

A novel method for component separation of extended sources in X-rays

MPE seminar, October 2022

Fabio Acero

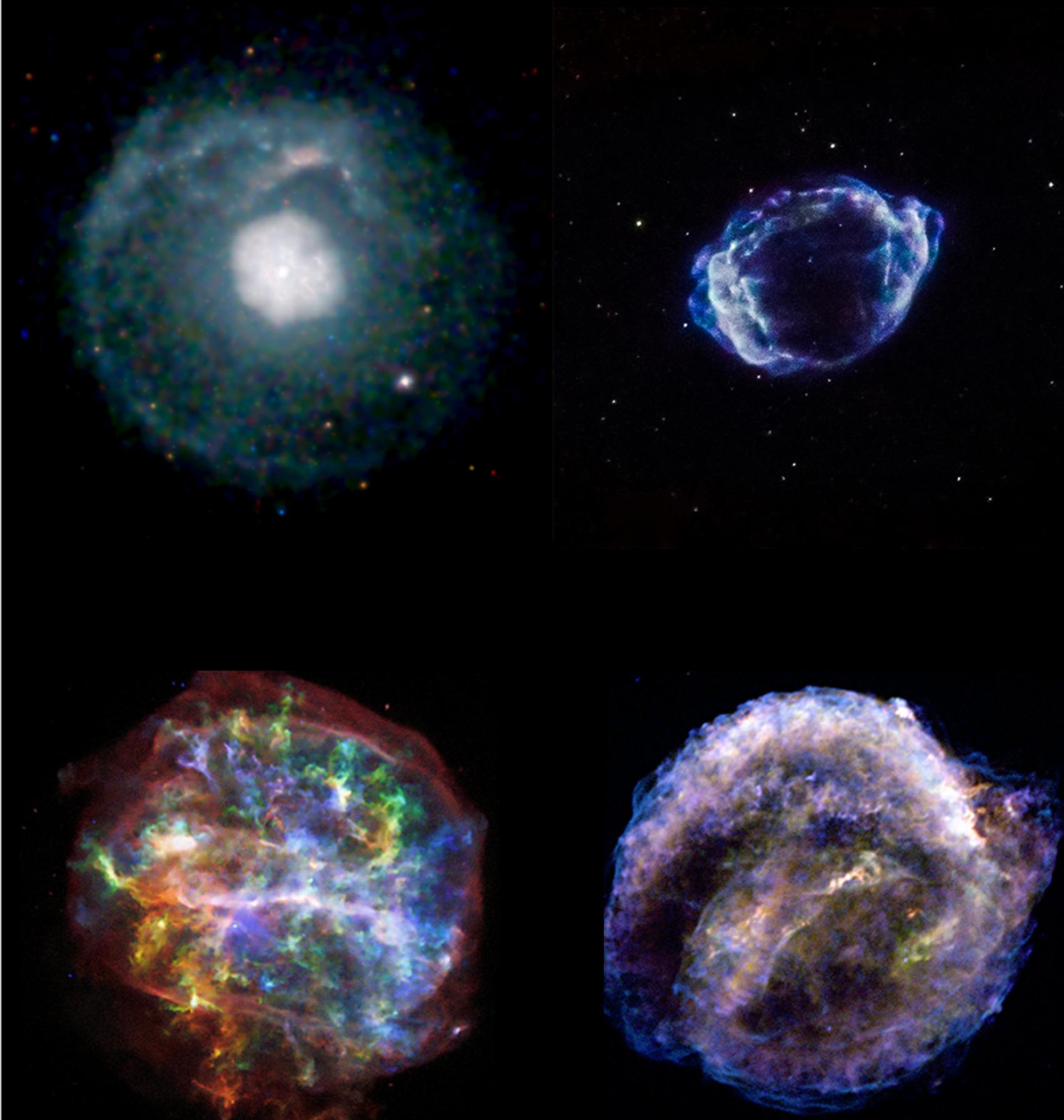
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Astronomy department, CEA/Saclay

 @fabacero

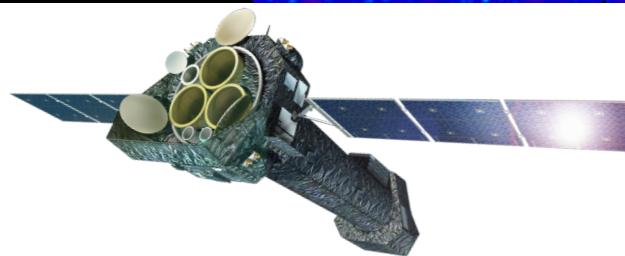
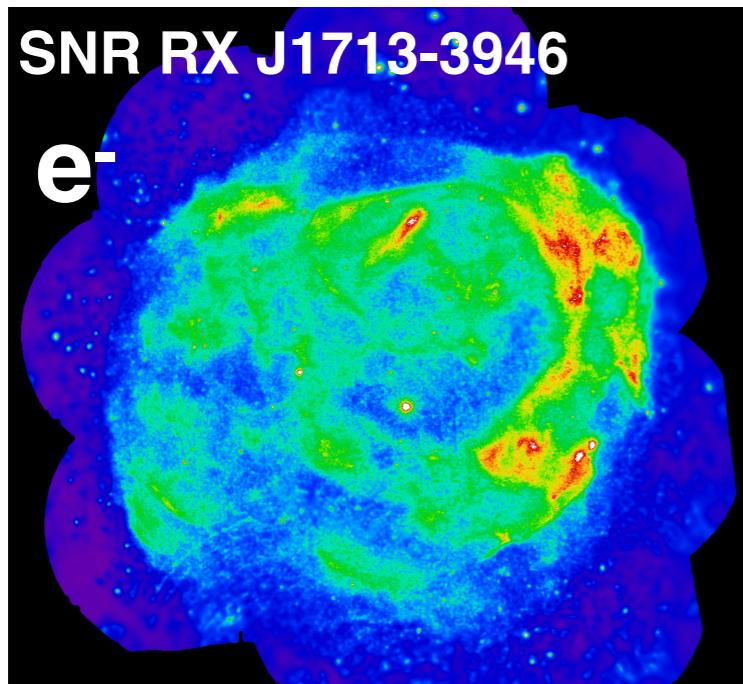


Chandra SNR gallery

My field of expertise : SNRs & PWNe from keV to TeV



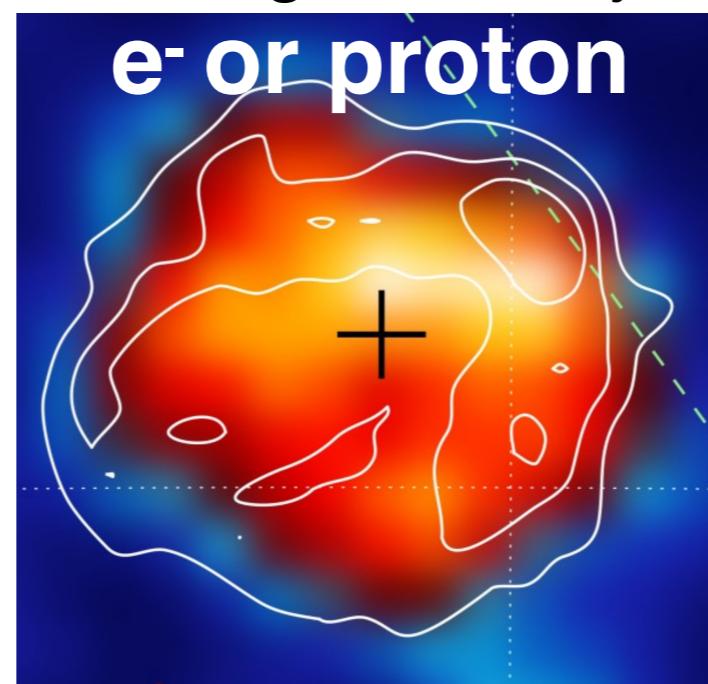
keV



XMM-Newton
NewAthena

Synchrotron

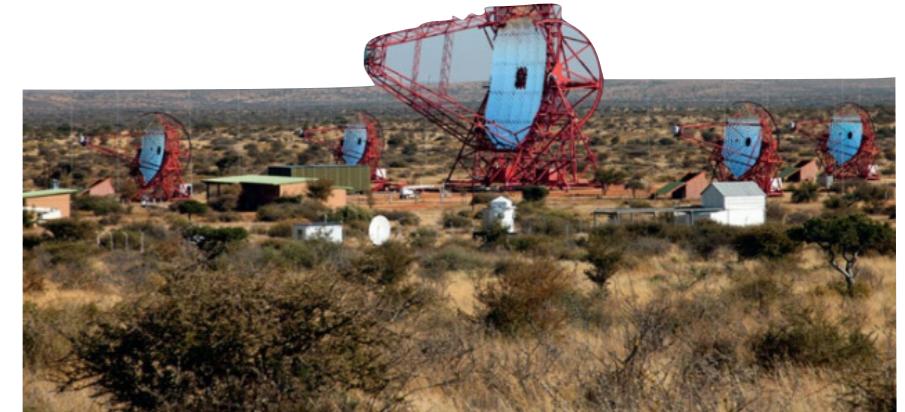
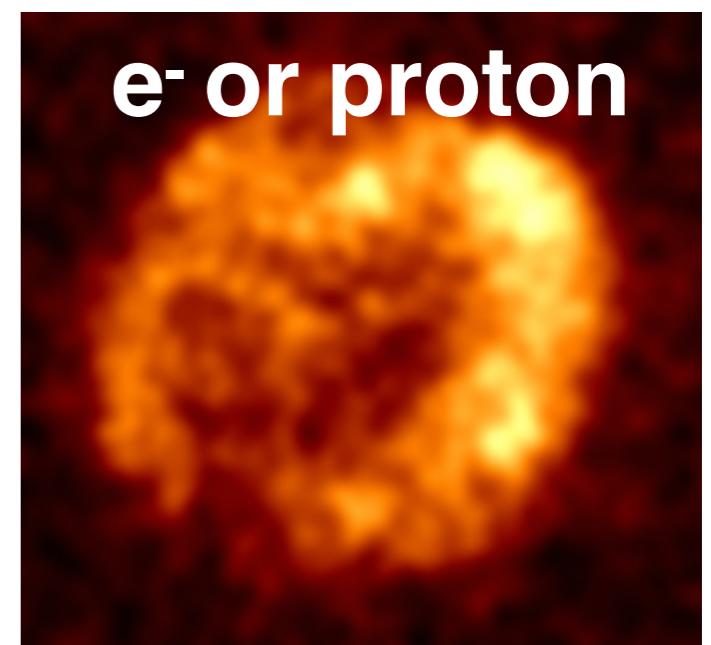
GeV gamma-ray



Fermi

Inverse Compton + Pi0 decay

TeV gamma-ray



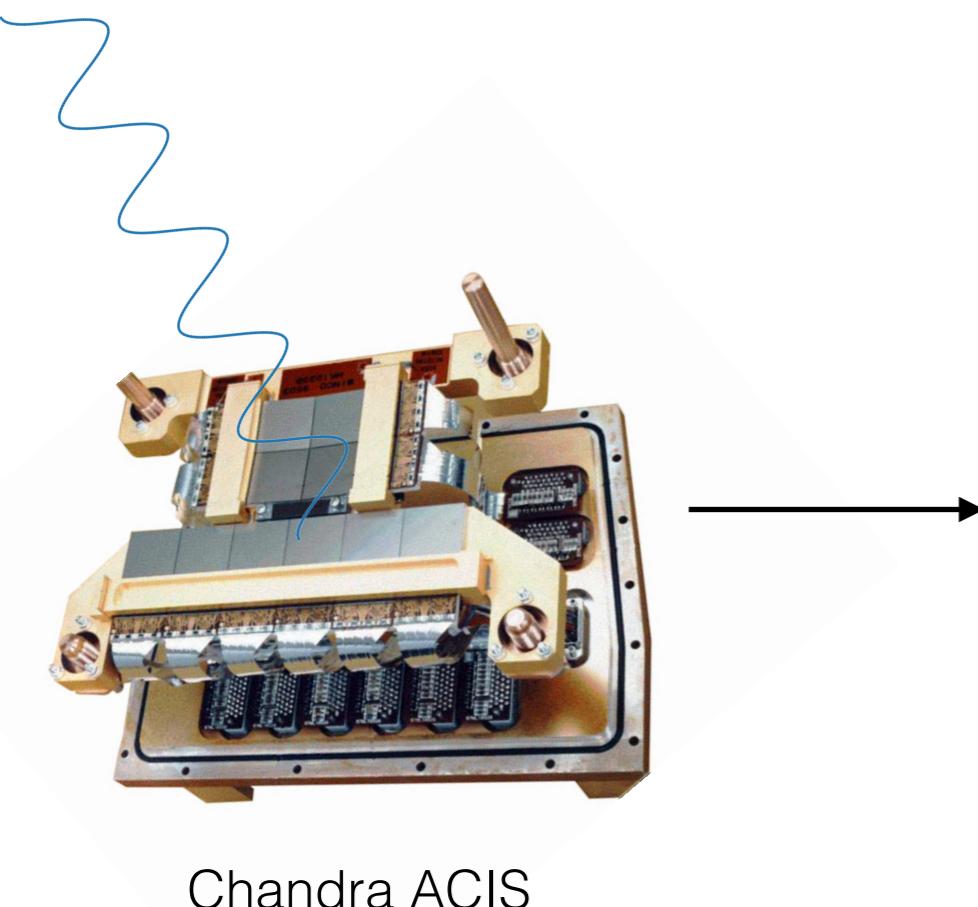
HESS + **CTA**

Outline

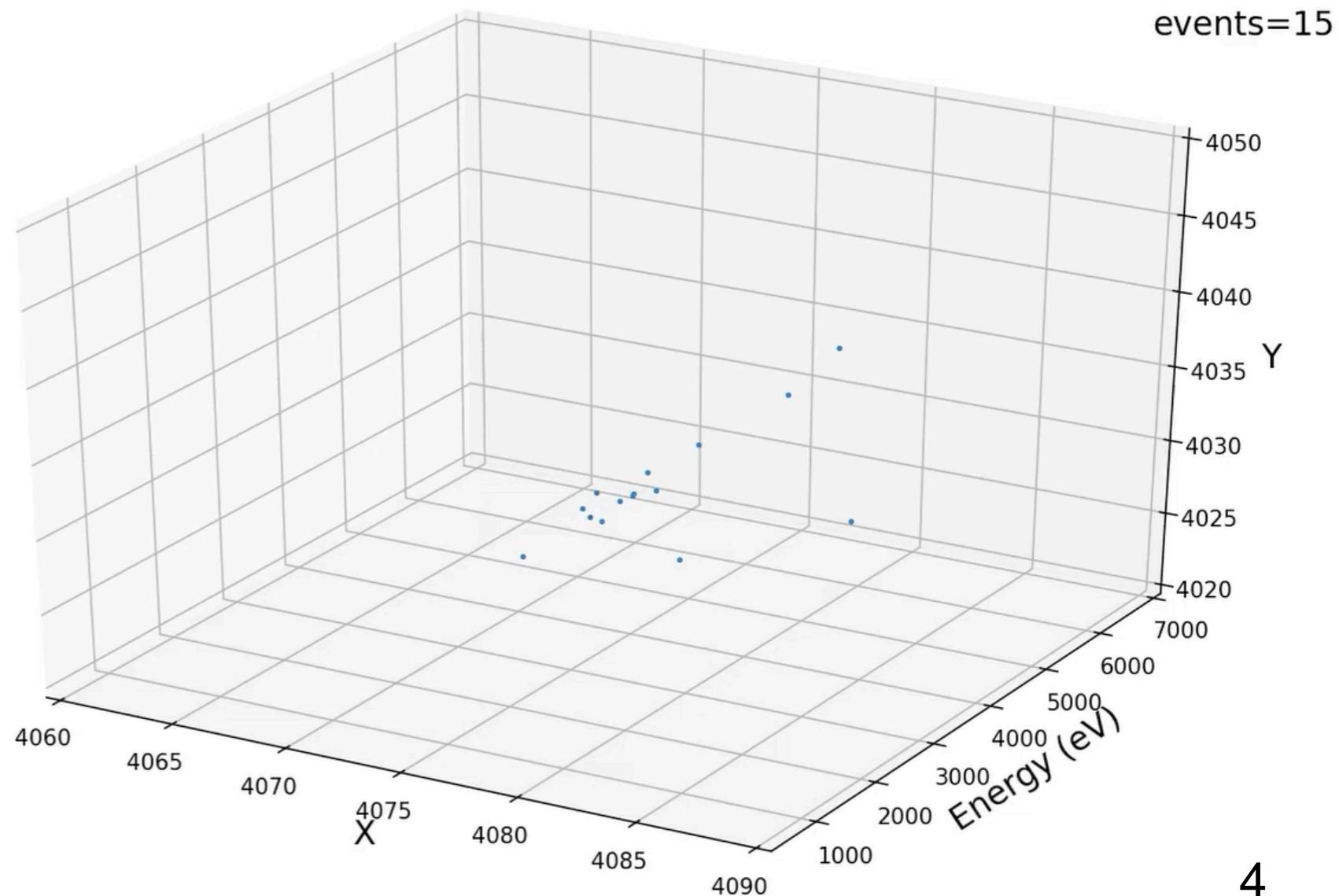
- **A few words on supernova remnants (SNRs)**
- **Science with spectro-imagers**
- **Challenges in X-ray data analysis & different existing workflows**
- **A new data analysis method using the 3D (X,Y,E) data**
- **Panorama of applications: Cassiopeia A & Tycho SNRs, Perseus cluster**
- **A benchmarking Athena dataset for testing new methods**

Spectro-imagers in high-energy

- X-ray spectro-imagers since Einstein (1978) and ROSAT (90)
- CCDs revolution with ASCA (93)
- Measure photon by photon:
 - X, Y, Energy, Time

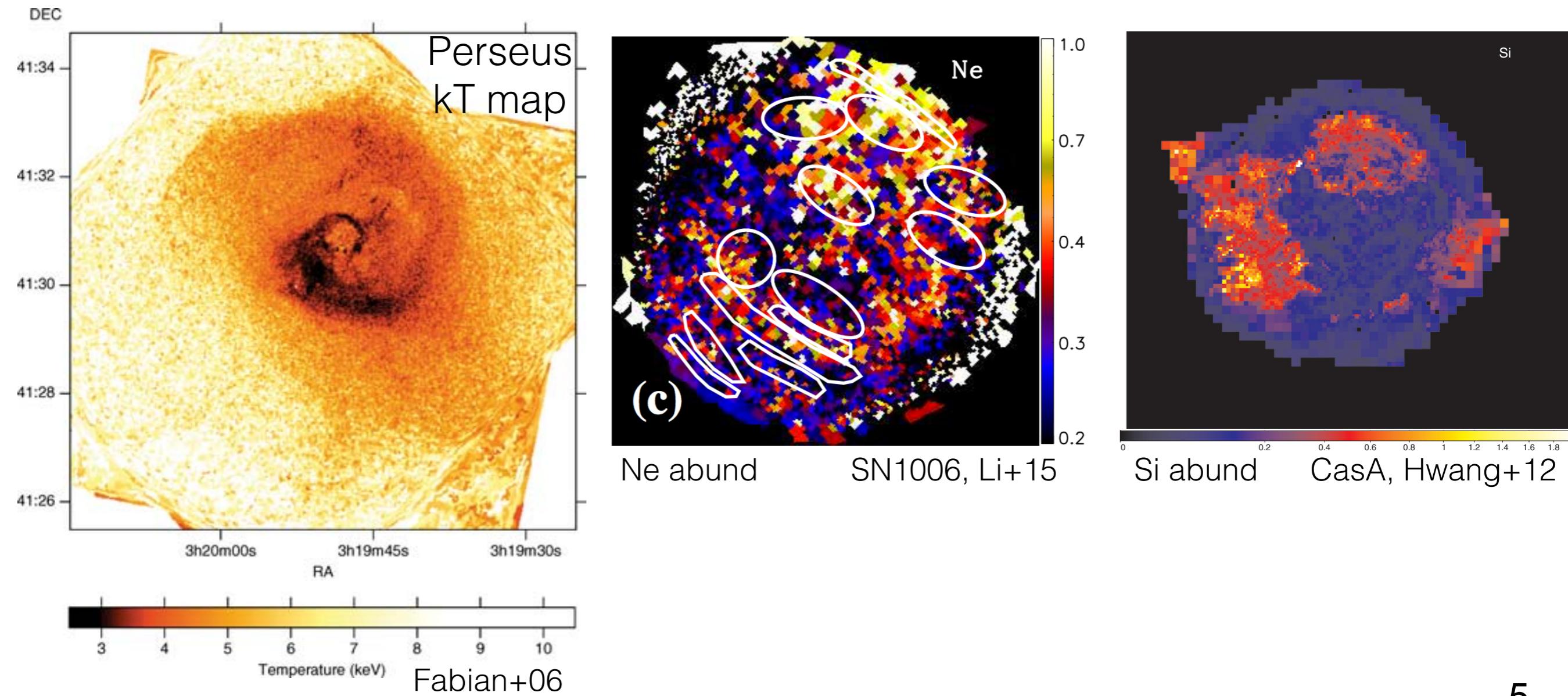


Chandra ACIS

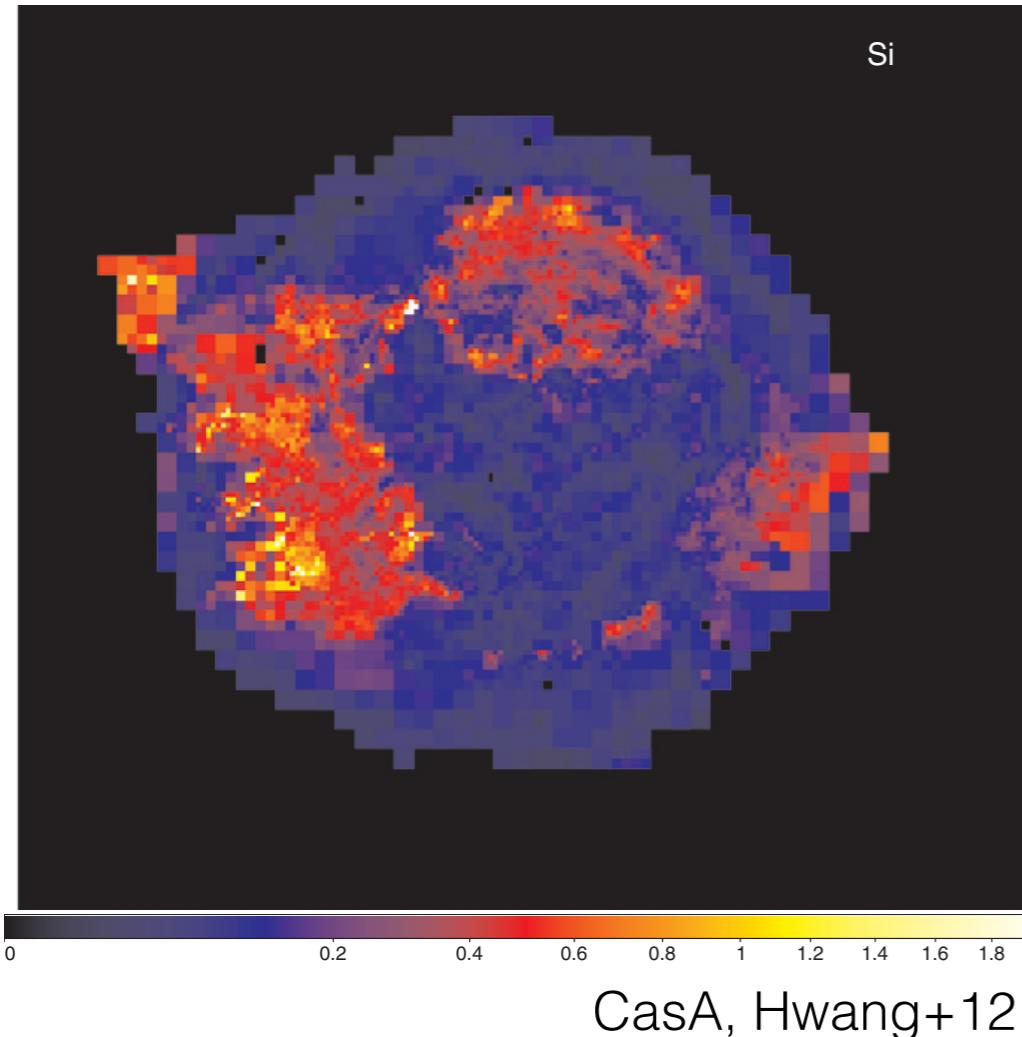


Science with spectro-imagers

- Allow us to isolate point sources or features from extended src
- Study spatial variations of physical parameters (kT, Index, ...) in :
 - galaxy clusters, galaxies, ISM, SNRs, PWNe



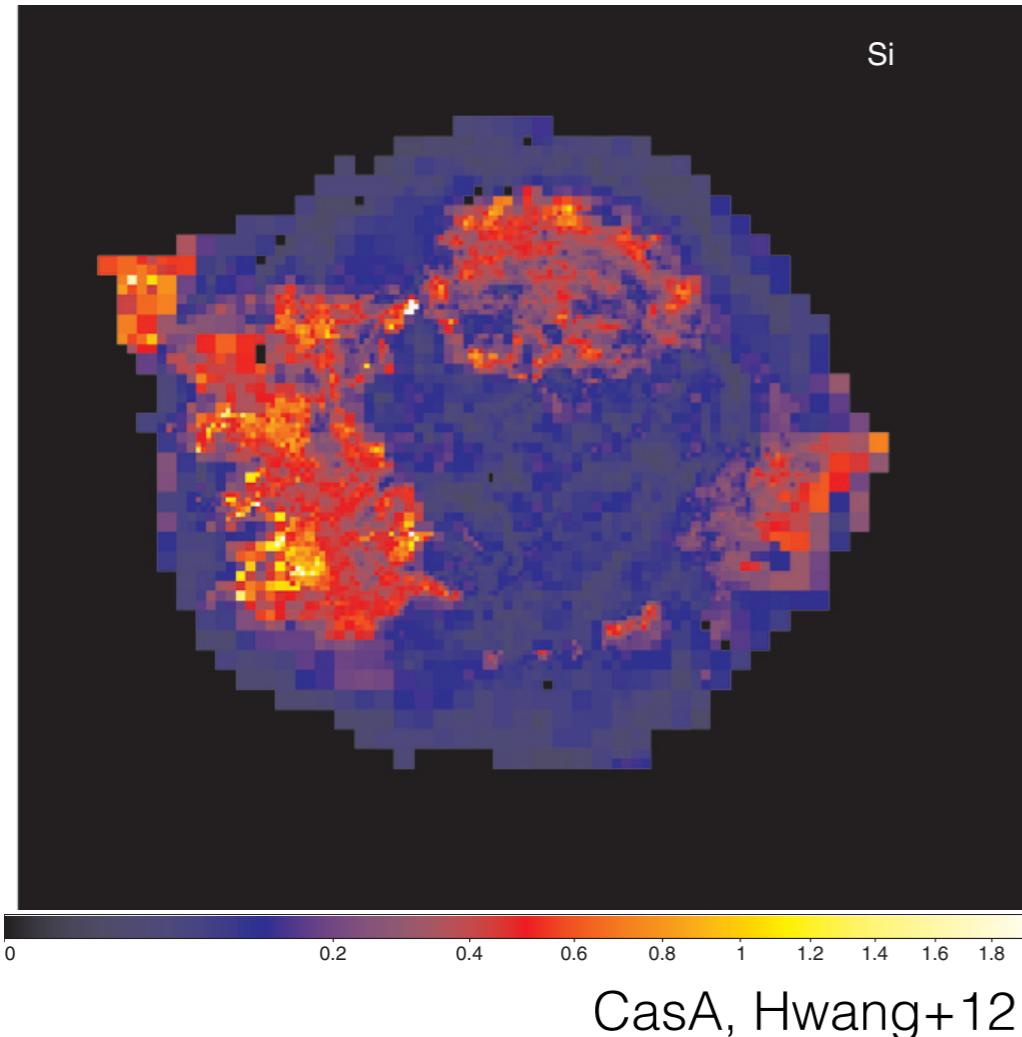
Challenges in data analysis



- **Multiple physical components entangled:**
 - Mixed/nested ejecta, synchrotron
 - projection effect
 - region definition impacts spectra
- **Adaptive tiling (Voronoi, contours):**
 - cells defined on surface brightness not physical components spatial distribution
 - cell definition for Si is not ideal for synchrotron emission
 - Painful analysis ($>10^4$ spectra to fit)

CasA dataset: >1 billion photons !

