

Scientific data process at CSNS

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IHEP, CAS



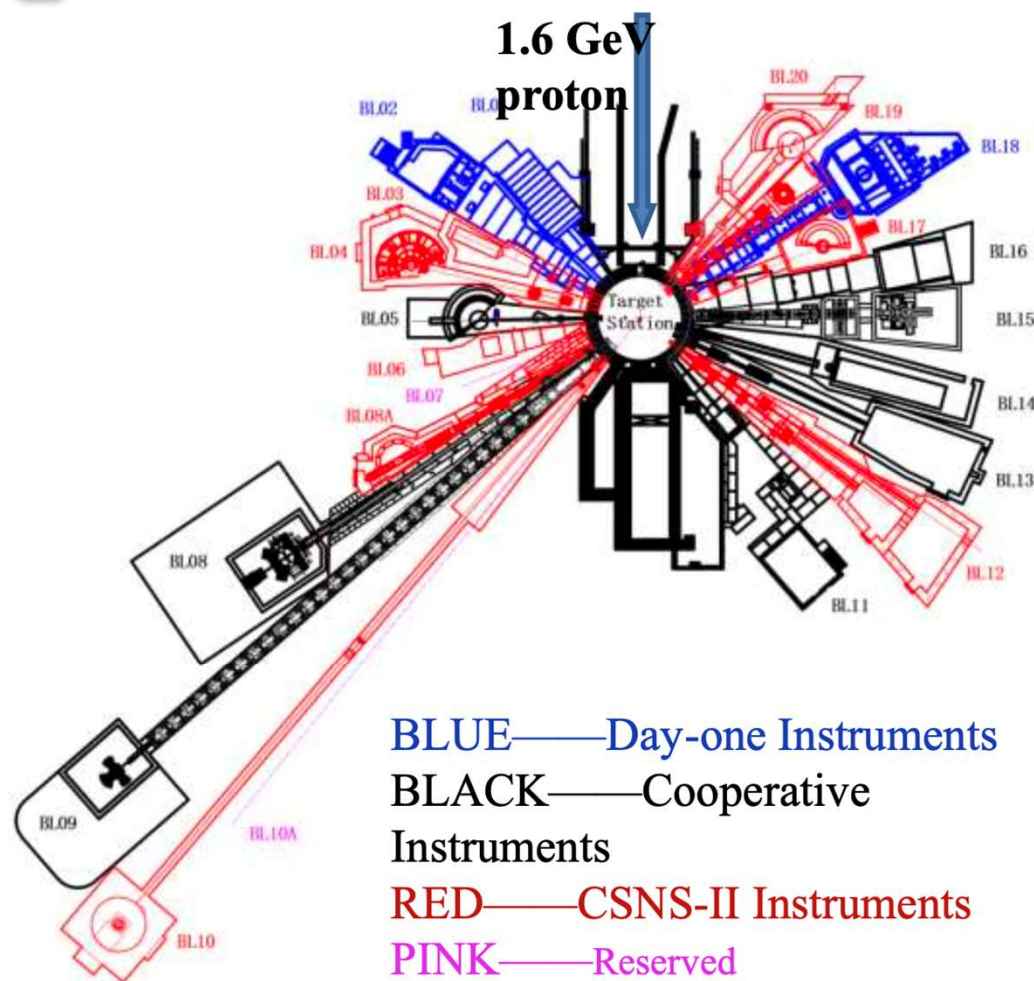
Introduction of CSNS



- 2001: conceptualization
- 2006: key technology research initiated
- 2011: construction began
- 2014: equipment installation and commissioning
- 2017: first neutron beam production
- 2018: project completion
- 2021: energy increase to 100 kW
- 2024: phase II construction initiated



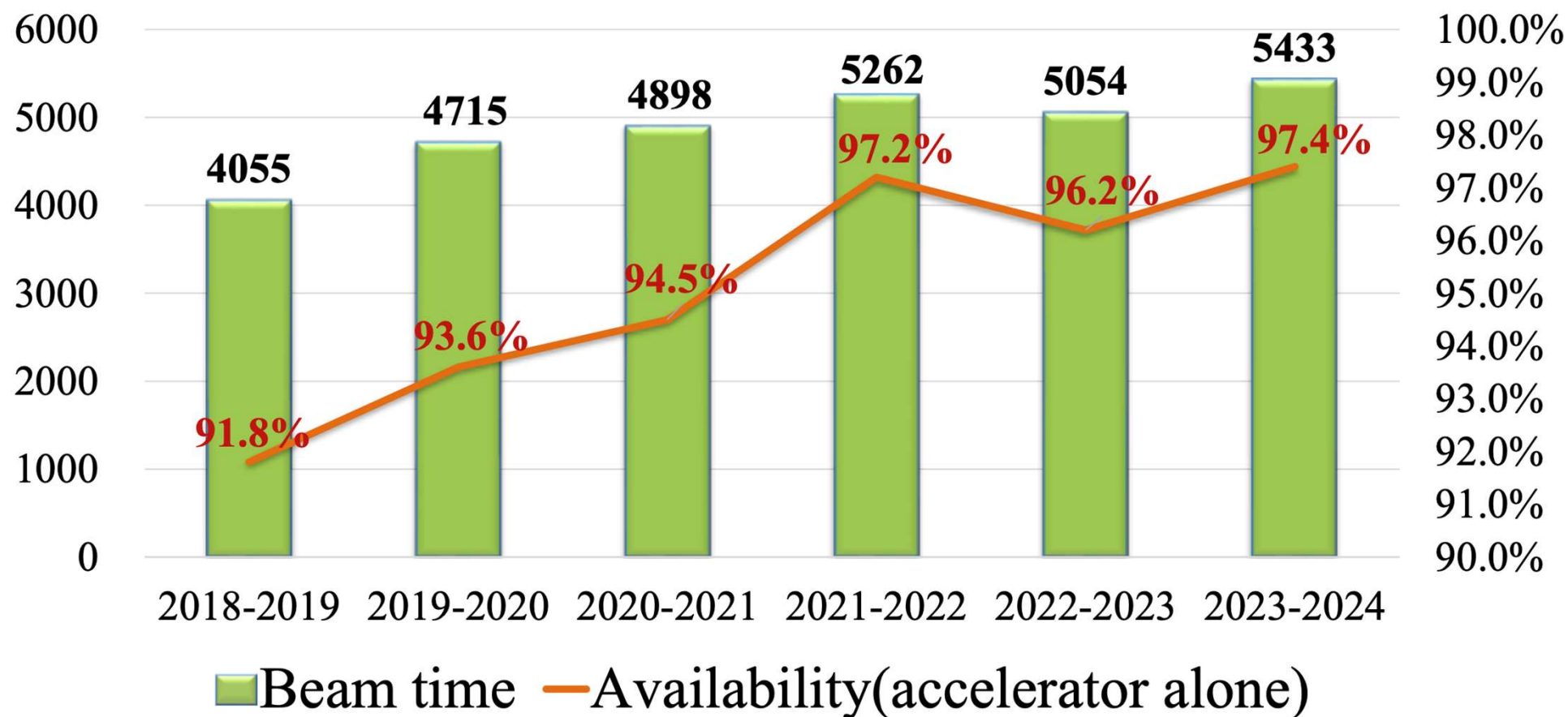
Neutron Instruments



Location	Instrument
BL01	Small Angle Neutron Scattering
BL02	Multiple Purpose Reflectometer
BL03	Liquids Neutron Reflectometer
BL04	Cold Neutron Inelastic Spectrometer
BL05	High Energy Direct Geometry Inelastic Spectrometer
BL06	Molecular Vibrational Spectrometer
BL07	Reserved
BL08	Engineering Material Diffractometer
BL08A	Neutron Technology Testing Station
BL09	High-resolution Neutron Powder Diffractometer
BL10	Neutron Backscattering Spectrometer
BL10A	Reserved
BL11	Atmosphere Neutron Irradiation Spectrometer
BL12	Neutron Physics and Application Instrument
BL13	Energy-resolved Neutron Imaging Instrument
BL14	Very Small Angle Neutron Scattering Instrument
BL15	High Pressure Neutron Diffractometer
BL16	Multi-Physics Instrument
BL17	Elastic Diffuse Scatting Spectrometer
BL18	General Purpose Powder Diffractometer
BL19	Single Crystal Neutron Diffractometer
BL20	PolArized Chopper Spectrometer

