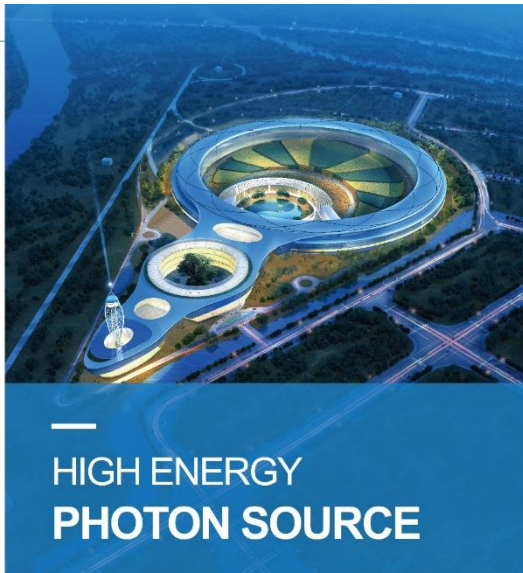


Institute of High Energy Physics

# Next-Generation Scientific Software System and AI-Driven Intelligence for Synchrotron Beamlines



**MAMBA**  
Data acquisition software

Yi Zhang  
2025/8/13

# Outline

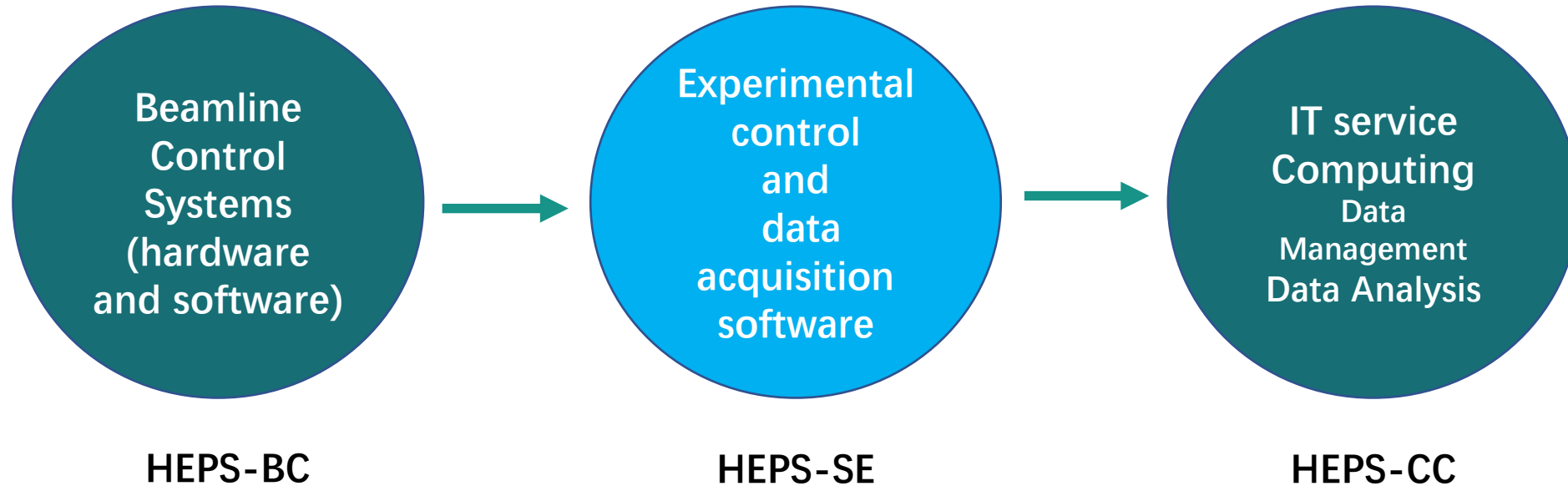
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- **The Mamba project**
- **Addressing big data challenge using AI/ML**
- **Collaborative efforts for intelligent light source**



# HEPS needs a systematic software solution

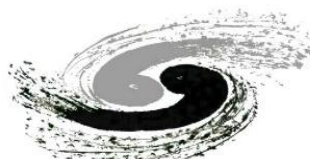
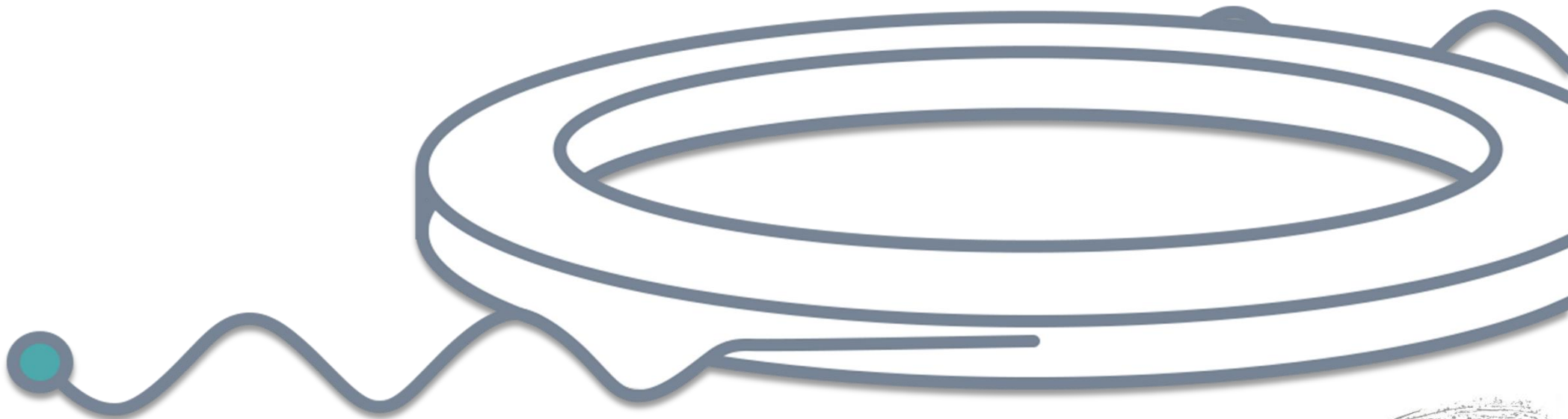
- ❑ Three dedicated HEPS teams for addressing the challenges in control, scientific software and computing



- ❑ Develop Control and acquisition software from scratch, no legacy issue
- ❑ Founded in 2020, HEPS-SE team are aiming to develop a systematic software solution in control and data acquisition for Phase I beamlines in HEPS



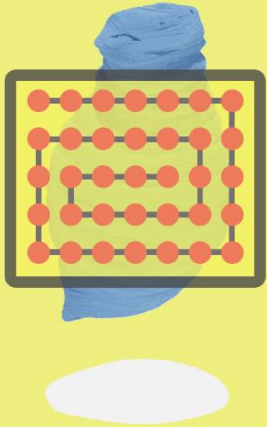
# *The Mamba Project*



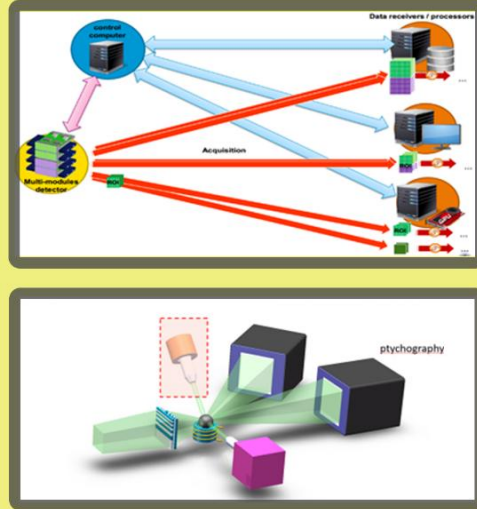


# Drastic increase in data and experiment complexity

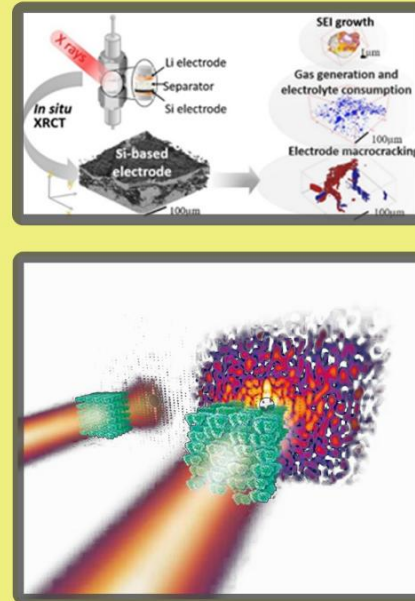
## 1 Nano & macro probe



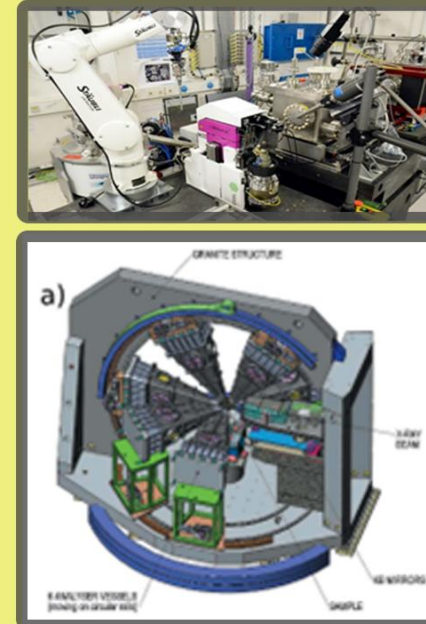
## 2 High throughput & Multi-modal



## 3 In situ & dynamic experiments



## 4 beamline automation & intelligent control

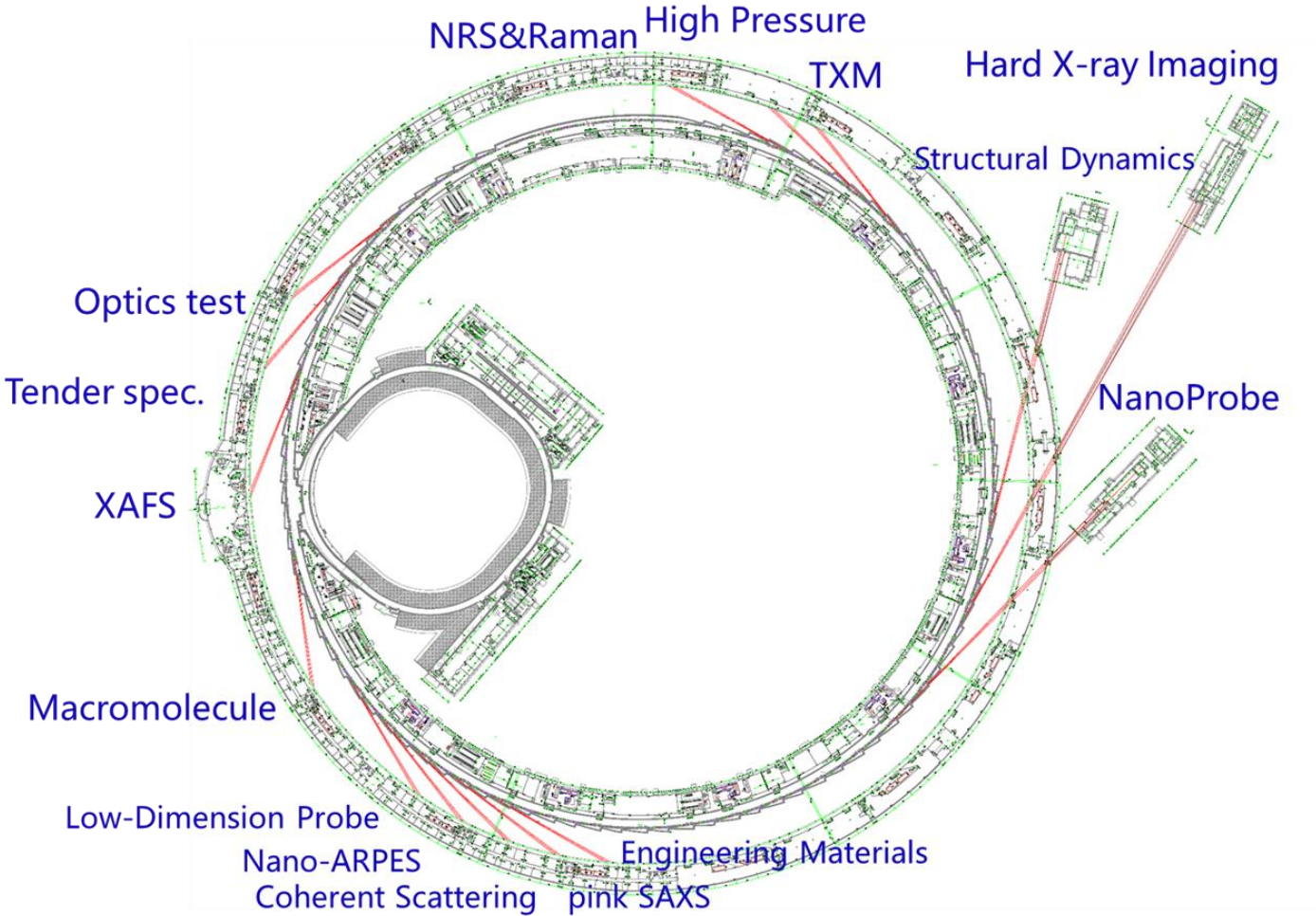


## 5 National data management policy



- X-ray flux orders of magnitude brighter,
- Detectors are orders of magnitude larger and faster, single beamline generate up to  $Pb$  /run,
- *In situ* and *dynamic* experiments require real-time feedback and autonomous control,
- Data and software infrastructure for big science project

# Heavy task for a young team

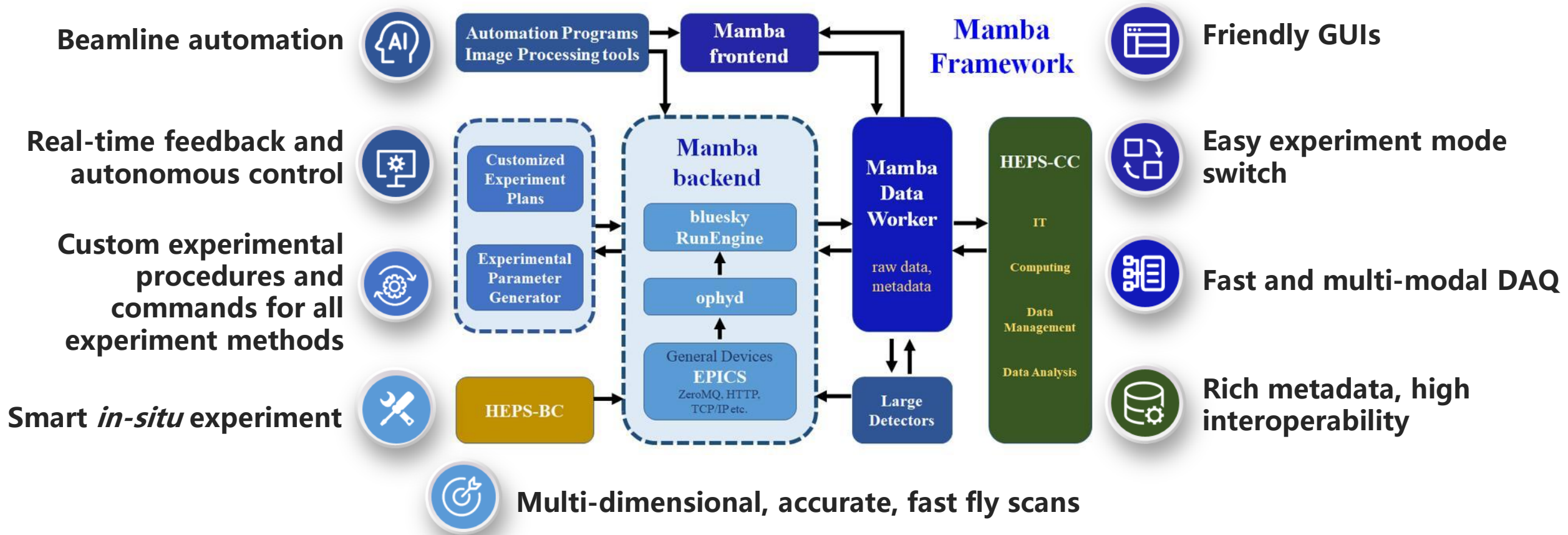


- ❑ 15 beamlines for Phase I project
- ❑ Multiple experimental modes and methods for single beamline
- ❑ Up to 30 suites of acquisition software delivered by 2025
- ❑ Limited personnel and lack of experience
- ❑ A systematic solution for all Phase I and future beamlines



# A new generation synchrotron experiment operating software system

*(Mamba)*

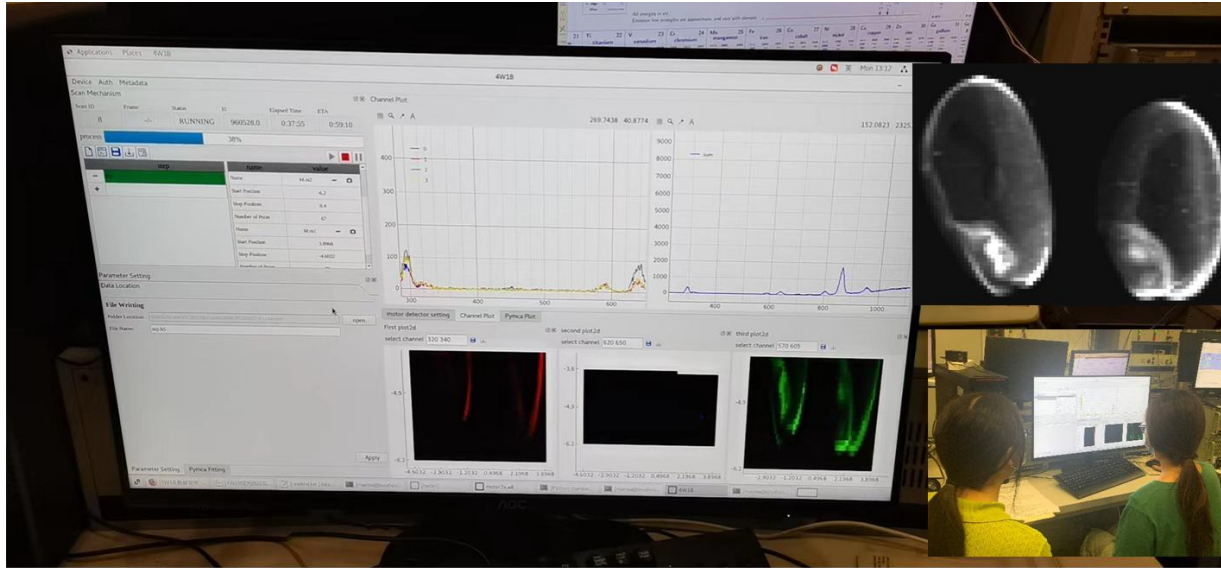


Mamba: a systematic software solution for beamline experiments at HEPS. *Journal of Synchrotron Radiation*, 2022



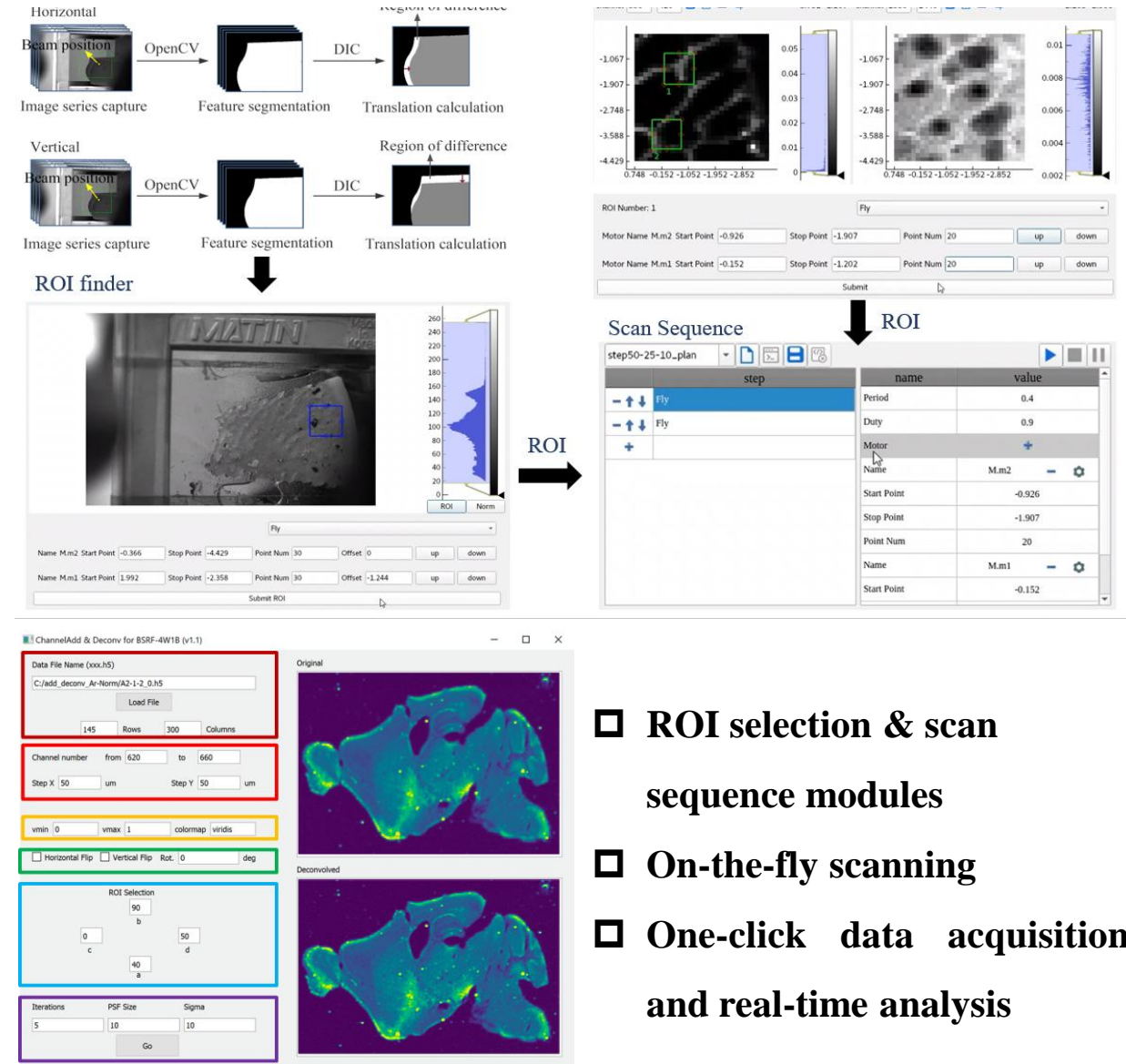


# Progress of *Mamba* project



## Software development & testing XRF mapping at BSRF

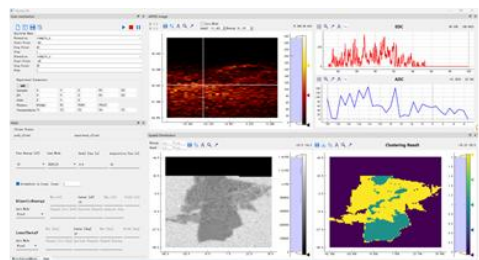
- Project start from April 2020
- *Mamba* was officially deployed and open to users at 4W1B beamline in July 2022



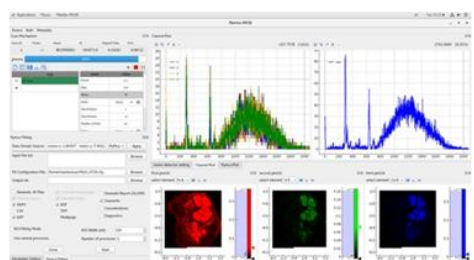
- ❑ ROI selection & scan sequence modules
- ❑ On-the-fly scanning
- ❑ One-click data acquisition and real-time analysis



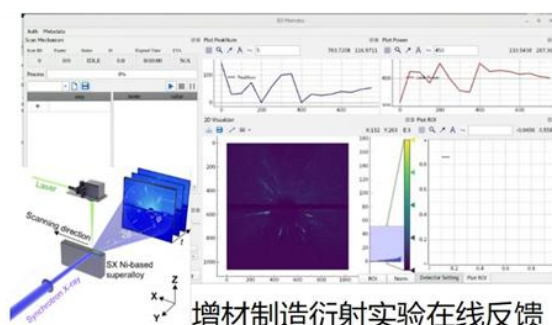
# Test and deployment of Mamba at HEPS



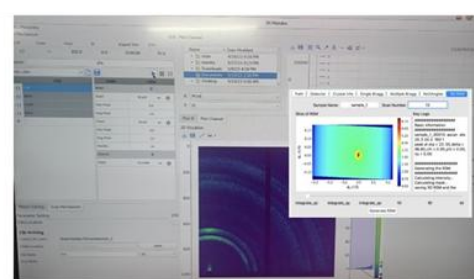
Nano-Arpes



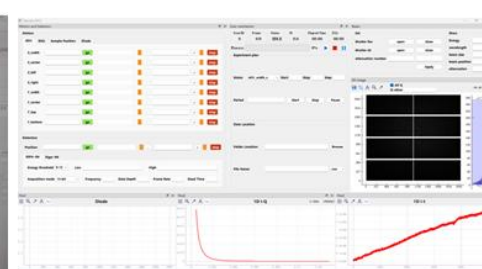
荧光“飞扫”



