McStas simulations of 15 T magnet and background prediction with Machine Learning

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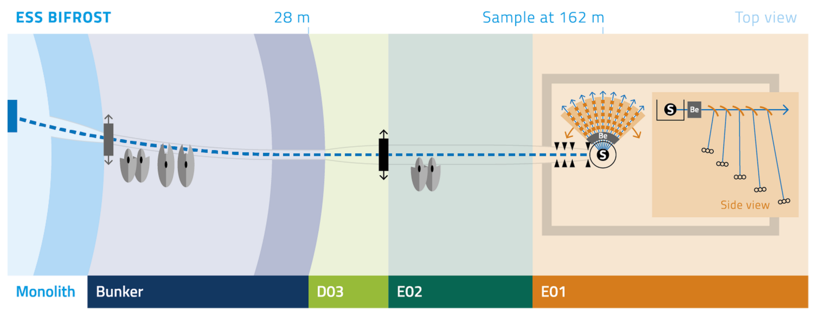
BIFROST at ESS

Indirect ToF spectrometer with multi-energy analysis [1]

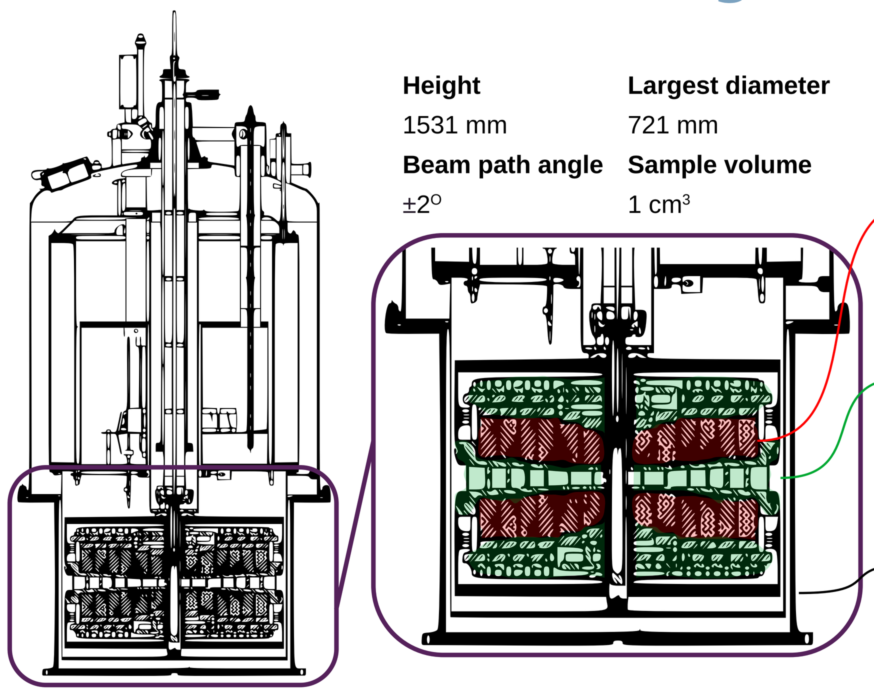


Magnetic fields
above 14 T

Temperature
down to 50 mK

Pressure
above 3 GPa

The 15 T Magnet



Height	**Largest diameter**
1531 mm	721 mm
Beam path angle	**Sample volume**
±2°	1 cm³

Magnet Coils
Add mass and large magnetic forces

Support structures
Withstand magnetic forces

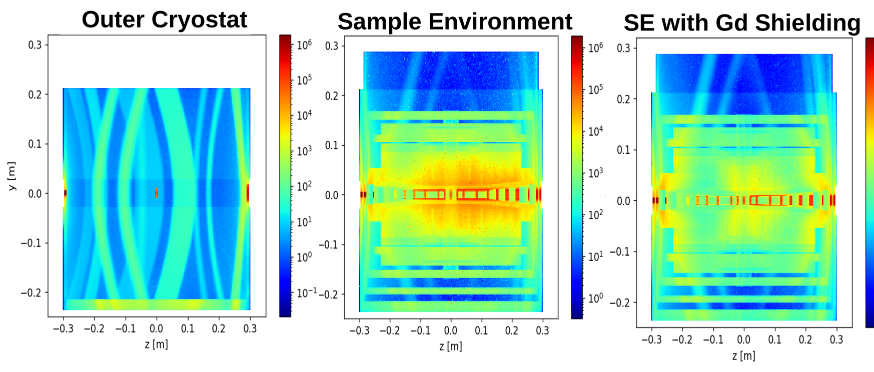
Cryostats
Maintain conditions in the sample environment

