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Event Mode Data Reduction & Analysis Method for the Time-of-Flight Spectrometer

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The Characteristics of Time-of-Flight Spectrometer Data

- Recently developed time-of-flight spectrometer
  - Large array of PSDs : total number of pixels : 10^4 ~ 10^5
  - Time resolution of electronics: Δtof < μsec
- Number of histogram elements
  - = [number of pixels] x [number of tof bins] ~ 10^8 or higher
  - In case of $CuGeO_3$ measured at J-PARC: ~ 3.0x10^9 (time bin size = 100 nsec)
  - About 98 % of the histogram elements are zero

Idea of Event Mode Data Process

- Big Size, but many of histogram elements are zero, if conserving the instrumental resolution.
  - Similar to large sparse matrix calculation, handling only non-zero matrix elements
- Data distortion during reduction process can be minimized, if conserving instrumental resolution
  - Time-of-flight to energy conversion
  - Position to momentum space conversion
- Question: Is it possible to do all of the data reduction processes in event mode ?

Inelastic TOF Spectrometer Data process

- Data Reduction
  - Normalization : Monitor, White-V, Mono-V
  - Detector Efficiency Correction,
  - k_i/k_f correction
  - Masking
  - Time-of-Flight to energy conversion
  - Converting to ($\mathbf{Q}$, ω) space
  - Background subtraction
- Data Analysis
  - $S(|\mathbf{Q}|, \omega)$, $S(\mathbf{Q}, \omega)$
  - 1D, 2D, 3D, 4D(?) visualization, analysis
- Each processes should be possible in event mode data.

Developing Environment

- Programming Language: Python
  - Python 2.6
  - Numpy, Scipy
    - Numerical calculation
  - Matplotlib
    - 1D, 2D plotting
  - PyQt4
    - Graphic User Interface
  - Supporting Multi Platform : MS Windows, Linux, Mac, etc..
- PC
  - Macbook Pro : 3.06 GHz(Core2Duo), 8 GBytes Memory
  - MacOS X 10.6 (64 bit OS) : Requires more than 4 Gbytes Memory

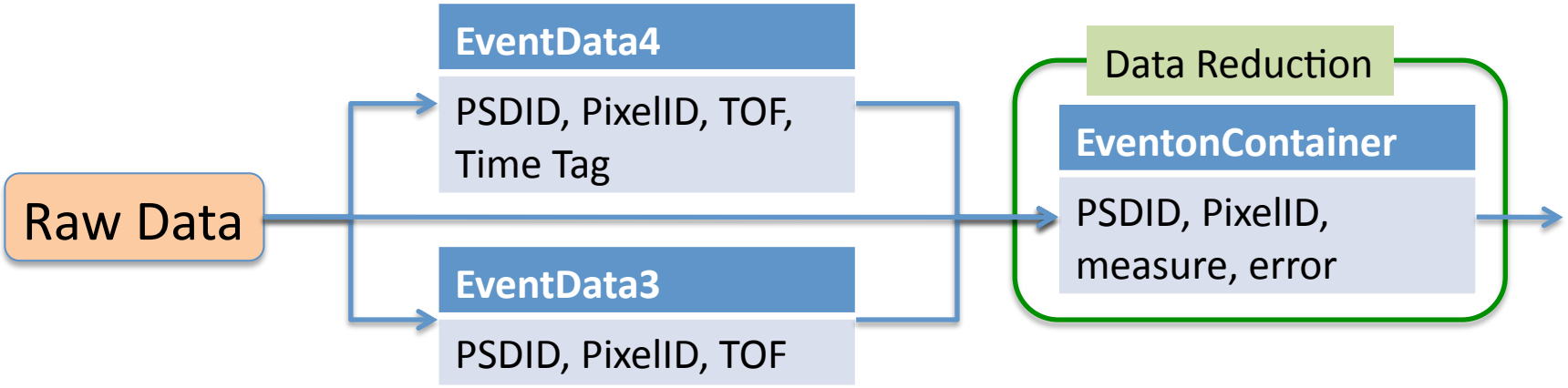
Python Module for Event Mode Data Process

