

# Single crystal data reduction of monochromatic-beam diffractometers at HFIR

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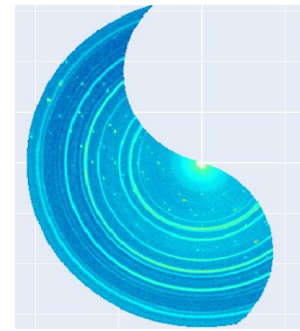
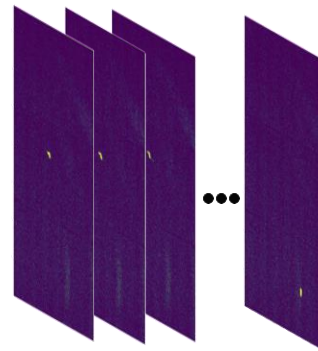
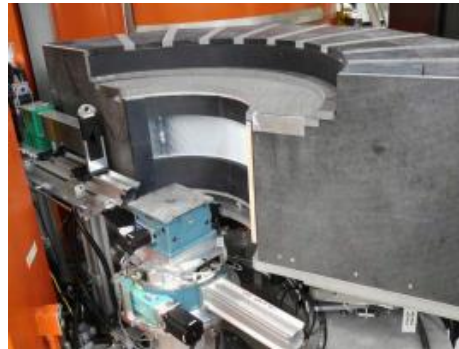
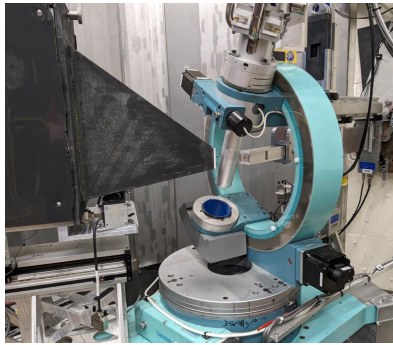
Single Crystal Neutron Diffraction Data  
Reduction and Analysis Workshop

ORNL, Jun 2024

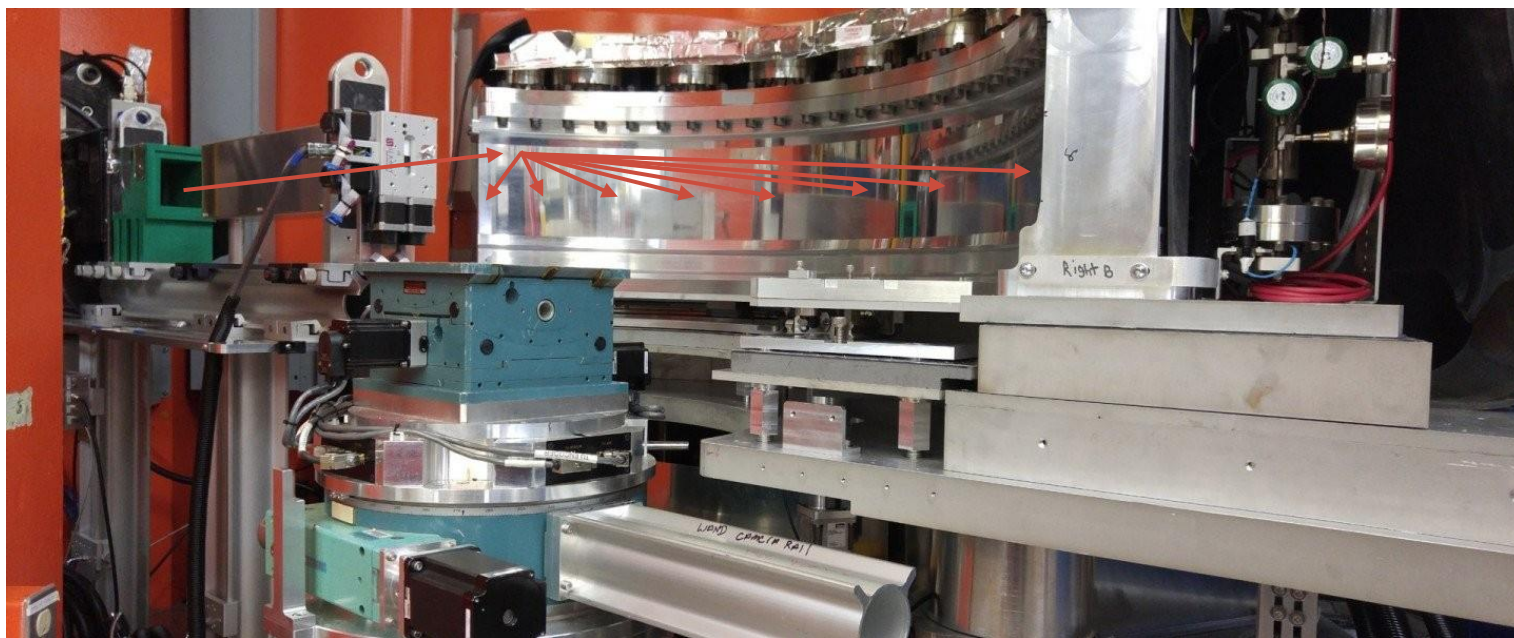
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# Outline