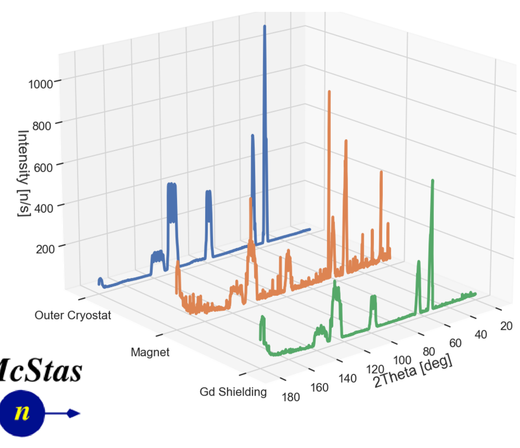
Motivation

Investigation and **prediction** of background scattering due to multiple scattering from the complex sample environment

Simulations of a 15 T Magnet

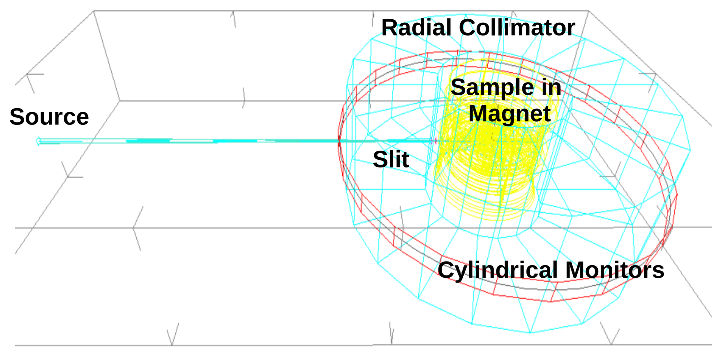
Layer-by-layer





Simulations made in McStasScript, using McStas Union [2,3]

Powder Diffraction Experiment [3,4]



Database of Simulation Results

Simulations were run on the ESS DMSC cluster

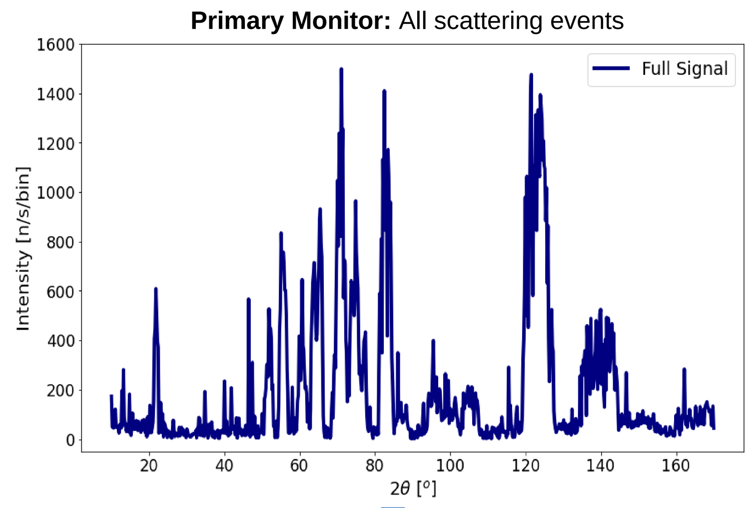
Produced over **24000** simulations based on 7 variable instrument parameters:

- Wavelength: λ, dλ
- Beam divergence
- Sample height/radius
- Sample – Detector distance
- Sample material

