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New Simulation Tools and Reproduction of CNCS results using Geant4

E. Dian,

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HAS Centre for Energy Research

European Spallation Source ESS ERIC

28 March 2017, ICANS XXII, Oxford

- The ESS detector challenge
 - All instruments in different design phases
 - Diverse set of requirements
 - Challenge: new detectors with several different designs
- Powerful simulation tools
- Application in detector design:
 - Background study for MultiGrid detector

**I'm an
end-user!**

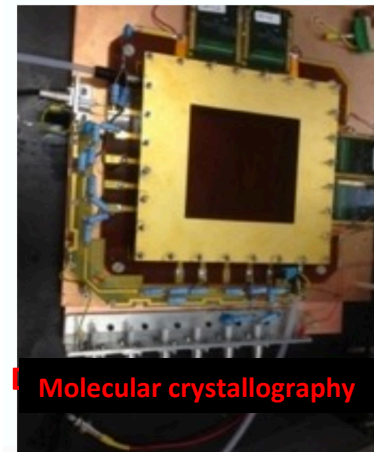
- Various detectors for various instruments at ESS
- All with **different designs**, all have to be **optimised** for respective instrument requirements
- Good measurement
=> high signal-to-background
- ESS: increased flux ✓
- Low level background
=> need to understand

**Effective and universal
simulation tool**

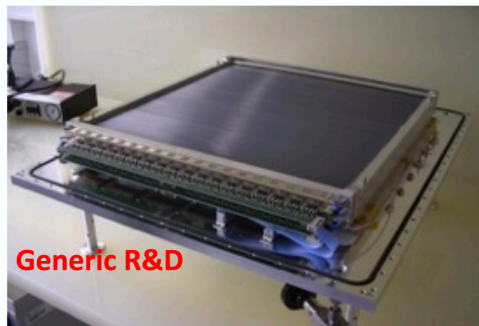
MultiBlade (ESS/Wigner/LU/LiU)



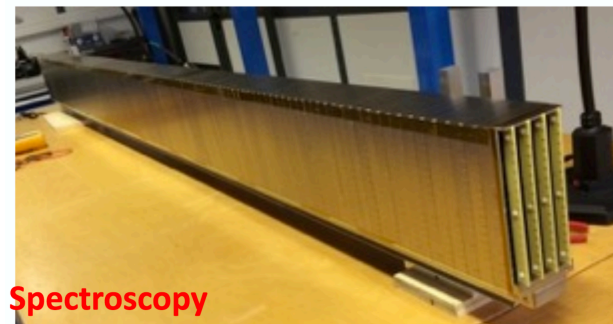
Gd-GEM (ESS/CERN/LiU)



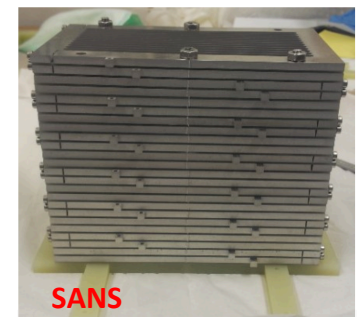
B-MWPC/ Macrostructures (ESS/FRM2)



MultiGrid (ILL/ESS/LiU)



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



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- All with **different designs**, all have to be **optimised** for respective instrument requirements

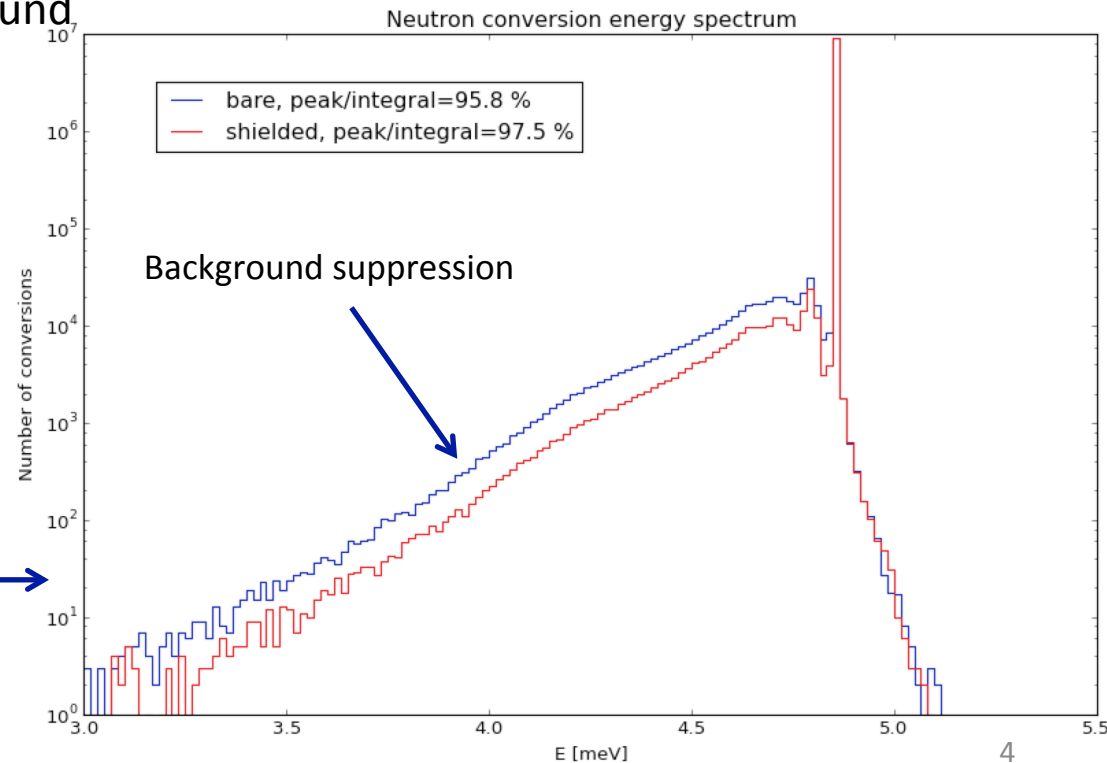
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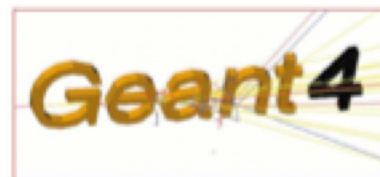
**Effective and universal
simulation tool**

Using scientific quantities
for optimisation

e.g. MultiGrid for inelastic instrument



- Several already existing simulation codes
- New or improved features needed:
 - Physics
 - Coherent scattering
 - Inelastic scattering
 - Single- and polycrystals...
 - And more
 - Communication
 - Visualisation
 - Ready-to use...



- **nxs library**

- Low-energy neutron scattering
- Polycrystalline materials
 - Coherent and
 - Incoherent neutron scattering

- <http://cern.ch/nxsg4/>

- examples, license details
- instructions for installation and usage
- usage of the code (including nxs and SgInfo) is **free for non-commercial purposes**



**NXSG4 makes nxs library
available as Geant4 extension**

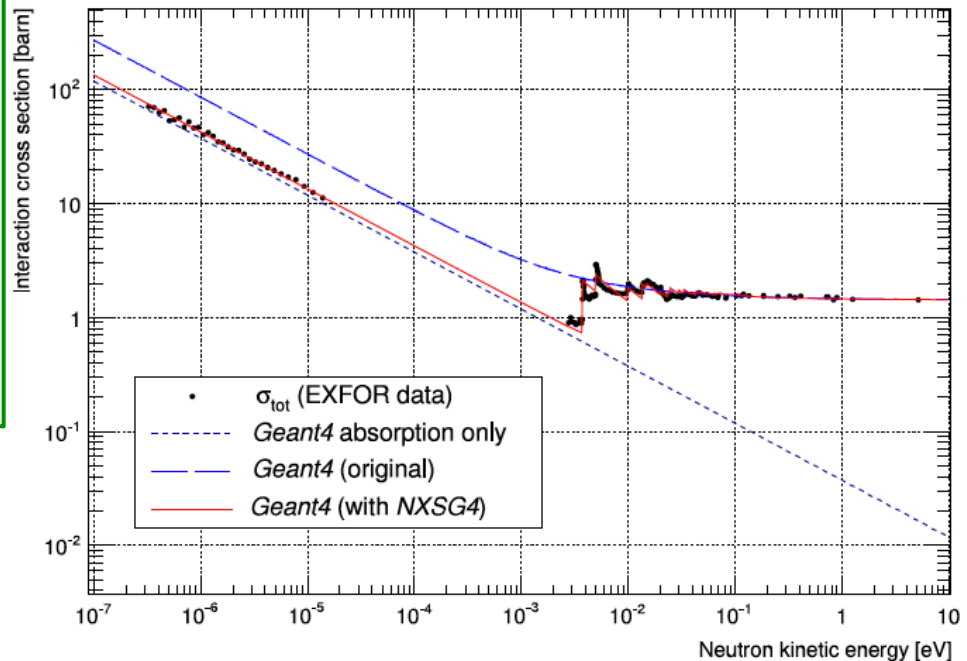
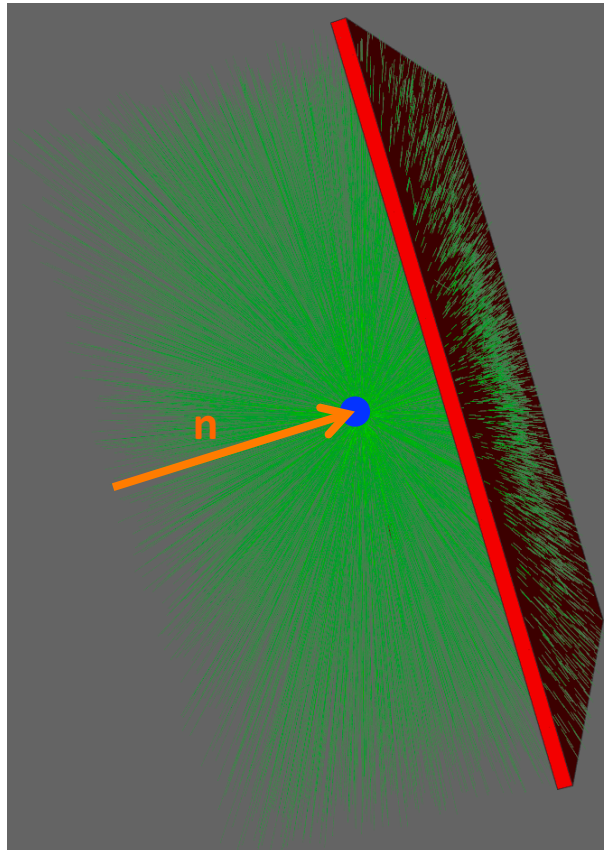


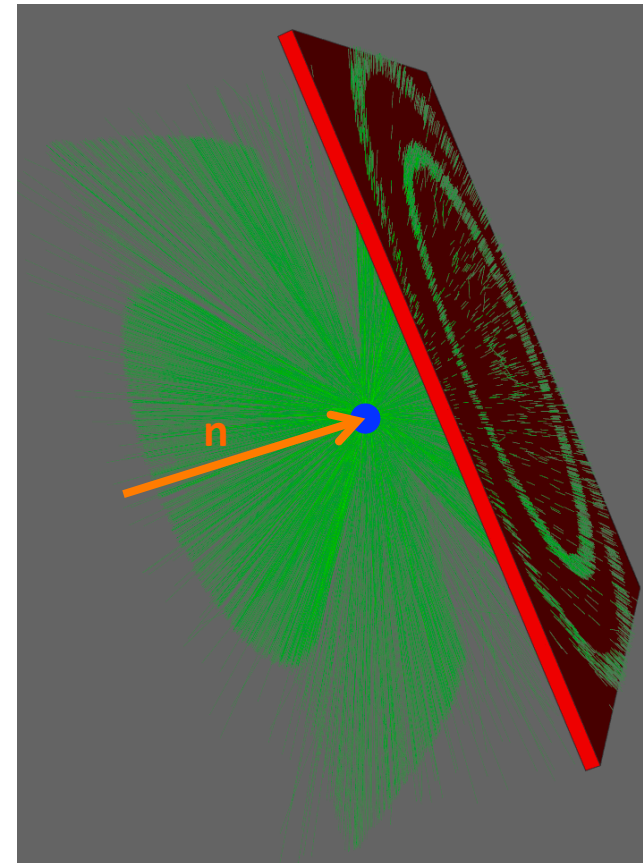
Fig. 4. Original and NXSG4-corrected cross sections for neutron interactions with aluminium in Geant4 compared to data [9].