- The instrument: specs and features
- The data: access, structure and format
- The software: visualization and reduction
- The future: next-gen experiment automation



# WAND<sup>2</sup> (HB-2C)



2-axis diffractometer with wide-angle detector bank

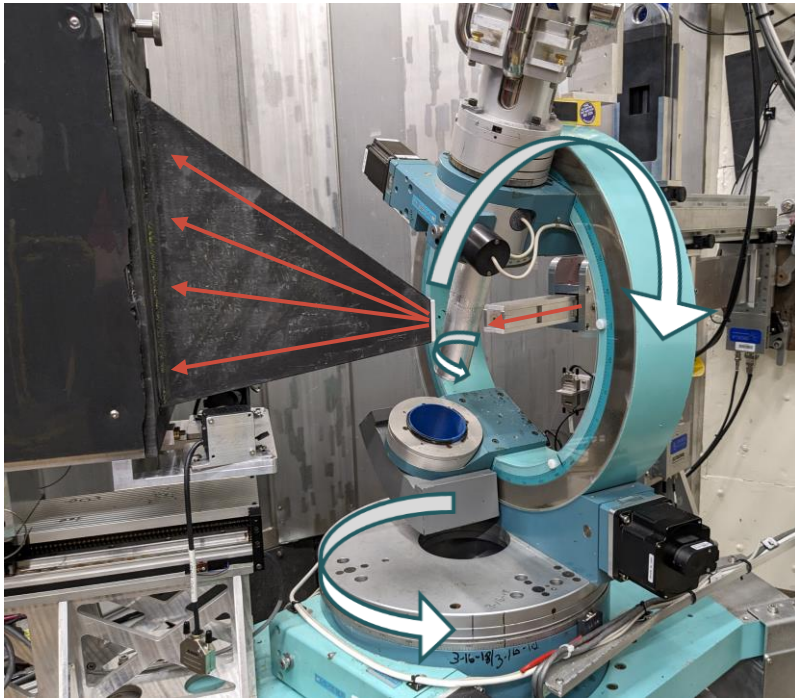
Detector: seamless 3He 2D-PSD  
(8\*480\*512 pixels, 0.4mm/pixel)

Horizontal coverage: 120 deg  
Vertical coverage: +/- 7.5 deg  
Detector Elevation: 100mm (0 to +15 deg)

Wavelength:  
 $\lambda = 1.5 \text{ \AA}$  (Ge 113),  
 $\lambda = 0.95 \text{ \AA}$  (Ge 115)