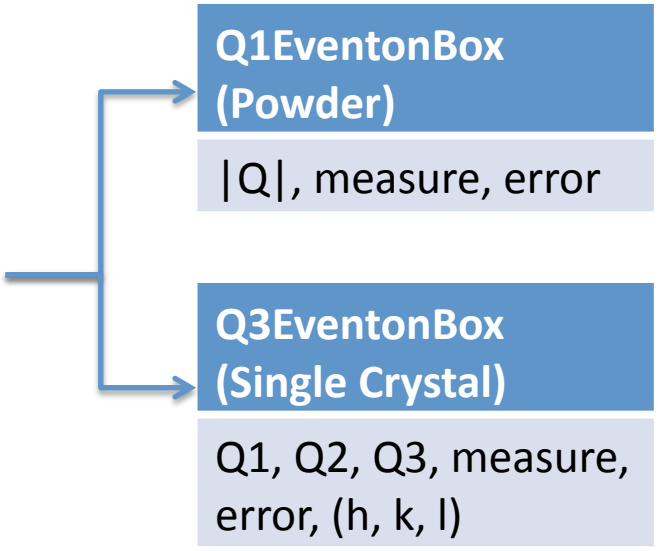
- Event mode data process
  - Classes for event data treatment
- 1D, 2D, 3D Histogram and Visualization
  - 1D least square fitting
- 4SEASONS@J-PARC event data & detector map file reading
- Single Crystal data process
  - UB matrix manipulation

Real Data Analysis

- CuGeO3 measurement data : Provided by J-PARC MLF
- CuGeO3 :
  - Measured @ 4SEASONS in J-PARC
  - Orthorhombic structure
  - one-dimensional Heisenberg antiferromagnet
- Multi Ei Method
- 176 PSDs, 128 Pixels/PSD = 22528 Pixels
- Histogram mode data analysis is published :
  - M.Nakamura, R.Kajimoto, Y.Inamura *et al.* J. Phys. Soc. Jpn. **78**(2009) 093002

Event Data : Data Class Flow





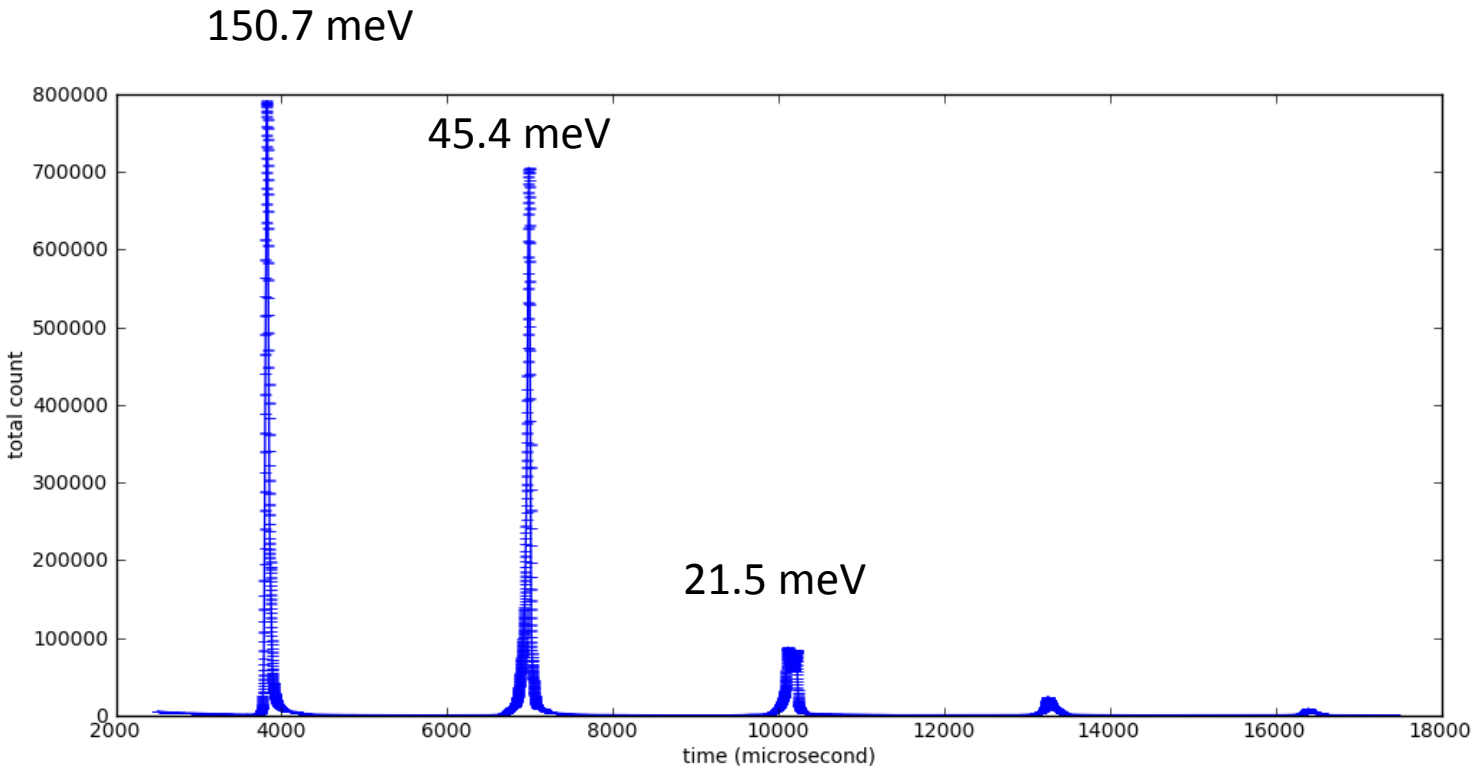
Measure : tof, Energy, wavelength, 1/tof, etc..