User hours and availability

➤ we provide over 5,000 hours of beam time every year

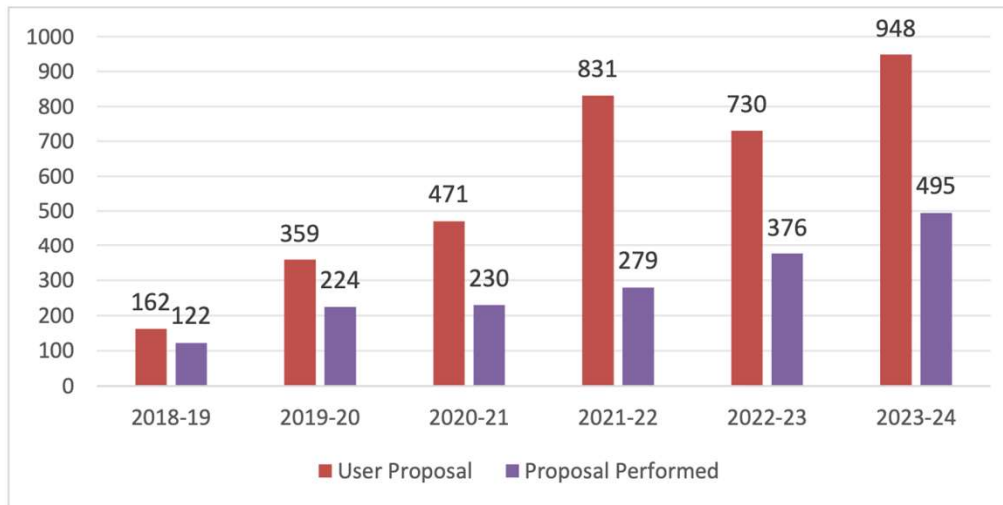




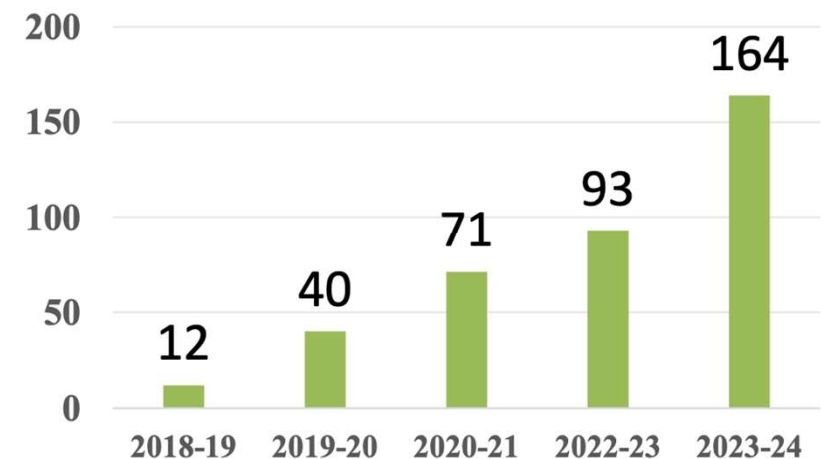
User program

<https://user.csns.ihep.ac.cn> (in both Chinese and English)

- Registration user: 8000+ (130+ abroad)
- A total of over 2,000 projects from ~240 units were completed, with industry users comprising approximately 10% of the total.
- Two rounds of proposal calls each year

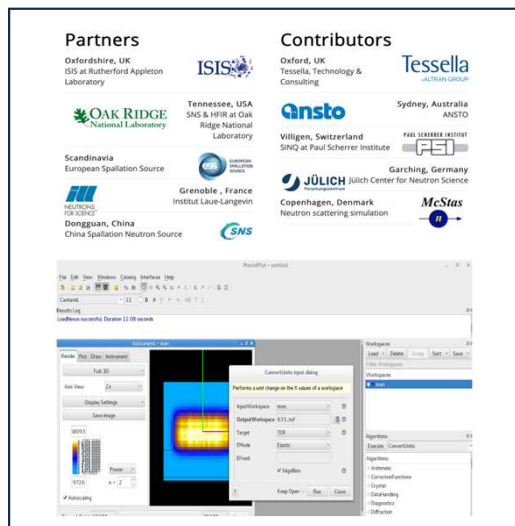
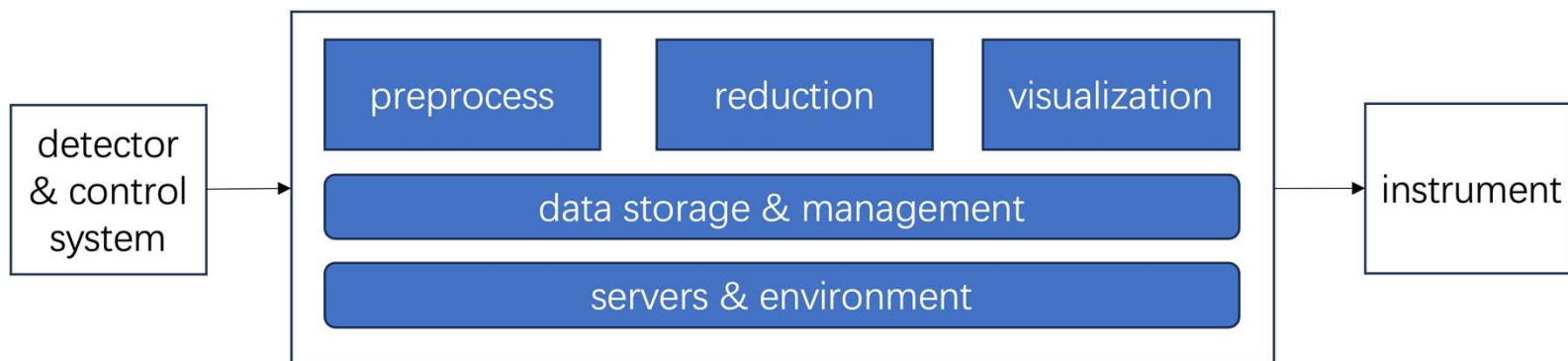