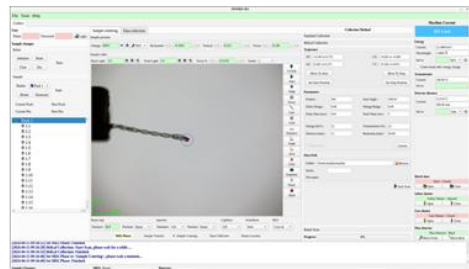
增材制造衍射实验在线反馈



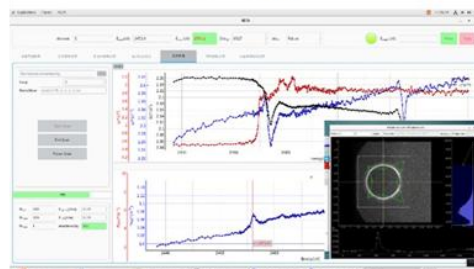
表面衍射



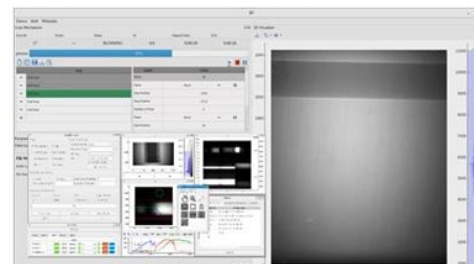
XPCS



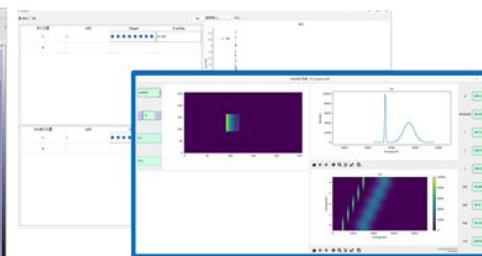
生物大分子



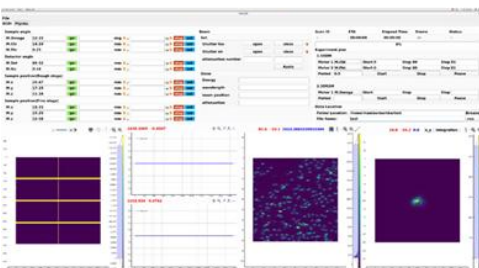
通用吸收谱与发射谱



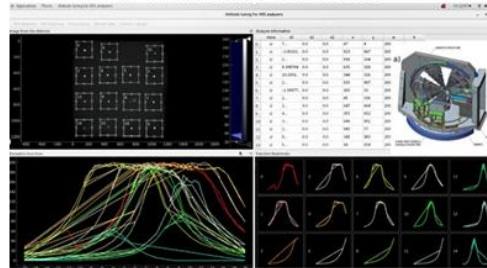
STXM & CT



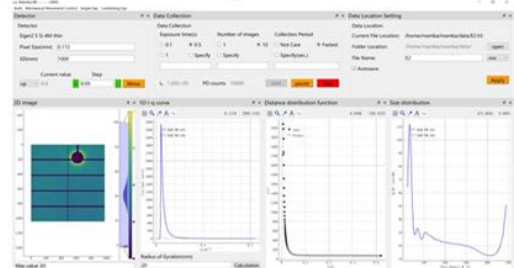
NRS/RIXS



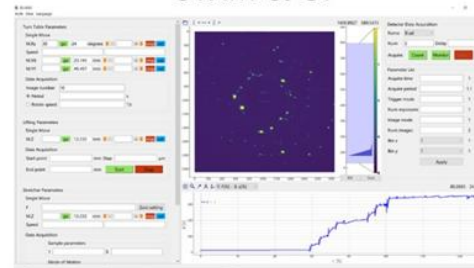
相干衍射成像



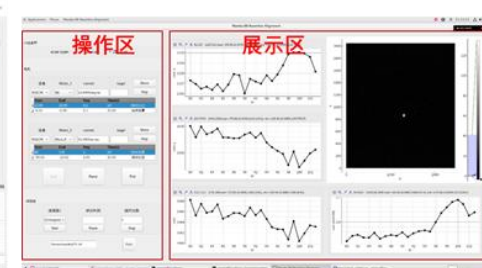
一键式拉曼谱仪调姿



SASX/WAXD联动



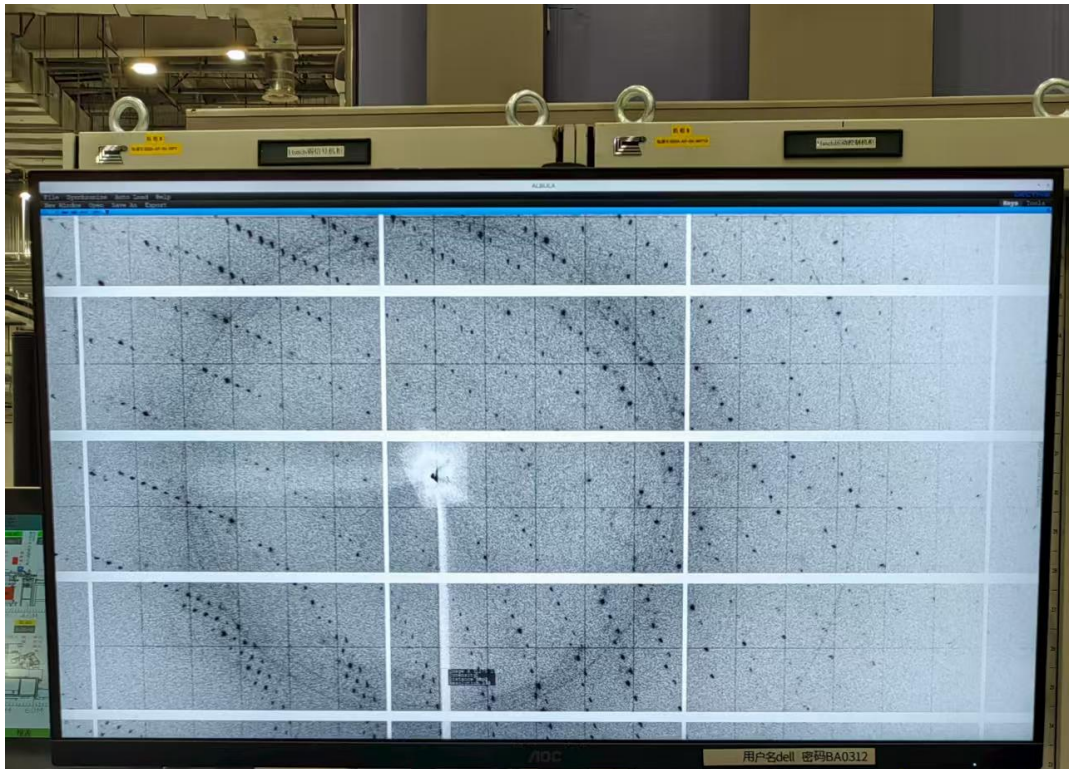
原位 3DXRD



束线调光

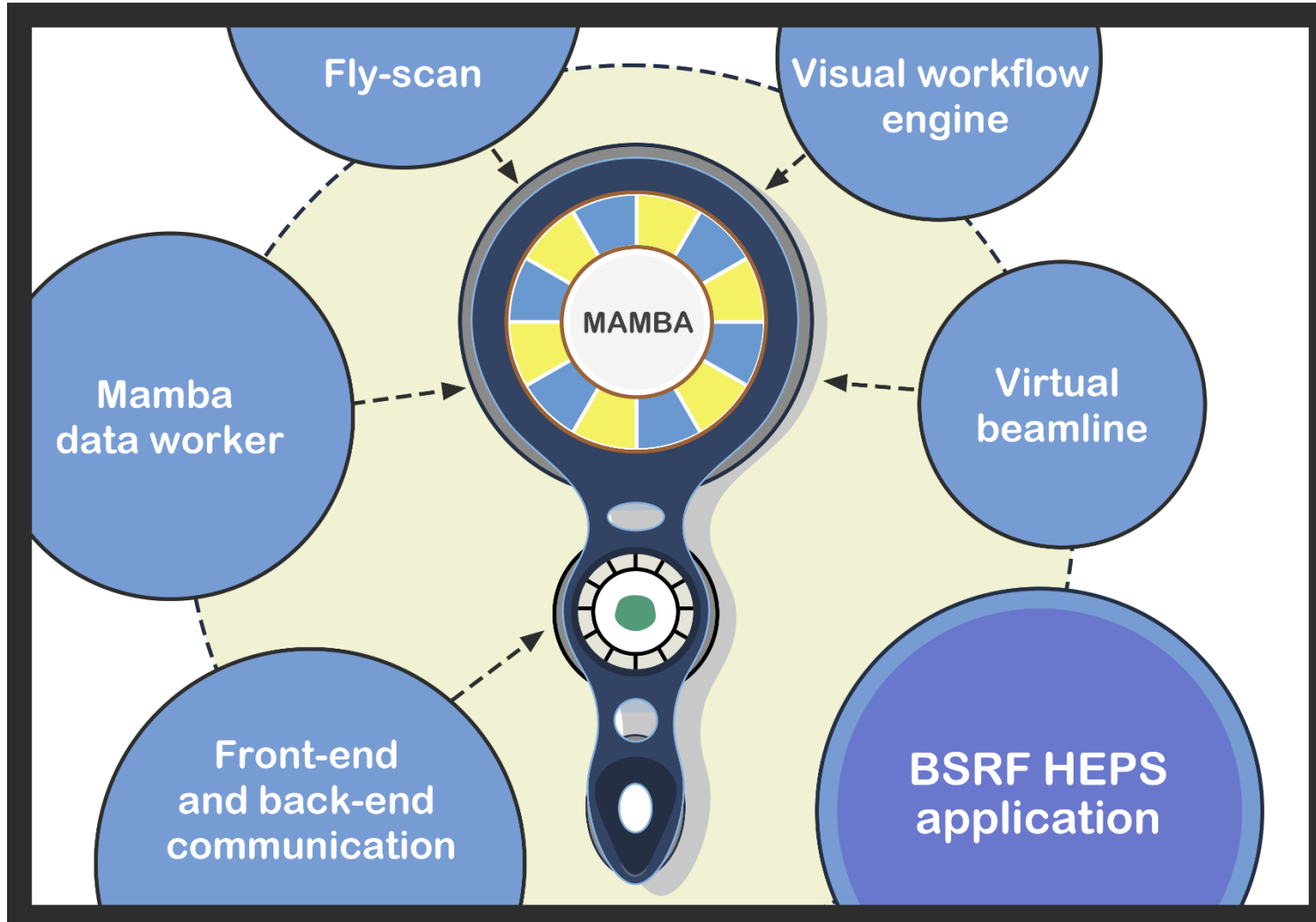






# Explore key techniques of new generation control and acquisition system

## ● Already



## ● On going

- ❑ Python IOC, Systematic detector integration and High-performance readout
- ❑ Beamline and experiment specific plan and GUI library
- ❑ Versatile attitude tuning framework and beamline automation
- ❑ Closed-loop control based on real-time data analysis
- ❑ AI-Enabled experimental control



Liu et al. *J. of Synchrotron Radiat.* **29**(3), (2022) ; Zhang et al. *J. of Synchrotron Radiat.* **30**(1), (2023) ; Li et al. *J. of Synchrotron Radiat.* **30**(6), (2023); Li et al. *Synchrotron Radiat. News*, (2023); Wang et al. *J. of Synchrotron Radiat.*, (2024);

# A systematic detector integration solution for HEPS

## □ Systematic -- work mainly done by HEPS beamline control team

Centralize management of developing detector IOCs;

EPICS-based integration and an extended ADGenICam;

ihep-pkg packaging system and ~/iocBoot conventions to simplify EPICS deployment and enhance .

### Main detector-like devices that need to be integrated

- Devices with *EPICS* IOCs that satisfy current requirements:
  - GenICam (GigE/USB3 Vision) industrial cameras: Hikvision, FLIR *etc*
  - Andor (sCMOS, CCD), marCCD, Merlin, Minipix, PICam, Pilatus
  - Keck-PAD, PCO, Photron, PVCAM; Mythen; Falcon Xn, Xspress 3
- Devices that require self-developed *EPICS* IOCs:
  - Specialized Imaging Kirana, Ximea
  - Self-made APD detector, iRay Mercur
- Devices that require high-performance integration modules:
  - Eiger, Lambda/Sparta, Rigaku XSPA, Hamamatsu
  - Tucsen, self-made Si-pixel detector
  - PandABox, multiple sensors (needing high-speed 0D readout)

## □ High-Performance

A QueueIOC framework for Python IOCs based on caproto;

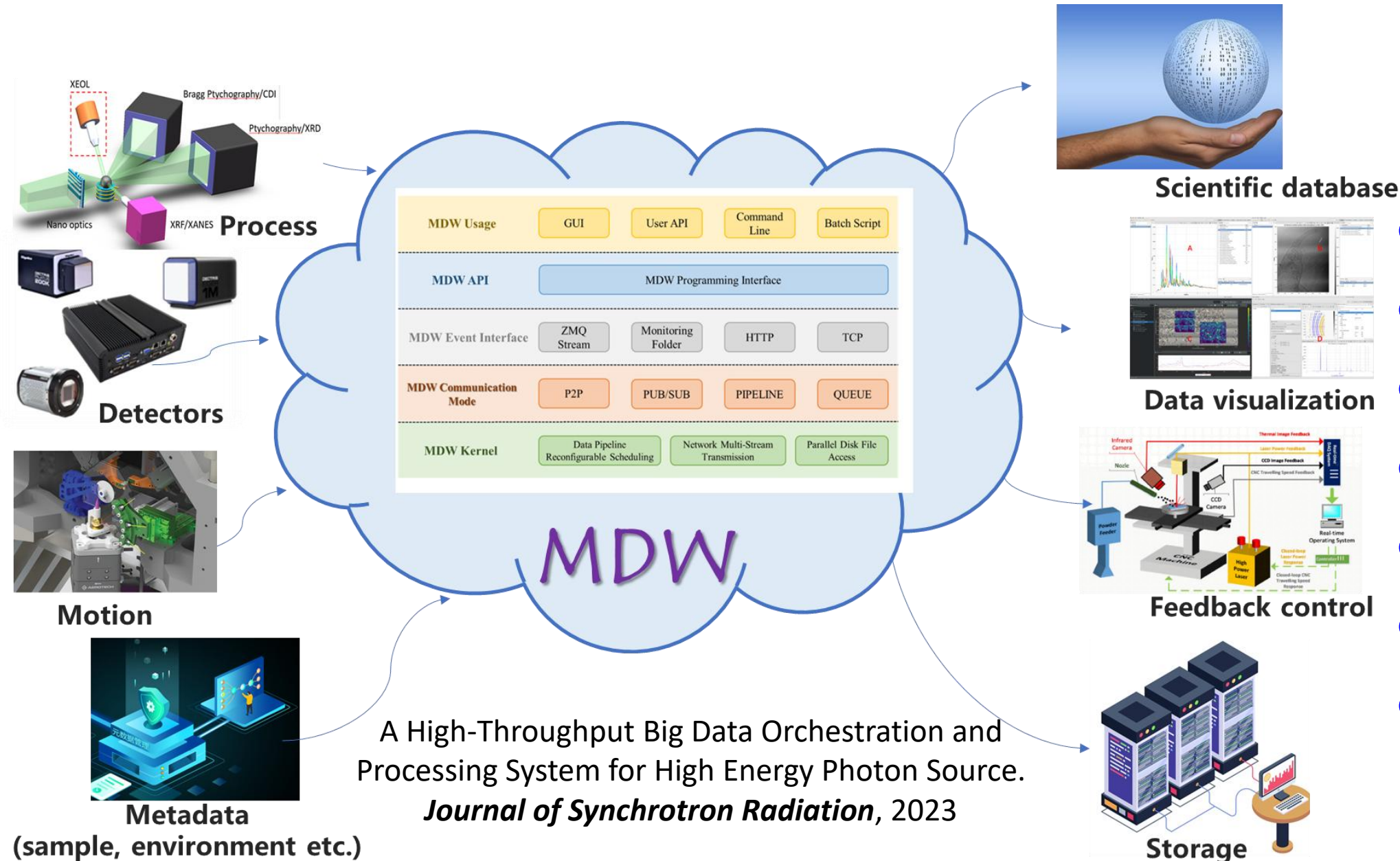
Simplify architecture and communication protocols leading to better performance than areaDetector.

**All 2D detector can be run in monitor mode**



# Mamba Data Worker for HEPS phase I experiments

- Tackles the exascale data acquisition and real-time processing challenge

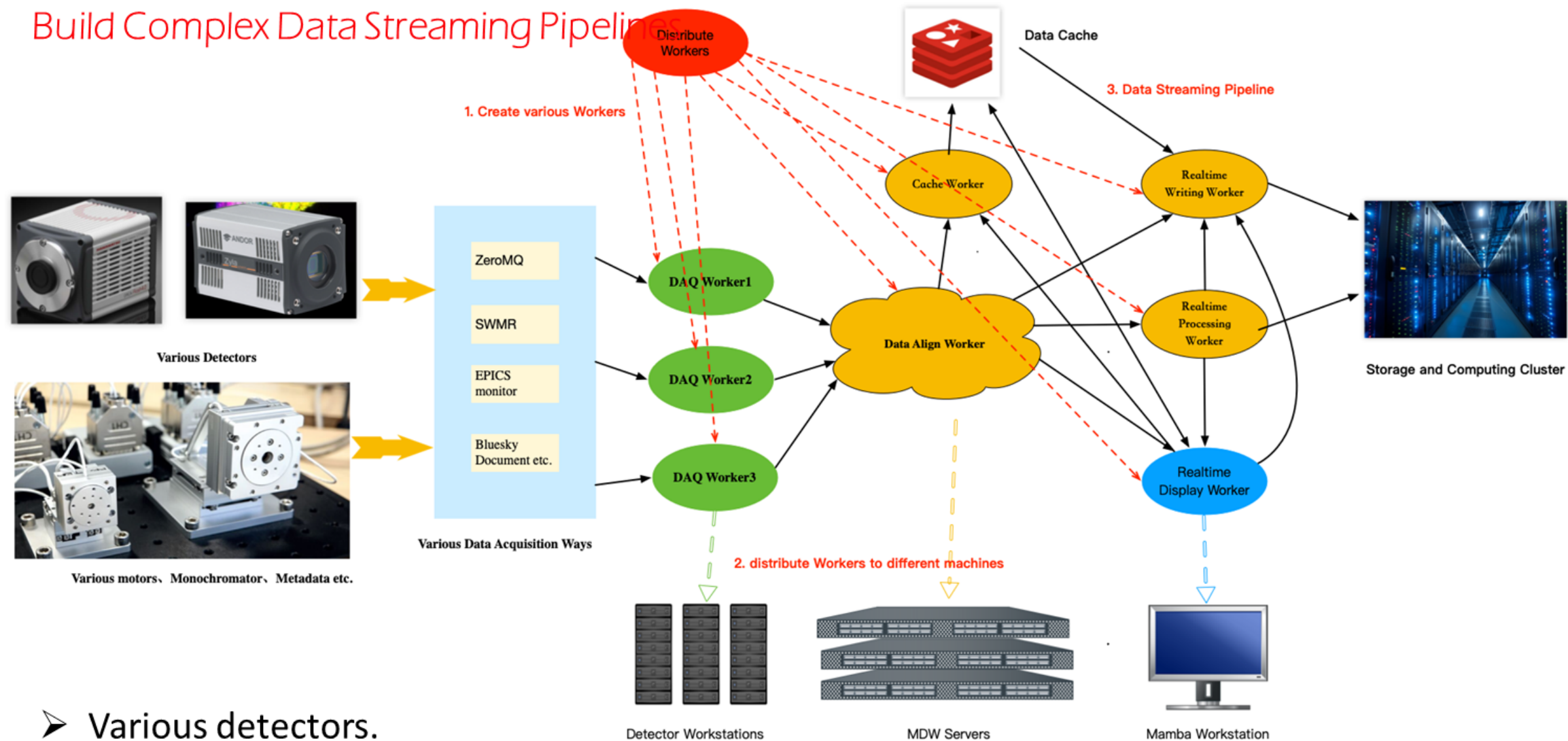


- DAQ
- Distribution
- Scheduling
- Assembly
- Reduction
- Disk writing
- Visualization

A High-Throughput Big Data Orchestration and Processing System for High Energy Photon Source.

*Journal of Synchrotron Radiation*, 2023

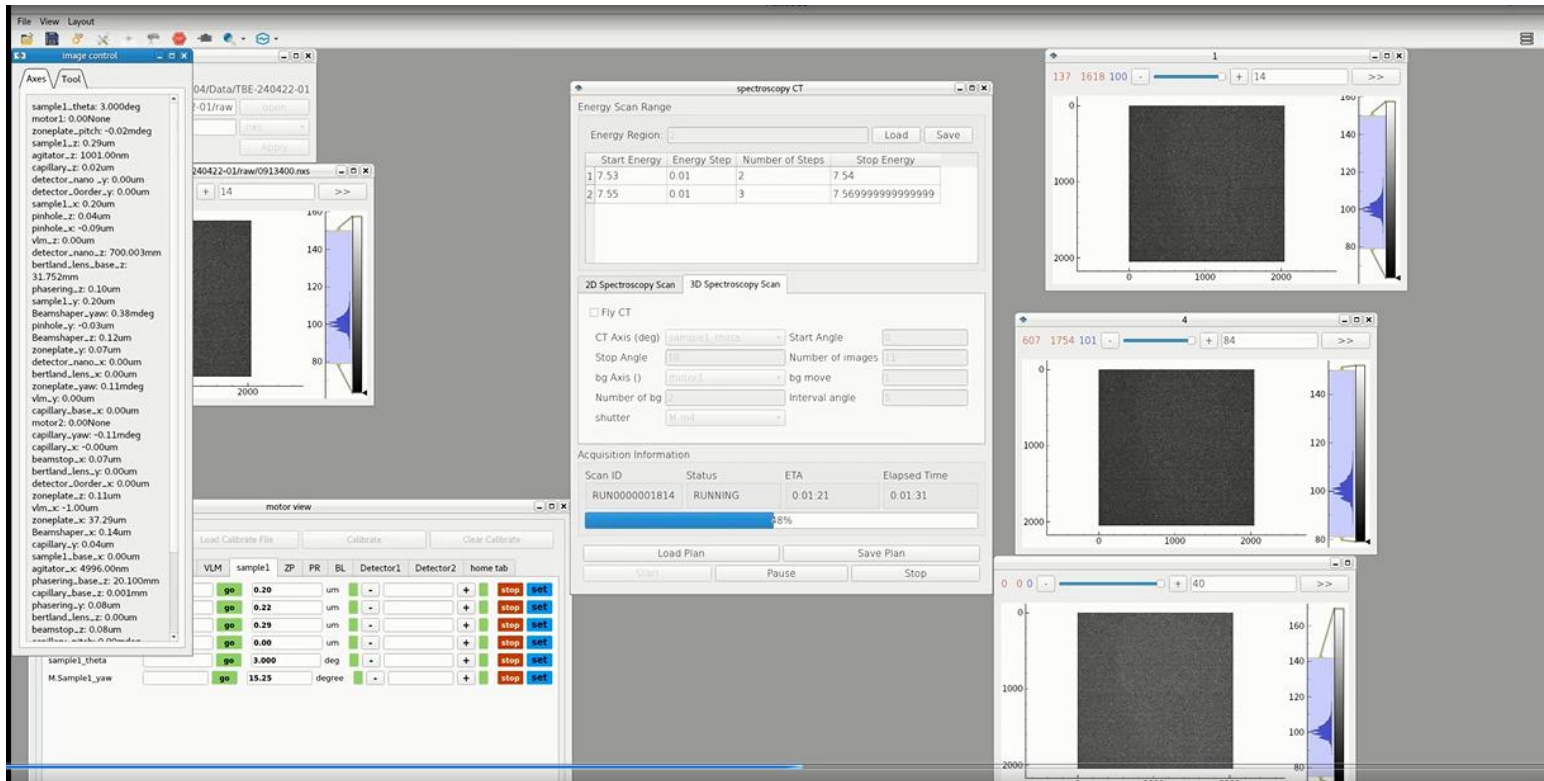
# Build Complex Data Streaming Pipelines



- Various detectors.
- Various scanning methods.
- Various data acquisition methods
- Various machines.
- Various data streaming paths

- Enable collaboration across terminals
- Ease of use

# Leading the way in making scientific data FAIR at China.



10个.hdf5  
300个dataset/hdf5  
Dataset:  
6144 x 6144

.hdf5

- 假设每300张（可调）存成一个data文件，
- 文件（1个master文件，10个hdf5文件）
  - ✓ ID21\_count(scan)\_Dhyana\_RunID\_master.h5
  - ✓ ID21\_count(scan)\_Dhyana\_RunID\_00000\_data.h5
  - ✓ ID21\_count(scan)\_Dhyana\_RunID\_00001\_data.h5
  - ✓ ...
  - ✓ ID21\_count(scan)\_Dhyana\_RunID\_00009\_data.h5

444\_0.nxs

- entry
- data
- instrument
- sample
- chemicalformula
- density
- description
- interestzone
- mass
- samplename
- sampleposition
- situation
- size
- type
- user
- beamtimeid
- contact
- endDate
- proposalcode
- proposalname
- startDate

HDView 3.1.3

Recent Files: /hepfs/hl/3W1/202210/Data/TB14-20221026-01/raw/br...

- ID21\_Projection\_2.nxs
- entry
- 元数据 nxs文件
- nx: file: metadata
- beamline
- beamtimeID
- end\_time
- experiment
- instrument
- instrument\_definition
- instrument\_file
- method
- proposal\_id
- run\_no
- sample
- start\_time
- size
- type
- user
- ID21\_Dhyana\_Projection\_2\_master.h5
- entry
- data
- data\_0000
- data\_0001
- data\_0002
- data\_0003
- data\_0004

图像大数据文件存储。每个文件5GB(100张)

Image subdata files: real image data

master file: image subdata link

图像数据 master文件

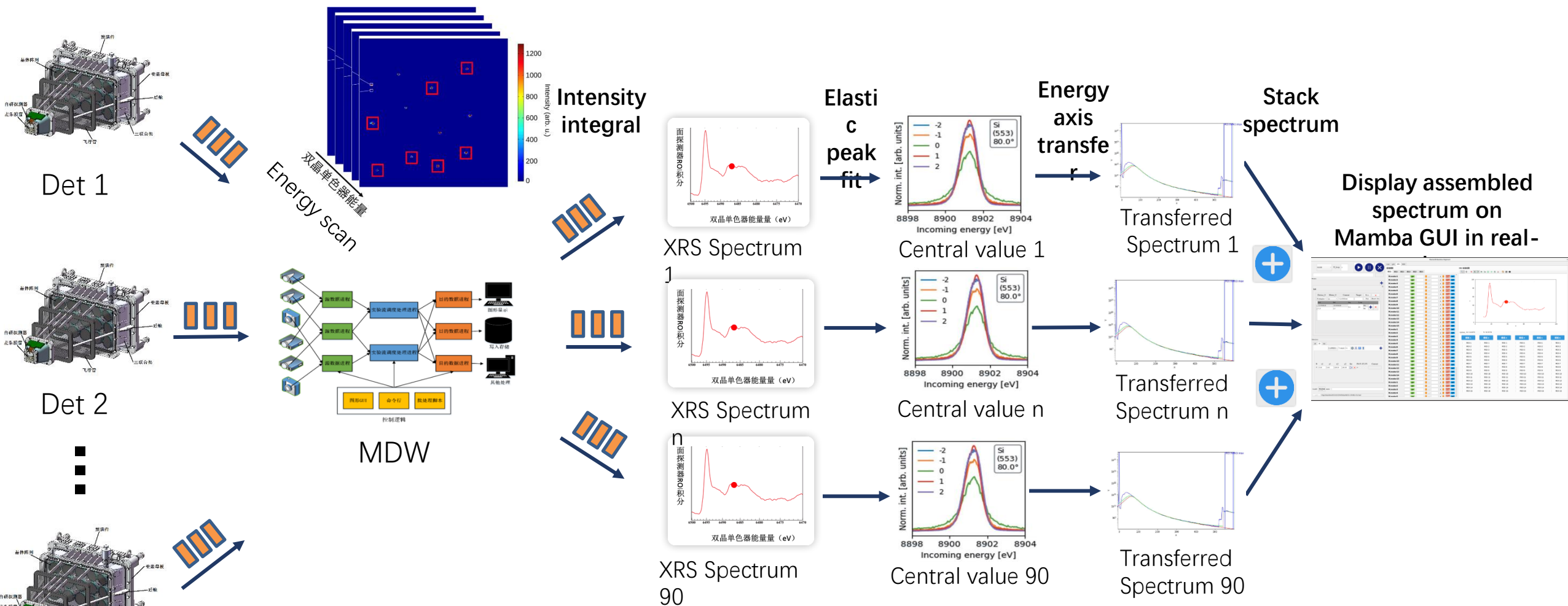
master文件外部链接到图像数据。

Single nxs file

nx+master+ data0+data1+...

- Unified data format and standards
- Data streaming for multi-modal experiments, easy data access from large dataset
- Each image and spectrum contain comprehensive metadata information, a flexible and automatic metadata collection mechanism

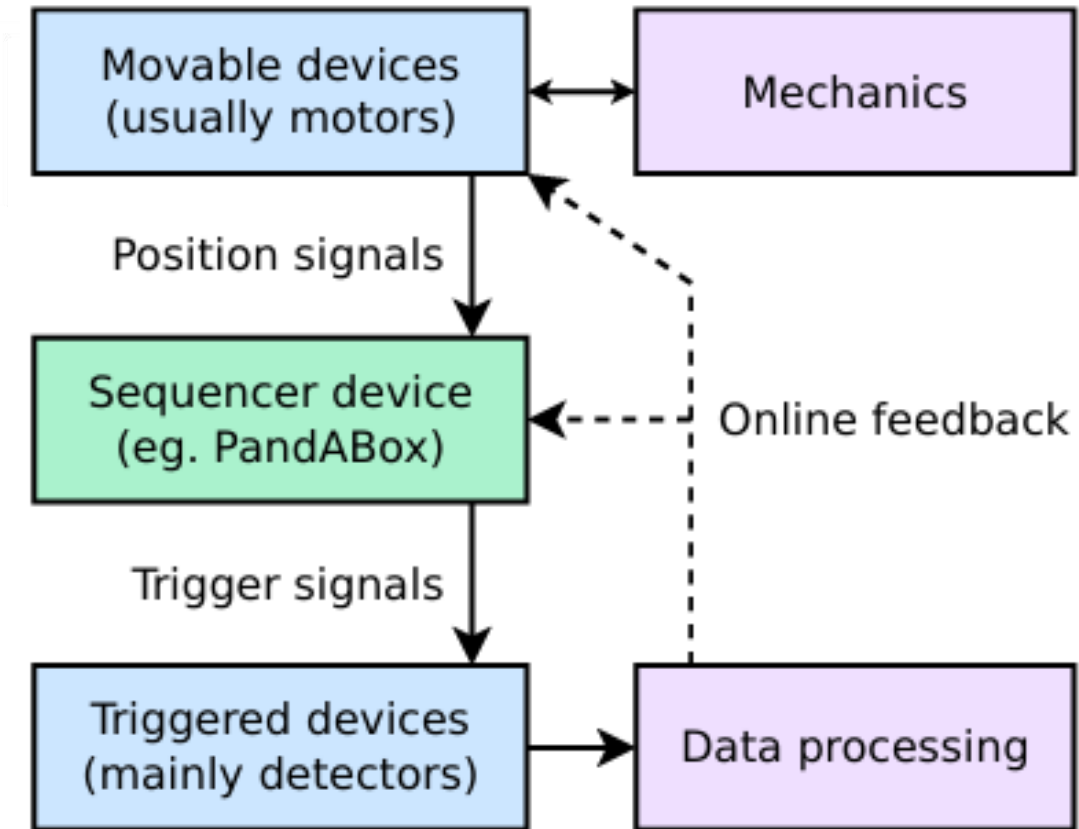
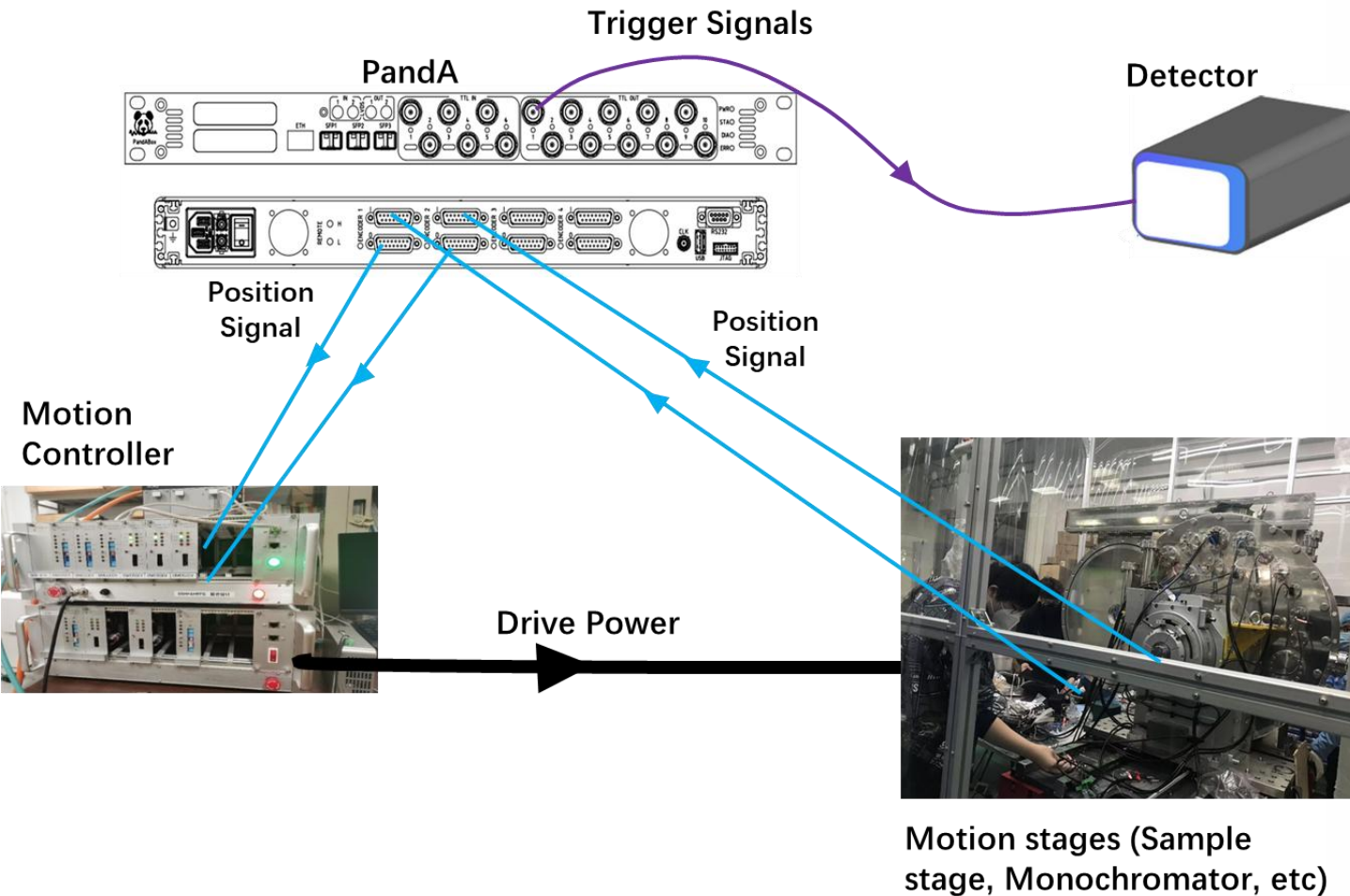




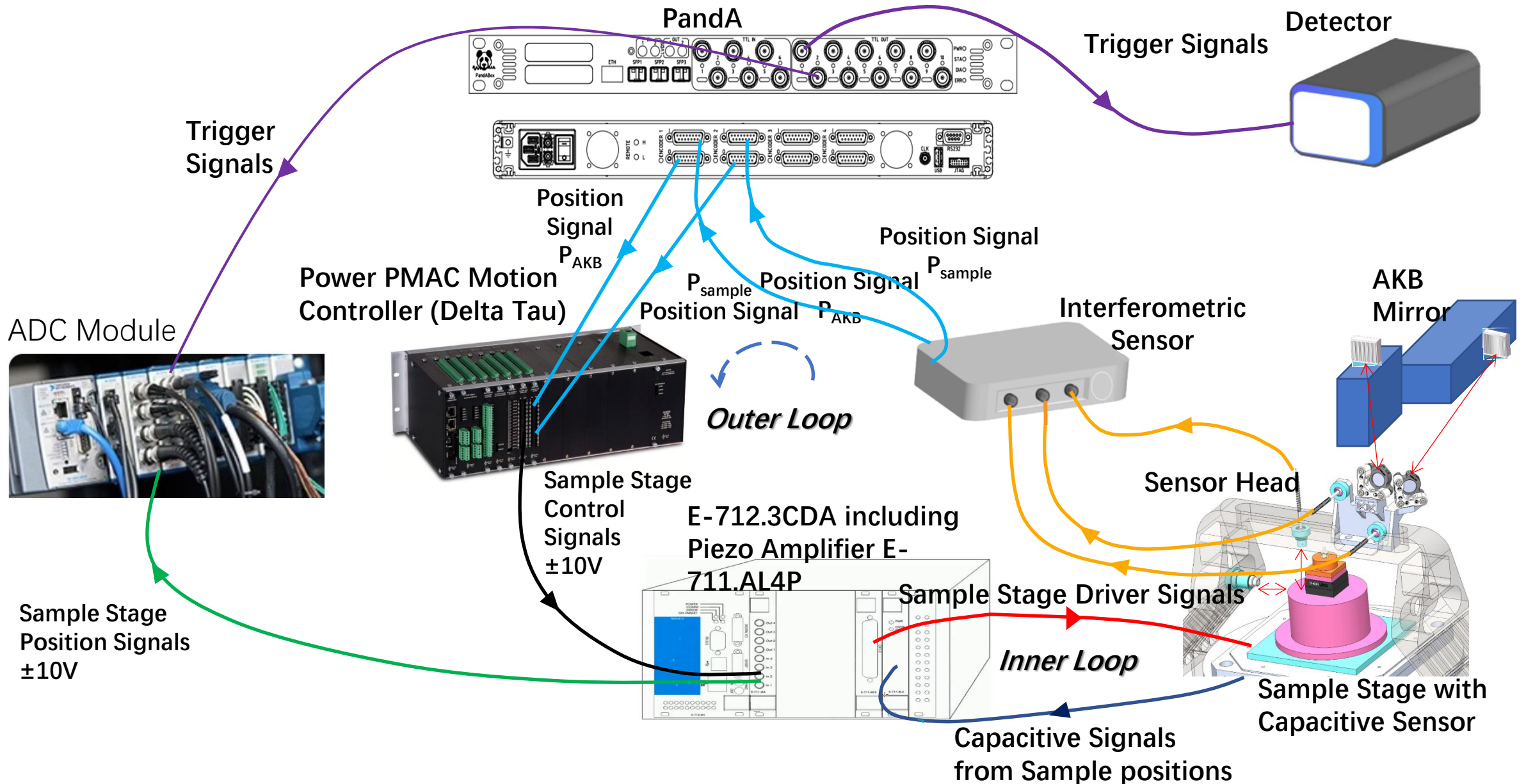
➤ Data assembling and manipulation pipeline for the XRS experiment at HEPS-ID33 Hard X-Ray High Resolution Spectroscopy Beamline

➤ We create this pipeline to transfer the images on the Raman spectrometer into 1D spectrum needed by the users, this pipeline includes several processing steps and is not necessarily straightforward to create.

