Virtual vs. real world experiments - validation of McStas components

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Abstract

In the neutron world, McStas [1][2] is becoming an important tool for optimising instrumentation, performing virtual experiments[3],[4] and data analysis purposes. To allow relevant comparison of virtual and real world experimental data, all included component models must undergo testing and validation to ensure the best possible agreement.

This poster presents highlight virtual experiment work, including comparative studies of experiments and virtual experiments, used for validation of McStas components.

Sample validation: Liquid metal (Indium) at IN22, ILL

Via the $S(q, \omega)$ scattering function, the McStas component `Isotropic_Sqw` can be used to model scattering from isotropic materials, e.g. liquids. Tabulated values of $S(q, \omega)$ from for instance ab initio or molecular dynamics simulations are used.

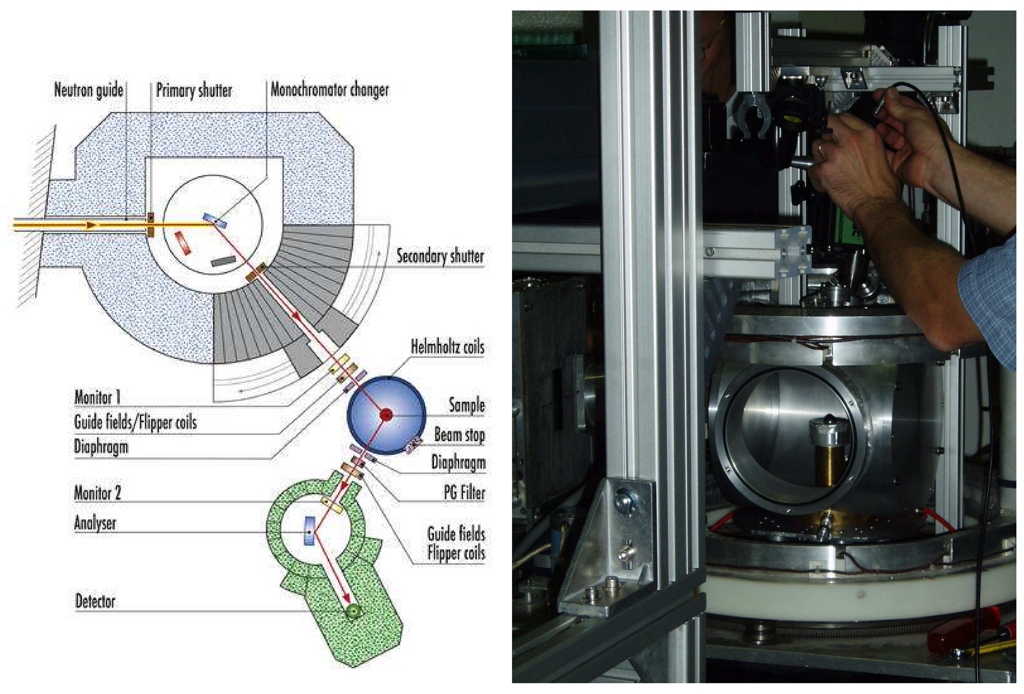

Figure 1: *LEFT: Schematic of the IN22 instrument. RIGHT: Special levitaion furnace used in the experiment.*

To avoid influence of sample environment on the signal from the liquid In, we used a special levitation device, see the figure. Ar gas was flowing through a B_4C nozzle, levitating the sample.

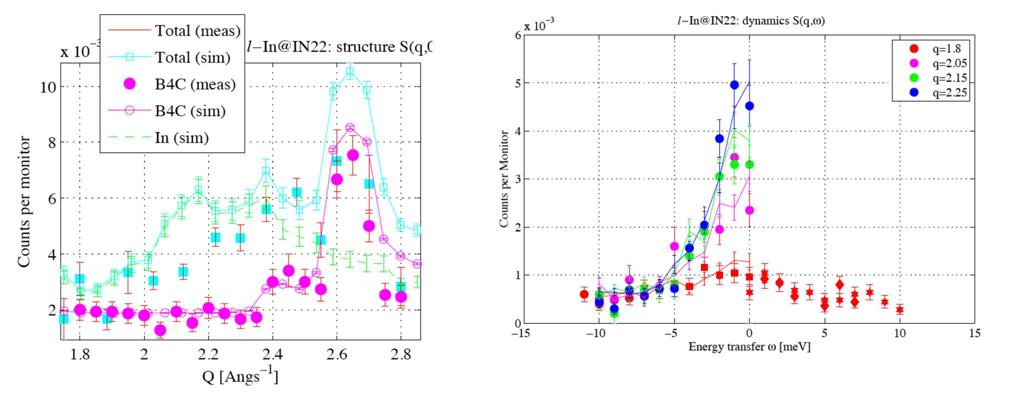

Figure 2: *LEFT: Simulated and measured scans of In liquid structure. RIGHT: Simulated and measured scans of In liquid dynamics.*

Apart from the expected signal from In, Bragg peaks of unknown origin were seen. Scattering from the highly neutron absorbing B_4C, unexpectedly had a large influence on the measured signal, revealed by simulation.