Challenges in data analysis

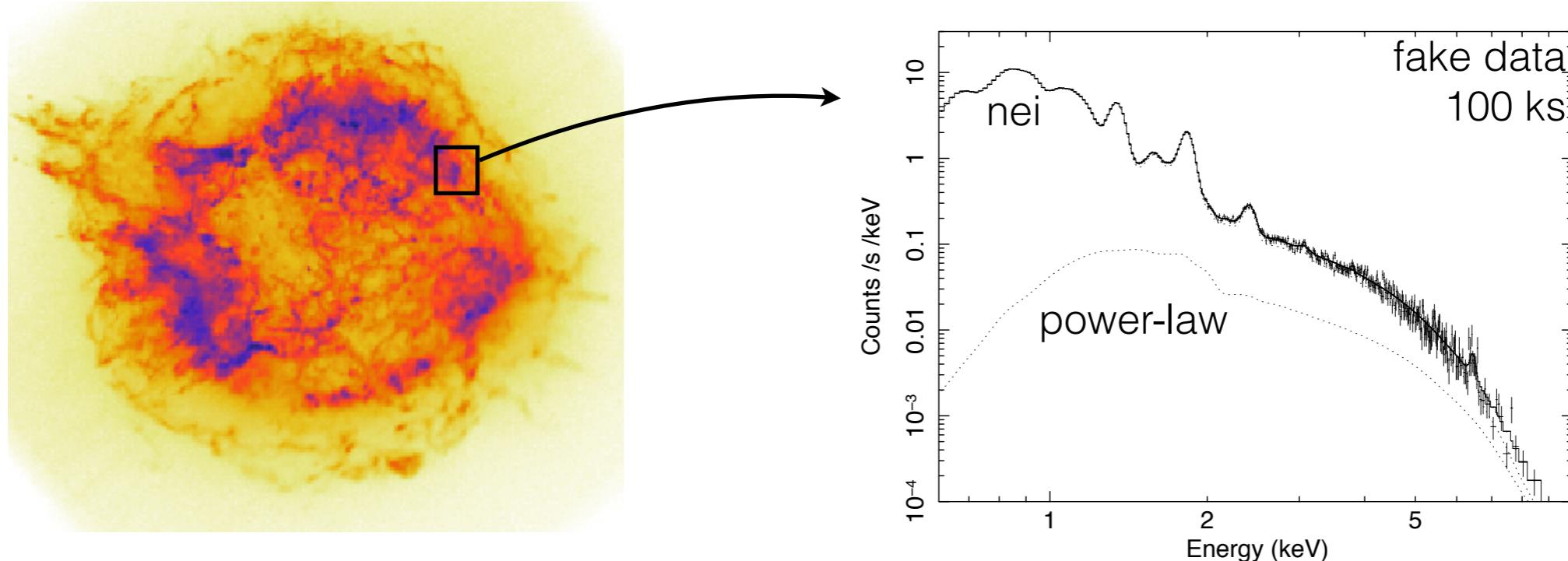


CasA dataset: >1 billion photons !

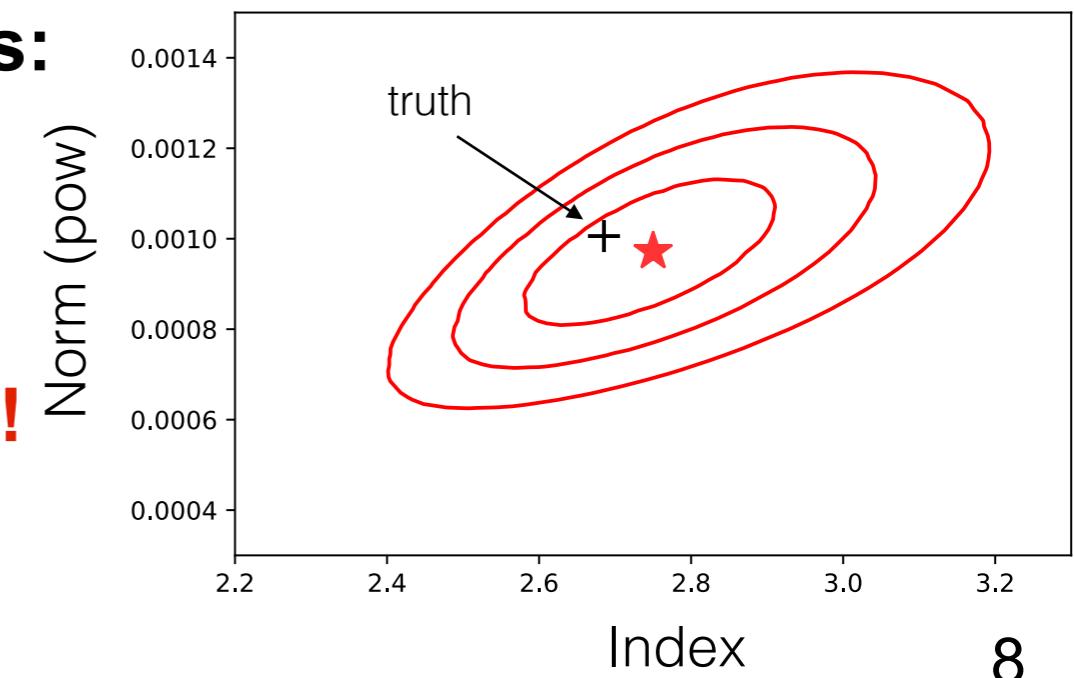
- **Multiple physical components entangled:**
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- **Issue: each cell is treated independently from its neighbors !**
 - 2D then 1D, not fully exploiting the data

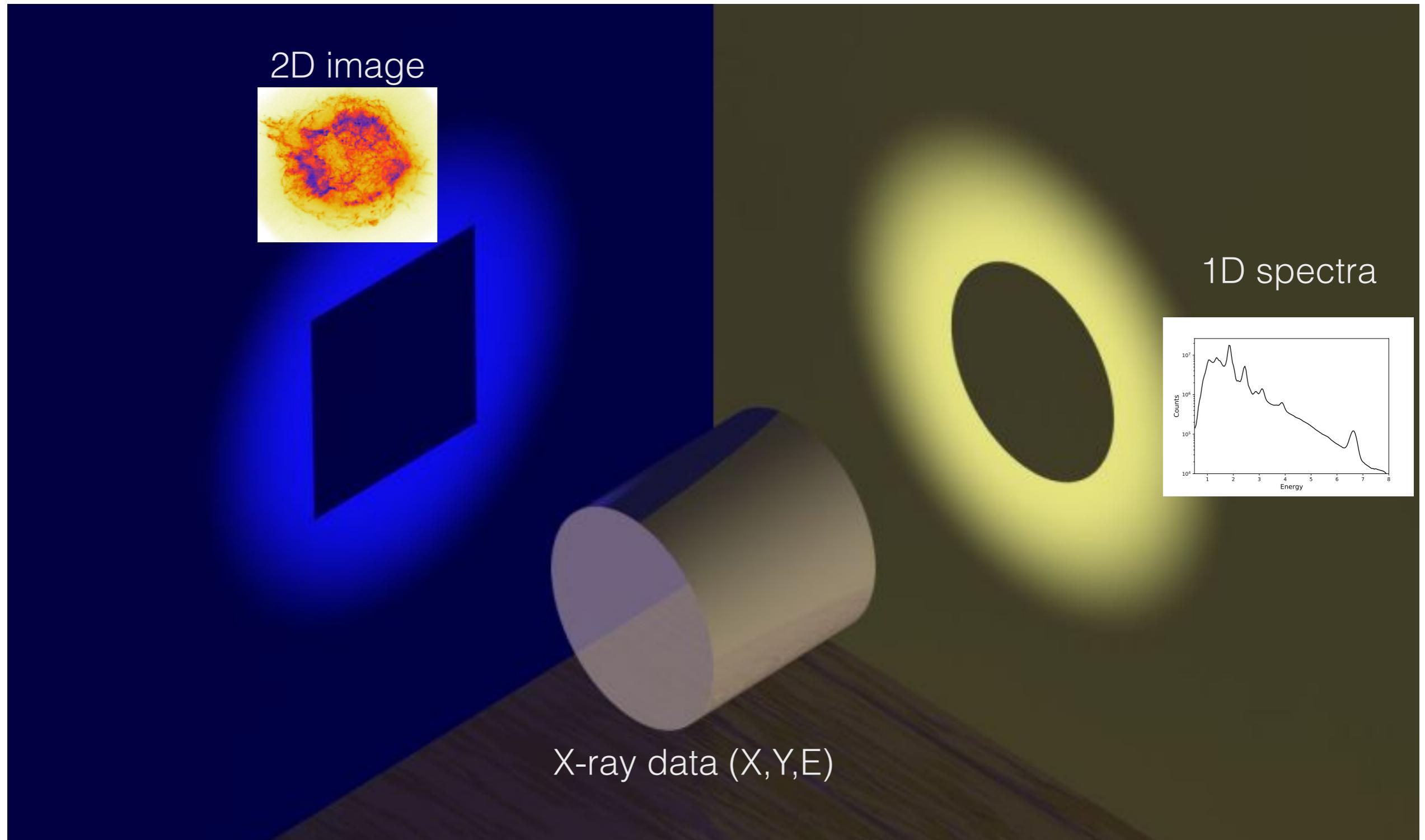
X-ray traditional workflow



- **Parametric fit. Compare models : $\chi^2(\text{nei})$ vs $\chi^2(\text{nei}+\text{pow})$**
- **Disentangling process is done in 1D using spectral signatures**
- **Hard to characterize faint components:**
 - **Degeneracy between Norm & Index**
- **Components have spatial signatures !**

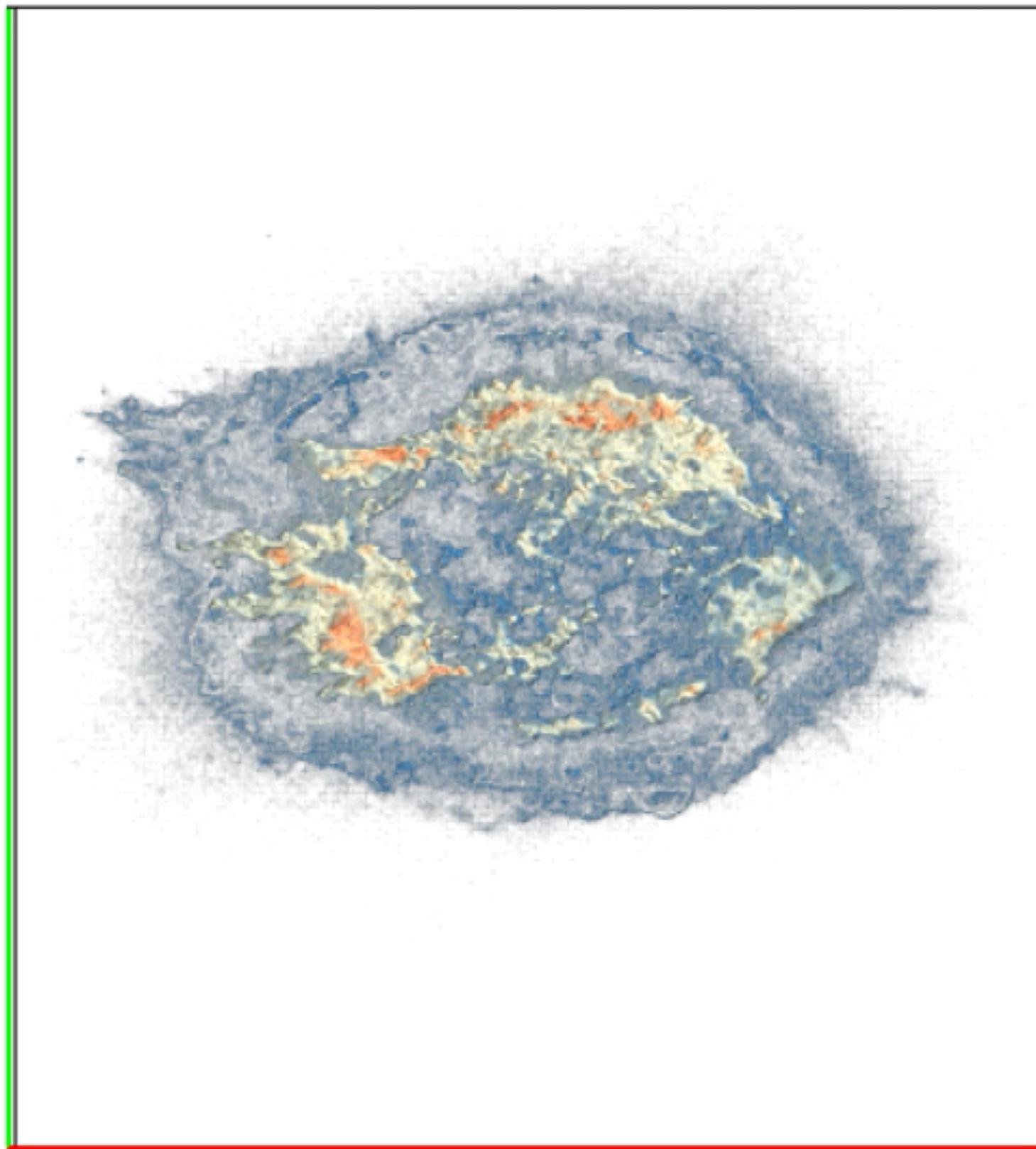


The spectro-imagers schizophrenia



A 3D view of CasA data

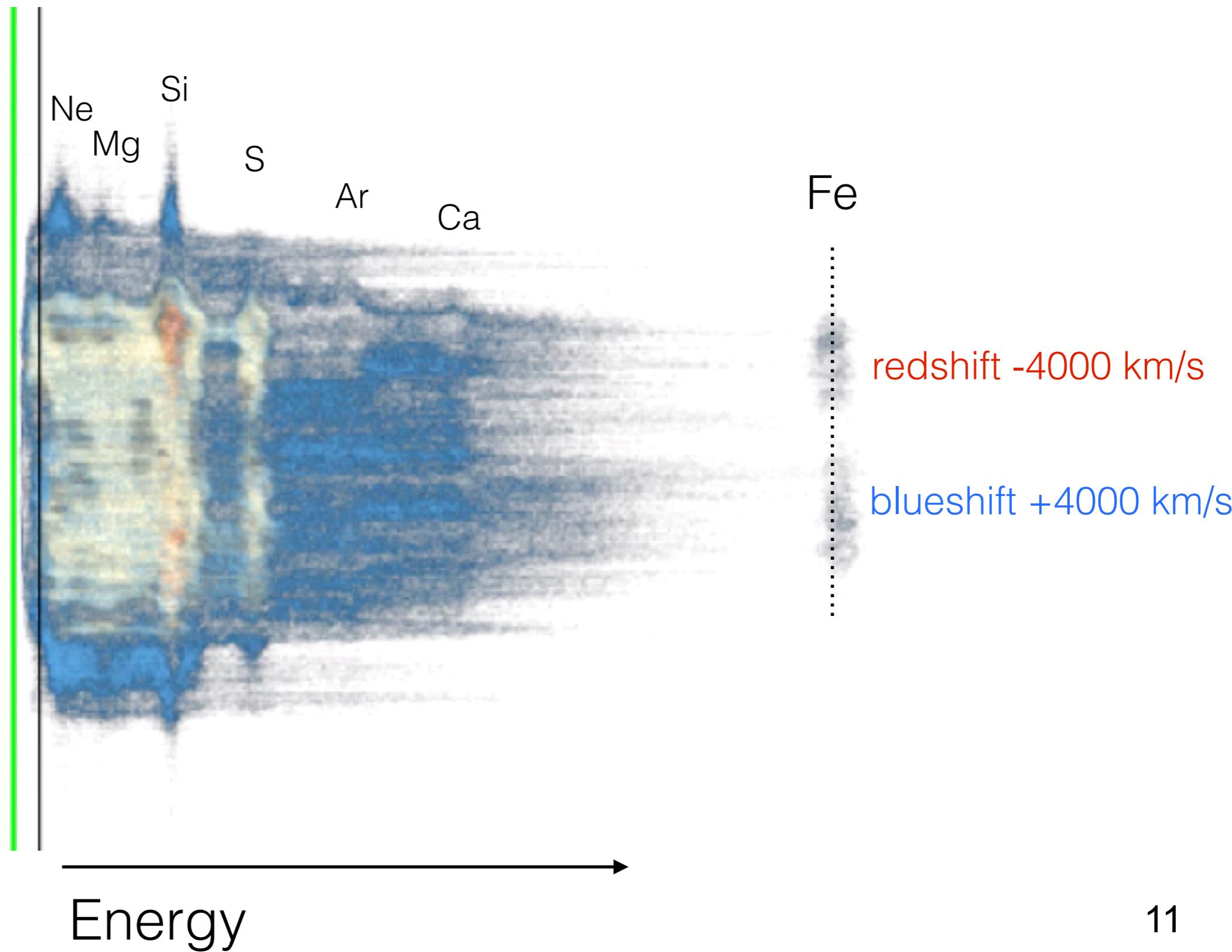
CasA Chandra X,Y,E cube



Data visualization
with vaex

A 3D view of CasA data

CasA Chandra X,Y,E cube

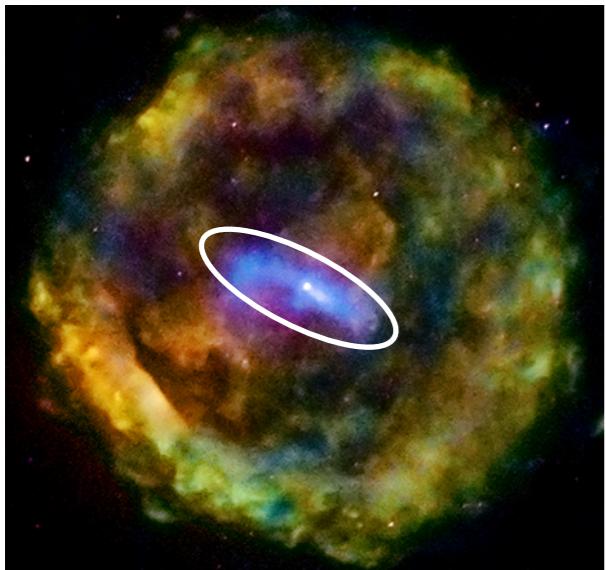


Status of high-energy workflows

2D then 1D

Spatial selection
then spectral analysis

a)



SNR G11.2-0.3

**Spectro-morphology
drawn by eye**

X-ray, TeV analysis

Issue:
ON region contains
SNR + PWN

Status of high-energy workflows

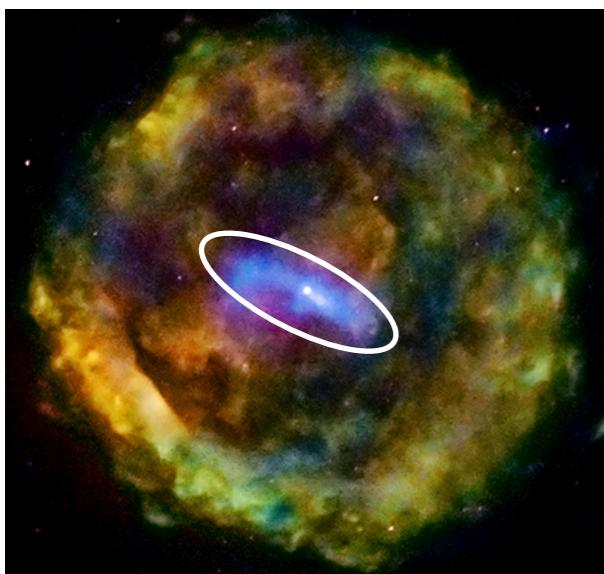
2D then 1D

Spatial selection
then spectral analysis

2D + 1D

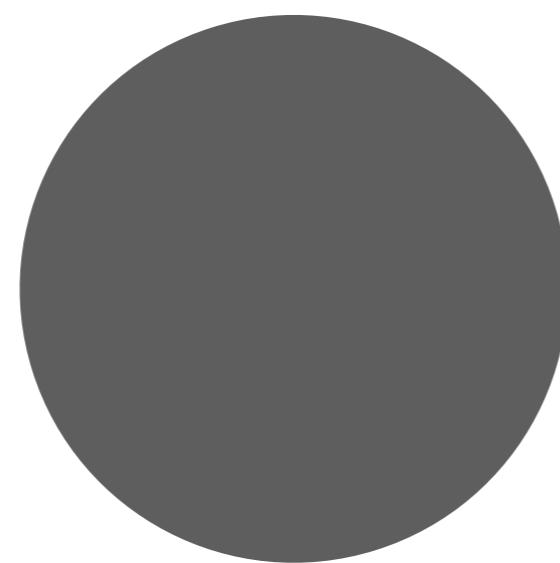
spatial + spectral
parametric analysis

a)



SNR G11.2-0.3

b)



* Spec1

+



* Spec2

**Spectro-morphology
drawn by eye**

**parametric morphology (gaussian, disk)
parametric spectra (Power-Law, etc)**

X-ray, TeV analysis

GeV analysis

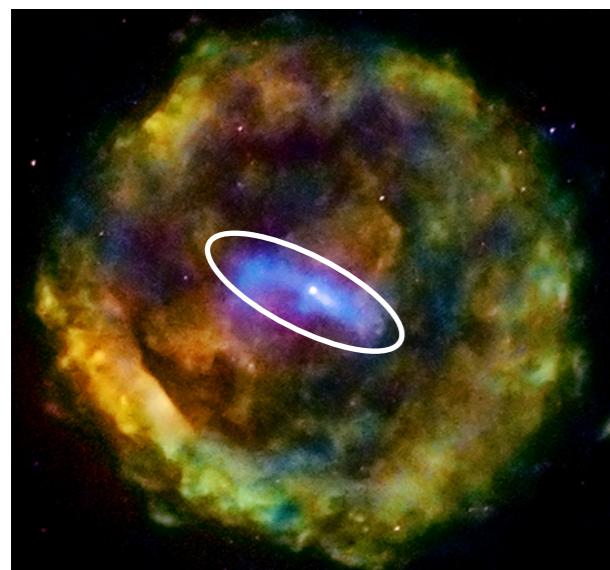
Issue:
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Issue:
Which morphology ?
Reality is not disk & gaussians