Geant4 simulation

Free-gas model Geant4
aluminum



NXSG4
aluminum



- **NCrystal**

- Neutron scattering on **single-** and **polycrystalline** materials
- detailed Bragg diffraction
- first principle inelastic model

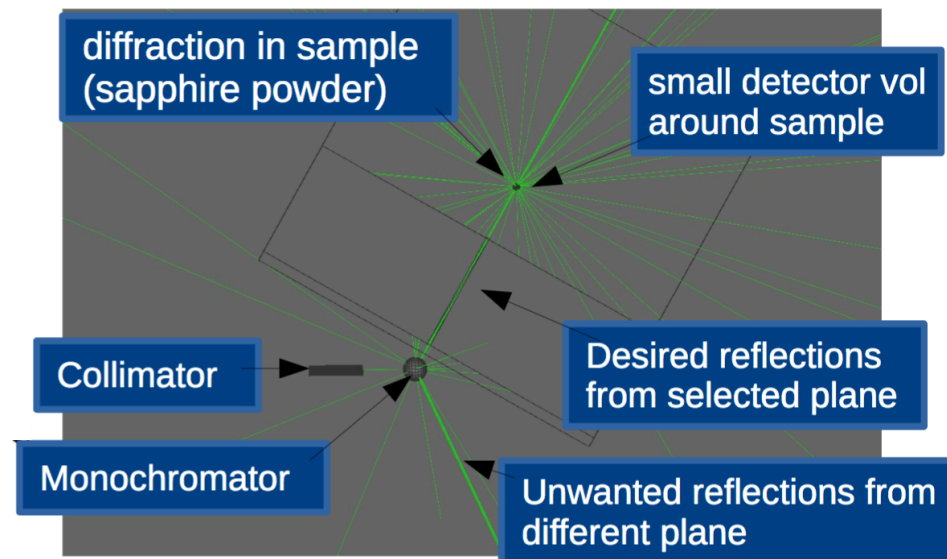
- C++
- open source

**Standalone NCrystal
tool coming soon**

See Xiao Xiao Cai's talk
Friday 09:55 (Neutronics 2)

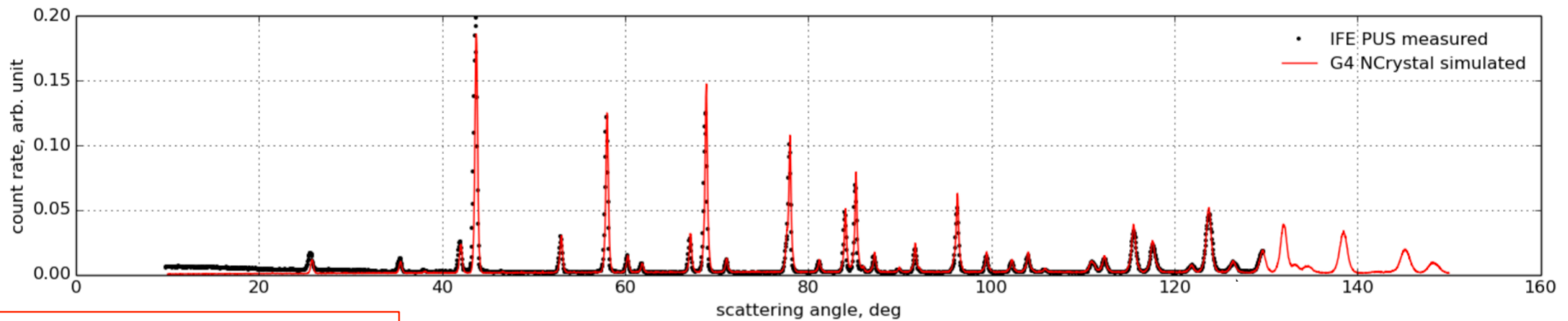
→ monochromators, analysers,
filters, powder samples

↓
full-instrument simulation



Geant4 simulation

Powder Diffractometer PUS at IFE, Norway



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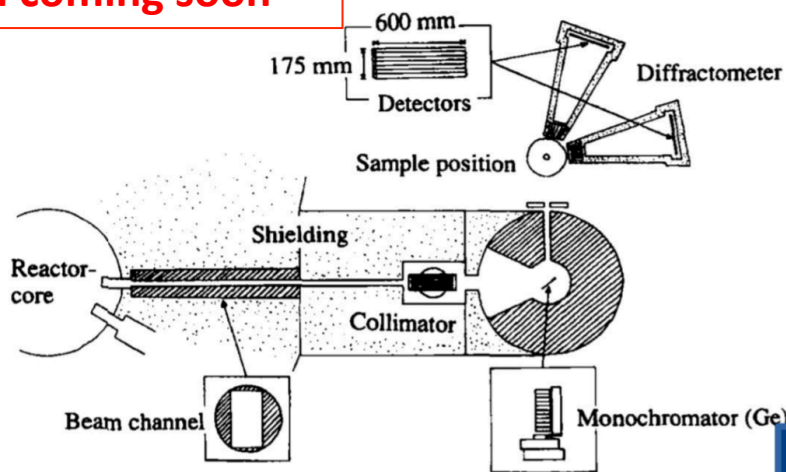
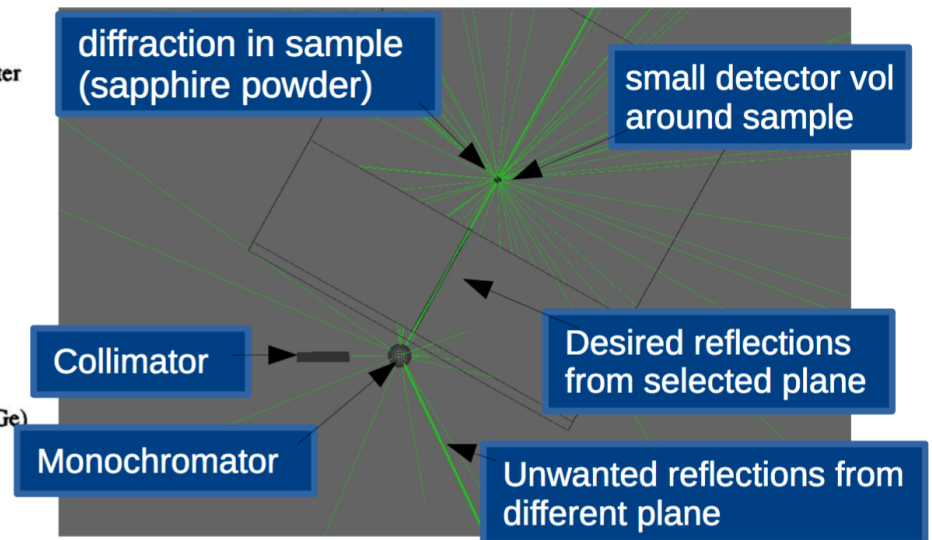
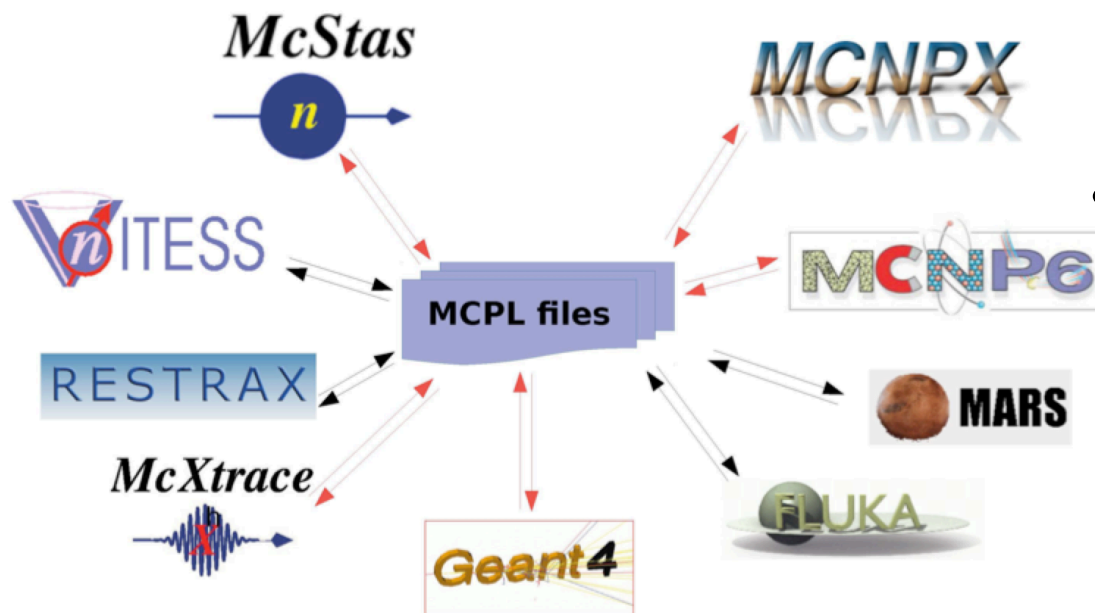


FIGURE 1 A schematic drawing of PUS.



Contact:

mcpl-developers@cern.ch



In **red** : already available now

Disclaimer: Non-exhaustive list of applications...

[arxiv:1609.02792](https://arxiv.org/abs/1609.02792)

<http://sine2020.eu/news-and-media/mcpl-a-new-format-that-simplifies-data-interchange-between-applications.html>

- **Monte Carlo Particle List**
 - <https://mctools.github.io/mcpl/>
 - Interchange particles with **all their properties** between MC packages
 - flexible yet efficient storage of particle-state information

**Best code for
best application**

- **Geant4 simulation framework**
 - Developed by ESS Detector Group
 - Used by other groups in ESS e.g. Accelerator Group, Shielding and Optics Group
 - Contains all afore mentioned tools:
 - Integrated
 - Transparent for end-user
 - Out-of-the-box usage
 - And more:
 - Effective build system
 - Python interface
 - Easy-to-handle histograms for analysis
 - 3D visualisation
 - Griff: an effective binary format for results
 - Powerful parameter scan without recompilation
- ↓
- Intuitive
 - User friendly

**I'm a happy
end-user!**

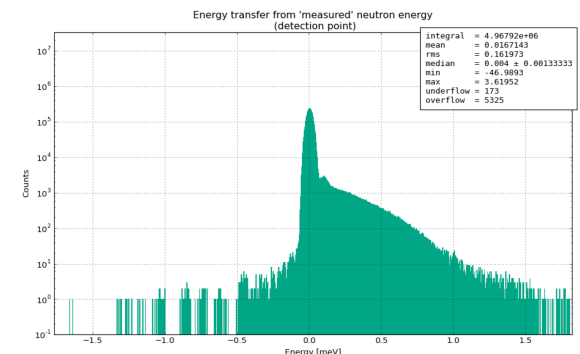
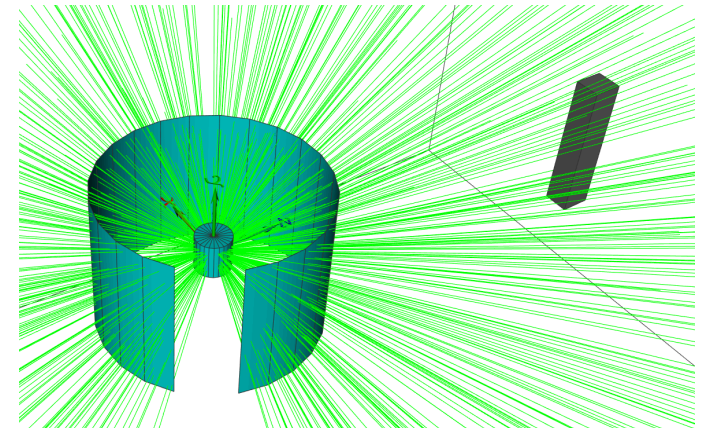
**Available, just
send a mail ☺**

Contact:

Thomas Kittelmann: thomas.kittelmann@esss.se

Xiao Xiao Cai: xcai@dtu.dk

Kalliopi Kanaki: kalliopi.kanaki@esss.se



Fast to develop new simulations

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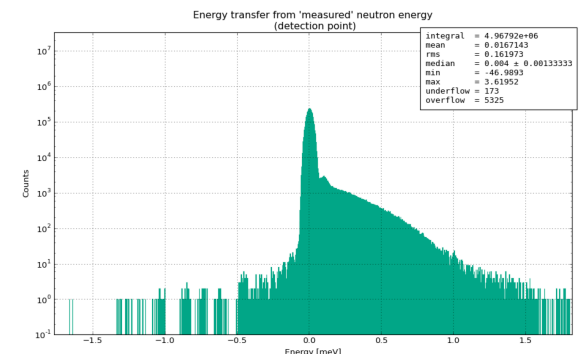
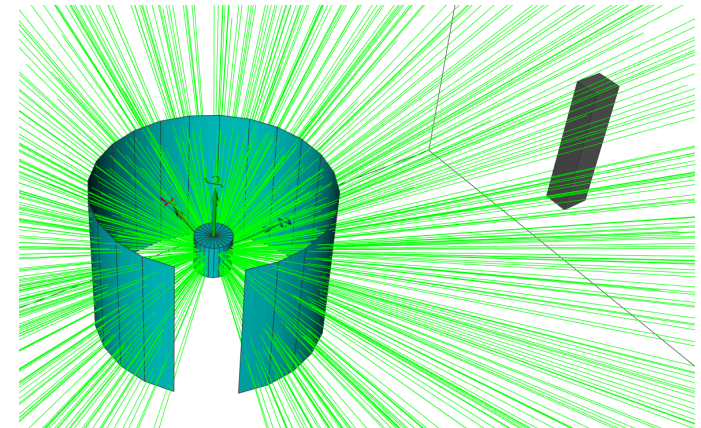
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Fast to develop new simulations

Now let's use it!

