Monte Carlo Simulations for Defining a Future Standard in Neutron Instrumentation

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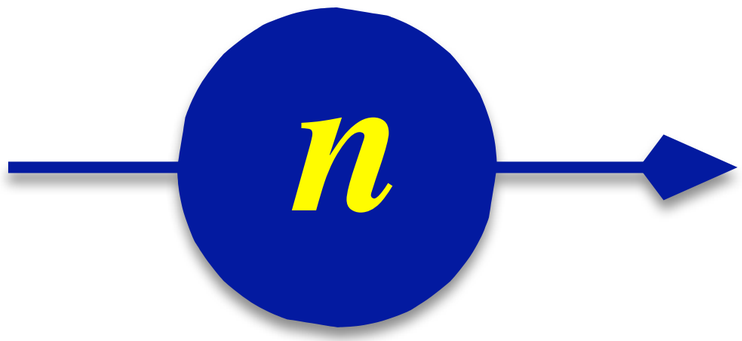
McStas

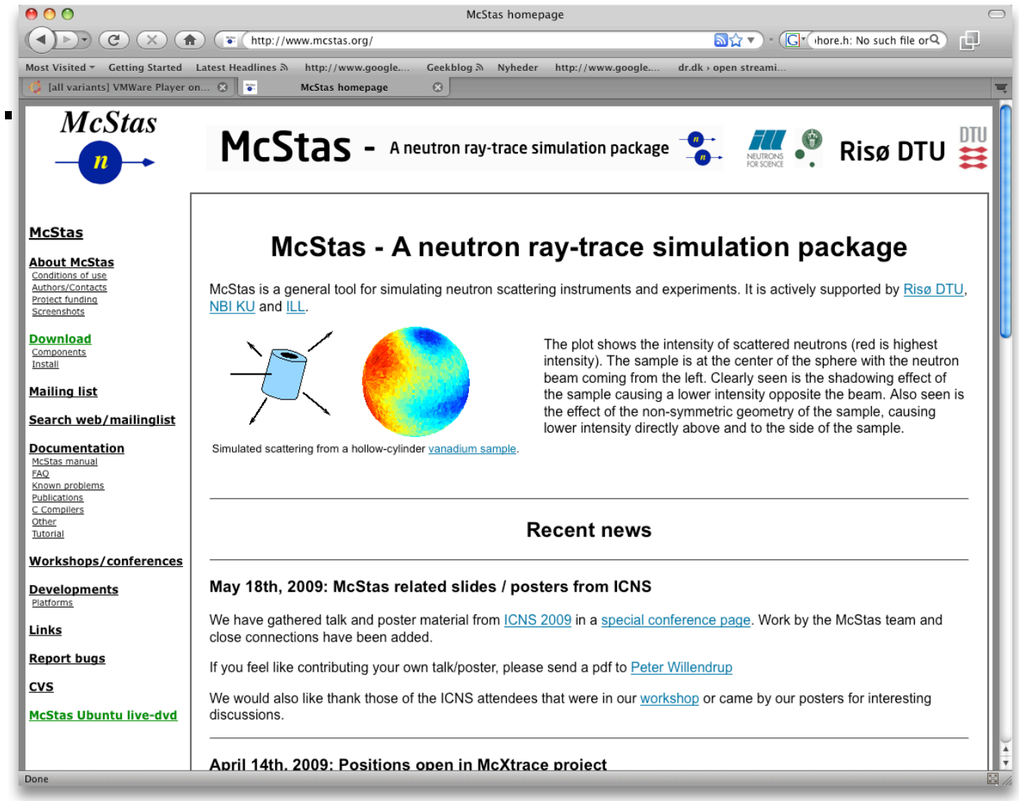


Agenda

- Brief McStas overview
- Validation strategies
  - Virtual experiments
  - Code intercomparisons
  - Validation experiments
- A future Instrumentation standard

McStas Introduction

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at RISØ DTU, KU and ILL, Grenoble.
- V. 1.0 by K Nielsen & K Lefmann (1998)
- Currently 2.5+1 people full time plus students



GNU GPL license
Open Source

Project website at
http://www.mcstas.org

neutron-mc@risoe.dk mailinglist

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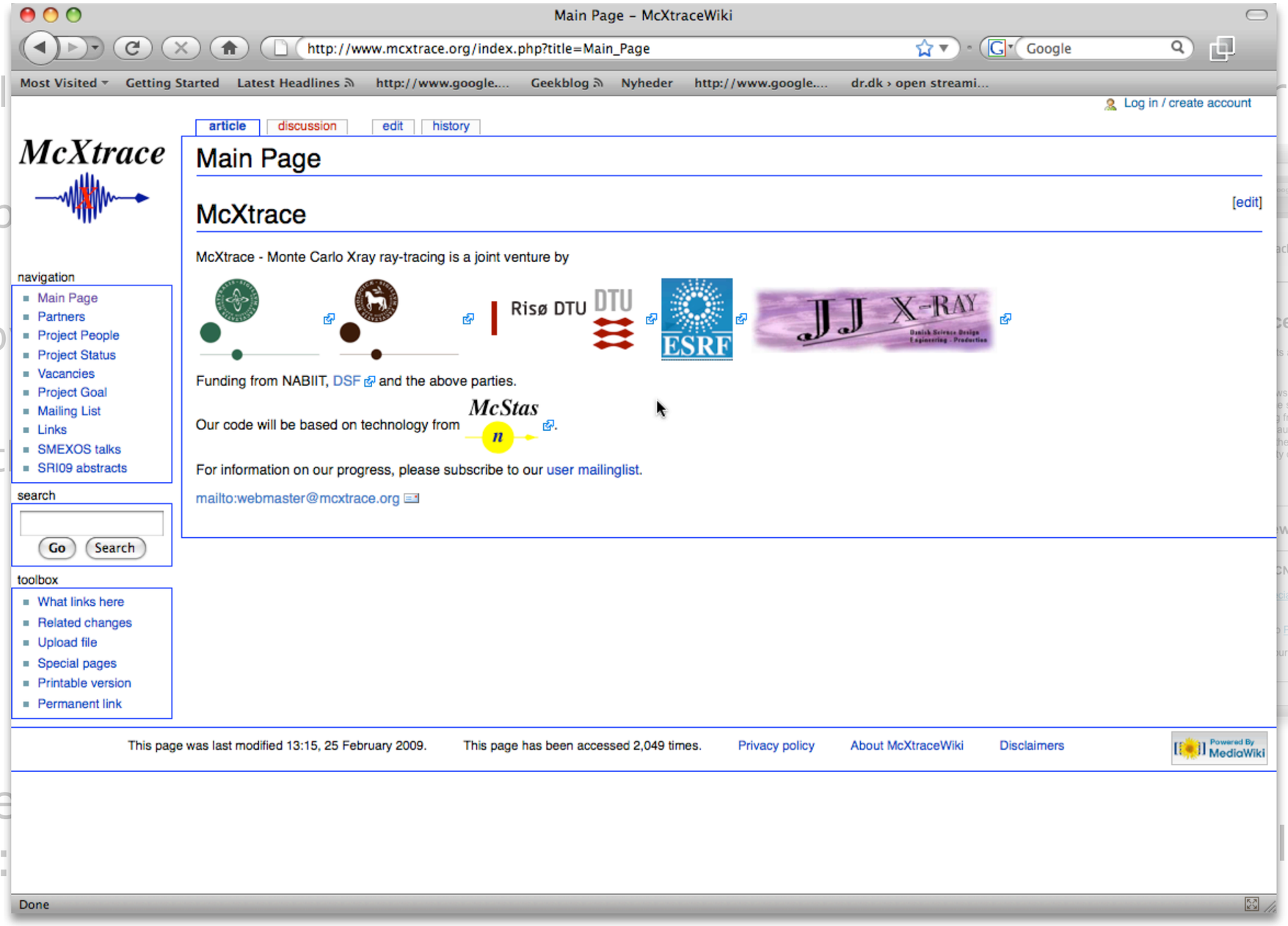
McStas Introduction

McXtrace - new startup (2009) in X-ray sim

- Flexible, general simulation utility for neutron scattering experiments.
- Original
- Develop
- V. 1.0 b
- Current