DMC @ PSI, $Na_2Ca_3Al_2F_{14}$

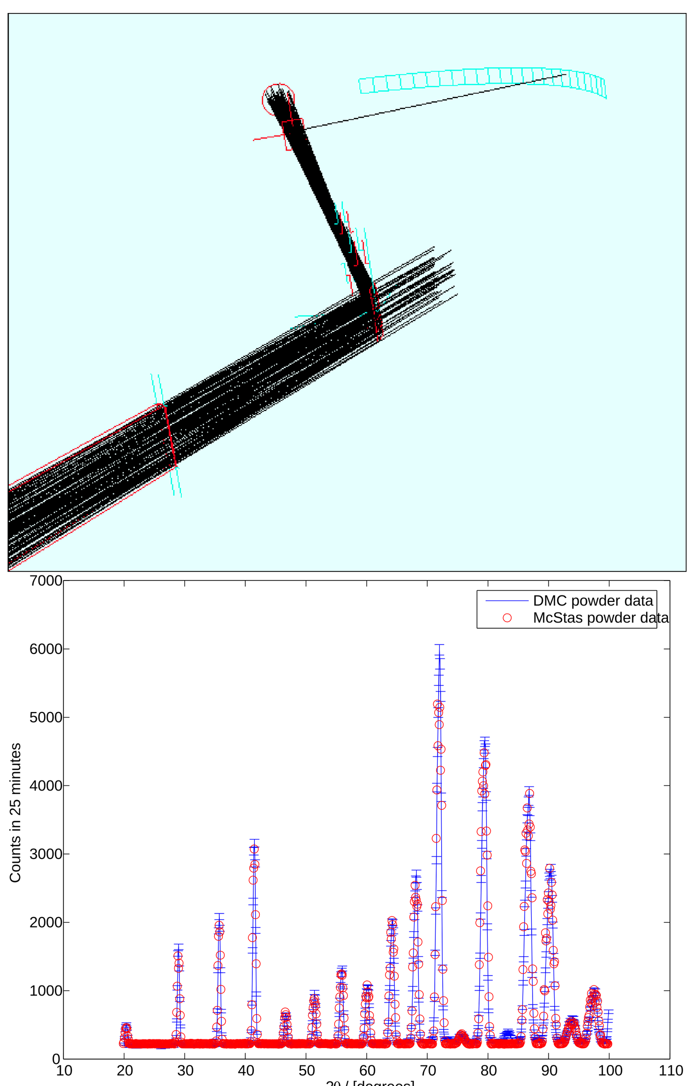

Figure 3: From [4] *DMC @ PSI instrument simulated using McStas. Left: 3D-display of the instrument. Right: Powder lines from $Na_2Ca_3Al_2F_{14}$. Comparison between virtual experiment and diffractometer data.*

RITA-II, PSI: Careful benchmarking of a RITA model

Linda Udby developed a very detailed model of the RITA-II instrument at PSI for her PhD thesis [5]. This paragraph shows benchmarks between simulation and experiments from this work.

Between monochromator and sample position at RITA-II, a selection of insertion collimators are available, nominally of collimation (10",20",40" and 80"). The actual collimation of the > 10" versions were measured, by inserting the 10" and placing the other ones at the sample position. Rocking curves were performed, giving a triangular-shaped peak per collimator.

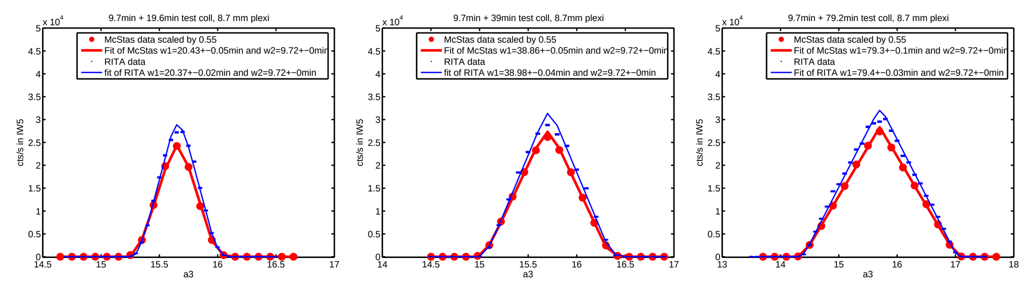

Figure 4: *RITA-2 TAS: Rocking curves of collimators (20",40",80")*

Carefully performing parameter variations of these collimations in simulated versions of the same scans, gave more accurate values than the nominal collimations.