- 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**

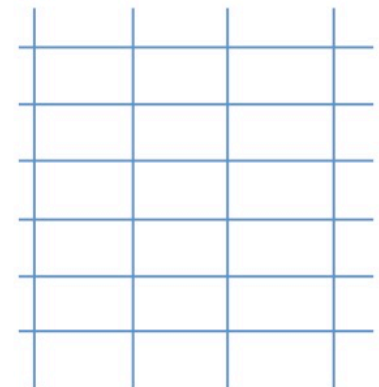
- Scattered neutrons (Geant4)
 - Elastic, inelastic
 - Coherent, incoherent

Great impact of Coding Framework!

General neutron activation study prepared with MCNP6 for ESS operation conditions

- Ar/CO₂ counting gas
- Aluminum-frame

E. Dian et al.
[arXiv:1701.08117](https://arxiv.org/abs/1701.08117)
submitted to ARI



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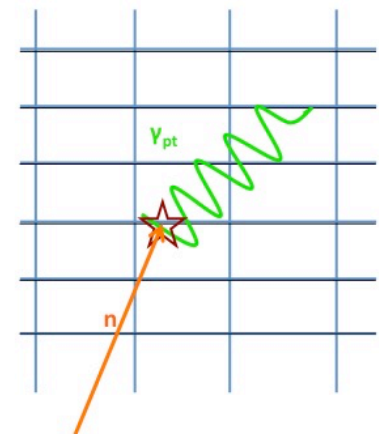
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Prompt gamma



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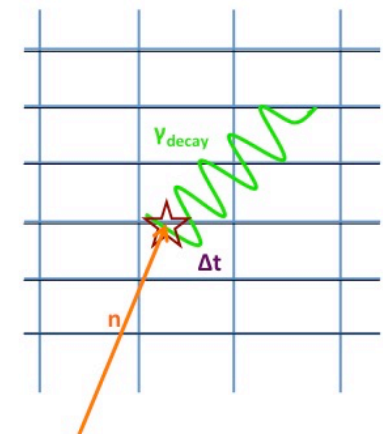
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Decay gamma



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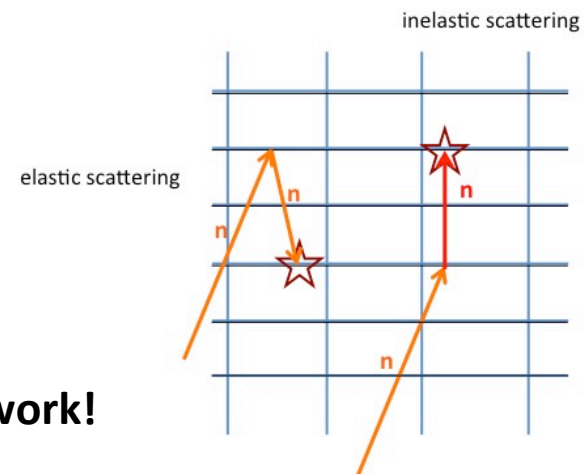
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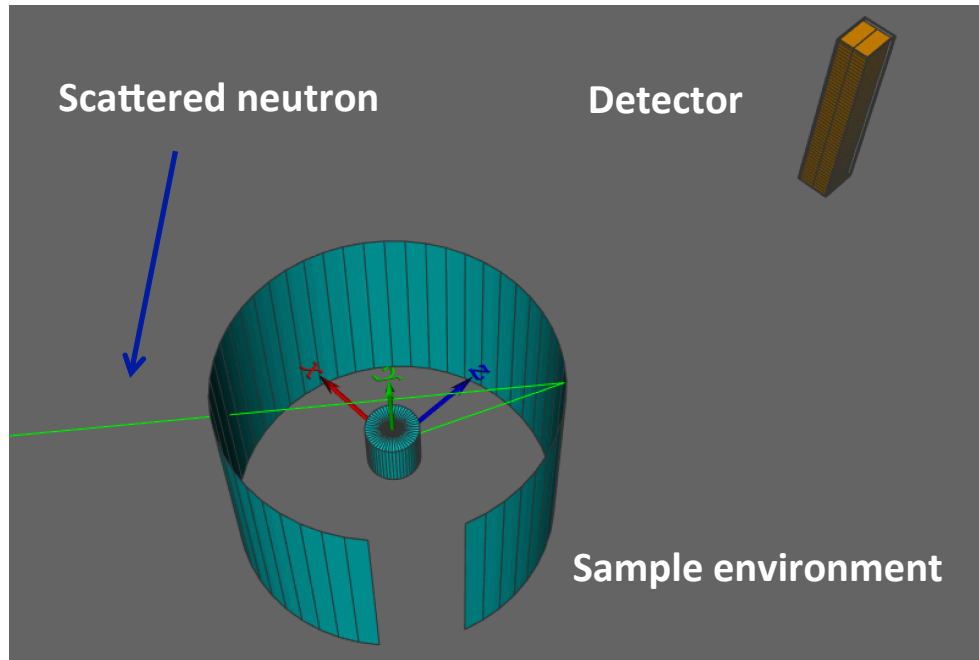
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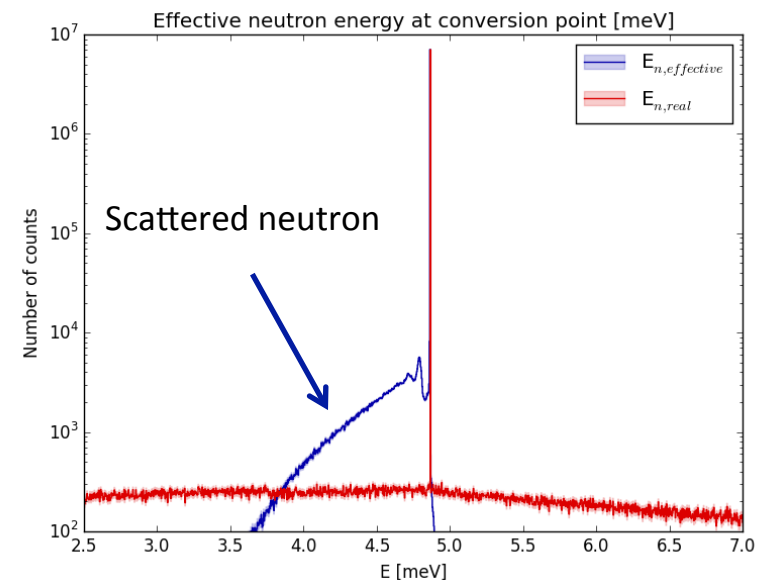


Scattered neutron background – power of simulation

- Follow the history of neutrons
- Study and distinguish background effects
- ↓
- Guidelines for detector design



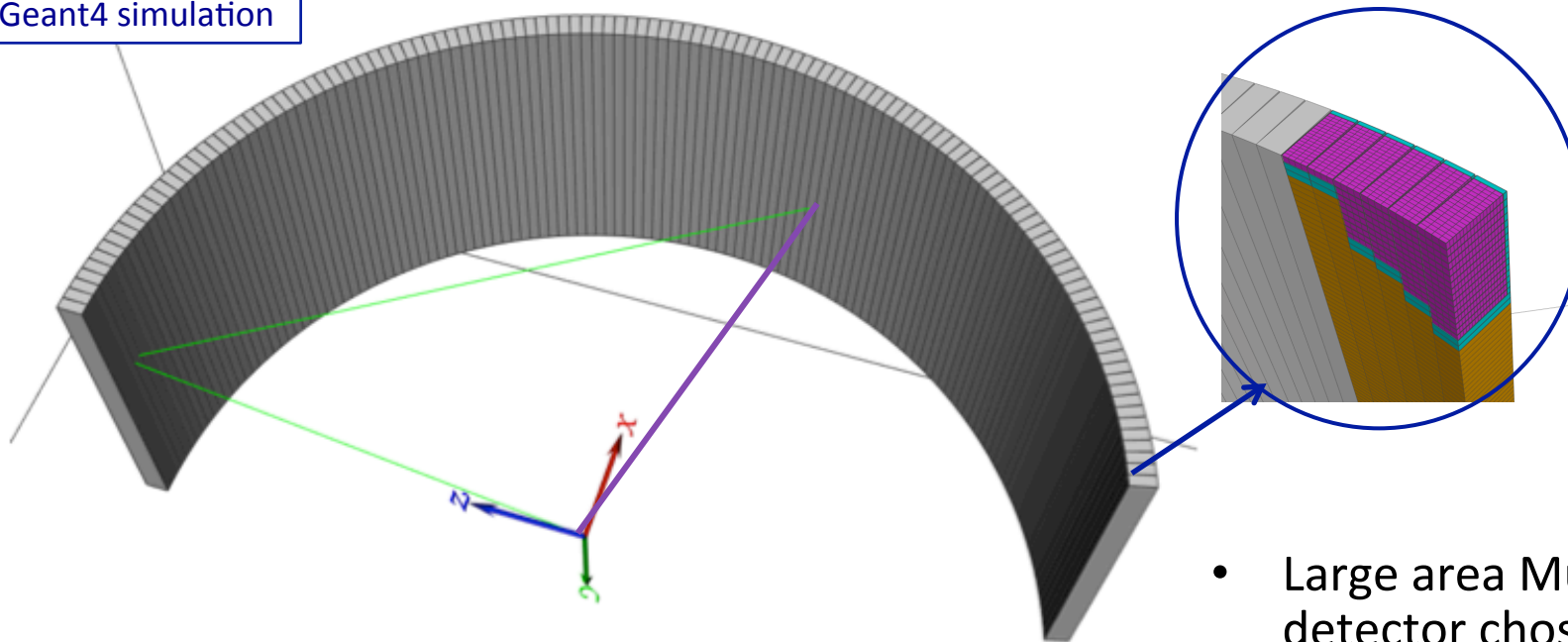
Realistic simulation



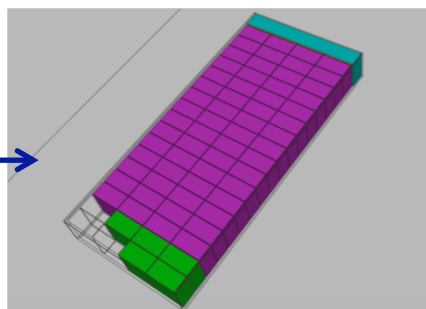
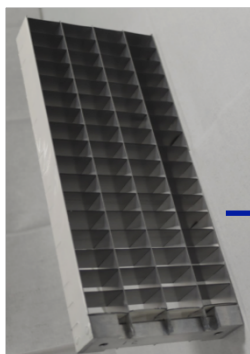
Real and measurable
neutron energy at
conversion point

Geant4 simulation

Geant4 simulation



- Large area MultiGrid detector chosen as example
- Chopper spectroscopy:
 - Low background is essential