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X-ray, TeV analysis

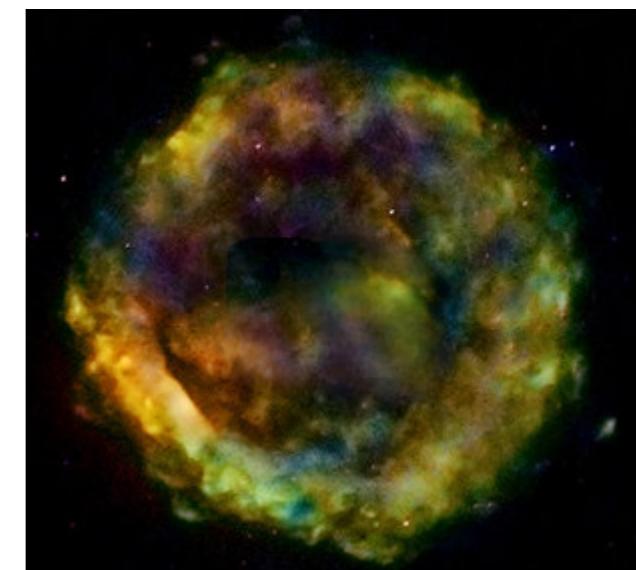
Issue:
ON region contains
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2D + 1D

spatial + spectral
parametric analysis



Component separation:
2D + 1D non parametric



**Non-parametric
morphology of spectral features**

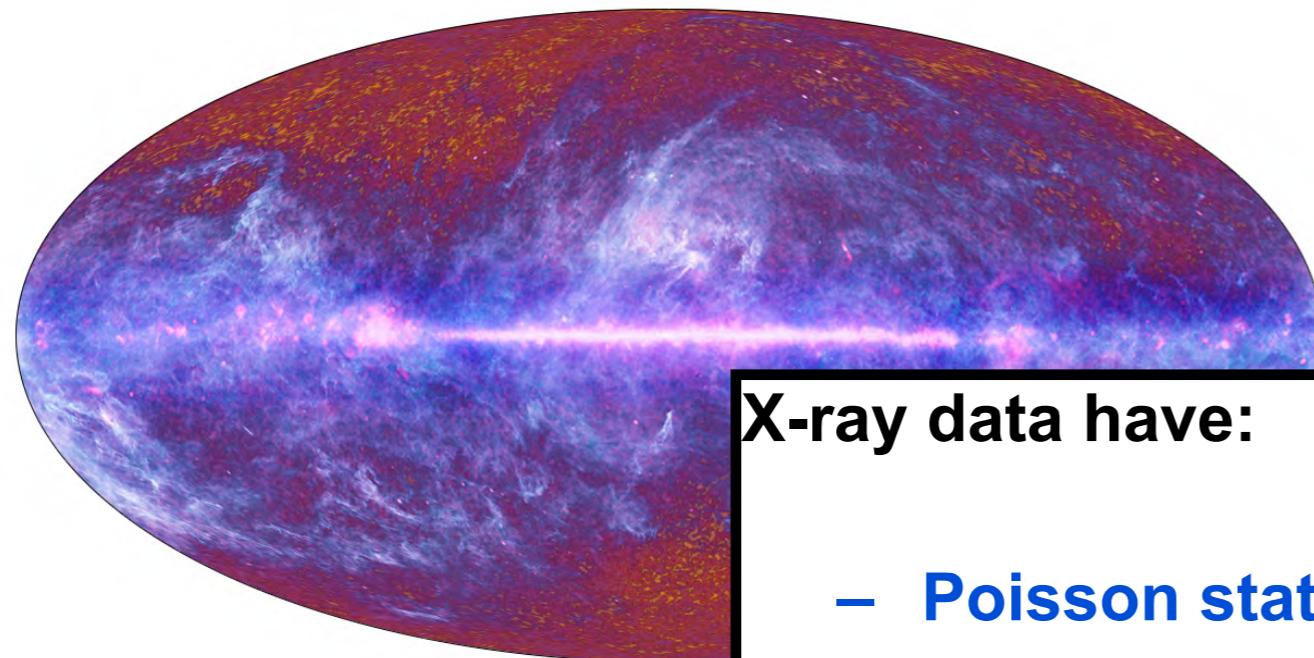
New method

disentangle components
with no morphology hypothesis

GeV analysis

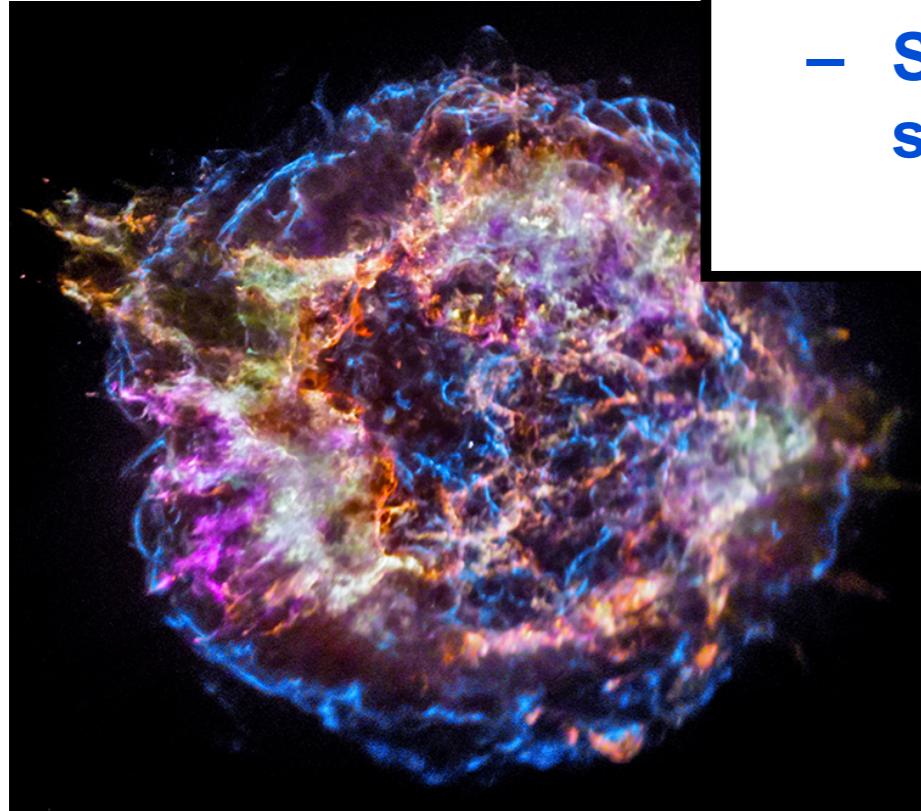
Issue:
Which morphology ?
Reality is not disk & gaussians

How to disentangle CMB from foregrounds

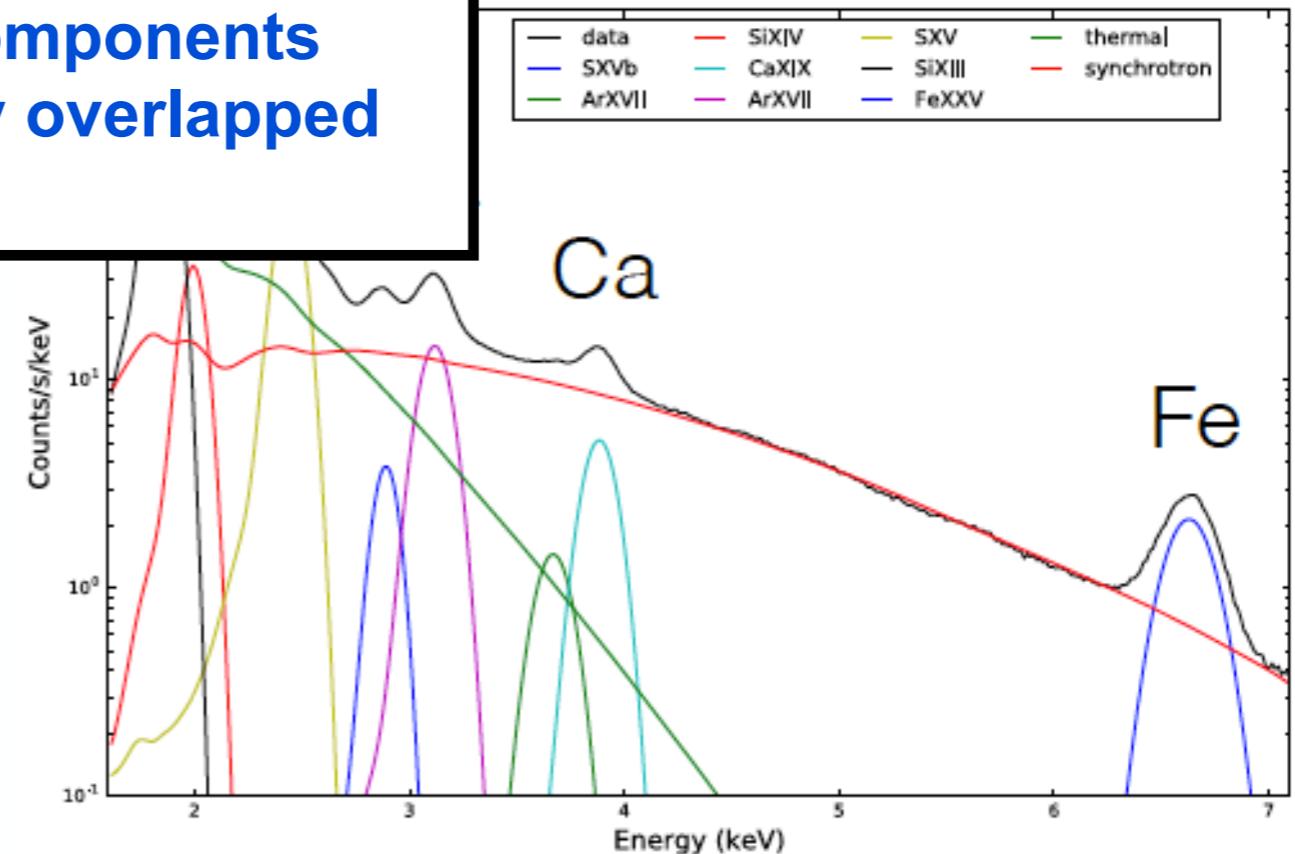
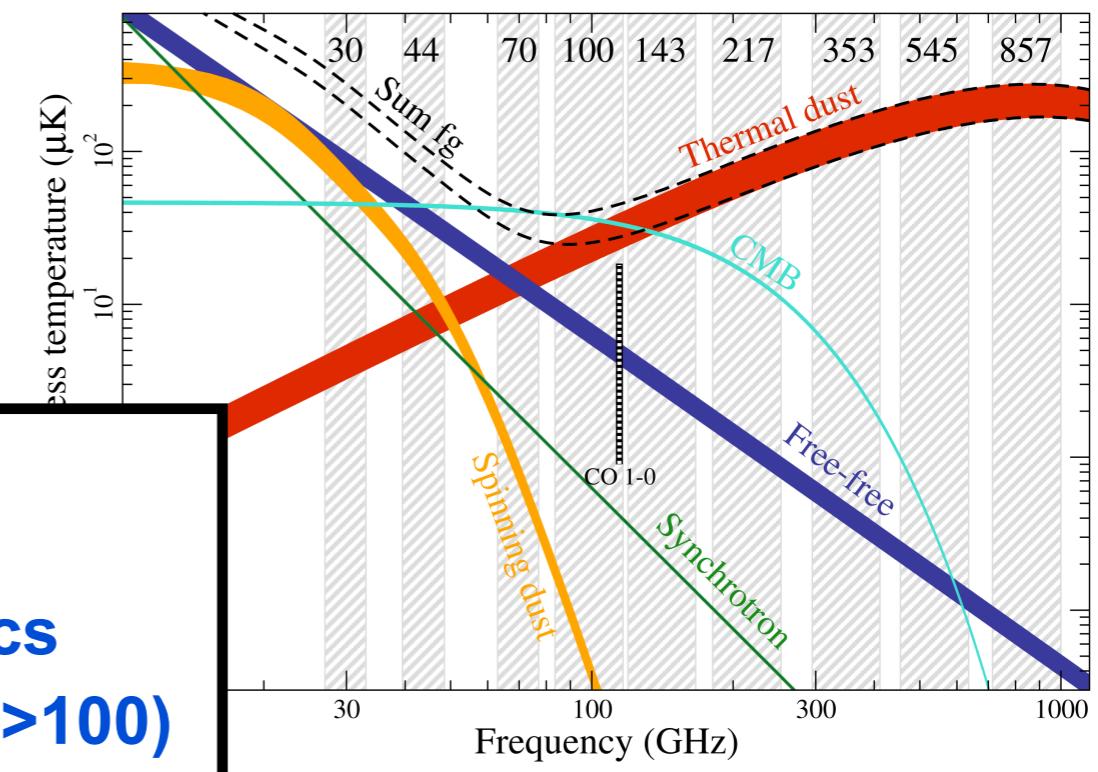


X-ray data have:

- Poisson statistics
- More channels (>100)
- High dynamic range
- SNR: components strongly overlapped

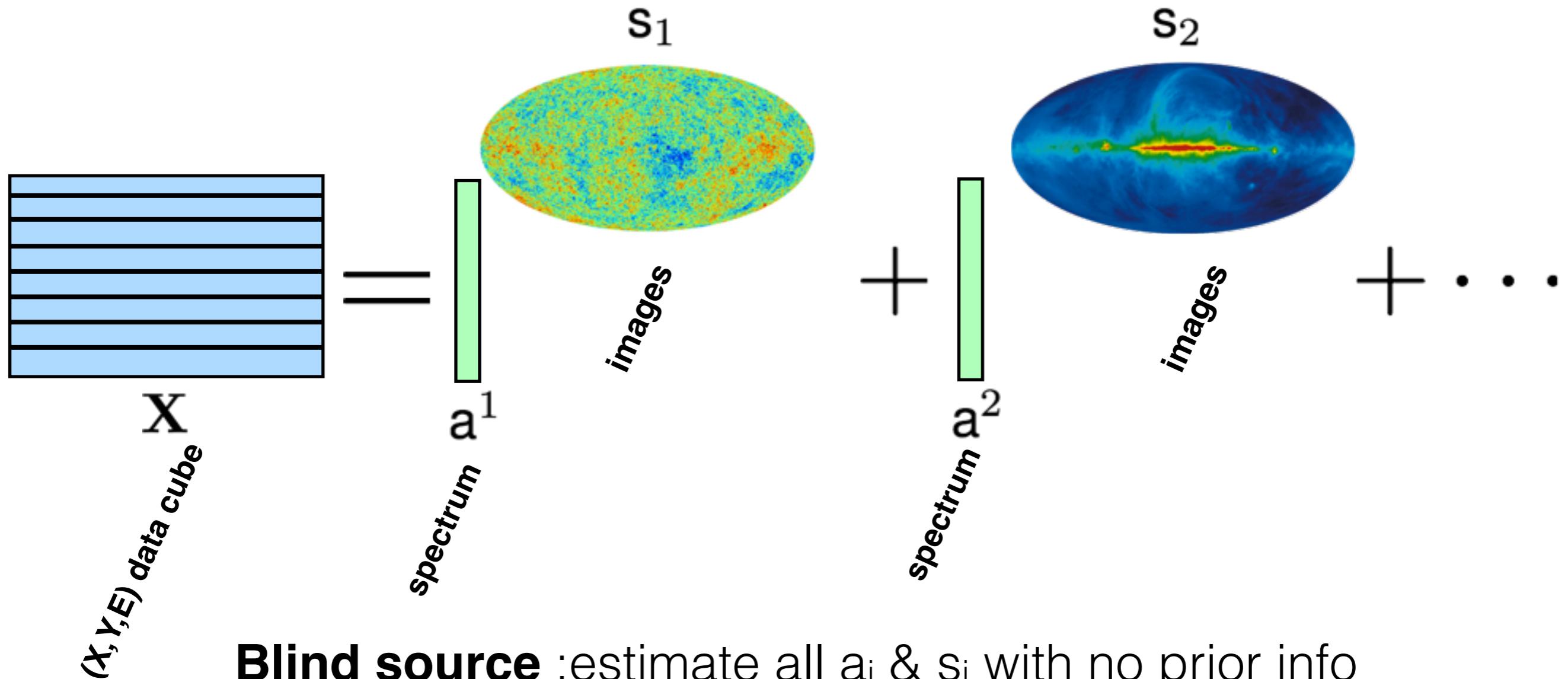


Core Collapse SN : Cassiopeia A



Generalized Morphological Component Analysis (Bobin et al. 2016)

Assumption: Linear combination of Spec*Image



Blind source : estimate all a_i & s_i with no prior info

Semi-blind : fix one spectral component (e.g. CMB)

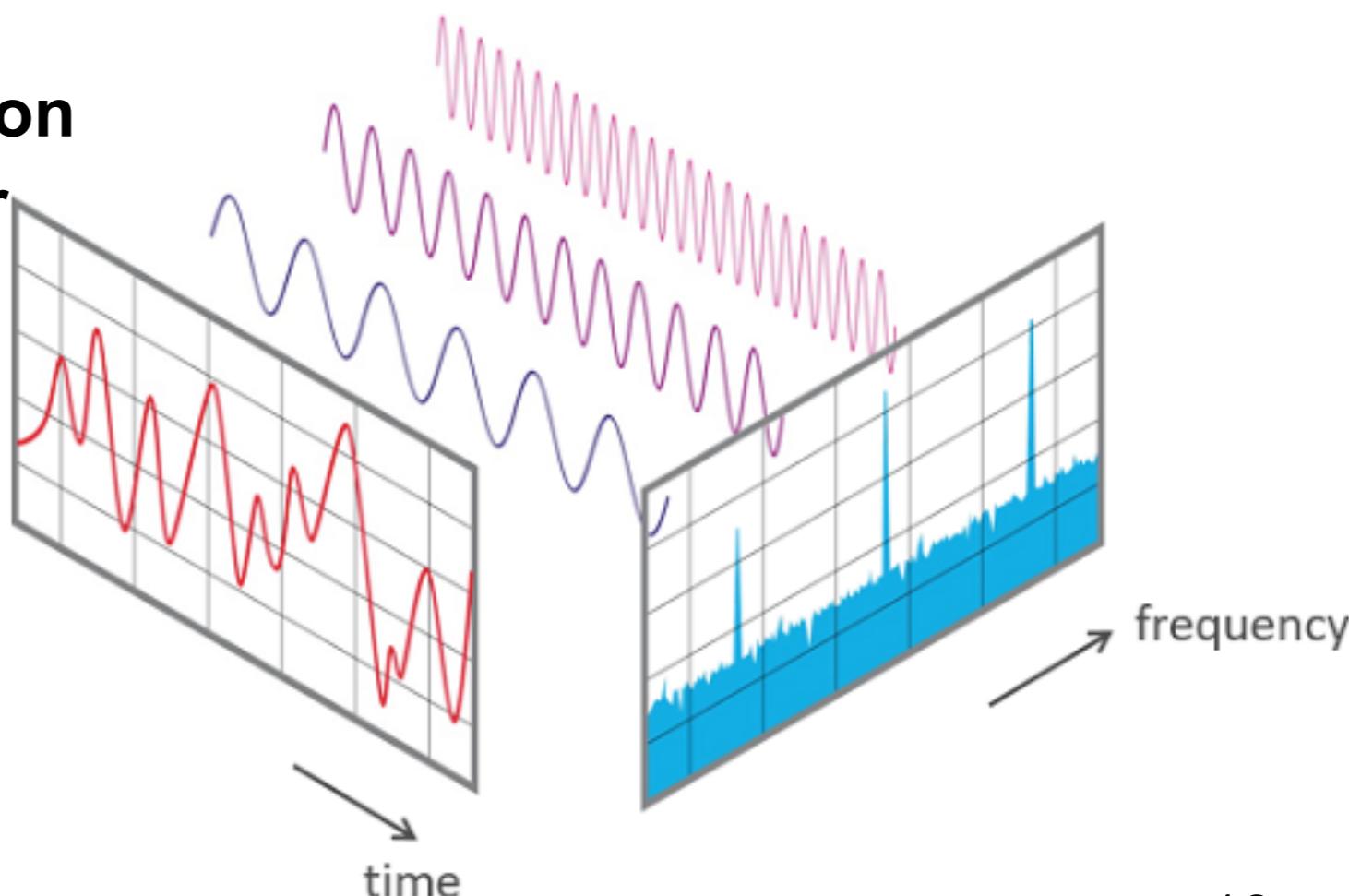
Limitation: morphology doesn't change with energy

Blind source separation: where is the magic ?

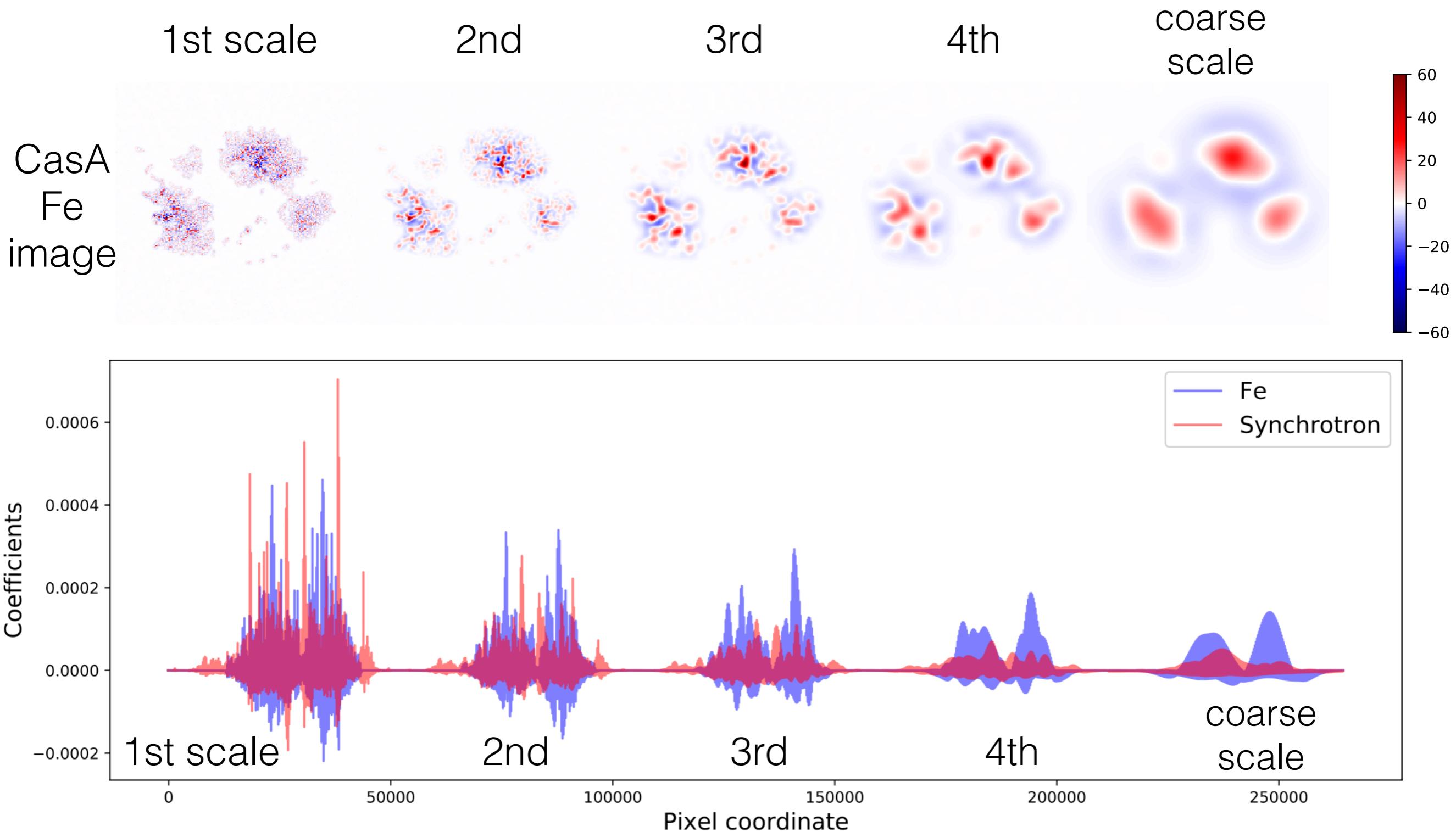
- Specify NO prior information (no spectral model, instrument response)
- Input :
 - Cube: 2D-1D data (X,Y,E)
- Output:
 - N cubes ($\text{Image}_i * \text{spectra}_i$), N fixed by user

Blind source separation: where is the magic ?

