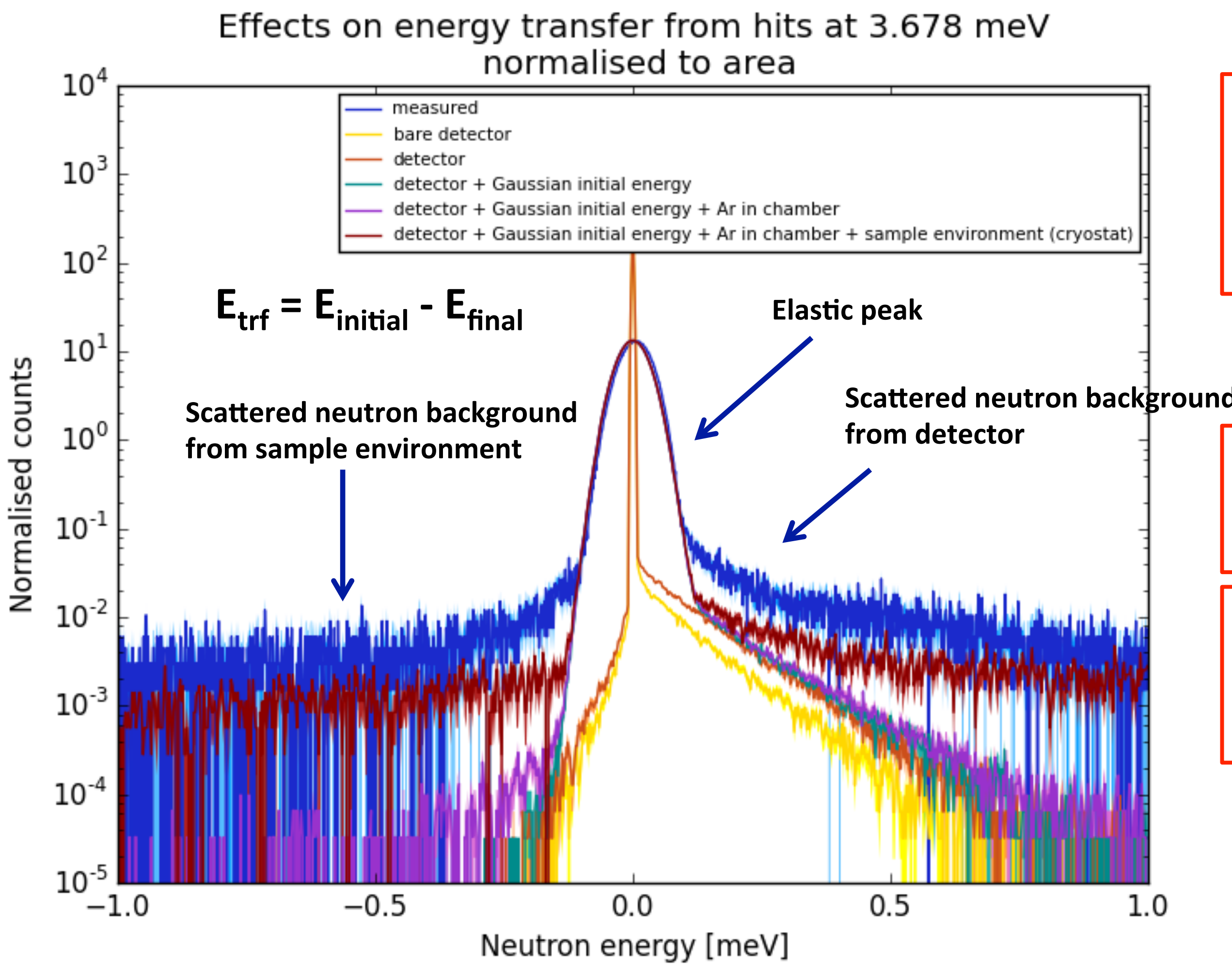
MultiGrid detector test at CNCS, SNS

Geant4 simulation

NXSG4



MultiGrid detector test at CNCS, SNS



Validation

Energy transfer reproduced with simulation at 3.678 meV

Distinguish different sources of background

Detailed analysis and quantification of background effects

Optimization

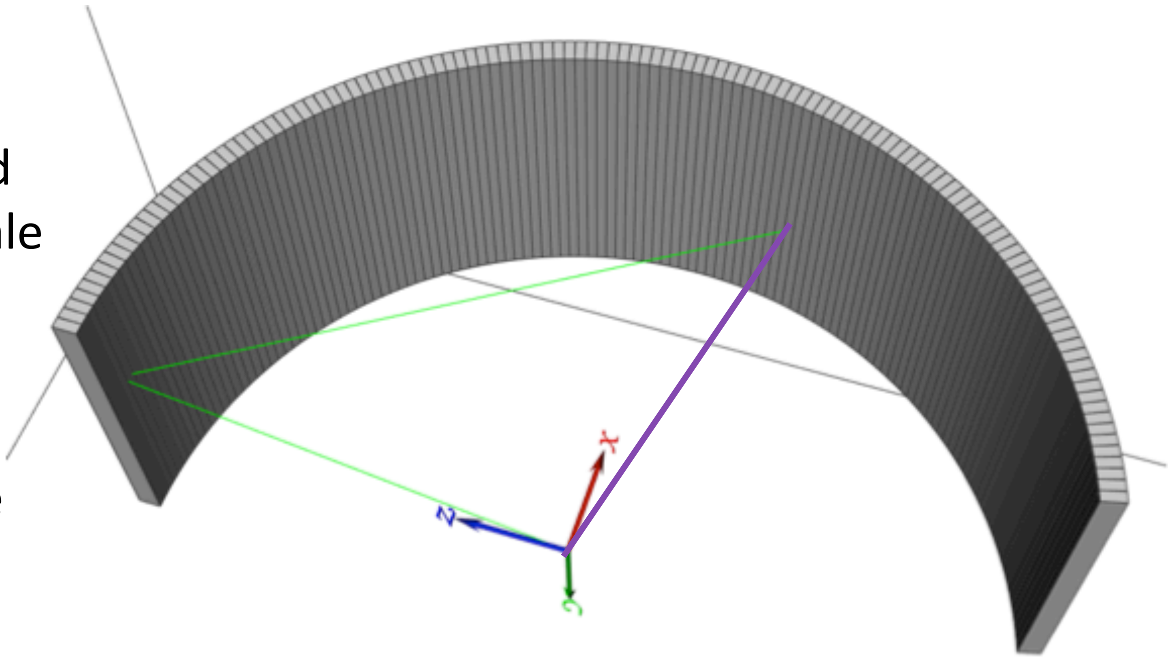
Conclusion

- Realistic Multi-Grid model built
  - reproduced measured results from IN6 and CNCS experiments
- Ready to use for optimization

→ **Instruments with better signal-to-background ratio by design**

↓

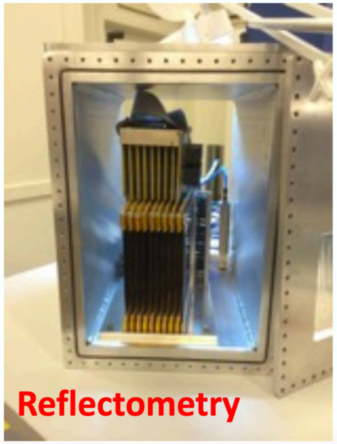
