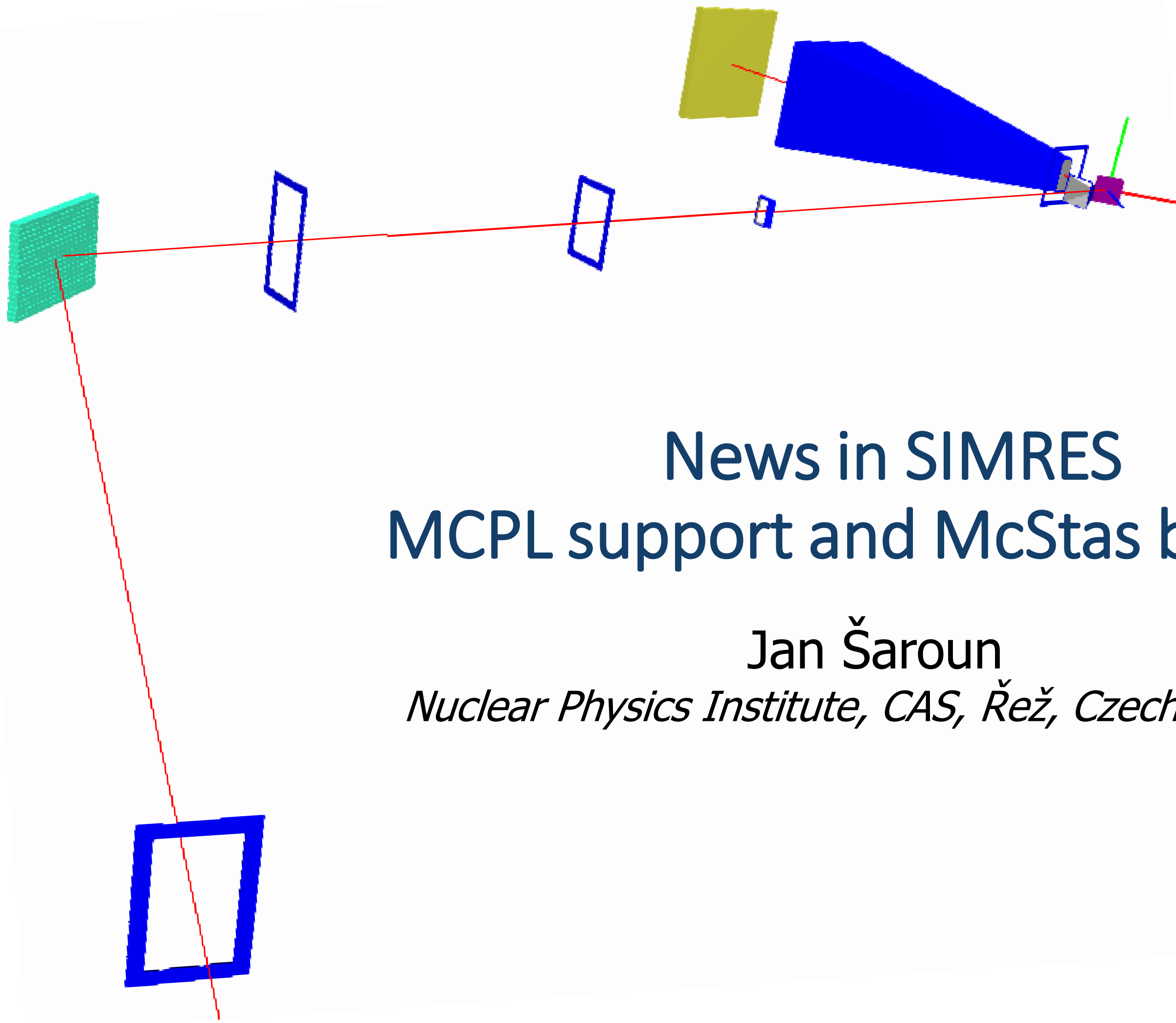

News in SIMRES
MCPL support and McStas bindings

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Introduction

Recent development in neutron simulation packages:

- Large and growing library of user contributed components in McStas
- Radiation transport (MCNP, Geant4): progress in simulation of neutron optics (guides)
- Vitess, SIMRES: other ray-tracing packages developed in parallel to McStas
  have features not available in McStas x miss many features that McStas has
- Monte Carlo Particle Lists (MCPL) – a great tool for putting everything together

(more details in the following talks)

Few facts about SIMRES:

✓ Developed from specialized tool (ResTrax for TAS) into general neutron ray-tracing program

✓ Desktop application with a friendly GUI (component editors, 3D view, scripting, commands for scanning and event analysis)

✓ Few but highly configurable and detailed components, quite general (most of current instruments can be simulated, monochromatic & ToF)

✓ Adaptive variance reduction + reverse tracing = much faster in many situations

✓ Difficult to add new components, limited options for sample models (good for powder diffraction)