Proje
http:



list

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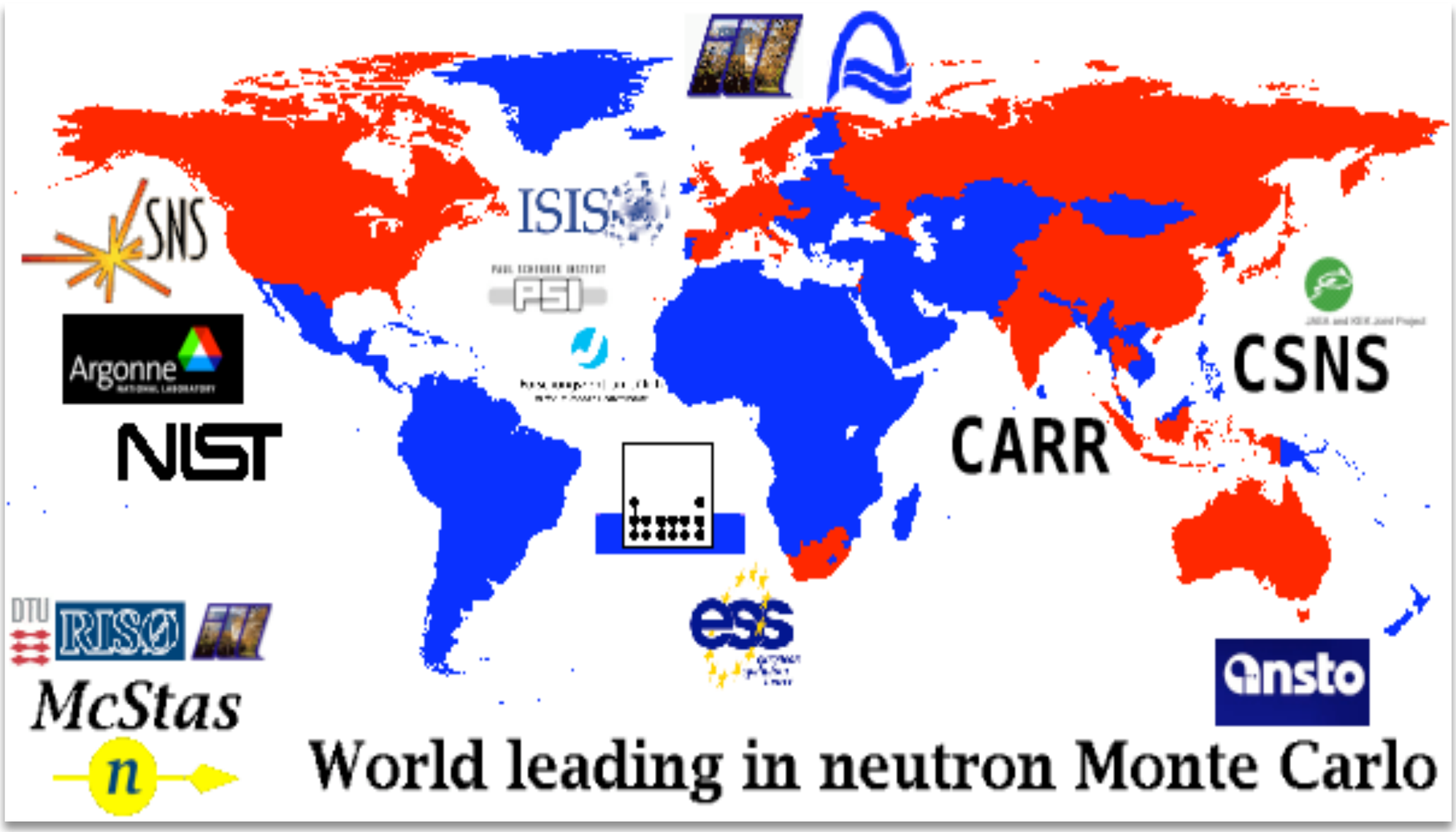
McStas Introduction

- Used at all major neutron sources



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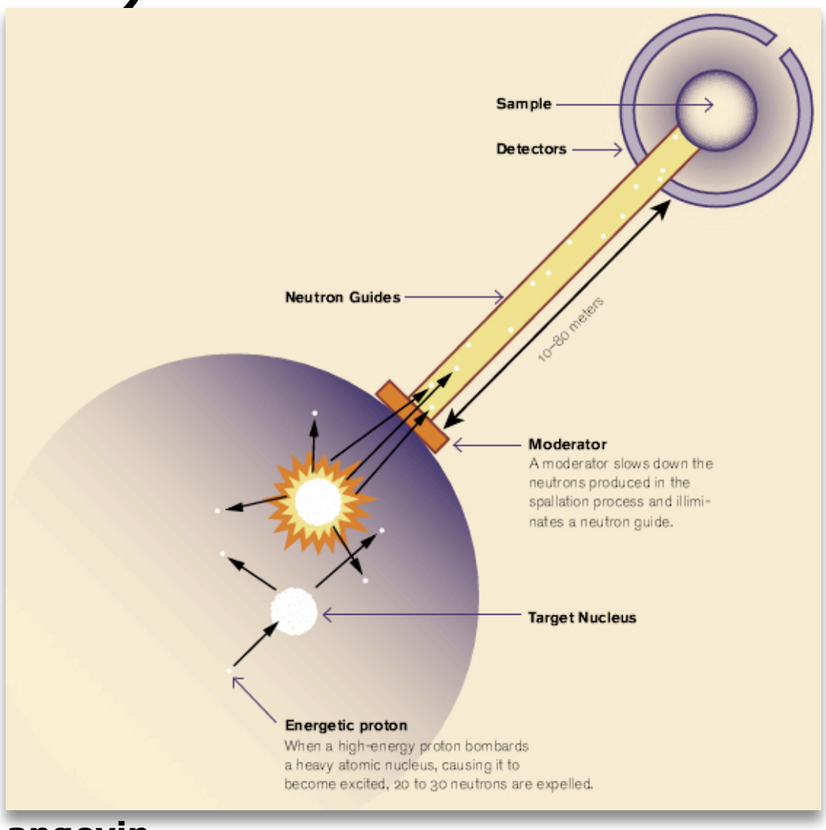
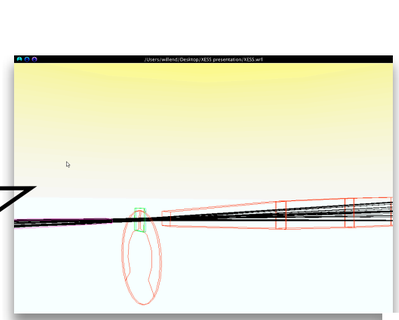
McStas overview

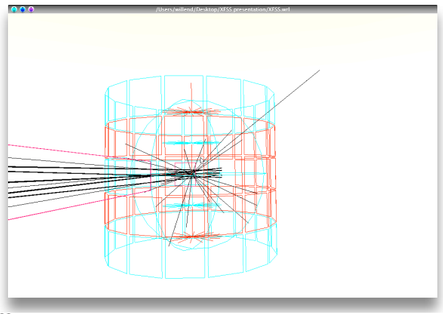
- Portable code (Unix/Linux/Mac/Win32)

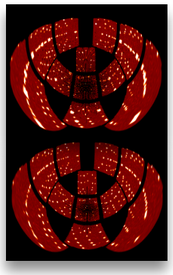
- 'Component' files (~100) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps

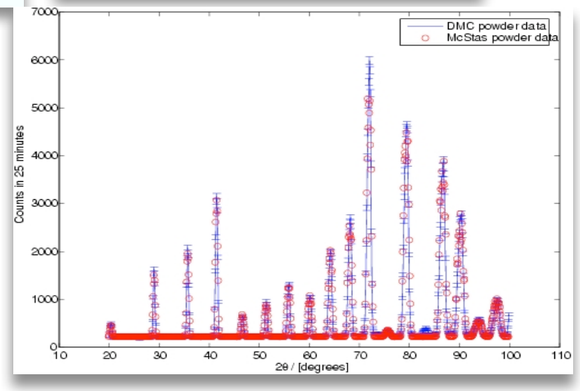


What is McStas used for?



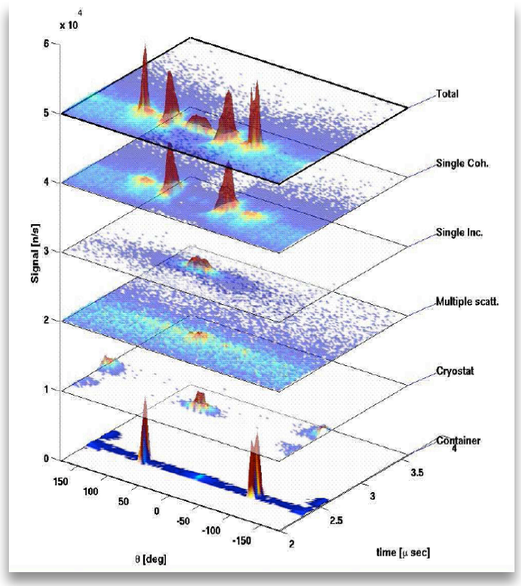


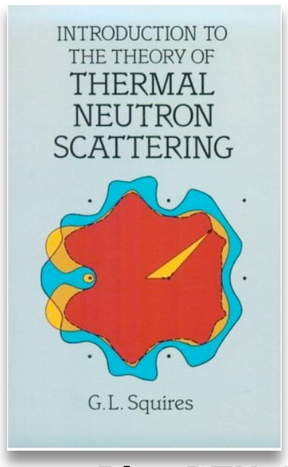


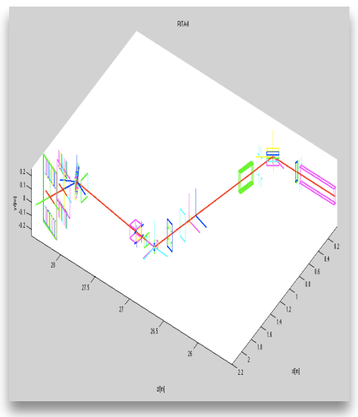


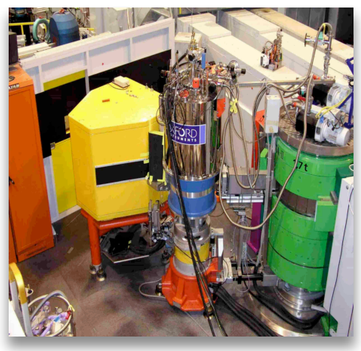
- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