- Predicament for background sources and levels in full-scale detector
- Shielding and design optimization in the level of grids, columns and full-scale detector



More on simulations…

- IKON13 next week
  - **Thursday, 28/9:** all day detector section
  - **16:00 Tänkartanken** (last talk before site visit):
    Joint talk of Hungarian student group of ESS Detector Group on detector modeling:

MultiBlade (ESS/Wigner/LU/LiU)

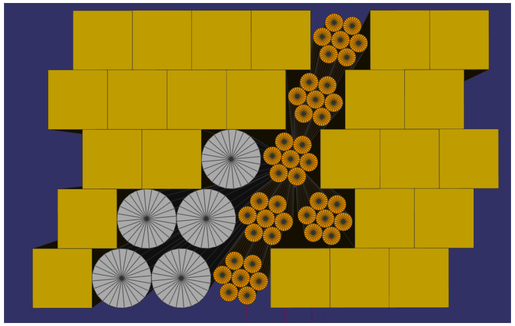


Eszter Dian[1,2] Gábor Galgóczi[3,4], Milán Klausz[1,2]

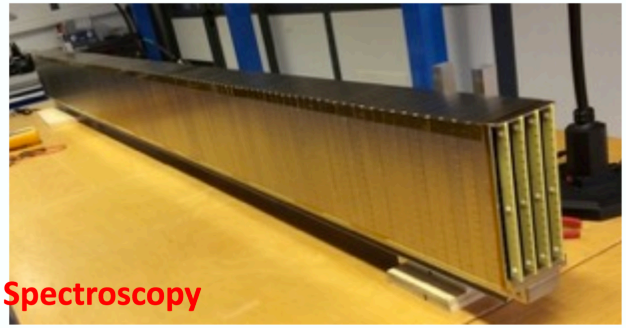
Multi-Grid **MultiBlade** **BCS&Bifrost**