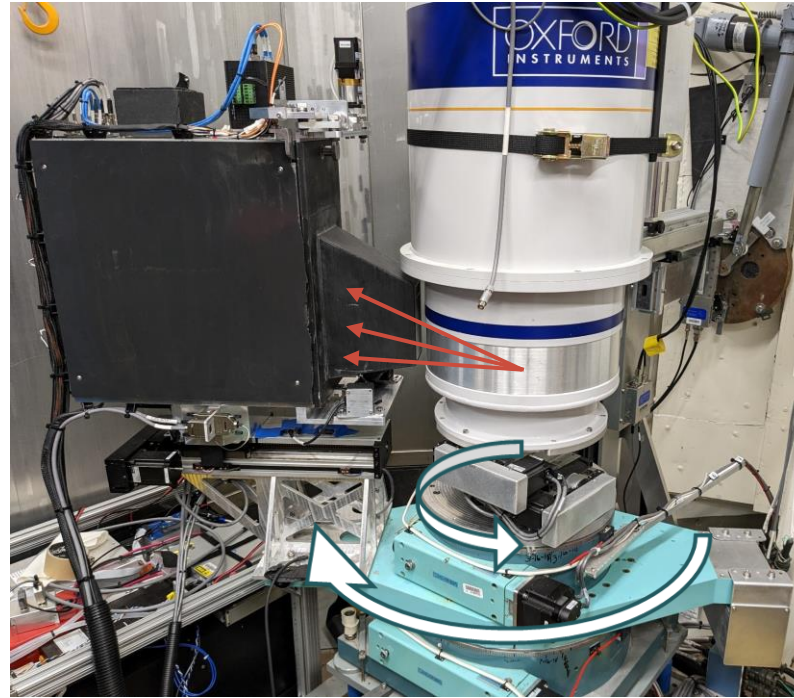
# DEMAND (HB-3A)

Four-circle mode



4 to 700 K  
Half-polarized option

Two-axis mode



40 mK (dilution)  
6 T (vertical magnet)

Detector: 3\*1 stack anger camera  
(3\*512\*512 pixels, 0.2mm/pixel)

Horizontal coverage: +/-8 deg  
Vertical coverage: -8/+40 deg

Four-circle mode:  
2theta range: 0 ~ 155 deg  
Omega range: 0 ~ 75 deg  
Chi range: -5 ~ 90 deg  
Phi range: -180 ~ 180 deg

Two-axis mode:  
2theta range: 0 ~ 155 deg  
Omega range: -180 ~ 180 deg

Wavelength:  
 $\lambda = 1.54 \text{ \AA}$  (Si 220),  
 $\lambda = 1.00 \text{ \AA}$  (Si 331),  
 $\lambda = 2.51 \text{ \AA}$  (Si 111)

# Data access

Analysis: (<https://analysis.sns.gov/>)  
(connection options: [https://analysis.sns.gov/connection\\_options.html](https://analysis.sns.gov/connection_options.html))

Download data to local: SFTP analysis.sns.gov on port 22

OnCat: (<https://oncat.ornl.gov/>)

DEMAND:

/HFIR/HB3A/IPTS-xxxxx/exp-xxx/Datafiles/\*.dat, \*.xml  
/HFIR/HB3A/IPTS-xxxxx/shared/autoreduce/\*.nxs

-raw data files  
-auto reduced files

WAND<sup>2</sup>:

/HFIR/HB2C/IPTS-xxxxx/nexus/\*.h5  
/HFIR/HB2C/IPTS-xxxxx/shared/autoreduce/\*.nxs

-raw data files  
-auto reduced files

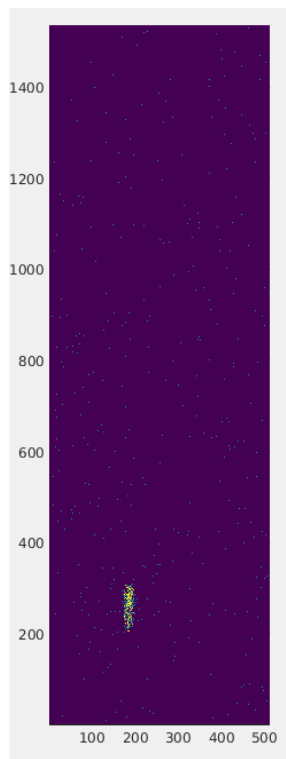
Useful resource:

<https://single-crystal.ornl.gov/>  
<https://docs.mantidproject.org/nightly/index.html>