# Fly-scan general event structure



# Fly-scan event structure based on Power PMAC



# Fly-scan hardware and event orchestrating structure

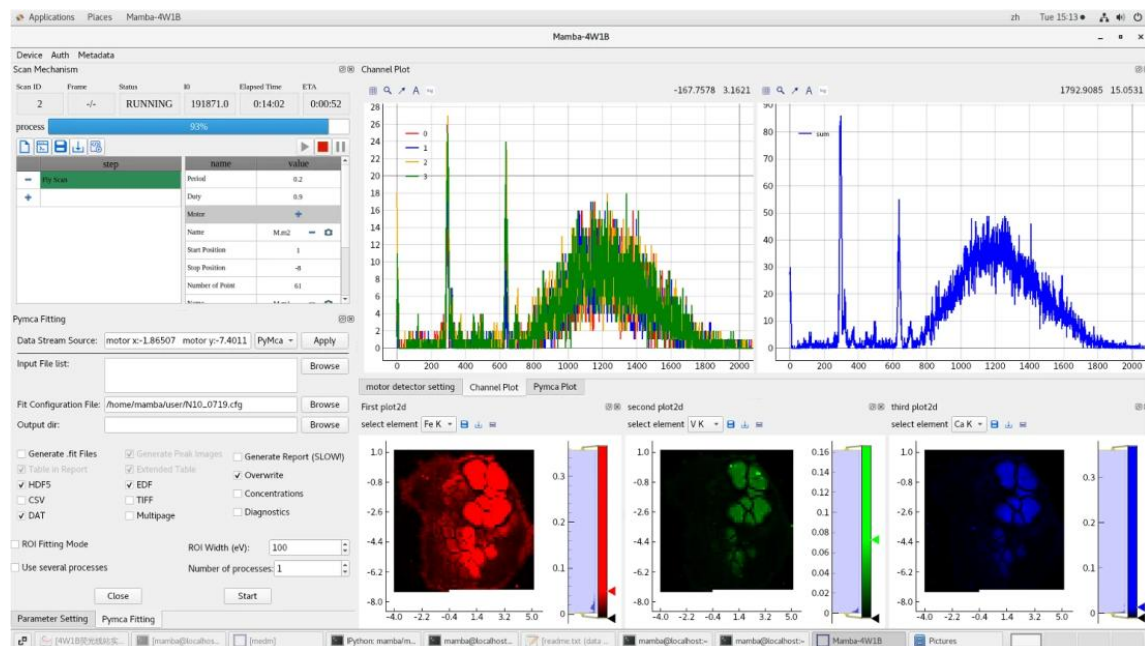
Scan Mode	Beamlines	Designed Structure
Fly Scan (11/15)	Hard X-ray Nanoprobe Multimodal Imaging Beamline	Structure based on Power PMAC
	Hard X-ray Coherent Scattering Beamline	
	Engineering Materials Beamline	General Structure
	Hard X-ray High Resolution Spectroscopy Beamline	
	High Pressure Beamline	
	Hard X-Ray Imaging Beamline	
	X-ray Absorption Spectroscopy Beamline	
	Low-Dimension Structure Probe Beamline	
	Tender X-ray Beamline	
	Transmission X-ray Microscope Beamline	
Step Scan (4/15)	Hard X-ray Nanoprobe Multimodal Imaging Beamline	Structure Based on Panda Box and GPIO in Power PMAC
	Hard X-ray Coherent Scattering Beamline	
	Hard X-Ray Imaging Beamline	Structure Based on Panda Box
	Pink Beam SAXS Beamline	Structure Based on Panda Box





# Fly-scan integration in Bluesky and Mamba

- ❑ Position based triggering
- ❑ Time based triggering
- ❑ Software based fly-scan
- ❑ Complex trajectory
- ❑ Online tuning fly-scan



- (a) *Mamba startup script fragment for PandaBox-based fly scans. ImagePlanner is a specialised MambaPlanner with friendly default settings for image data handling.*
- ```
U.planner = ImagePlanner(U)
U.planner.extend(PandaPlanner(
    D.panda and D.adp are Bluesky encapsulations for the control and data interfaces of
    PandaBox, respectively; the latter is based on the EPICS module ADPandaBlocks. div
    requires a fragment to contain at most 12216 frames of data from Xspress3. h5_tols
    requires the HDF5 file acquired from Xspress3 to contain exactly the expected number
    of frames at the end of each line during a fly scan.
    D.panda, D.adp, divs = {D.xsp3: 12216}, h5_tols = {D.xsp3: 0},
    enc_tols requires that for every motor involved in a fly scan, the difference between its
    raw position and its encoder position does not exceed 25 pulses at the beginning of the
    scan, in order not to disrupt the sequencer program used.
    enc_tols = {m: 25 for m in M.values()},
    vbas_ratios requires that the speed of a motor to be at least 2 times its starting speed,
    because otherwise the speed setting would be disregarded by the motion controller (Kohzu
    ARIES, used at the 4W1B beamline of BSRF).
    vbas_ratios = {m: 2.0 for m in M.values()},
    configs sets Xspress3 to be triggered by external TTL signals during a fly scan.
    configs = {D.xsp3: {"cam.trigger_mode": 3}}
))
P = U.planner.make_plans()
An example for grid fly scans, which intentionally mimics Bluesky's grid_scan().
#P.fly_grid([D.xsp3], M.m2, -1, 1, 3, M.m1, -4, 4, 5, duty = 0.5, period = 0.5)
```
- (b) *Mamba startup script fragment for Bubo-based software fly scans.*
- ```
U.planner = ImagePlanner(U)
U.planner.extend(BuboPlanner(D.bubo, h5_tols = {D.xsp3: 0}))
An example for software-based grid fly scans, similar to the PandaBox-based interface above.
#P.sfly_grid([D.xsp3], M.m2, -1, 1, 3, M.m1, -4, 4, 5, pad = 0.5)
```



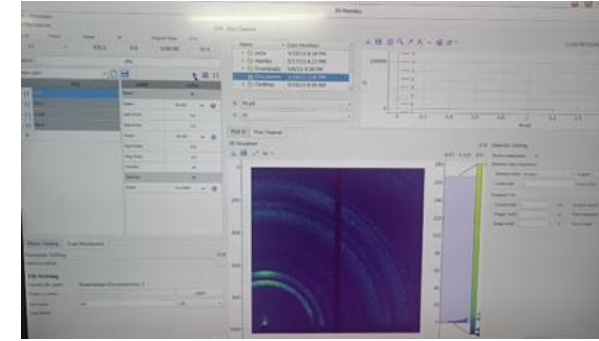
P.-C. Li, C.-L. Zhang, ..., Y. Liu\*. Synchrotron Radiat. News, 2023

P.-C. Li, C.-L. Zhang, ..., Y. Liu\*. Radiat. Detect. Technol. Methods, 2023

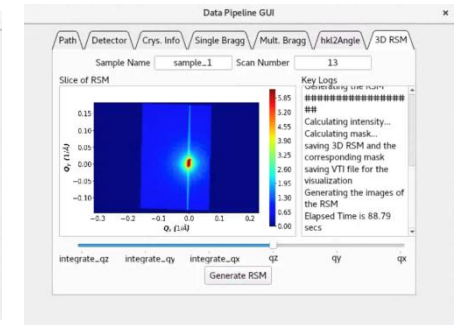
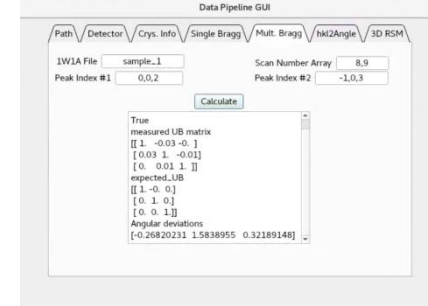
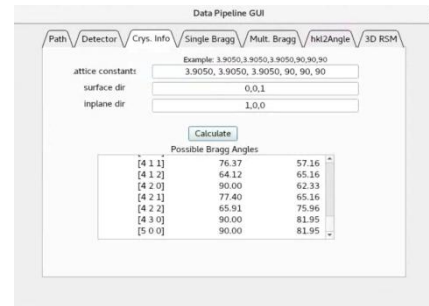
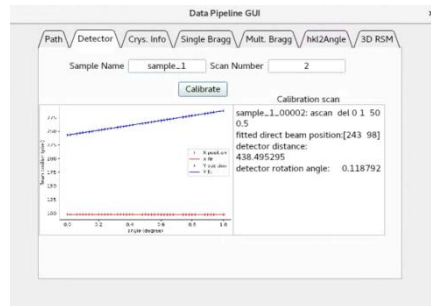
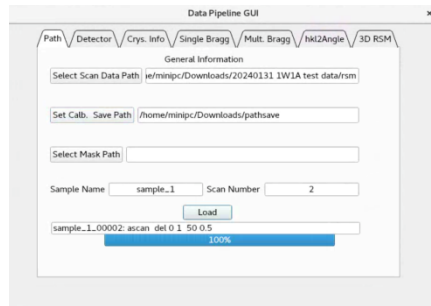


# Beamline and experiment specific plan and GUI library

- ❑ At HEPS-B9: implemented 6-circle diffractometer control in bluesky

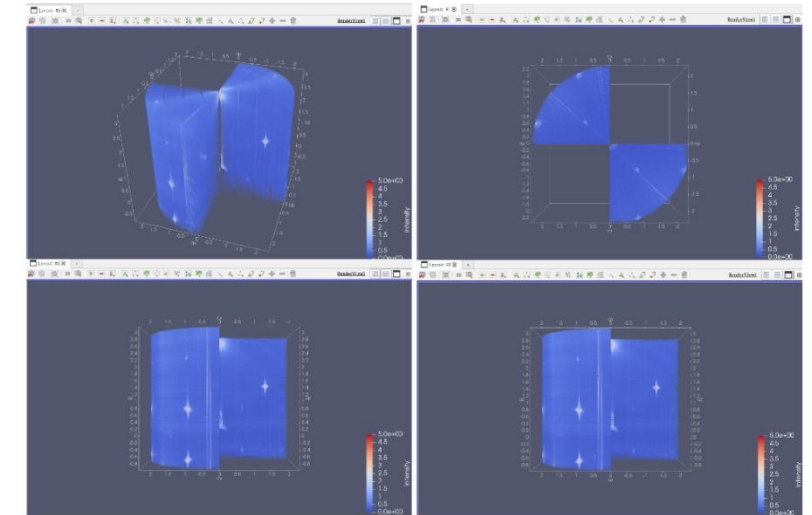


- ❑ UB matrix calculation GUI based on PyCXIM (collaboration with Dr. Zhe Ren)

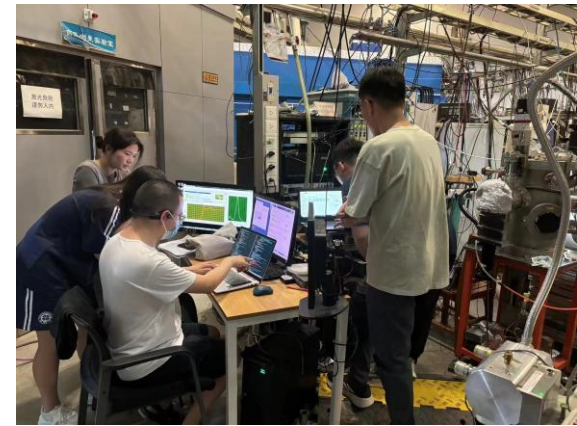
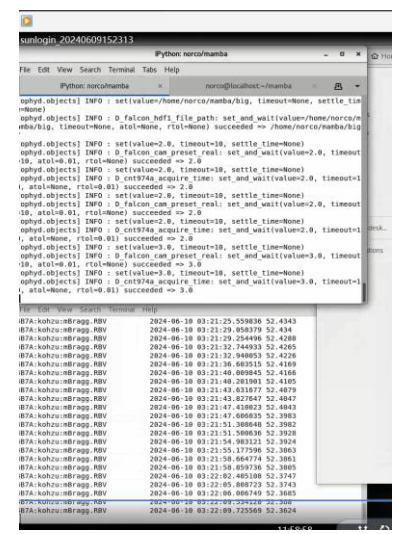
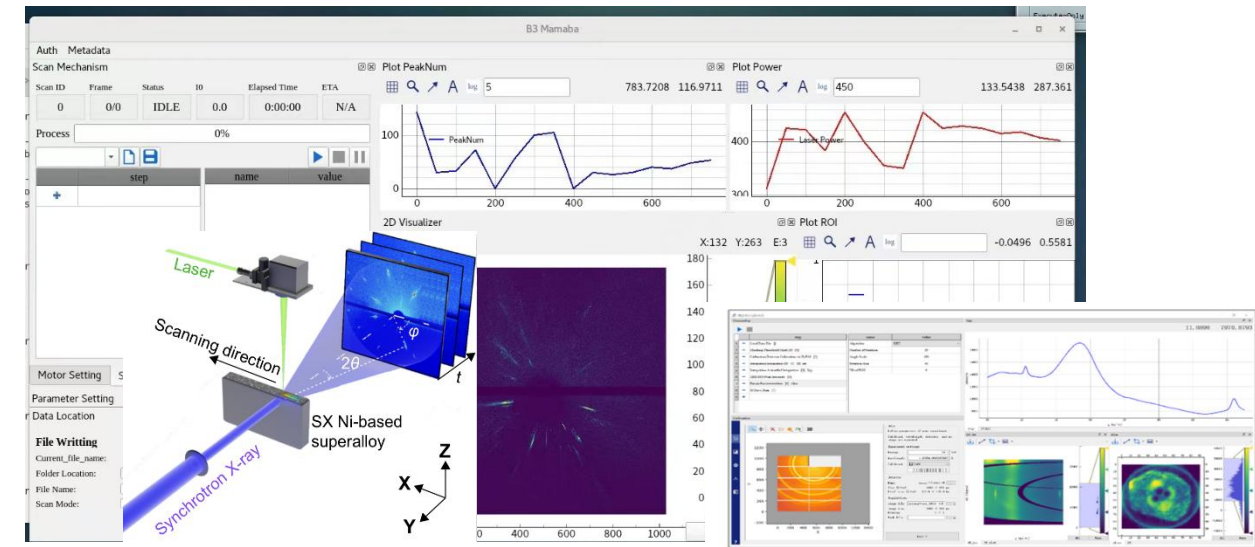
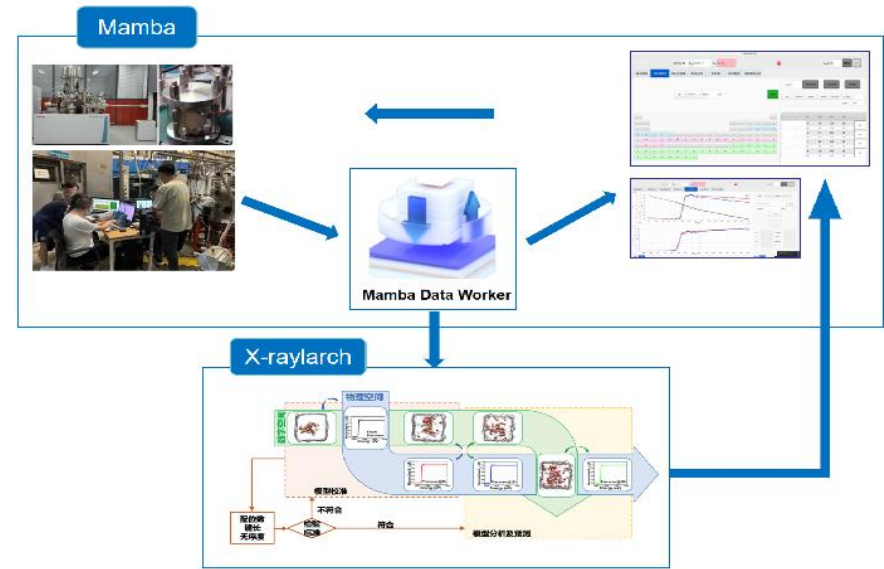
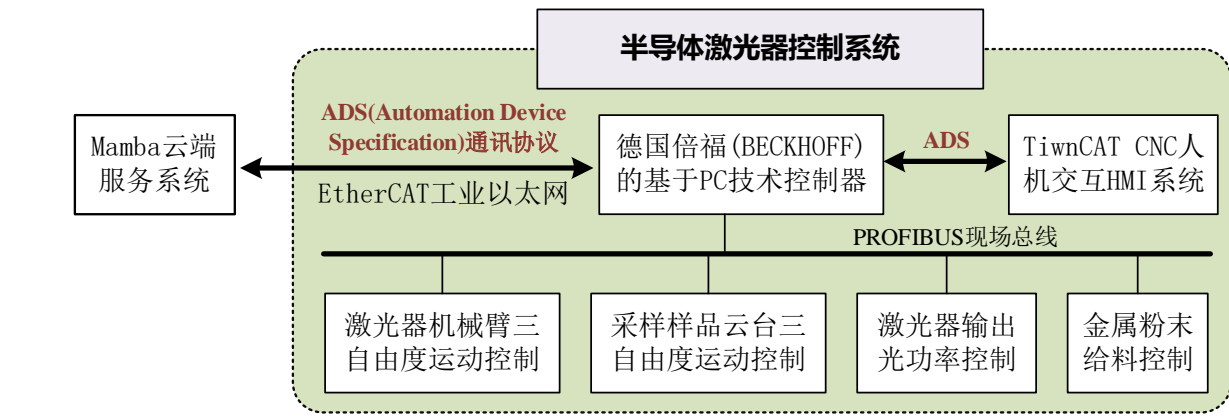


- ❑ Integrating the PyCXIM algorithms into the beamline-specific plans of *Mamba*

- ❑ High-resolution large-scale 3D reciprocal space reconstruction for real-time visualization and analysis



# ❑ Closed-loop control based on real-time data analysis



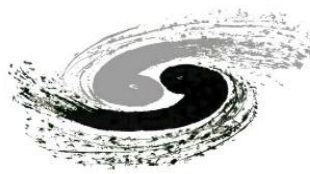
❑ Proof-of-concept test on real-time feedback control technology of metallic additive manufacturing

❑ Proof-of-concept test on performing digital twin experiments (dynamic XAFS)



Experimental automation via good software design,  
Beamline intelligence empowered by AI/ML .

# *Addressing big data challenge using AI/ML*





# A new research paradigm at fourth-generation synchrotron

## ● “Large-scale scientific software framework + AI for Science”

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Comment | Published: 18 May 2022

### Exascale image processing for next-generation beamlines in advanced light sources

[Yuhui Dong](#) , [Chun Li](#), [Yi Zhang](#), [Pengcheng Li](#) & [Fazhi Qi](#)

[Nature Reviews Physics](#) **4**, 427–428 (2022) | [Cite this article](#)

Compared to other data-intensive scientific fields, users in light source facilities come from various research backgrounds, and do not necessarily have the knowledge and computational resources to handle such big data. Therefore, a common approach is to incorporate state-of-the-art image processing algorithms into the integrated large-scale data acquisition and analysis software framework developed for the next-generation synchrotron and XFEL facilities. These ambitious software projects, such as Bluesky (NSLS-II, APS), Mamba (HEPS) and Karabo (Eu-XFEL), are designed to interface naturally with the new scientific algorithms and programs. They are being developed to provide a universal platform to collect, manage, visualize and process big data. The power of these platforms will be further

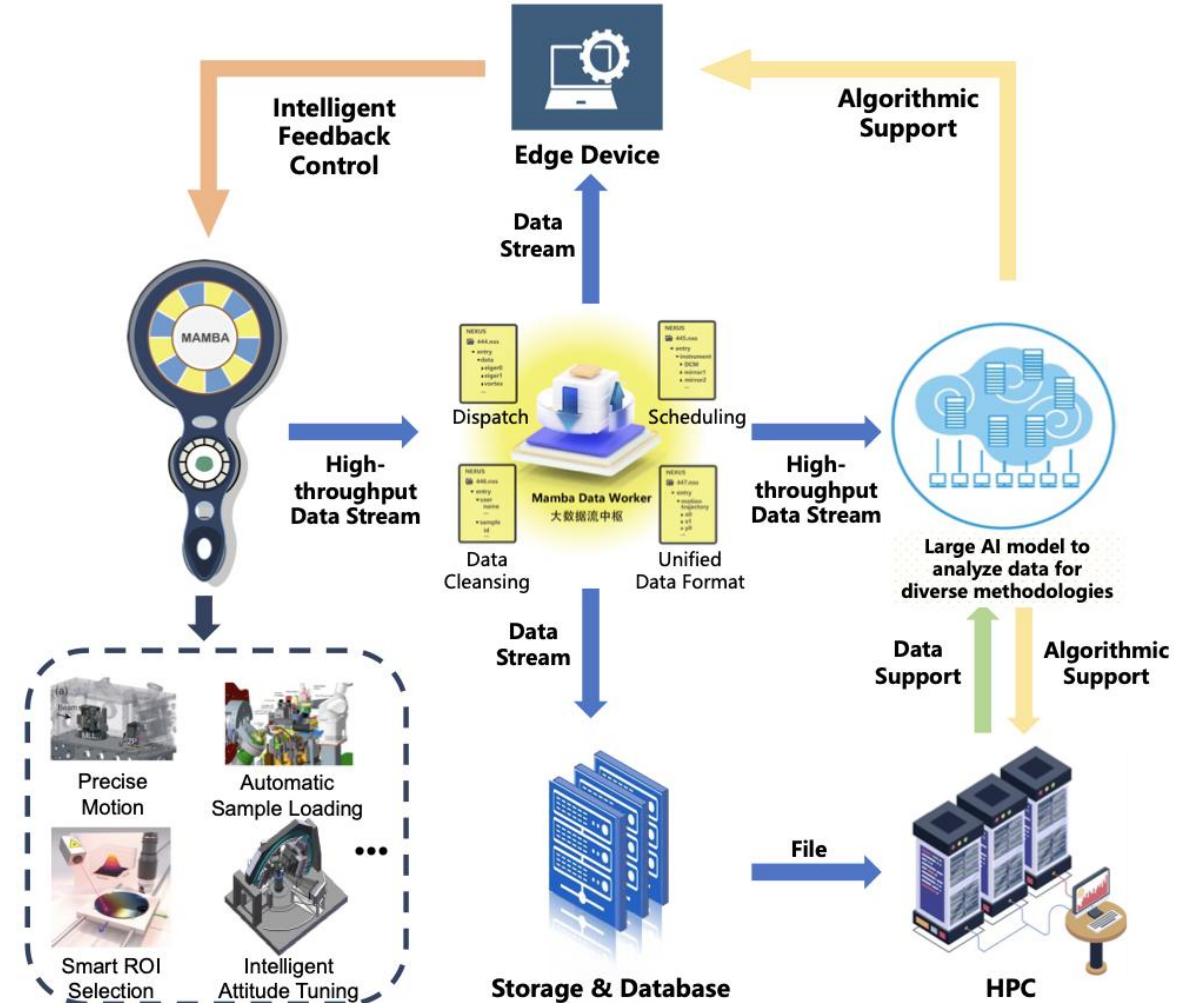
Integrating image processing algorithms into data acquisition software framework addresses the big data challenge

- Leveraged by the unified software ecosystem, data will flow seamlessly between various application nodes, further empowering algorithms
- The software framework will provide a broad stage for the algorithm application at wide range of sciences

# AI facilitated big scientific project at intelligent light source

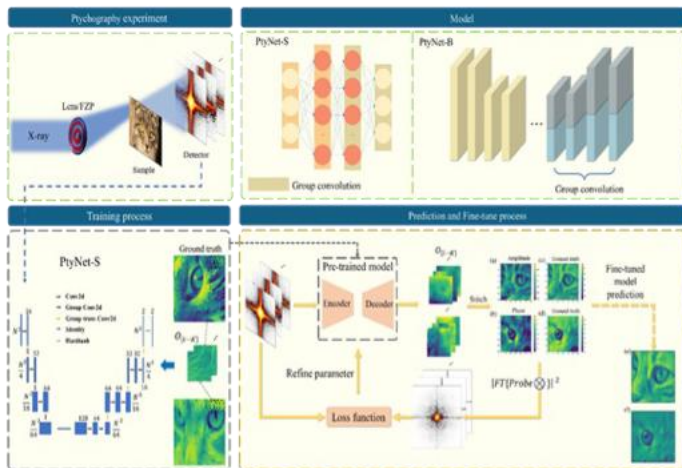
- **The light source is becoming one of the largest scientific data source**

- ❑ DL-empowered full-stack DAQ and analysis pipeline for synchrotron experiments
- ❑ Mamba data worker for big data science
- ❑ Domain specific big AI model
- ❑ Intelligent cluster of scientific infrastructures



# “AI for Science” applications in diverse methodologies

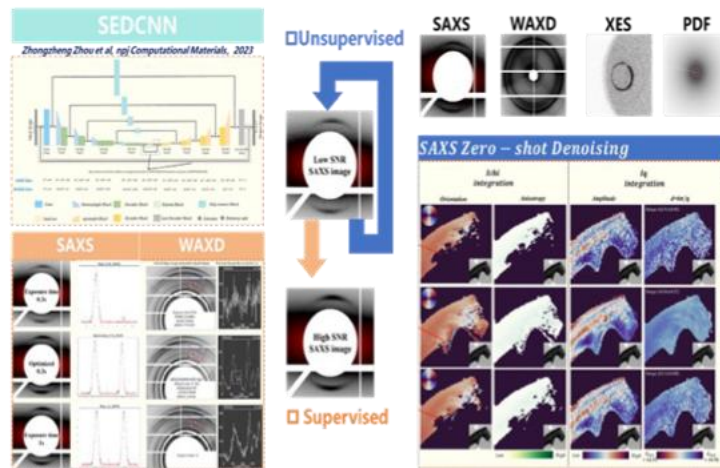
## Large AI model solves ptychographic phase retrieval problem