- Specify NO prior information (no spectral model, instrument response)
- Input :
 - Cube: 2D-1D data (X, Y, E)
- Output:
 - N cubes ($\text{Image}_i * \text{spectra}_i$), N fixed by user
- Where is the magic ?
- Find a sparse data representation
- A 1D analogy would be Fourier



Wavelet Starlet transform



GMCA: algorithm

$$X = AS + N = \sum_{i=1}^n A_i S_i + N$$

data cube *spectrum* *image* *additive noise*

- Equation has an infinite number of solution (ill-posed inverse problem)
 - Example: $4 = a * b$ cannot be solved without constraints
 - Constraint: a & b are positive integers. Solution: (2,2) & (4,1)
- Each cube slice (image) is transposed in the wavelet domain (X: 4D array)

GMCA: algorithm

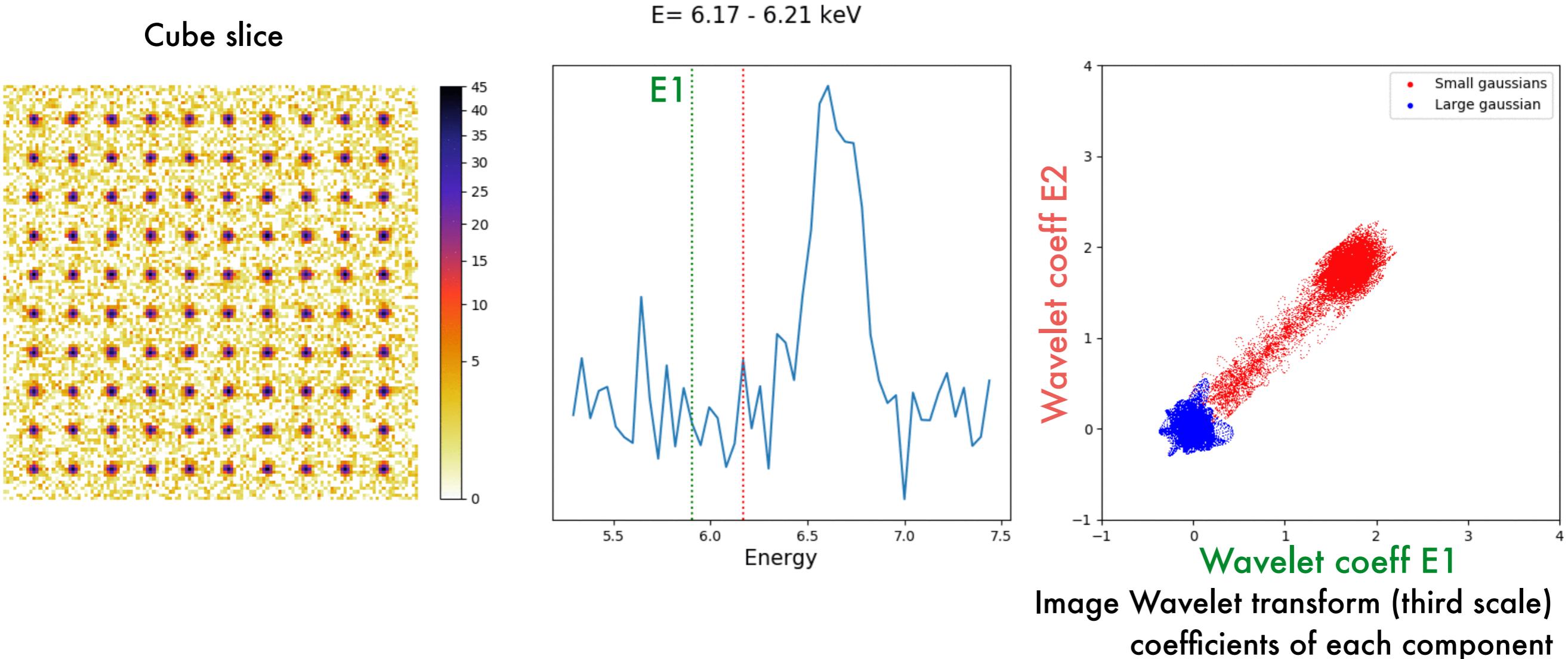
$$\min_{A,S} \sum_{i=1}^n \lambda_i \|S_i\|_p + \|X - AS\|_F^2$$

sparsity constraint term data fidelity term
(Poisson likelihood for X-rays)

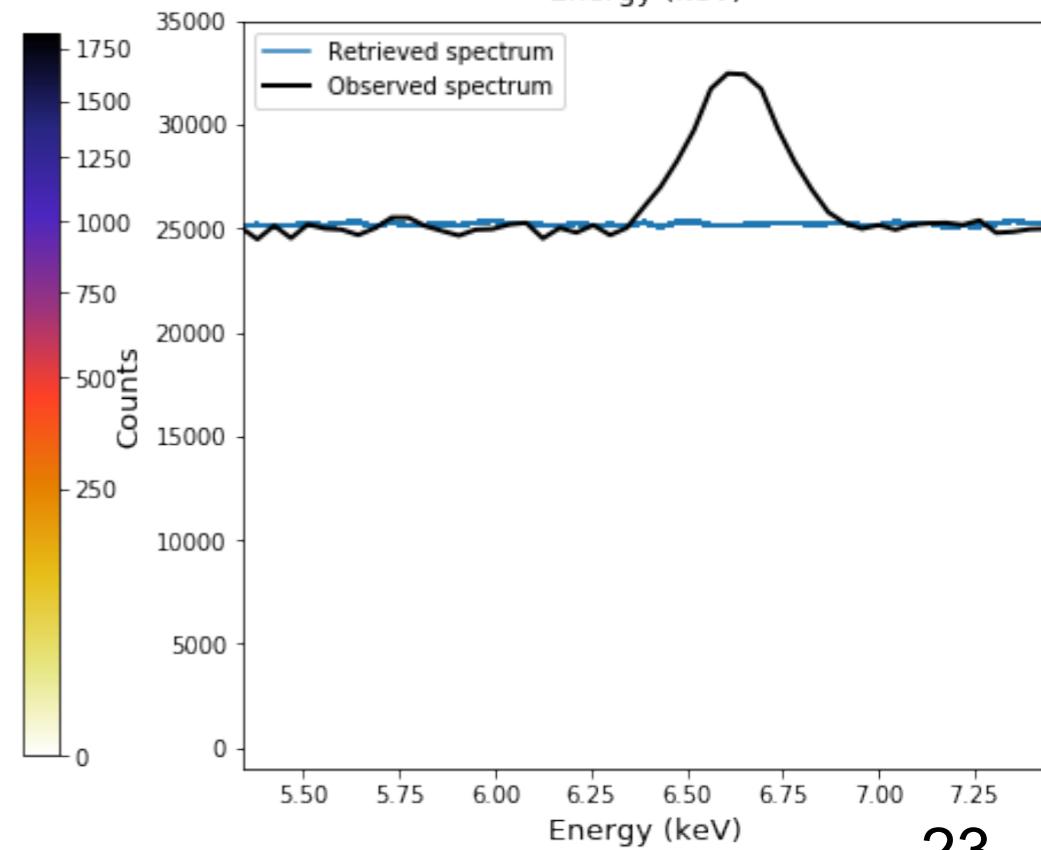
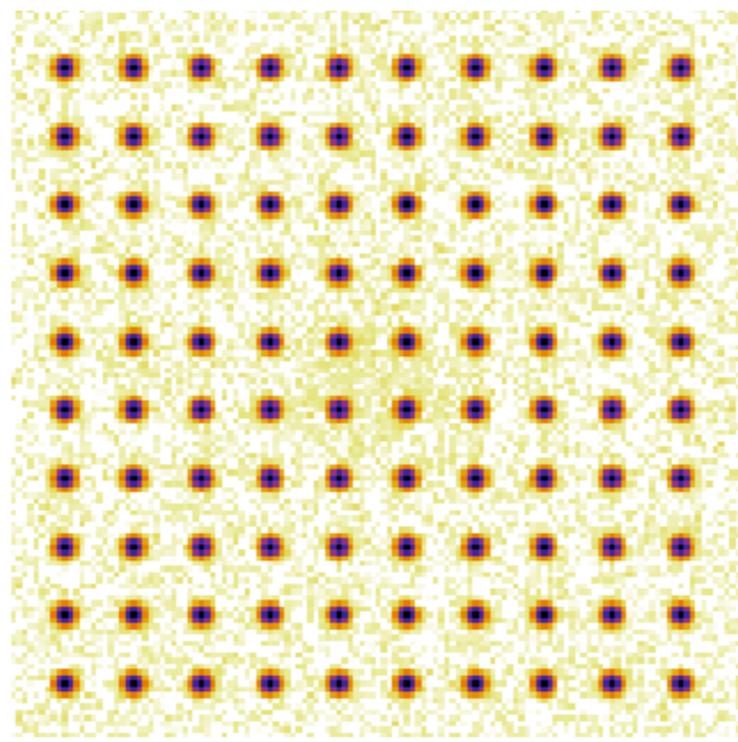
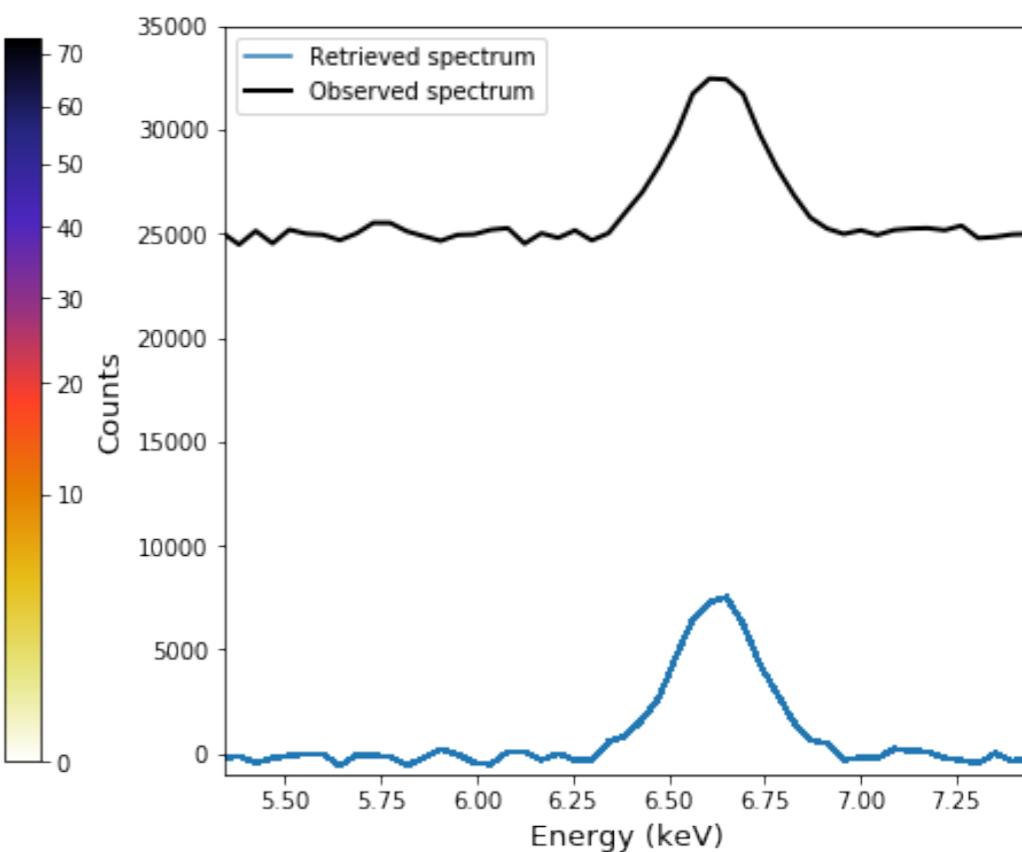
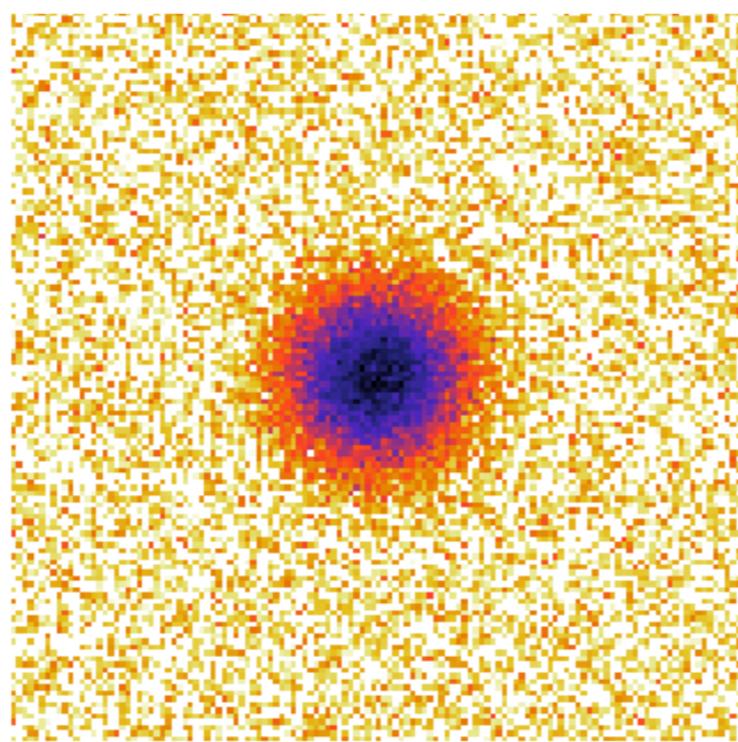
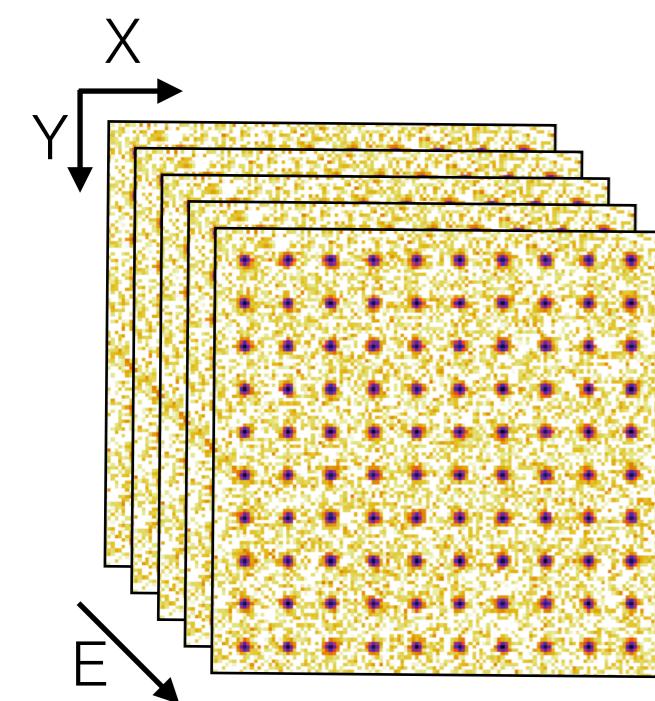
- Here we constrain sparsity of the images (S_i) in the wavelet domain
- Alternatively estimate S for fixed A , then A for fixed S

GMCA : example

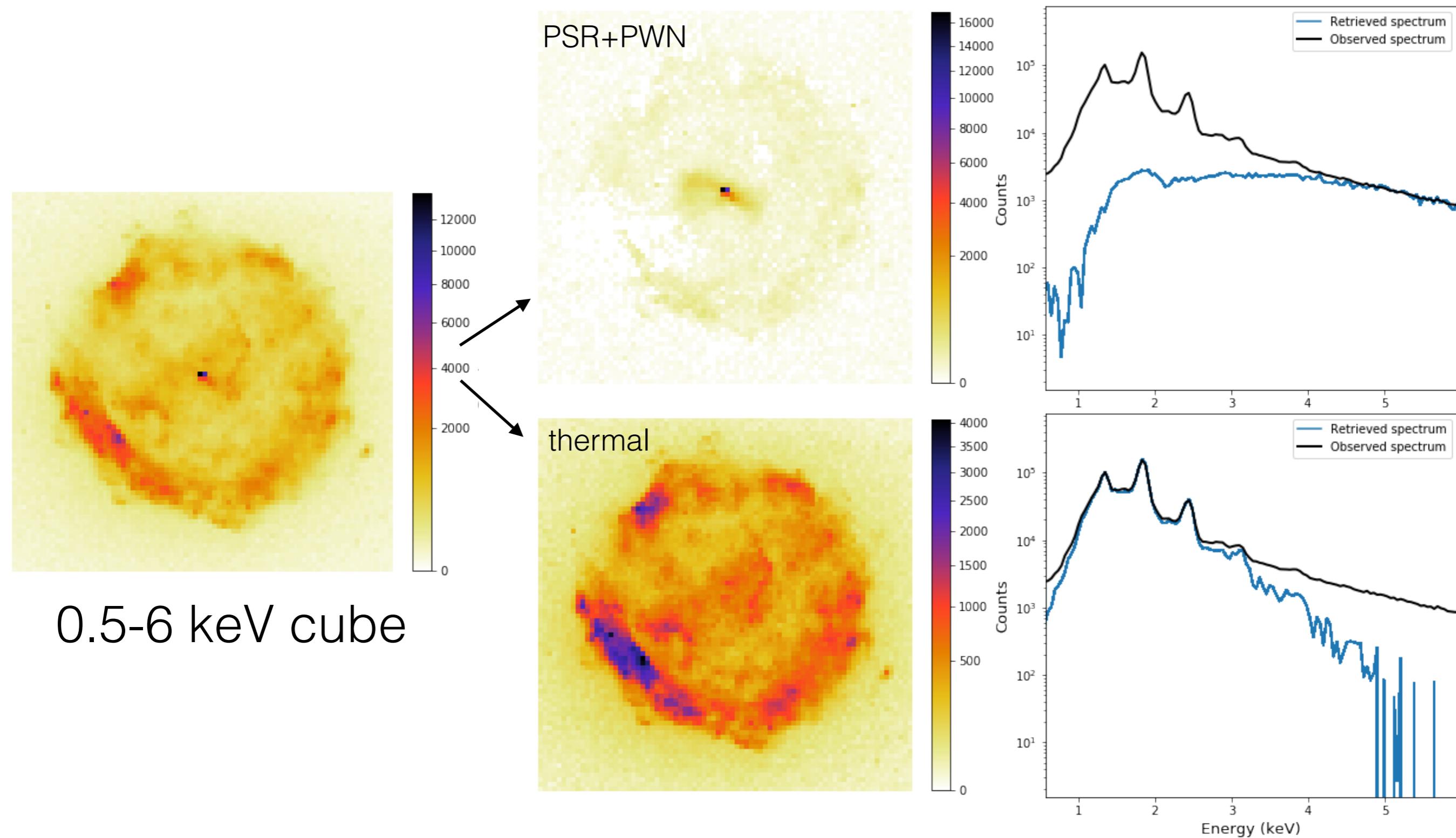
- In a way GMCA is an unsupervised ML clustering algorithm