-Single crystal diffraction website  
-MANTID online document

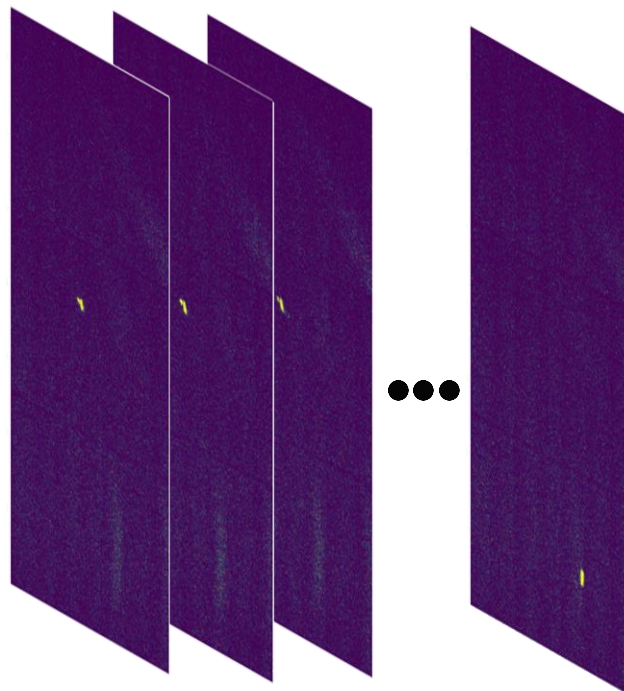
# Data structure and format

DEMAND .xml file  
(raw data)



$\omega, 2\theta, \chi, \phi, \dots$   
 $\lambda, focus, \dots$   
 $T, H, \dots$

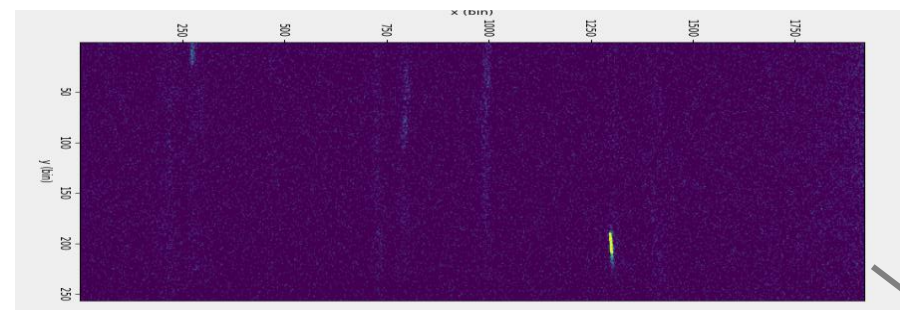
DEMAND .nxs file  
(auto reduced)



$\omega, 2\theta, \chi, \phi, \dots$   
 $\lambda, focus, \dots$   
 $T, H, \dots$

+ time

WAND<sup>2</sup> .h5 file (raw data)