They all support :

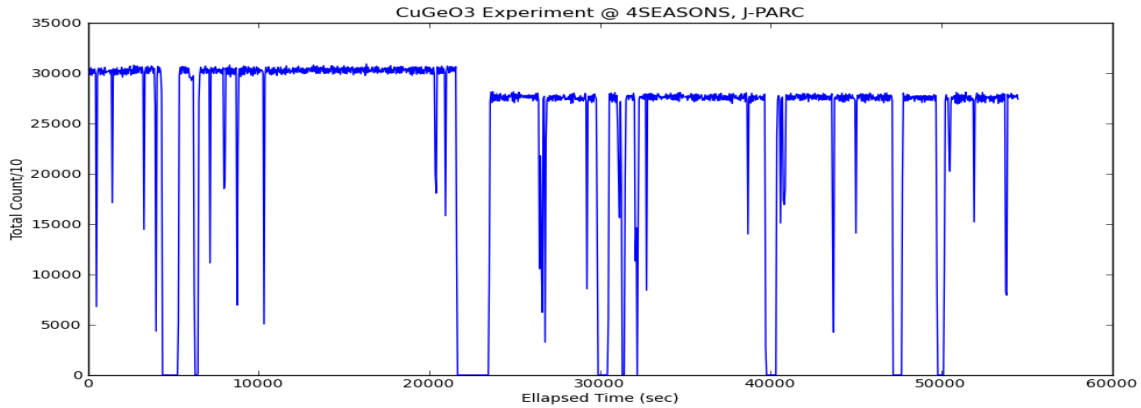
- Simple operation : +, - , x, /
- Merging multiple data of same class
- Normalization
- Error propagation
- Histogramming, Visualization