A. Khaplanov et al.

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

Validation

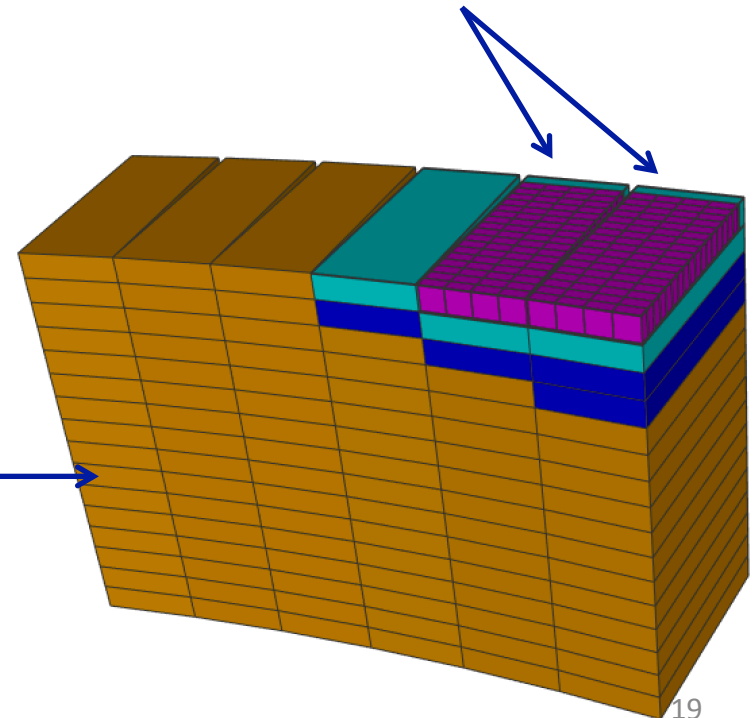
In-beam test of the Boron-10 Multi-Grid neutron detector at the IN6 time-of-flight spectrometer at the ILL

A. Khaplanov et al.

<http://iopscience.iop.org/article/10.1088/1742-6596/528/1/012040/pdf>

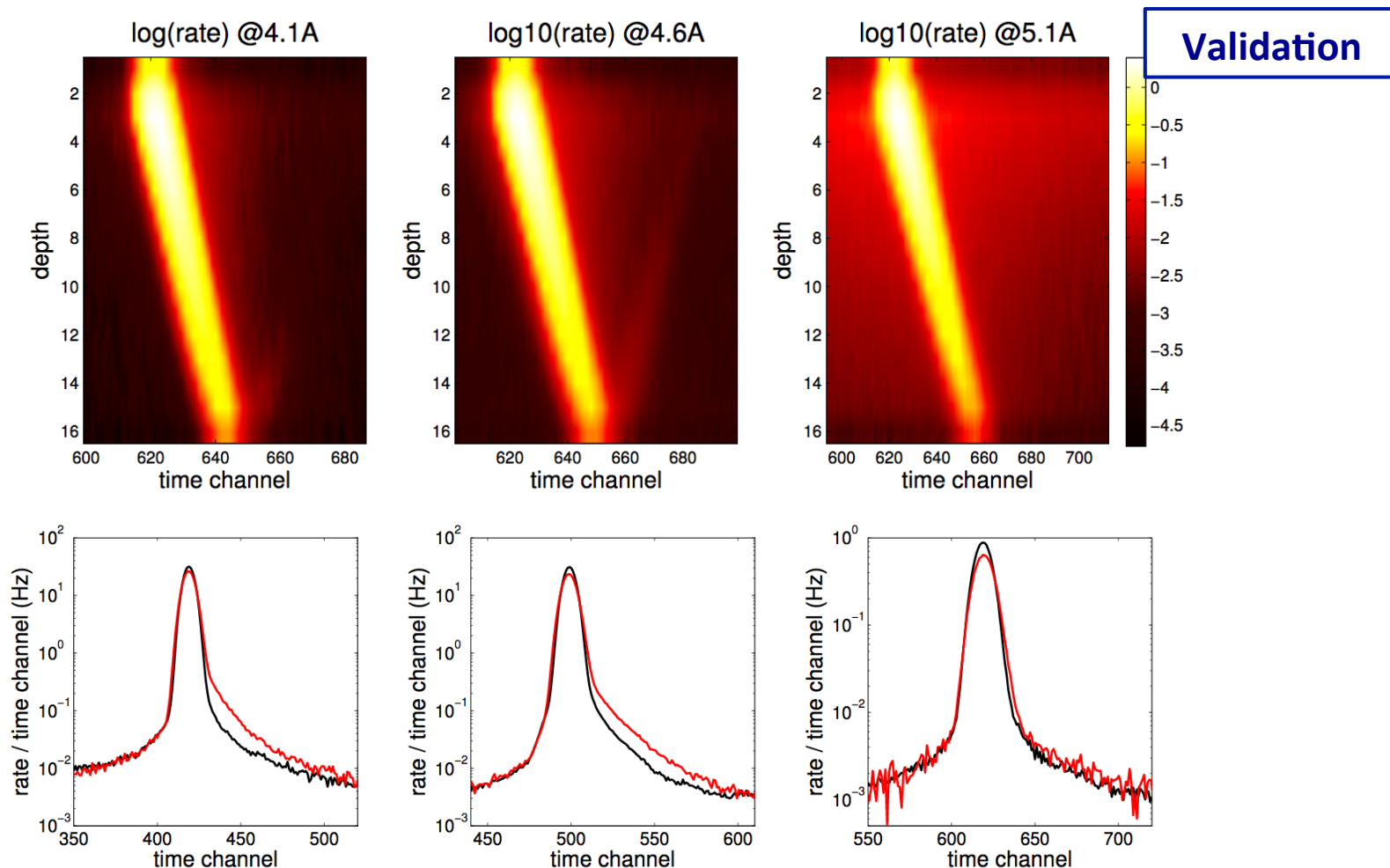


No shielding on the rear wall of grids



MultiGrid detector test at ILL

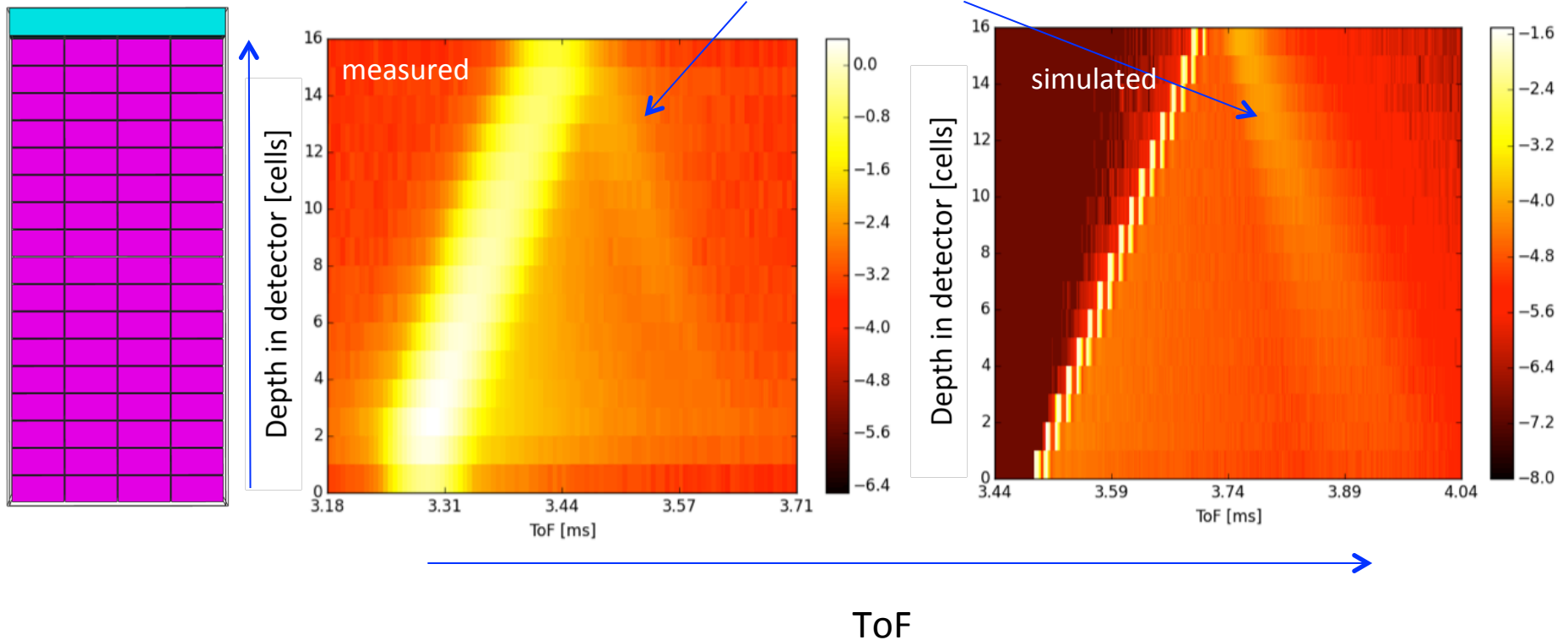
Measured data (ToF, depth of detection)



Geant4 simulation

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

Validation



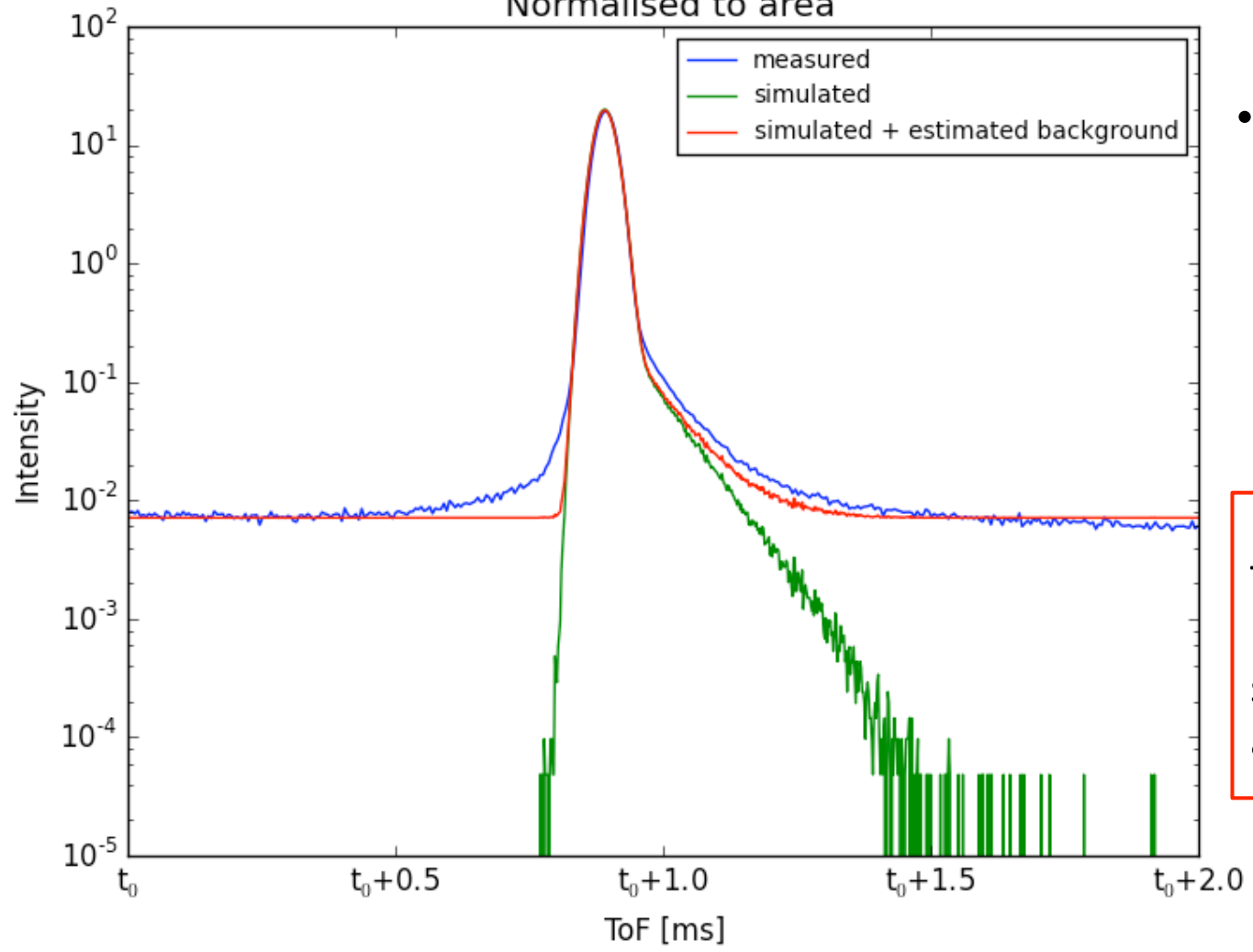
Measured ToF-depth characteristic and backscatter phenomena reproduced with simulation at 4.1 and 4.6 Å