Aim

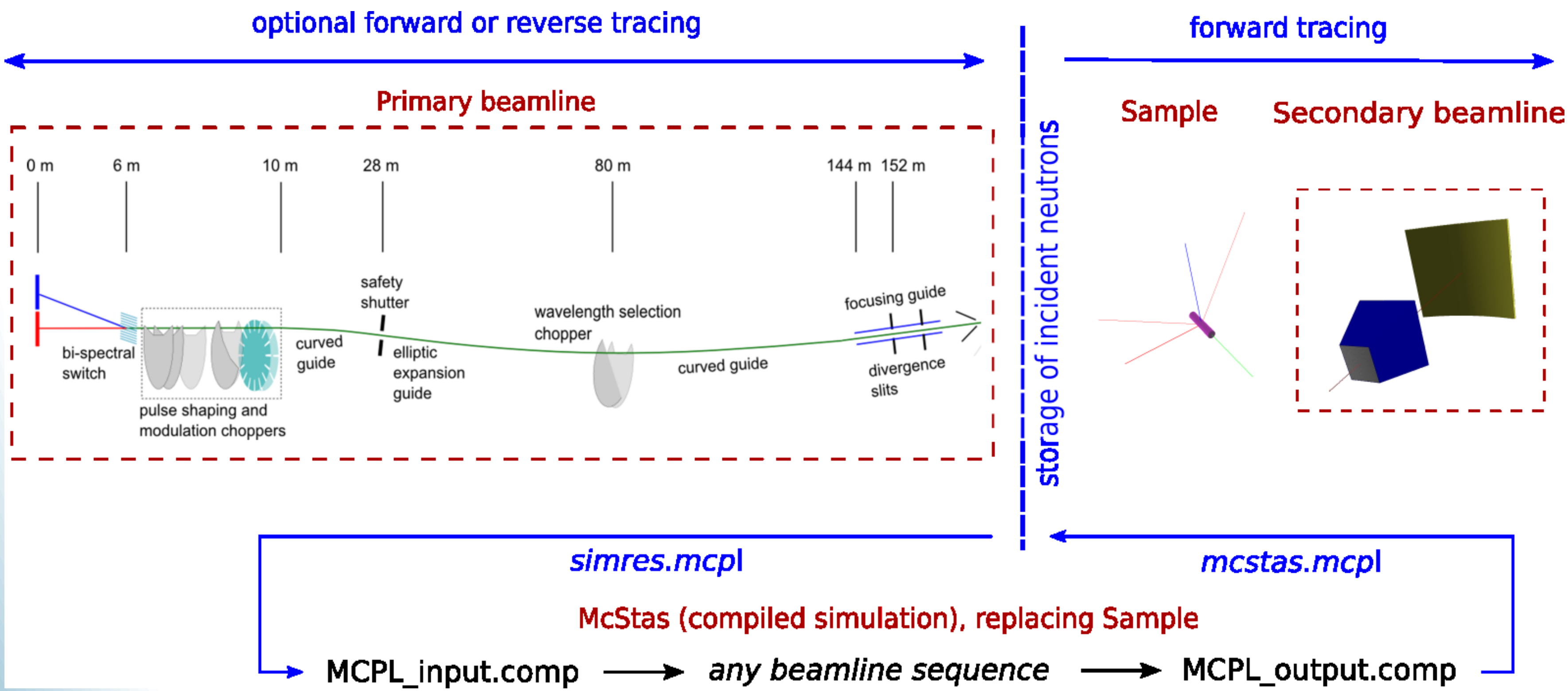
Employ MCPL to combine McStas and SIMRES in a single simulation
& exploit the synergy effects:

- ✓ Much higher simulation speed provided by SIMRES in many configurations involving samples & other bottle necks
- ✓ Employ the large McStas library of samples (and other components)
- ✓ Benefit from high configurability allowed by the McStas meta-language framework.

Newly implemented in SIMRES:

- ✓ MCPL import & export to/from SIMRES monitors
  NOTE: includes guide surfaces, scattering events in a sample, back-trace monitors, ...
- ✓ Possibility to launch McStas simulation from SIMRES, exchange instrument parameters & neutron lists
- ✓ Control of a combined simulation SIMRES -> McStas (-> SIMRES)

How does it work



- ✓ Independent on McStas environment
  Only instrument executable is needed ...
- ✓ A very general meaning of “*Sample*”
  = anything between the primary and secondary sections of the SIMRES instrument