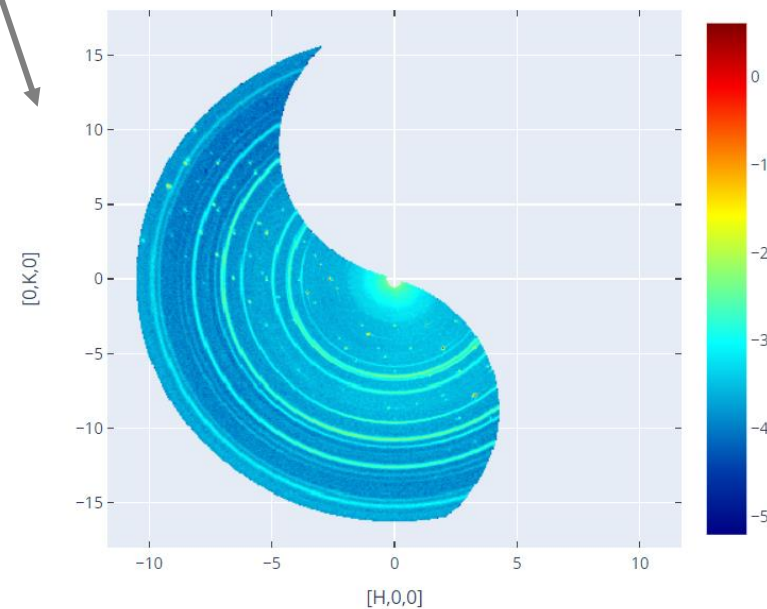


Events

$t_1$ , pixel ID 1,  
 $t_2$ , pixel ID 2,  
 $\dots$   
 $t_N$ , pixel ID N,

N counts

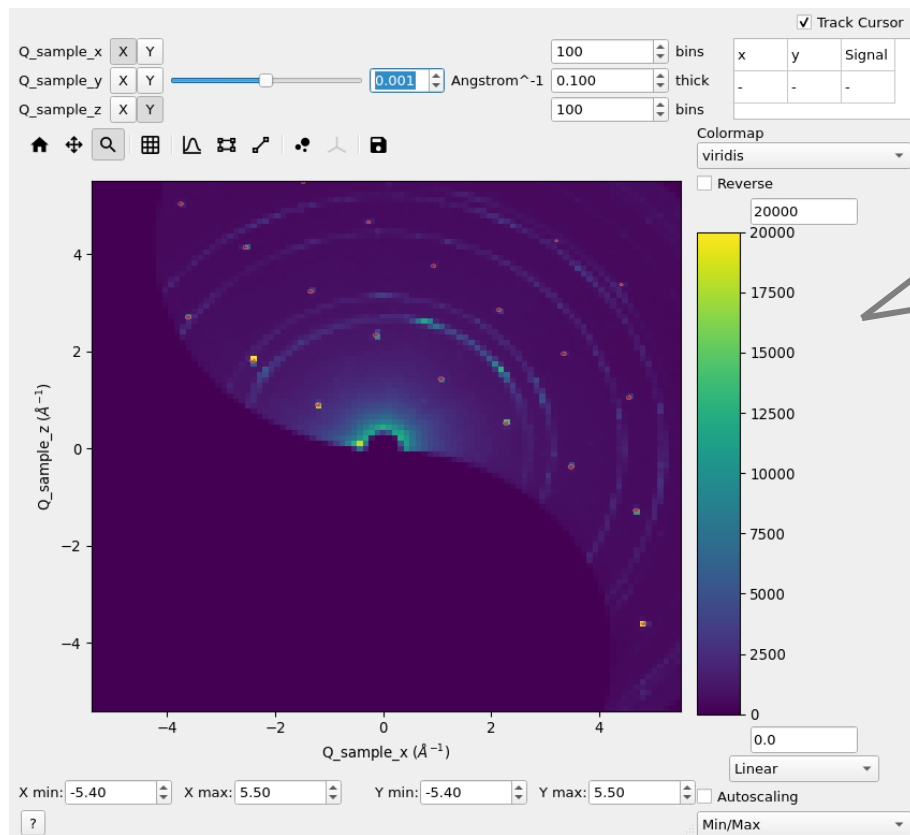
WAND<sup>2</sup> .nxs file (auto reduced)