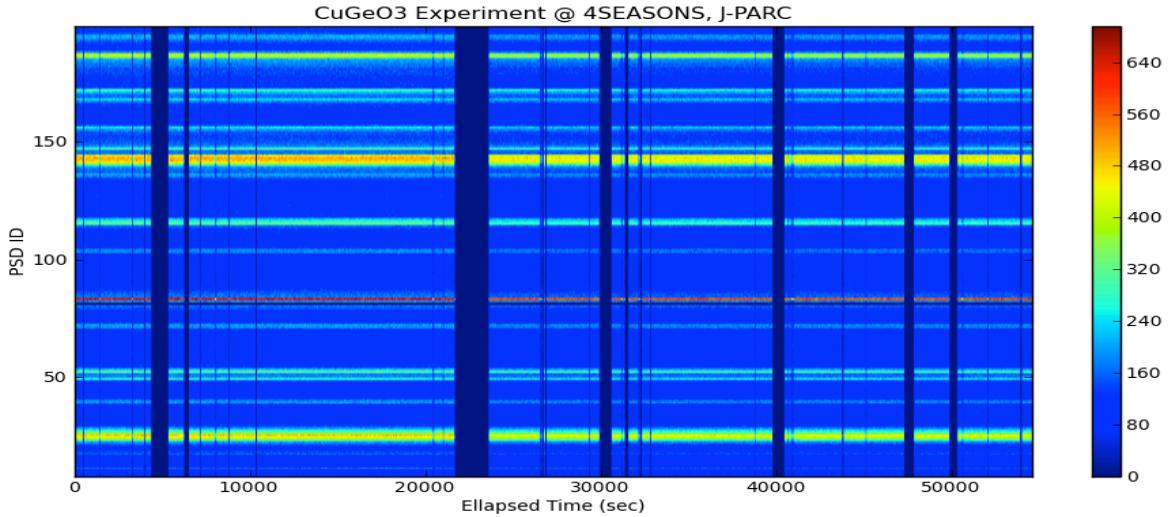
Multi Ei Measurement

Total Neutron Counts = 1.1×10^8



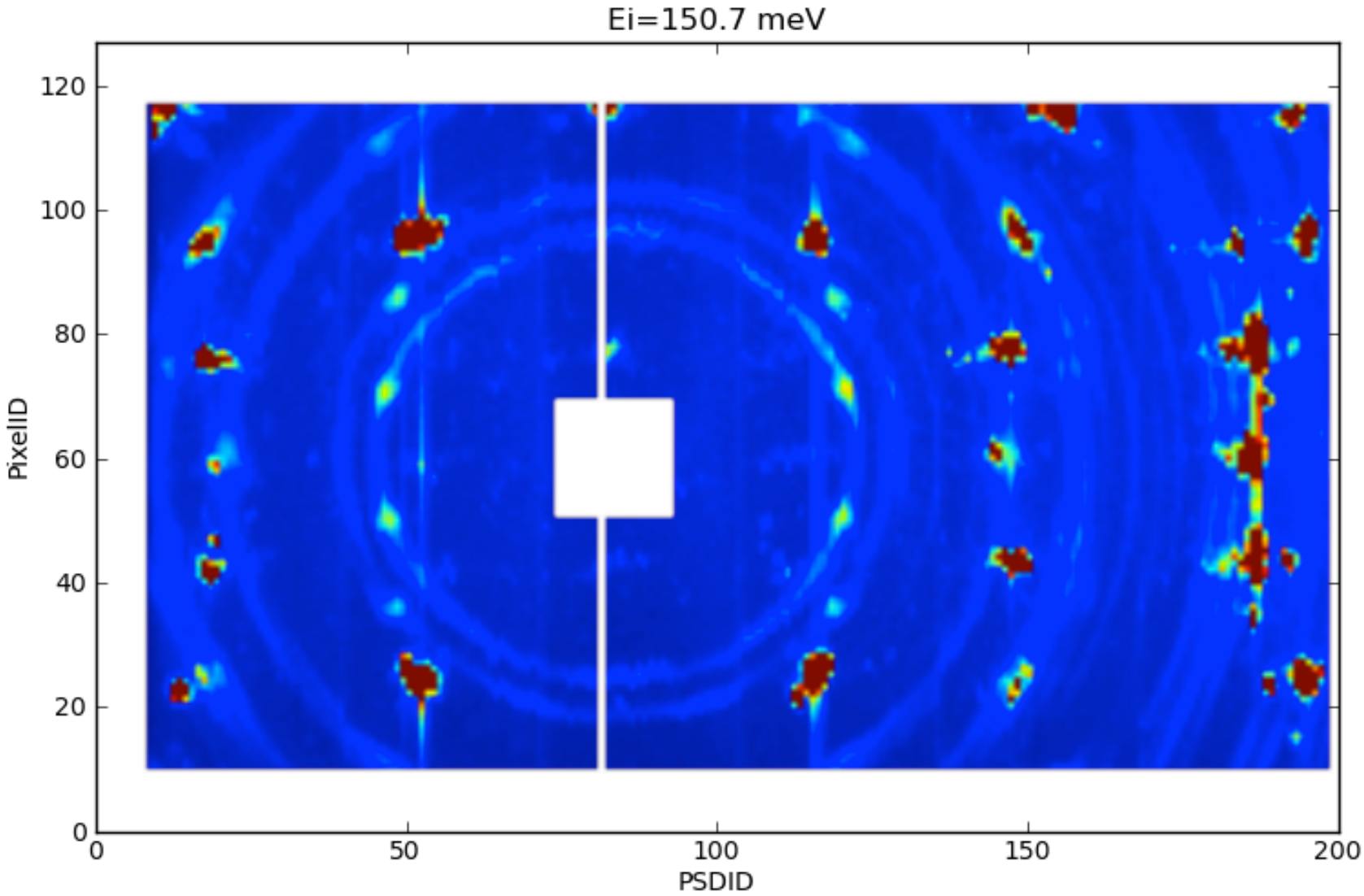
Data Check – elapsed time





- From *EventData4* class
- One can easily select or eliminate specific time region