MultiGrid detector test at ILL

Measured and simulated ToF spectra

Geant4 simulation


Measured and simulated tof spectra at 4.6 Å
Normalised to area



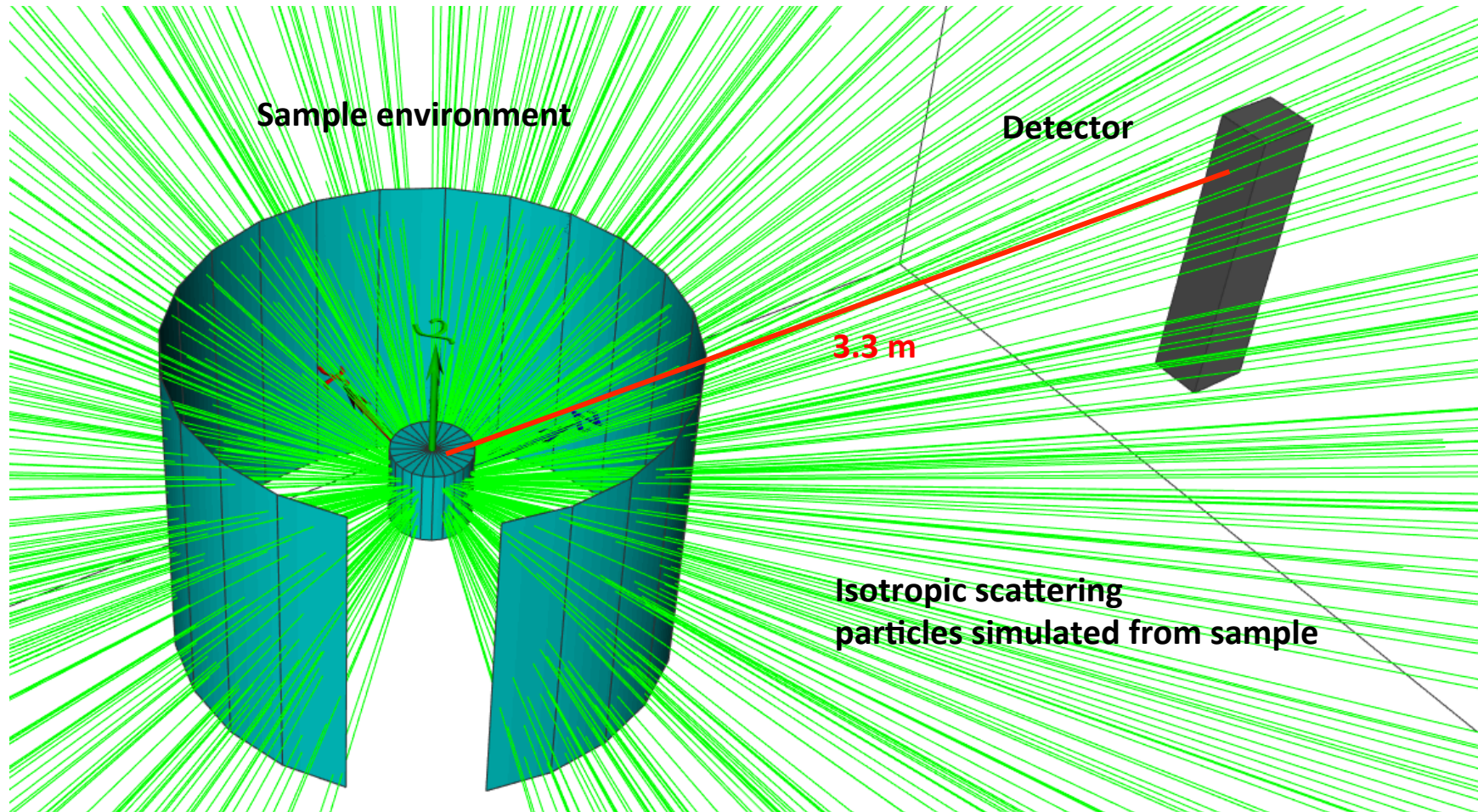
Validation

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

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

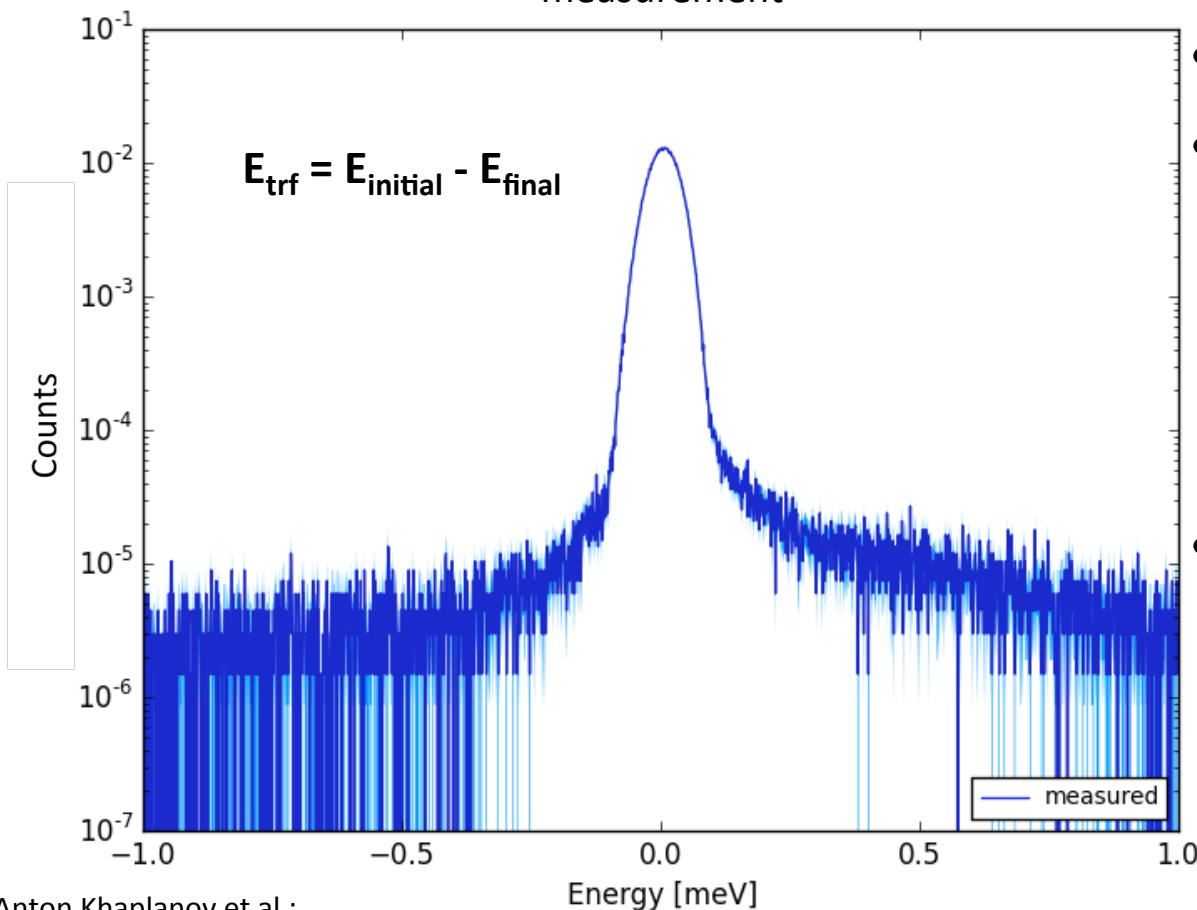


Geant4 simulation



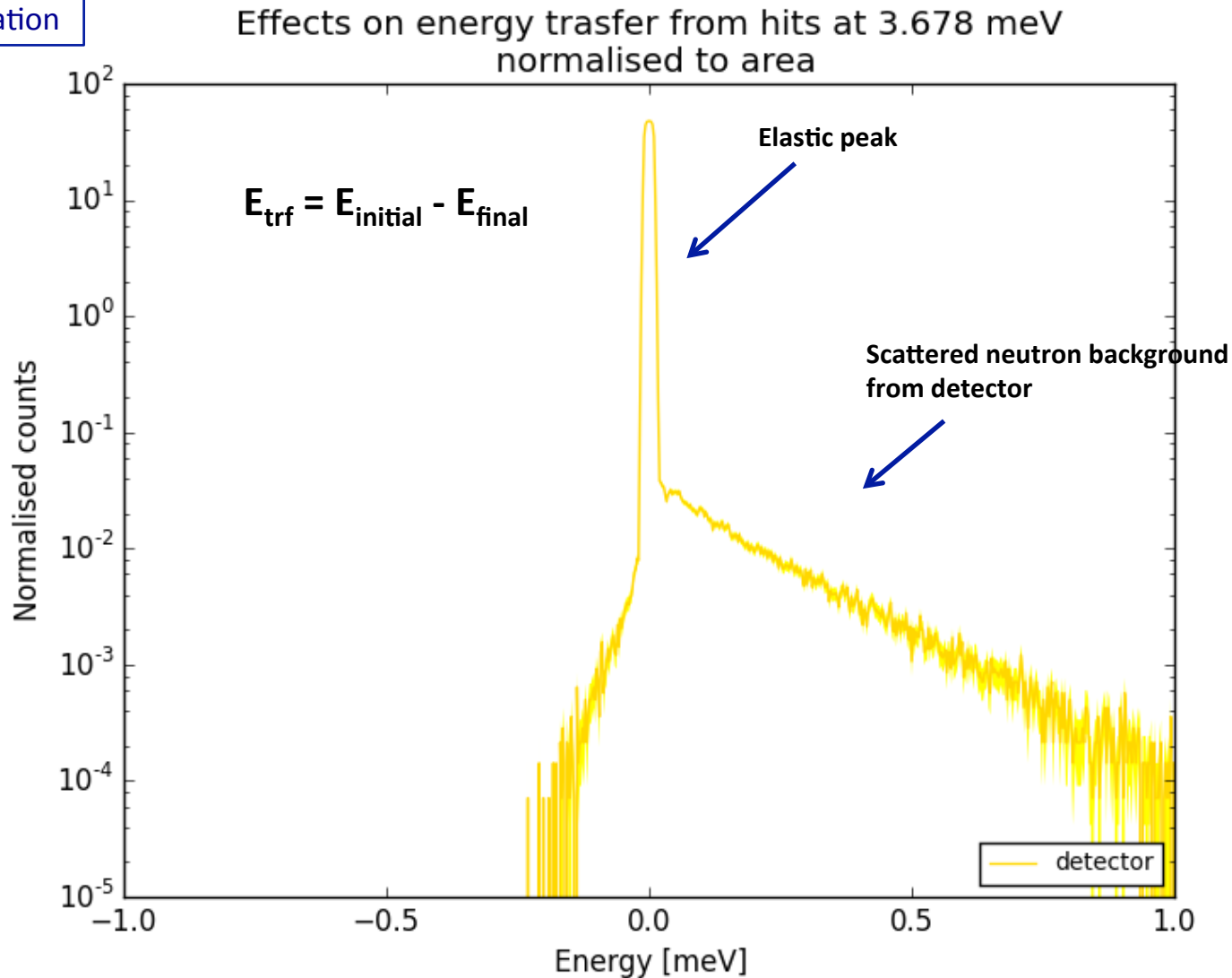
Derived energy transfer at 3.678 meV from
measurement

See Anton Khaplanov's talk
Today 12:10 (Detectors 1)