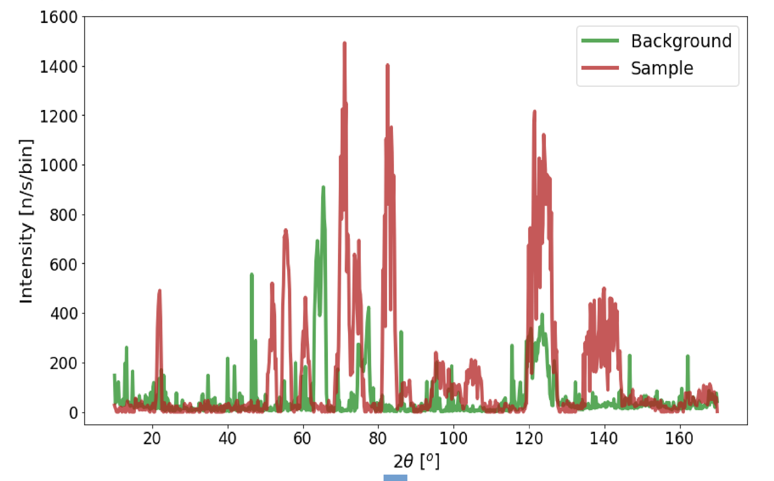
Sampled from random uniform distributions

Example: Simulation of a $La_{2-x}Sr_xCuO_4$ sample with λ = 1.475 Å

Primary Monitor: All scattering events



Sample Monitor: Neutrons scattered only once and by the sample
Background Monitor: All remaining scattering events



Features

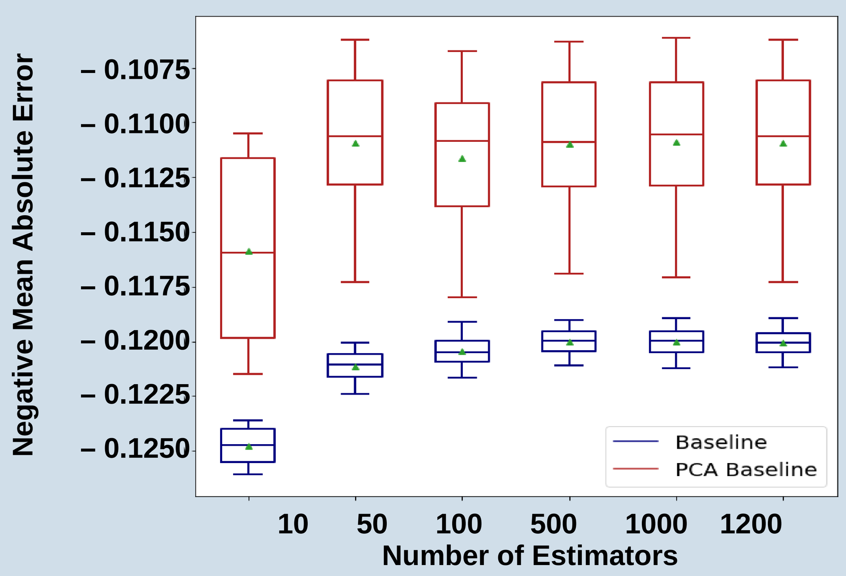
Target Values

What data predicts background better?

Exploration with a Random Forest ...

Dimensionality Reduction

High-dimensional *or* reduced features?



High-dimensional	**PCA** Principal Component Analysis
807 features	81 features

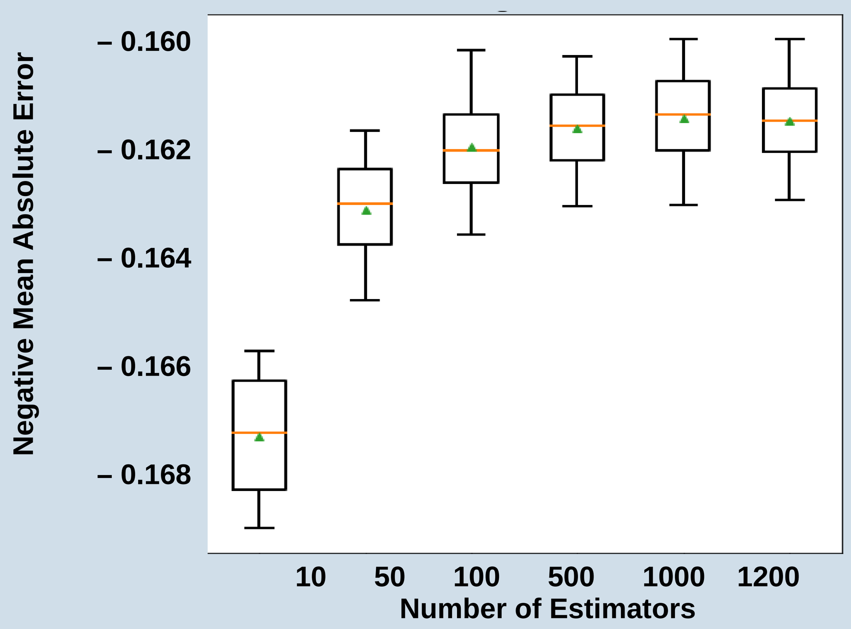
- 7 Instrument parameters
- 800 Intensity/angle values

- 89.96% of initial features
- 94.45% of information

Input: PCA

Information – Complexity trade-off

High-dimensional *or* reduced target values?