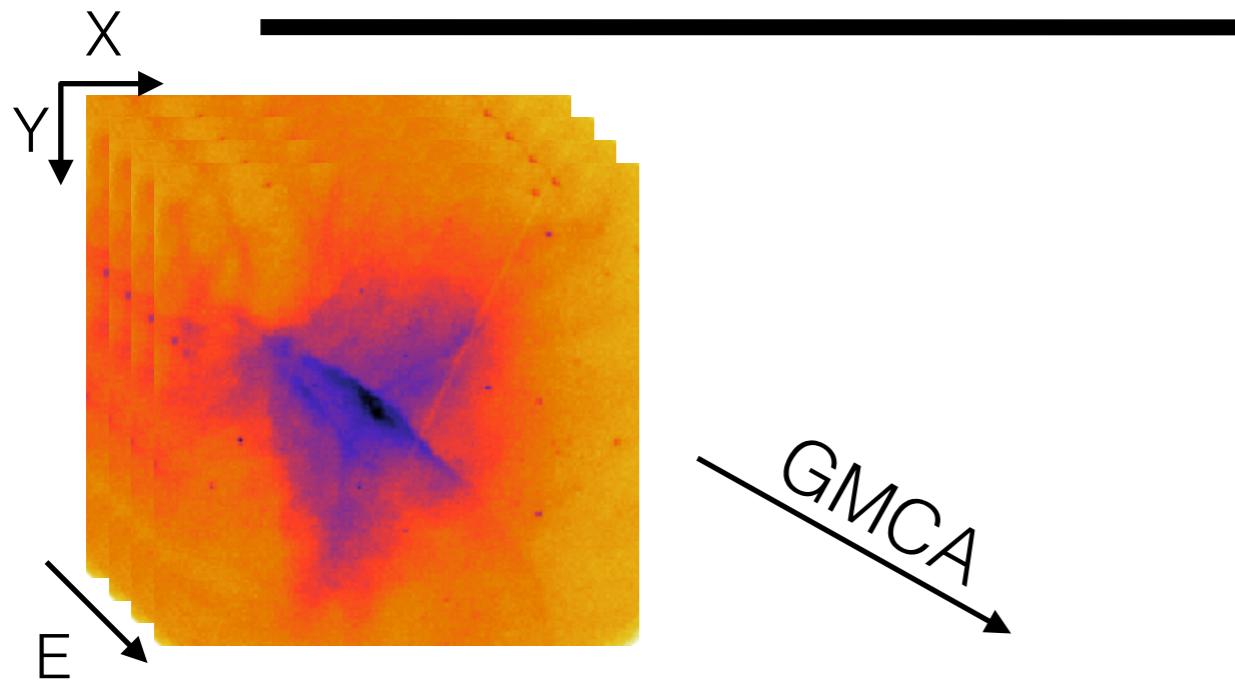
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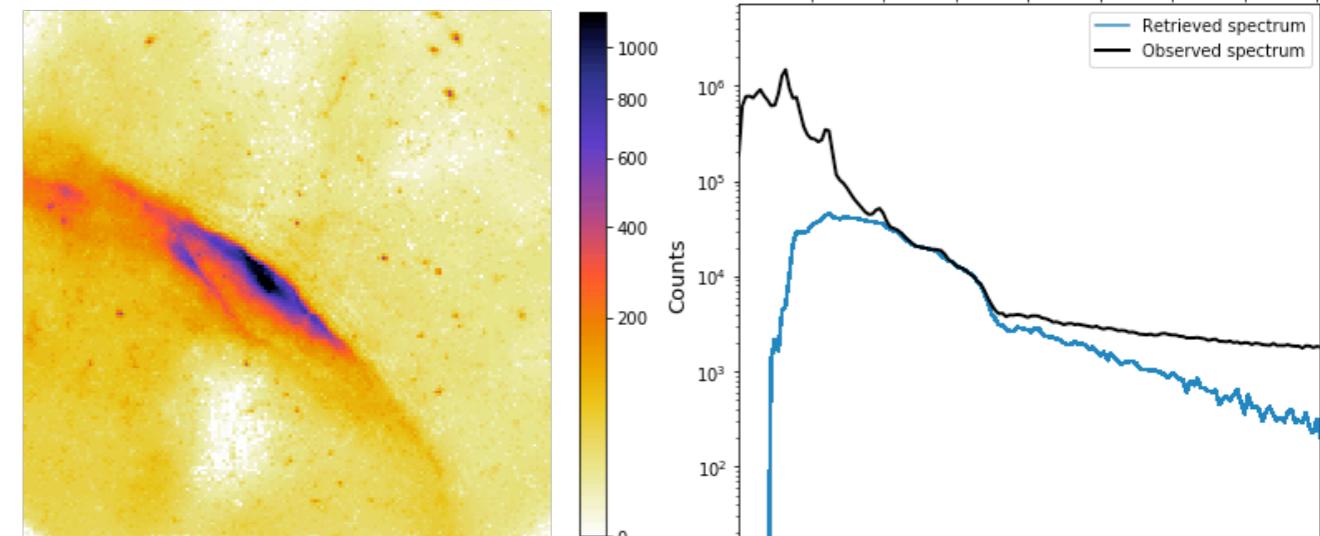
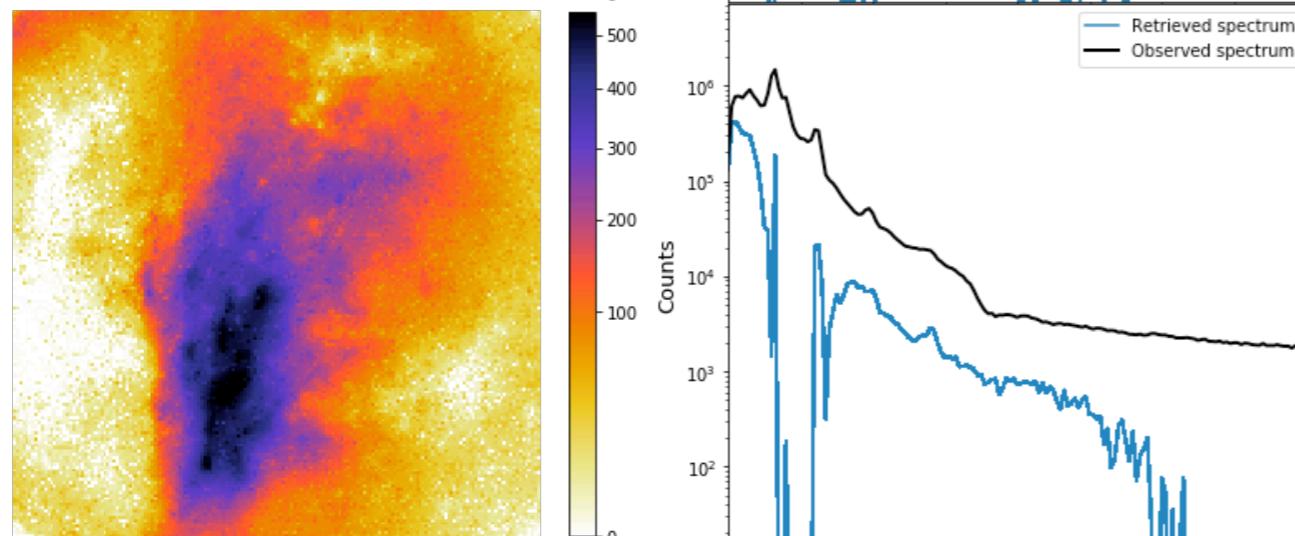
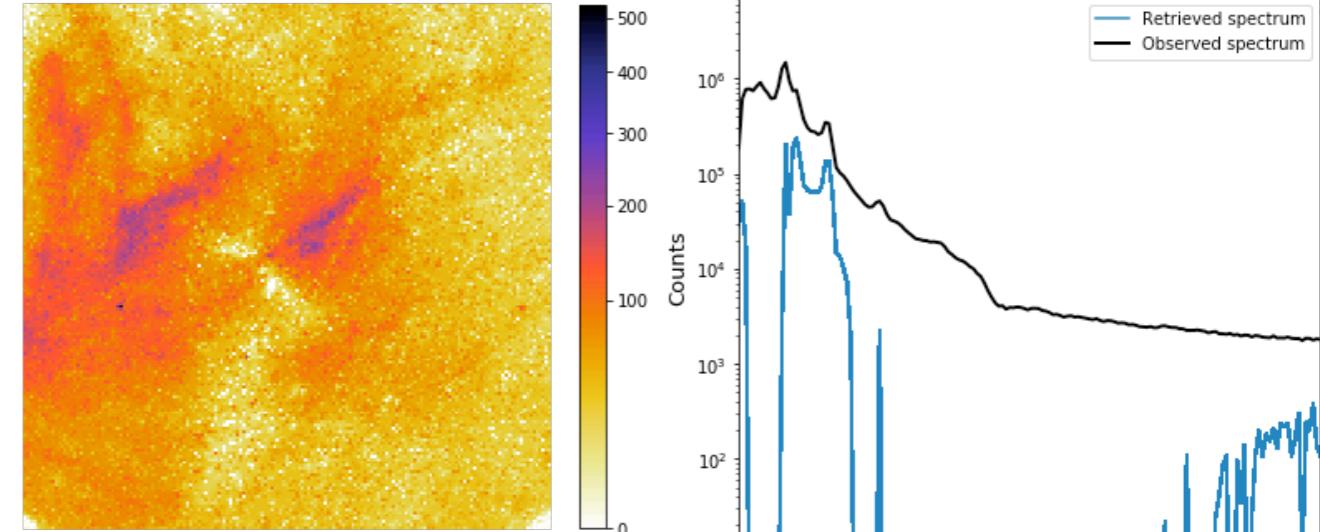
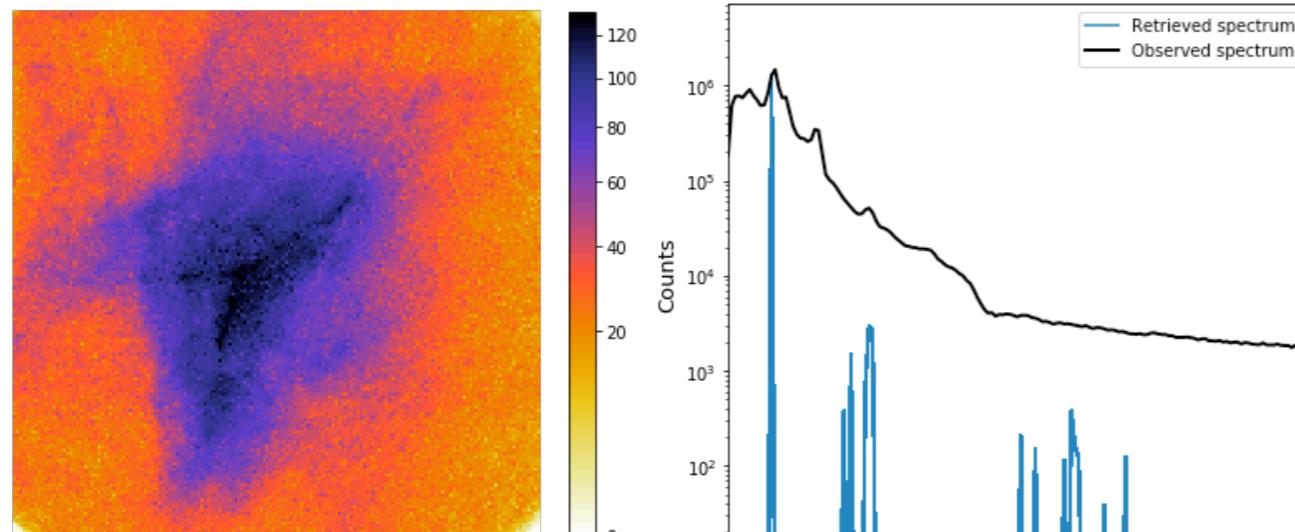
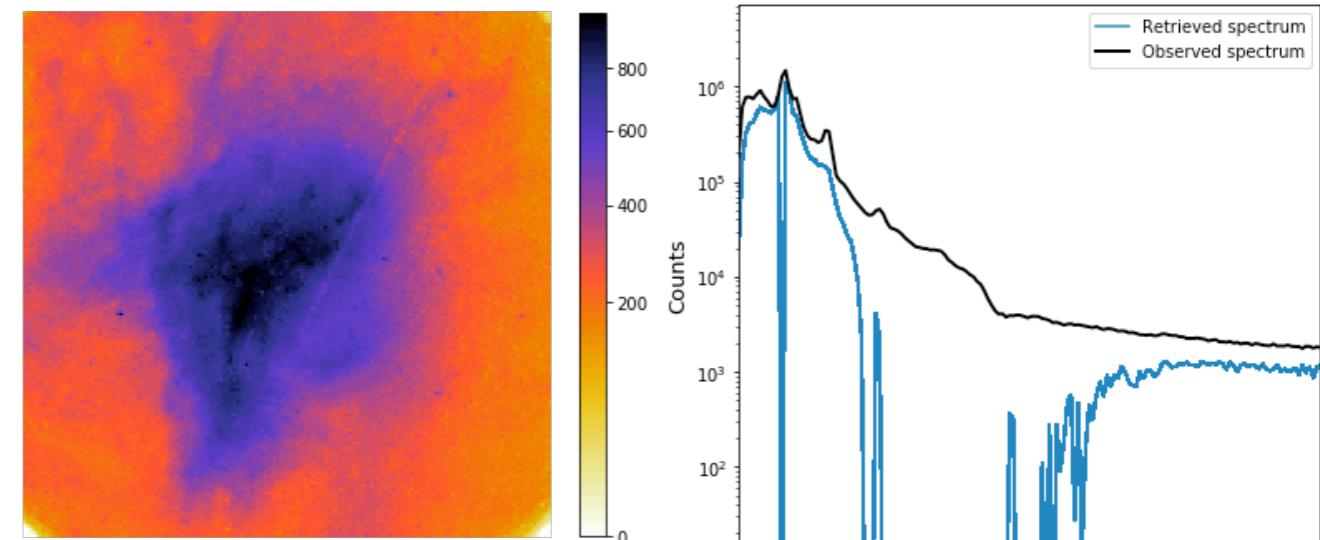
Real case applications: Chandra G11.2-0.3



Real case applications: eROSITA EDR Vela region

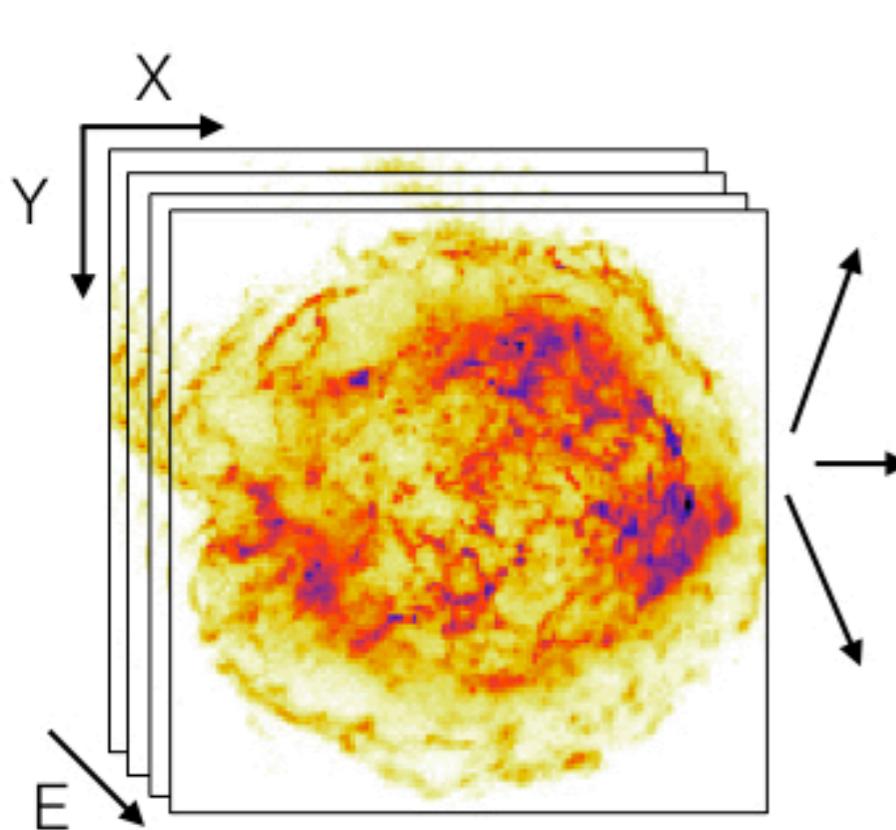


GMCA



Application to real data: Cassiopeia A

- Chandra 1 Ms 5-8 keV:

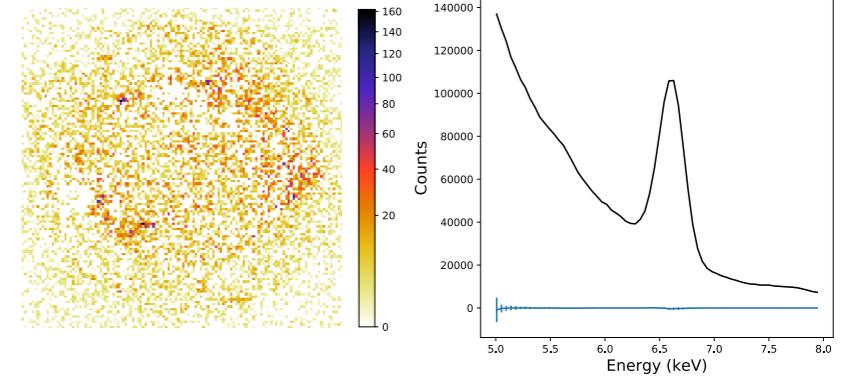
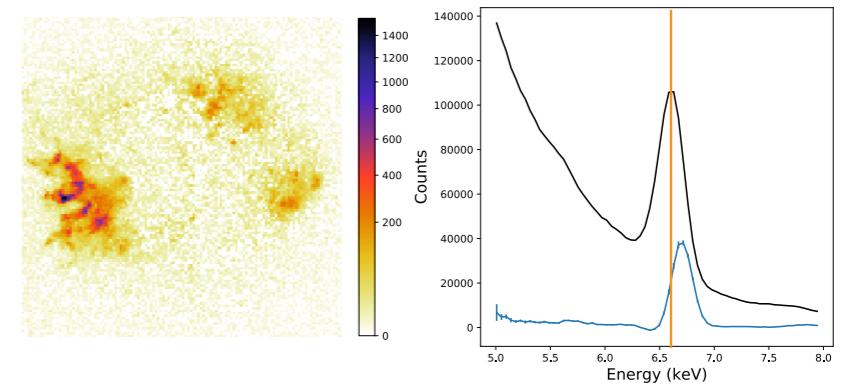
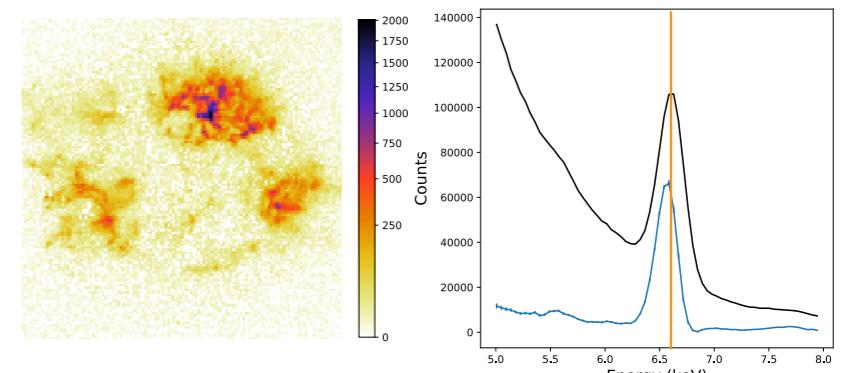
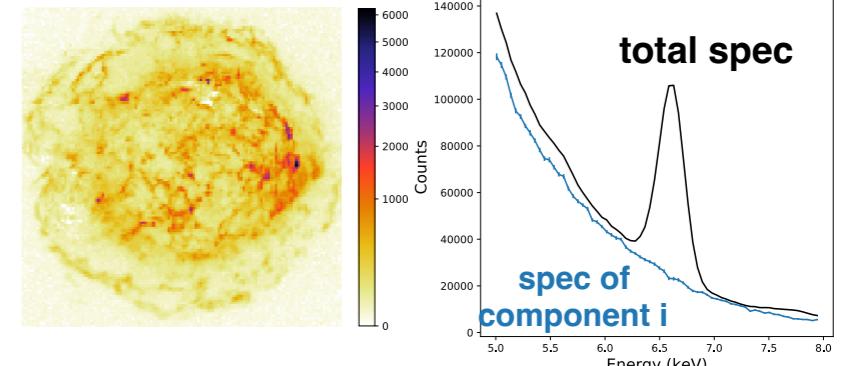


Synchrotron

Red-shifted Fe structure

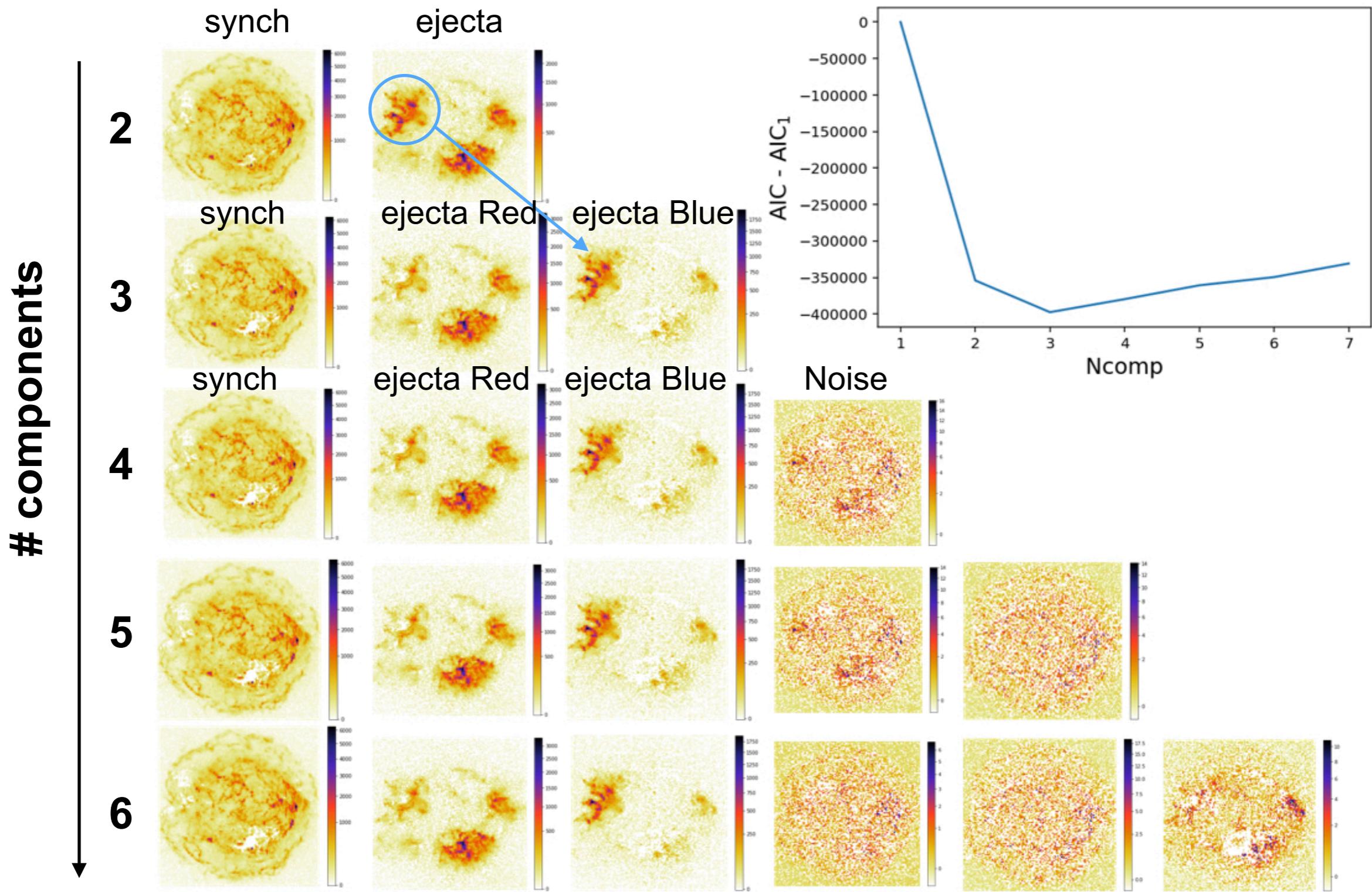
Blue-shifted Fe structure

Noise



Akaike information criteria for choosing N component

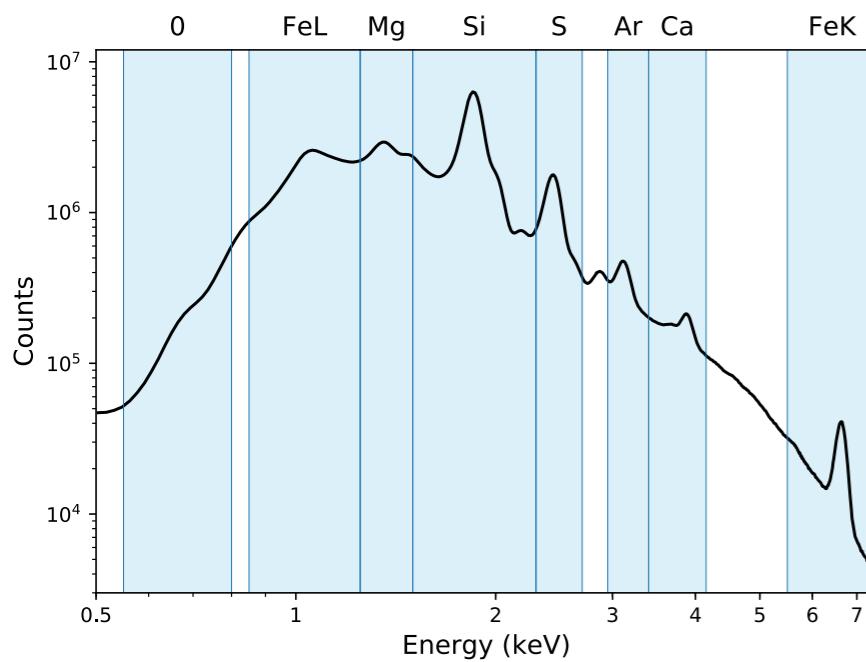
- Is my separation better with more components ?