User proposal VS. Proposal proved

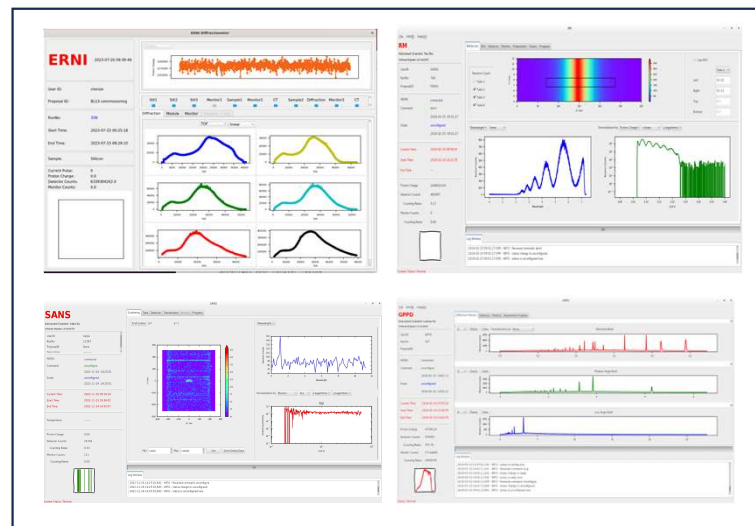


User publication

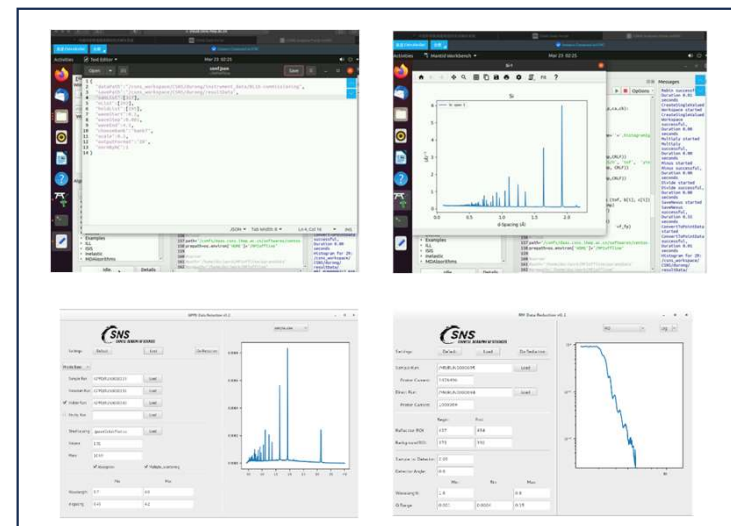
Software at CSNS



joined Mantid in 2019

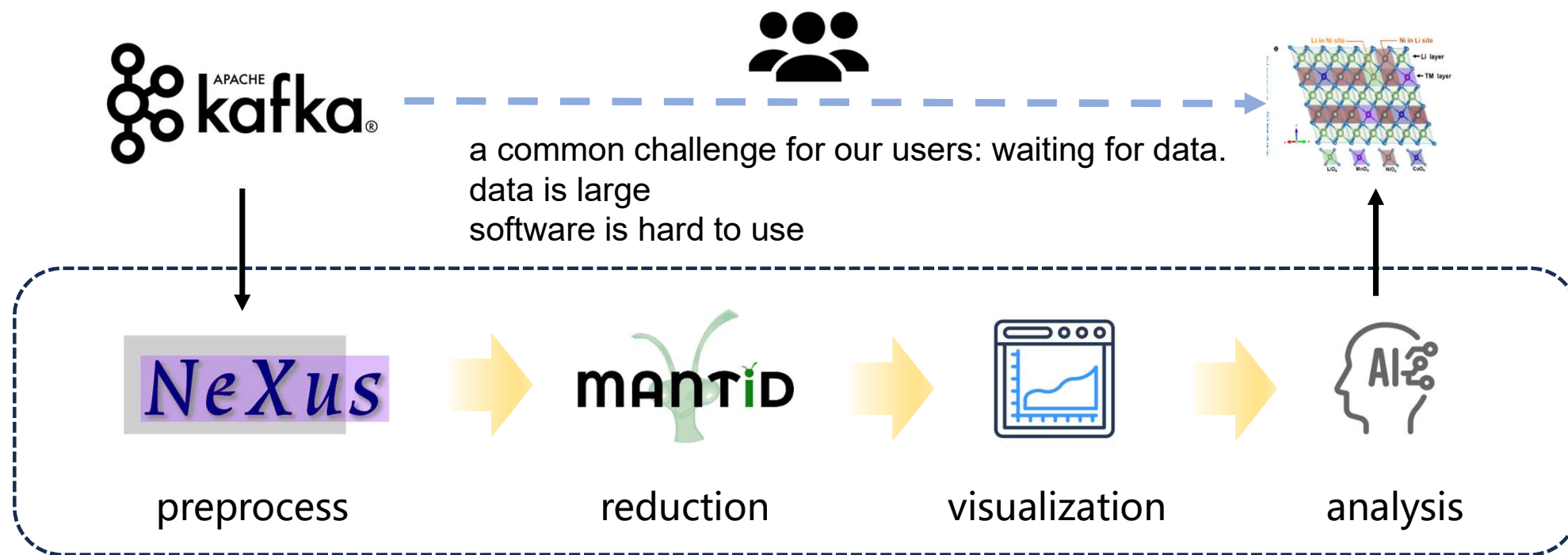


online software



offline software

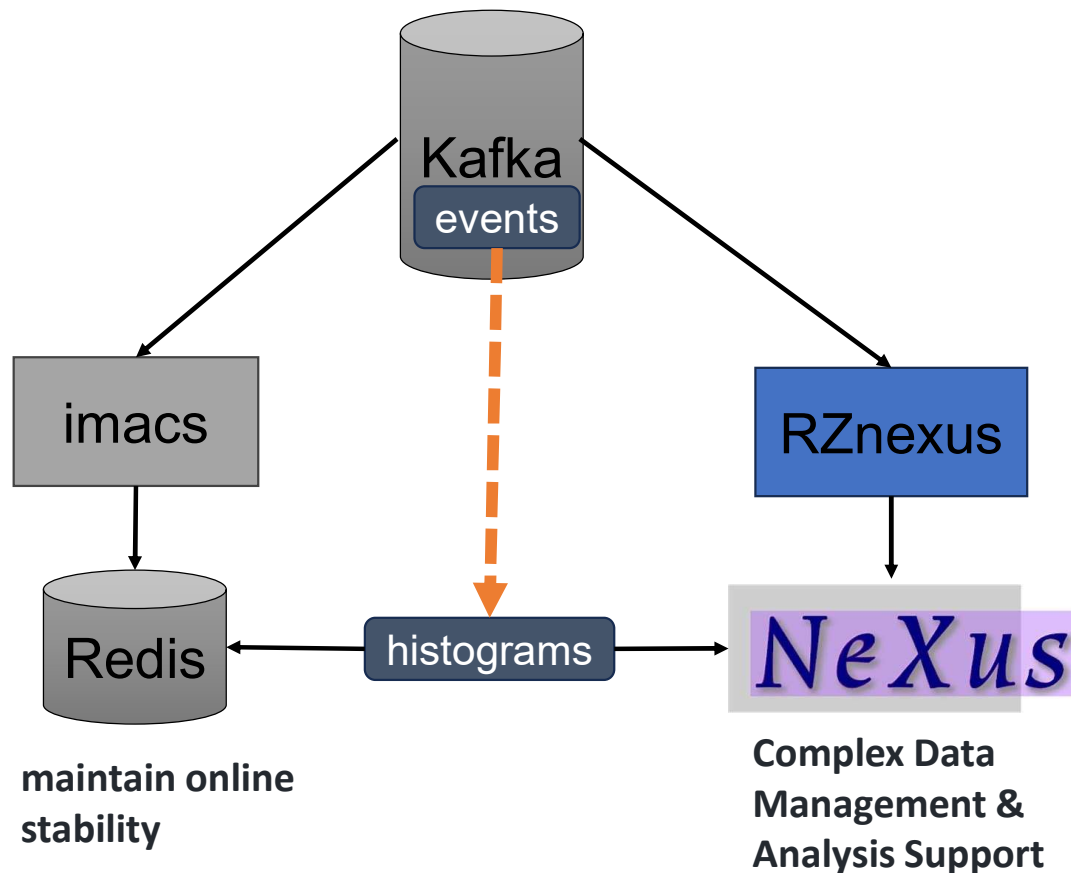
New version of framework



speed up the entire process
Let scientists focus on their science, not on the data

The current RZera only integrates these solutions to make the key steps much faster and smoother. Our ultimate goal is to connect everything into a start-to-finish pipeline.

- convert neutron 'events' into histograms

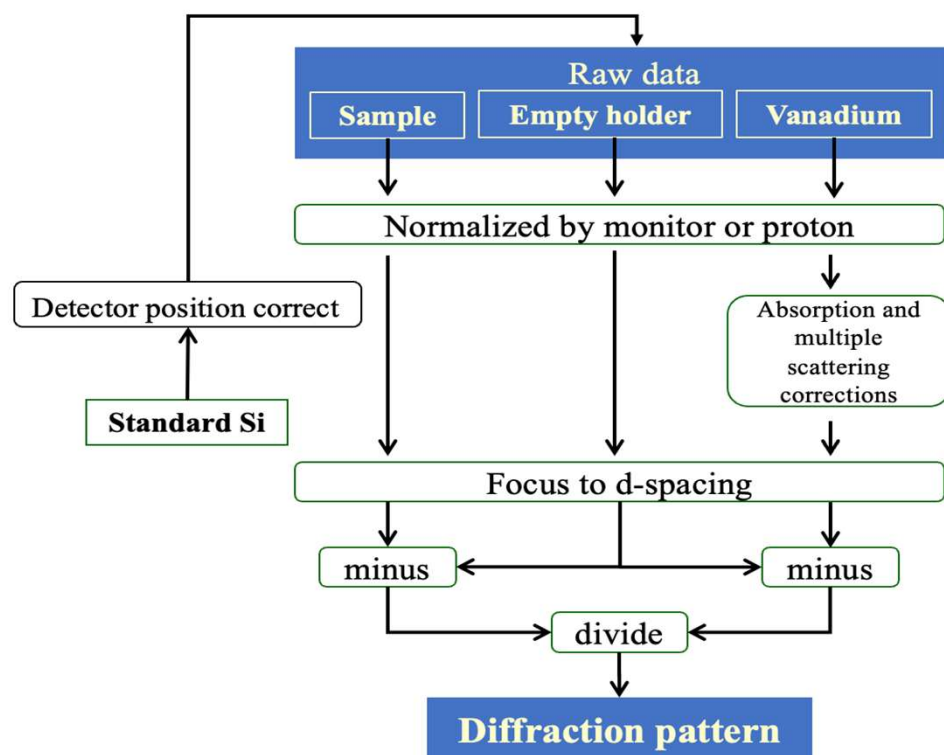


It's designed for large data volumes.
The speed can now match the detector's maximum counting rate.