(KU 2005-2009)









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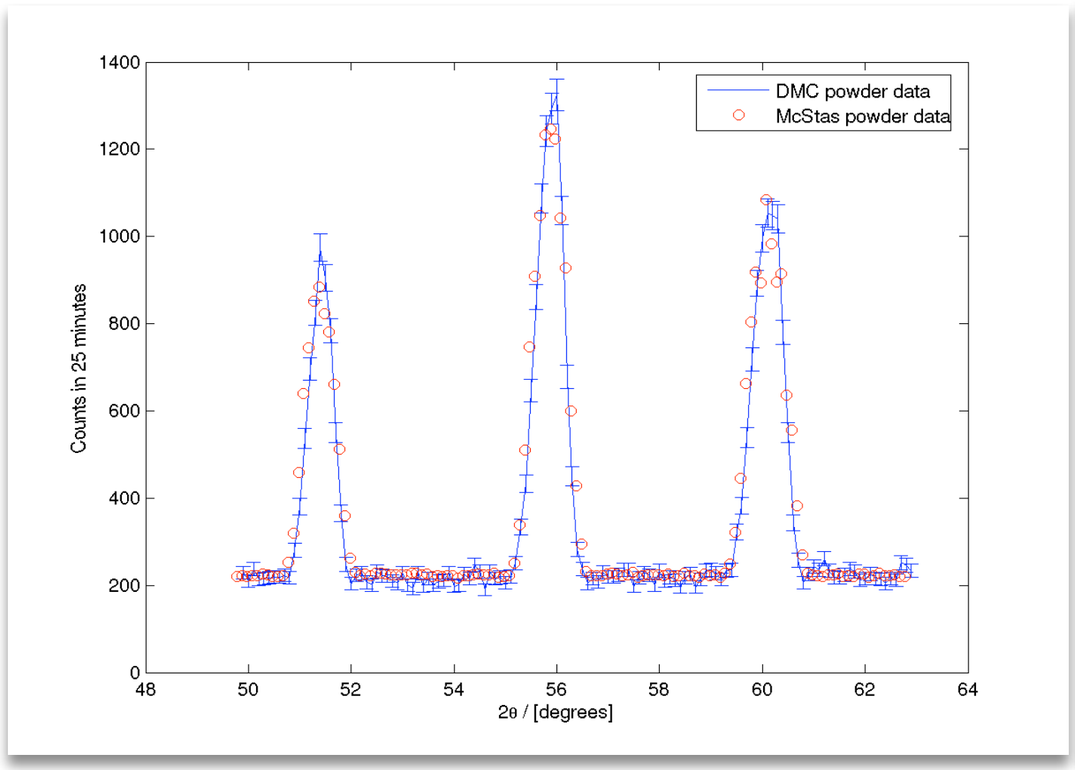
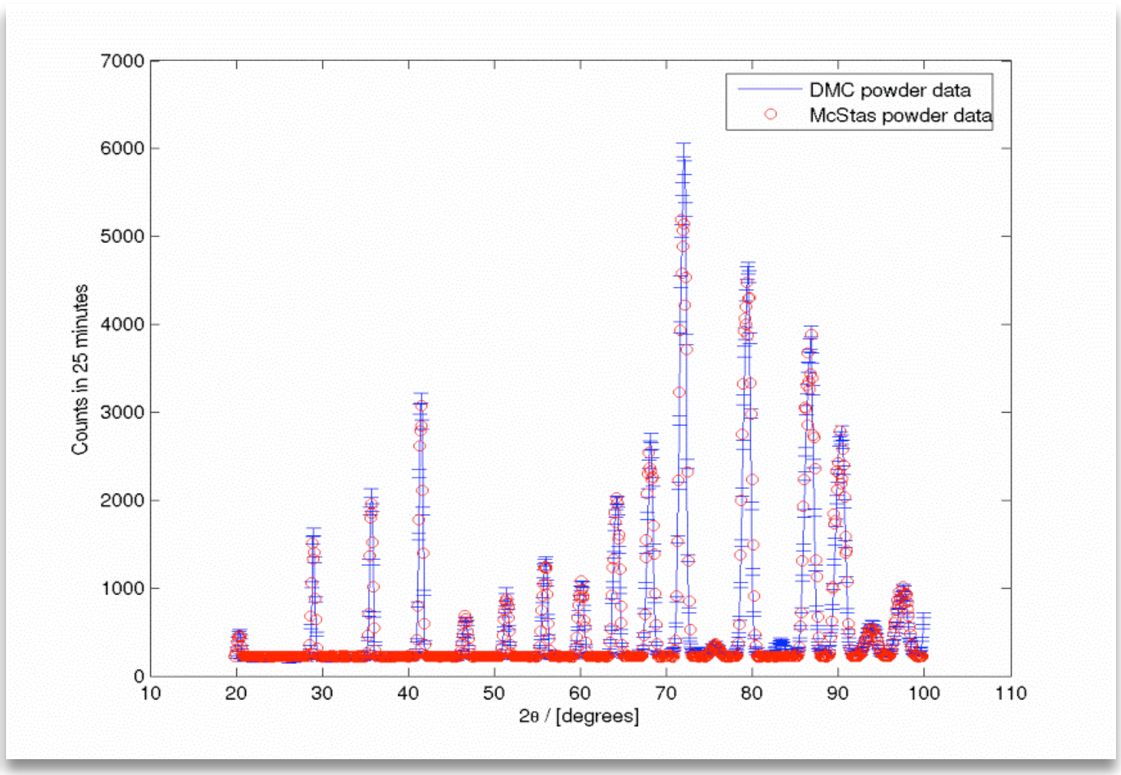
Virtual experiments, definition

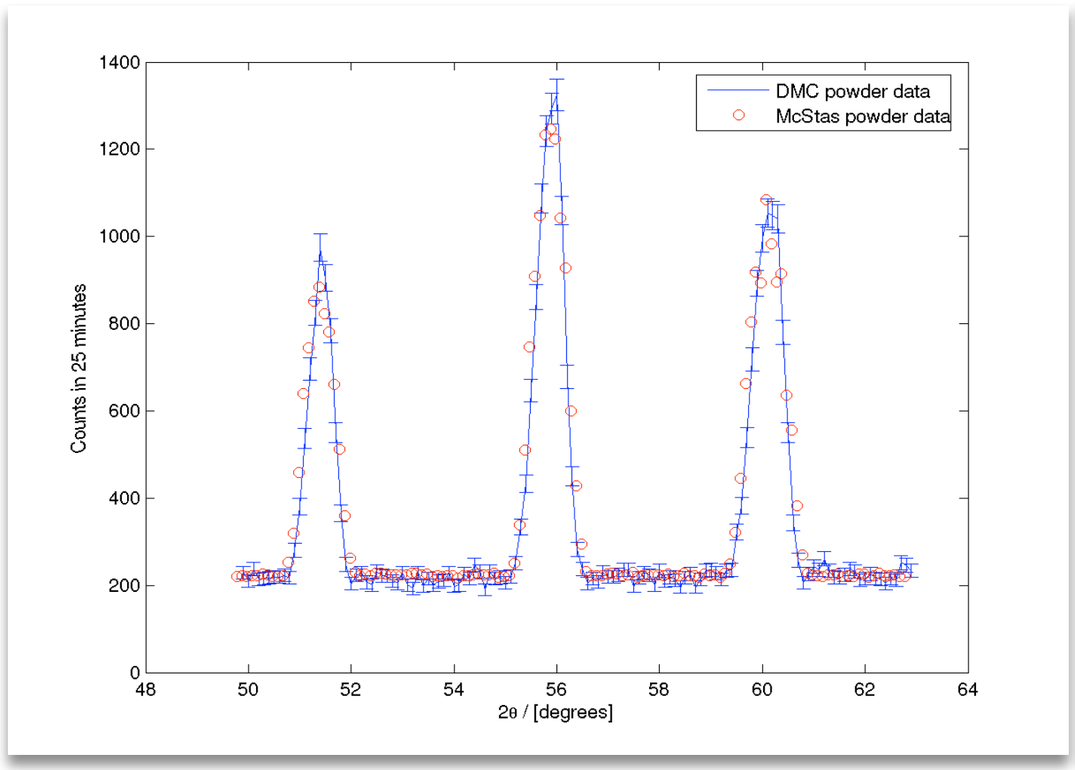
- Simulation of a complete experiment
- … from source to detector
- Ideally controlled like real experiment.
- Data analysed by ”real” analysis programs