Samples: Powder (Al_2O_3) at RITA-II, PSI

To verify alignment of the instrument (specifically absolute energy definition and 2θ, powder line scans of Al_2O_3 (1 0 2) were performed in + and - configuration respectively.

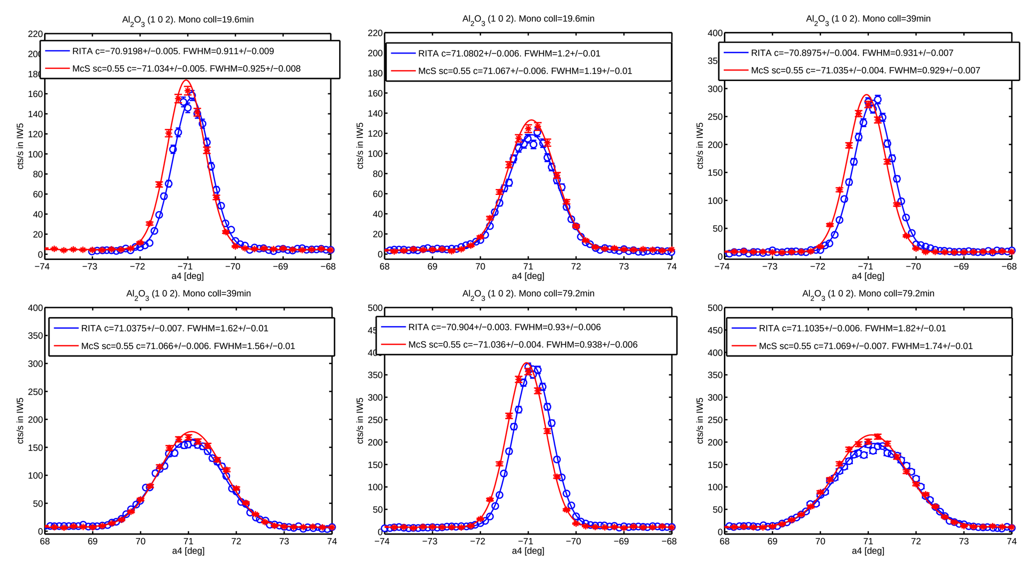

Figure 5: *RITA-II TAS: Simulated and measured powder lines from Al_2O_3. Scaling factor of 0.55.*

Simulations are in almost perfect agreement with the measurements, apart from the same factor of 0.55 as applied above.

Samples: Perfect Single Crystal (Ge)

A perfect single crystal (in shape of a Ge wafer) was placed a the sample position, for determination of the mosaicities of the individual analyzer blades. At energy transfer $\hbar\omega = 0$, an a4 (2θ) scan was performed.

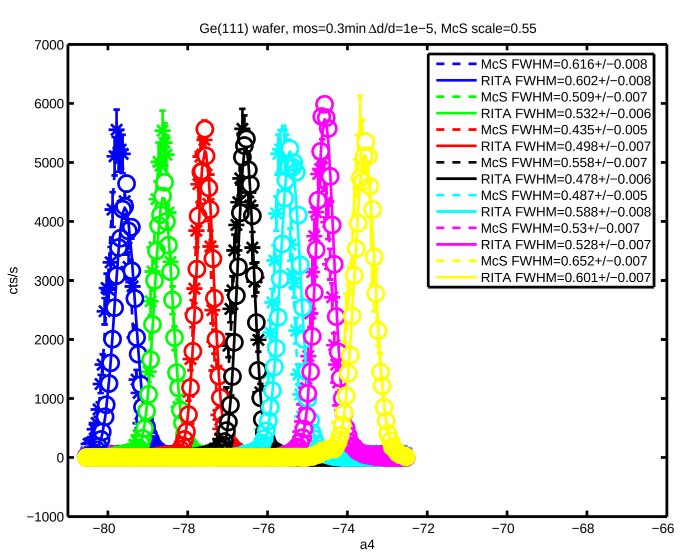

Figure 6: *RITA-II TAS: Simulated and measured Bragg position of Ge (111) (wafer), as diffracted by blades of the multi-analyzer. Scaling factor of 0.55.*

Again, agreement between measurements and simulation is convincing, apart from the scaling factor of 0.55 as mentioned above.