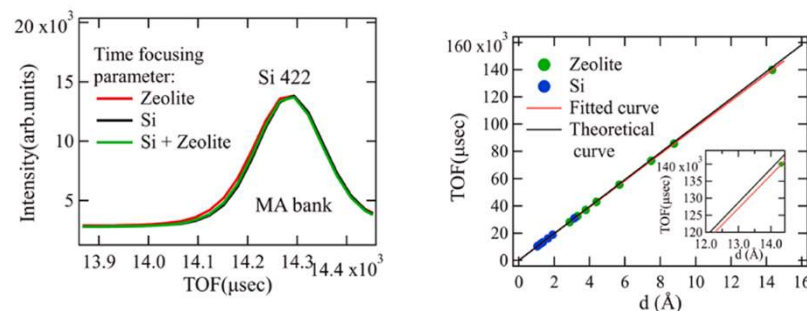
- ✓ **Unified Configuration:** quick integration of new instruments
- ✓ **Multi-threaded operation:** fast processing of high-volume data
- ✓ **Automatic Task Allocation:** conserve resources
- ✓ **Automatic Monitoring:** detect issues

Reduction: powder diffraction

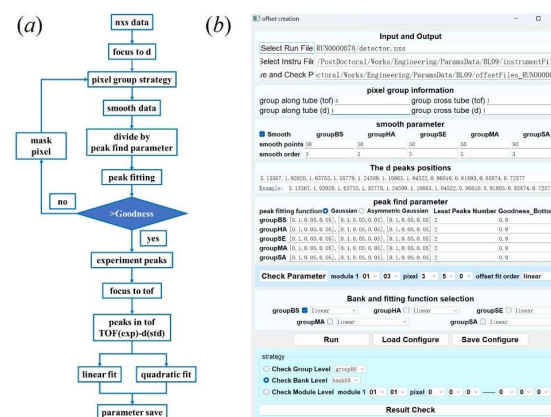
- This workflow is not a one-time, fixed process.



- A new function of advanced time focusing correction



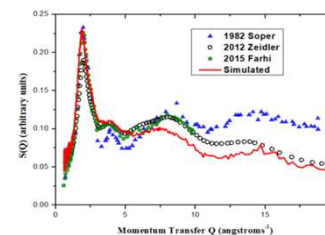
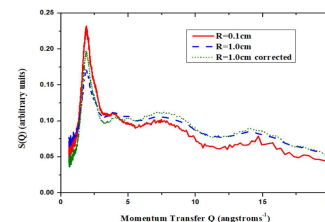
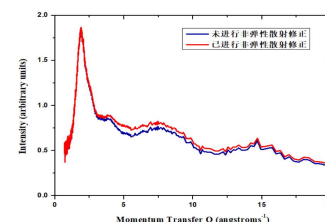
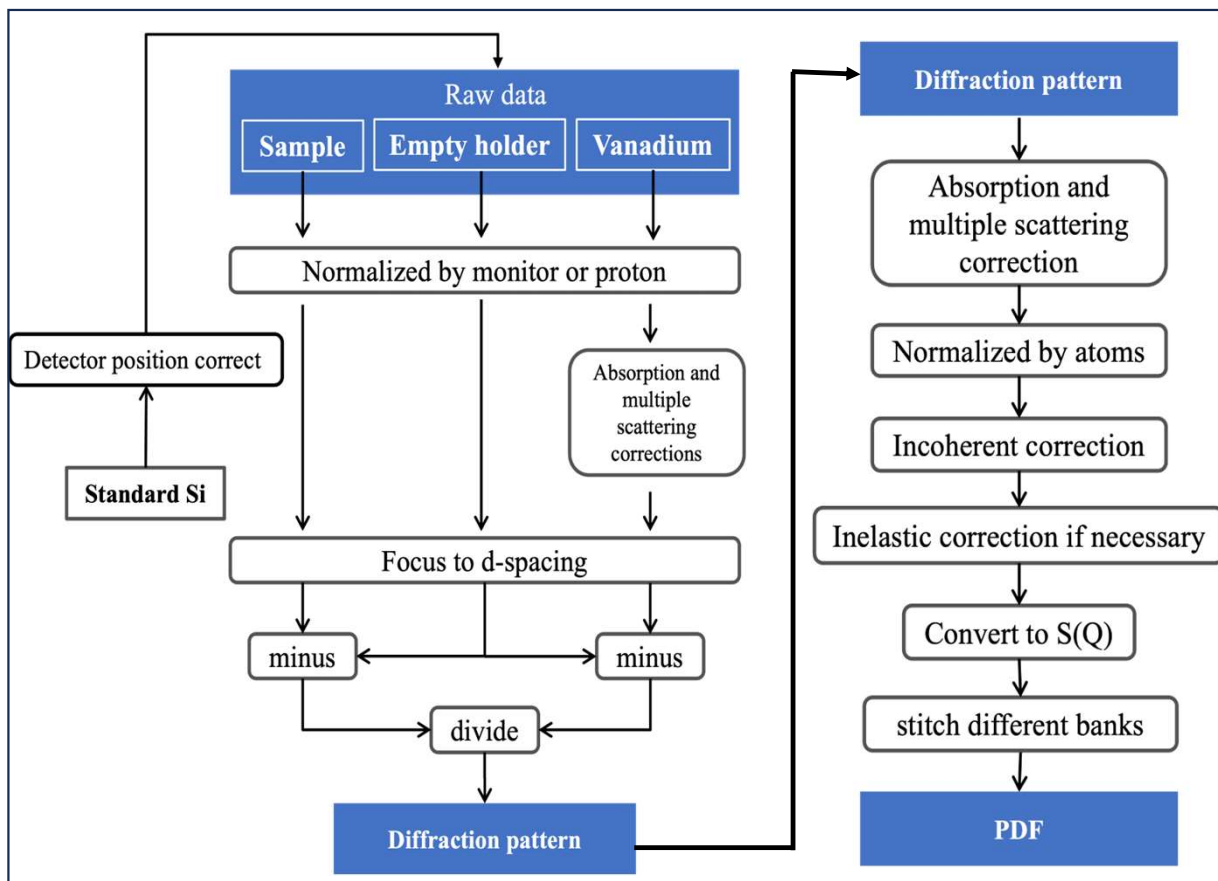
multi-peak fitting of silicon and zeolite



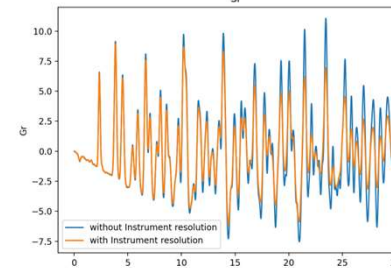
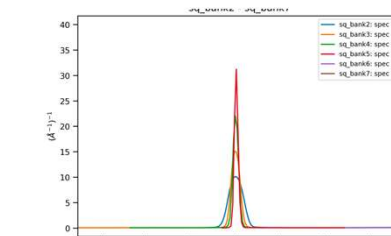
user-friendly function with a clear, step-by-step interface