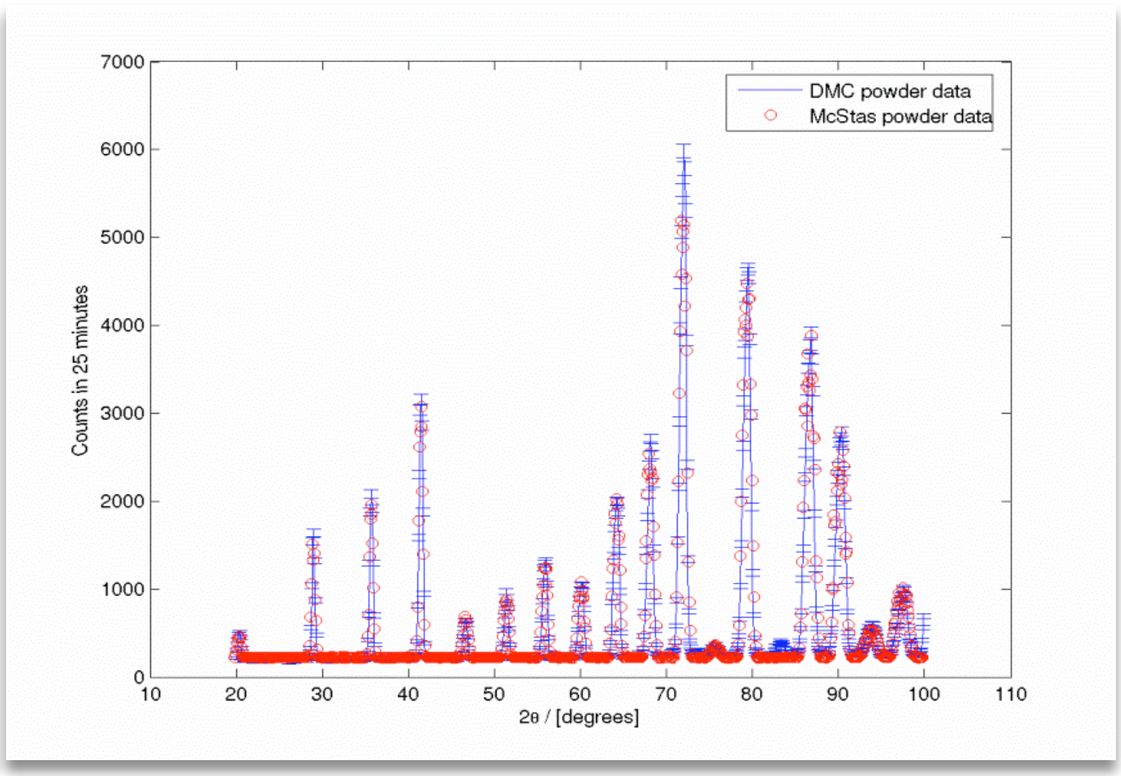




Tests and cross comparisons

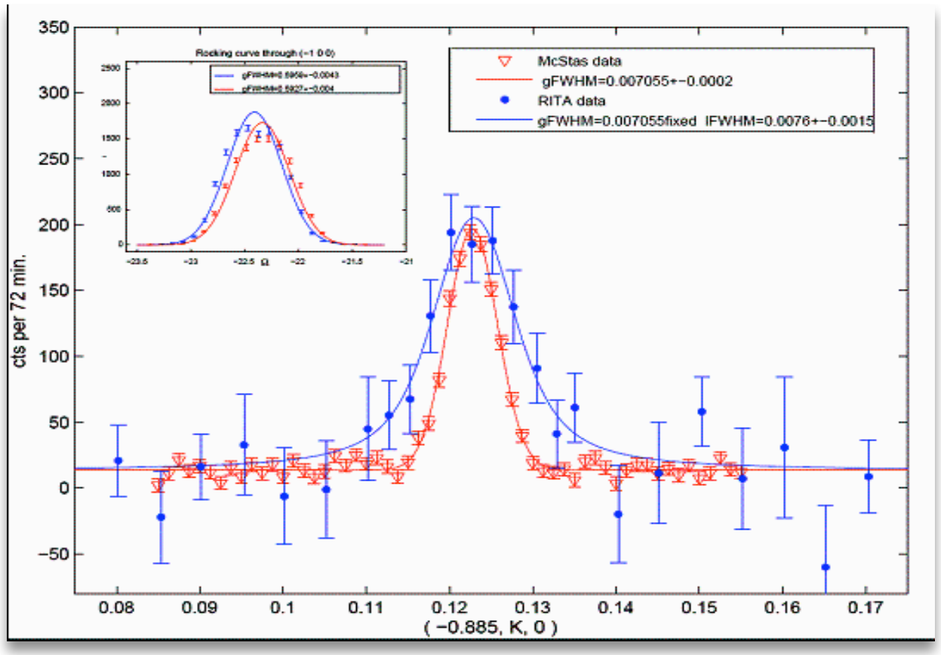
- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agree very well with other packages (NISP, VitESS, IDEAS, RESTRAX, ...)
- Experimental line shapes are within 5%
- Absolute intensities are within 10-30%
- Common understanding: McStas is reliable



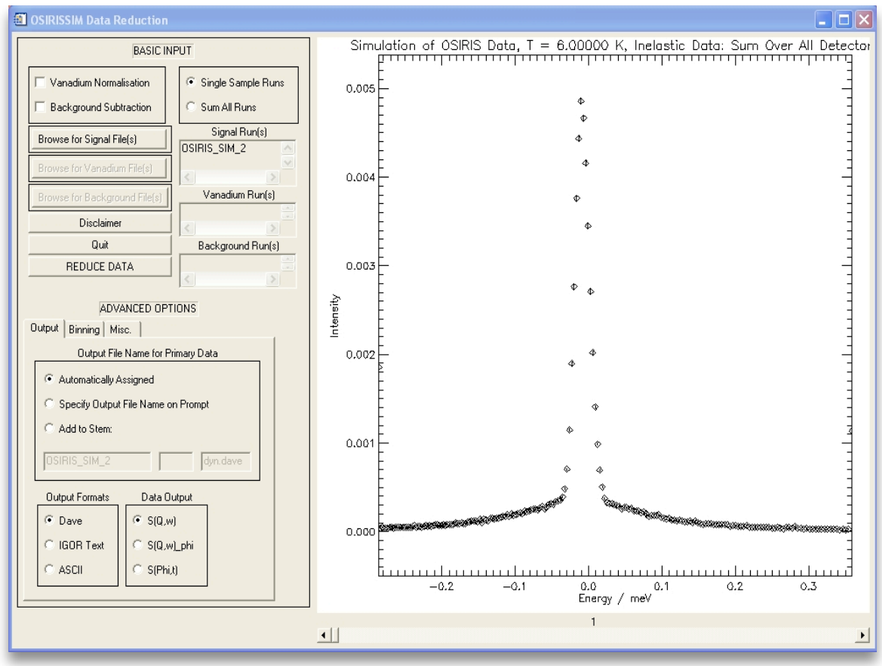


Virtual experiments, analysis

- VE data has been used to test data analysis programs
- … and to check resolution effects