[1]Hungarian Academy of Sciences, Centre for Energy Research
[2]European Spallation Source ESS ERIC
[3]Wigner Research Centre for Physics
[4]Institute of Physics, Eötvös Loránd University,

PTI Boron-coated straws



MultiGrid (ILL/ESS/LiU)

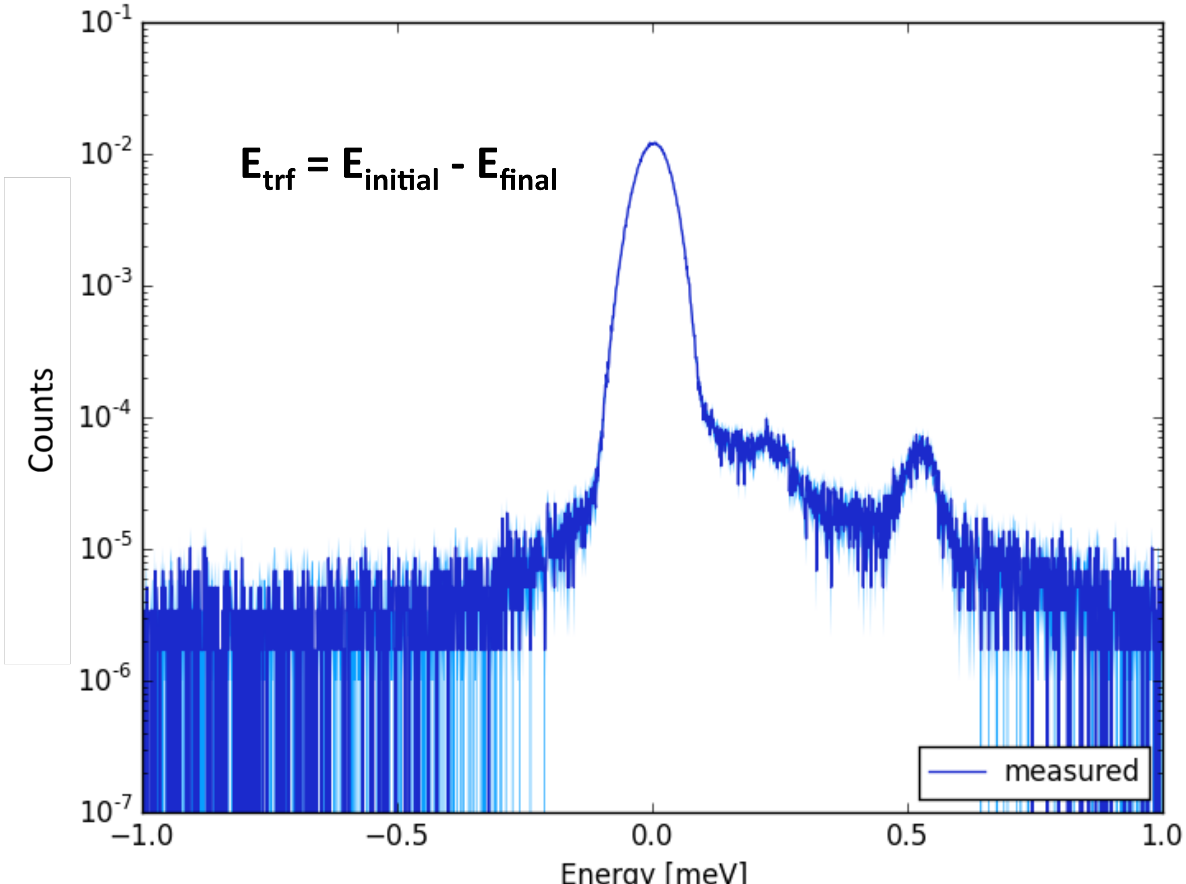


Thank you for your attention!

Backup slides

MultiGrid detector test at CNCS
[Anton Khaplanov]

Derived energy transfer at 3.807 meV from measurement



- Chopper spectroscopy
- Measured quantities:
  - ToF
  - detection-coordinates

↓

- Energy transfer:

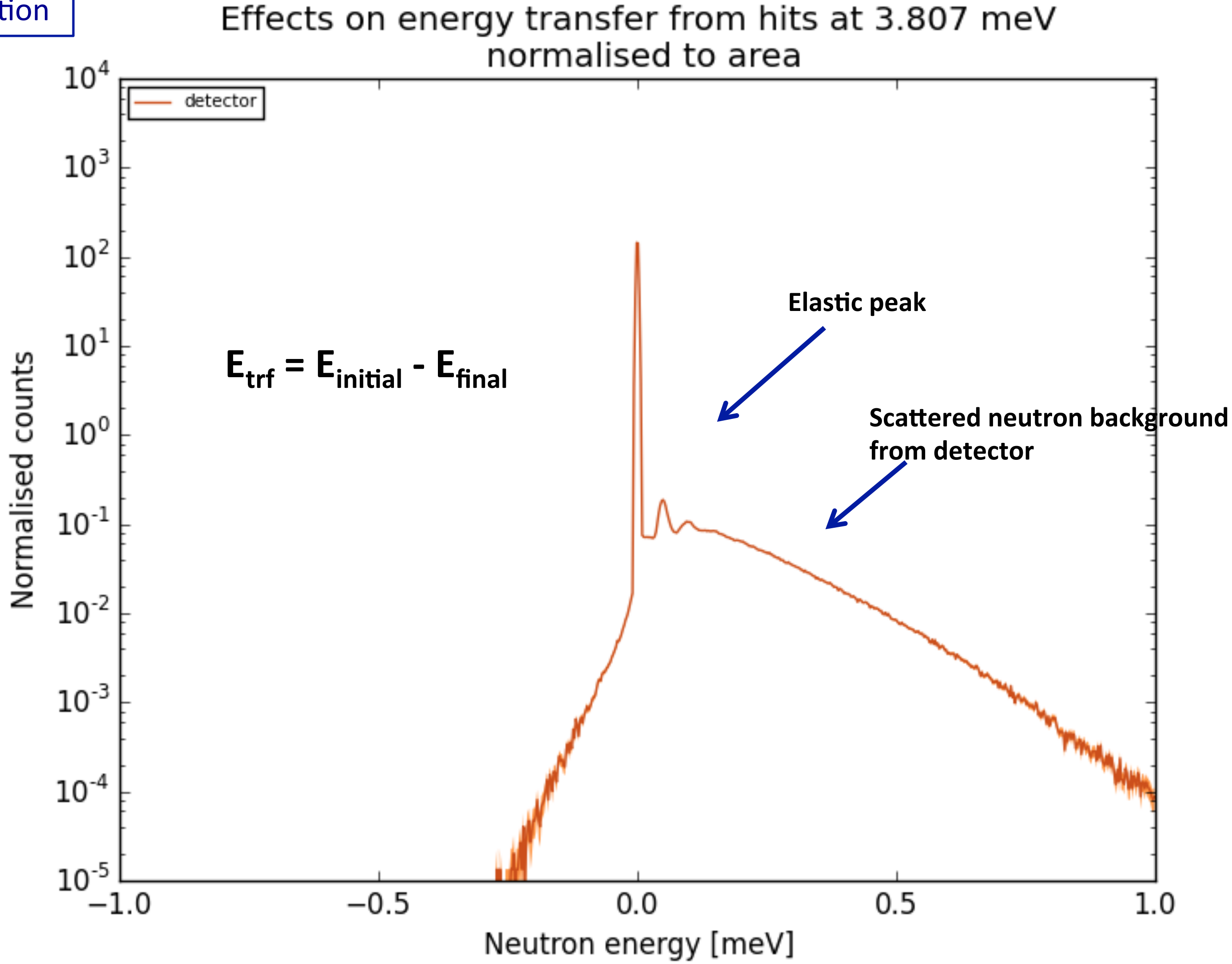
$E_{trf} = E_{initial} - E_{final}$

Anton Khaplanov et al.:
Multi-Grid Detector for Neutron Spectroscopy: Results Obtained on Time-of-Flight Spectrometer CNCS
Submitted to JINST arXiv:1703.03626