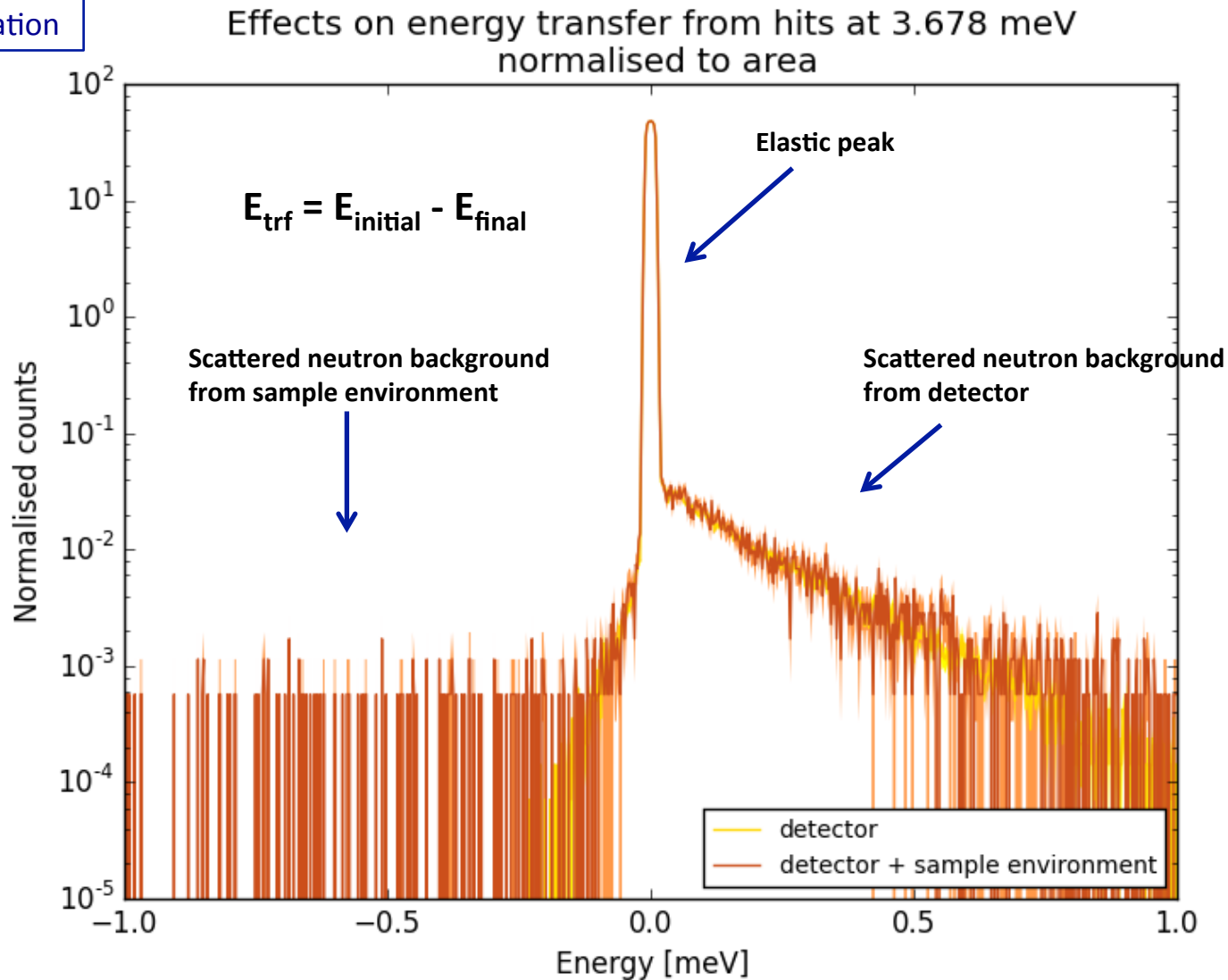


- Chopper spectroscopy
 - Measured quantities:
 - ToF
 - detection-coordinates
- ↓
- Energy transfer:
 $E_{\text{trf}} = E_{\text{initial}} - E_{\text{final}}$

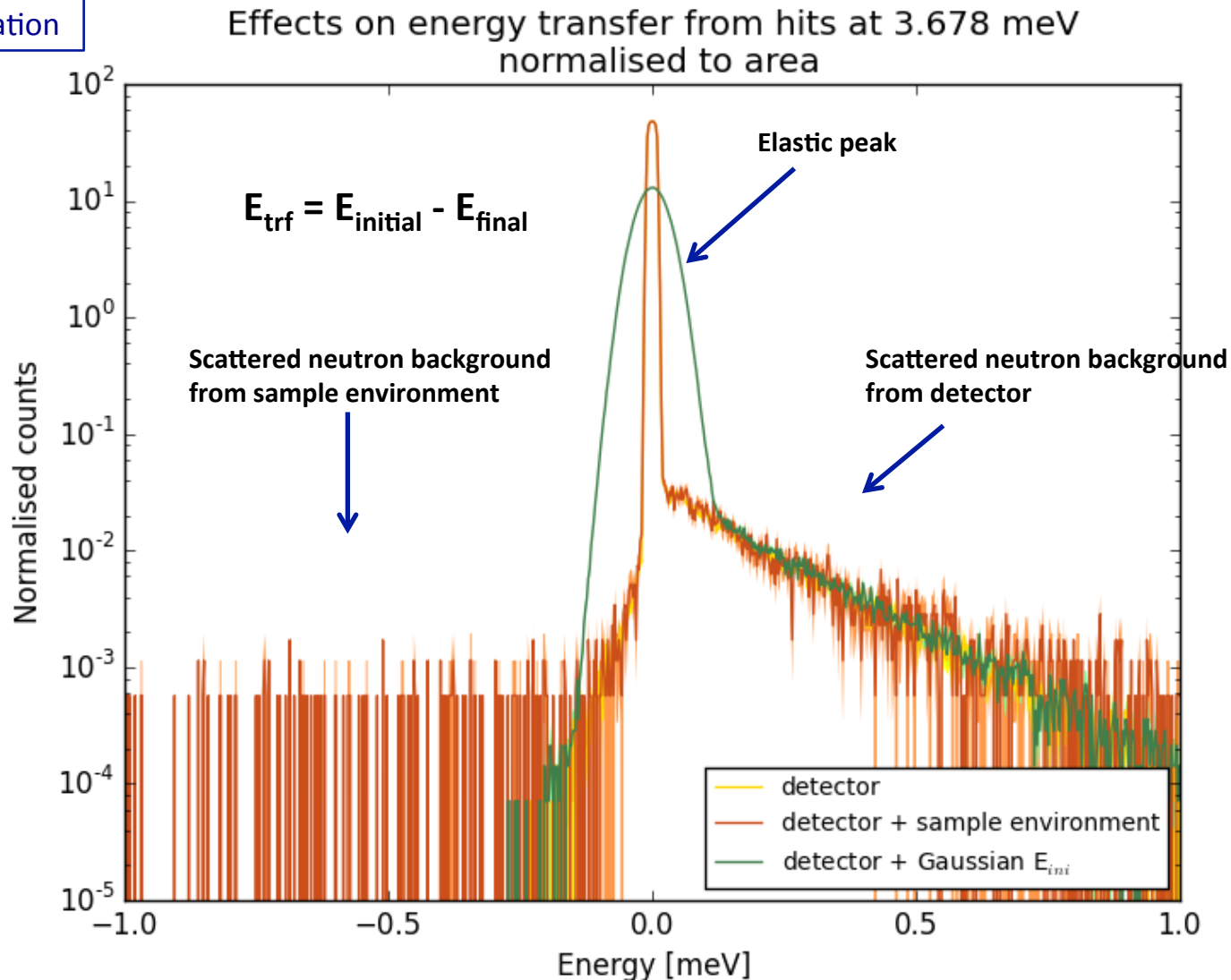
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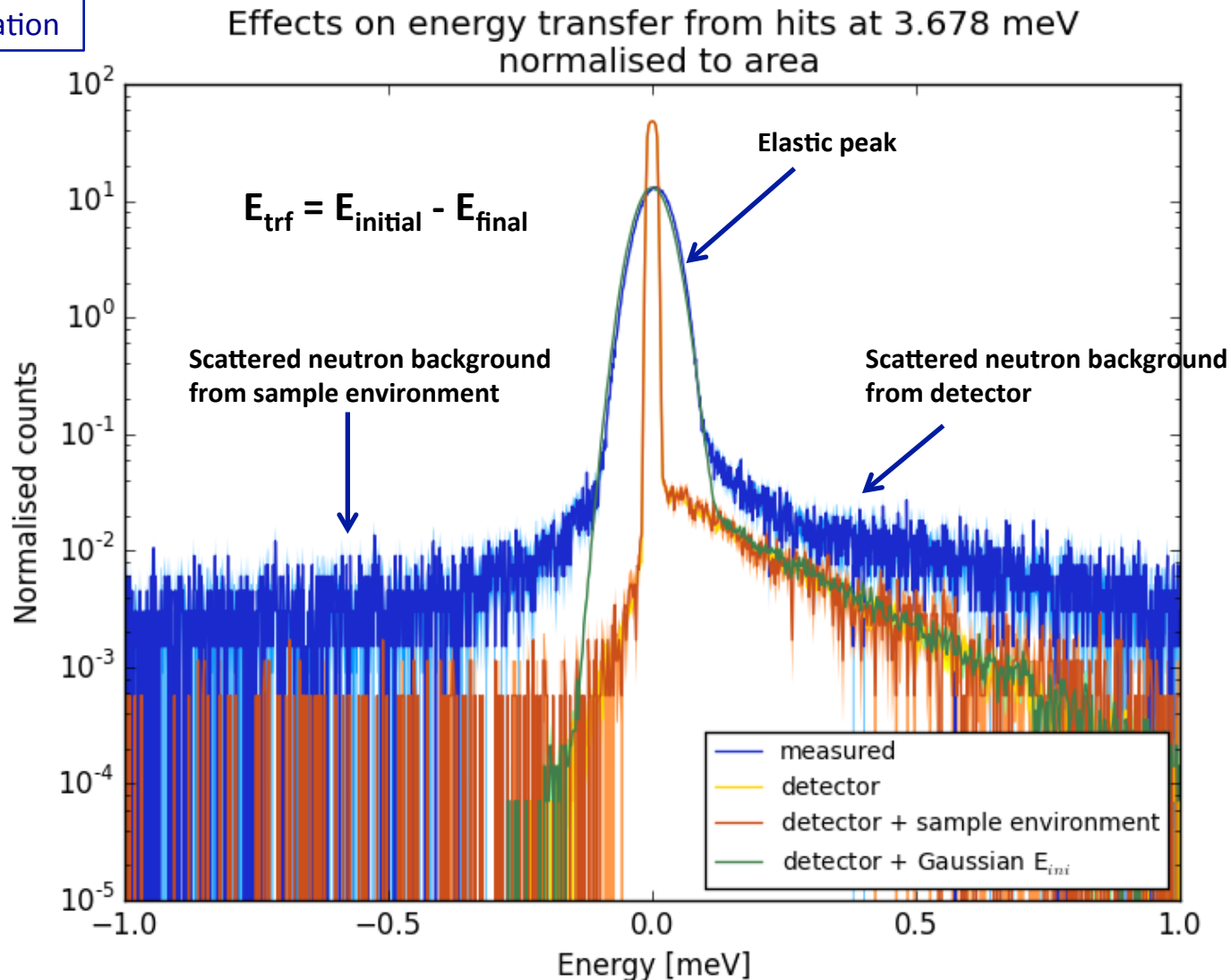
Geant4 simulation