Reduction: total scattering

- The absolute scattering intensity to calculate the Pair Distribution Function (PDF)



merging the $S(Q)$ data from different detector banks

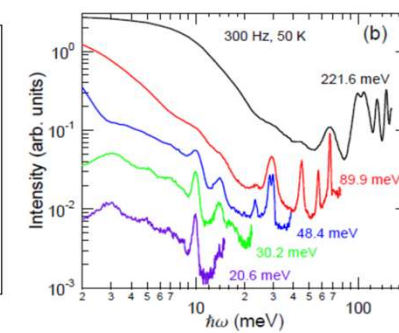
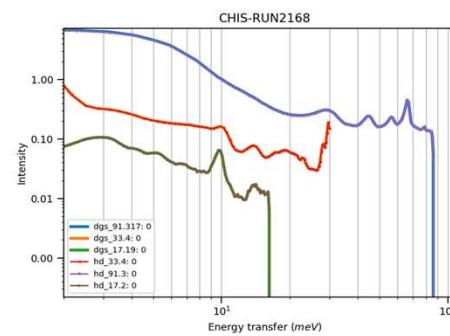
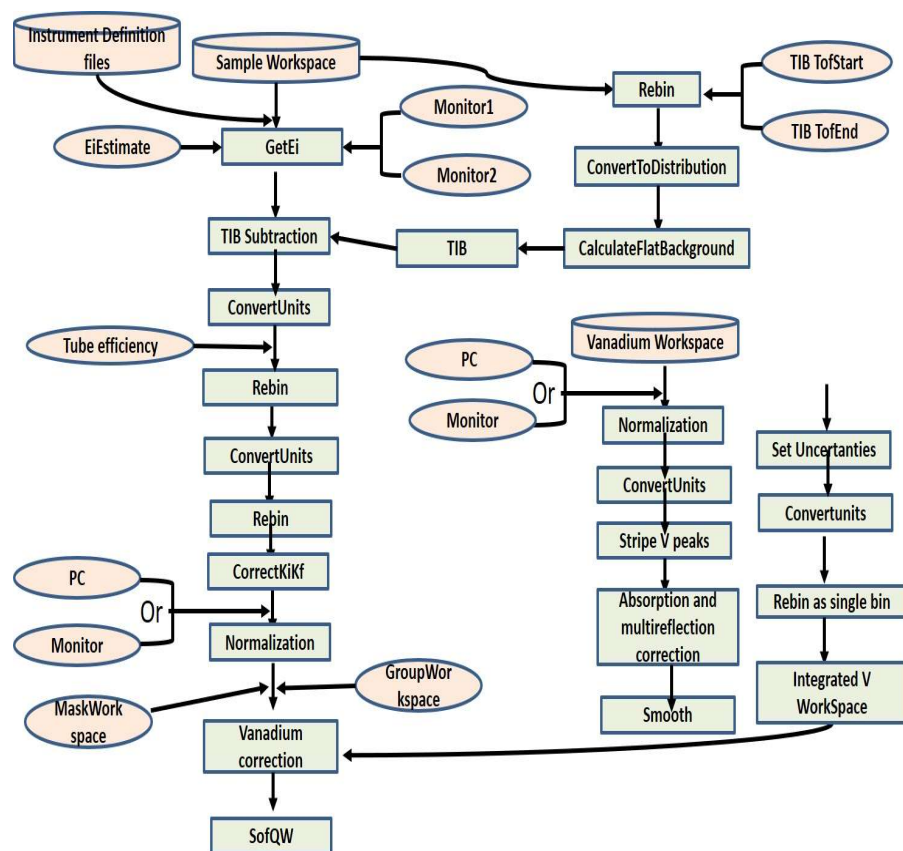


It not only corrects for detector resolution effects but also fully automates the PDF calculation.

Wang, S., et al. (2024). Journal of Applied Crystallography.

Reduction: inelastic scattering

➤ Workflow based on DGS reduction algorithm in Mantid



DgsReduction input dialog

Top-level workflow algorithm for DGS reduction.

Sample Setup:

- SampleInputFile: [Browse]
- SampleInputWorkspace: [Browse]
- SampleInputMonitorWorkspace: [Browse]
- DeCalFilename: [Browse]
- IncidentEnergyGuess: 30.89625
- TimeZeroGuess: 38.23599
- Monitor1Specid: [Browse]
- Monitor2Specid: [Browse]
- EnergyTransferRange: -15.0, 15.28.5
- HardMaskFile: [Browse]
- GroupingFile: [Browse]
- ShowIntermediateWorkspaces: [Check]

Data Corrections:

- RelocateDetectors: [Check]
- UseIncidentEnergyGuess: [Check]
- SoftPhiElasticDistribution: [Check]

Buttons: Keep Open, Run, Close

CSNSdirectgeometry input dialog

Inelastic scattering reduction for HD

Sample: BL05/RUN0002168/detector.nxs [Browse]

Instrument: /Users/kobude/paramsData/BL... [Browse]

Toffset: 0

multiEI: 33.91

DoEICorrection: [Check]

DoVanadium: [Check]

Vanadium: BL05/RUN0002225/detector.nxs [Browse]

Flux Normalization:

- DoFluxNormalization: [Check]
- FluxNormalizationType: Monitor

Mask or Group:

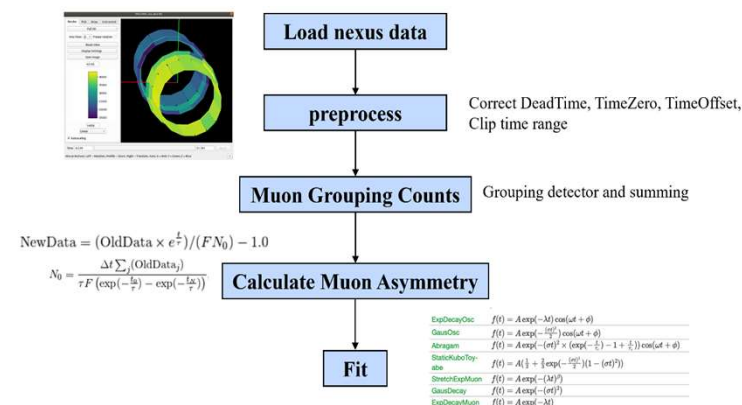
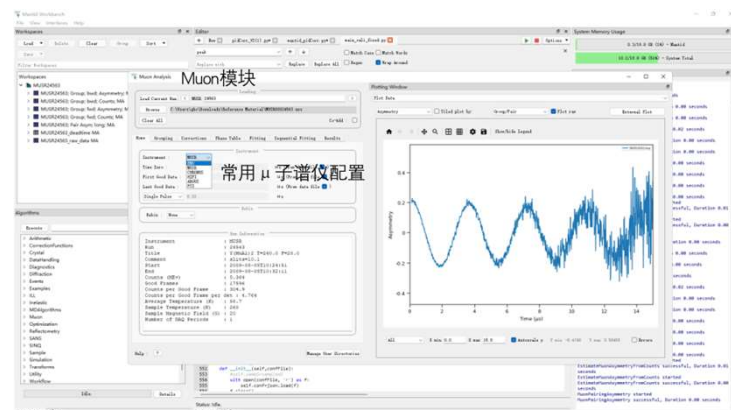
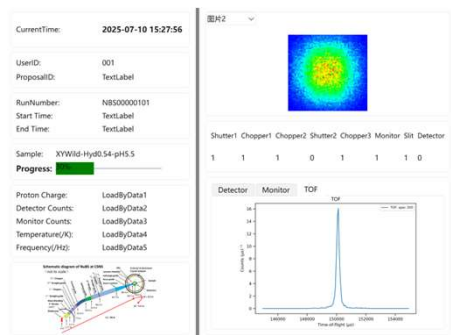
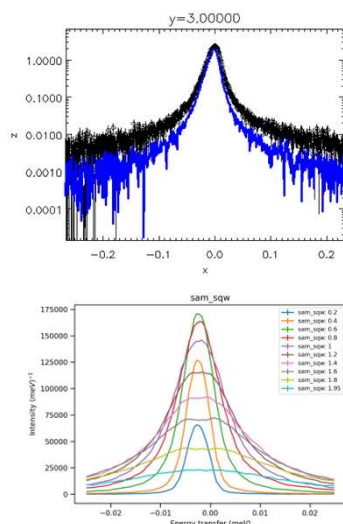
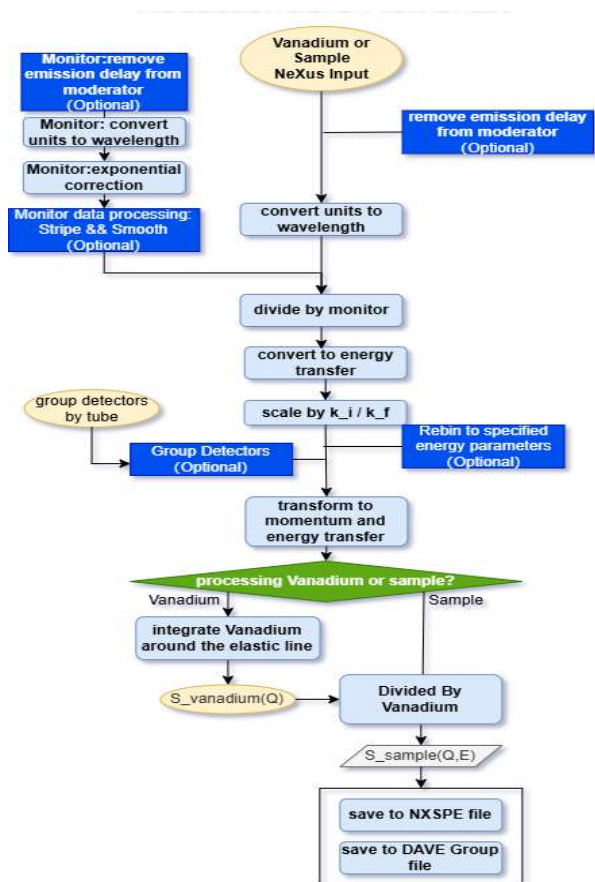
- DoMask: [Check]
- MaskFile: ers/kobude/HD_2024/mask_202410.xml [Browse]
- DoGroup: [Check]
- GroupFile: ers/kobude/HD_2024/group_degree.xml [Browse]