MultiGrid detector test at CNCS, SNS

Geant4 simulation

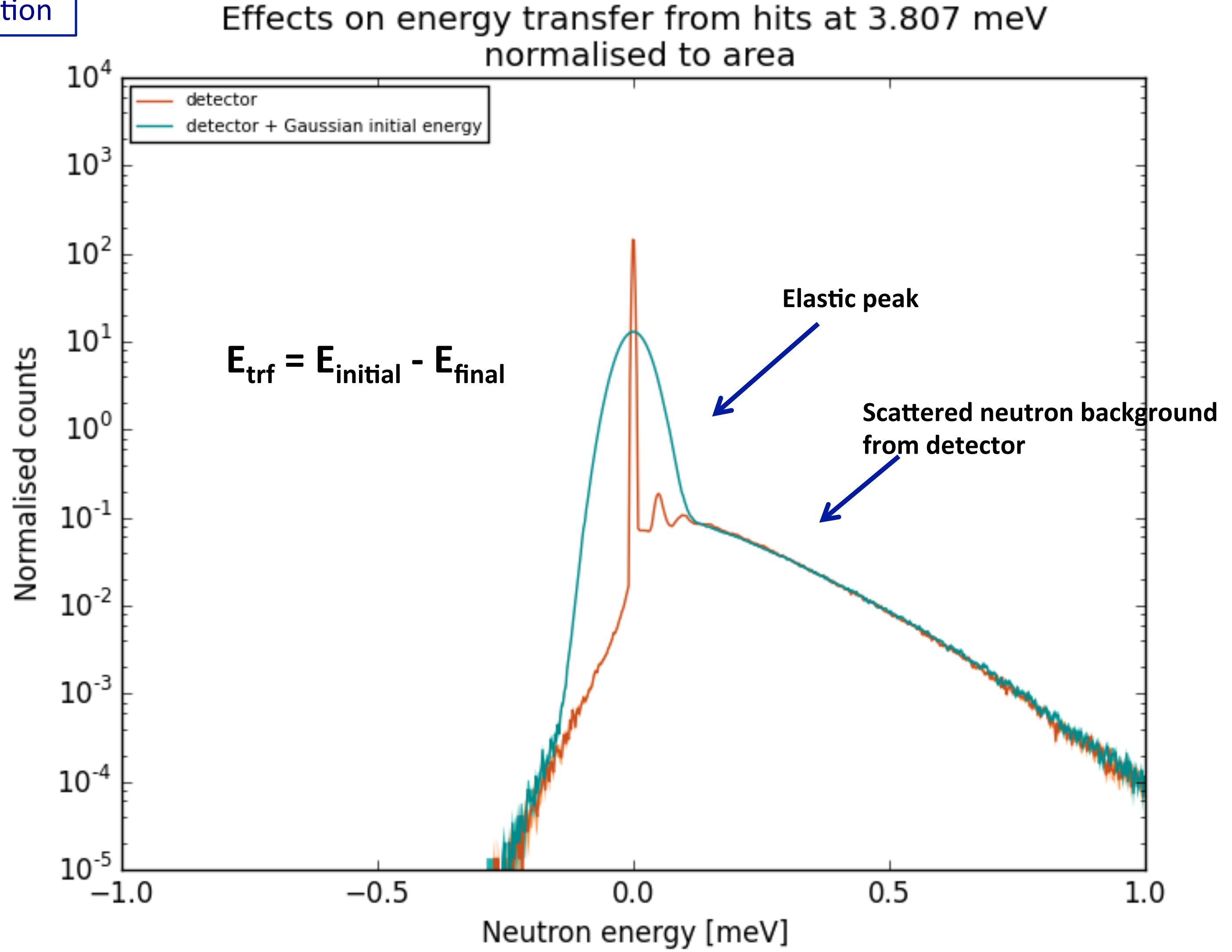
NXSG4



MultiGrid detector test at CNCS, SNS

Geant4 simulation

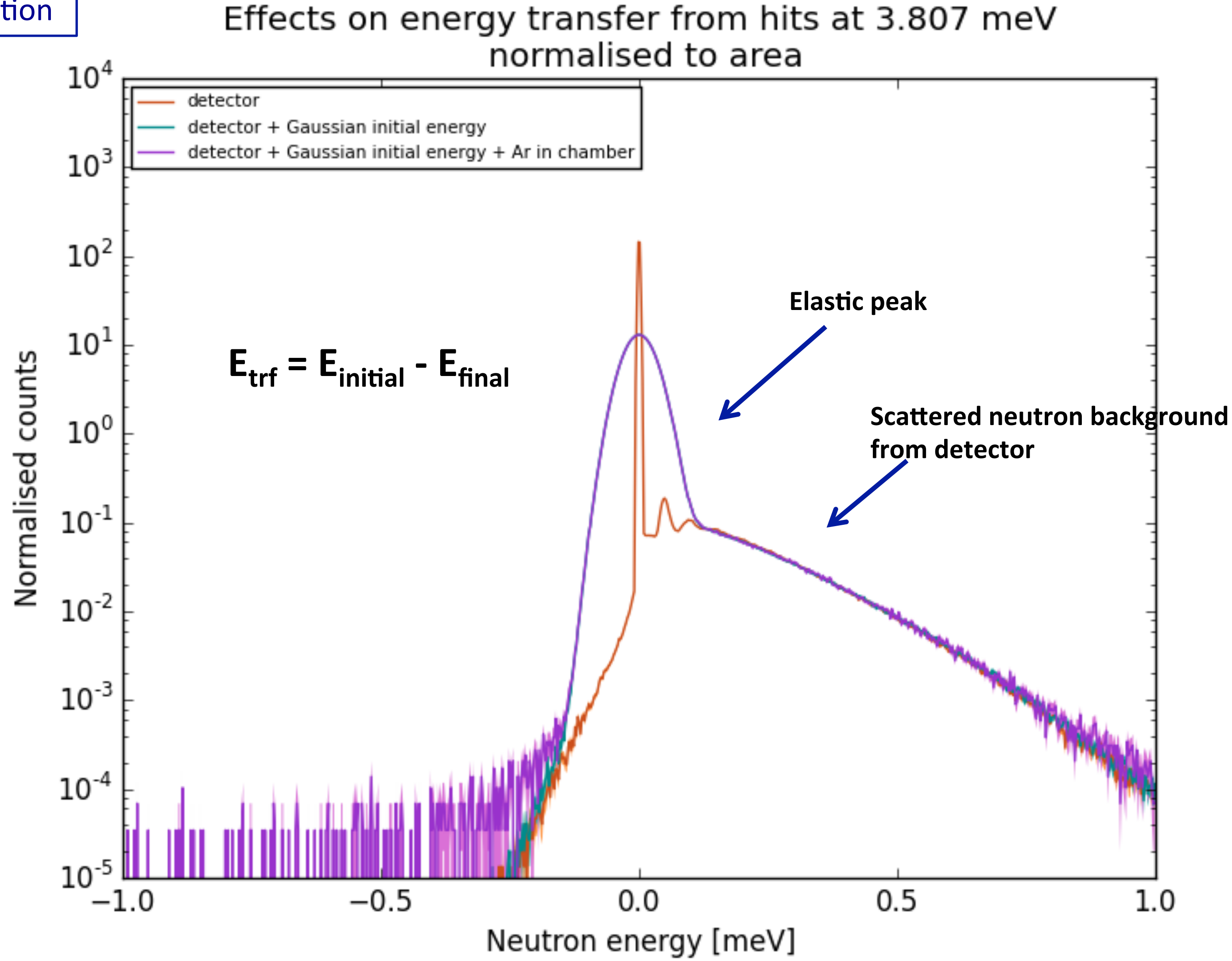