Simple McStas code: *SIMRES -> McStas -> SIMRES*

```
DEFINE INSTRUMENT SIMRES_MCPL_SCRYST(string input="simres.mcpl",
int repetition=1, string export="mcstas.mcpl")

TRACE

COMPONENT Origin = Progress_bar()
AT (0, 0, 0) ABSOLUTE

/* MCPL import */
COMPONENT src = MCPL_input(filename=input, repeat_count=repetition,
polarisationuse=0, doubleprec=1, ...)
AT( 0,0,0) RELATIVE PREVIOUS

/* Sample axis, position is relative to the SIMRES monitor */
COMPONENT Sample_axis = Arm()
AT (0, 0, 0.04) RELATIVE src

/* SAMPLE. Other components can be placed before or after the sample. */
COMPONENT sample = Single_crystal(xwidth=0.003, yheight=0.003, zdepth=0.003,
mosaic = 30, reflections="SiO2_quartza.lau")
AT(0, 0, 0) RELATIVE Sample_axis

/* MCPL export. This is where SIMRES will continue */
COMPONENT vout = MCPL_output(filename=export, doubleprec=1, ...)
AT(0, 0, 0) RELATIVE Sample_axis

END
```

obligatory parameters
required setting

imported from SIMRES monitor

... neutron goes back to the SIMRES monitor

Simple McStas code: *SIMRES -> McStas*

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COMPONENT sample = Single_crystal(xwidth=0.003, yheight=0.003, zdepth=0.003,
mosaic = 30, reflections="SiO2_quartza.lau")
AT(0, 0, 0) RELATIVE Sample_axis

/* DETECTOR. */
COMPONENT xymon = PSDcyl_monitor(nr=360, ny=100, filename="cylmon.dat", ...)
AT (0, 0, 0) RELATIVE Sample_axis

END
```

obligatory parameters
required setting

imported from SIMRES monitor

Tracing stops here

Use cases

Engineering diffractometer BEER@ESS

1. Standard medium resolution strain mapping
   An experiment with a small gauge volume of 1x1x3 mm3 in duplex steel.
2. High resolution strain mapping employing the beam modulation method.
3. Single crystal diffraction
   Measurement of a small single crystal (α-SiO2) using a white beam on BEER.
4. Simultaneous diffraction and SANS measurement
   A rod sample in axial strain geometry (typical for thermo-mechanical loading experiments).

Event based analysis of lattice strain distributions

Deconvolution method employing particle lists

- Treatment of pseudo-strains and strain gradient smearing in a steel tube
- Test on synthetic data for STRESS-SPEC@FRMII and BEER@ESS

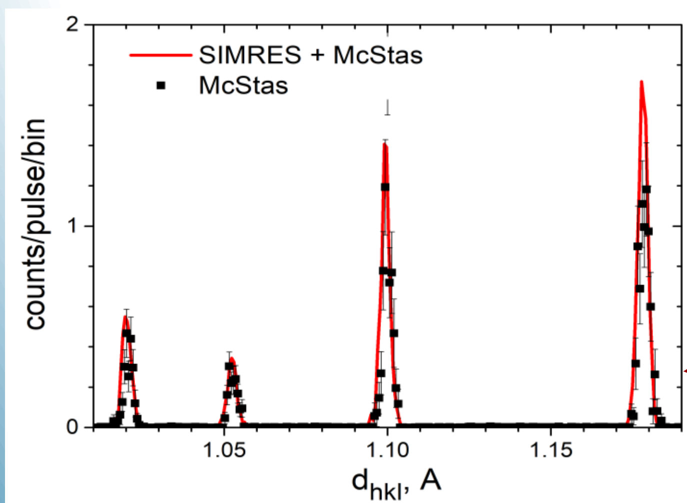
Medium resolution strain mapping

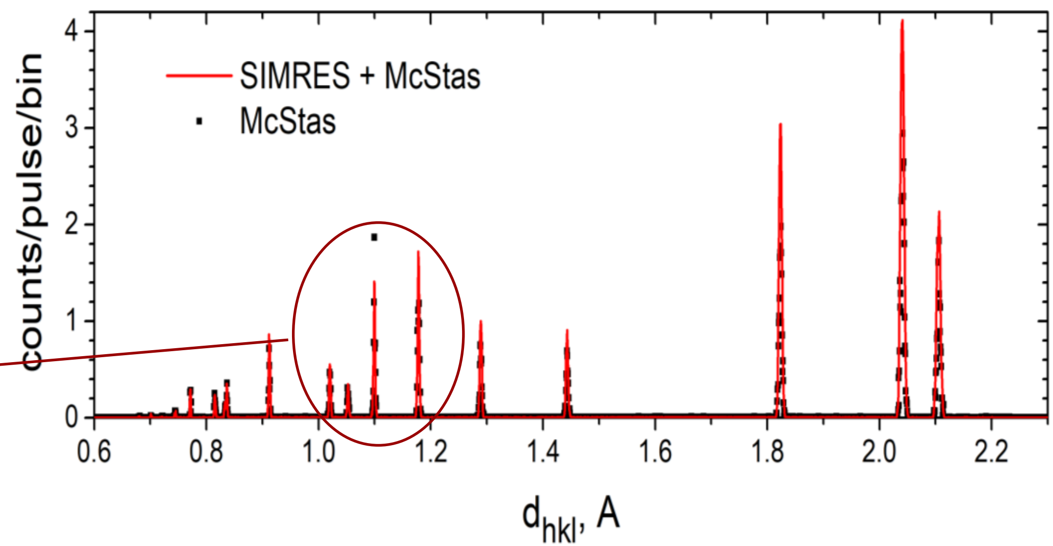
The engineering diffractometer BEER (ESS)

Using McStas components:

```
PowderN
ExactRadialCollimaor
NPI_tof_dhkl_detector.comp
```

- **Source**: bi-spectral, W2 beamport of ESS
- **Resolution choppers**: a pair of choppers,280 Hz in optically blind mode.
- **Wavelength bandwidth**: from 1 Å to 3 Å.
- **Primary collimation**: vertically focusing neutron guide, primary slit 1x3 mm^2
- **Sample**: rod (diameter=10 mm, length = 50 mm), duplex steel, axial strain geometry
- **Secondary collimation**: Radial collimator with gauge FWHM = 1 mm (ENGIN-X setup).
- **Detector**: cylindrical, resolution 2x5 mm

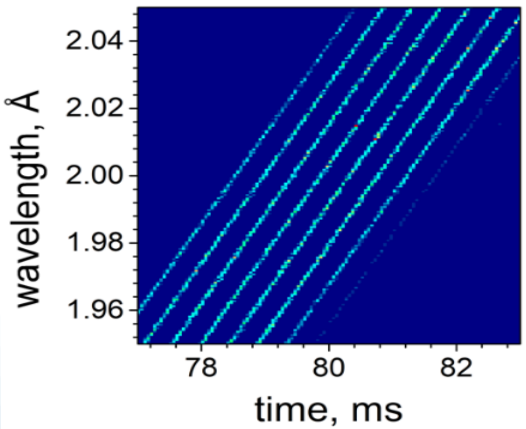




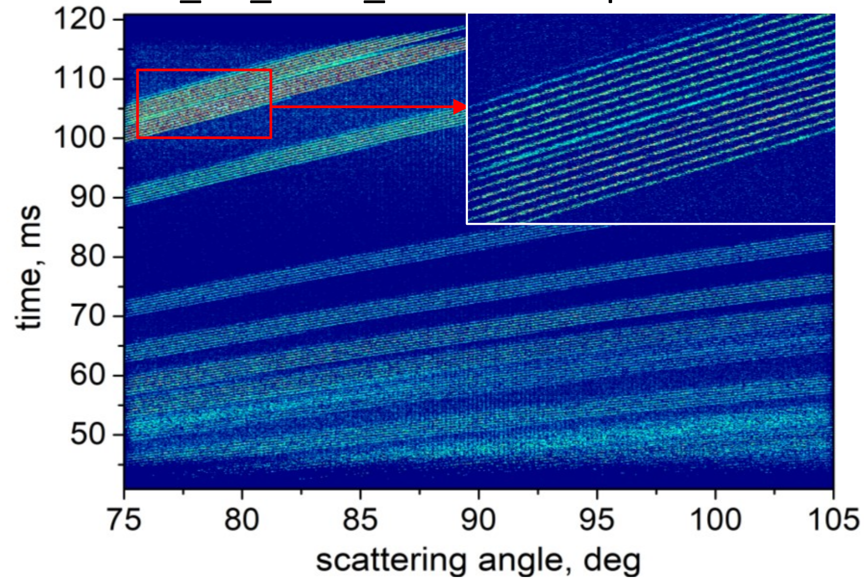
	Rel. error (primary beam)	Computing time