X.Y. Pan et al. *iScience*, 2023

X.Y. Pan et al. *Acta Physica Sinica*, 2023

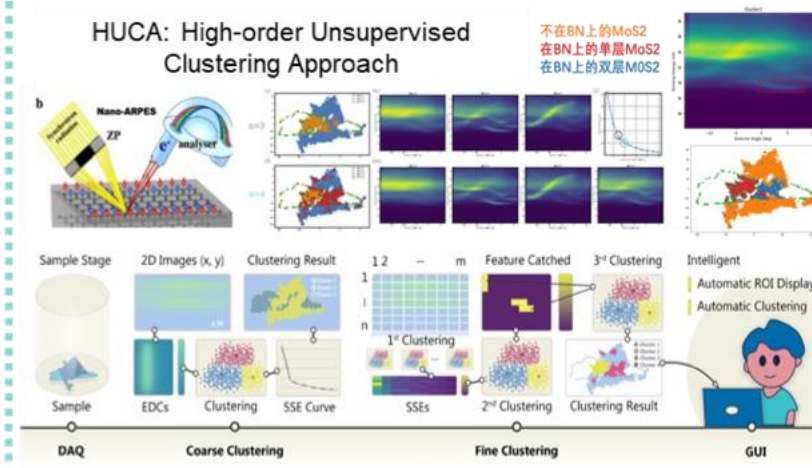
## Physics-informed denoising solution



Z.Z. Zhou et al. *npj Comp. Mater.*, 2023

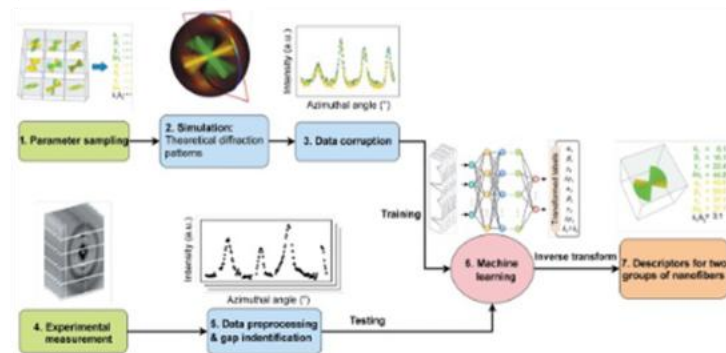
Z.Z. Zhou et al. *Journal of Appl. Crystallogr.*, accepted

## Clustering of Nano-ARPES experimental spectra



L.Z. Bian et al. *Commun. Phys.*, under review

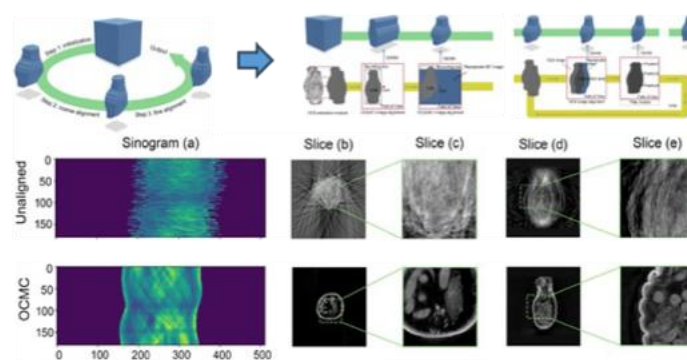
## Physical information retrieval from massive diffraction data using machine learning methods



M. Sun et al. *IUCrJ*, 2023

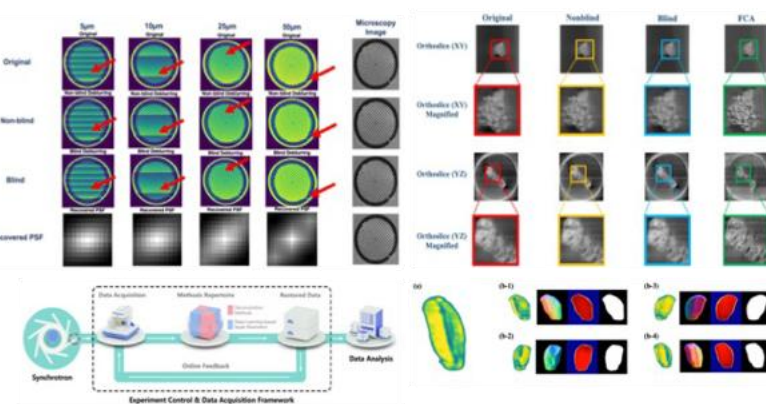
X. Zhao et al. *IUCrJ*, 2024

## End-to-end image misalignment correction method for tomography



Z. Zhang et al. *iScience*, 2023

## Deconvolution and super-resolution pipeline

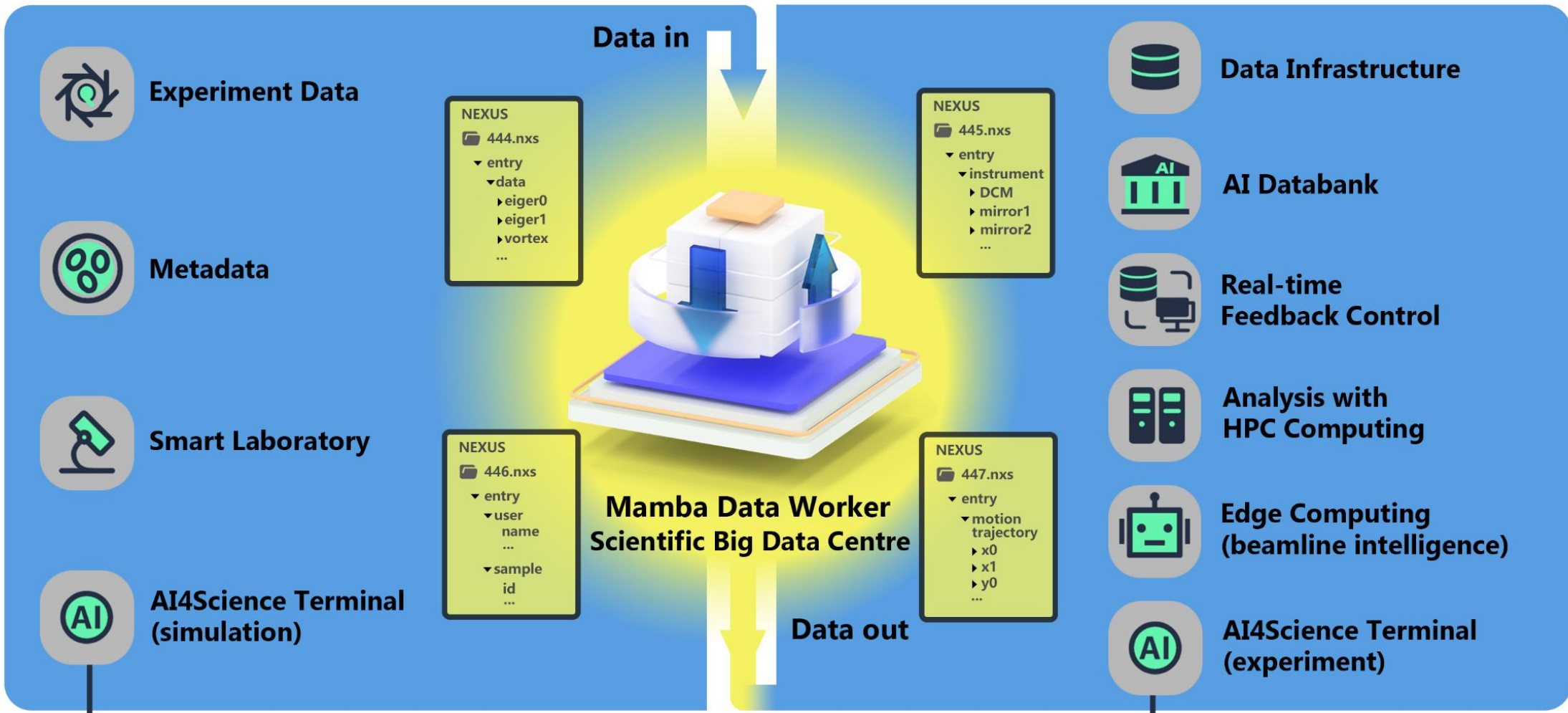


C. Li et al. *Nucl. Sci. Tech.*, accepted



# Mamba Data Worker for intelligent light source

- Enables new scientific opportunities



Digital Twins: Merge simulation and experiment data

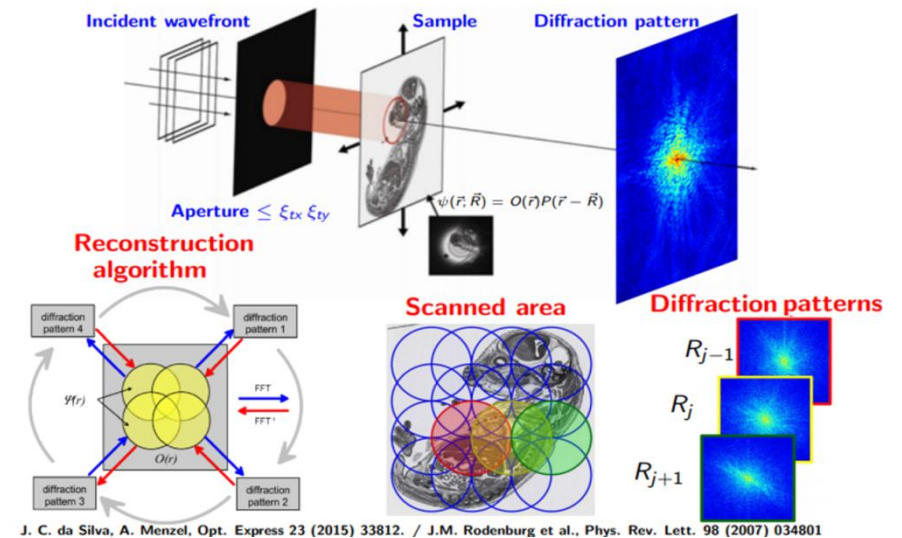
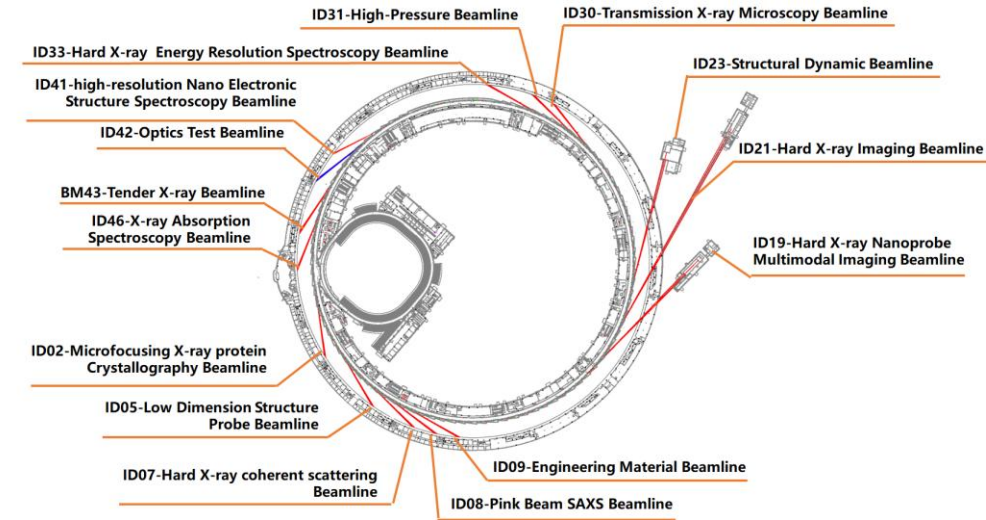
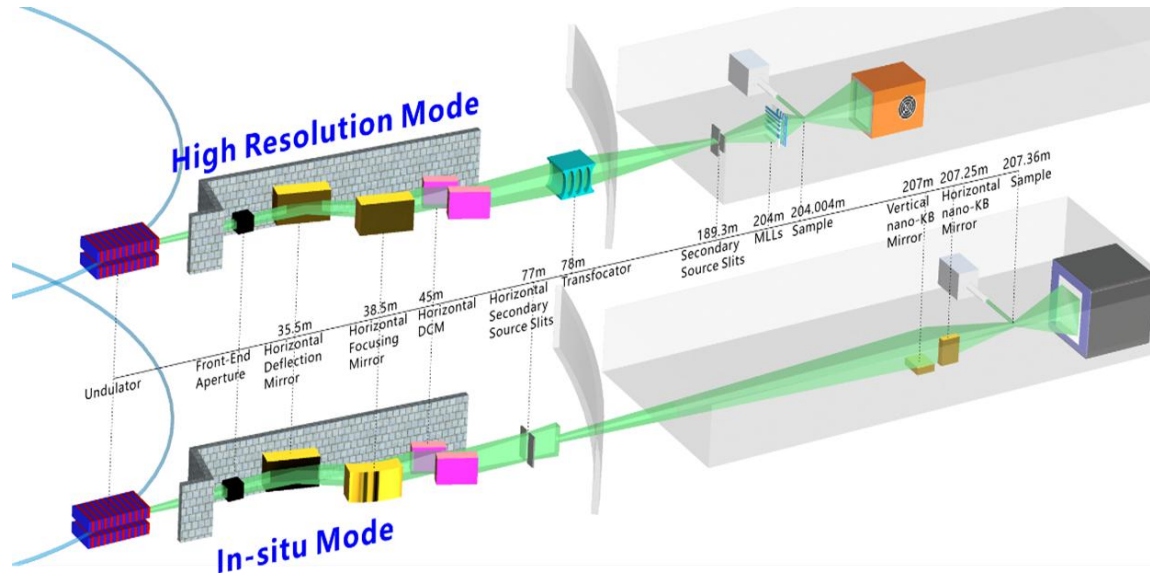
- Beamline intelligence 束线智能
- AI4Science Terminal 智慧终端



# Data-driven beamline intelligence applications : beamline alignment

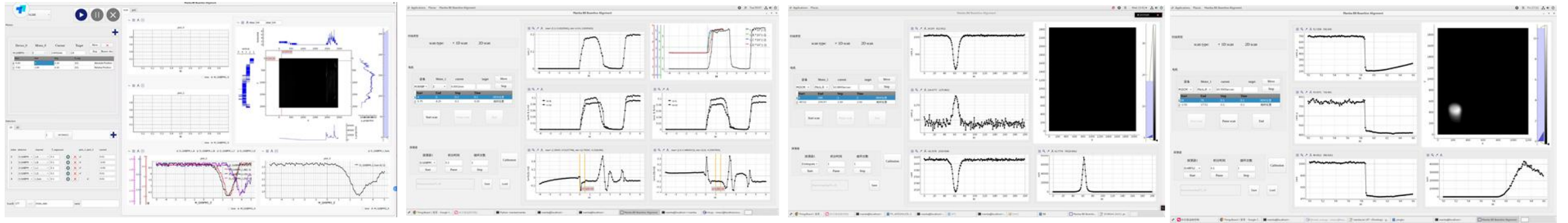
## Requirements Analysis

- ❑ Many last-minute requests with tight deadlines.
- ❑ A large number of micro/nano beamlines.
- ❑ The critical dependence of experiments on precise beam alignment.
- ❑ The necessity for immediate feedback during operation.
- ❑ A strong push towards automating processes.

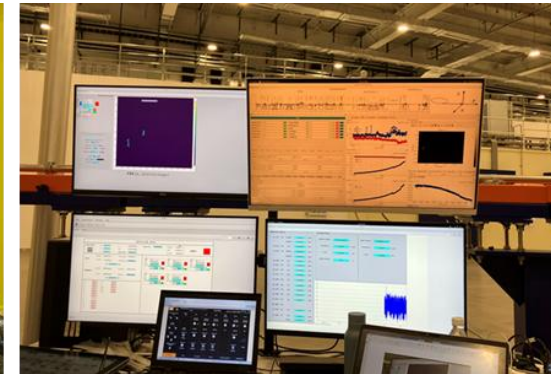
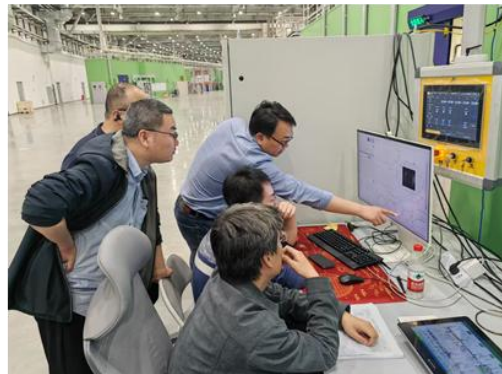
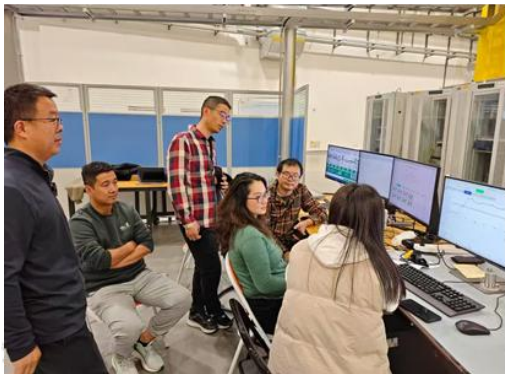
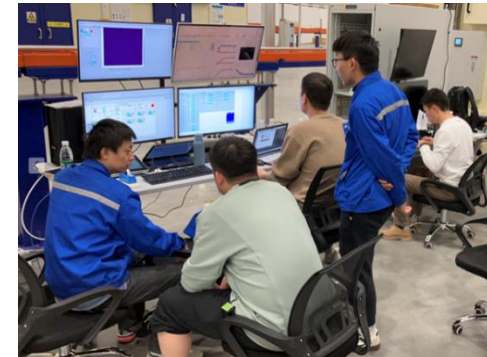
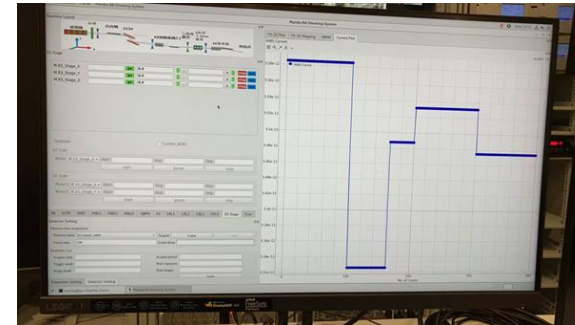
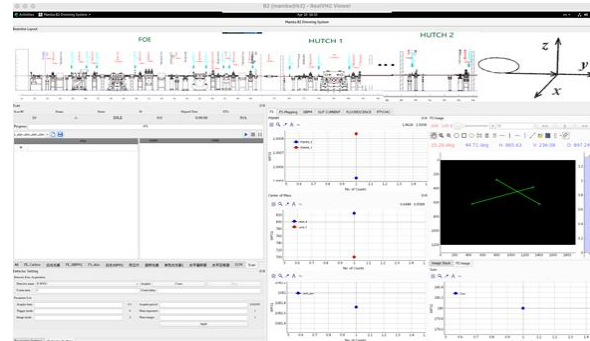




# Data-driven beamline intelligence applications : beamline alignment

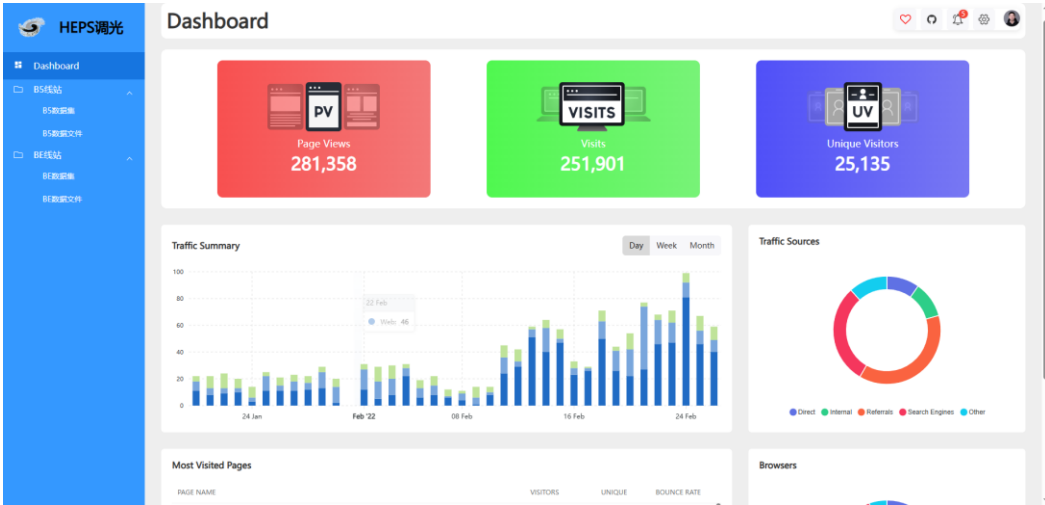
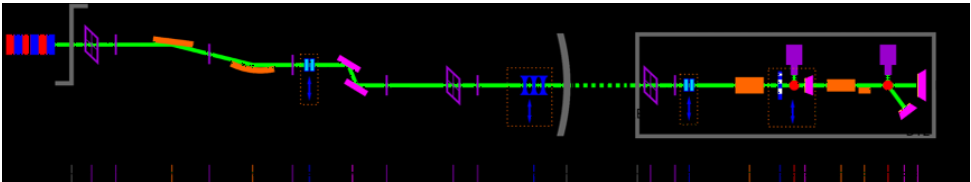


**Step1:**  
Beamline commissioning  
software



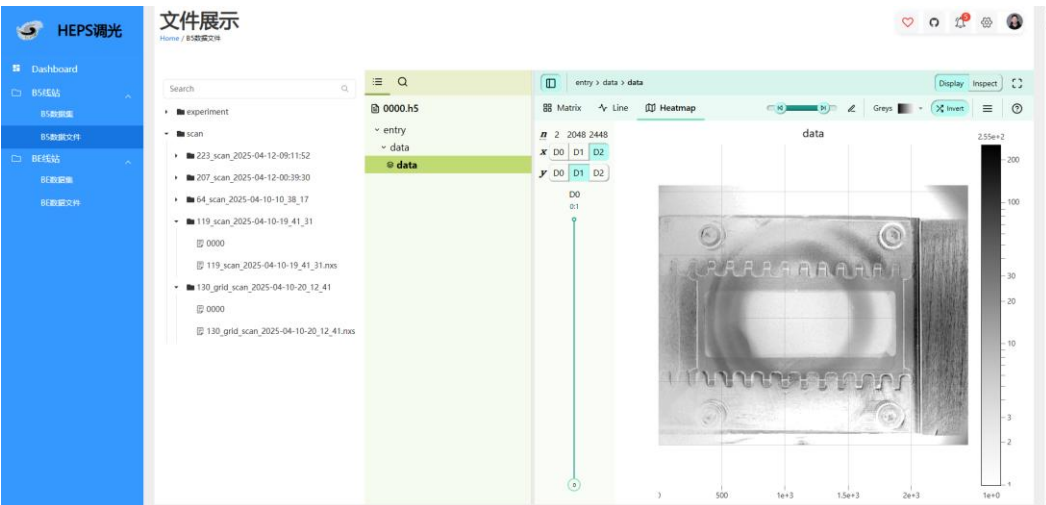
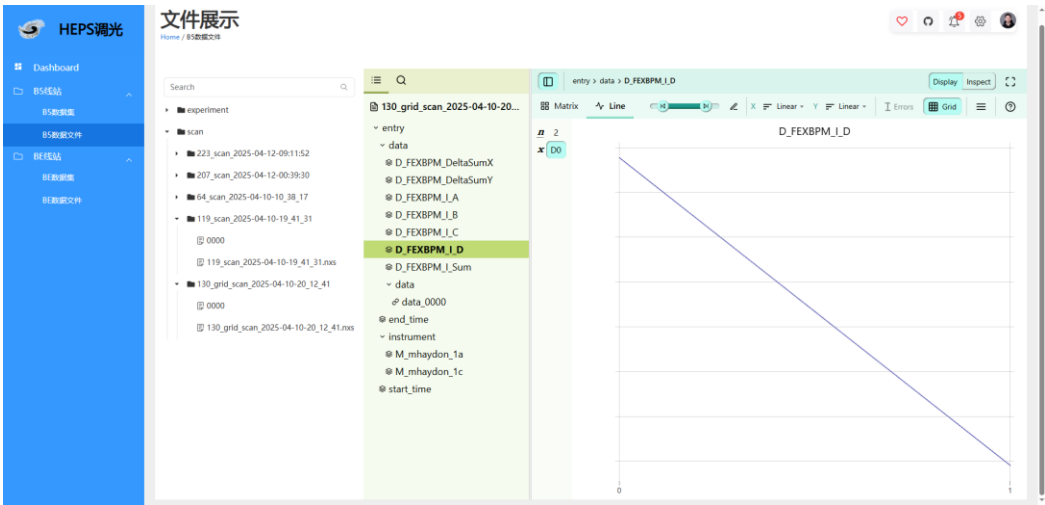
# Data-driven beamline intelligence applications : beamline alignment

## Step2: Collecting Beamline commissioning data

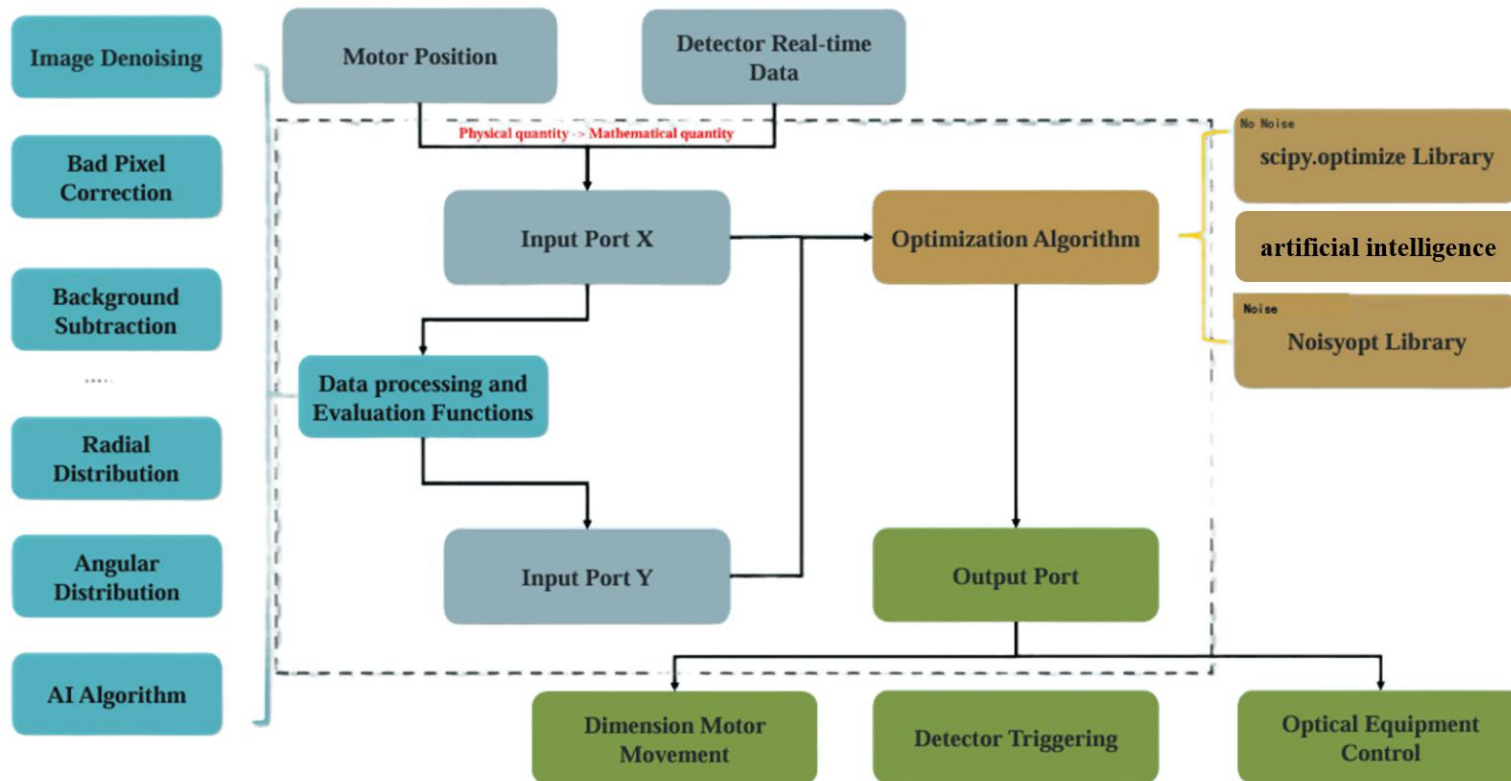


数据展示

Beamline ID	ID	姓名	邮箱	备注	数据收集量	开始时间	结束时间	操作
BT202411190001	PR202311001	Alice Johnson	alice.johnson@example.com	Initial calibration dataset	1	2024-11-11T14:35:00	2024-11-15T18:20:00	查看
BT202411190002	PR202311002	Bob Smith	bob.smith@example.com	Test sample 1	2	2024-11-11T09:00:00	2024-11-15T16:45:00	查看
BT202411190003	PR202311003	Catherine Brown	catherine.brown@example.com	Background data acquisition	3	2024-11-19T10:15:00	2024-11-19T11:45:00	查看
BT202411190004	PR202311004	Daniel Wilson	daniel.wilson@example.com	Sample test dataset	4	2024-11-19T14:00:00	2024-11-19T16:00:00	查看
BT202411190005	PR202311005	Eve Thompson	eve.thompson@example.com	Calibration and alignment data	5	2024-11-19T08:30:00	2024-11-19T10:30:00	查看
BT202411190006	PR202311006	Frank White	frank.white@example.com	Sample run 2	6	2024-11-19T11:00:00	2024-11-19T13:30:00	查看
BT202411190007	PR202311007	Grace Hall	grace.hall@example.com	Optimization dataset	7	2024-11-19T15:00:00	2024-11-19T17:00:00	查看
BT202411190008	PR202311008	Henry Clark	henry.clark@example.com	Final data collection	8	2024-11-19T09:45:00	2024-11-19T11:15:00	查看
BT202411190009	PR202311009	Ivy Lewis	ivy.lewis@example.com	Control experiment data	9	2024-11-19T13:45:00	2024-11-19T14:45:00	查看
BT202411190010	PR202311010	Jack Martin	jack.martin@example.com	Verification dataset	0	2024-11-19T10:00:00	2024-11-19T12:30:00	查看



## Step3: A Unified Framework for Attitude Tuning



### Input/Output ports

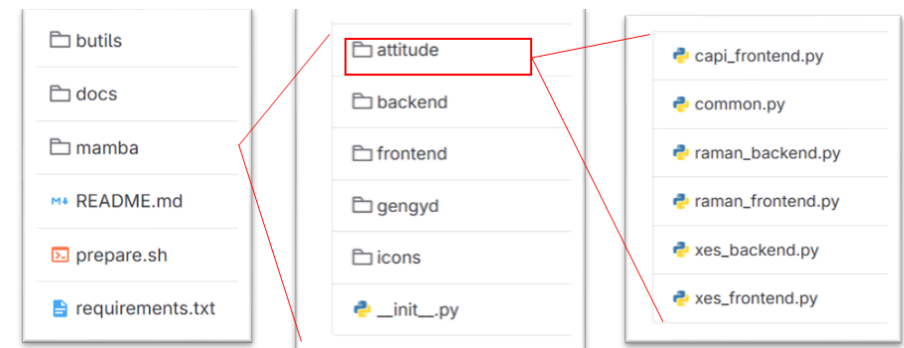
Physical quantity -> Mathematical quantity

### Data Processing and Evaluation Functions

Optional, scalable (Image Denoising、Bad Pixel Correction、Background Subtraction、Radial Distribution、Angular Distribution and AI .)