NXSG4



MultiGrid detector test at CNCS, SNS

Geant4 simulation

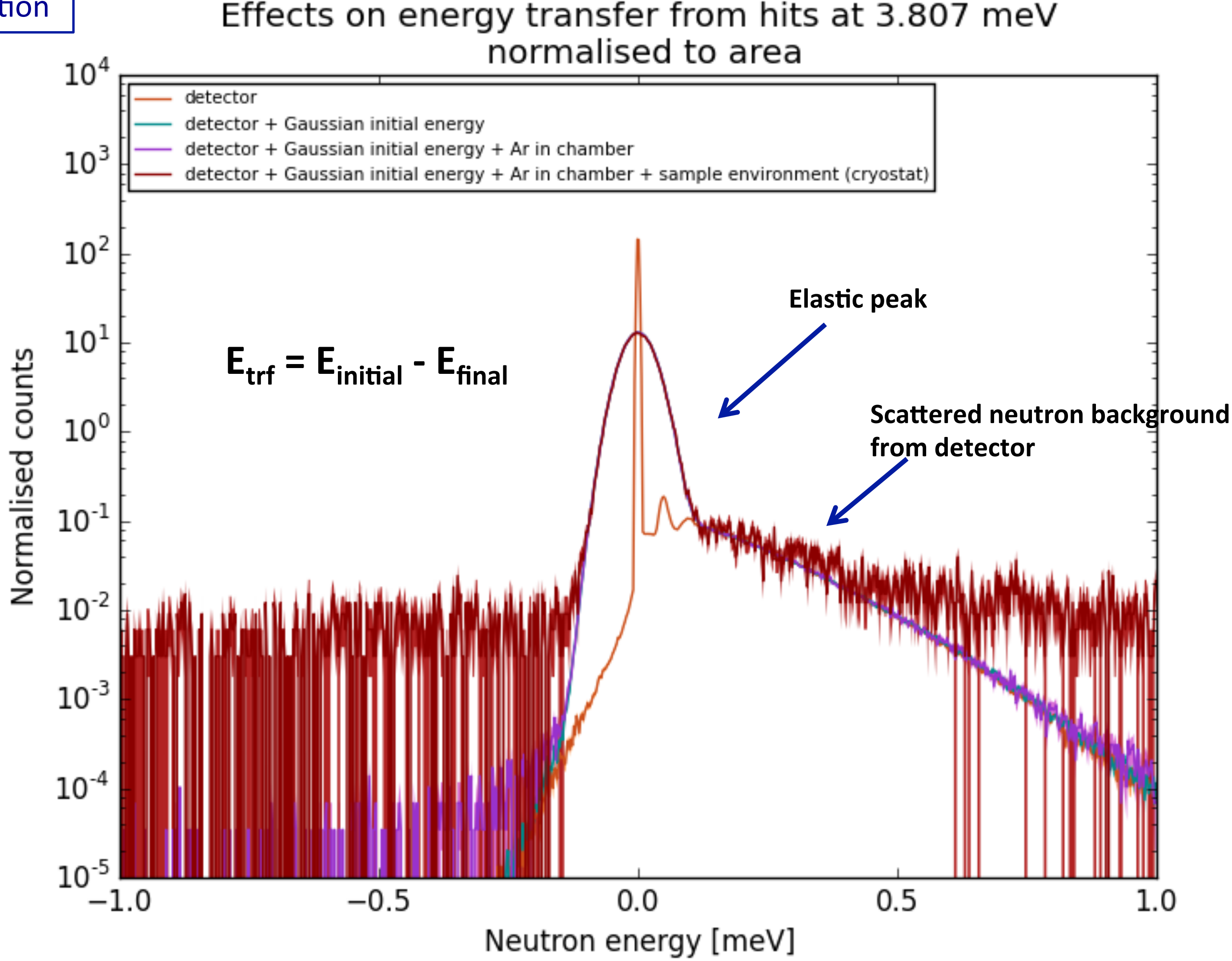
NXSG4



MultiGrid detector test at CNCS, SNS

Geant4 simulation