SIMRES + McStas	1.1 %	56 s
McStas	1.8 %	1110 s

BEER in modulation mode

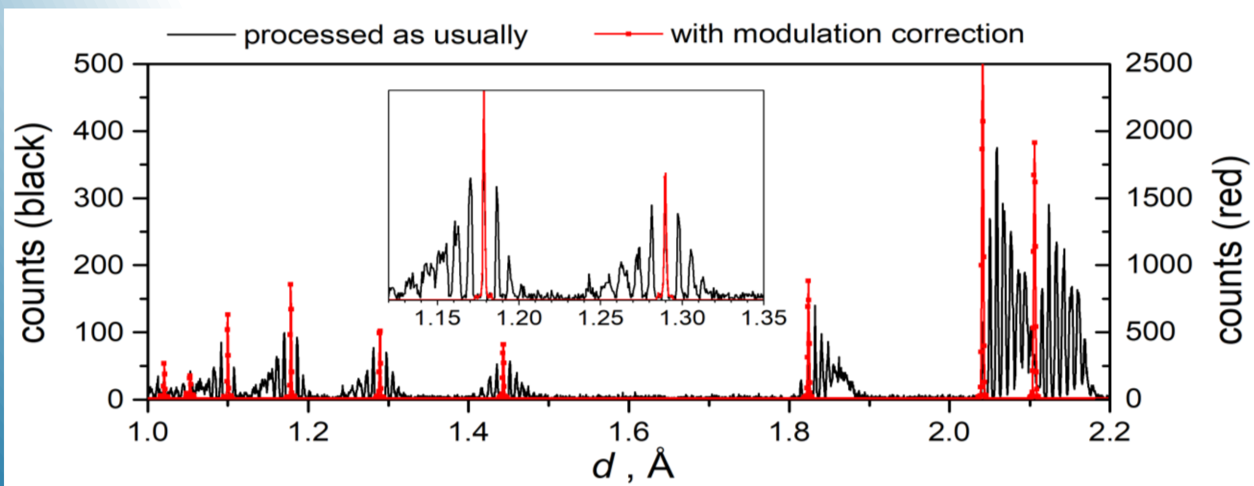
Modulated primary beam by SIMRES



Scattering pattern by PowderN and NPI_tof_theta_monitor.comp in McStas



Modulated data – event processing by McStas NPI_tof_dhkl_detector.comp

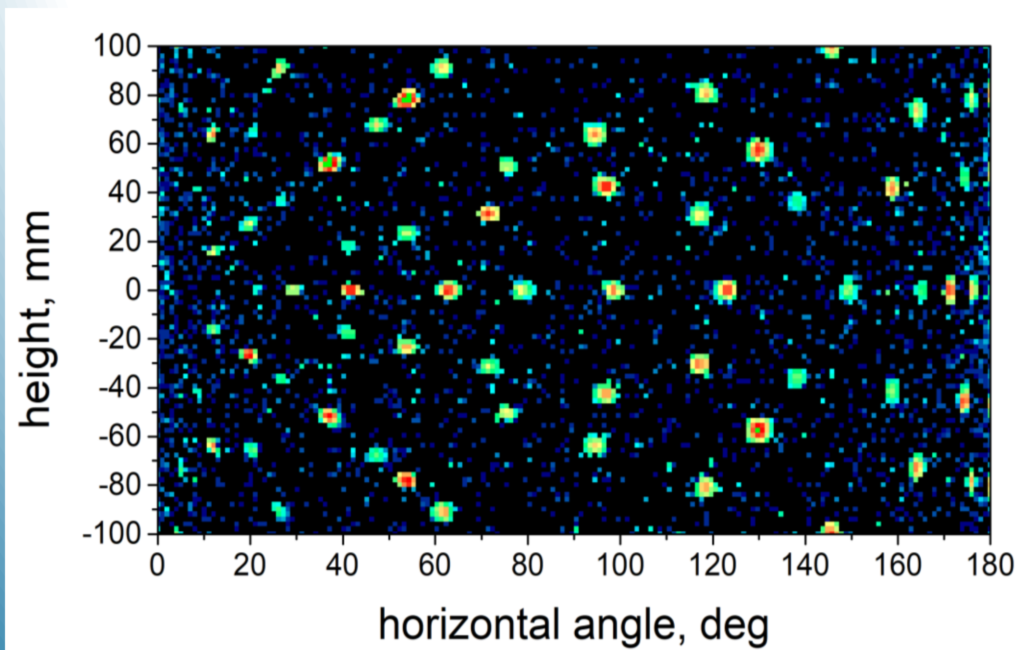


- *black*: standard processing
- *red*: reconstructed diffractogram

Single crystal diffraction

Using `Single_crystal.comp` of McStas

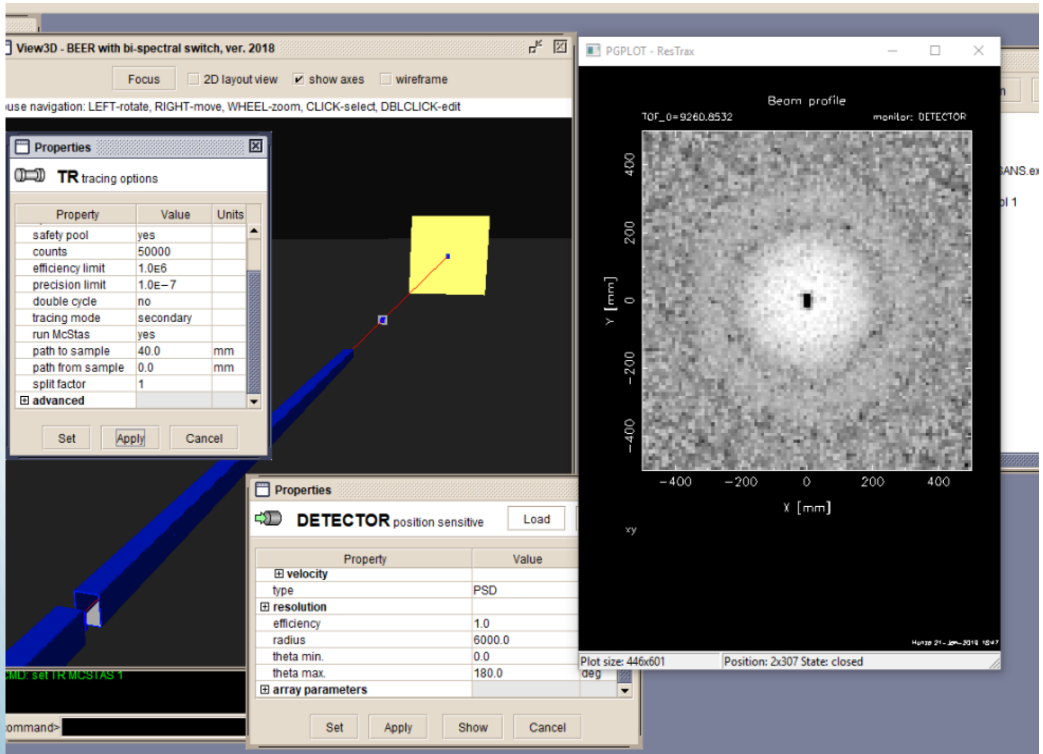
- **Choppers**: switched off (white beam).
- **Wavelength bandwidth**: from 0.5 Å to 2.7 Å.
- **Primary collimation**: divergence slit 15x15 mm (6 m before the sample) primary slit 4x4 mm^2 at 50 mm the sample.