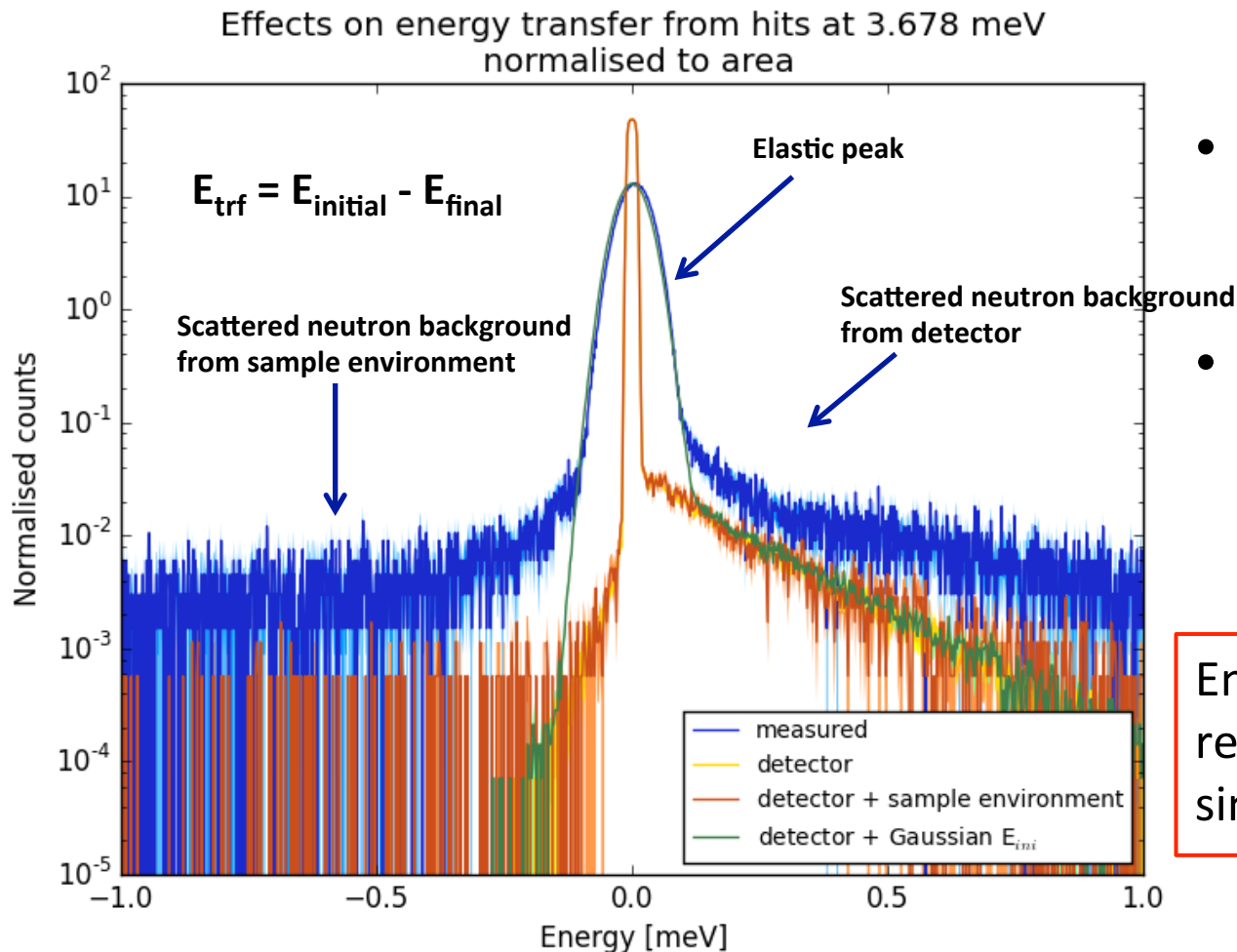


Geant4 simulation



Geant4 simulation



**Validation**

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

Energy transfer reproduced with simulation at 3.678 meV



Summary

- **Great progress in neutron scattering simulation**
 - **Improved modeling** for neutron scattering on crystalline material (NXSG4, NCrystal)
 - **Effective particle interchange** (MCPL)
 - Easy to combine MC codes
 - ESS Coding Framework, where all tools are combined

↓

 - **Full-scale instrument** simulation can be done with a single application



**A powerful neutron
simulation toolkit
developed**

- Realistic MultiGrid model built
 - reproduced measured results from IN6 and CNCS experiments
- Ready to use for optimisation



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

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Use the Force, Luke!



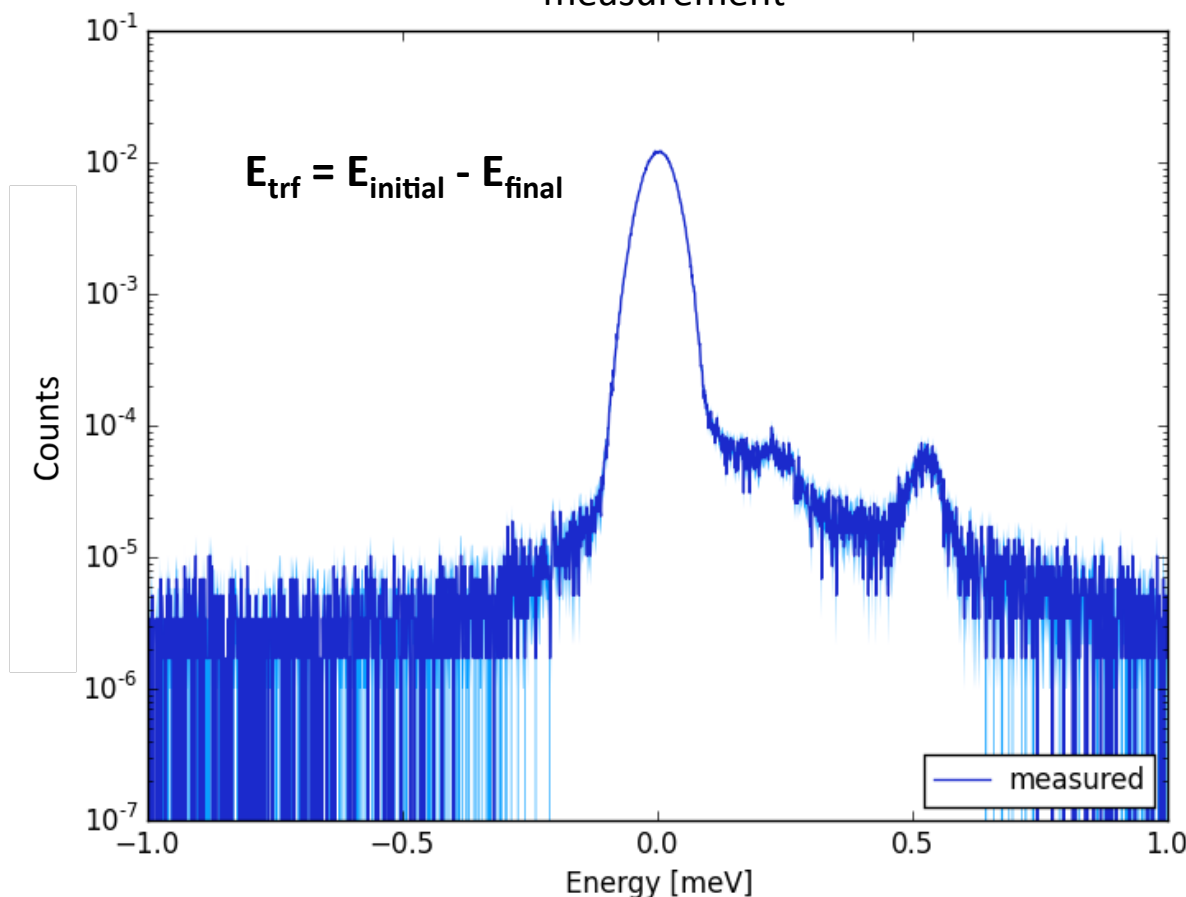
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Thank you for your
attention!



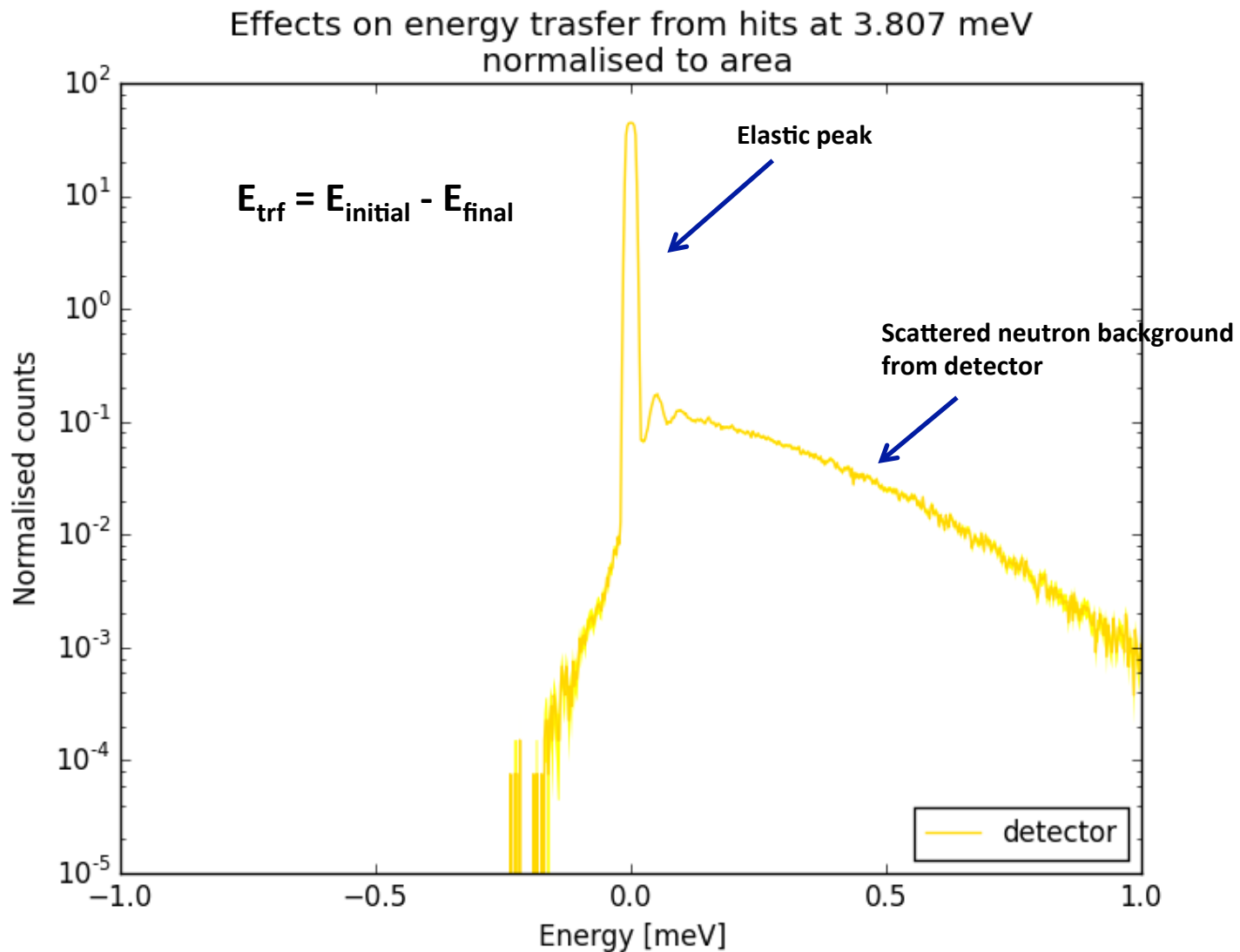
**Thanks to the collaborators for all the prepared
tools and materials,
and for making my life easier!**