Data Check : 2D Image plot (PSDID-PixelID)



Data Process in this test

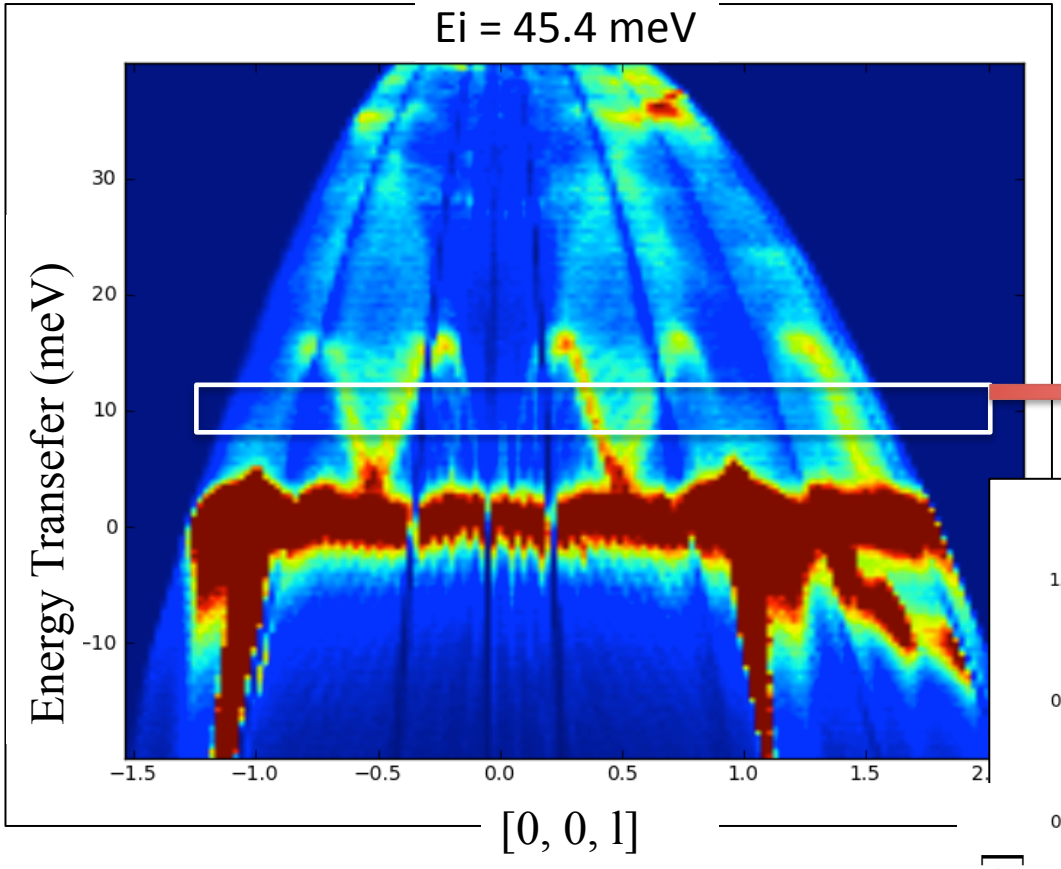
- Data Process
  - Read Raw Data (multiprocessing, time resolution = 100 nsec)
  - Reading detector information file and assigning detector position of pixel
  - Masking (Eliminate bad psd/pixel data)
  - Divide the data by E_i (3 E_i) and assign Ei
  - Time-of-flight to Energy transfer conversion
  - Ki/kf correction
  - (**Q**, E) space conversion
  - Assign UB matrix
  - Save 3 single crystal data(Q3EventonBox) using cPickle
- They all takes about 14 min in my laptop