- **Sample**: α-SiO2 cube 3x3x3mm^3, mosaicity 30’ (data file `SiO2_quartza.lau`)
- **Detectors**: cylindrical (`PSDcyl_monitor`) and 4PI (`PSD_monitor_4PI`) monitors, and 1x1m^2 ^{3}He detector at 90^o (`PSD_Detector`).



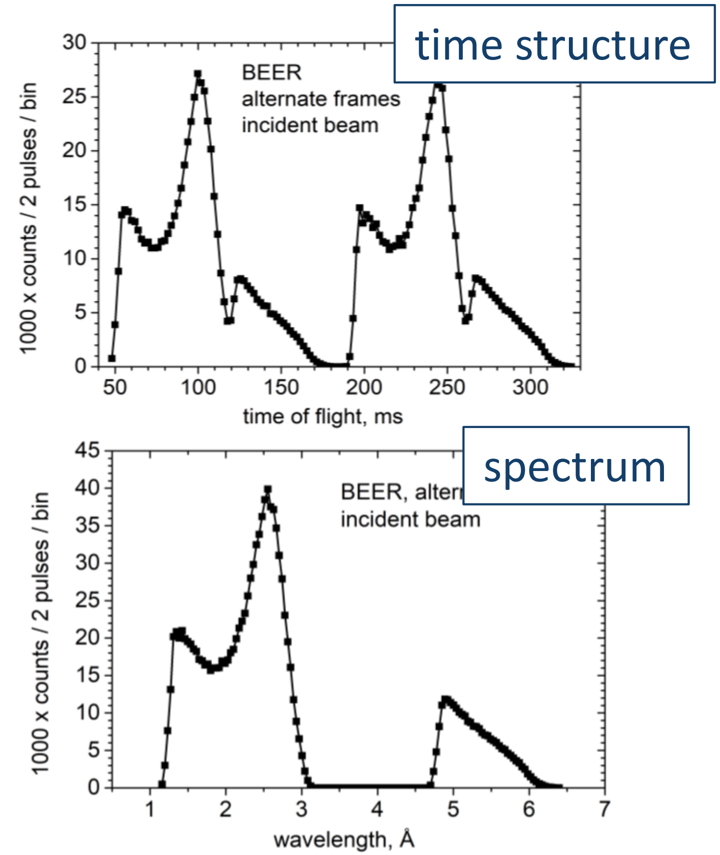
Single crystal diffraction pattern (α-SiO2) recorded by the SIMRES detector.

- Primary beam simulated by SIMRES.
- Sample simulation redirected to McStas.
- The secondary beam traced by both McStas and SIMRES.

Simultaneous diffraction and SANS measurement



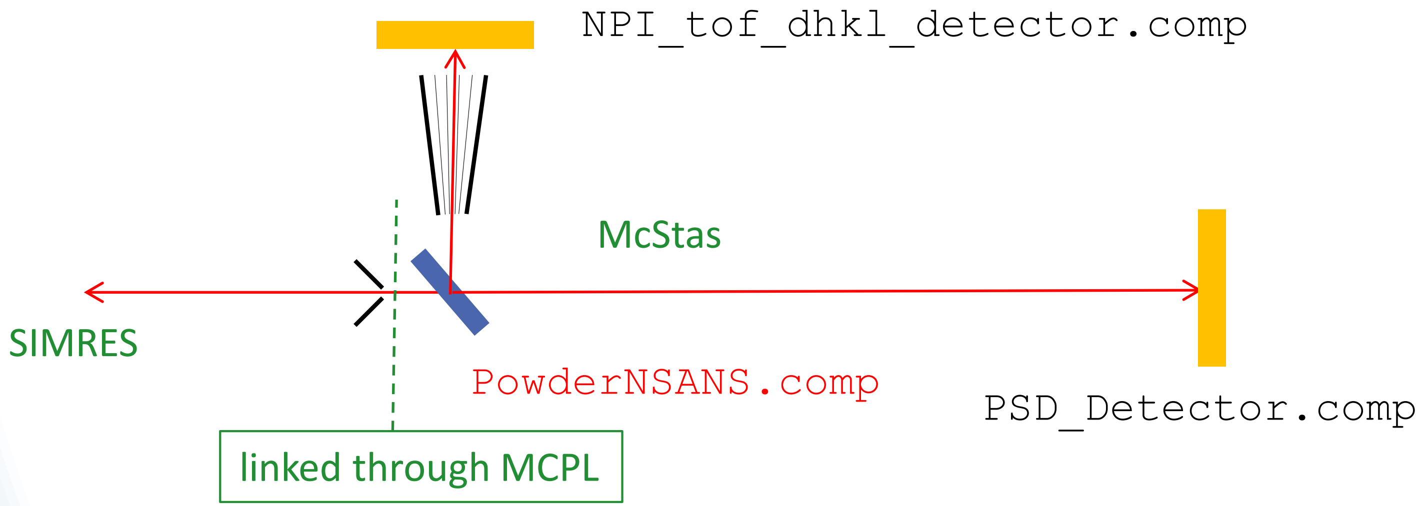
BEER, alternating frame mode

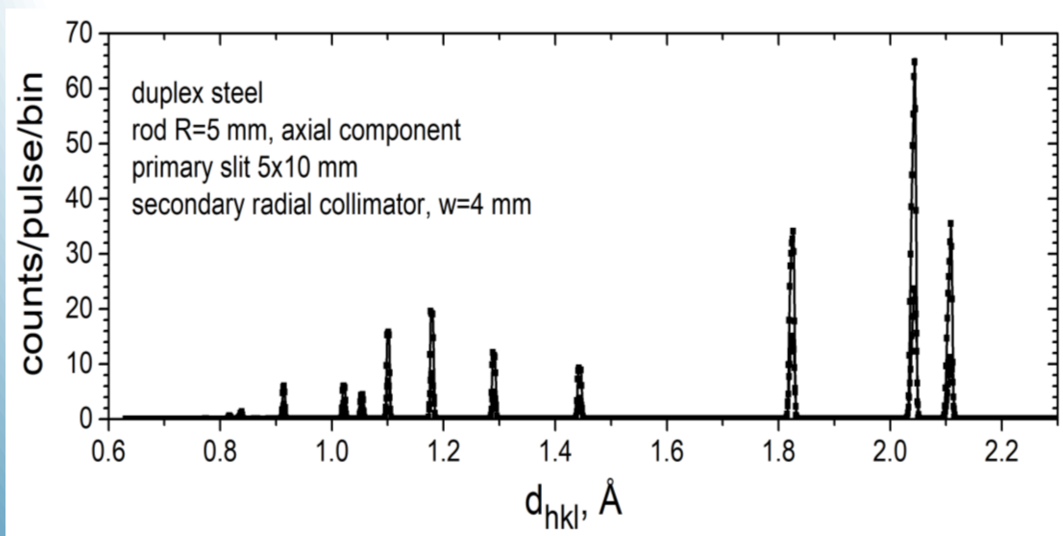