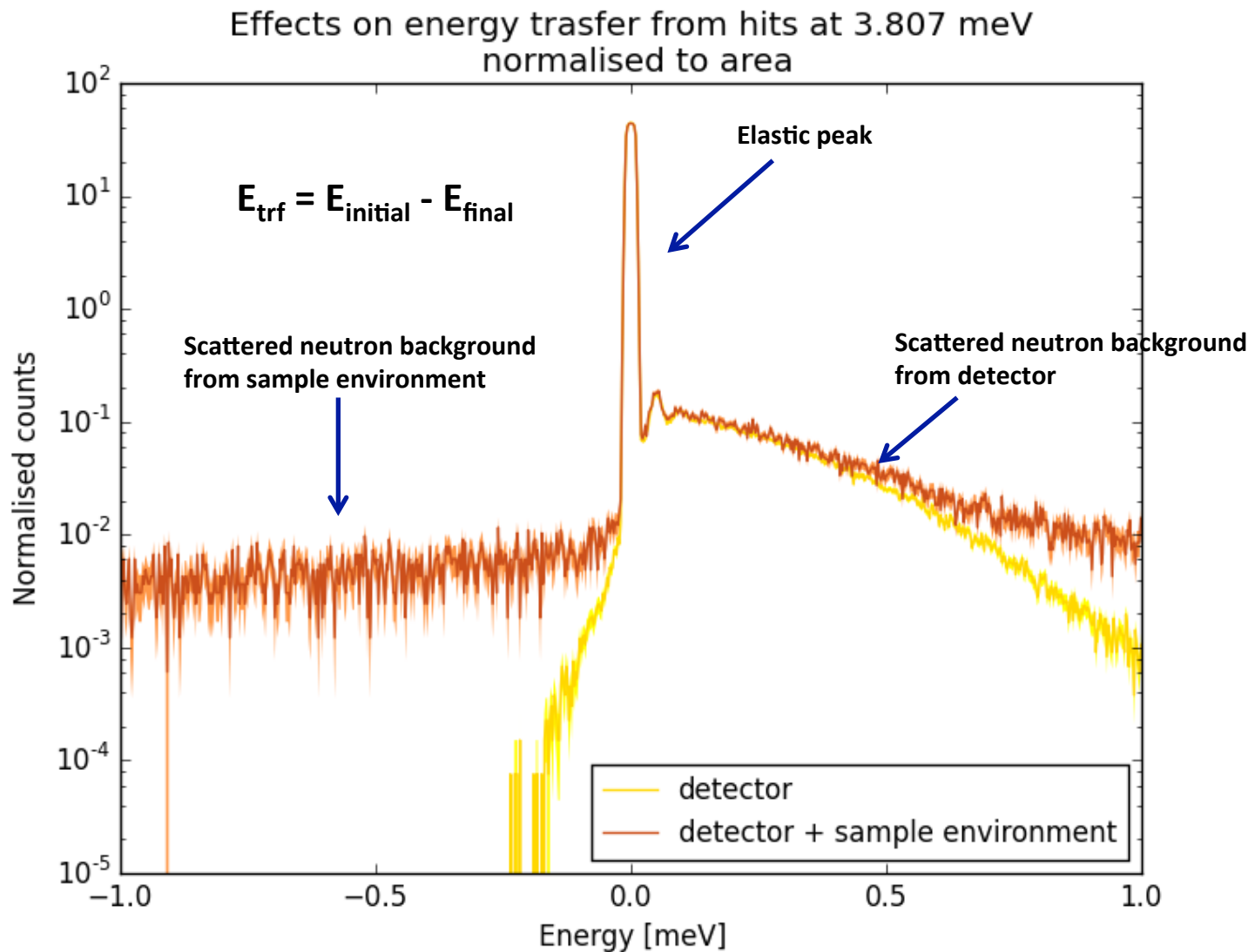
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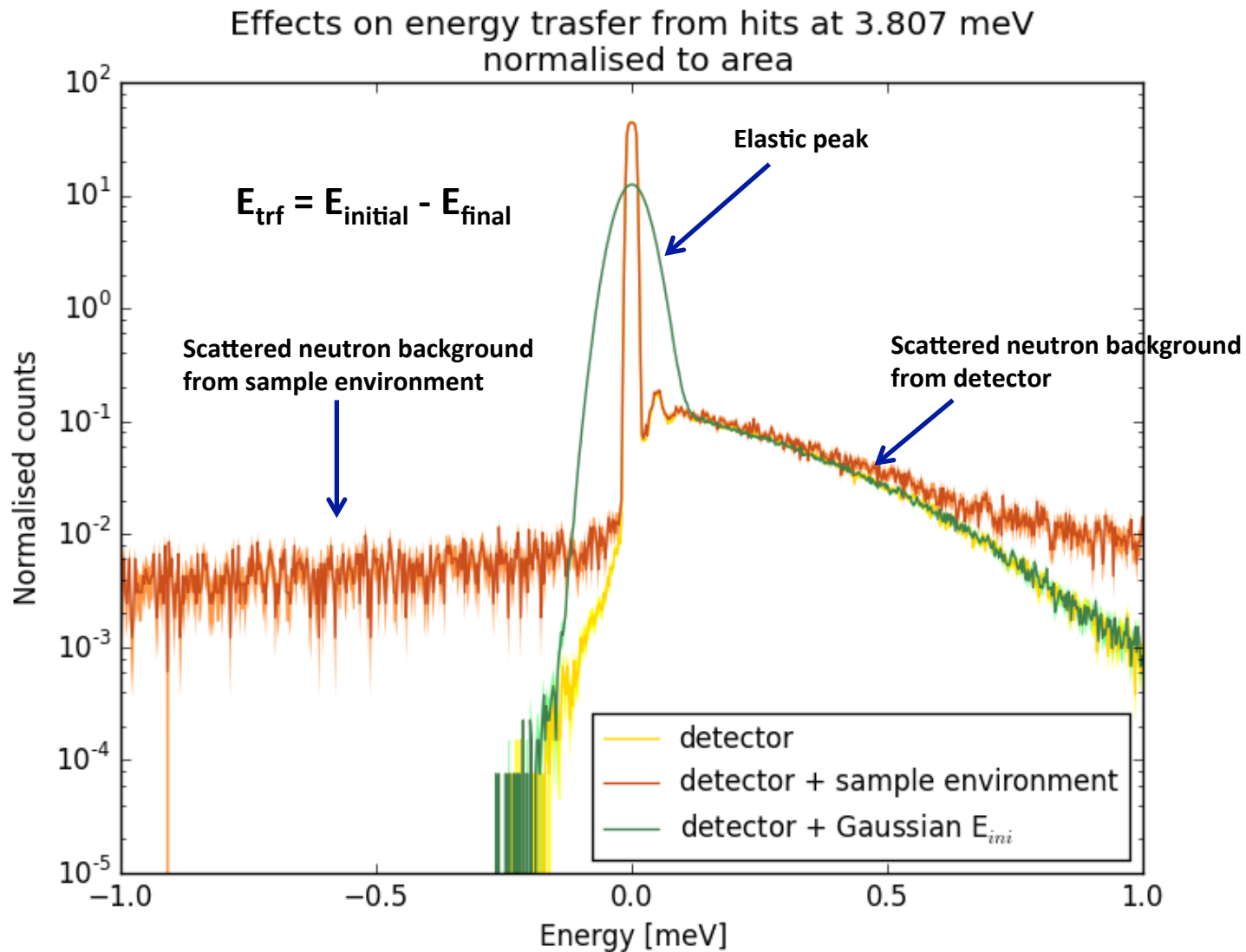


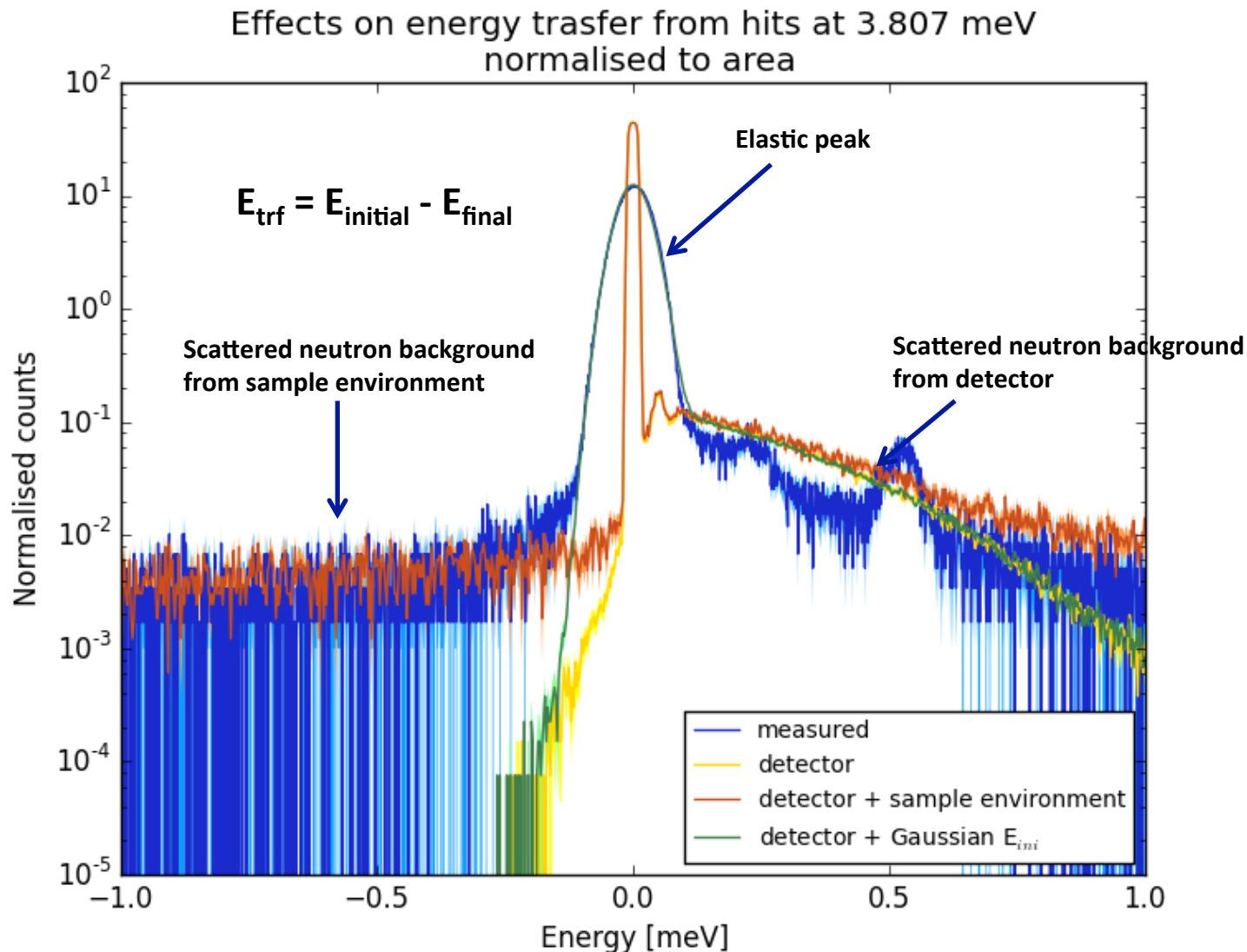
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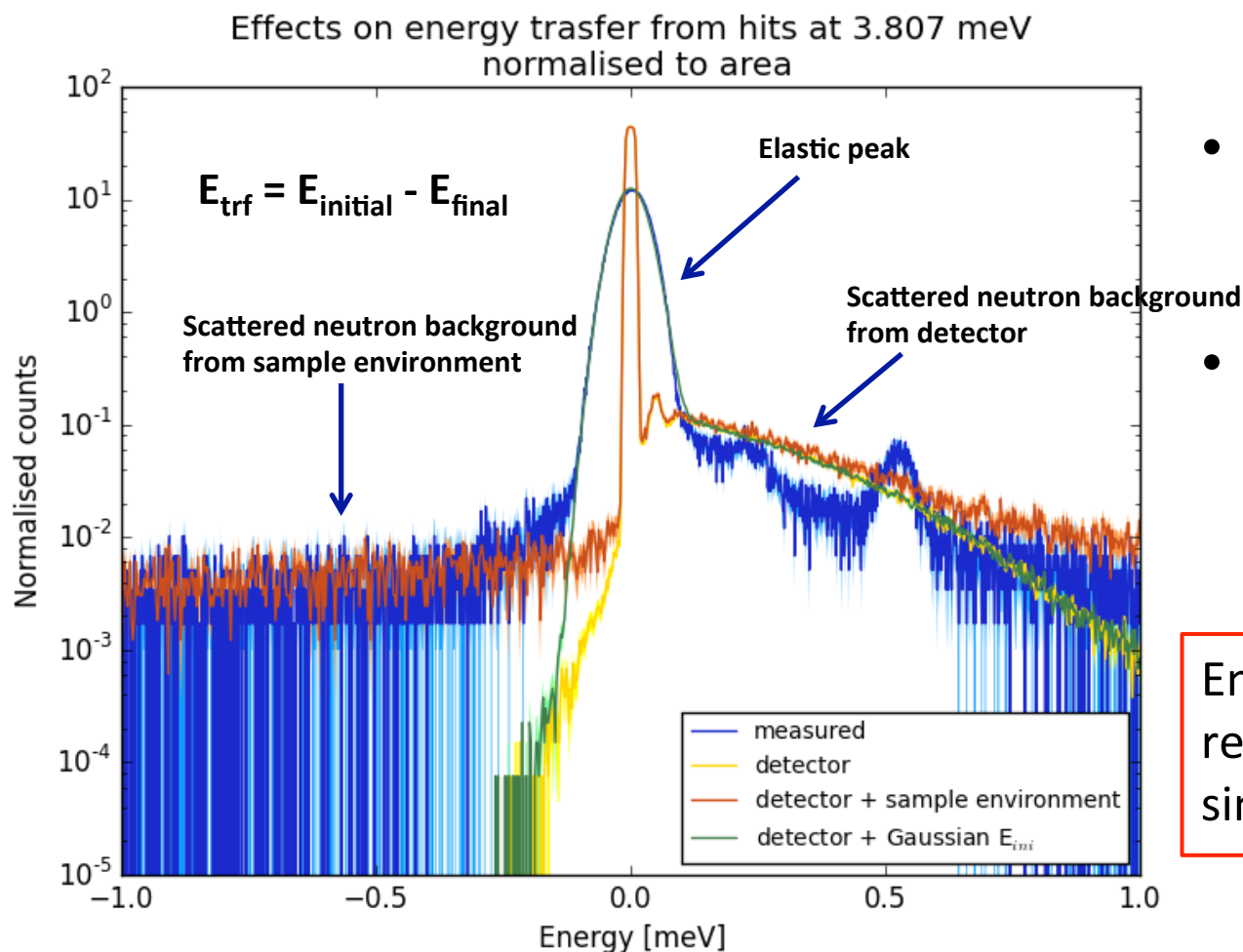
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