MomentumTransferBins: 0.5, 0.01, 8

Buttons: Keep Open, Run, Close

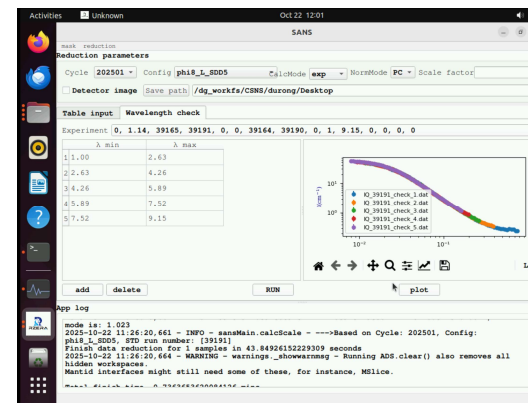
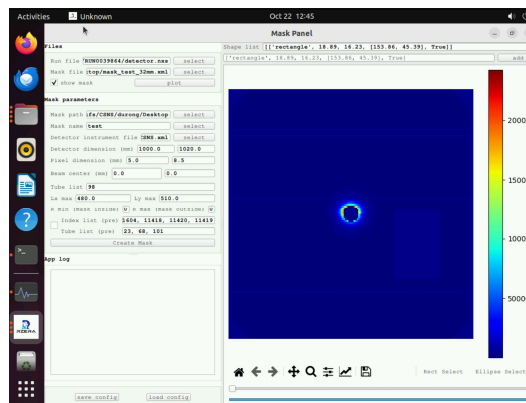
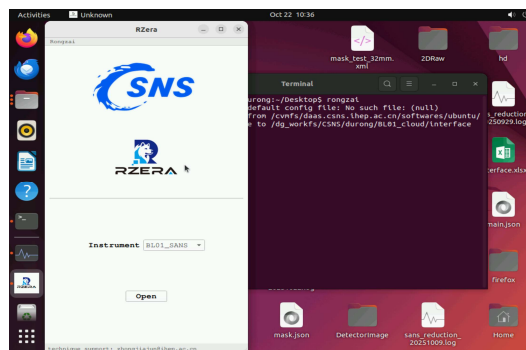
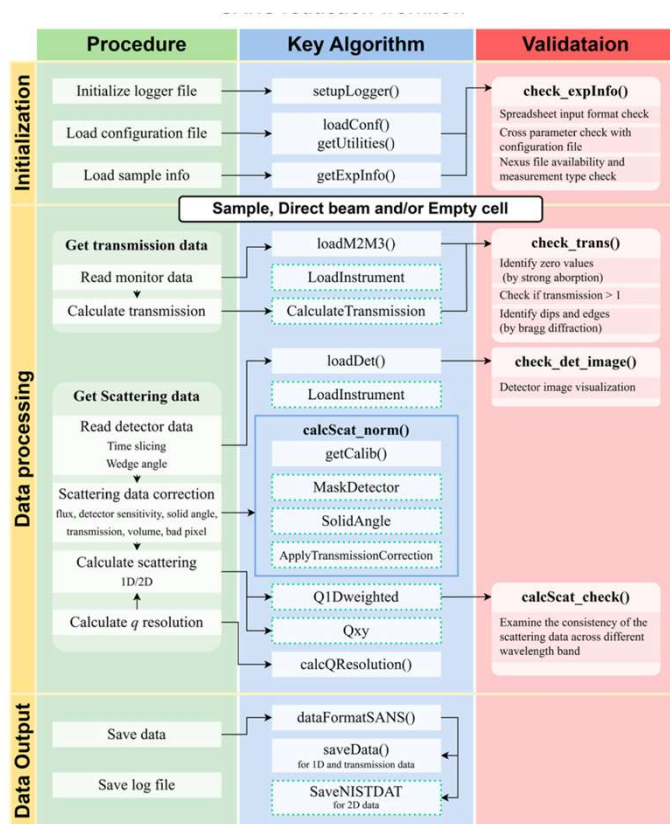
Reduction: Phase II

- Use McStas simulations and process them through existing workflows in Mantid



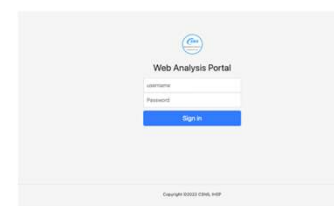
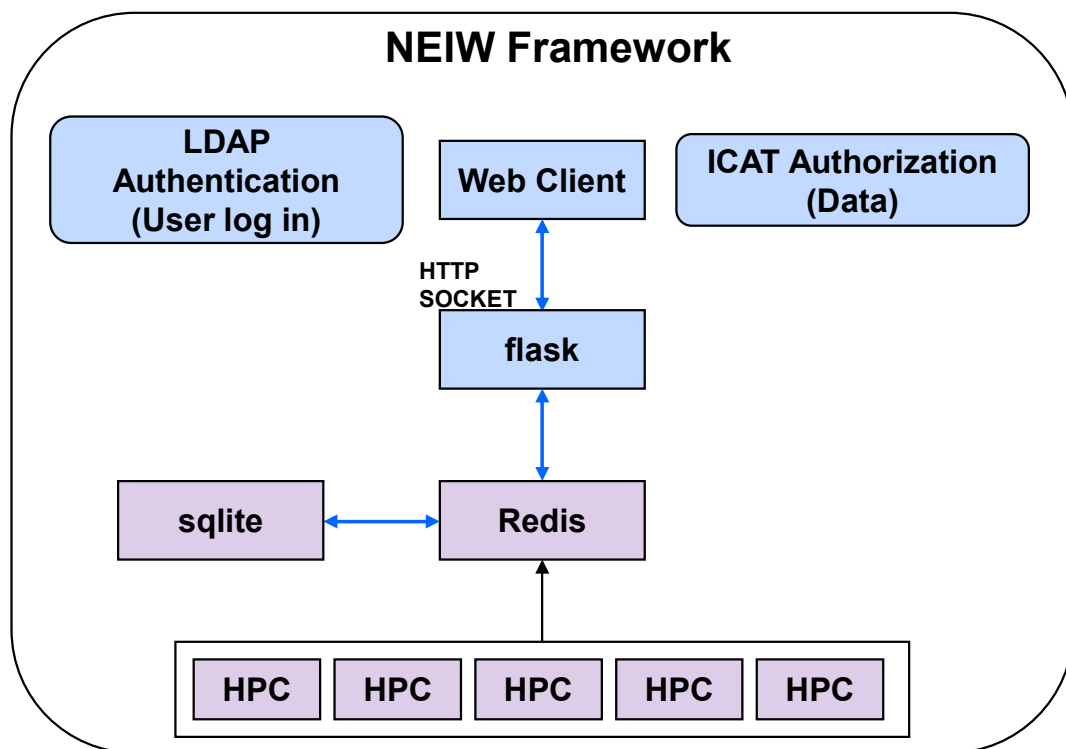
Visualization: SANS