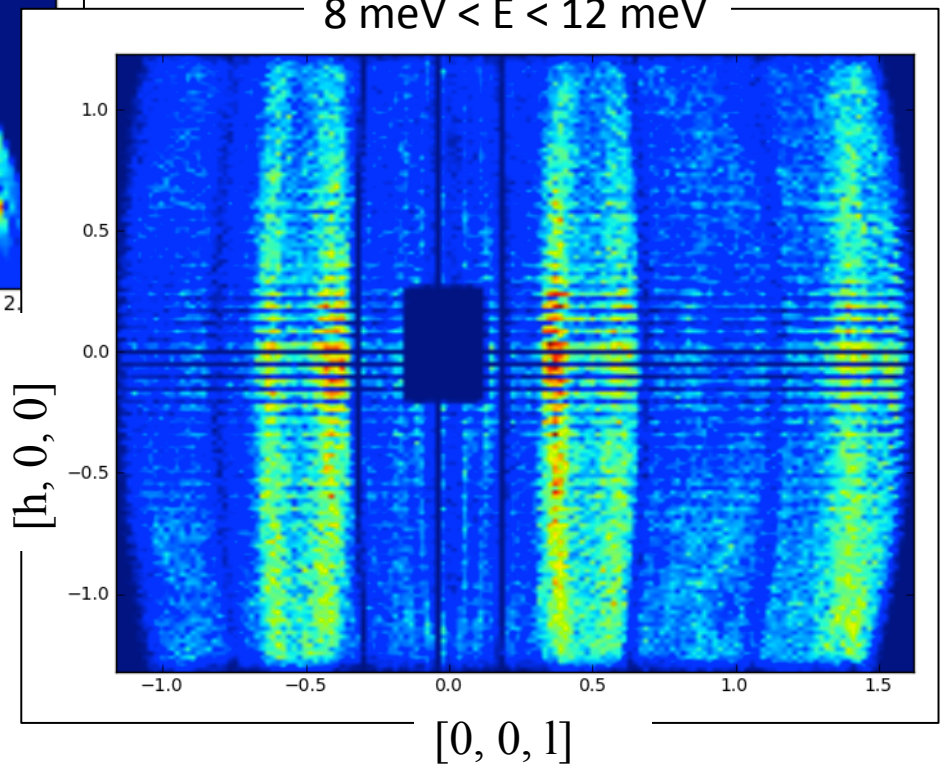
Data Size : Histogram vs Events

ΔE/Ei	Ei = 150.7 meV			Ei = 45.4 meV		
	Number of Histogram Element (10^6)	Number of Event (10^6)	Ratio	Number of Histogram Element (10^6)	Number of Event (10^6)	Ratio
0.0001	363.2	12.9	0.036	333.3	11.0	0.033
0.0005	72.6	11.8	0.162	66.7	9.1	0.137
0.001	36.3	8.6	0.238	33.3	7.1	0.212
0.005	7.3	3.7	0.512	6.7	3.6	0.543
0.01	3.6	2.2	0.601	3.3	2.3	0.679