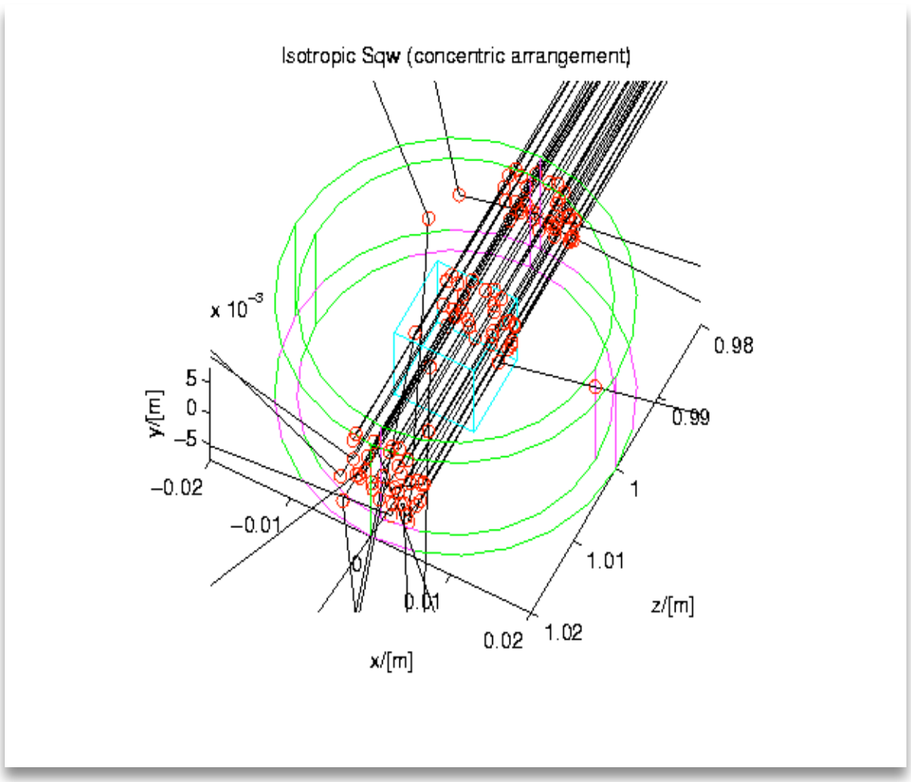
L. Udby, Risø-DTU

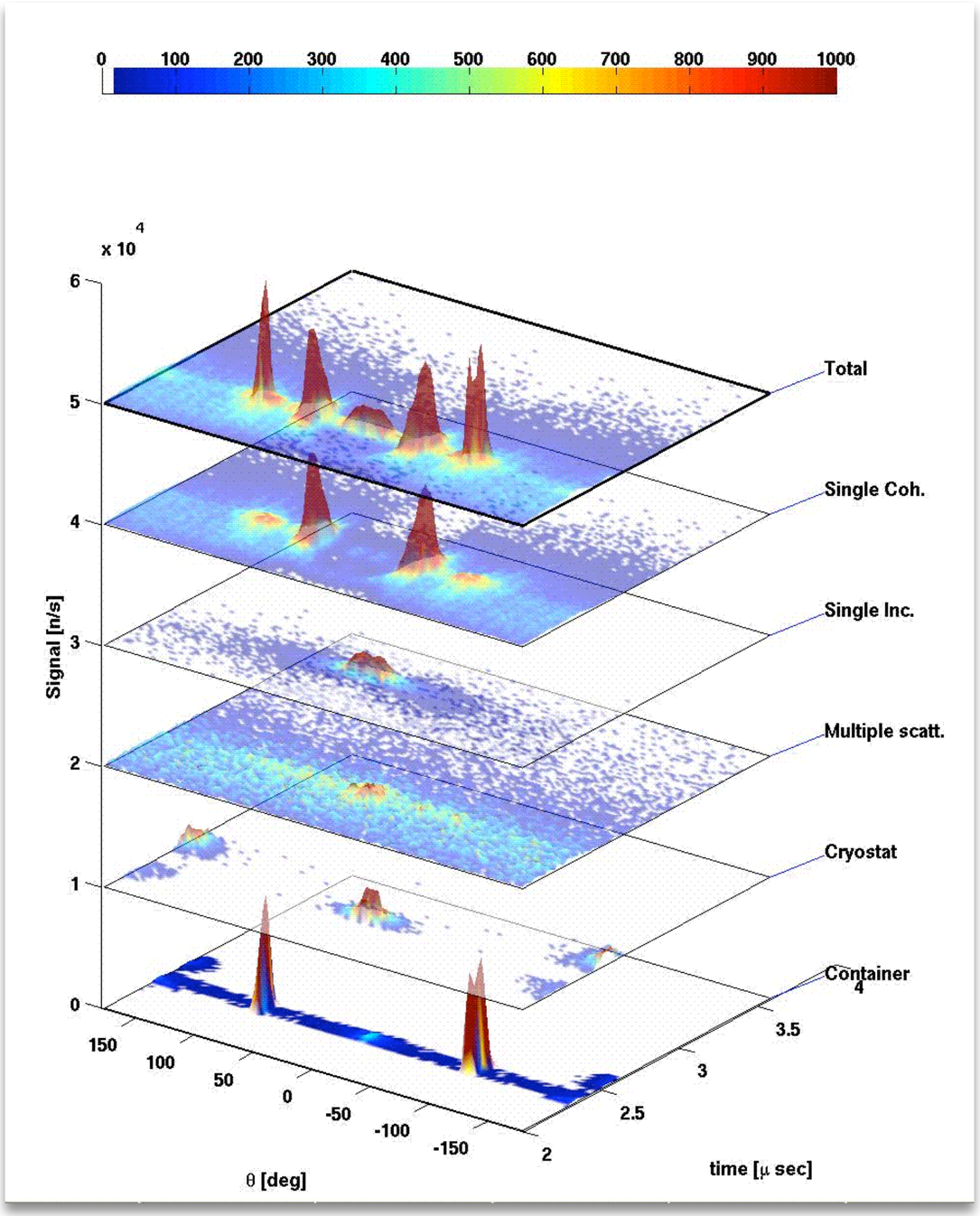


P. Tregenna-Piggott, PSI

Virtual experiments, analysis

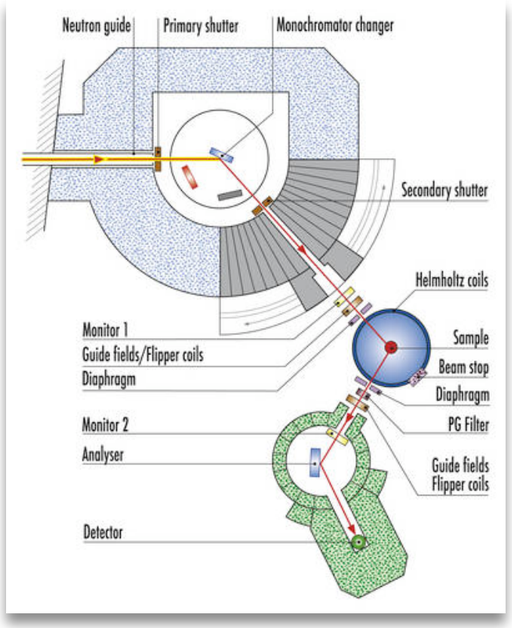
- Virtual TOF exp. at IN6, ILL
- Liquid Ge sample
- Coherent / incoherent
- Multiple scattering
- And sample environment
- All contributions can be separated by VE !