### Optimization Algorithms

Feature-rich, widely supported, high maturity

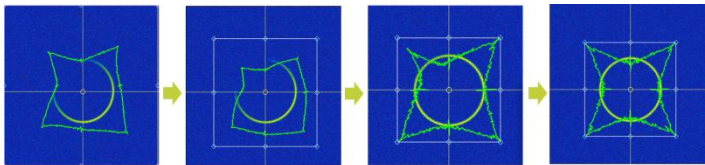




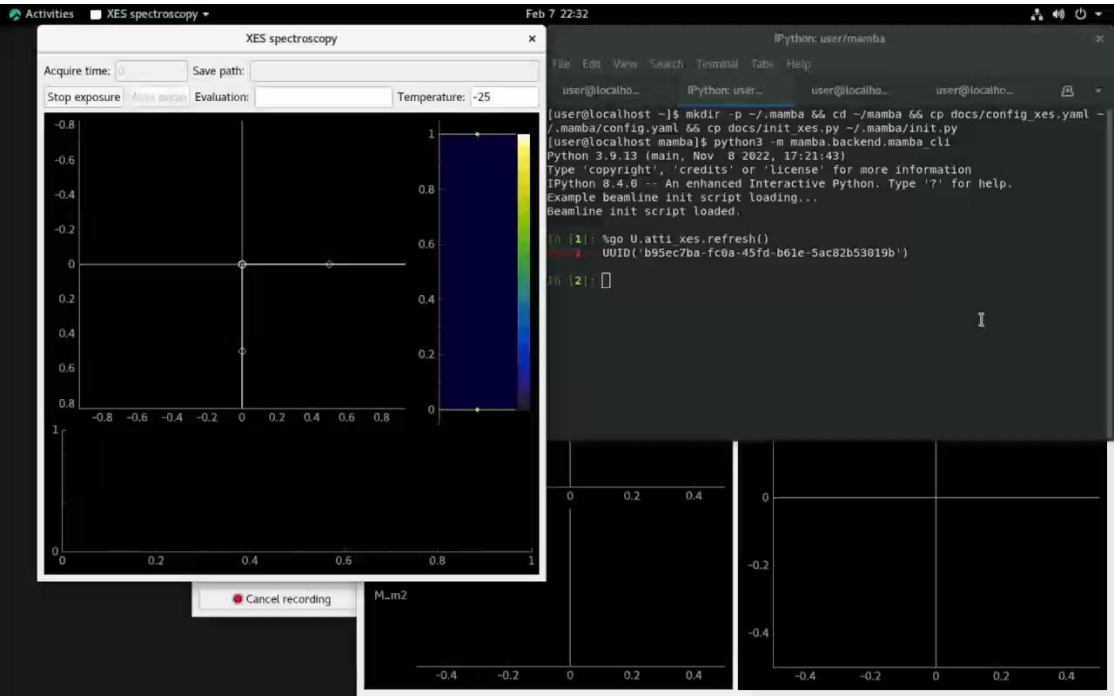
# Step3: A Unified Framework for Attitude Tuning

## General Attitude Tuning: XES Spectrometer

- ❑ Performing Bragg reflection on the analyzer of the vonHamos spectrometer on the 4W1B of BSRF will produce a circular pattern.  
(pitch/tilt & yaw/pan angles)
- ❑ General Attitude Tuning software is used to optimize the shape of the circle.

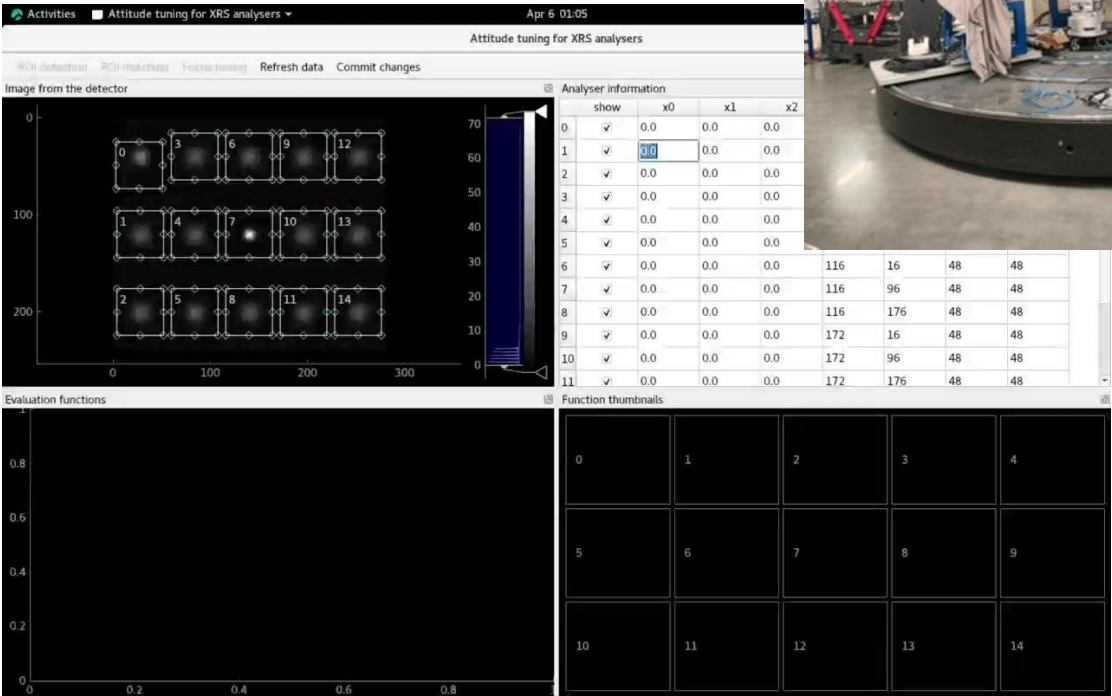


XES Spectrometer Attitude Tuning Process



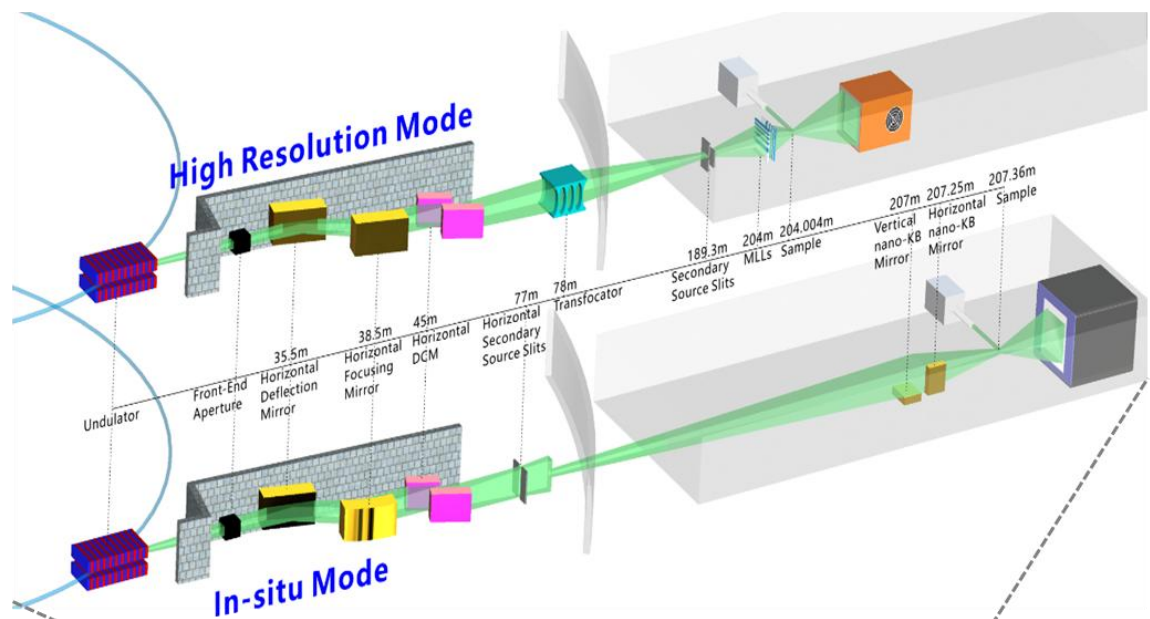
## Specialised Attitude Tuning: XRS Spectrometer

- ❑ Proof-of-concept test on the automatic attitude tuning of analyzer crystals of HEPS Raman spectrometer.  
(90 analyzer crystals, 270 motions , and 6 detectors)
- ❑ Specialized attitude tuning software is used for spot identification, allocation and focus adjustment.

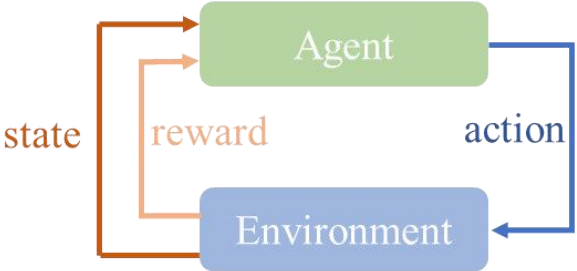
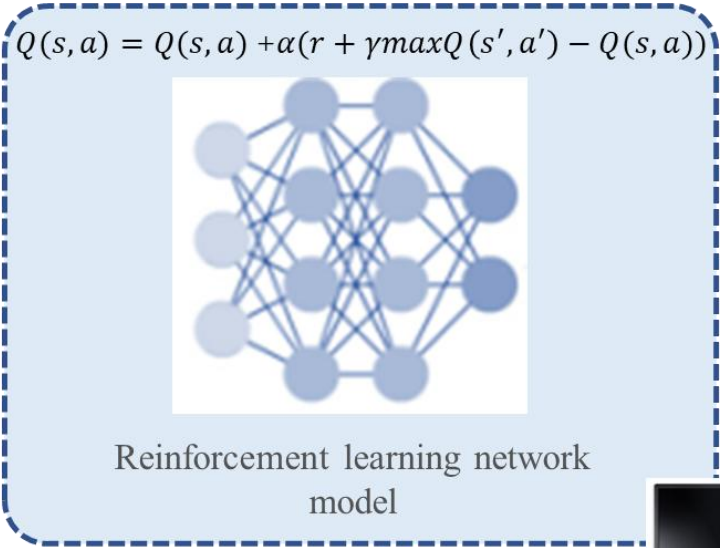


Step4: algorithm development and deployment

Fast Intelligent Autofocus Alignment Of Digital Twin System For Beamline Stations



Realtime online X-ray focusing system

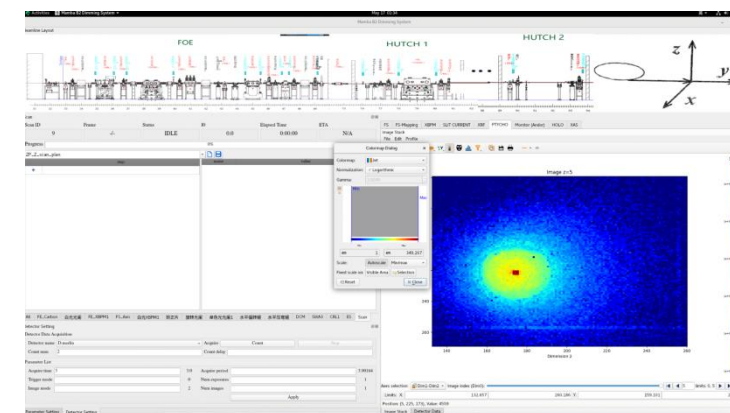
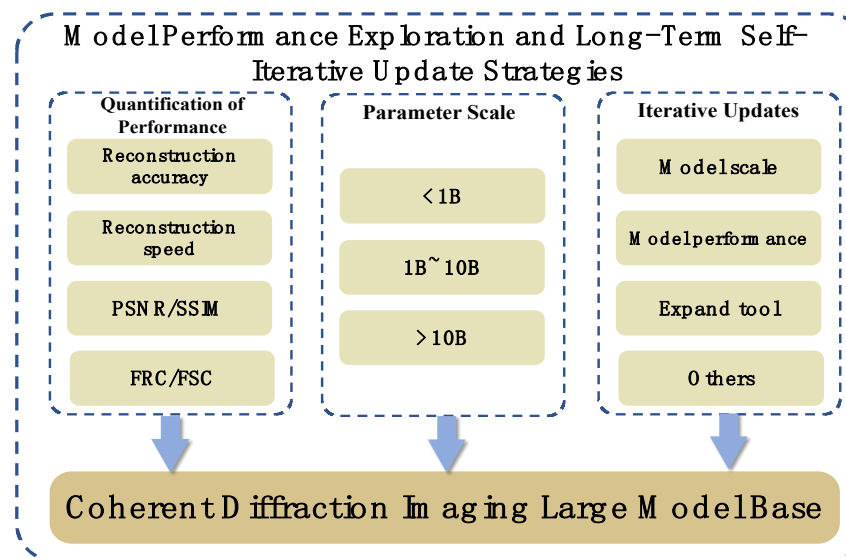
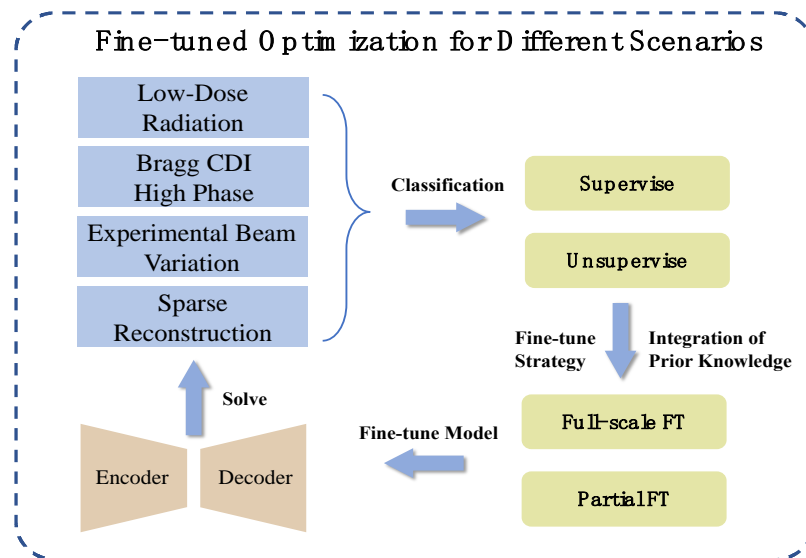
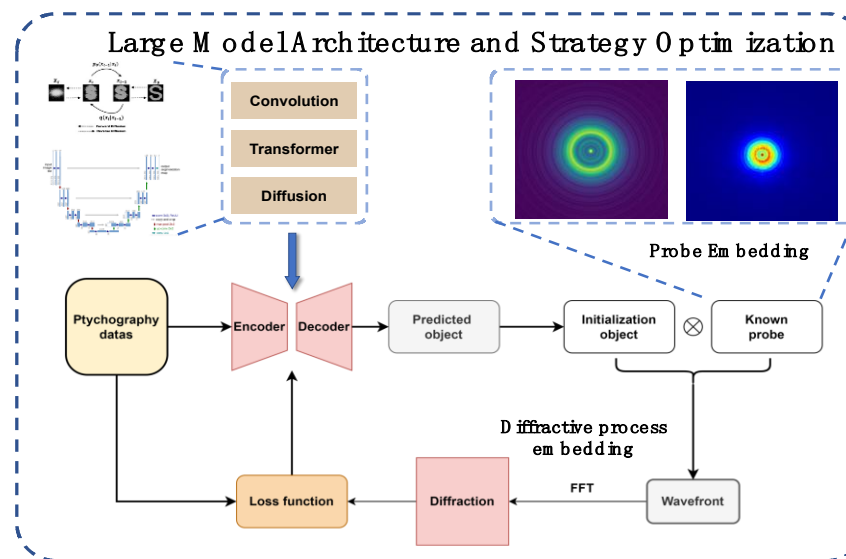
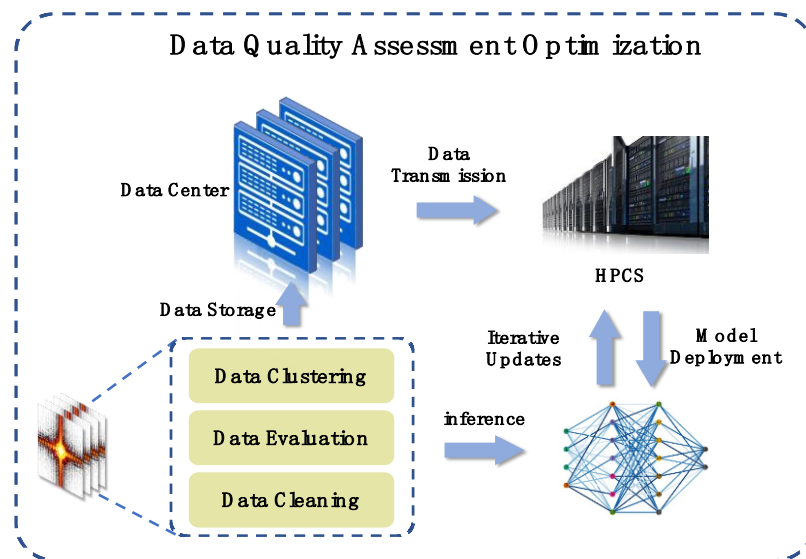


Virtual digital twin system for autofocus alignment

Further optimize training

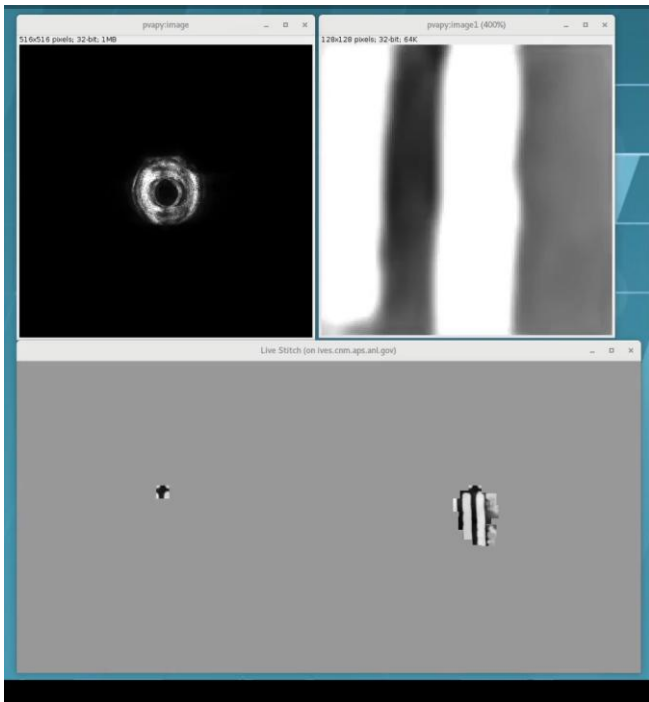
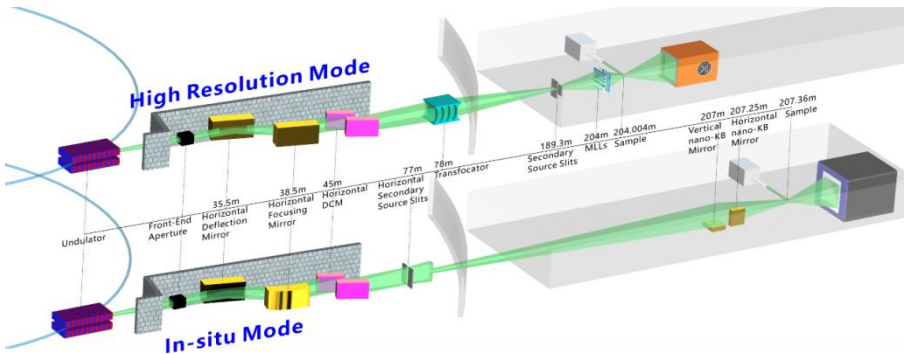
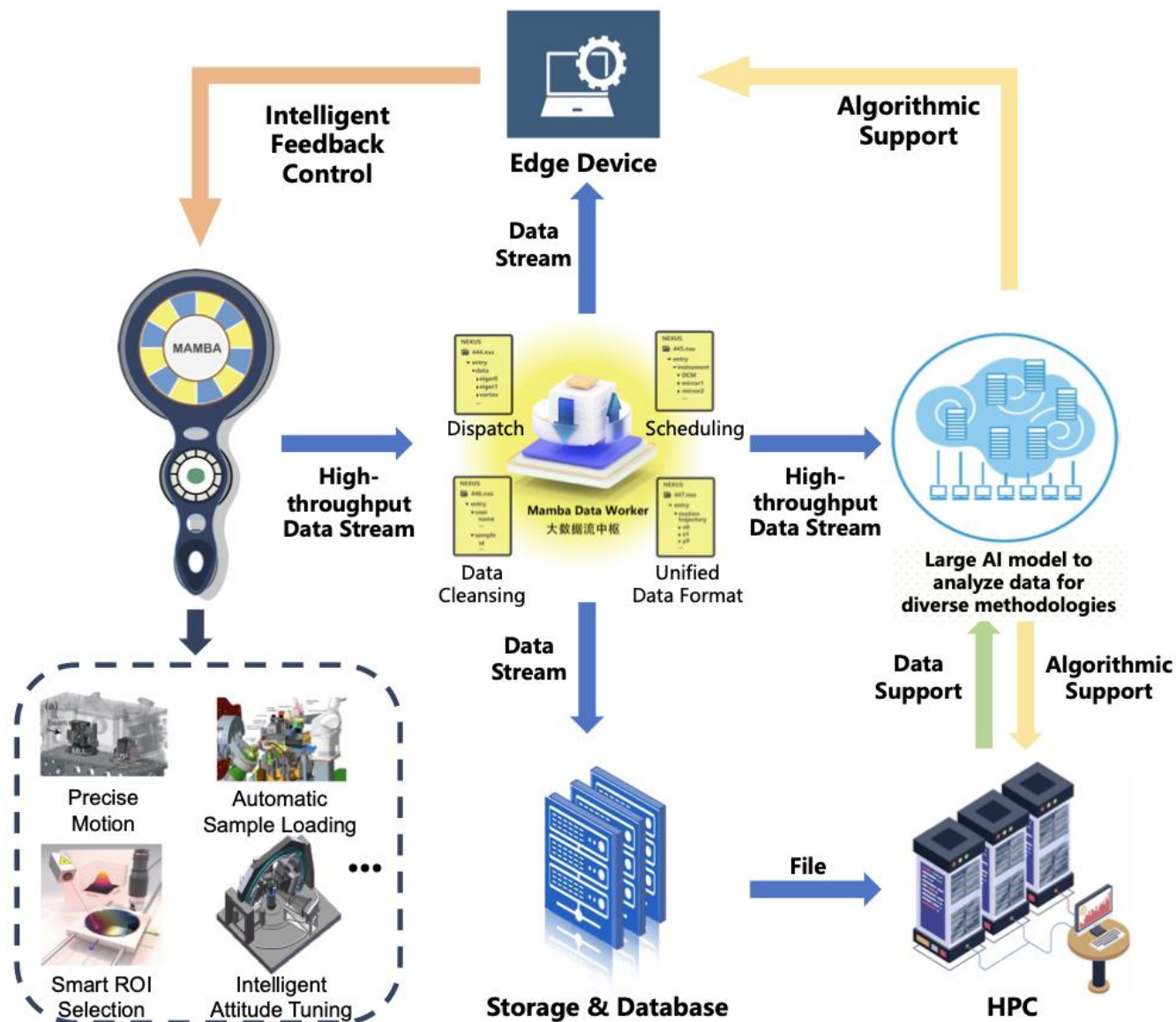
# Step5: Developing Domain specific big AI model

- Real-time data analysis and online feedback control capabilities
- Deployable to edge devices from various beamlines
- Iteratively updated with data accumulating at long-term





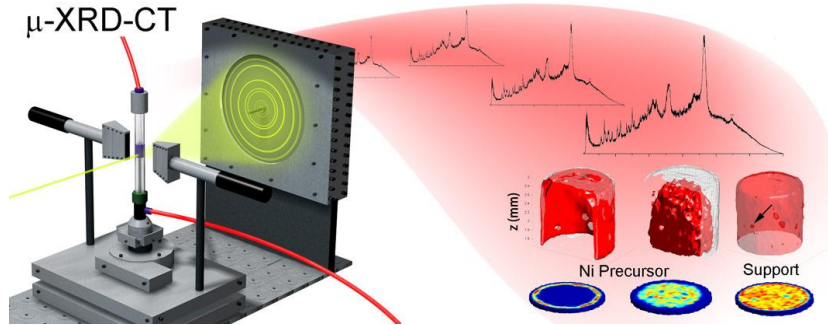
# Step6: Beamline auto-piloting



# Algorithms-driven SAXS/WAXD technique development

Multidimensional SAXS/WAXD is becoming a routine method

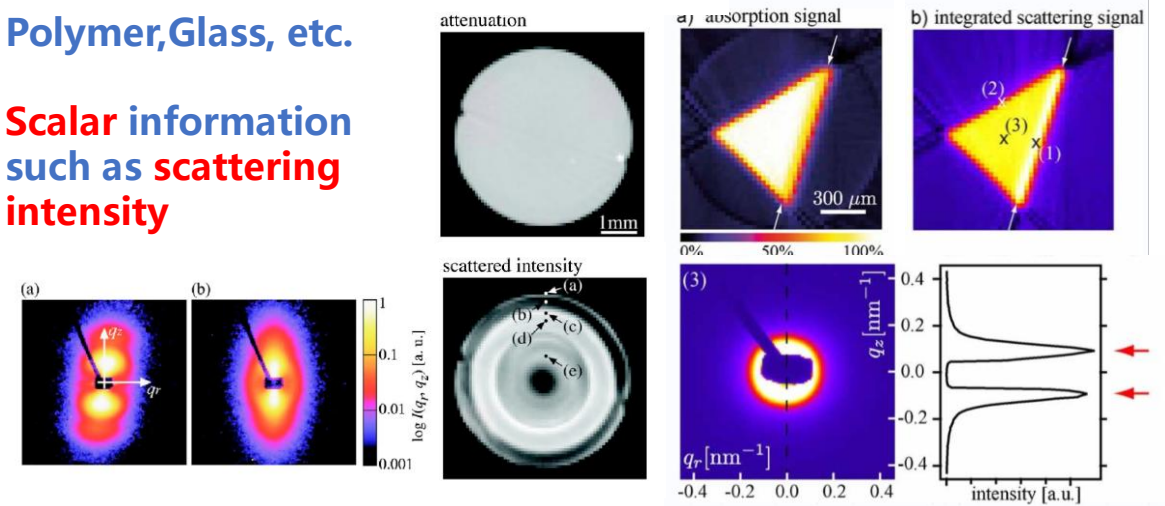
**Powder samples**  
(catalysts, rocks,  
minerals, etc.)