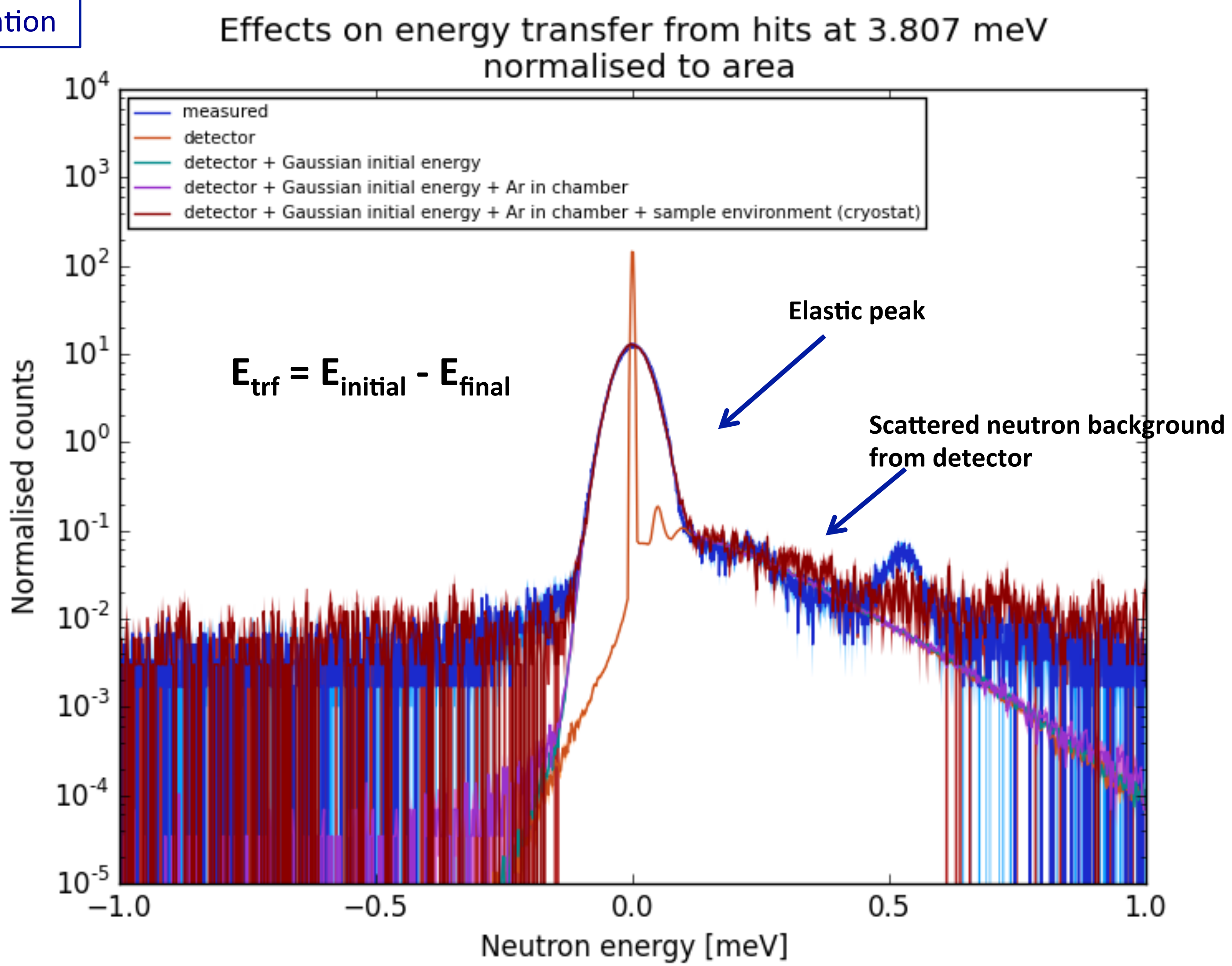
NXSG4



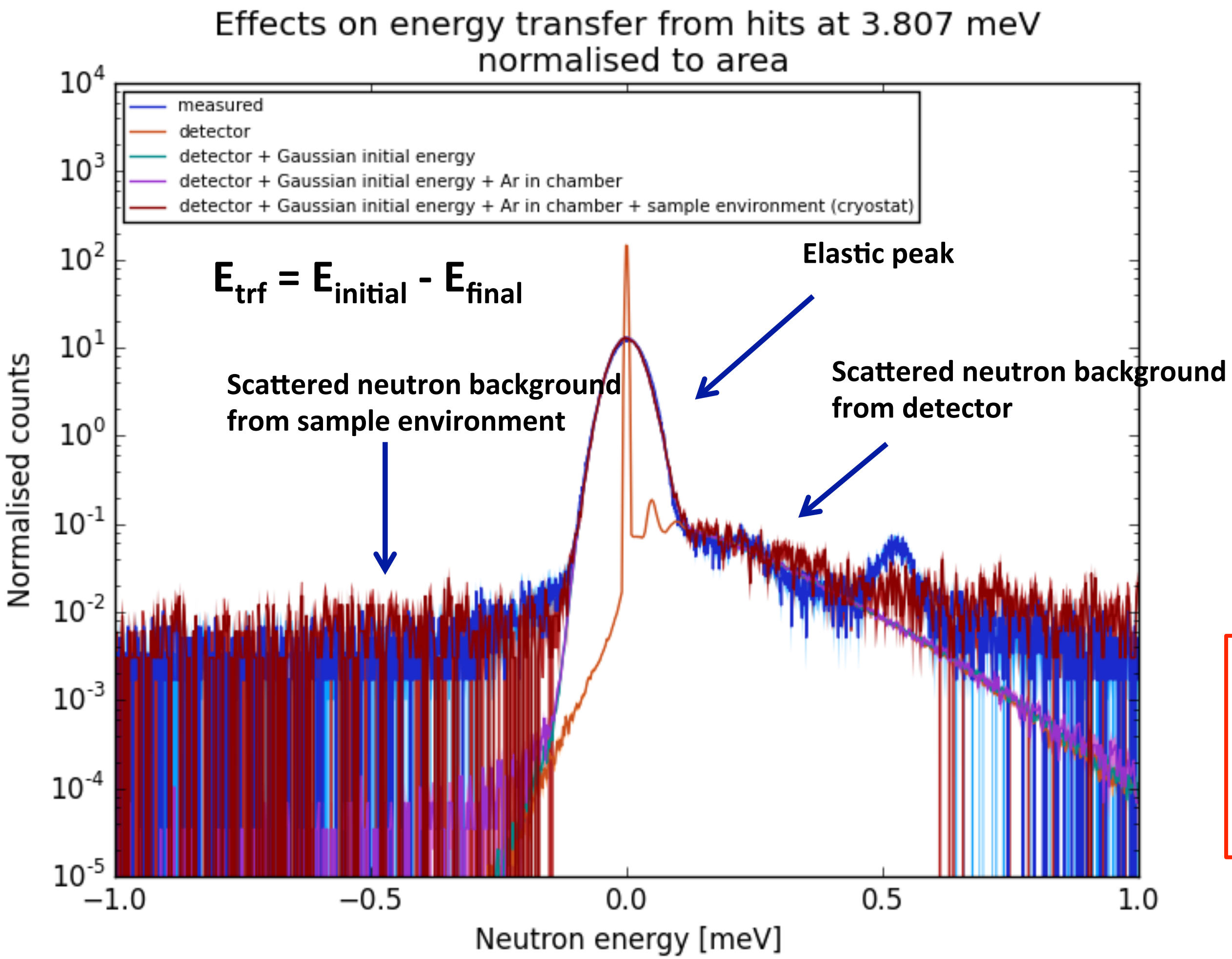
MultiGrid detector test at CNCS, SNS

Geant4 simulation

NXSG4



MultiGrid detector test at CNCS



- Distinguish different sources of background
- Detailed analysis and quantification of background effects

Energy transfer reproduced with simulation at 3.807 meV ✓

676548

Thank you for your attention!