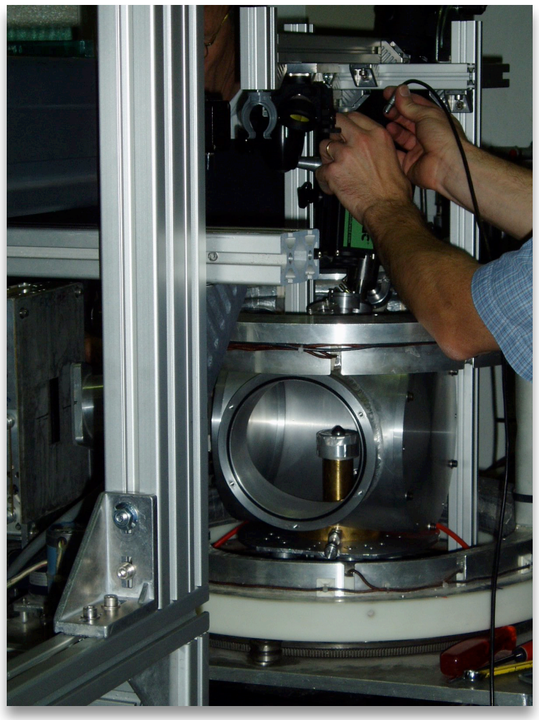


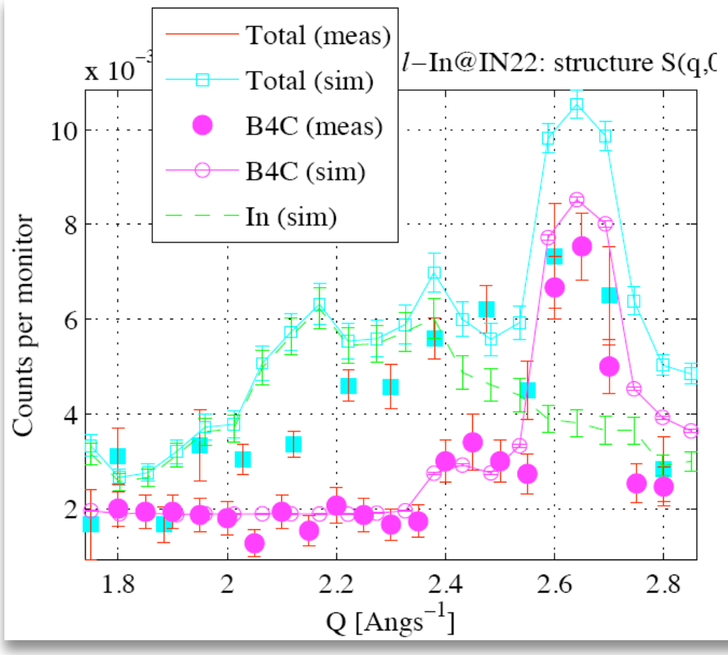


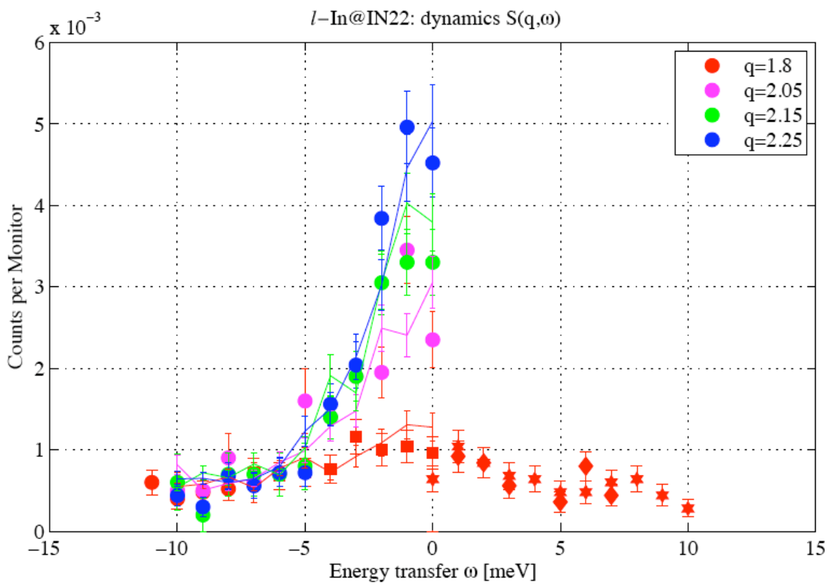
Recent experiments and VE's

- IN22, Liquid In, levitation furnace



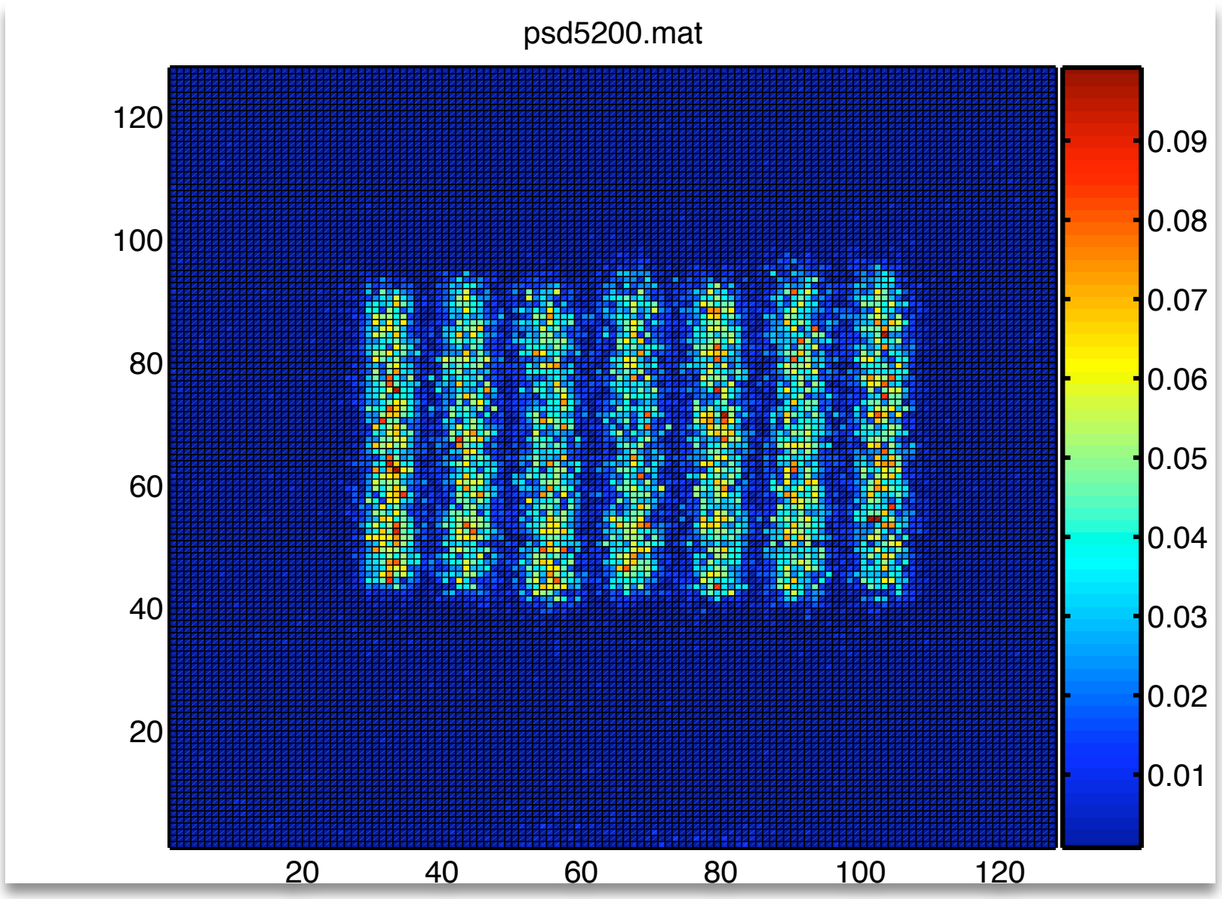


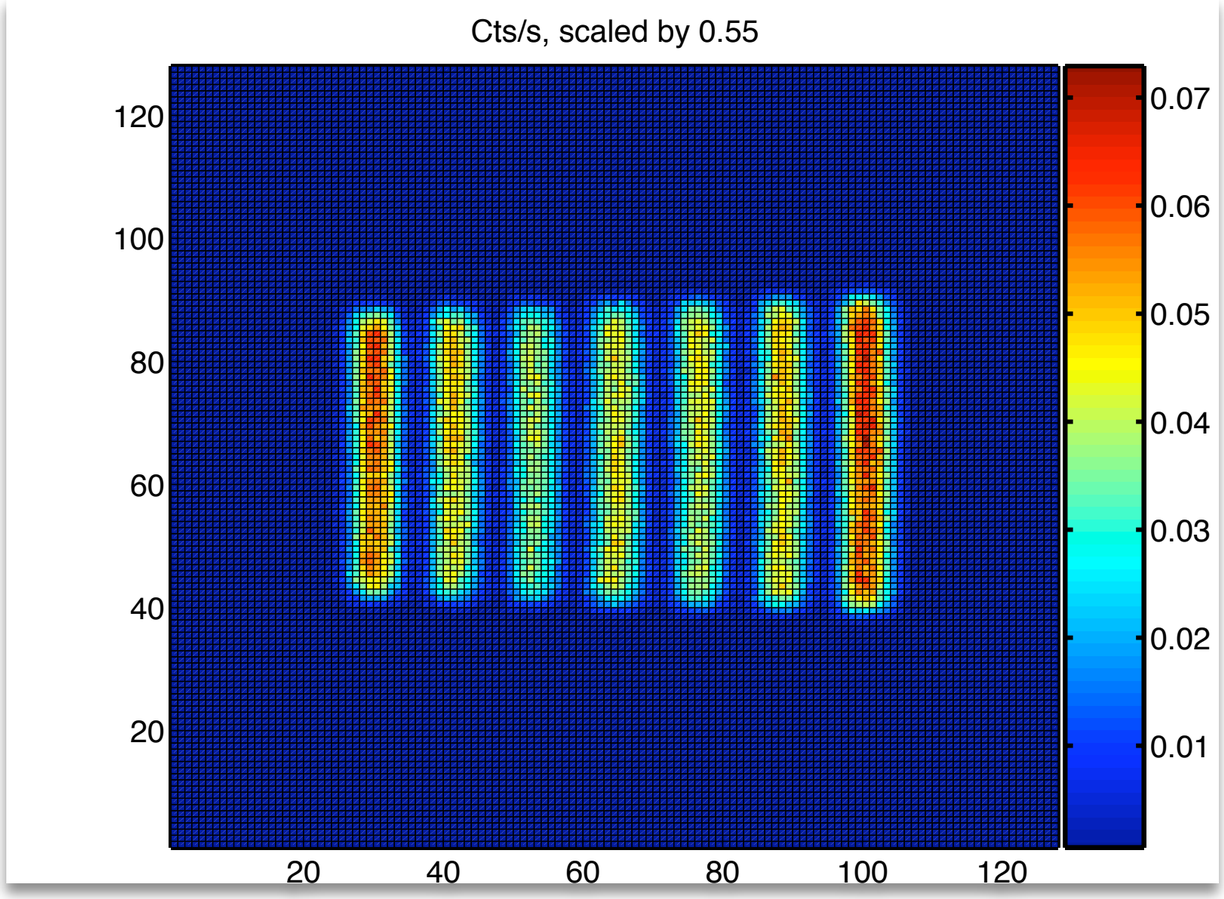




Recent experiments and VE's

- RITA-II, PSI - V (incoh)