## SAXS-CT

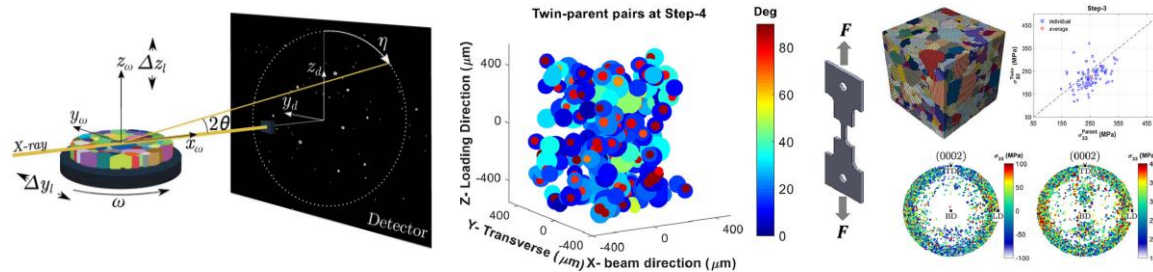
**Polymer, Glass, etc.**

**Scalar information**  
such as **scattering**  
**intensity**

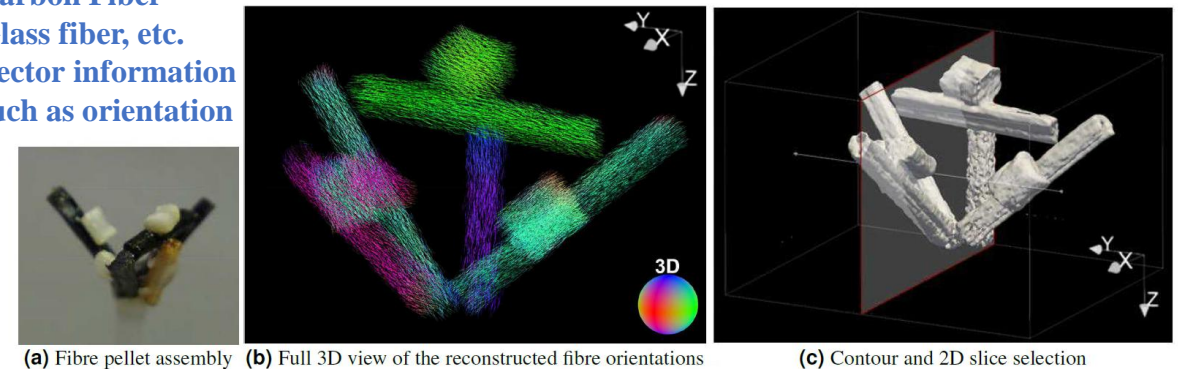


## 3D XRD

**Metal**



**Carbon Fiber**  
**Glass fiber, etc.**  
**Vector information**  
such as **orientation**



J. M. Feldkamp, et al. Phys. Status Solidi A, 2009

Tao Hu, et al. Macromolecules, 2020

Jisoo Kim, et al. Scientific Reports. 2021

N. Axel Henningsson, et al. J. Appl. Cryst., 2020

Hamidreza Abdolvanda, et al. Acta Materialia. 2020

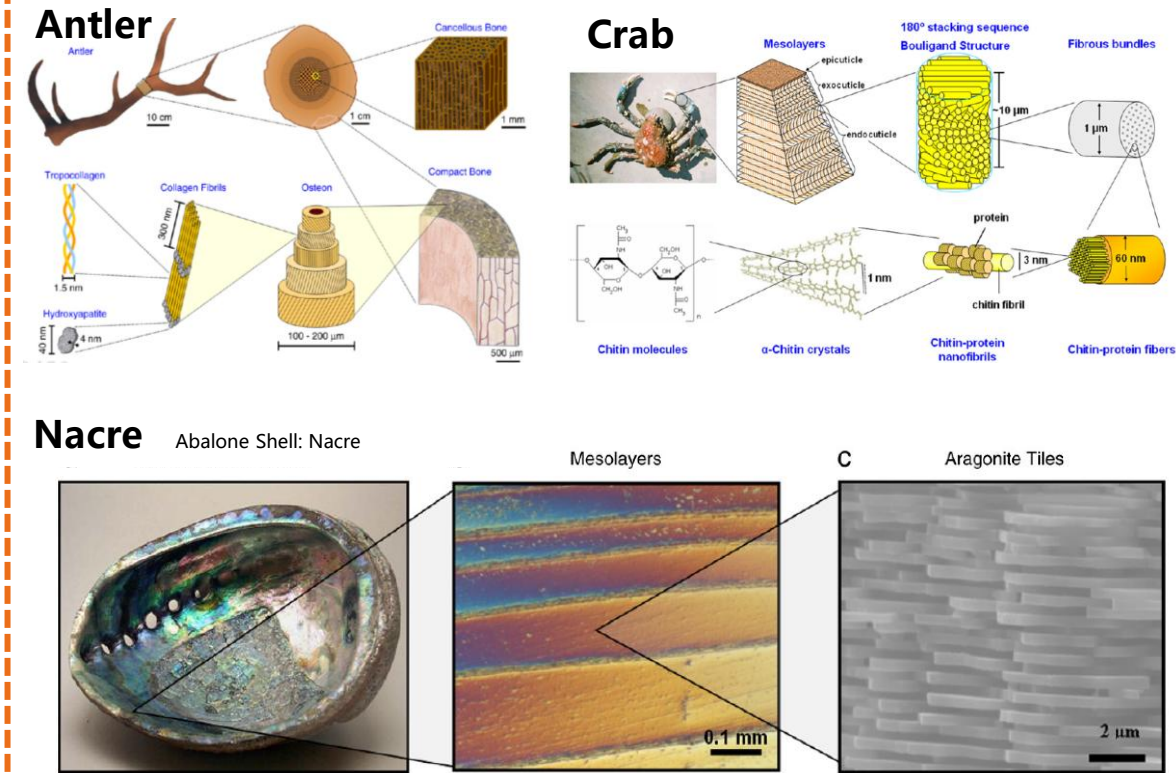




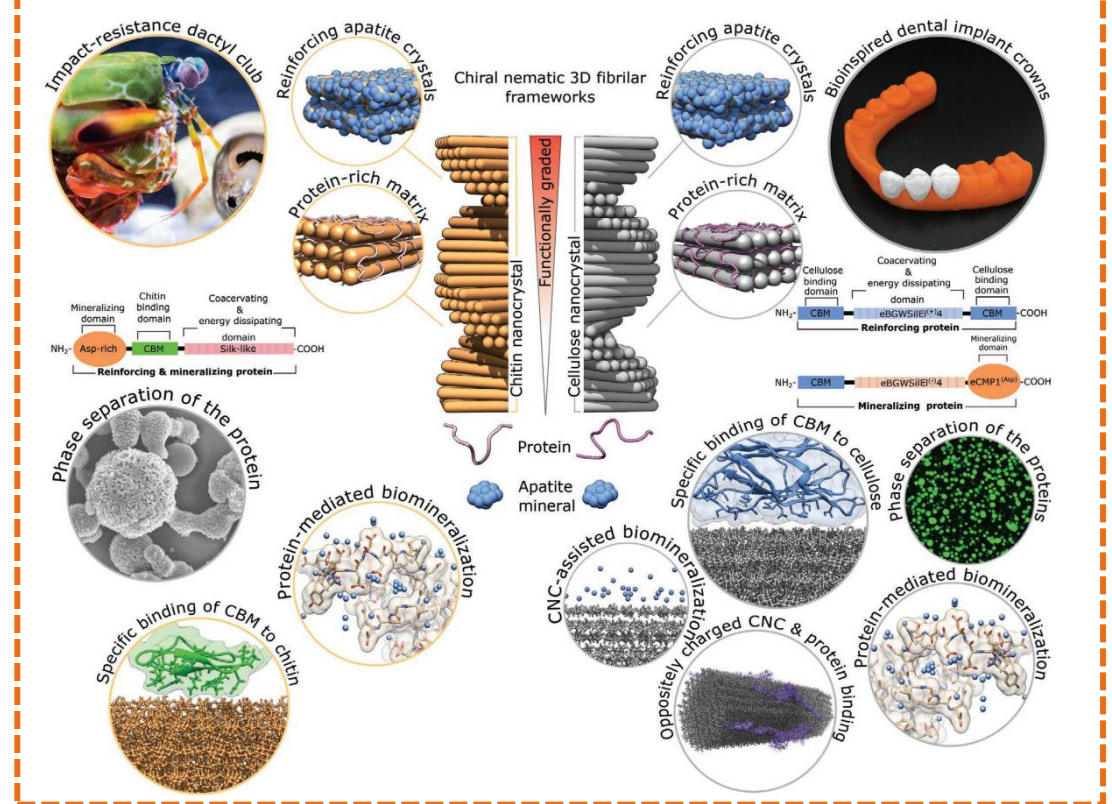
# Algorithms-driven SAXS/WAXD technique development

## 3D characterization of anisotropic fiber orientation

### Natural Material



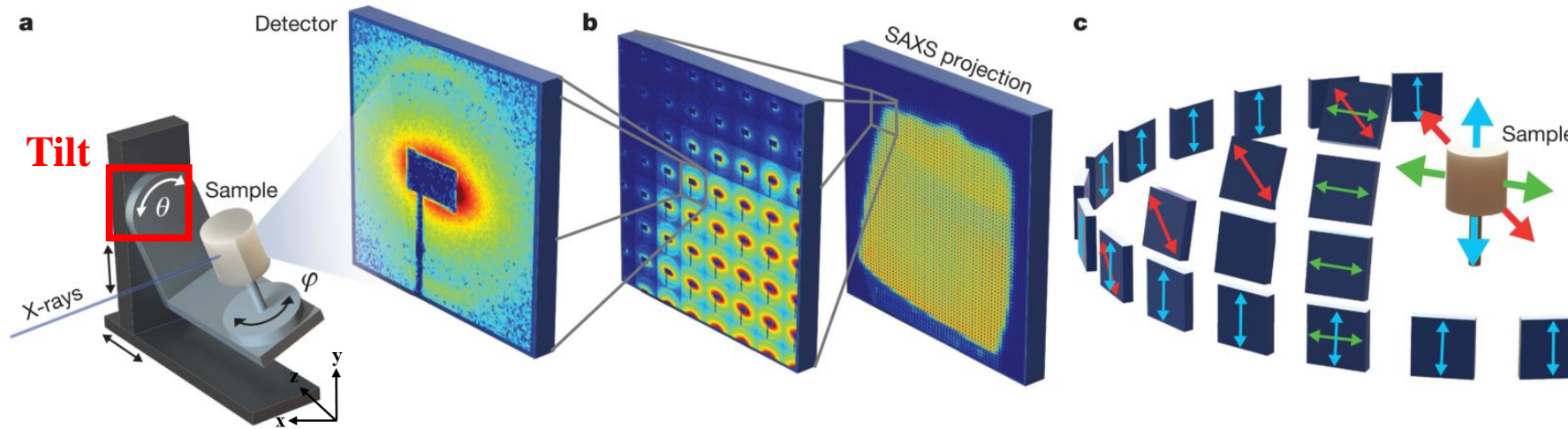
### Biomimetic Material



**Anisotropic fiber orientation is directly related to the anisotropic mechanical properties of materials, but there is a lack of suitable characterization methods.**

# Algorithms-driven SAXS/WAXD technique development

## Bottleneck of 6D SAXS/WAXD : Timeliness of sample scanning



How to **avoid time-consuming Tilt angle scanning** and directly use 3D scanning data to replace 4D scanning, to achieve 6D SAXS/WAXD tomography:

- ❑ Improve the efficiency of 6D SAXS/WAXD experiments and reduce the experimental time by an order of magnitude.
- ❑ Reduce the amount of experimental data.
- ❑ Implement *in-situ* experiments setup.

**For anisotropic materials, SAXS/WAXD tomography does not meet the rotational invariance required for CT reconstruction.**

**Sample Size :  $3 \times 4 \text{ mm}^2$**

**Beam Size:  $50 \times 50 \text{ } \mu\text{m}^2$**

**Exposure time: 50 ms**

**Patterns Number :  
1,376,352**

**Time consumption:  
40 h**

**Rotation range:  $0-360^\circ$**

**Tilt range:  $0-68^\circ$   
(10 tilt angles)**

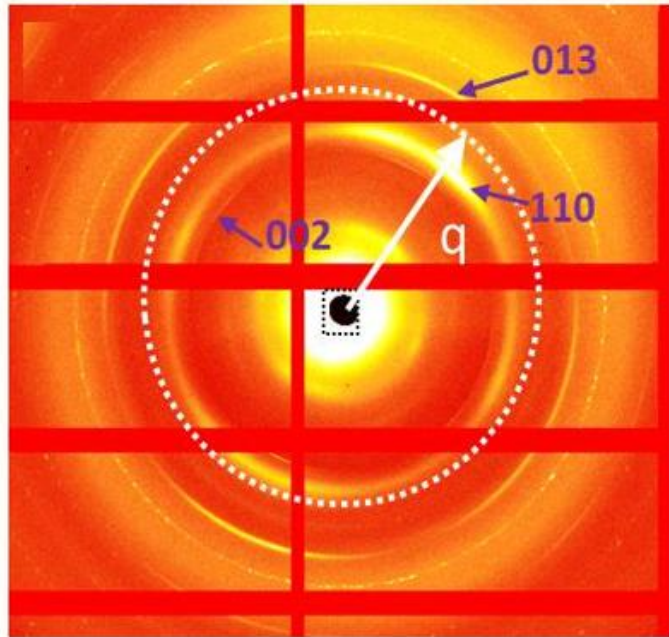




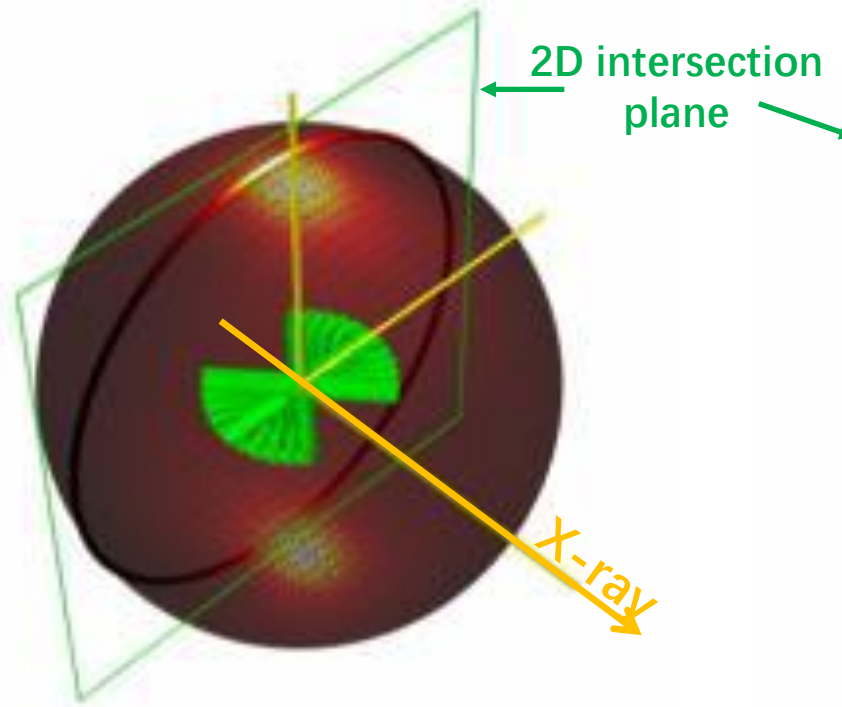
# Algorithms-driven SAXS/WAXD technique development

Can the scanning process of reciprocal space be simplified?

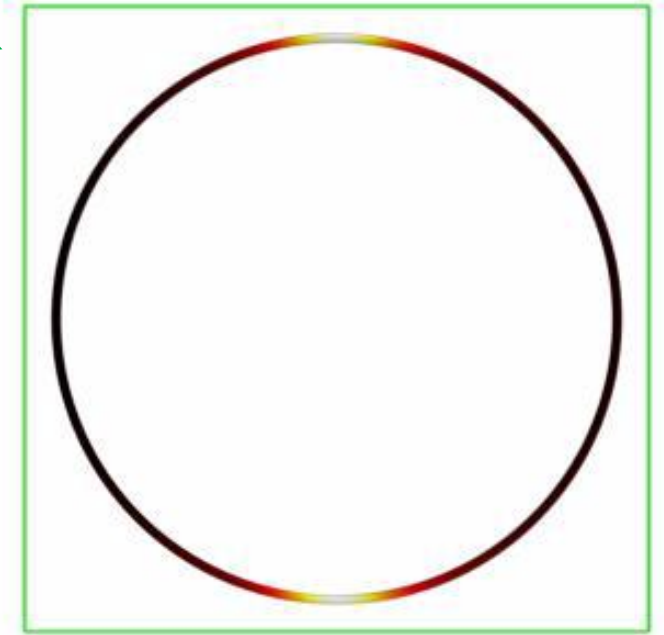
Are there 3D information hidden behind 2D WAXD pattern? The QS(110) change with fibre orientation parameters ( $\gamma, \Delta\gamma$  (2D),  $\alpha, \beta$  (3D)) variation



2D WAXD pattern



Intensity distribution changes on QS(110) sphere



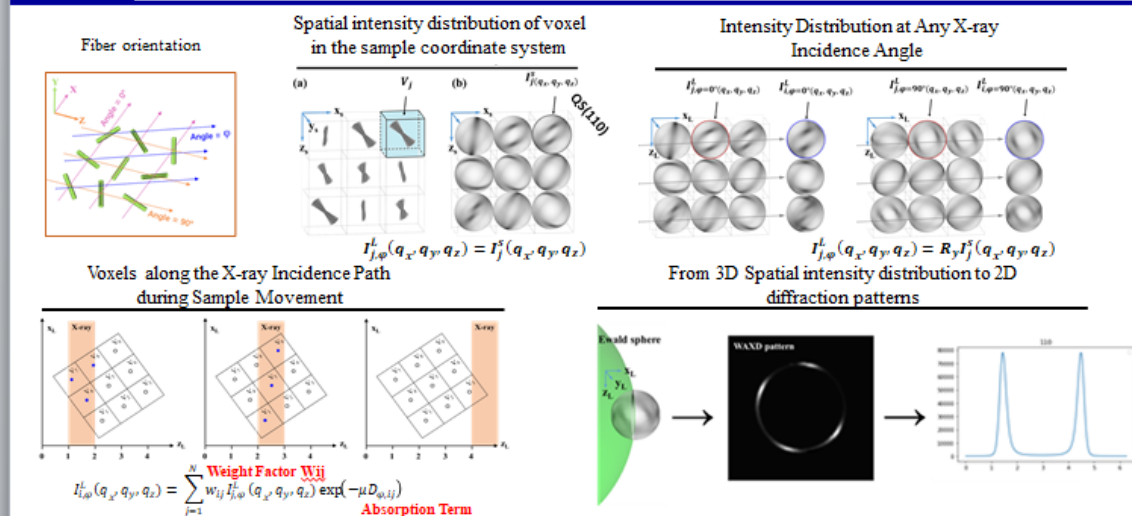
2D diffraction ring





# Algorithms-driven SAXS/WAXD technique development

## Step 1: Simulating 6D WAXD Tensor Tomography Dataset



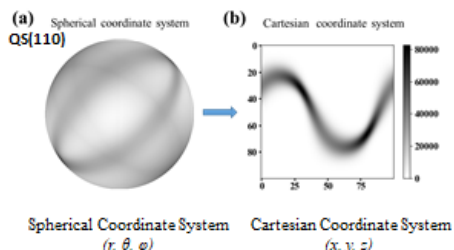
SRI 2024

12

## Step 3: Reconstruction

### Tensor Reconstruction :Distributed Reconstruction Strategy

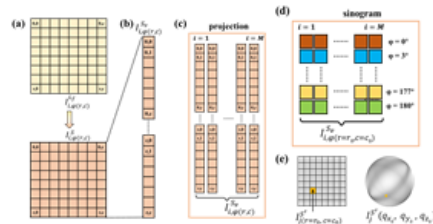
Step 1: Transforming 3D Reciprocal Space from Spherical Coordinate System to Cartesian Coordinate System



Dimensionality Reduction from 3D Reciprocal Space to 2D Tensor

Step 2: Point-by-point CT reconstruction

Step 3: Stitching point-by-point to form a three-dimensional voxel space image.



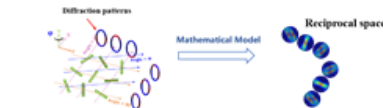
The sinogram formed by the intensities at the same position  $(x_0, y_0)$  of  $I_{i,\varphi}^t(q_x, q_y, q_z) \rightarrow$  FBP reconstruction, the intensity of each voxel at the position  $(x_0, y_0)$ .

6D reconstruction achieved through CT reconstruction methods.

15

## Step2: From 2D patterns to 3D QS(110)

### 3D Inverse Space Prediction and Numerical Optimization of Diffraction Data



Traversal  $\rightarrow$  Basin-hopping Algorithm

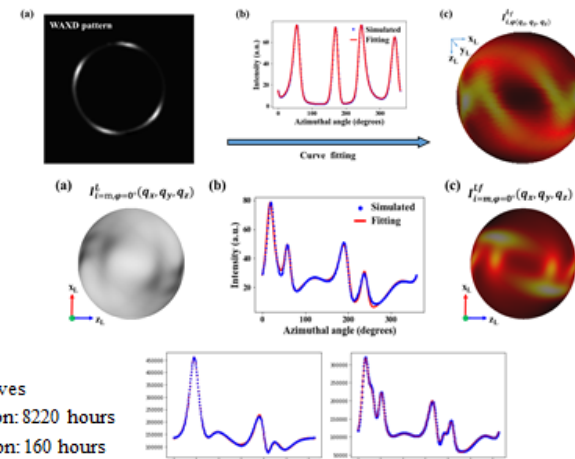
#### Basin-hopping Algorithm:

- Results: Simulation curve and fitting curve with  $R^2 = 99.1\%$ , correlation coefficient (PCC) between simulated  $QS(110)_{i,\varphi}^t$  and fitted  $QS(110)_{i,\varphi}^{tf}$  is 0.91
- Advantages: Setting iteration count, callback function, boundary conditions, etc., to accelerate finding the optimal solution of the function.

Fitting 1051 curves

CPU computation: 8220 hours

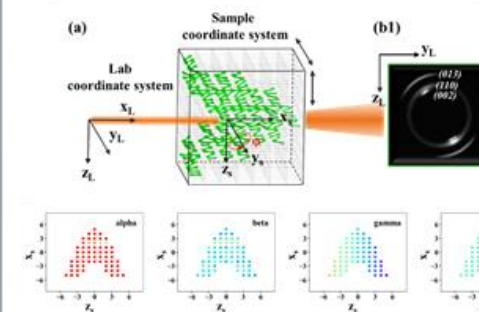
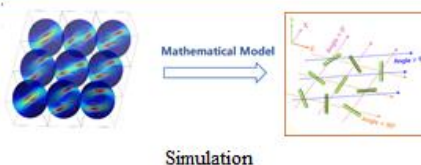
GPU computation: 160 hours



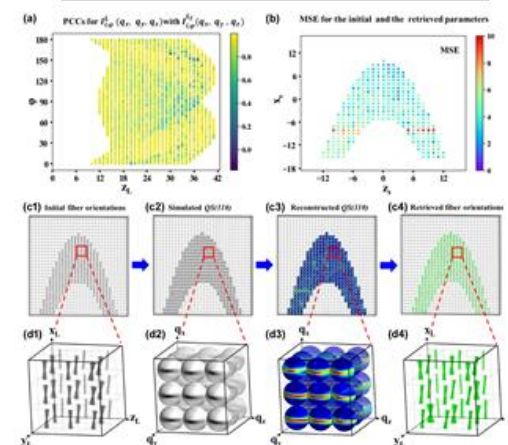
SRI 2024

13

## Step 4: Fiber Orientation Parameter Extraction



Result

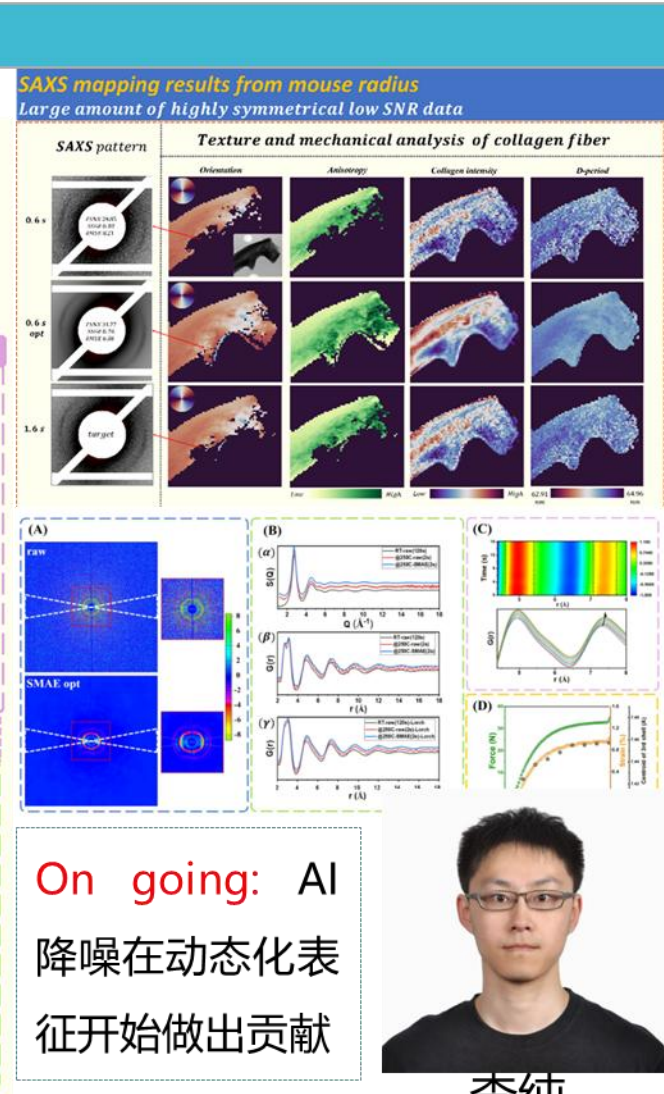
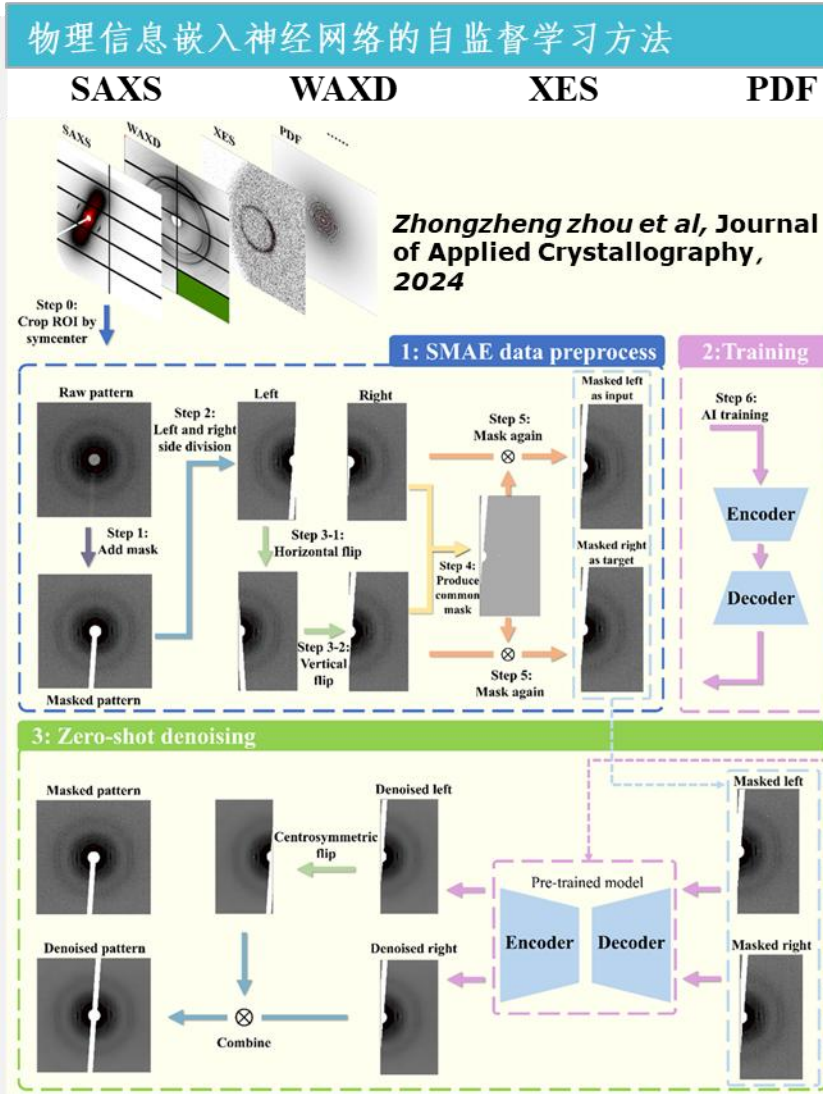
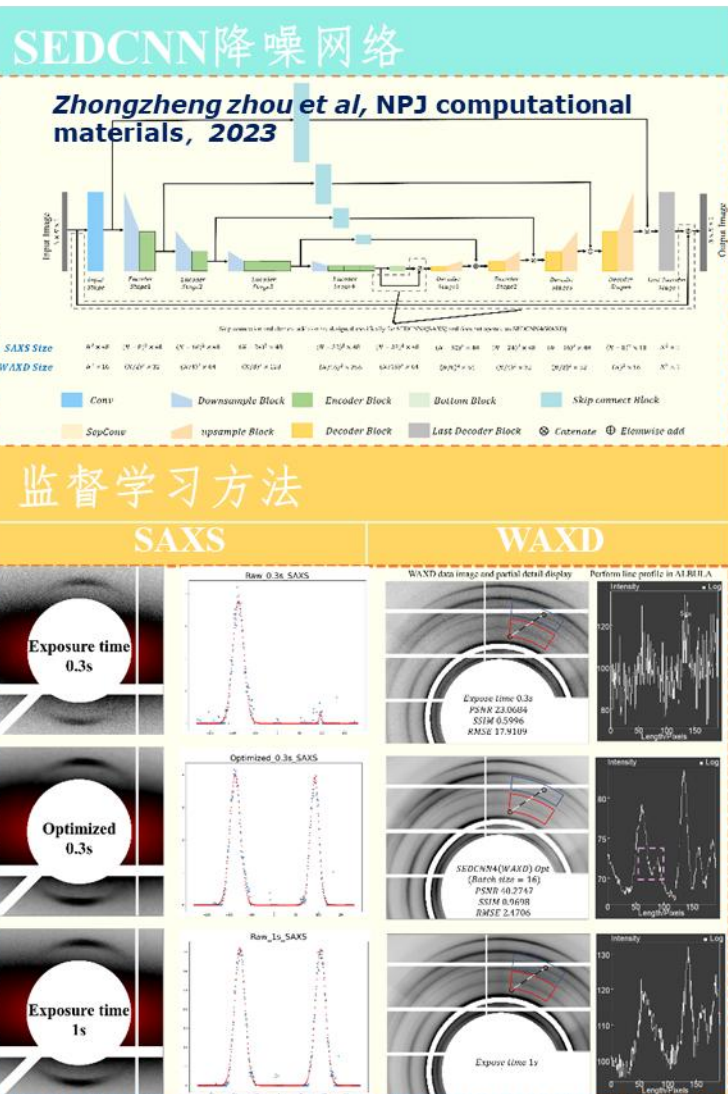


16



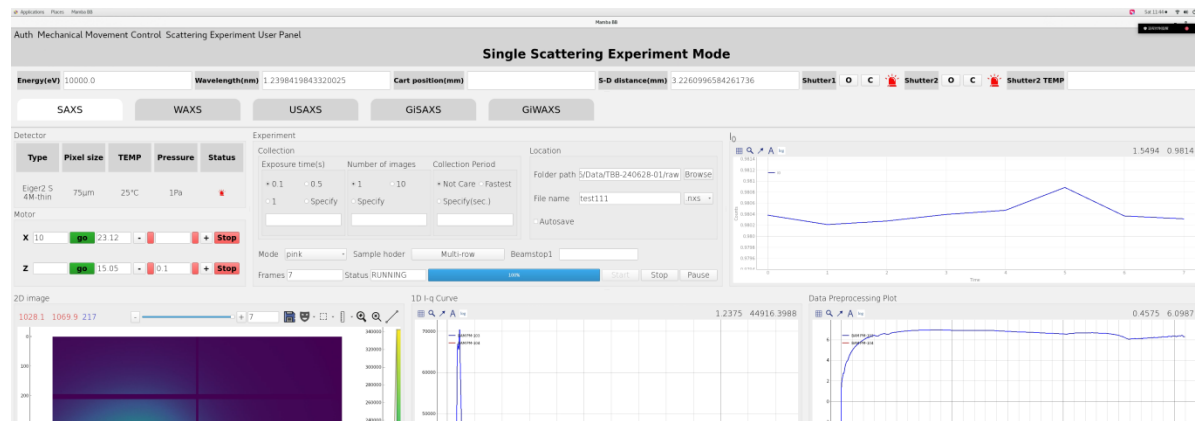
# Algorithms-driven SAXS/WAXD technique development