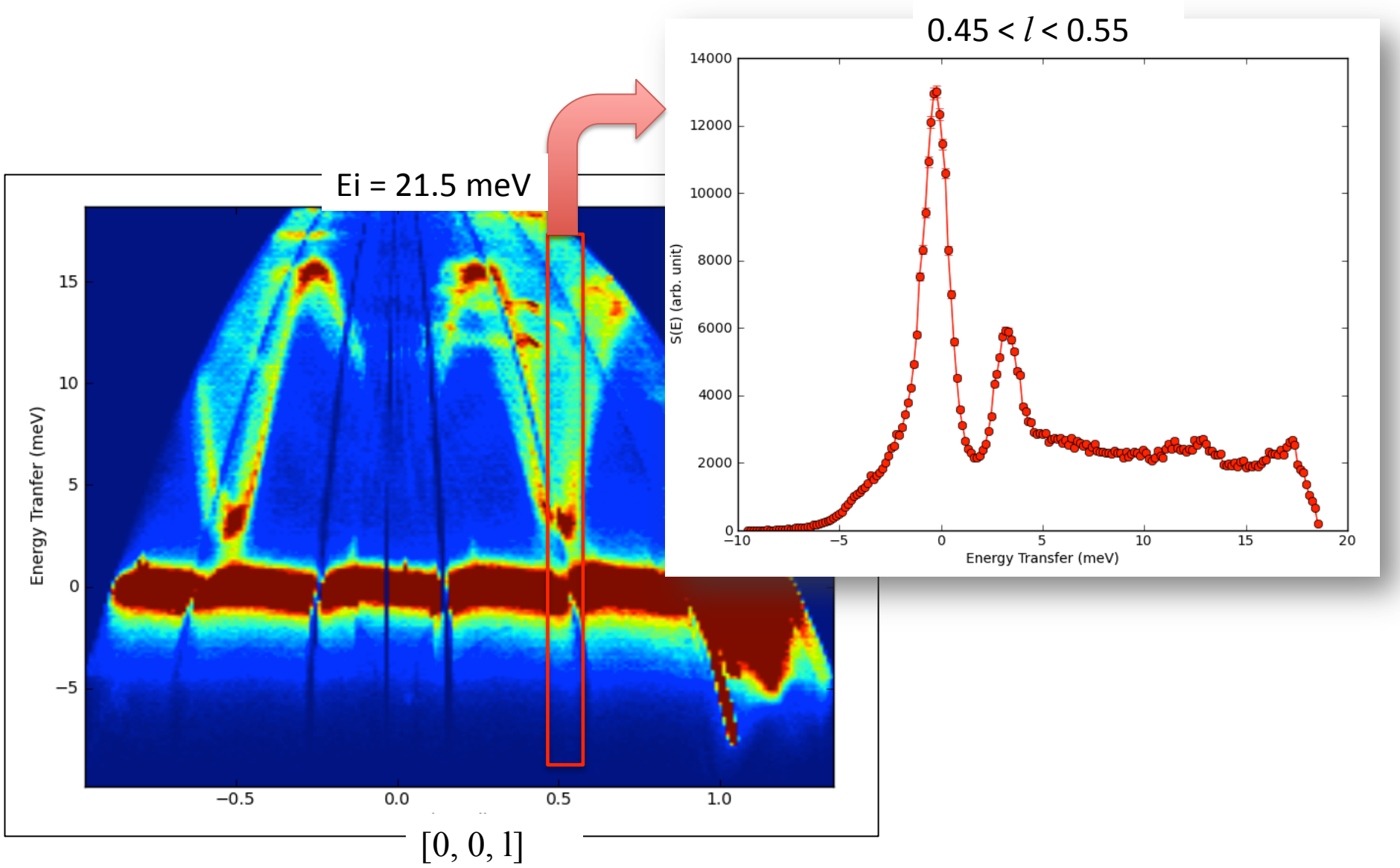
- Number of event ≈ Number of histogram element with non-zero value, if same energy bin size.
- High resolution histogram is very sparse -> need for event mode

Analysis Example : 1D Antiferromagnet





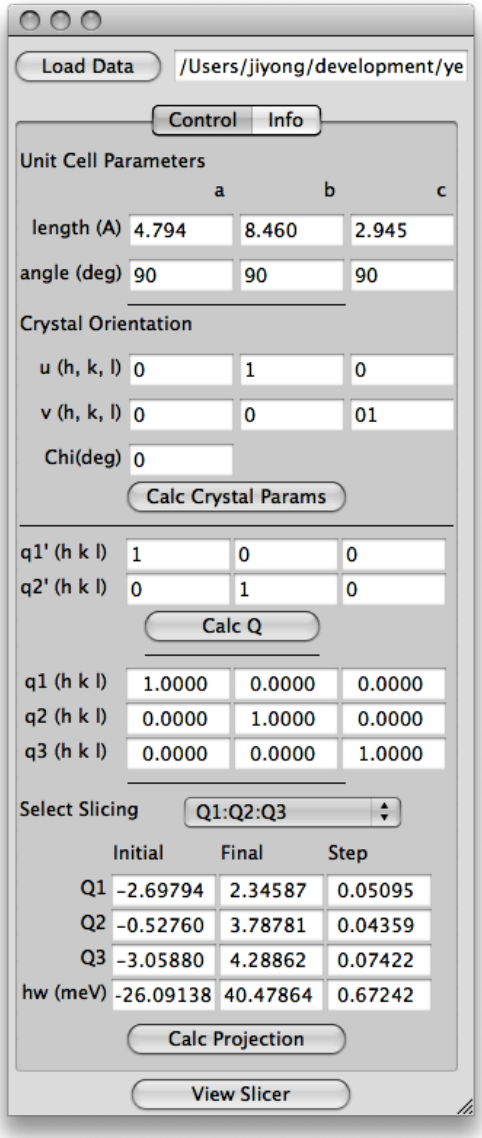
Example : Spin Gap (ΔE = 2.5 meV)