- The standalone sansRZ software for our SANS instrument.
- ✓ It uses the powerful and trusted algorithms from Mantid
- ✓ Designed for our instrument's architecture and user community
- ✓ It handles data quickly and includes features to help users spot potential data issues early on.



➤ web interface for diffractometer

utilize SLURM for resource scheduling to accommodate various users



#	Title	Proposed	Submitted	Created	Actions
211	BLM commissioning	BLM commissioning	BLM	2021-01-16 07:45:47	View
212	BLM calibration	BLM calibration	BLM	2021-01-16 07:45:47	View
218	基于中子衍射技术对材料性能进行表征	基于中子衍射技术对材料性能进行表征	PM2101000001	2021-01-16 07:45:47	View
219	LiAlH ₄ D-HO 体系下制备的纳米材料性能表征	LiAlH ₄ D-HO 体系下制备的纳米材料性能表征	PM2101000001	2021-01-16 07:45:47	View
219	基于中子衍射技术对材料性能进行表征	基于中子衍射技术对材料性能进行表征	PM2101000001	2021-01-16 07:45:47	View
219	基于中子衍射技术对材料性能进行表征	基于中子衍射技术对材料性能进行表征	PM2101000001	2021-01-16 07:45:47	View

Wave End: 4.5

Scale Factor

V-Hold: 0.5

Sample-Hold: 0.5

Choose bank, if None, calculate all banks

BankName:

d Rebin:

Reduction

Plot bank data

bank2 bank3

bank4 bank5

bank6 bank7

qmin: 2

qmax: 30

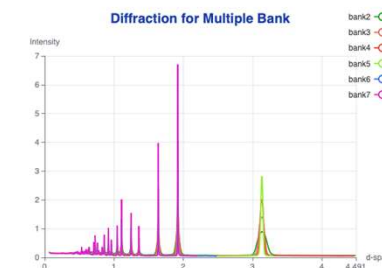
rmin: 1.1

rmax: 25

SoQType: S(Q)

PDFType: G(r)