## Measure faster by x-ray denoising method

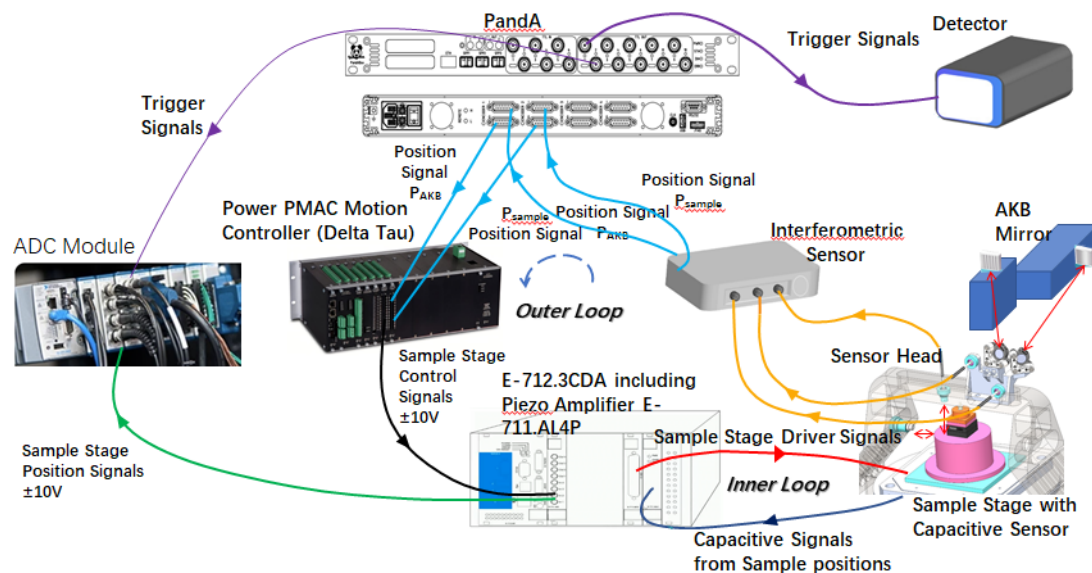


# Algorithms-driven SAXS/WAXD technique development

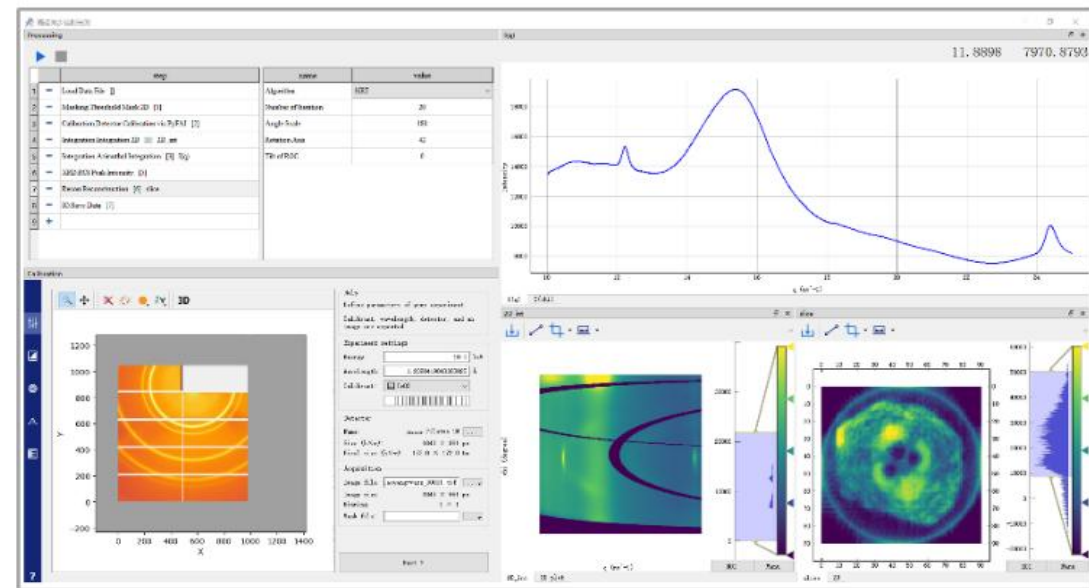
Data quality assurance by Mamba soft



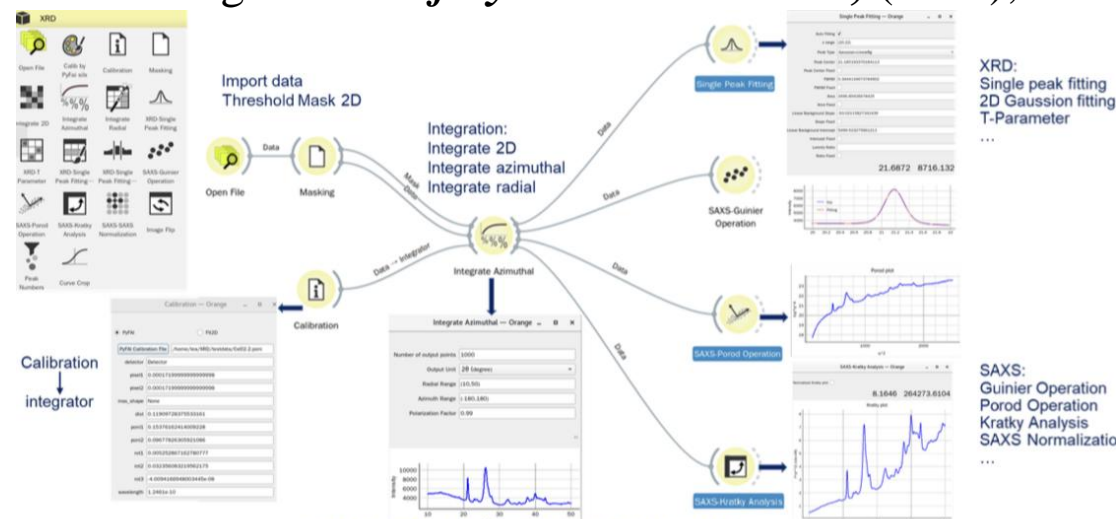
Fly-scan event structure based on Power PMAC



□ Fly-scan



Wang et al. *J. of Synchrotron Radiat*, (2024);



同时显示积分后的多种数据处理结果

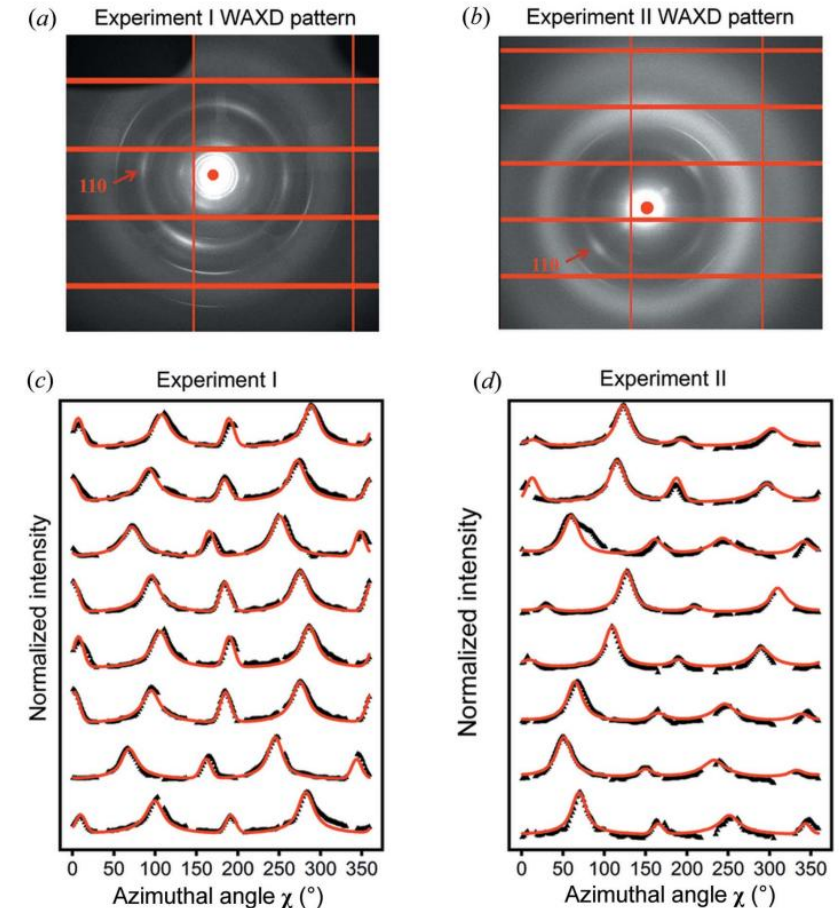
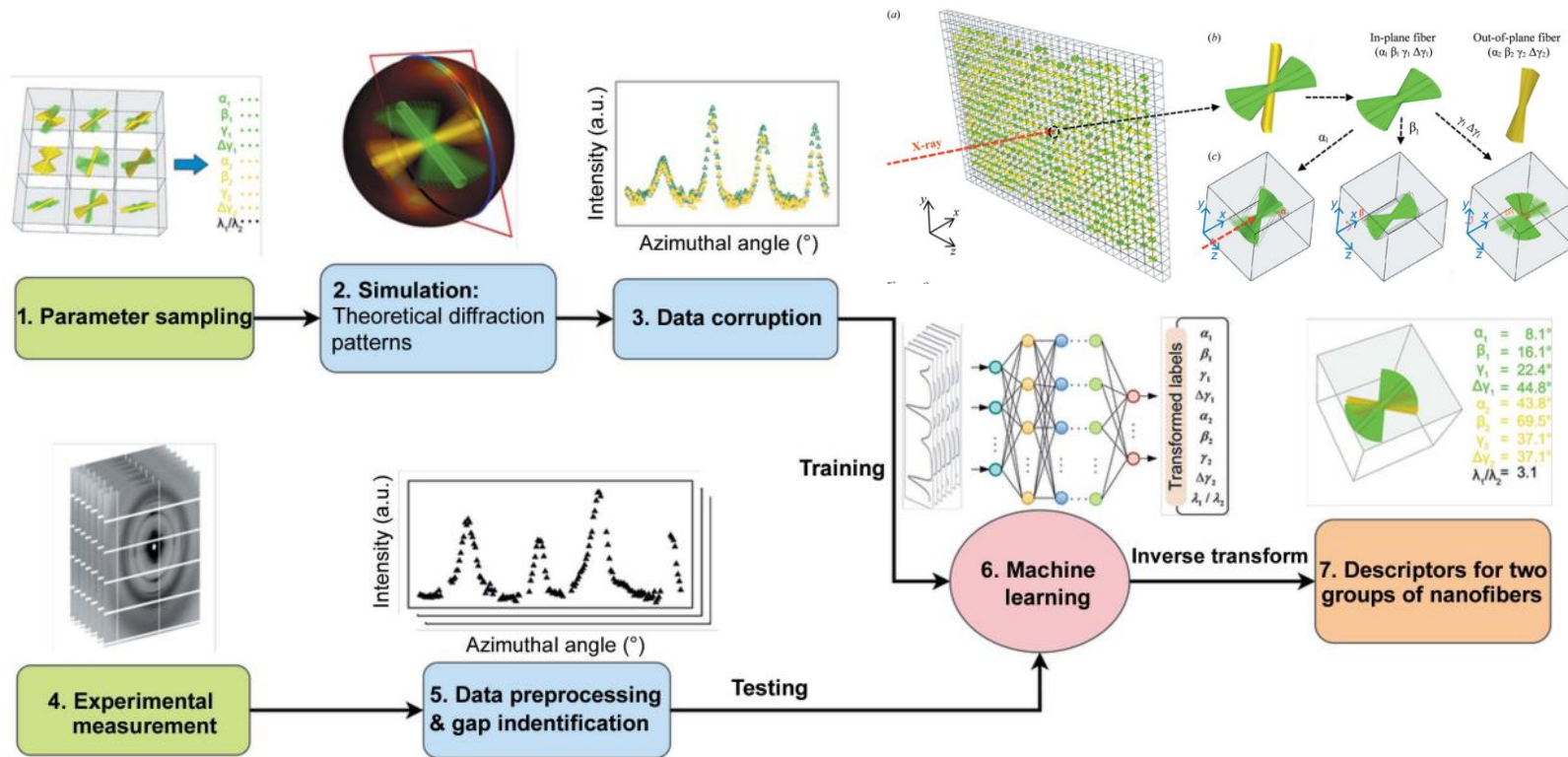
□ Real-time data analysis



# Algorithms-driven SAXS/WAXD technique development

Faster data analysis using AI

## Learning for Extracting Physical Information from Massive Diffraction Data

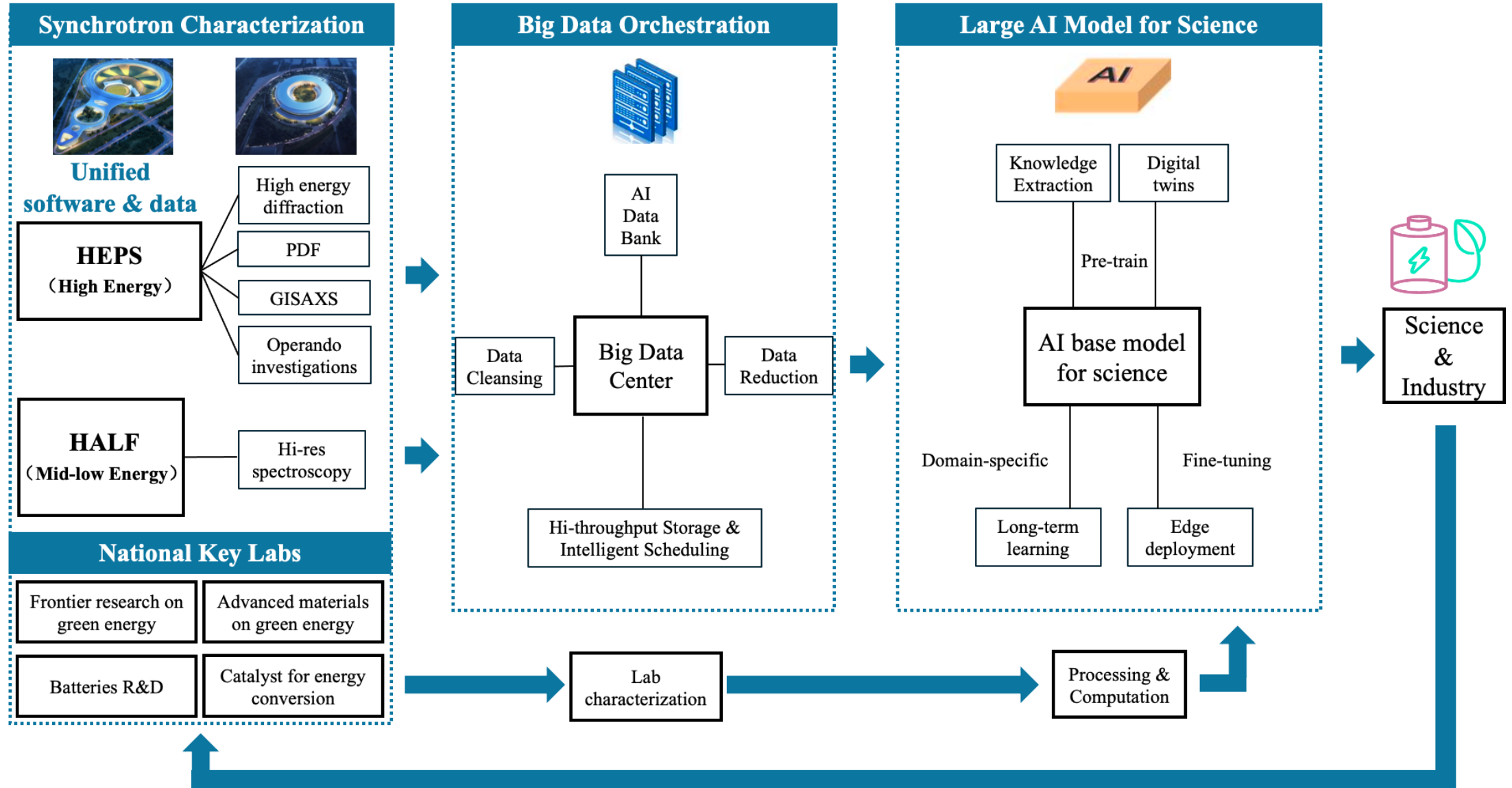


Efficient Data Acquisition Rate of One Million Frames per Hour, with Data Processing Time Less than 10 s.

Sun, M.<sup>#</sup>, Zheng Dong<sup>#</sup> et al. IUCrJ (2023)



# Intelligent cluster of scientific infrastructures



# *Collaborative efforts for intelligent light source*





# Our Team

- Building an all-round scientific software and algorithm development group



**Complex device  
control**



**Experiment  
process control**



**MAMBA**



**Area-specific  
algorithms**



**Big data  
acquisition and processing**



**User client  
development**



**Artificial Intelligence**



**Welcome to join our team**



# Domestic and international collaboration



Funding from:

- National Key Research and Development Project of China;
- Chinese Academy of Sciences;

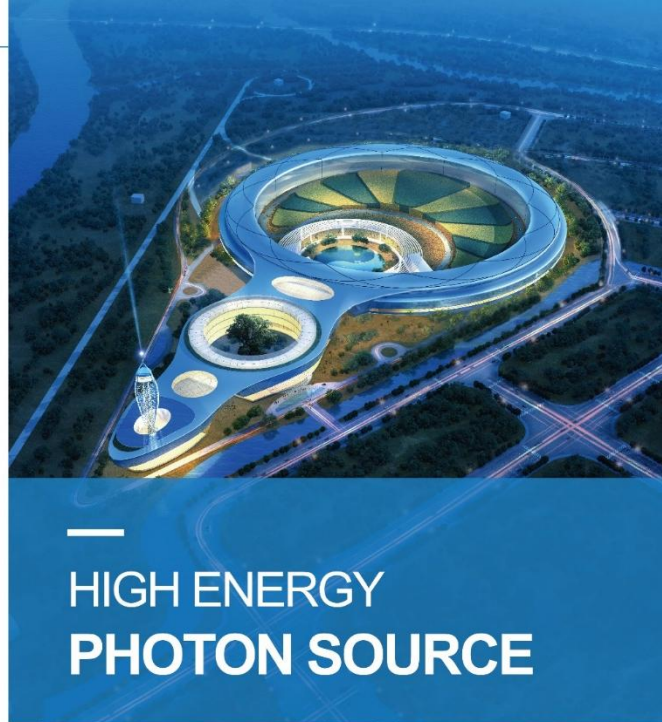
We are planning to form and develop a nation-wide united scientific software solution in China.

Internationally, we are looking for collaboration from other synchrotron sources.





## *Mamba* and *HEPS* Grow together

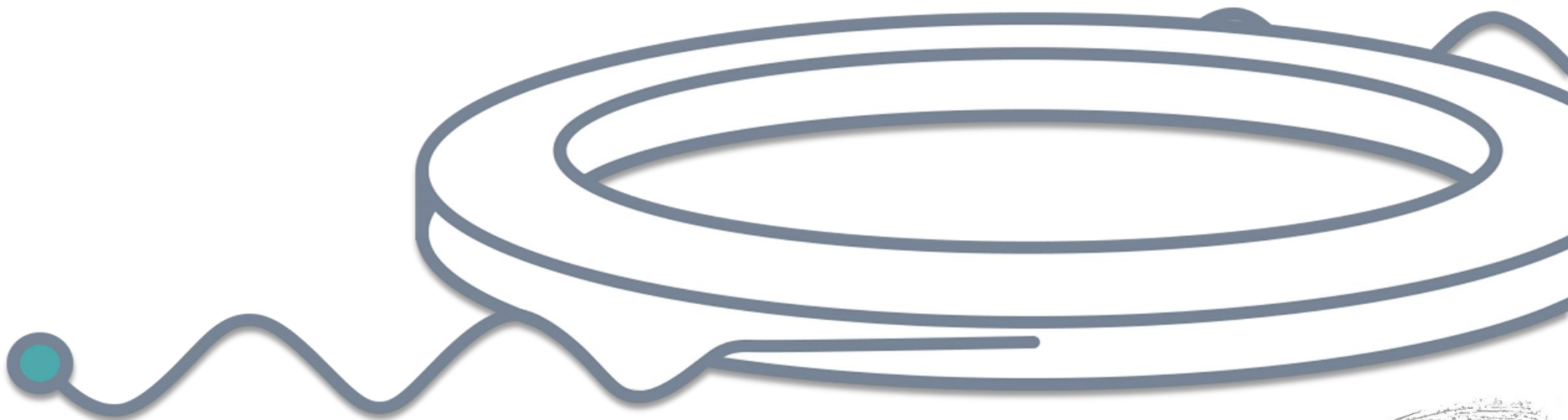


The full potential of the HEPS will be realized by coupling the intrinsic capabilities of the facilities with advanced Mamba system





# Device and motion control

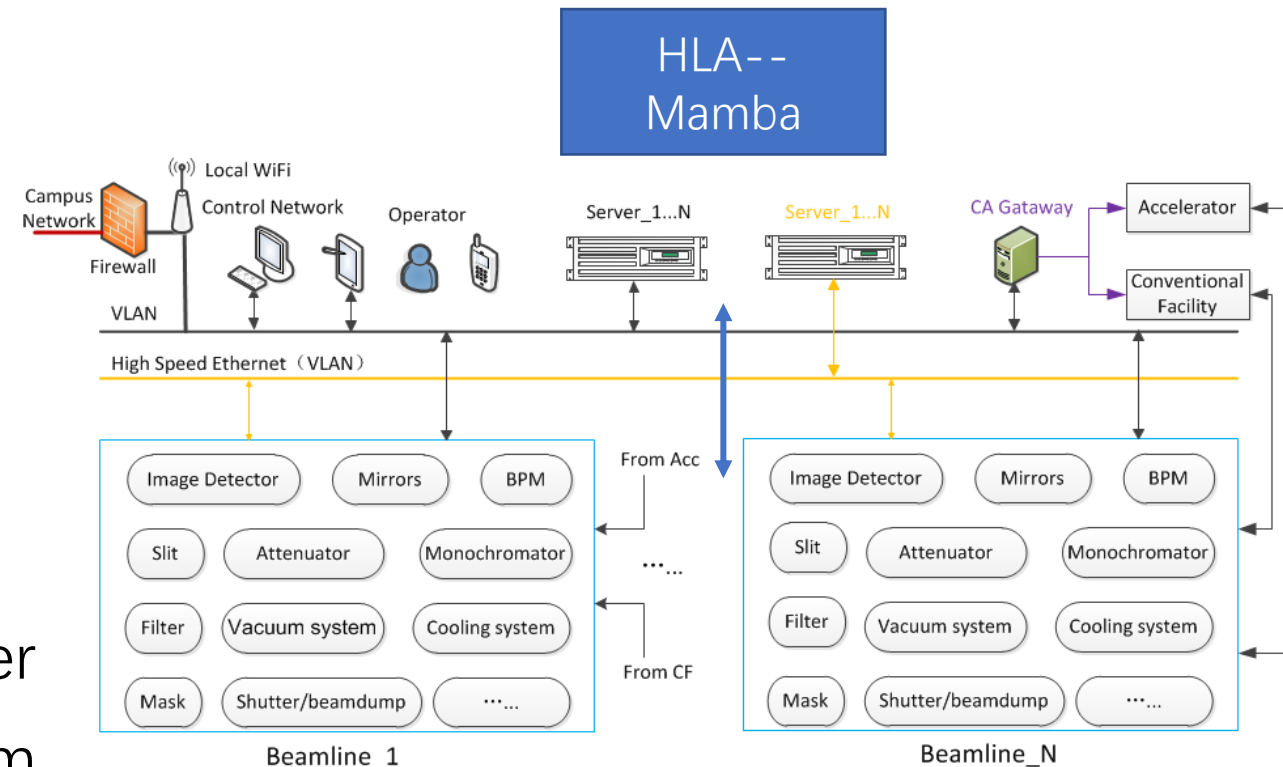


# Beamline control system

- Control tasks
  - “14+1” beamlines
    - Achieve the desired X-ray
    - Ease the scientist at experimental endstations
    - Control and monitor all the equipments of beamlines
    - Detect the position of X-ray beam
    - Protect the people/equipment from hazard, and send alarm and issue information.
    - Provide friendly OPIs, robust and efficient communications tools and rich application tools
    - Archive and retrieve the data of beamline

# Beamline control system

- The controlled equipment
  - Mirror and crystal bender
  - Monochromator
  - Beam Position Monitor
  - Image Detector
  - Low current measurement device
  - Slit, Shutter, Mask, Attenuator, Filter
  - Cryo-cooling/water-cooling system
  - Vacuum devices, etc.



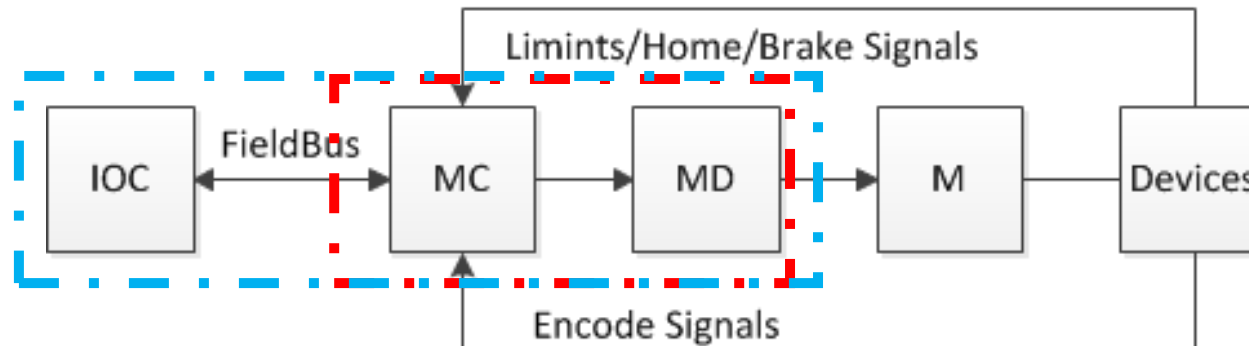


# Beamline control system

- Design Principles of the Control System
  - Stability
  - Availability
  - Reliability
  - Flexibility
  - Extendibility
  - Real Time

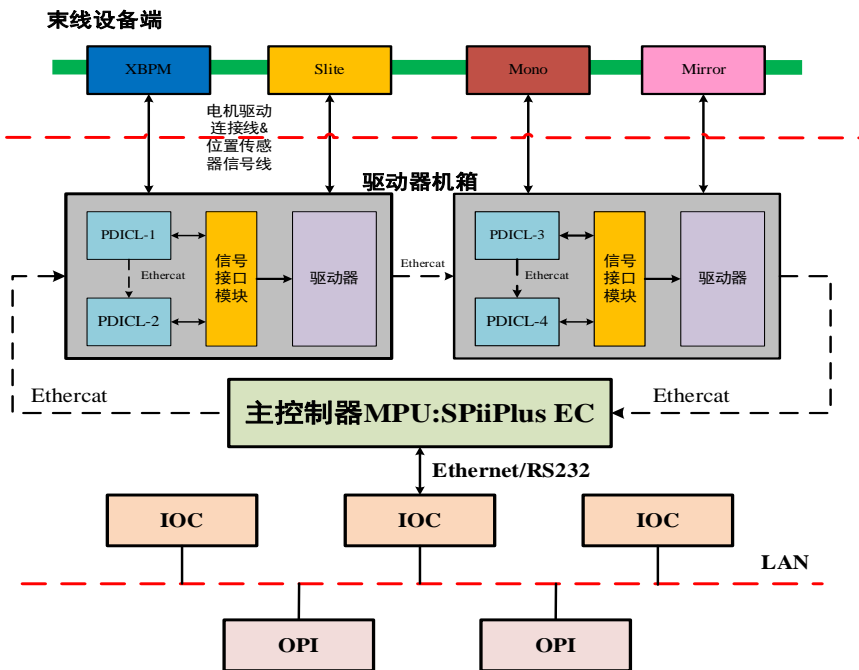
# Beamline control system

- Motion control system
  - Drive the optical elements (such as mirror, slit, attenuator, monochromator, filter, etc.) to get satisfied X-ray beam.
  - Critical subsystem of the beamline control system
  - Supporting various motor types
    - **step motor**, servo motor, piezo motor and so on



# Beamline control system

- Motion control system
  - Self-developed a set of motion control system
  - Drive two-phase and five-phase step motors