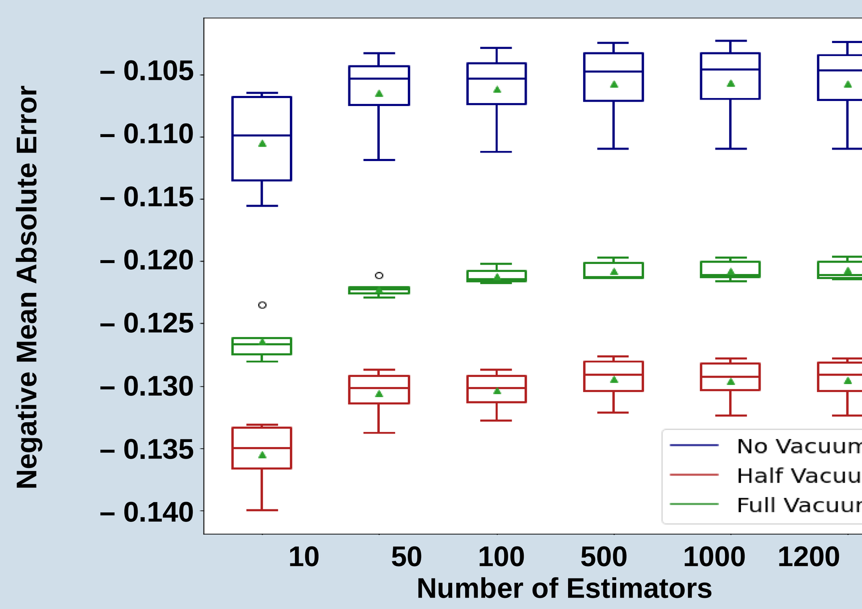
Target Values: Normalised intensity within 10° – 170°

800	**160**
5 bins/degree	1 bin/degree
MAE = 0.161	MAE = 0.111

Output: 160 values

Bias Exploration

Include background measurements in the training sample?