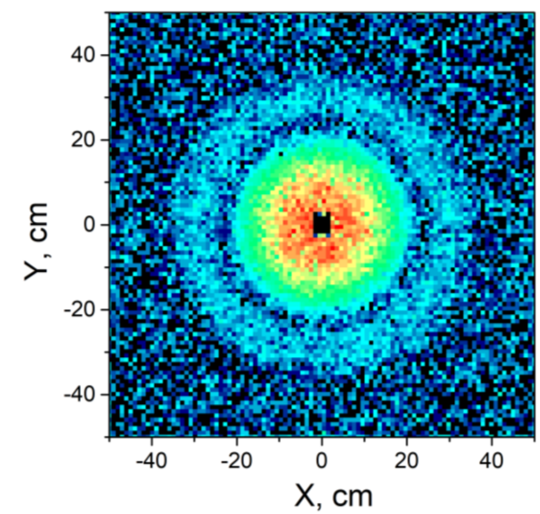
- Screenshot of the SANS pattern shown in the SIMRES
- SANS sample simulated by McStas.

- Time structure and spectrum of the primary beam simulated
- Used as MCPL input to the subsequent McStas simulation of the sample and secondary beamline.

Simultaneous diffraction and SANS measurement







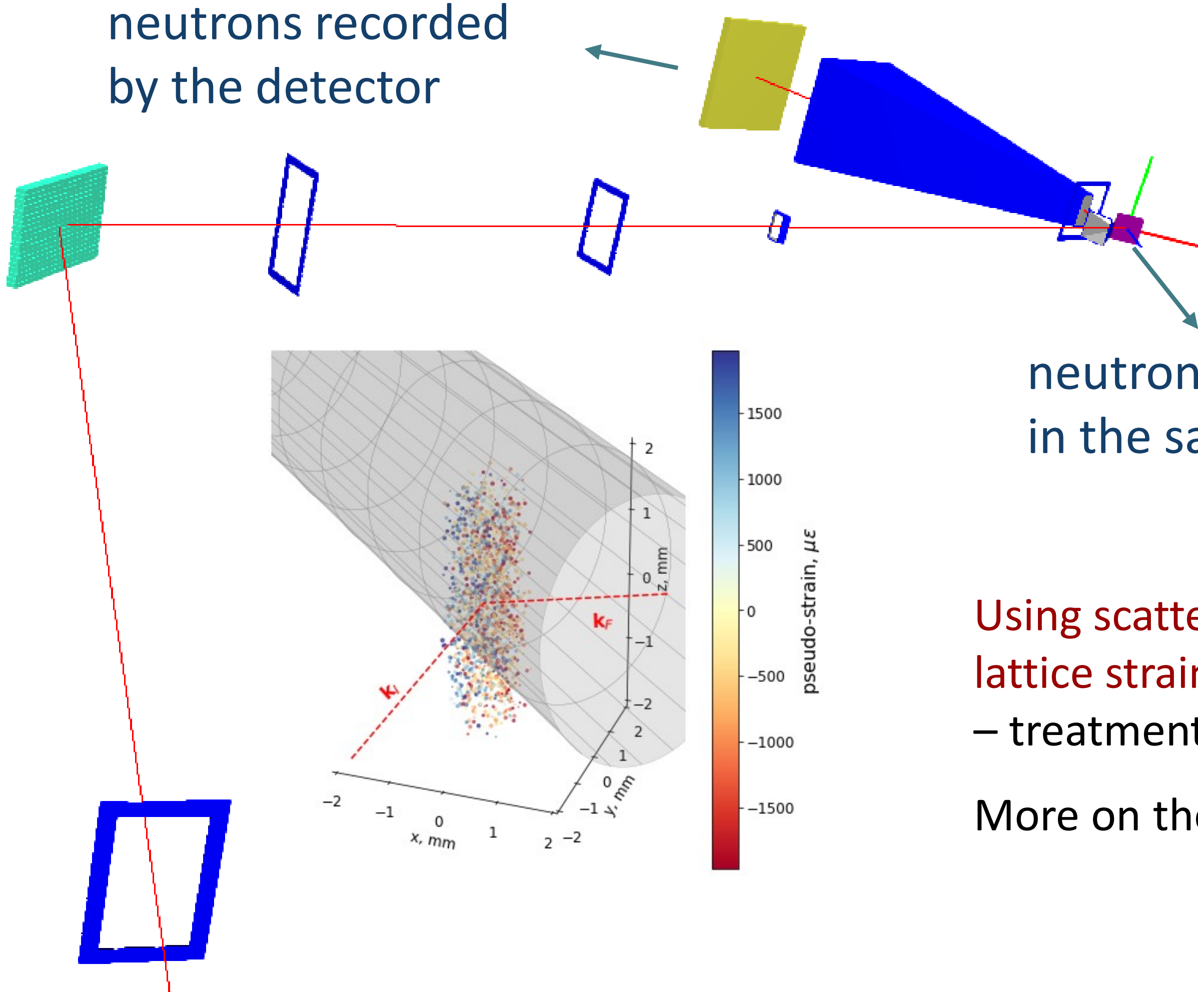
Diffractogram and SANS pattern produced simultaneously by McStas.
Primary beam simulated by SIMRES.

Scattering event lists

MCPL file 1

Data analysis software employing **scattering event list**

neutrons recorded by the detector



MCPL file 2

neutrons recorded in the sample

Using scattering event lists to analyse lattice strain ditributions
– treatment of pseudostrain effects

More on the ECNS poster, Tue 2/7/2019

Conclusions

Benefits

- ✓ Higher simulation speed by more than an order of magnitude,
- ✓ Wider library of components which can be used to configure the instrument model,
- ✓ Combining components available only in SIMRES or McStas
- ✓ No extra effort needed for code porting and maintenance.

Limitations

- ✓ Ray tracing algorithm of SIMRES does not permit to employ McStas sources
- ✓ Parallel computing: not available in SIMRES.
  No principal obstacle for McStas to employ paralel computing on its part of the ray-tracing job (?)

Thank you for your attention