Recent experiments and VE's

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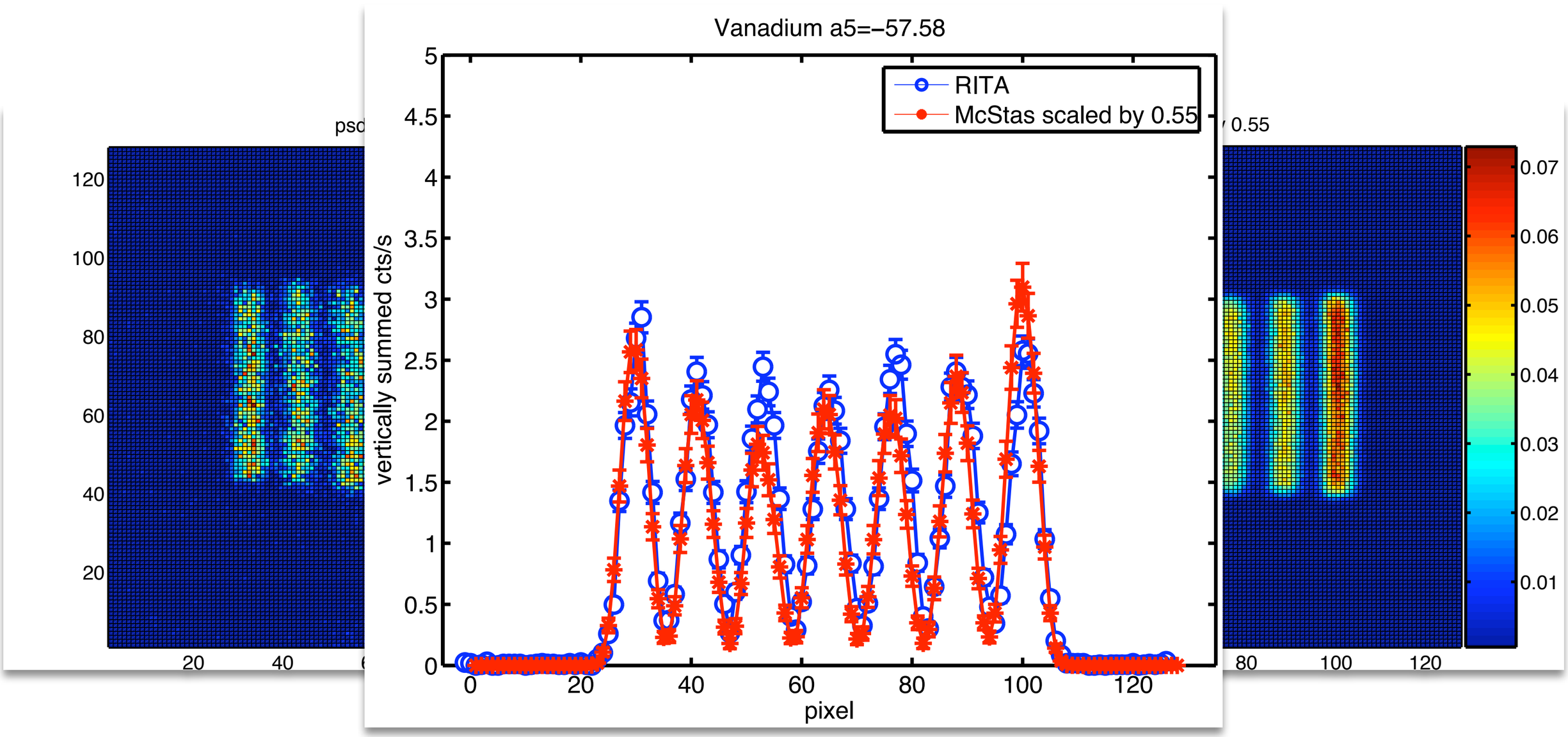
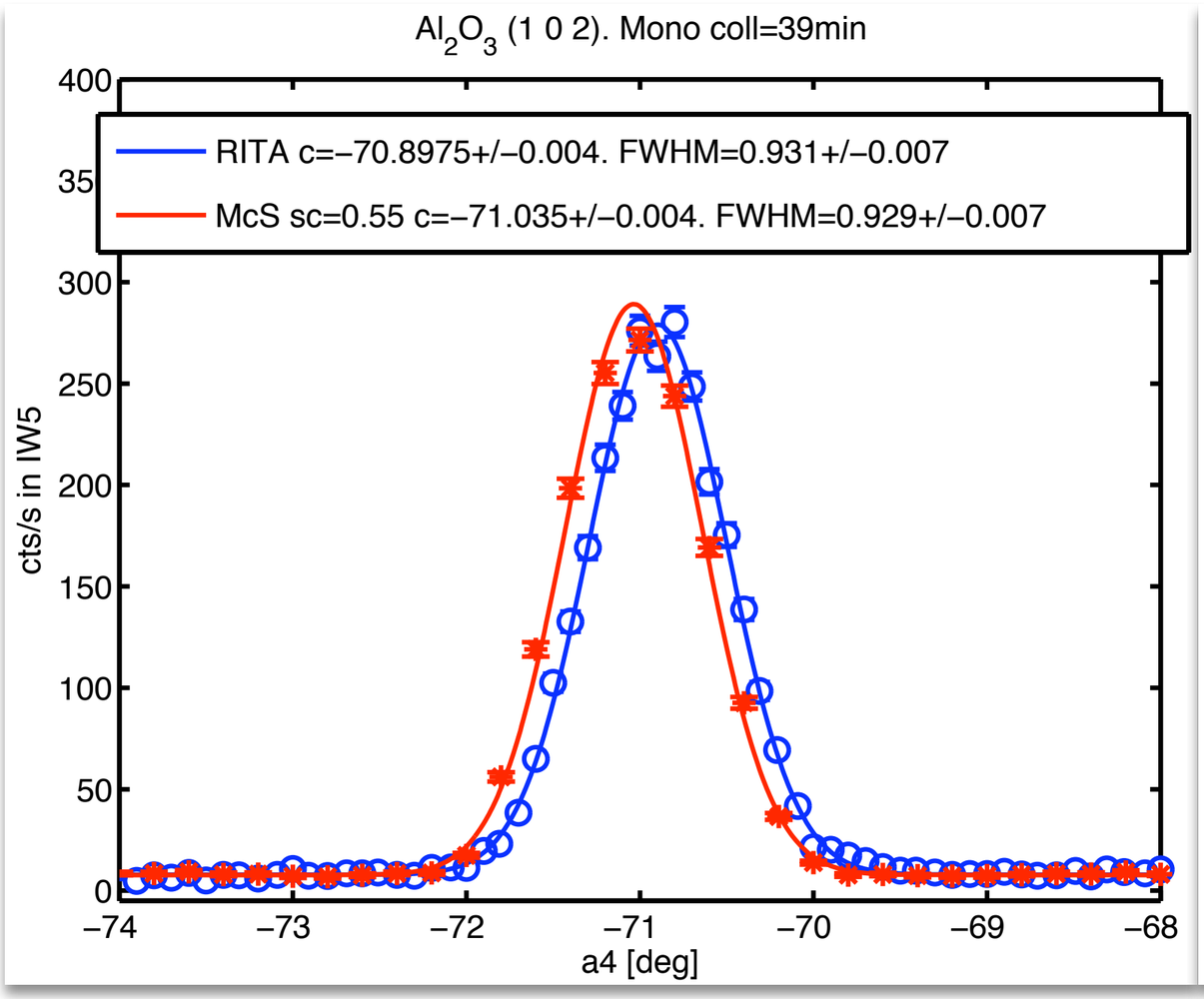
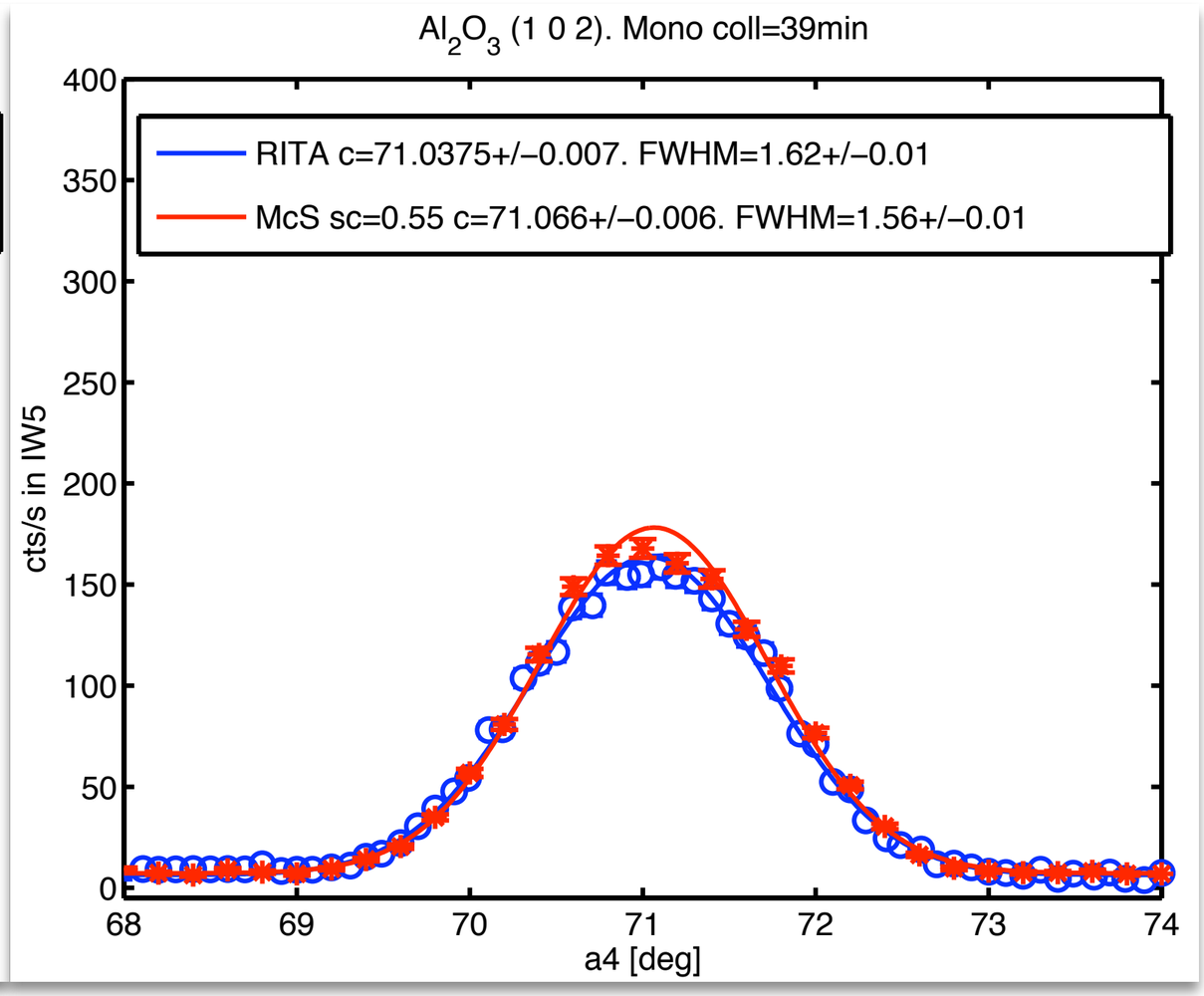