# Data reduction in MANTID (reciprocal space)



## Qx-Qy-Qz plot (unindexed reciprocal space)



## Peak list

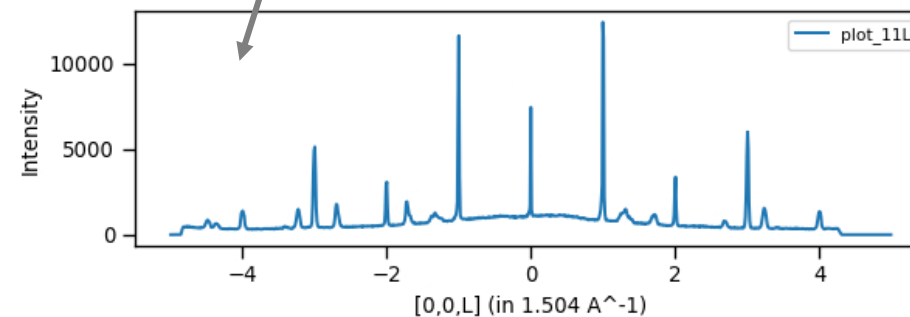
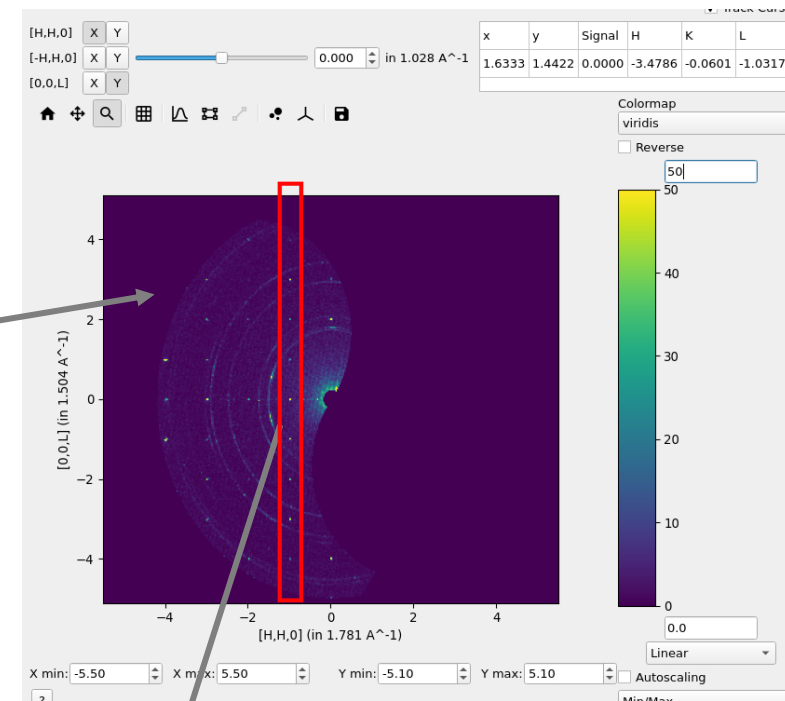
Peak Actions  
bragg Add Peaks Remove Peaks

Workspace: bragg

Concise View

RunNumber	h	k	l
1 0	-2.99156	-2.99470	-1.00347
2 0	-2.99331	-2.99841	-0.00337
3 0	-2.99558	-2.99787	0.99717
4 0	-1.99729	-1.99588	-2.00287
5 0	-2.00040	-1.99573	-1.00109
6 0	-1.99908	-1.99923	-0.00110
7 0	-1.99722	-1.99873	1.00085
8 0	-1.99860	-1.99977	2.00123
9 0	-1.96403	-1.96343	2.97290
10 0	-1.00012	-0.99574	-3.00020
11 0	-0.99953	-0.99828	-2.00002
12 0	-1.00233	-0.99522	-1.00099
13 0	-1.00135	-1.00102	-0.00047
14 0	-0.99823	-1.00323	1.00179
15 0	-0.99836	-1.00082	2.00264
16 0	-1.00221	-1.00101	3.00450
17 0	-1.00343	-1.00173	4.00200

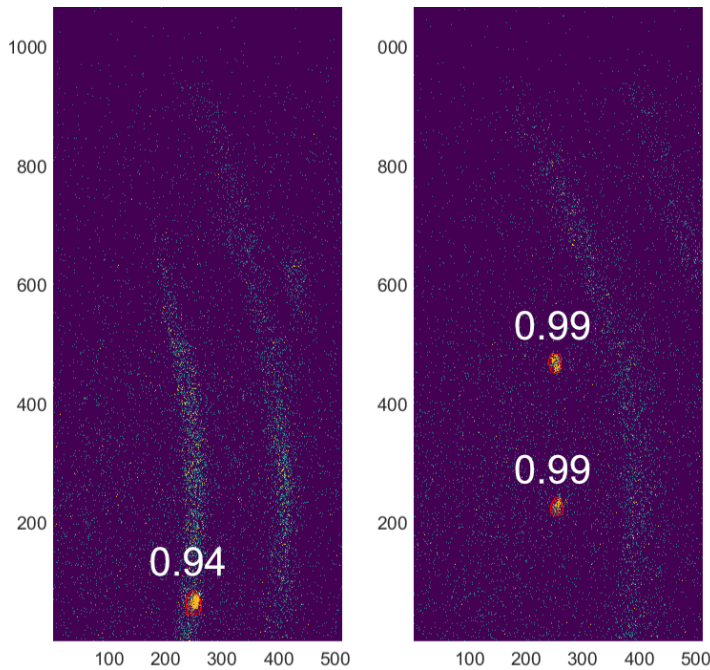
## HKL-plot (indexed reciprocal space)