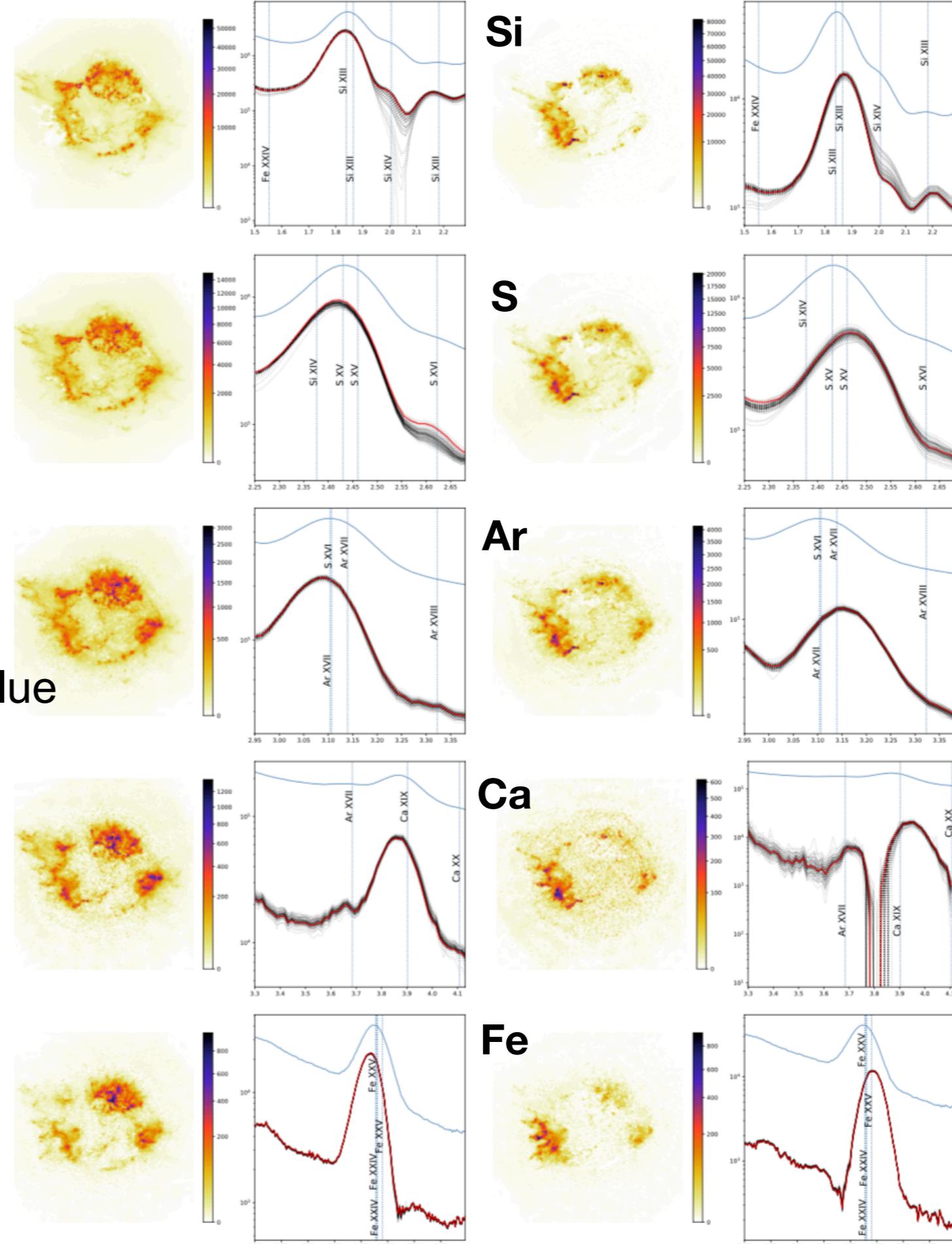
3D assymmetries in CasA

Picquenot, Acero, et al., 2021

GMCA on Chandra 1 Ms subcubes



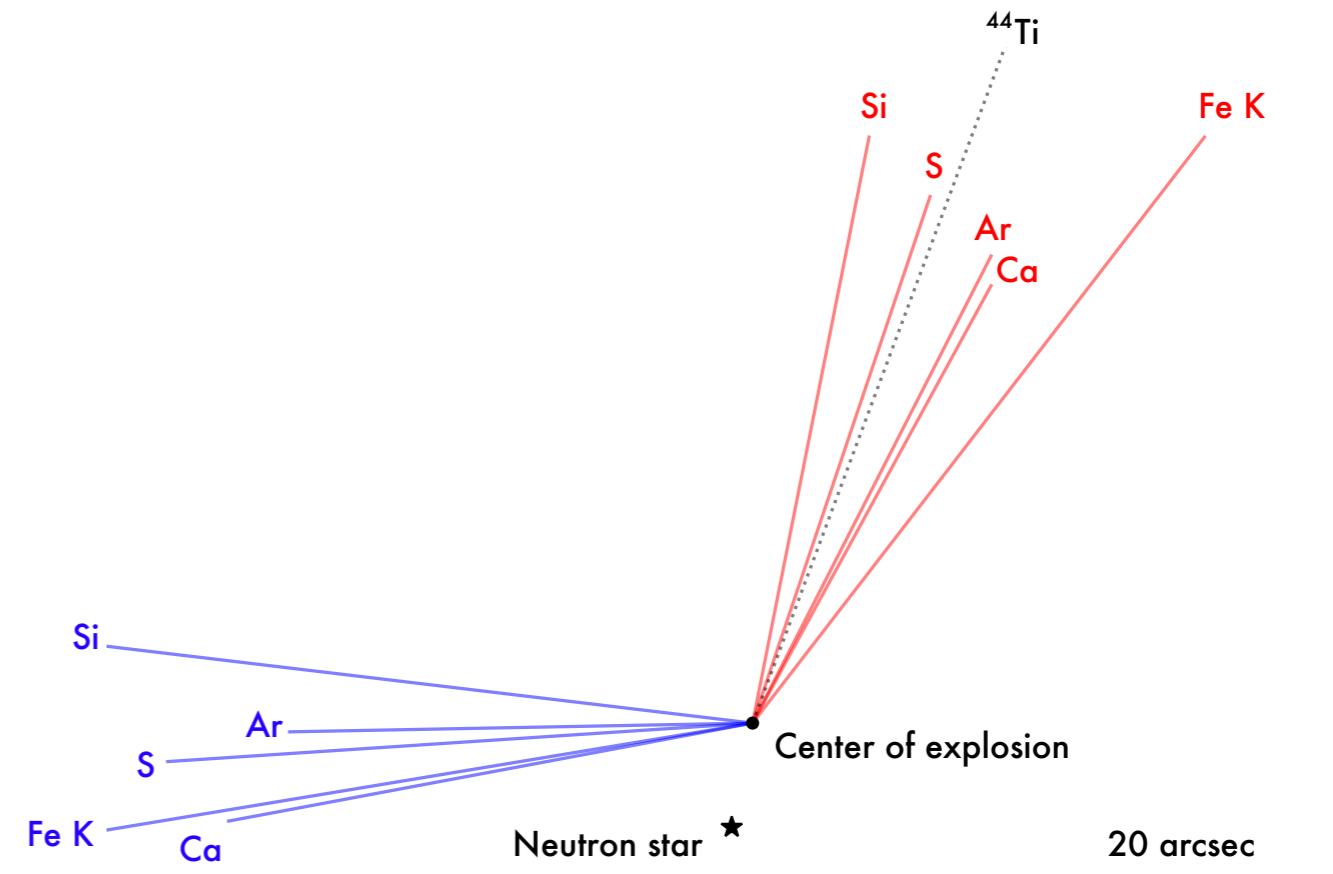
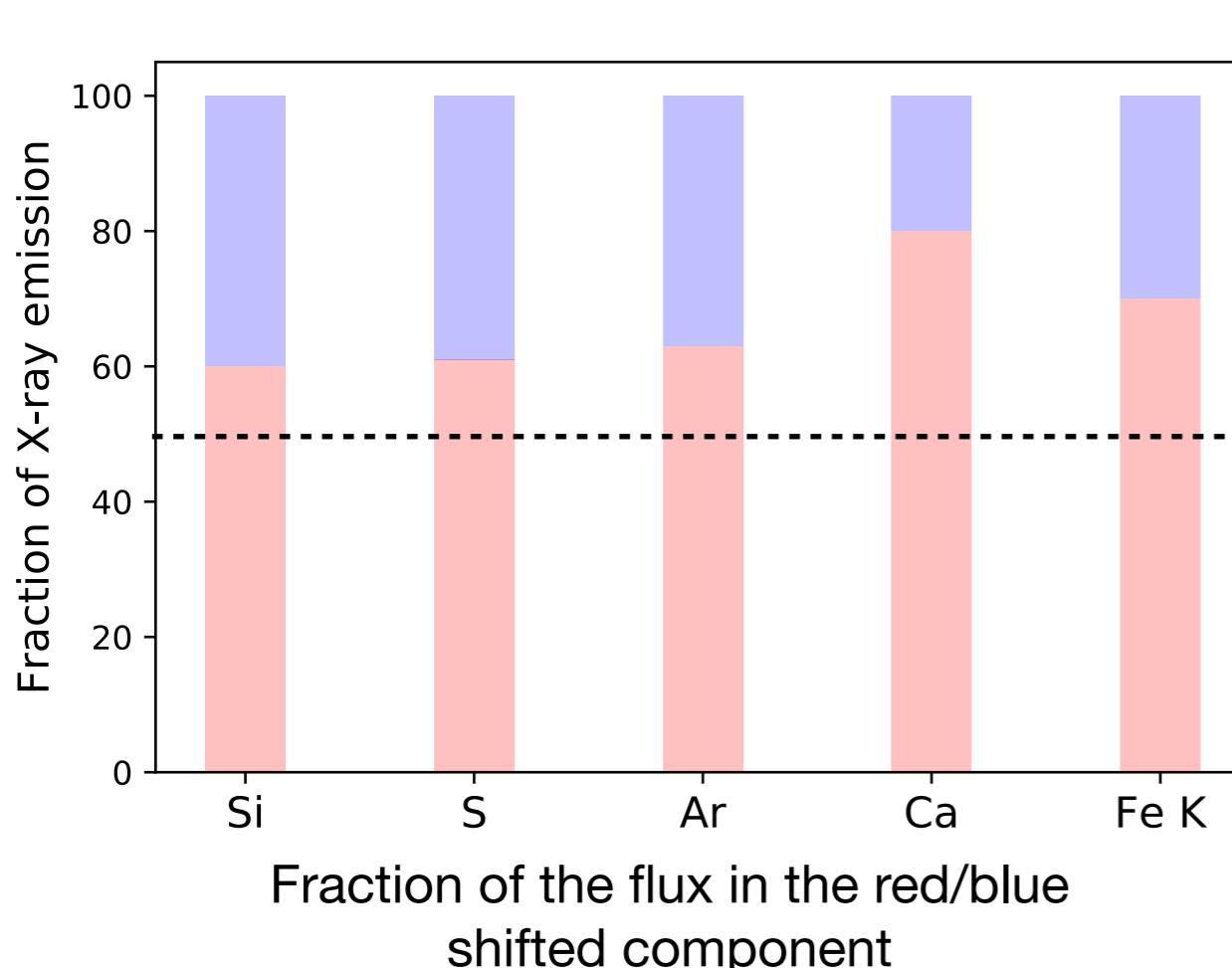
Red-shift



- For the Si, S, Ar, Ca, FeK bands two components that we interpret as red/blue shifted line emission from ejecta
- 3D X-ray maps element by element
- Study assymmetries in the explosion

3D asymmetries in CasA

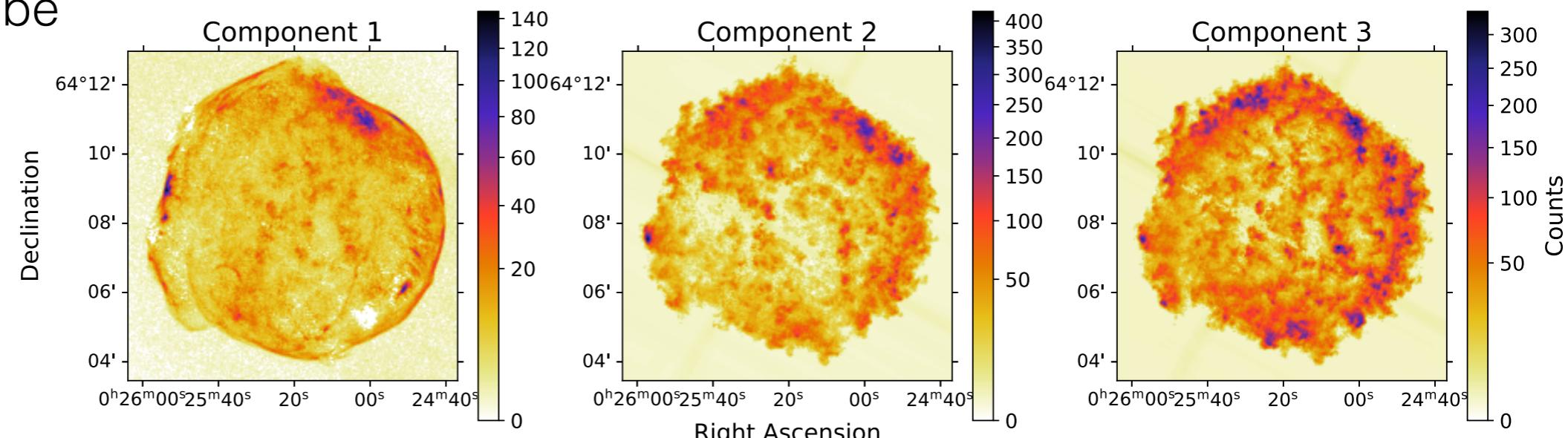
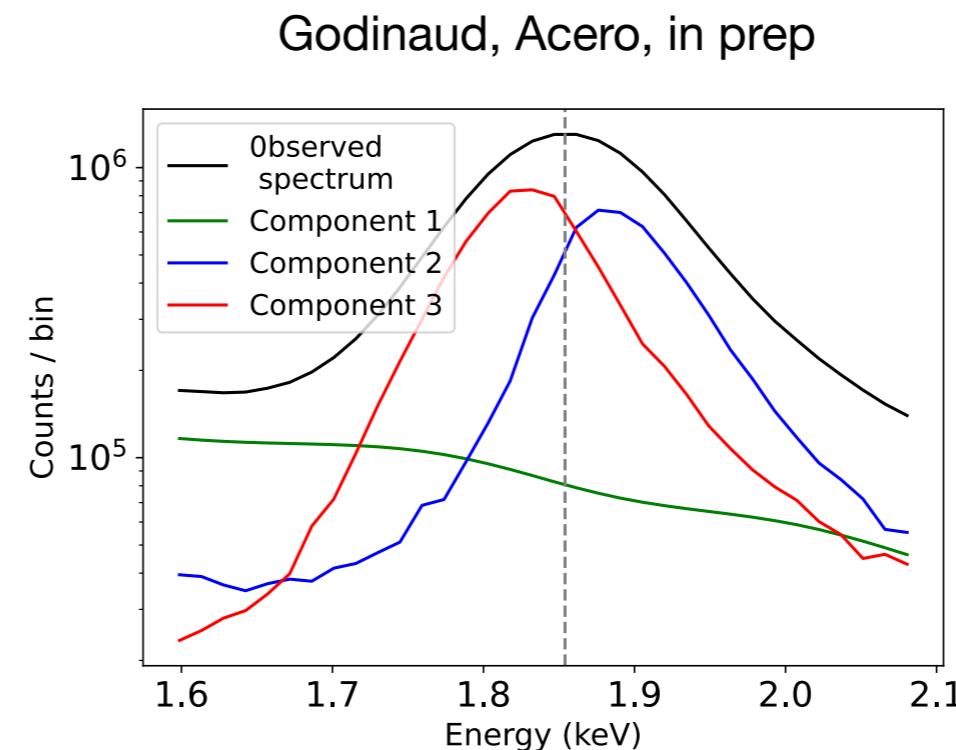
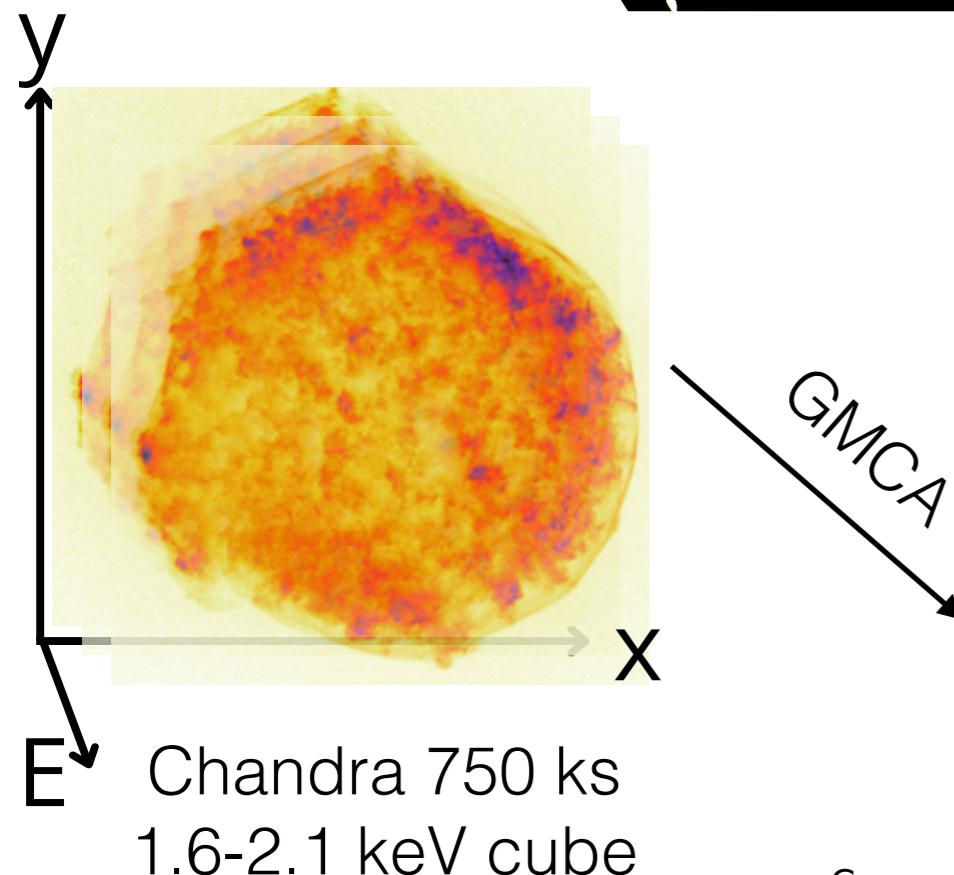
- Most of the X-ray emission is red-shifted. Similar to ^{44}Ti
- Most of the material is expelled on the opposite direction of NS



Picquenot, Acero, et al., 2021

Red/blue shifted components are
not in opposite directions
disfavoring jet/counter jet explosion

Tycho SNR: asymmetries with 3D vector fields



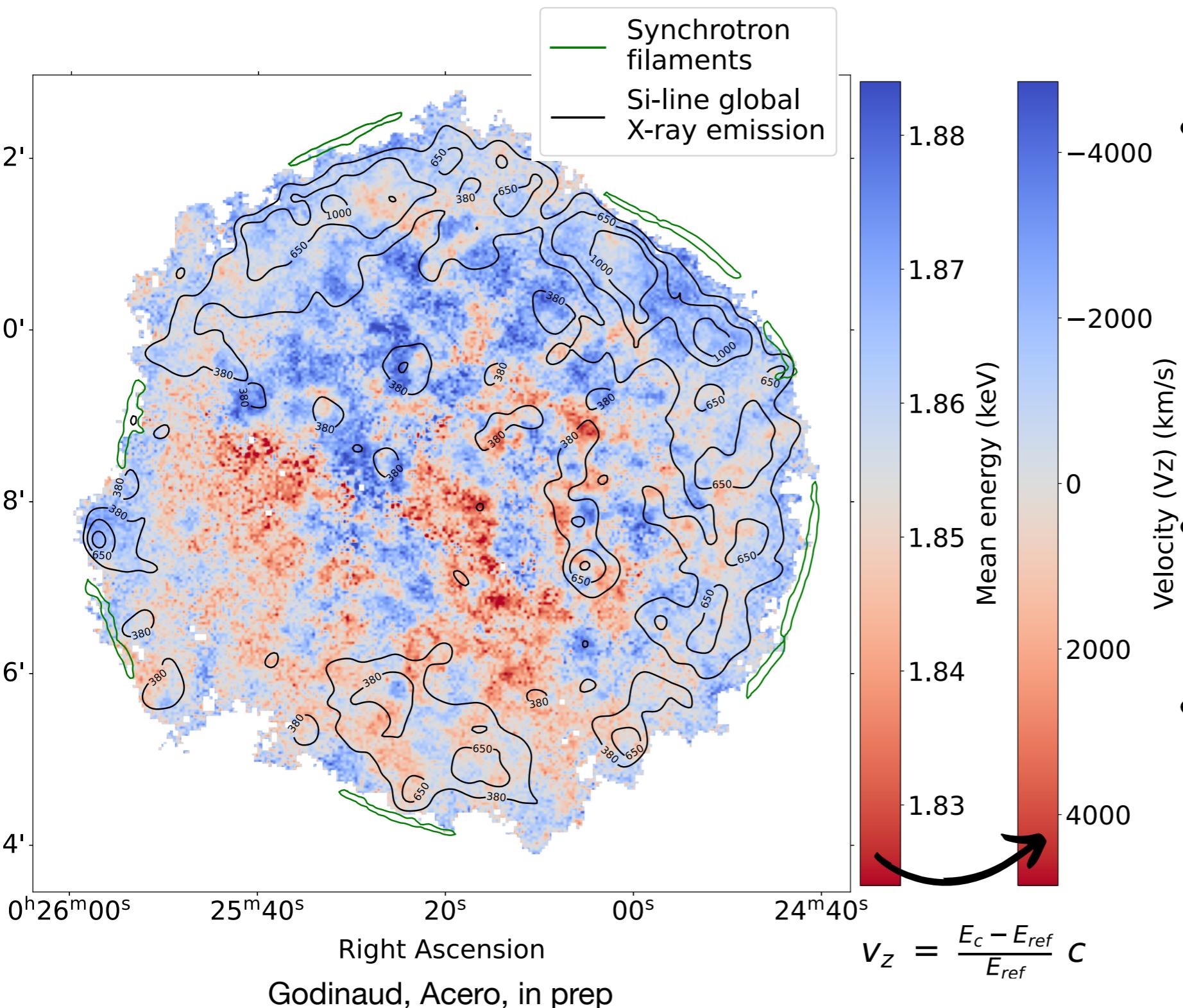
Components that
we interpret as:

Synchrotron

**Blue-shifted
ejecta**

**Red-shifted
ejecta**

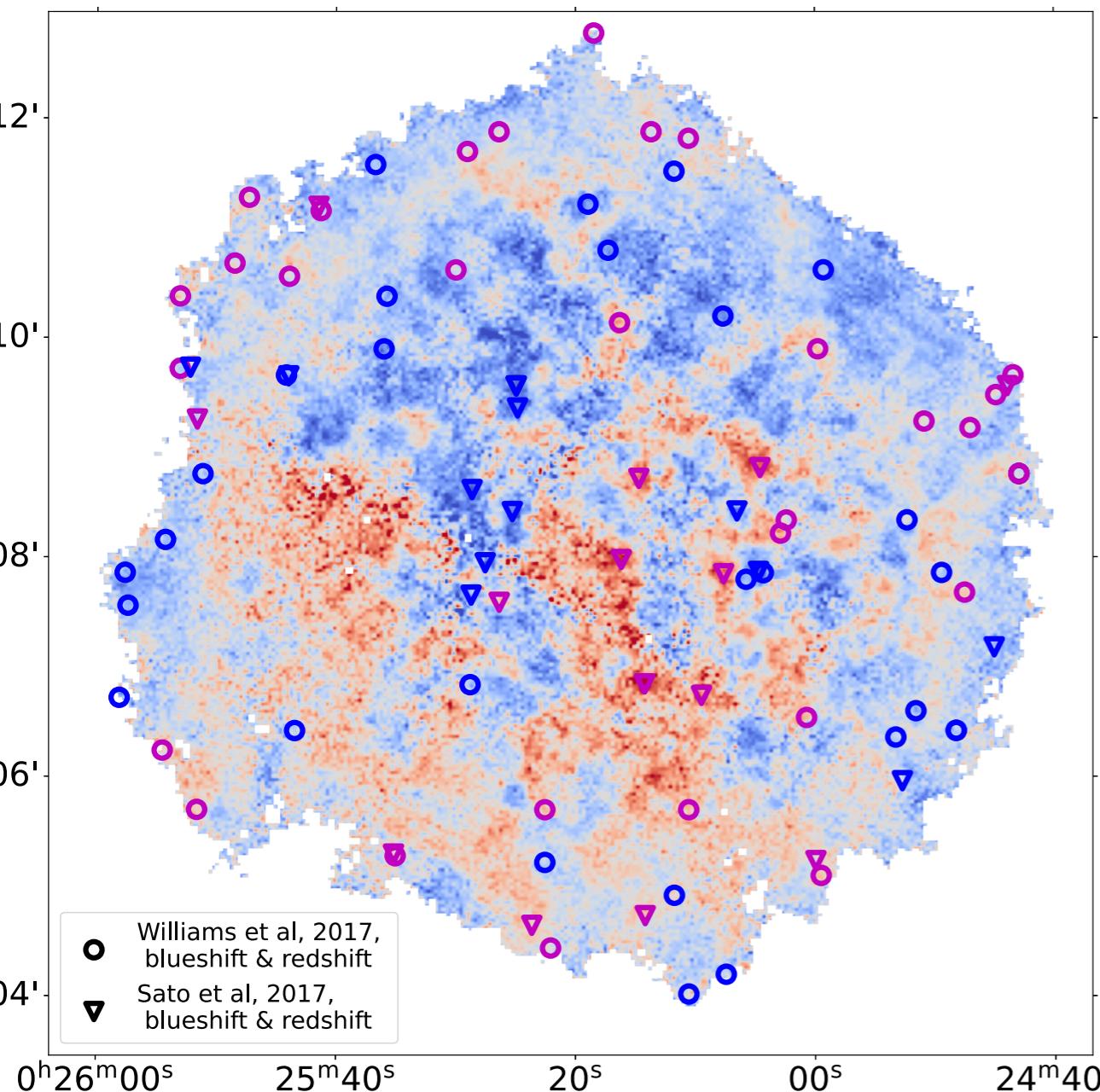
Tycho SNR: ejecta velocity along the line of sight (V_z)



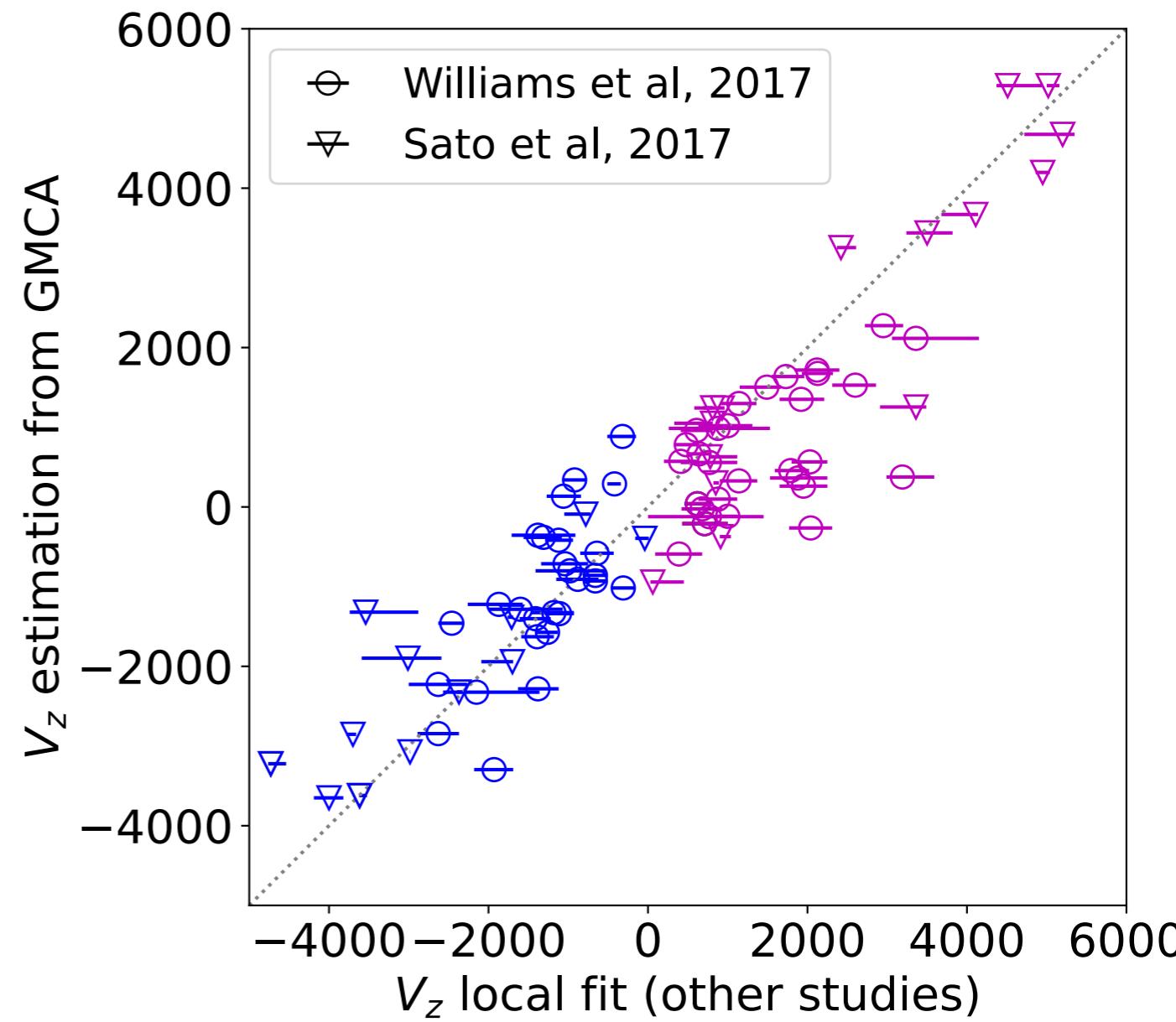
- Idea: Use GMCA components (red/blue) as a basis to reconstruct the energy centroid in each pixel
- Complete coverage + pixel level
- Clear asymmetry of ejecta North/South