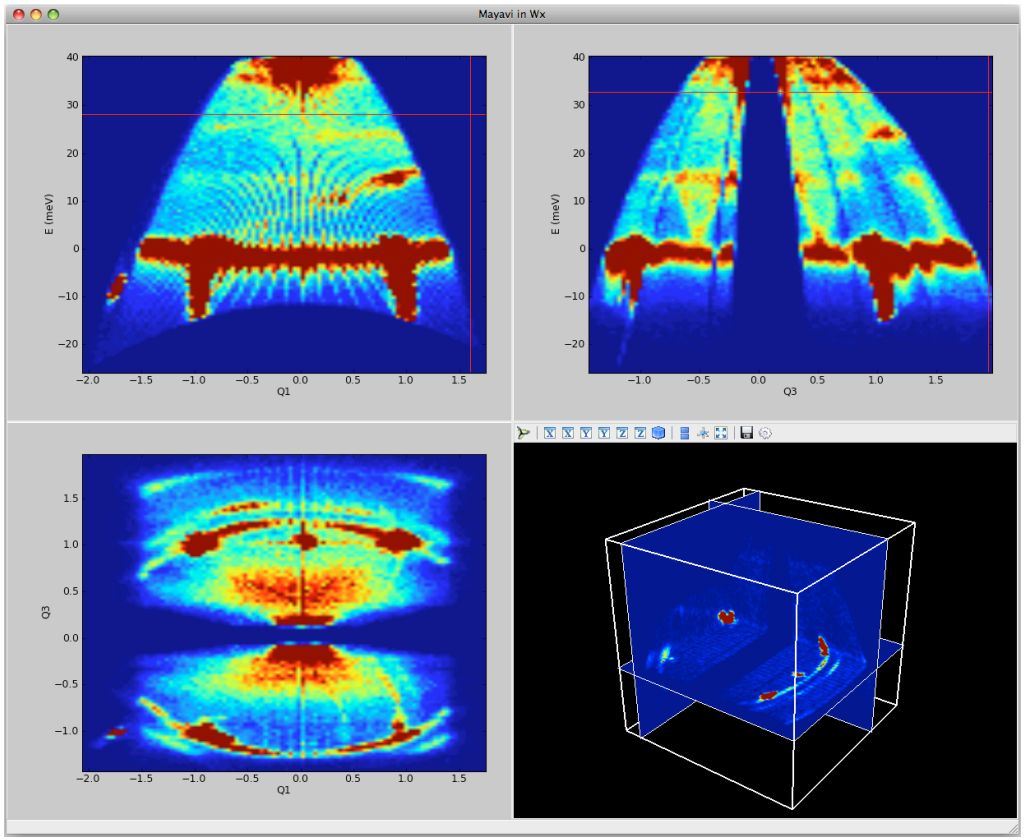


Interactive Data Analysis Example (in ipython)

```
In [47]: data3  #Ei = 21.5 meV
Out[47]: <neweventtype.Q3EventonBox object at 0x11d17ac10>

In [48]: data3=data3[data3.measure>-10.0] #selecting measure range

In [49]: his3=np.histogram2d(data3.measure, data3.l, weights=data3.weight,
    bins=[200,200])

In [50]: imshow(his3[0], origin ='lower', aspect='auto', extent=[his3[2][0],
    his3[2][-1], his3[1][0], his3[1][-1]])
Out[50]: <matplotlib.image.AxesImage object at 0x11d1bd590>

In [72]: m3=data3[(data3.l>0.45) & (data3.l<0.55)] #selecting momentum range

In [73]: his3=np.histogram(m3.measure, weights=m3.weight, bins=200)

In [74]: his4=np.histogram(m3.measure, weights=m3.error**2, bins=200)

In [75]: x3=0.5*(his3[1][1:]+his3[1][:-1])

In [77]: errorbar(x3, his3[0], yerr=np.sqrt(his4[0]), fmt='ro-’)
```

3D slicer (In Previous Version)





- Real time visualization : Slicing, Adding along specified axis.
- Not yet implemented in current version.
  - Fail to install Mayavi2 in 64 bit Mac OSX (Snow leopard)

Future Improvement

- Developing the data process module
  - Absolute normalization : (mb/meV/sr/f.u. unit)
- Speed up the process
  - C/C++ implementation
  - Algorithm optimization
- Development of GUI

Conclusion

- Event mode data reduction and analysis is the more effective method than histogram method
- I guess it can be applicable to other kinds of instruments : Diffractometer, SANS, etc..