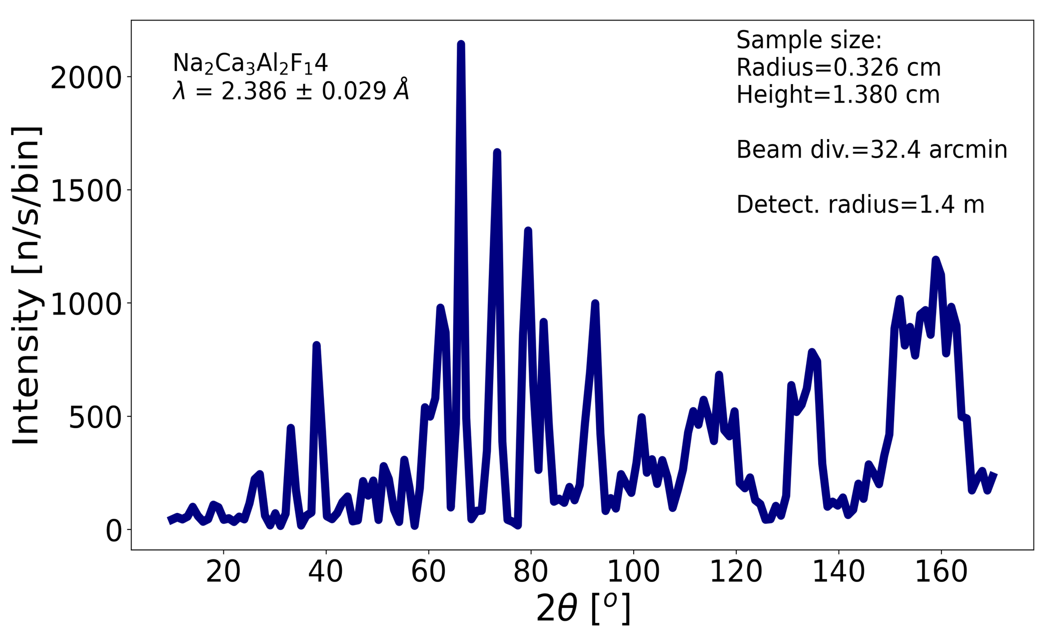


0%	**50%**	**100%**
MAE = 0.105	MAE = 0.129	MAE = 0.121

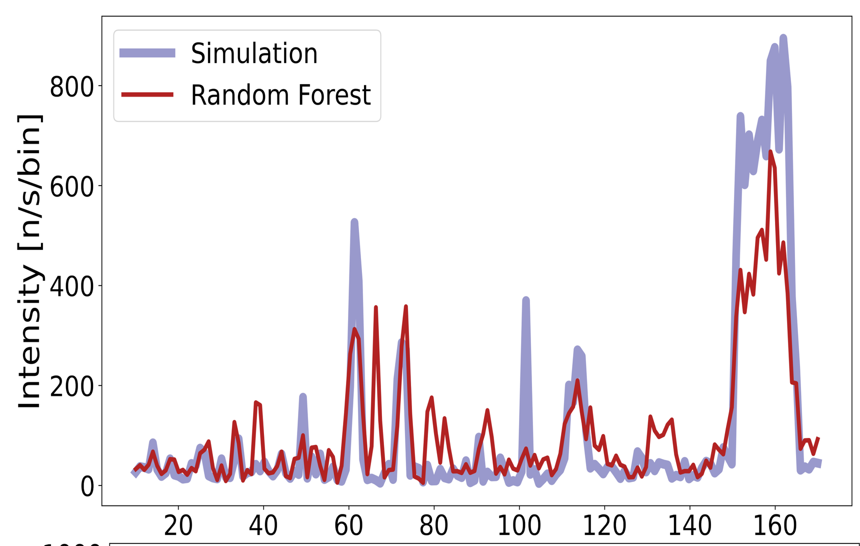
No Backround

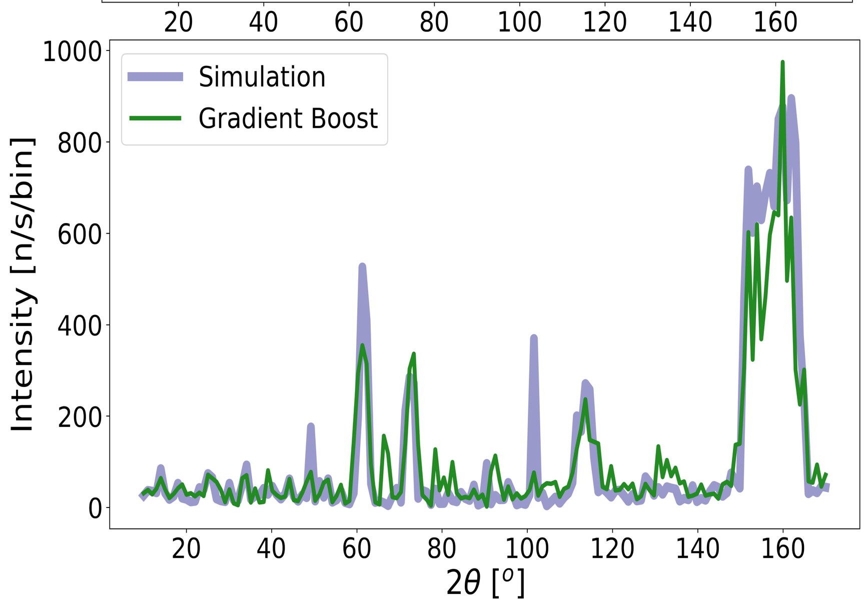
Random Forest vs Gradient Boost

Simulation

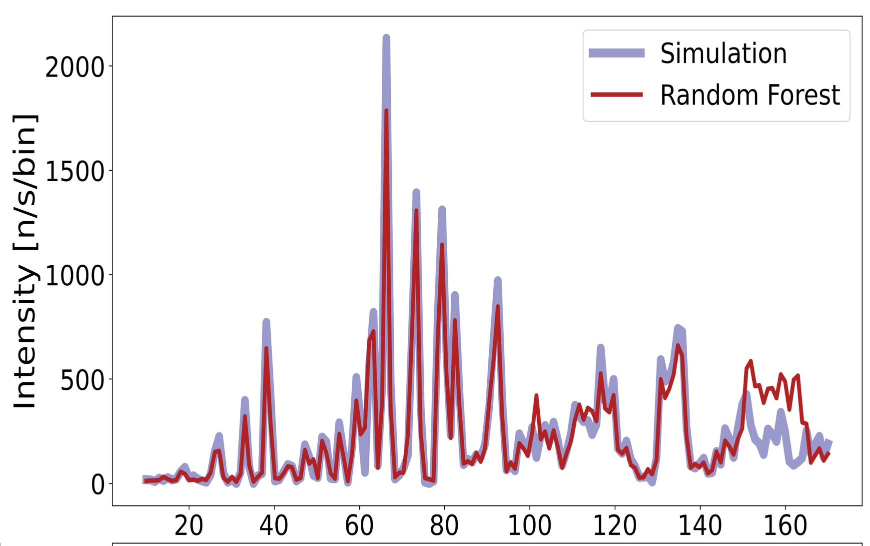


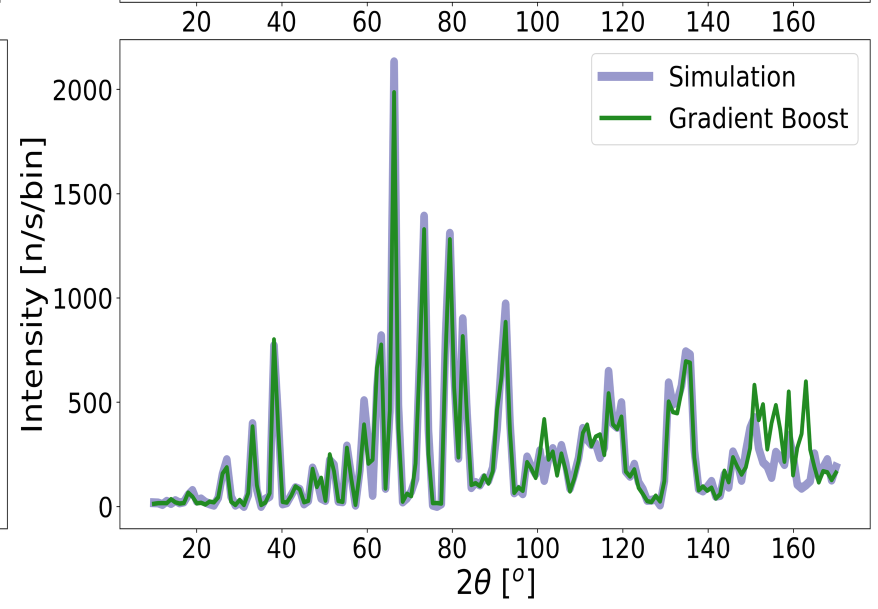
Predicted Background





Predicted Sample





Overall Performance

Model	Random Forest	Gradient Boost
MAE	0.1215	0.1192

What's Next?

- Simulation improvements
- Database restructuring
- Neural Network and Deep Learning models
- Material-agnostic models

EUROPEAN SPALLATION SOURCE

References

1 K.H. Andersen et al. "The instrument suite of the European Spallation Source". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 957 (2020), p. 163402. ISSN: 0168-9002. DOI: https://doi.org/10.1016/j.nima.2020.163402. URL: https://www.sciencedirect.com/science/article/pii/S0168900220300097.

2 Mads Bertelsen. "Software for simulation and design of neutron scattering instrumentation". PhD thesis. University of Copenhagen, Faculty of Science, Niels Bohr Institute, Nano . . ., 2017.

3 Peter Kjær Willendrup and Kim Lefmann. "McStas (i): Introduction, use, and basic principles for ray-tracing simulations". In: *Journal of Neutron Research* 22.1 (2020), pp. 1–16.

4 Peter Kjær Willendrup and Kim Lefmann. "McStas (ii): An overview of components, their use, and advice for user contributions". In: *Journal of Neutron Research* 23.1 (2021), pp. 7–27.