Cross checking V_z with other spectral studies

- Comparison of our method with dedicated spectral analyses



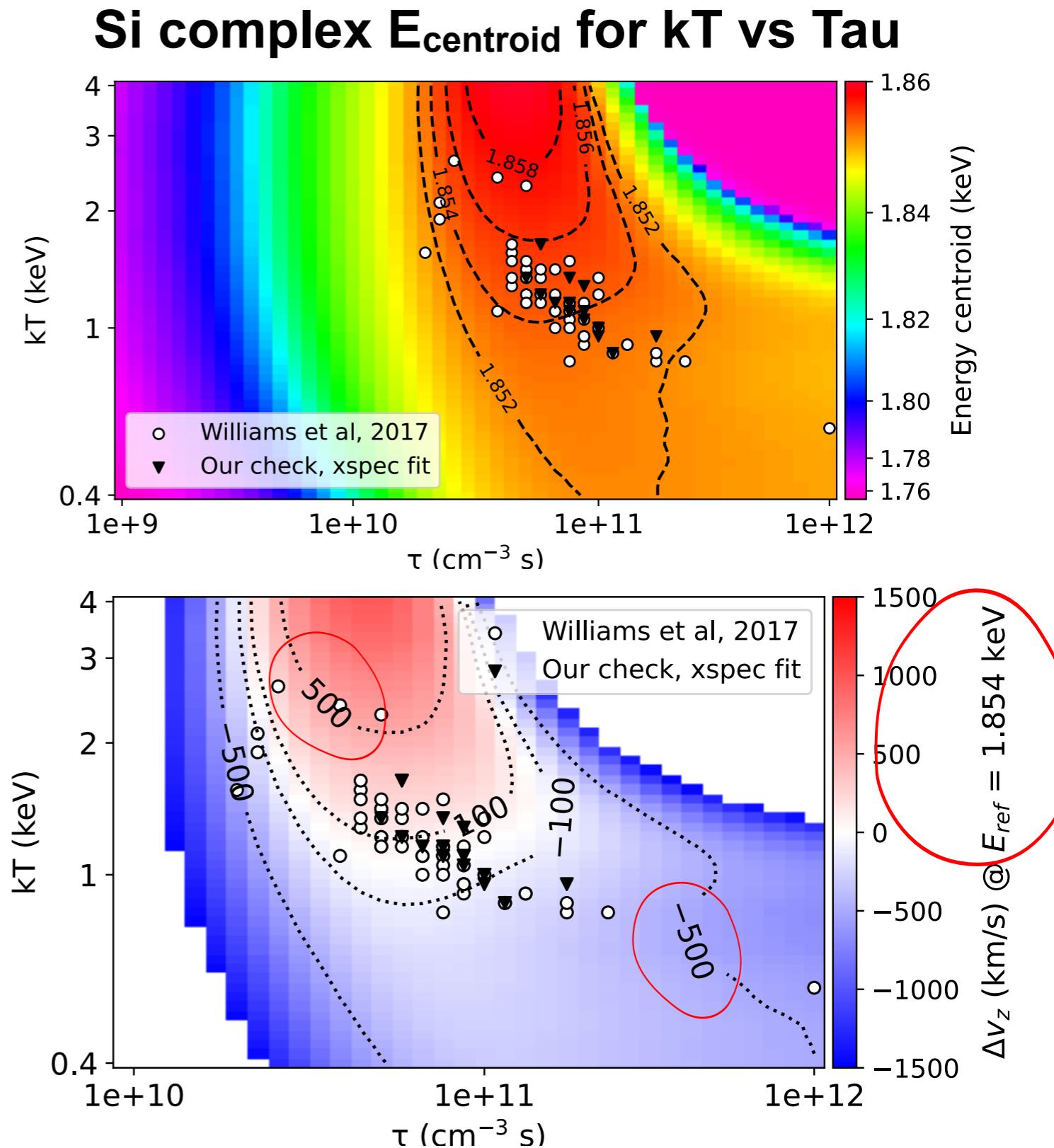
Previous studies have ~50 regions



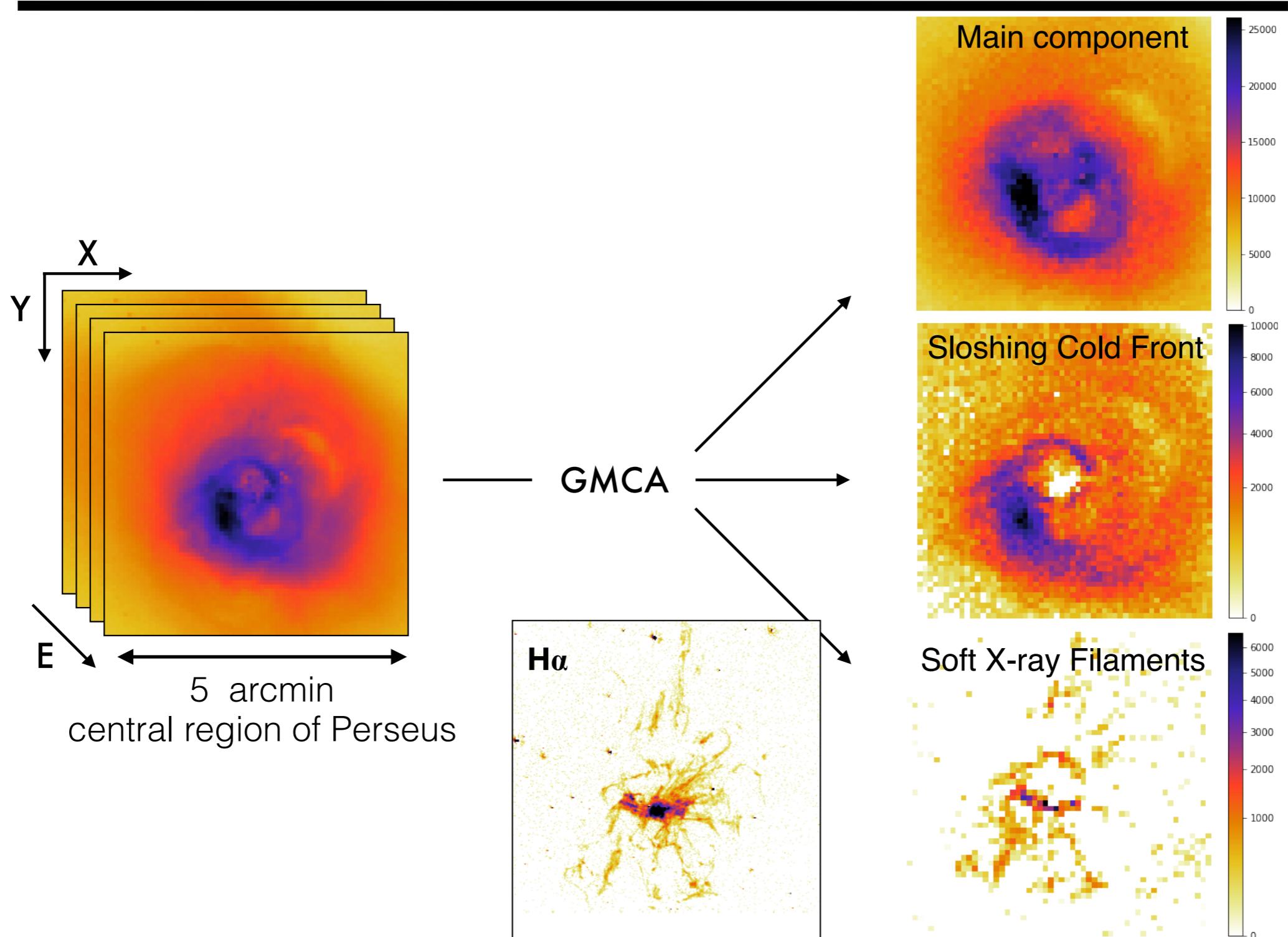
Good agreement between our V_z proxy and dedicated spectral fitting

Impact of choosing an energy of reference vs kT and Tau

- We take the mean corresponding energy centroid at 1854 eV
- Small impact of the variation of E_{ref} for V_z (maximal values of 500 km/s)



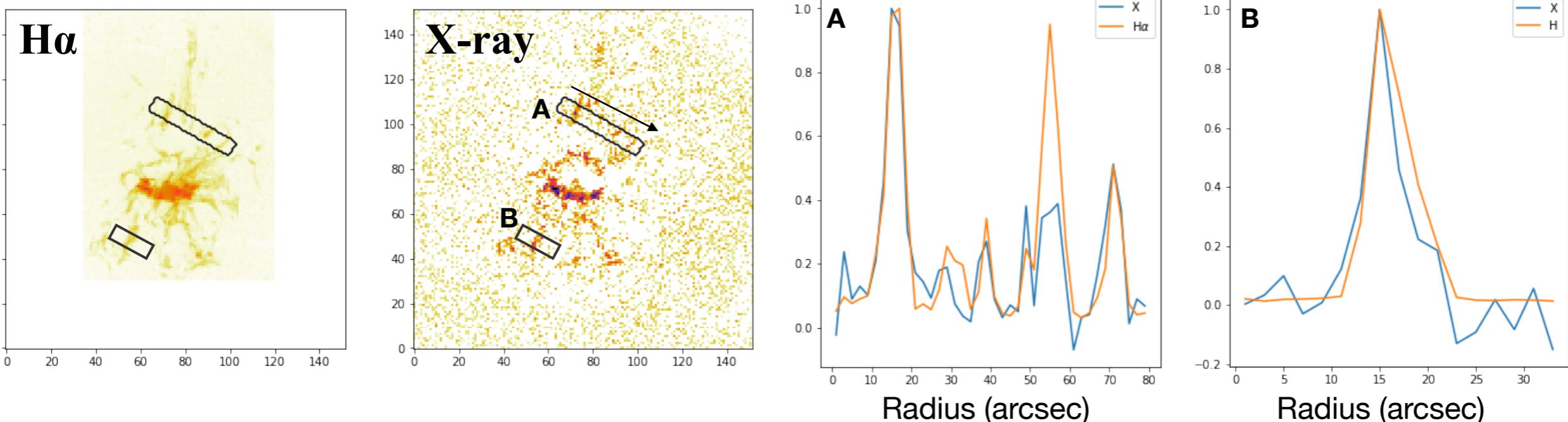
Galaxy cluster: Perseus 0.5-3 keV



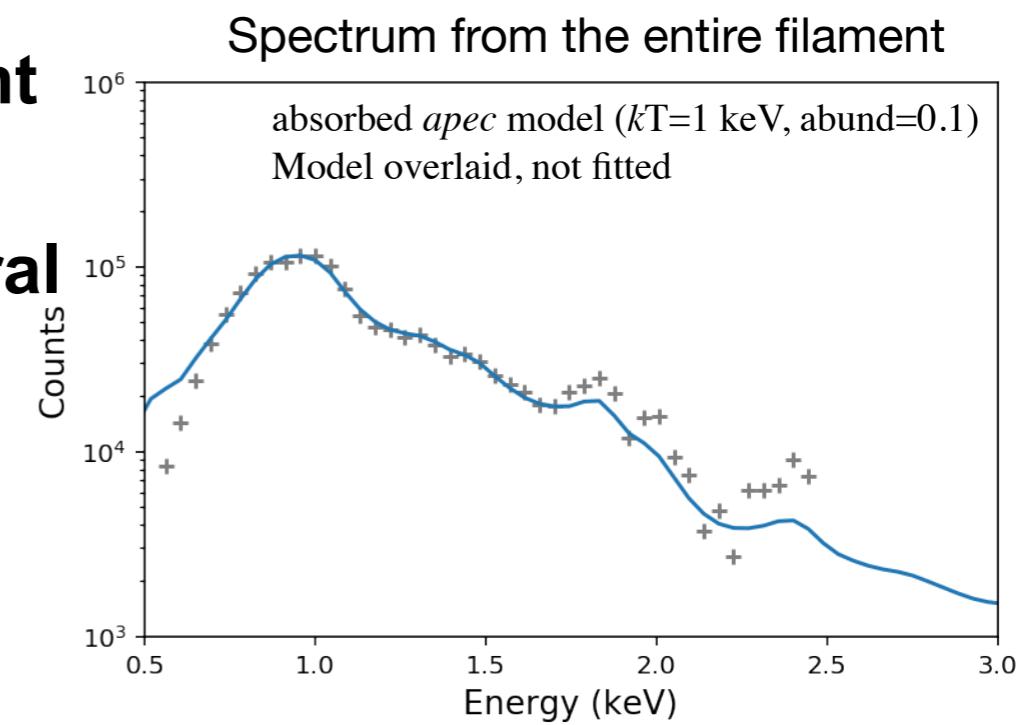
First time imaging of X-ray filaments
Ability to obtain image+spectrum

X-ray/Halpha morphological comparison

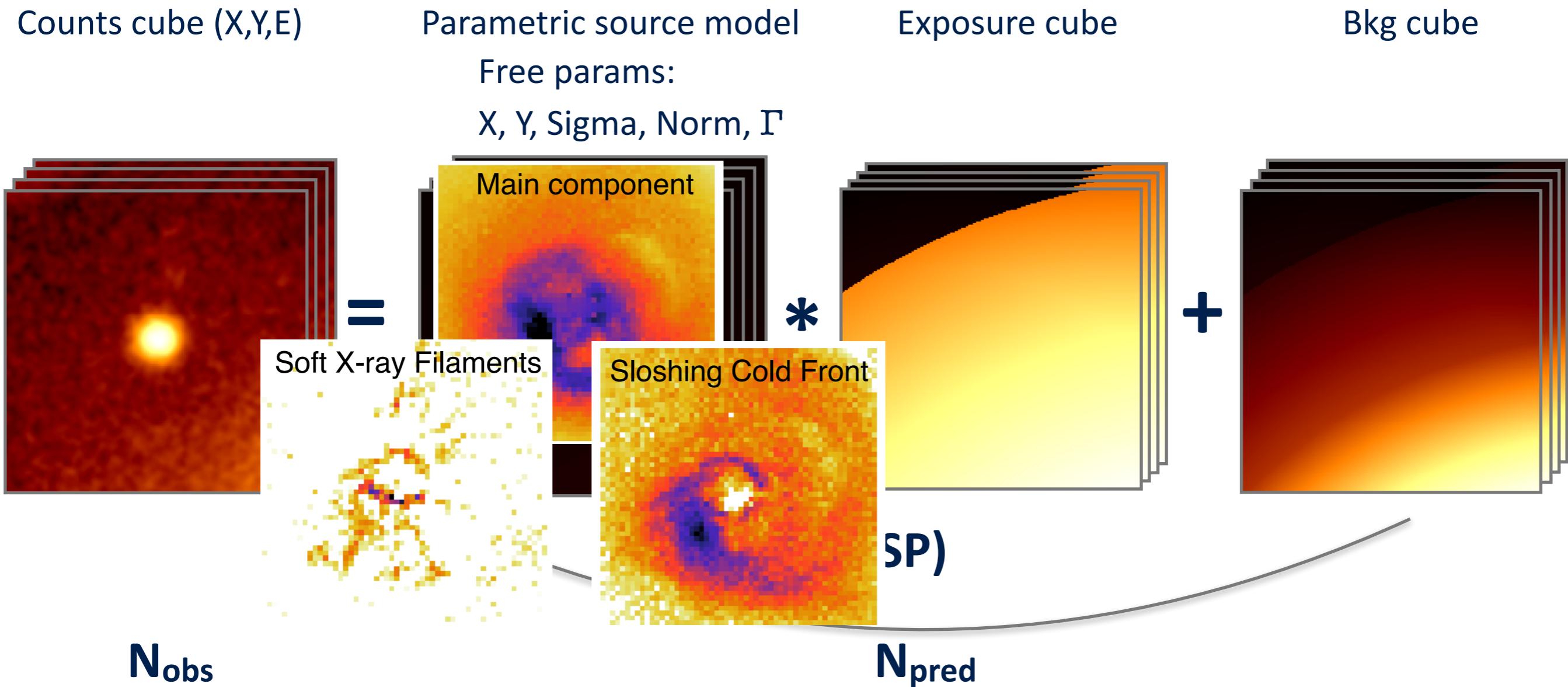
- Same width filament width in H α and X-rays



- Mist of condensing gas. Not a stratified filament
- Similar abundance to intracluster gas
- Infalling matter from cluster gas not from central Galaxy outflow
- Thermal radiation from the cooling gas



A 3D analysis for classical fitting of each Perseus component



- Minimization of $-\text{LogLikelihood}(N_{\text{pred}}, N_{\text{obs}})$
- Replacing spatial parametric model with GMCA spatial templates

eROSITA analysis of EDR 30 Doradus

Collaboration with C. Maitra, M. Sasaki, J. Knies, P. Maggi

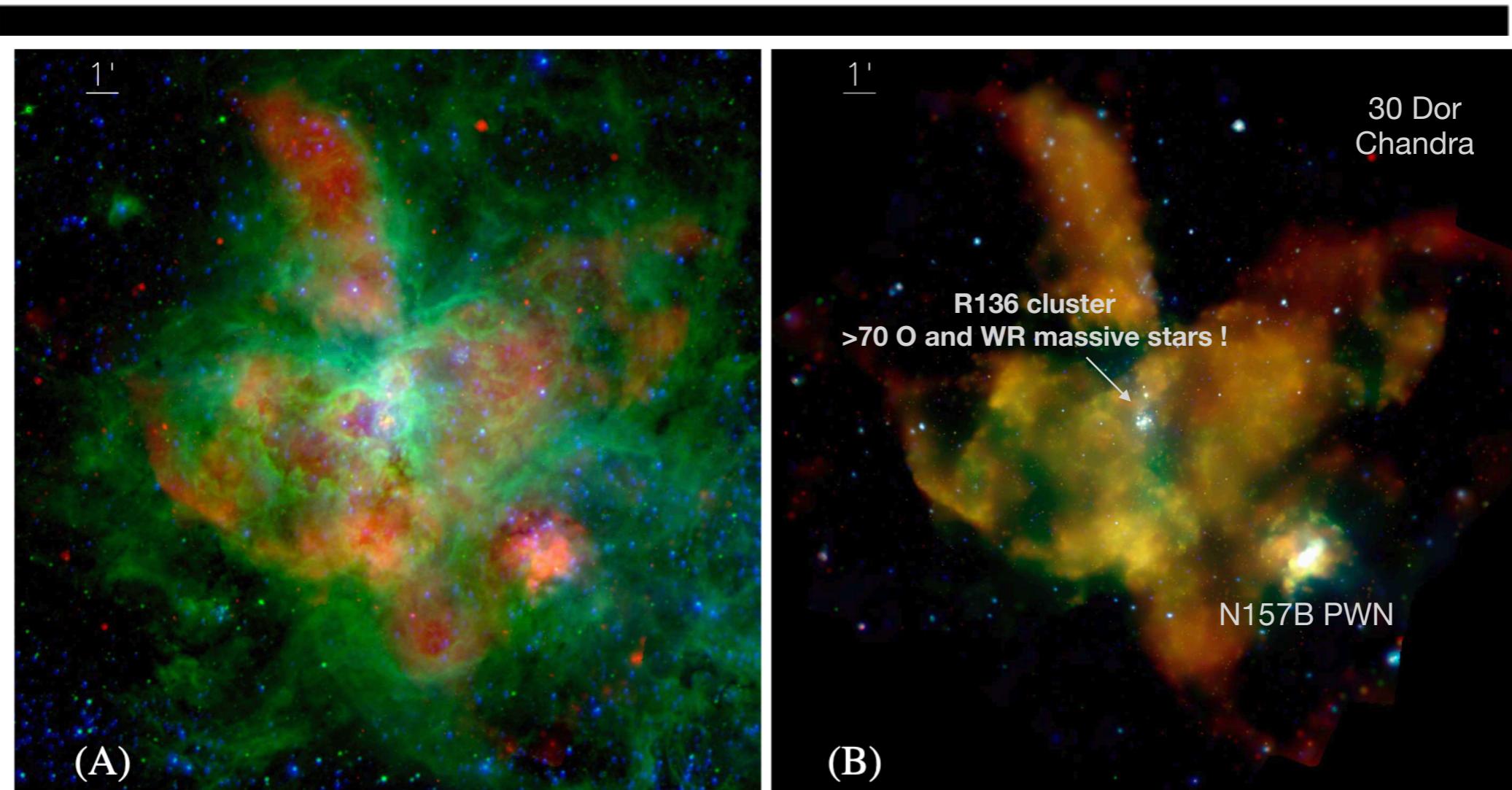
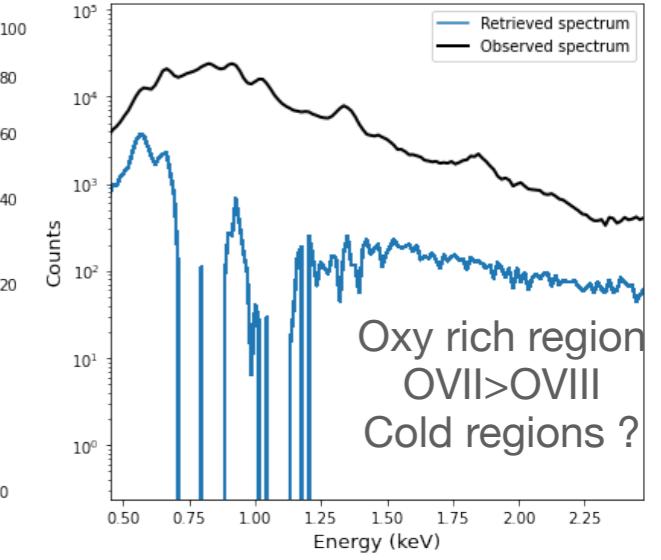
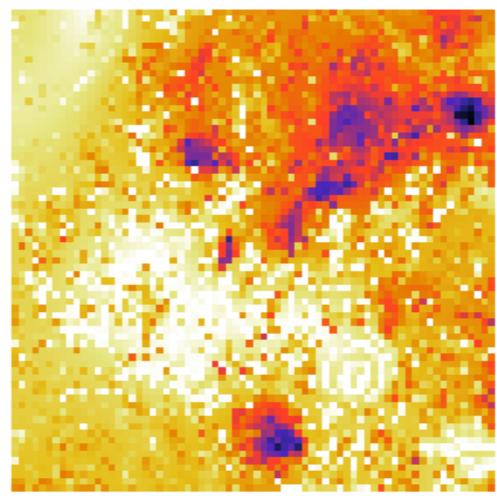
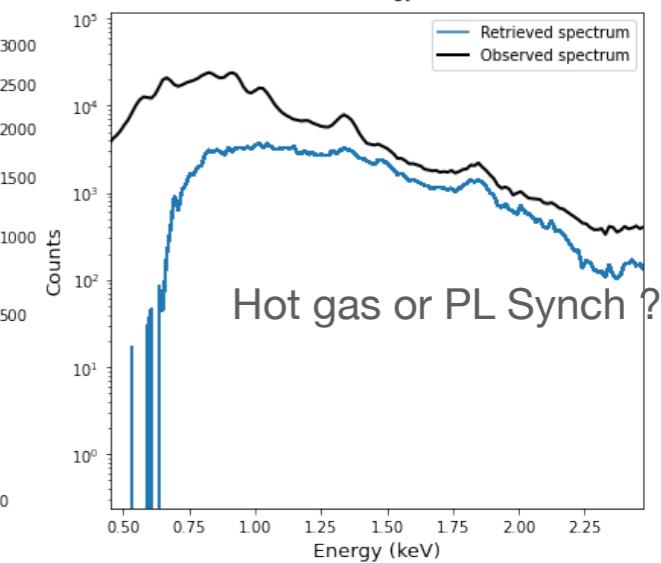
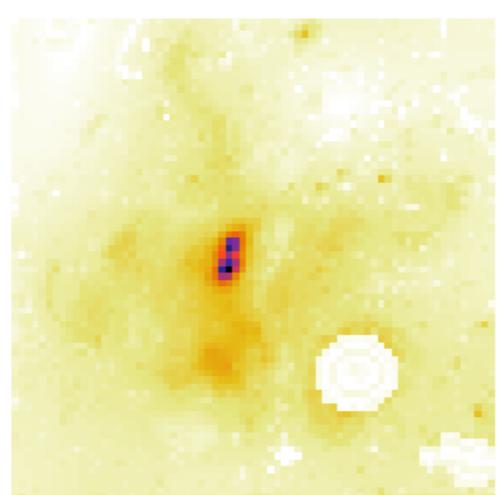
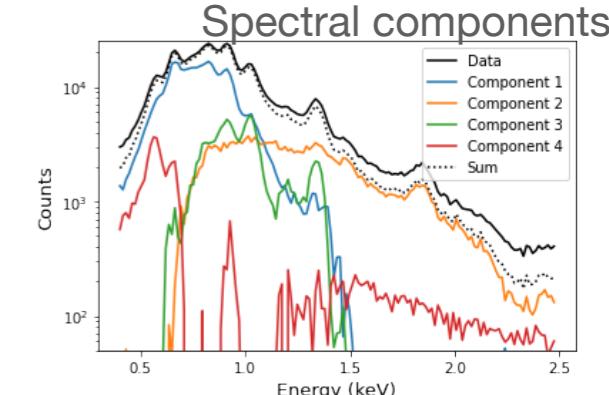
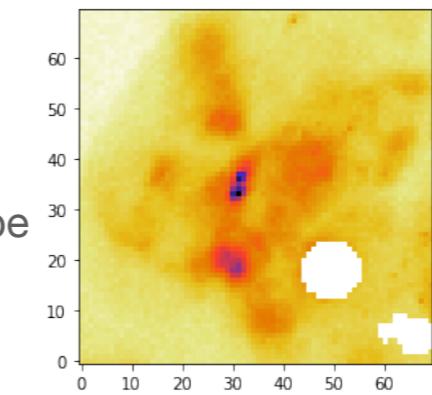
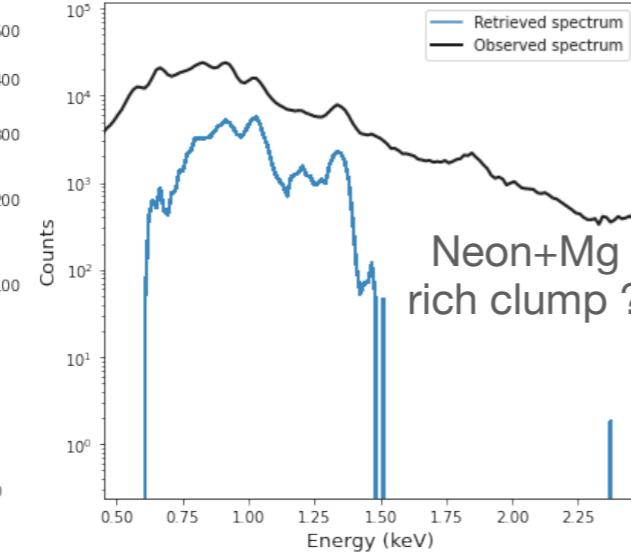
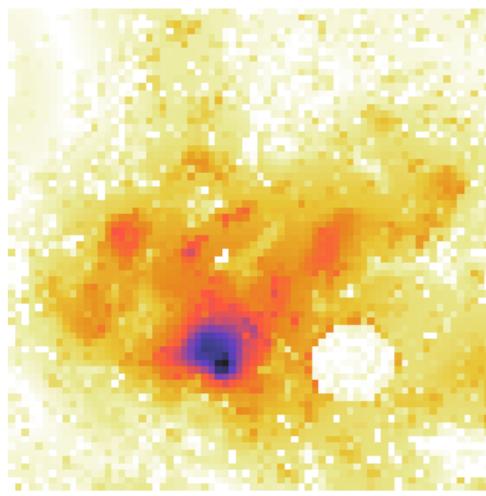
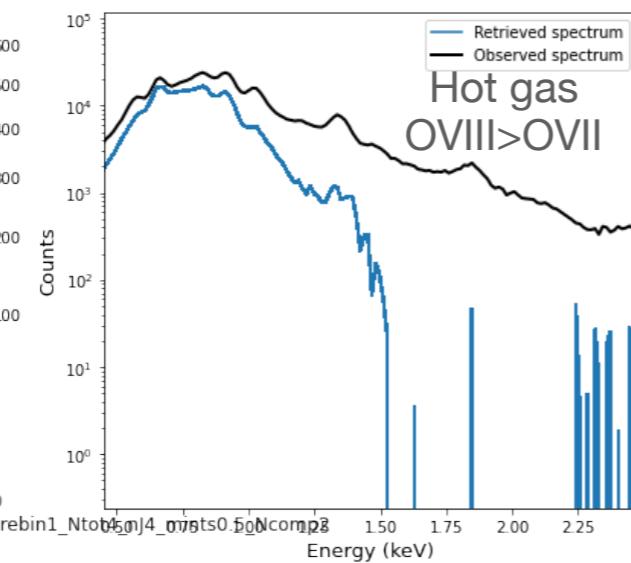
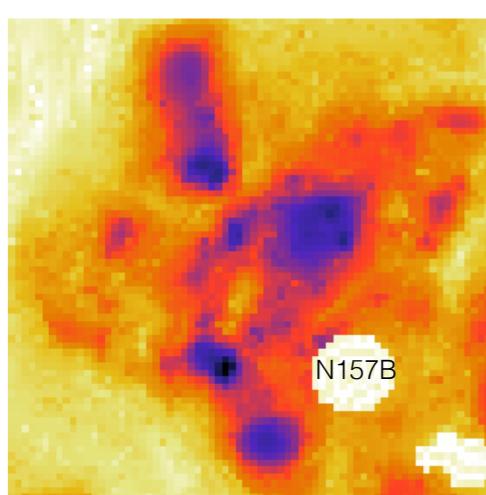