Recent experiments and VE's

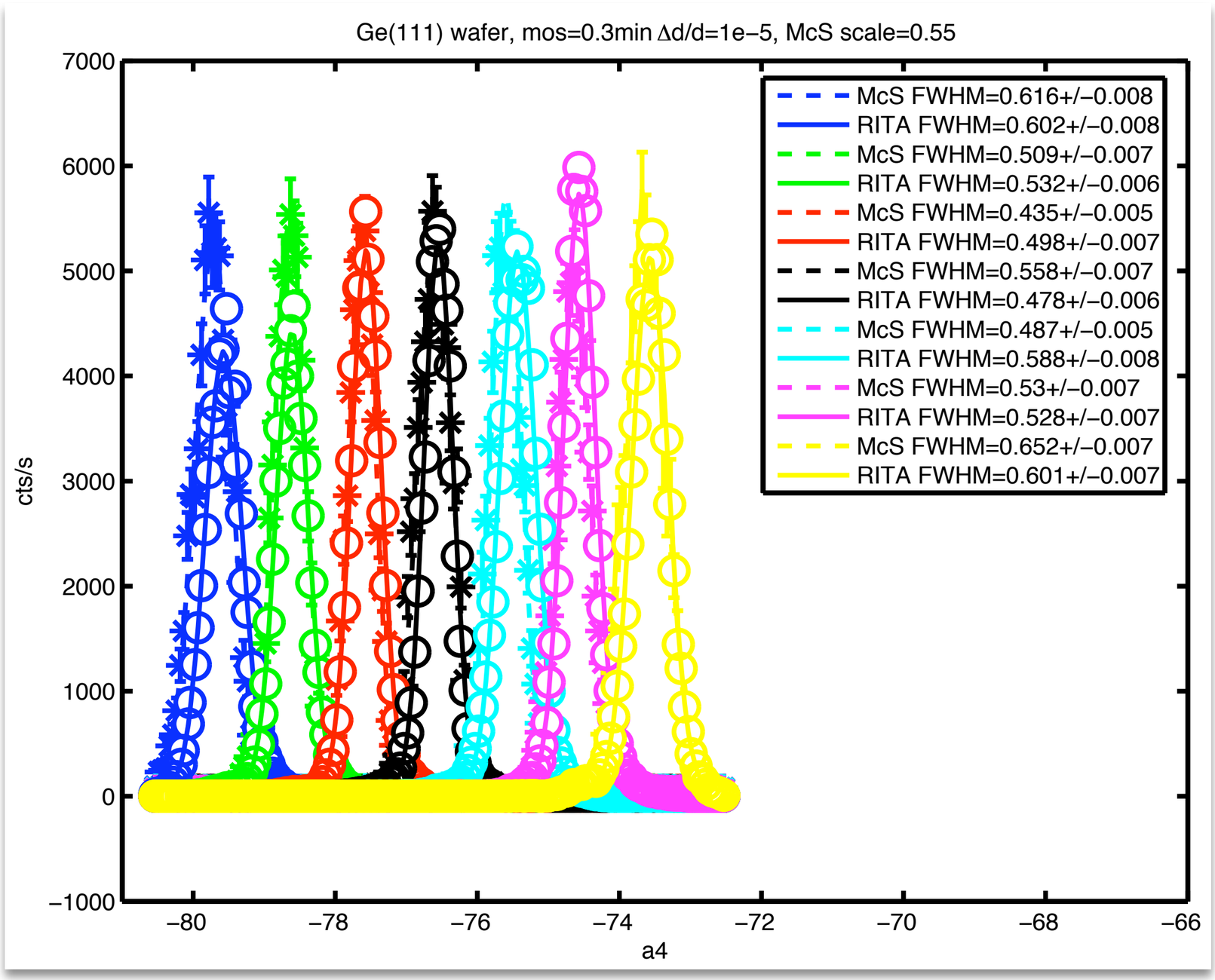
- RITA-II, PSI - Al_2O_3 powder





Recent experiments and VE's

- RITA-II, PSI - Ge wafer (perfect single crystal)



Instrumentation standard - I

- McStas:
  - extensively used for instrumentation
  - has wide portfolio of components, including sample models
  - is well suited for virtual experiments
  - is in agreement with the other MC codes
  - reproduces experimental conditions and results
    - (linewidths within 5%, intensities 10-30%)

- Virtual experiments are useful for
  - performing key experiments during design
  - benchmarking analysis codes
  - user training and education
  - data analysis

- Monte Carlo (e.g. McStas) is useful in the whole lifetime of an instrument - from design phase to operation mode

Instrumentation standard - II

- Special focus areas in the McStas 2.x series:
  - Code standardization
    - (Uniform parameter naming, PROP_DT, intersect_ used everywhere)
  - Component unit testing (at least one test instrument pr. component)
  - Continuous comparison with experiment

- In the future:
  - Facilities should set up MC-based infrastructures for:
    - Performing VE's prior to experiment (beam-time estimates, feasibility studies, resolution estimates)
    - New approaches to data analysis
  - The developed instrument models should be passed on from instrument designer to beamline scientist, to the beamline user
  - MC codes (McStas) could be used to study decrease in instrument performance
    - Key experiment performed at start of cycle
    - Compare with simulation
    - Utilize simulations to pin-point cause of performance decrease

Summary/Conclusion

- Monte Carlo (e.g. McStas) has all needed features to establish an ISO-like standard for neutron instrumentation:
  - Definition of geometries and physical properties of beamline components, sample environments and samples
  - Realistic source descriptions via input from e.g. MCNP models
  - Is used in all major instrumentation efforts
  - Has validated components
  - Gives easy access to VE methods for
    - Key experiments
    - Beamtime / statistics estimates
    - Analysis code benchmarks
    - User training
    - Data analysis

- All we need is a method for knowledge transfer -> Contribute back to McStas!