RITA-II @ PSI, instrument resolution / data analysis

Taking the work from [5] further, the instrument model was utilized for data analysis [6]. The instrument model was further evaluated and finally used to determine that a peak was not resolution limited, determined with better precision than more traditional methods[7].

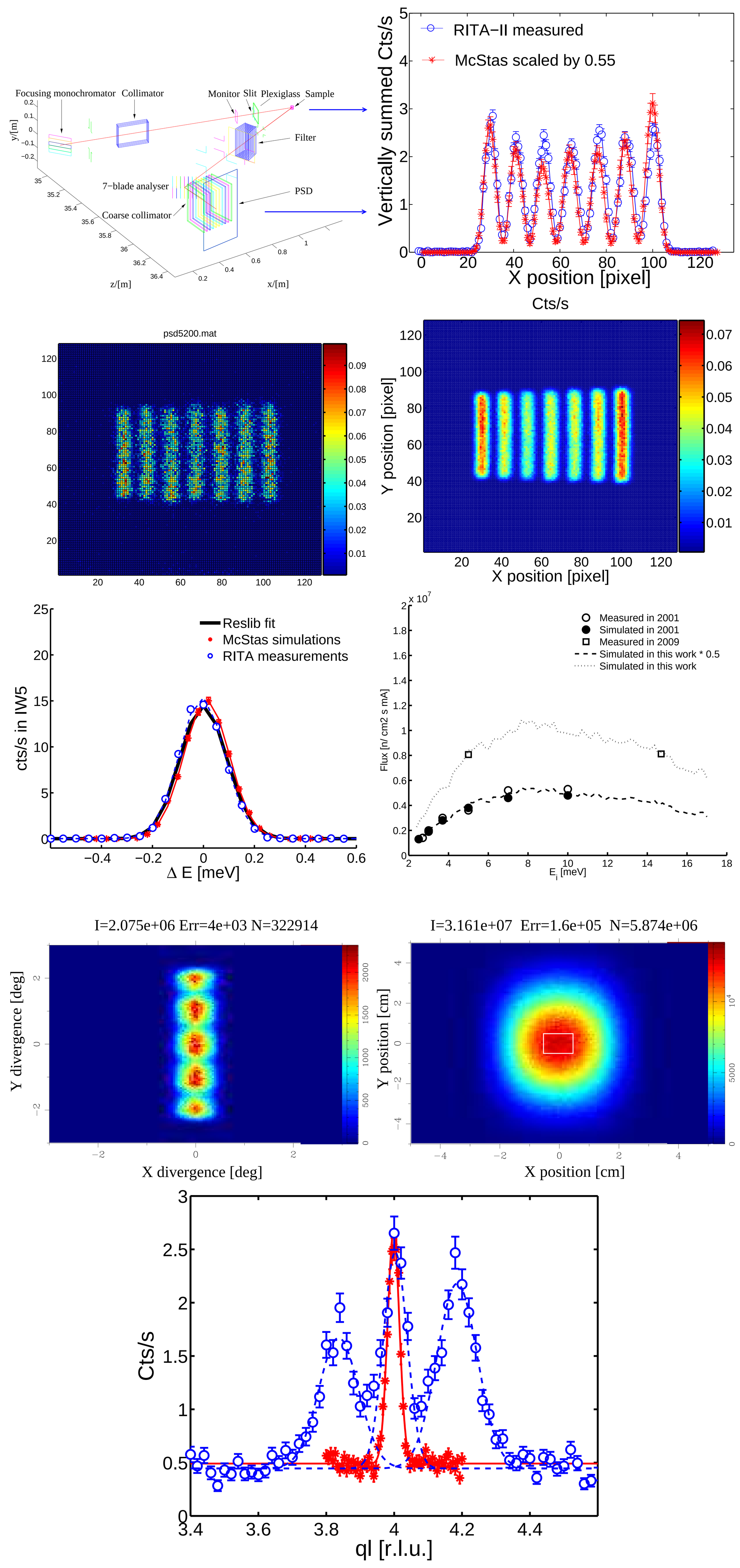

Figure 7: From [6] *RITA-II @ PSI instrument simulated using McStas. A detailed study of instrument and resolution function, applied to data analysis.*

References

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