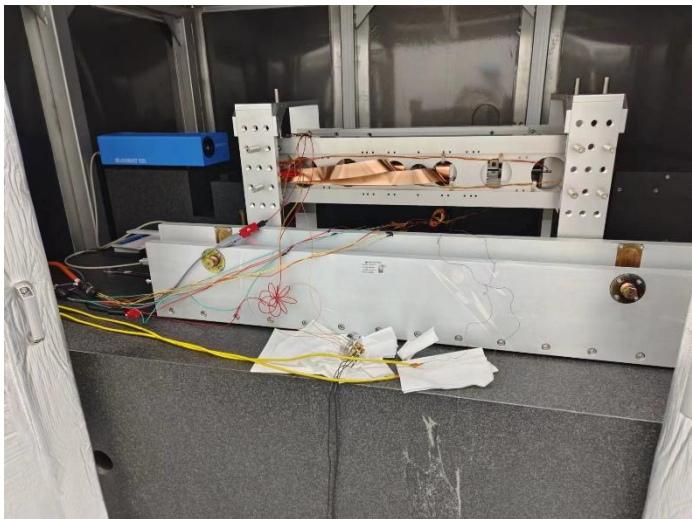
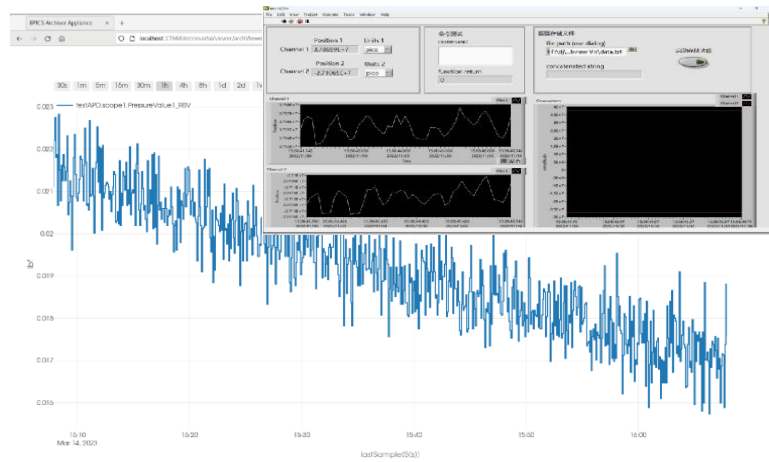
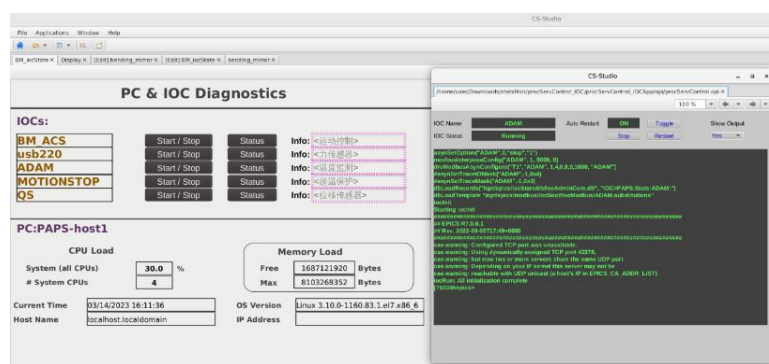
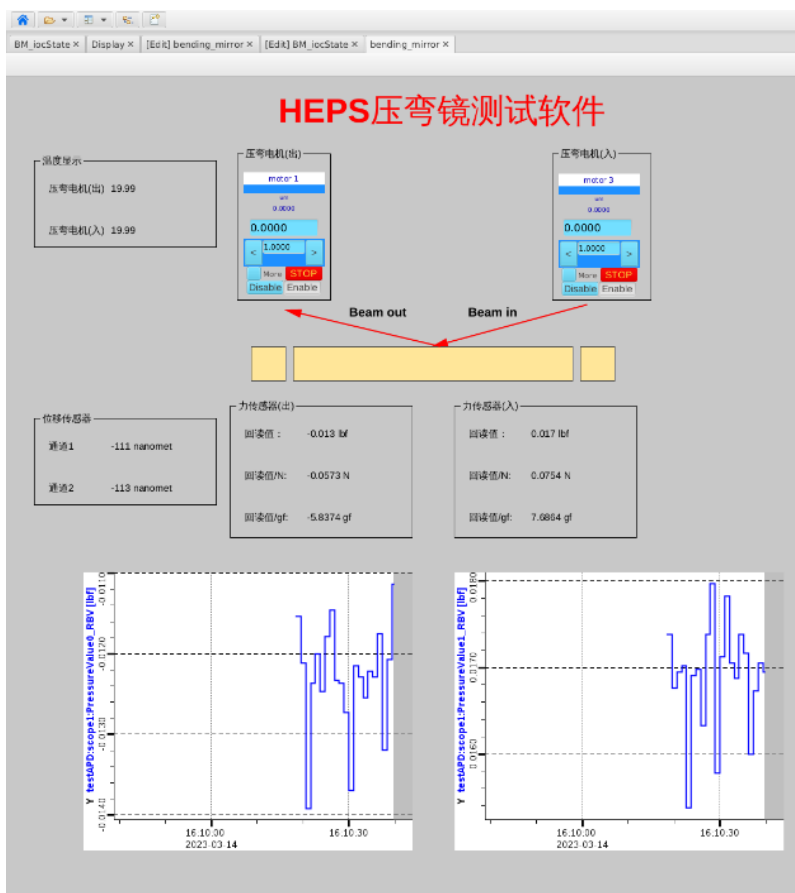
# Beamline control system





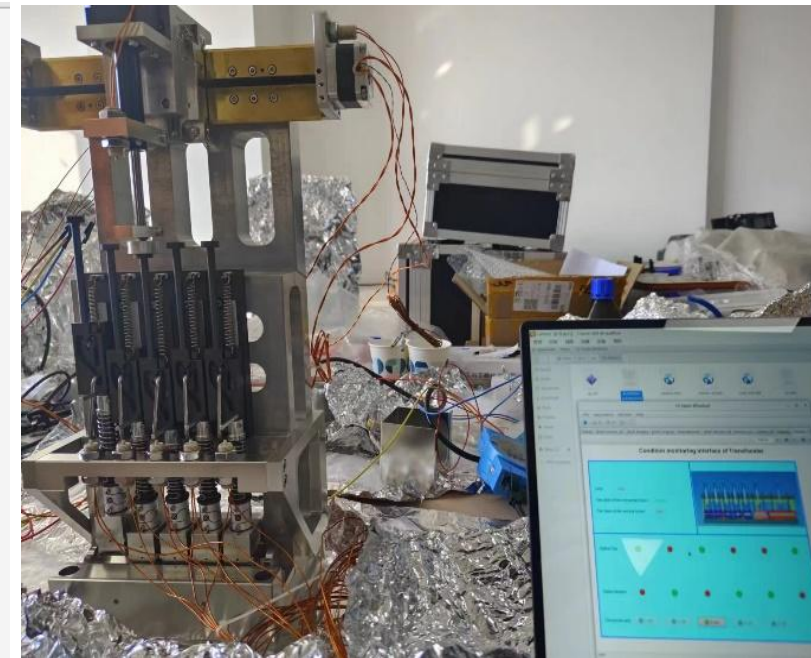
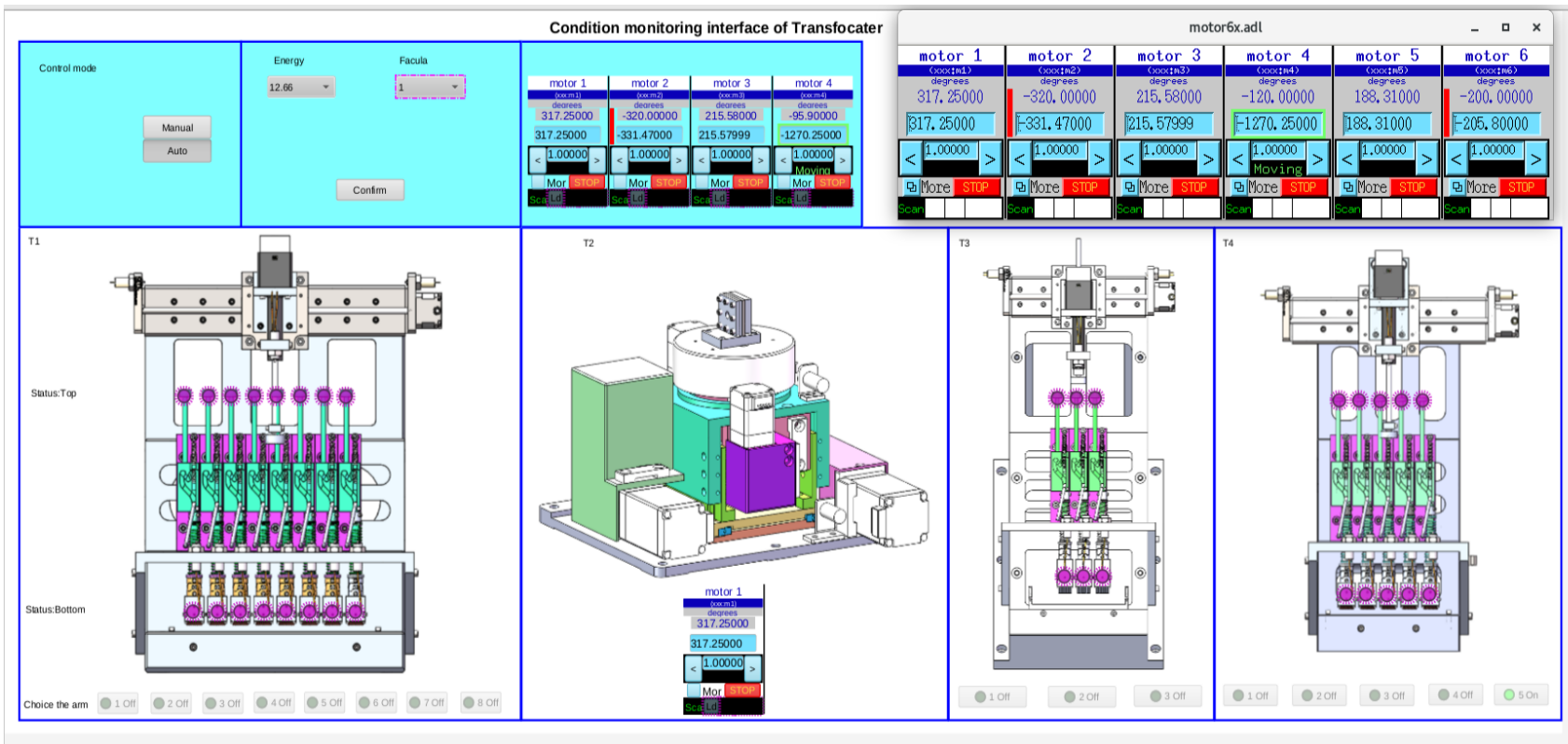
# Beamline control system

- Motion control system used at PAPS



# Beamline control system

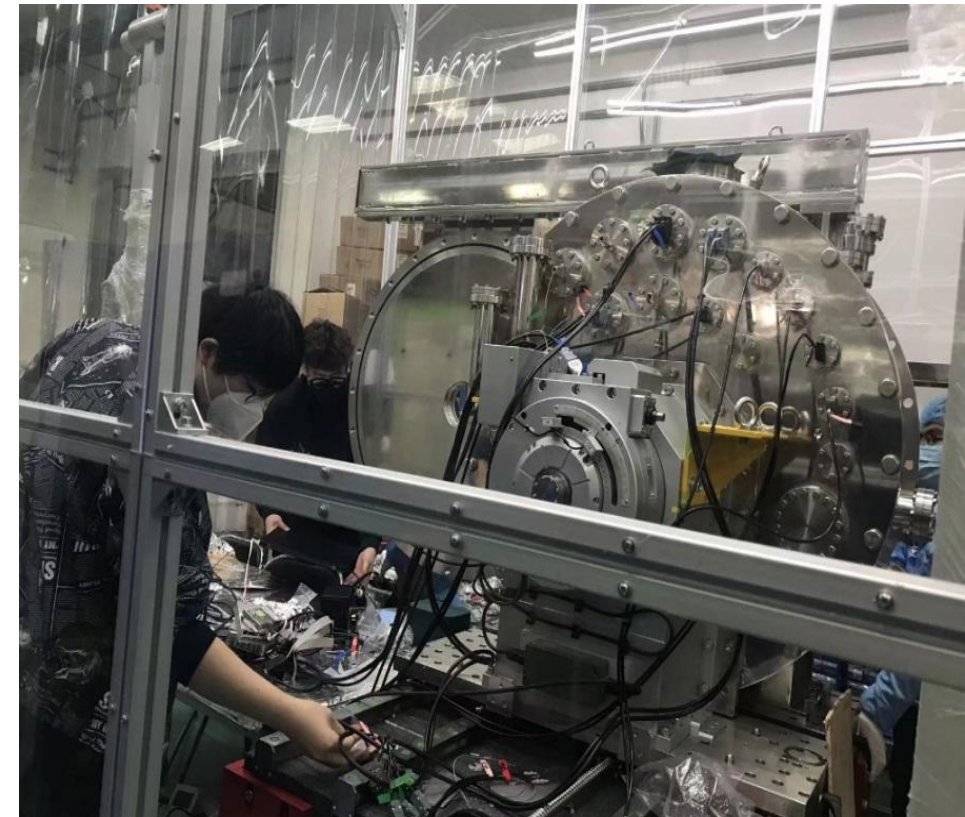
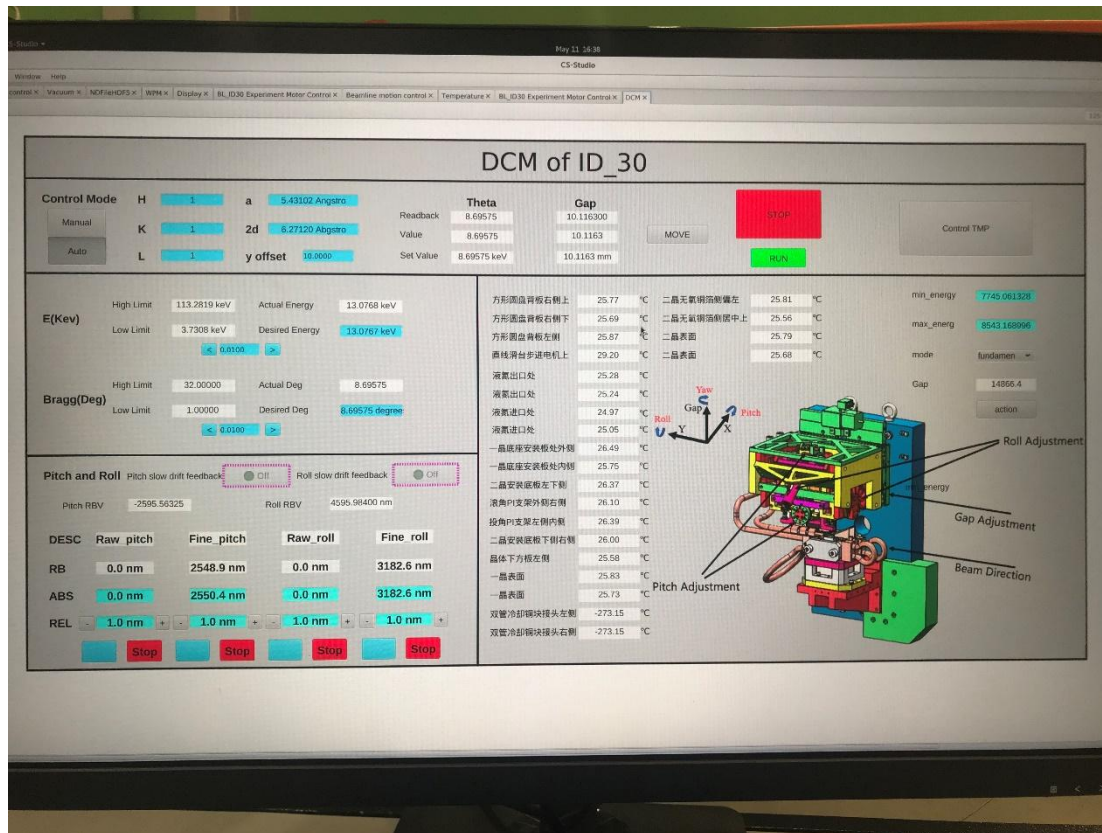
- Transfocator motion control





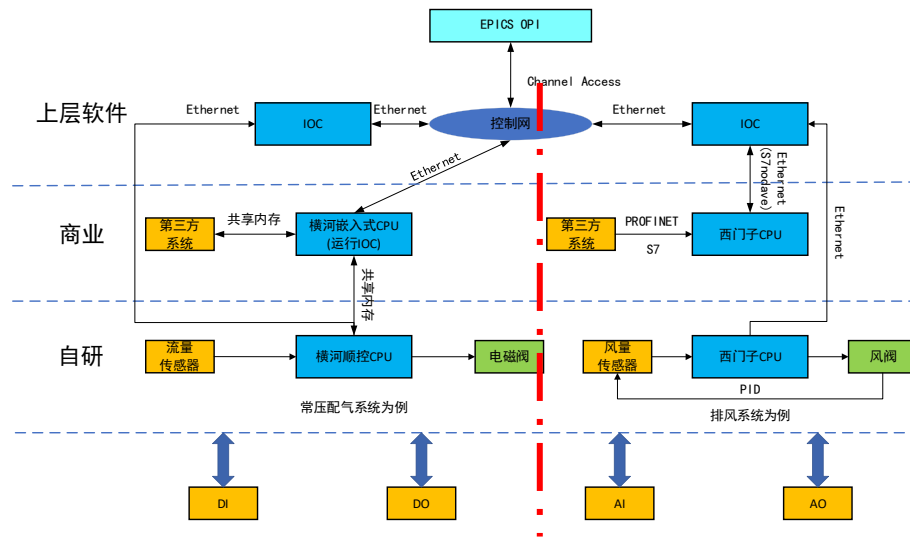
# Beamline control system

- DCM motion control system

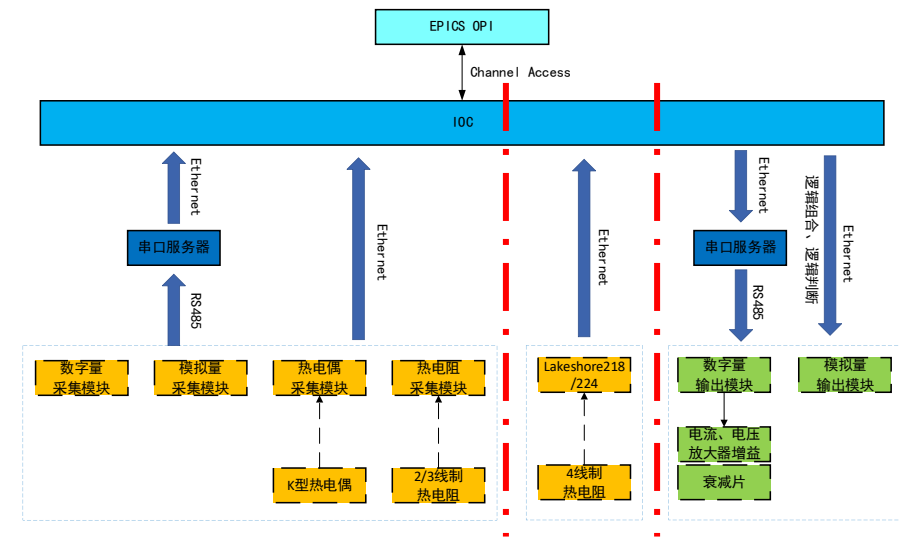


# Beamline control system

- Control system based on PLC and intelligent IO module
  - PLC: gas distribution system, hutch exhaust system, etc.
  - Intelligent IO module: temperature, shutter, discrete IO control

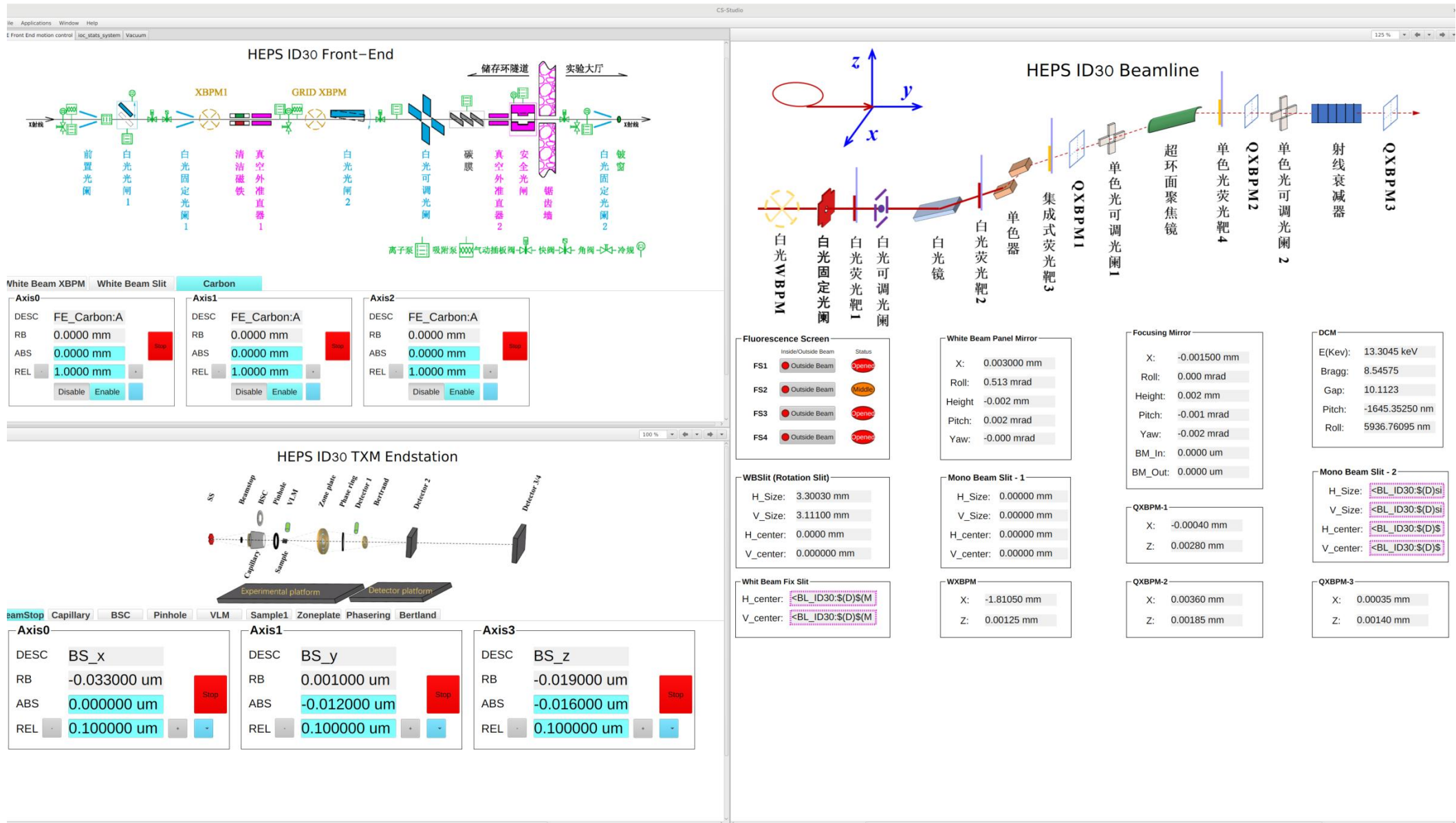


The structure of PLC control system



The structure of discrete IO control

# BE beamline control system





# BE beamline control system

FileApplicationsWindowHelp

DCM

67 %

DCM of ID\_30

Control Mode

H1a5.43102 Angstrom

Theta8.54575

Gap10.112250

STOP

Control TMP

ManualK12d6.27130 Angstrom

Value8.54575

MOVE

AutoL1y offset10.0800

Set Value8.54575 keV

10.1123 nm

RUN

E(Kev)

High Limit113.2819 keV

Actual Energy13.3045 keV

Low Limit3.7308 keV

Desired Energy13.3045 keV

8.8398

8.8398

Bragg(Deg)

High Limit32.00000

Actual Deg8.54575

Low Limit1.00000

Desired Deg8.54575 degree

8.8398

8.8398

Pitch and Roll

Pitch slow drift feedback

Roll slow drift feedback

Pitch RBV-1445.35250

Roll RBV5936.76095 nm

NEW\_pitchPI\_pitch0.000002542.4500000.000003182.600000

NEW\_rollPI\_roll0.000001.000000.000001.00000

MoreSTOPMoreSTOPMoreSTOPMoreSTOP

AbortAbortAbortAbort

24.90 °C

24.79 °C

24.94 °C

27.46 °C

24.73 °C

24.70 °C

24.57 °C

24.64 °C

25.60 °C

24.86 °C

25.32 °C

25.09 °C

25.32 °C

24.95 °C

24.69 °C

24.94 °C

24.83 °C

273.15 °C

24.92 °C

24.64 °C

24.89 °C

24.80 °C

二晶无氧铜箔右侧上

二晶无氧铜箔右侧中

二晶表面

液氮出口处

液氮出口处

液氮进口处

液氮进口处

一晶底座安装板处左侧

二晶安装板处左侧

液氮内支架左侧右侧

二晶安装板下侧右侧

晶体下方板左侧

一晶表面

双管冷却铜块接头左侧

双管冷却铜块接头右侧

方形圆盘右侧上

方形圆盘右侧下

方形圆盘左侧

直线滑台步进电机上

液氮出口处

液氮出口处

液氮进口处

液氮进口处

一晶底座安装板处左侧

二晶安装板处左侧

液氮内支架左侧右侧

二晶安装板下侧右侧

晶体下方板左侧

一晶表面

双管冷却铜块接头左侧

双管冷却铜块接头右侧

Roll Adjustment

Gap Adjustment

Beam Direction

Pitch Adjustment

Vacuum

70 %

PumpFS

IP-10.00E0

IP-20.00E0

IP-30.00E0

WBM

FS

IP-40.00E0

IP-50.00E0

DCM

FS

IP-60.00E0

IP-70.00E0

Beamline Map

BE XBPM

FE-XBPMFE-XBPM Settings&DrawsIP: 10.8.54.2前端区距光源20825mm

WXBPMWXBPM Settings&DrawsIP: 10.8.54.3FOE距光源33855mm

QXBPM1QXBPM1 Settings&DrawsIP: 10.8.54.4FOE距光源46797.5mm

QXBPM2QXBPM2 Settings&DrawsIP: 10.8.54.5Hutch距光源55620.5mm

QXBPM3QXBPM3 Settings&DrawsIP: 10.8.54.6Hutch距光源58942.4mm

SlitsSlits Settings&DrawsIP: 10.8.54.7Hutch距光源56000mm

History data ( Free to Add )

Beamline Map

FE-XBPM

CHA0.00nA

CHB0.02nA

CHC0.06nA

CHD0.08nA

SUM0.16nA

DELTA-UD-0.12nA

DELTA-LR /SUM-0.757225nA

DELTA-LR0.00nA

DELTA-UD /SUM-0.012048nA

plot count

plot curr

plot delta/sum

SET5.00V

Read4.99V

ON / OFFOn

BIAS VOLTAGE (5 ~ 150V)

WXBPM

0.10nA

0.09nA

0.10nA

0.10nA

0.39nA

-0.01nA

-0.03nA

0.02nA

0.05nA

plot count

plot curr

plot delta/sum

5.00V

4.99V

On

QXBPM1

1.80uA

2.56uA

3.02uA

0.98uA

8.36uA

0.37uA

0.04uA

-2.81uA

-0.34uA

plot count

plot curr

plot delta/sum

5.00V

4.99V

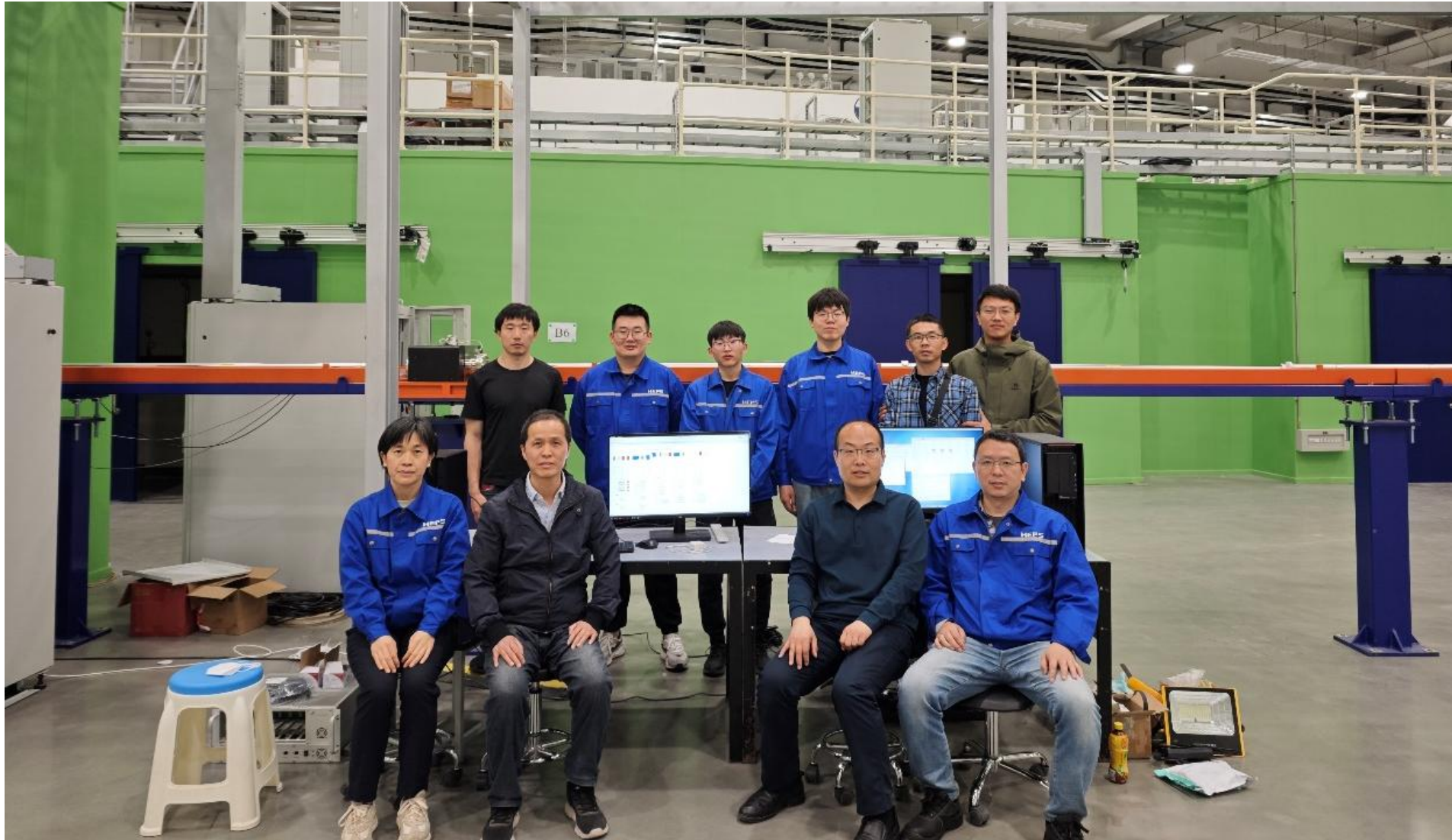
On

# Beamline control system

- 7 beamline control systems have already been delivered
  - BE, BD, B7, B8, BF, BB and B4

[illegible]

# Control Team







Thanks for your attention!