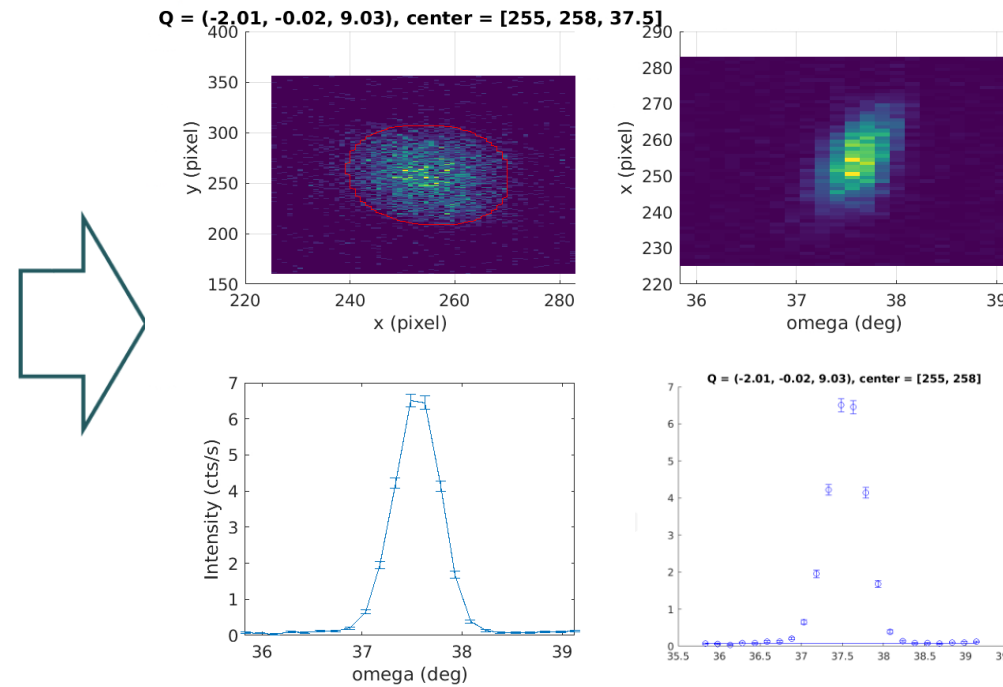
# Data reduction in ReTIA (detector space)

ReTIA is a MATLAB package for reducing detector image data. (currently work for DEMAND)