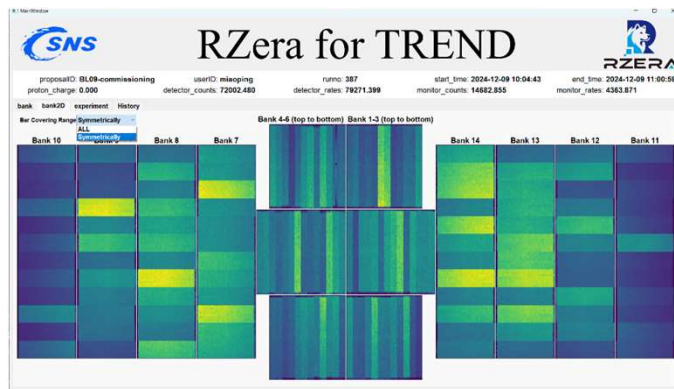
PDF



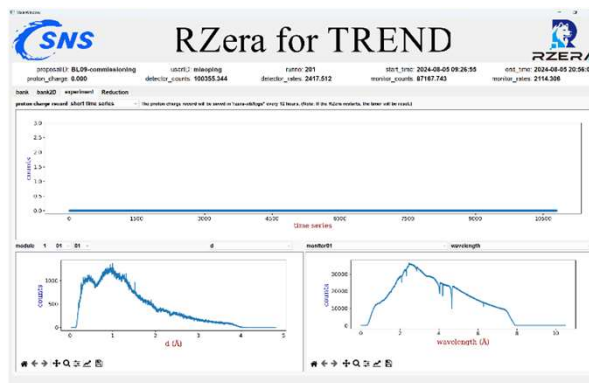


Visualization: online

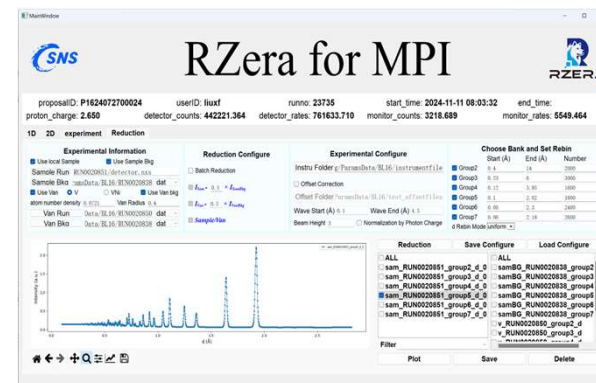
➤ Presented Information



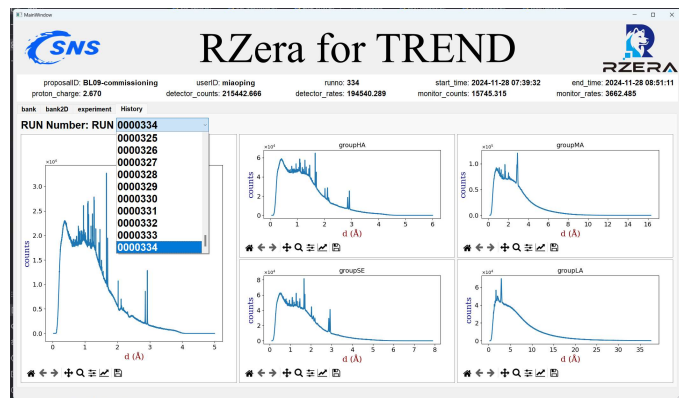
2D detector image



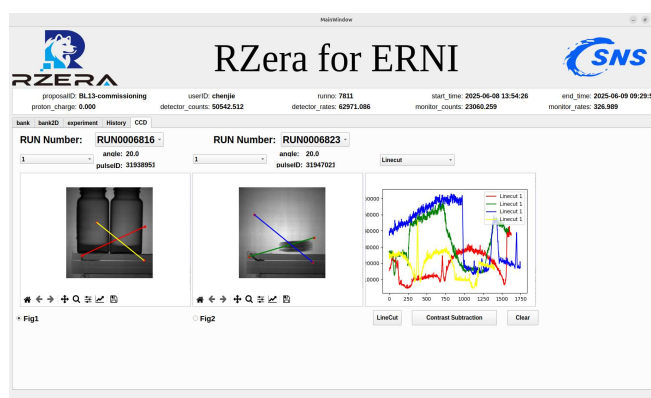
Monitor data, Proton charge



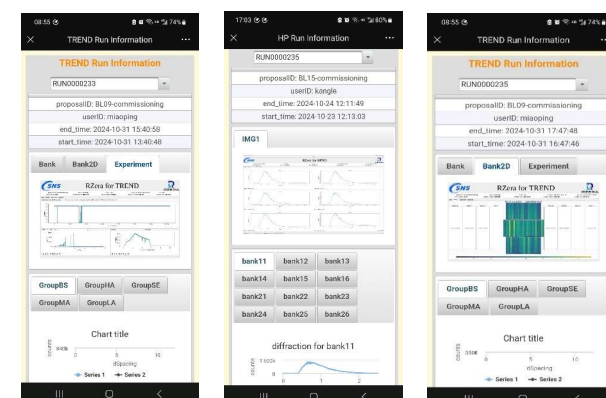
1D reduced data



history data

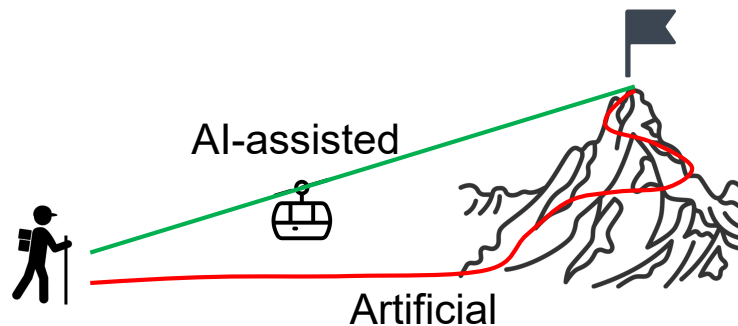


Line Cutting Analysis on imaging data



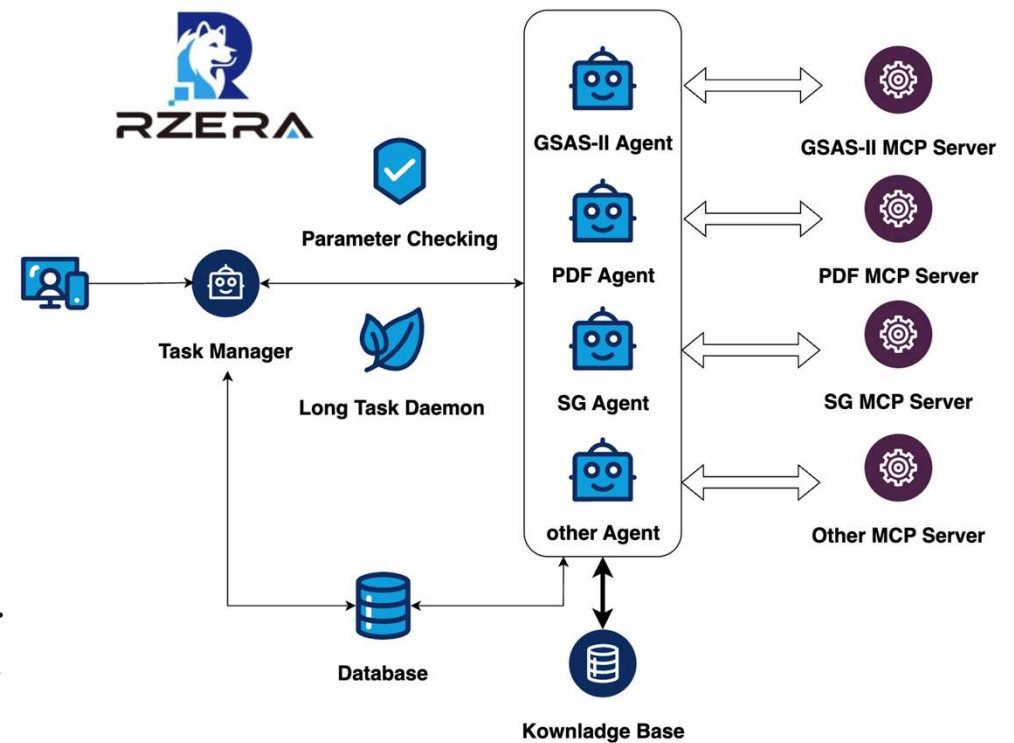
live status through WeChat

- data analysis: Use AI to accelerate scientific discovery.



Solution: An AI Partner

- **Conversational:** It understands your questions.
- **Process-Aware:** It navigates complex workflows.
- **Knowledgeable:** It leverages scientific expertise.



➤ diffraction refinement and PDF fitting in Rongzai Agent

正在分析您需要处理的数据，请稍后...

数据处理失败，原因：在RUN0021905里面没有找到实验信息文件

处理一下BL16 的RUN0021905实验数据，用Si的cif文件，按你的想法做一次衍射精修

处理一下BL16 的RUN0023568实验数据，用Si的cif文件，按你的想法做一次衍射精修

正在分析您需要处理的数据，请稍后...

数据处理失败，原因：处理中子衍射数据时，必须明确指定需要处理的探测器组

处理一下BL16 的RUN0023568实验数据，使用group5，用Si的cif文件，按你的想法做一次衍射精修

正在分析您需要处理的数据，请稍后...

group5组的中子衍射数据精修任务已提交...

group5组的中子衍射数据精修任务已完成!

报告生成成功!

实验报告

用户: Wang Hao 单位: CSNS 谱仪: BL16

中子衍射数据分析报告

实验信息

样品化学式: Si₁

实验RUN号: RUN0023568

实验时间: 2024-10-16T20:58:32+00:00 --- 2024-10-17T20:24:29+00:00

所选择的刻度数据分别是:

- 钽: RUN0023567
- 空盒: RUN0023566

波长范围: 0.1到4.5埃

归一条件: monitor

中子衍射第group5组精修结果

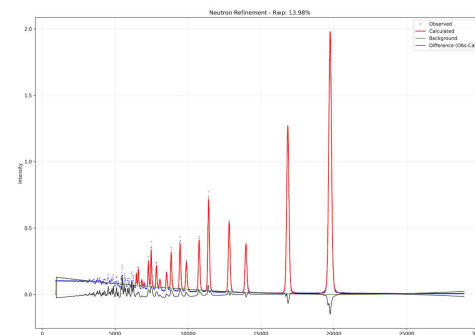
精修后的结构文件

8. refine_cif_url:

This is an early prototype.
We are building a scientific
knowledge base.

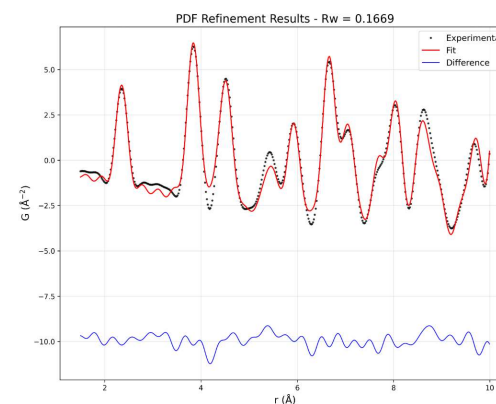
Rongzai Agent: an intelligent,
knowledge-guided assistant

精修后的中子衍射图像



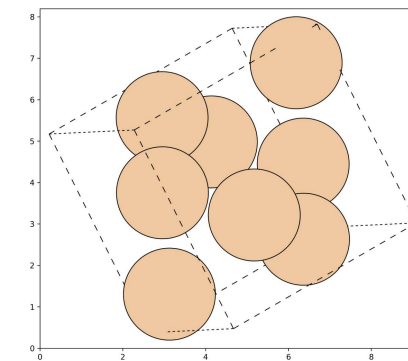
报告文件已上传至<https://nsls1.llnsl.gov/np22/files/file-df911839784685834348379893cd5/preview>

精修后的图像



精修后的结构文件

8. refine_cif_url:

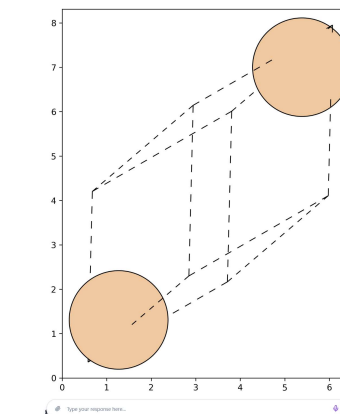


精修后的晶格参数

0.35421108119540 a, 0.35421108119540 b, 0.35421108119540 c 0.000 0.000 0.000 90.000 90.000 90.000

精修后的Rwp

32.99934240172177





RZera = Rongzai Era

Acknowledgments

This work is supported by the National Key R&D Program of China (Grant No. 2023YFA1610000). The raw experimental data was provided by the multi-physics instrument (BL16) of CSNS. Rong Du is grateful to Rongzai for her valuable inspiration and spiritual support.

I would like to thank Rongzai for providing inspiration and spiritual support



Thank you!