Auto-detection peak on detector image



Auto-indexed and optimized peak scans



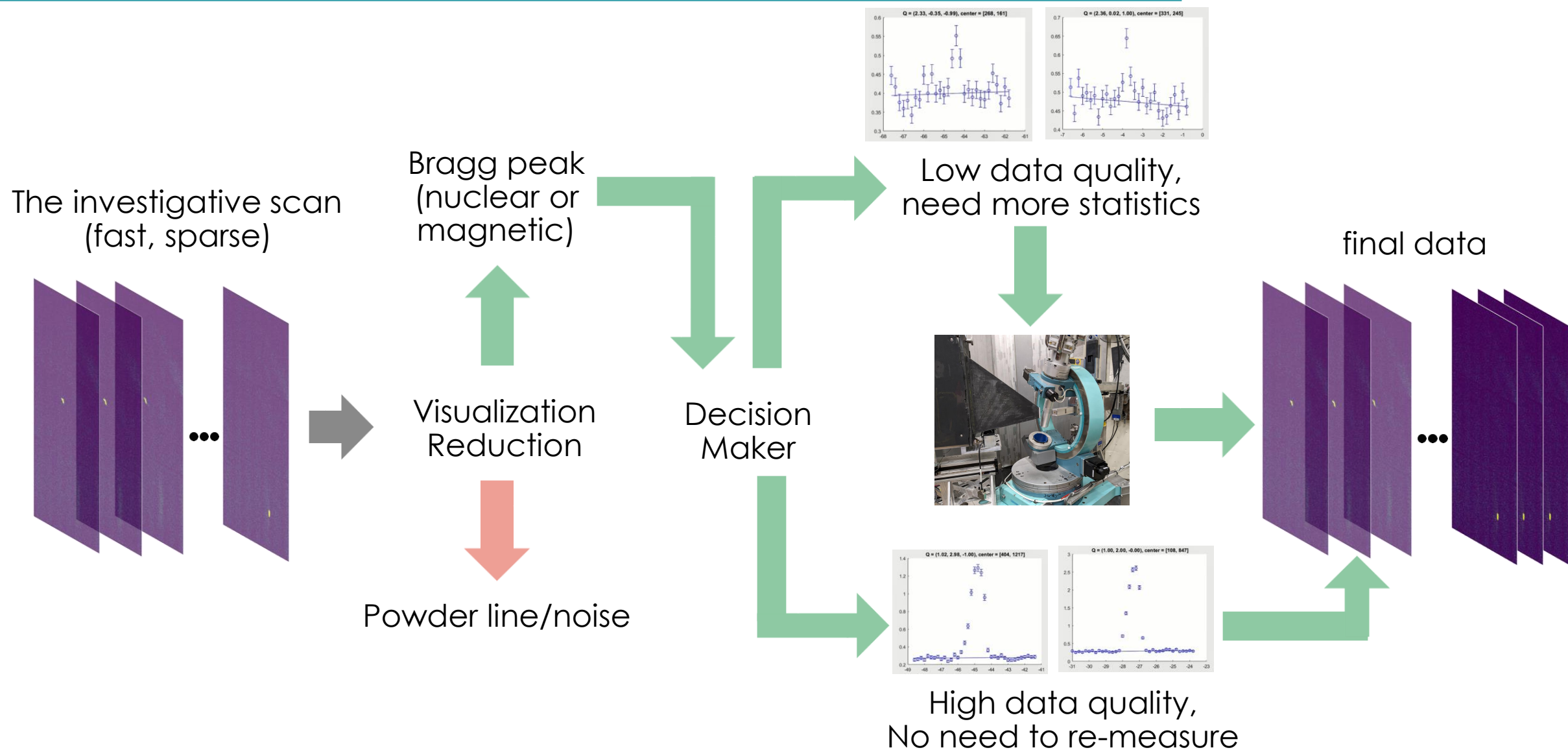
Reduced intensity

```

Crystal
(314, 2f8.2, i6, 6f8.0)
1.5424 0 0
-4 0 0 0.11 0.05
-4 0 1 25.72 0.14
-4 0 2 16.82 0.11
-4 0 3 38.97 0.18
-4 -0 4 67.24 0.25
-4 -0 5 12.48 0.10
-3 -2 -1 0.12 0.05
-3 -2 3 0.00 0.05
-3 -2 4 0.11 0.05
-3 -2 5 0.61 0.05
-3 0 -0 1.34 0.05
-2 -2 -1 0.17 0.05
-2 -2 -0 131.23 0.56
-2 -2 1 0.06 0.05
-2 -2 2 7.20 0.07
-2 -2 3 0.36 0.05
-2 -2 4 19.39 0.12
-2 -2 5 0.22 0.05
-2 -2 6 38.60 0.19
-2 -1 -0 0.24 0.05
-2 -1 1 0.27 0.05
-2 -1 2 0.61 0.05
    
```



# Next step: automated single crystal diffraction experiment



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# THANK YOU!