Figure 1. Multi-wavelength montages of 30 Doradus: (A) 0.5-2 keV (red), H α (green), and UV (blue); (B) *Chandra* images in the 0.5-1 keV (red), 1-2 keV (green), and 2-8 keV (blue) bands. The H α image was taken with the 4m telescope at Cerro Tololo Inter-American Observatory ([Chu & Kennicutt 1994](#)), while the UV image was from the GALEX survey.



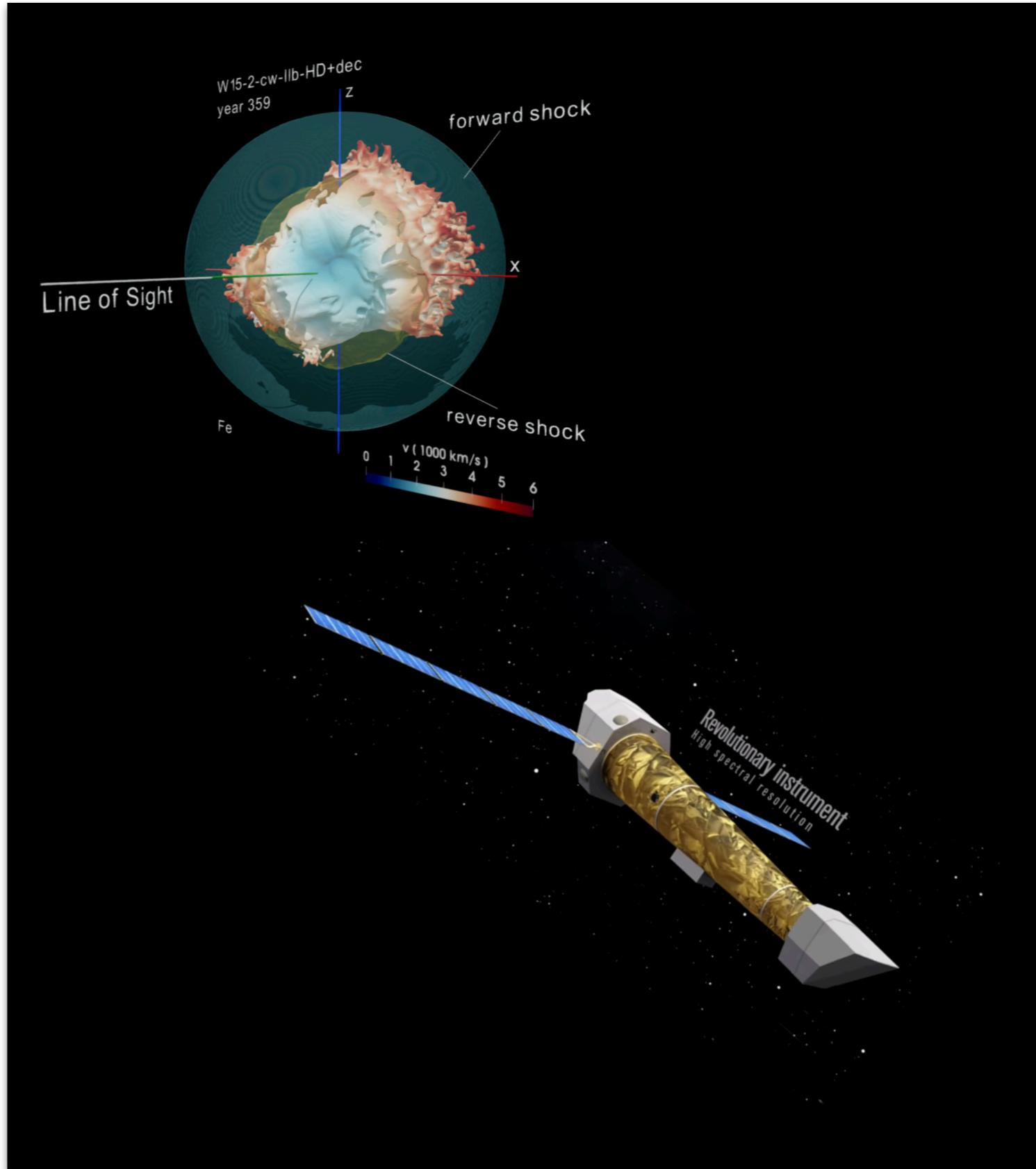
eROSITA analysis of 30 Doradus: 4 components

Collaboration with C. Maitra, M. Sasaki, J. Knies, P. Maggi



From numerical simulations to synthetic X-ray observations

The case of Athena X-IFU

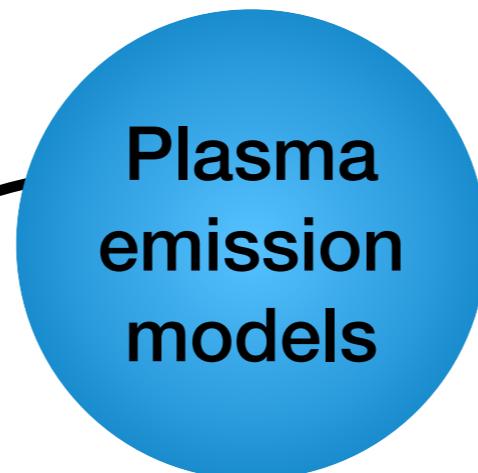
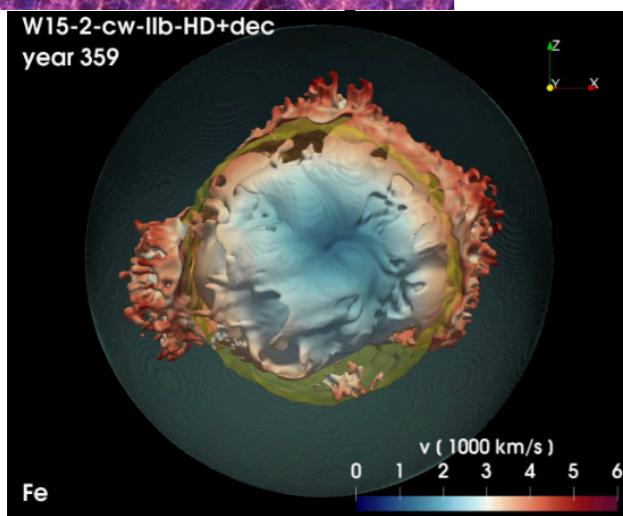
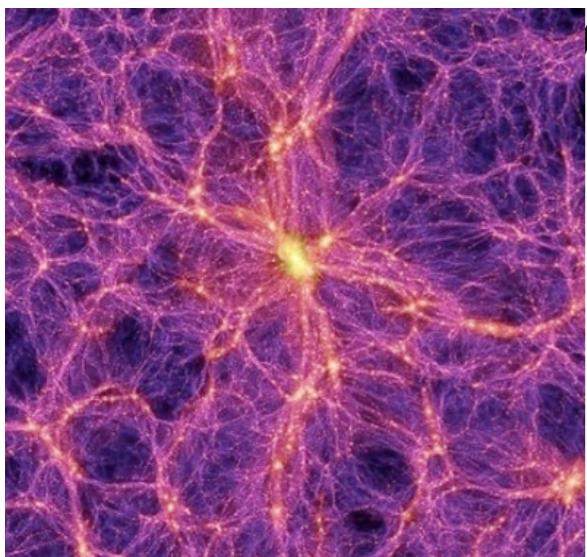


Pipeline for X-ray simulations of extended sources

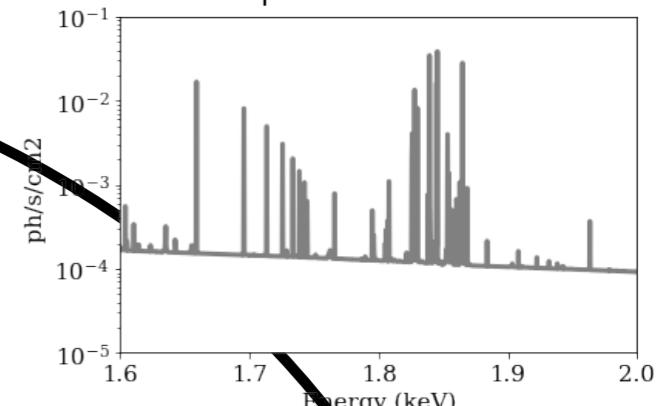
Collaboration with C. Kirsch, J. Wilms

Numerical simulations

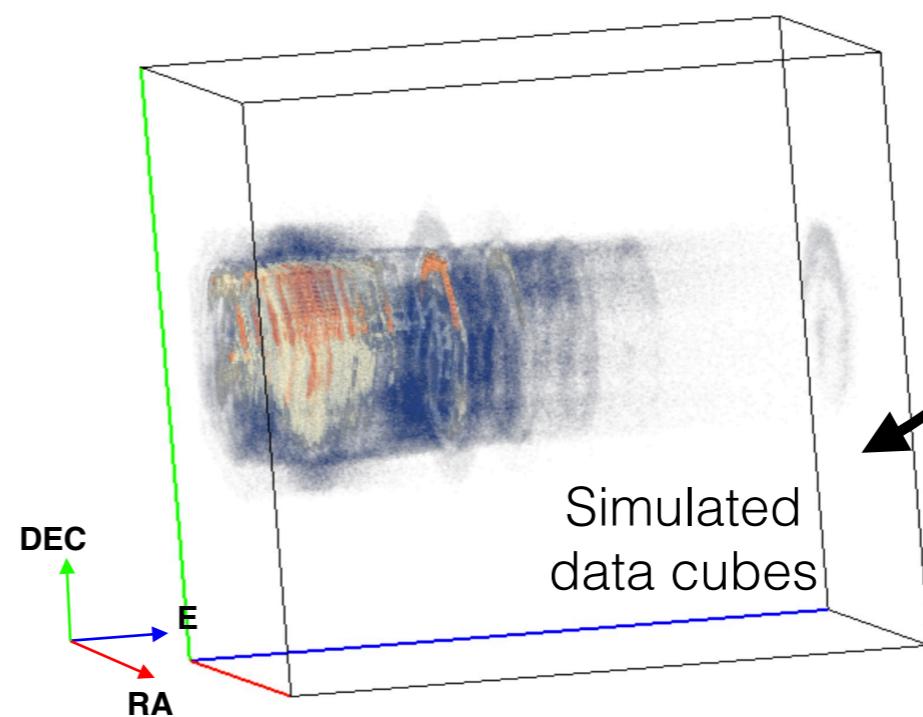
Temperature, density, velocity



X-ray flux hypercubes (X,Y,Z,E)
No parameter table



Simulation of X-ray telescopes with
instrument performance

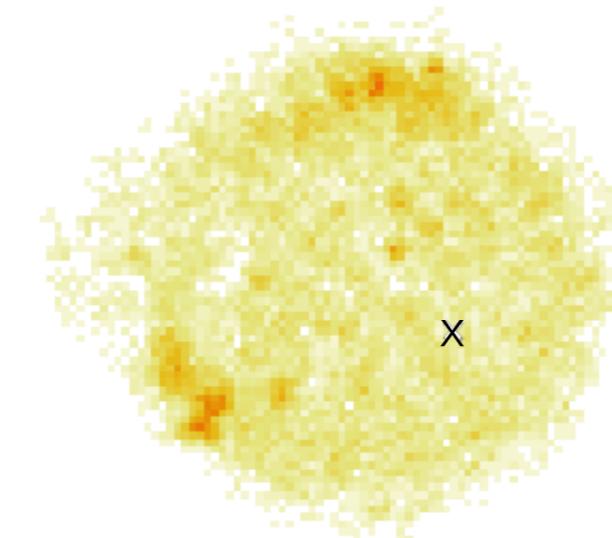


Tomography slicing through the cube @ Si lines

3D numerical simulation of a
CasA-like SNR (Orlando et al.)

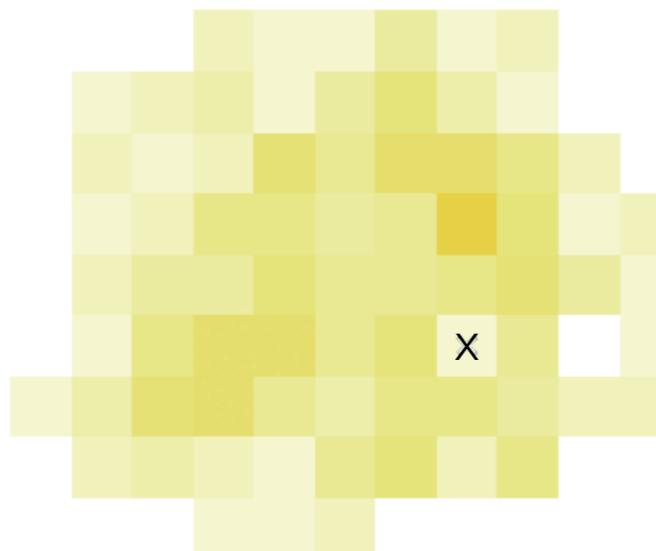
Viewed by in **10 ks** by
XIFU 4'' pixels
FWHM=5''

Athena X-IFU



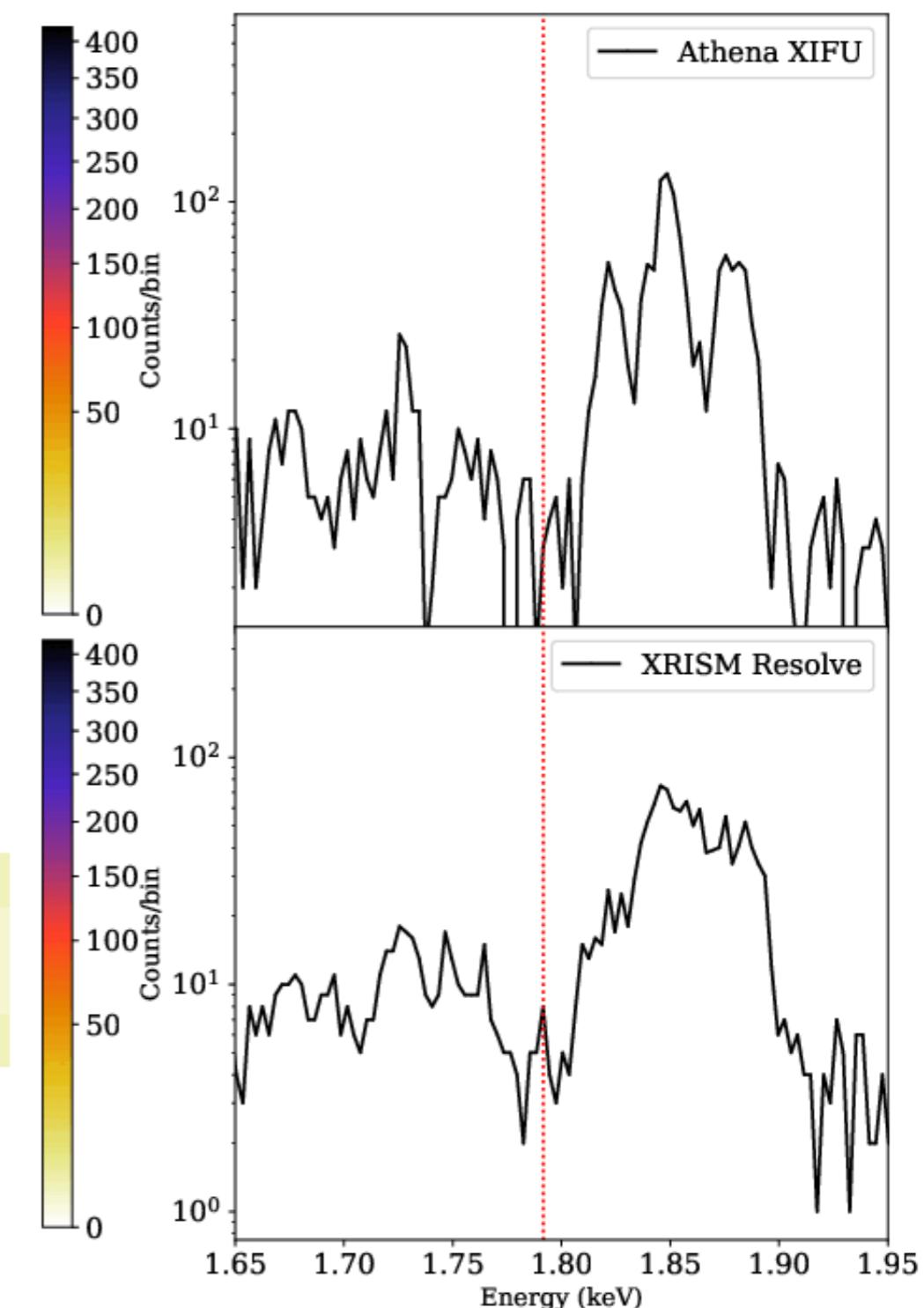
XRISM Resolve 30'' pixels
FWHM=1.5 arcmin

XRISM Resolve

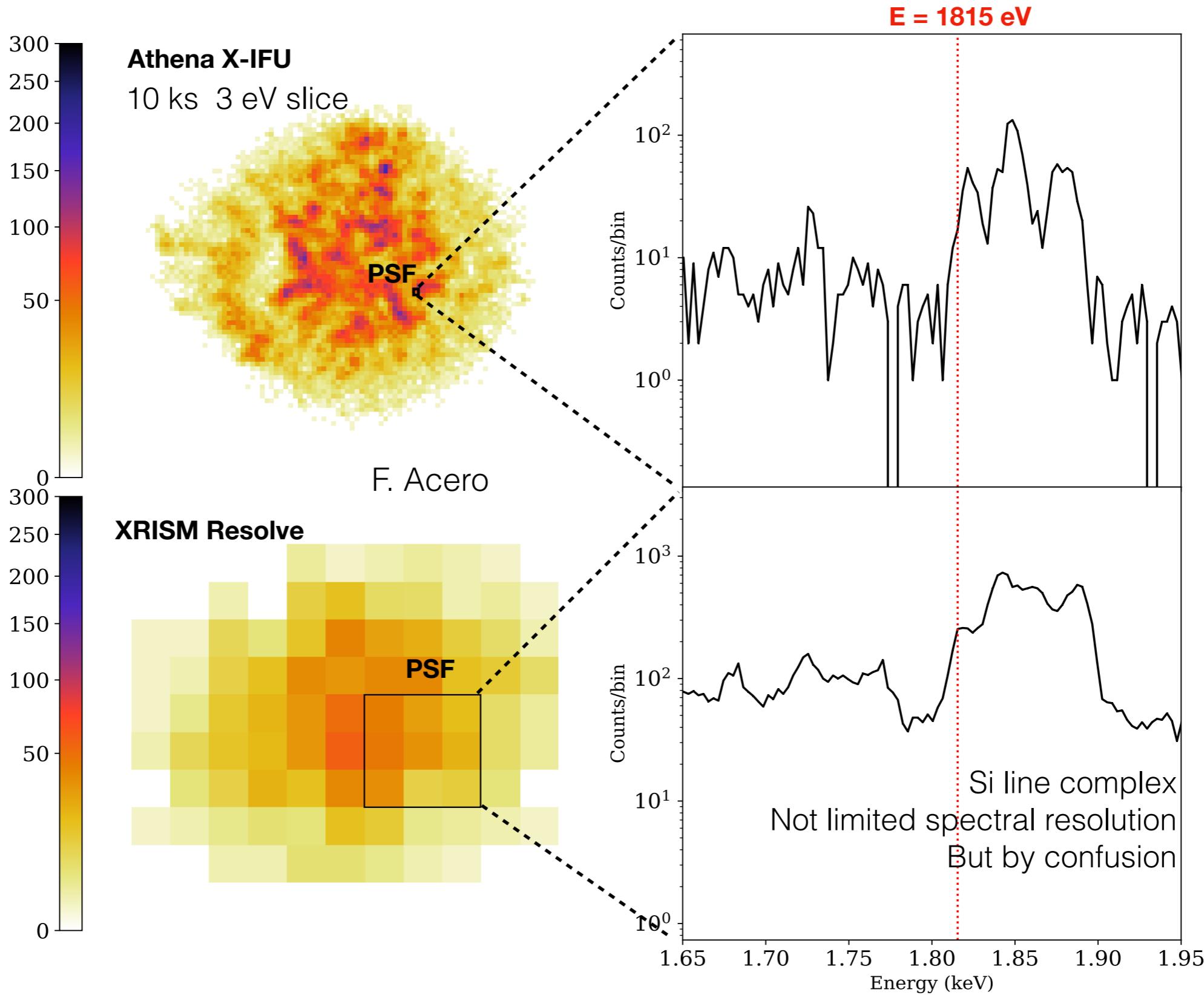


E = 1.791 keV

Spectra for one instrument pixel



The need for HR imaging for HR spectroscopy



Conclusion

- Wealth of information in deep X-ray observations but analysis methods have stalled in the last 20 years
- GMCA: a blind source separation method for X/Gamma-rays
 - Exploit the 2D-1D info from spectro-imagers (MUSE, Fermi, CTA)
 - Applicable to SNR, PWN, clusters, galactic center or time cubes (X, Y, T)
- GMCA retrieves the overlapping physical components with morphological spectral diversity
 - eROSITA provides very large mosaic and great spectral resolution. In several degree scale image, great spatial resolution & high statistics !
- Caveats:
 - Each component is Spec*Image. No spatial variation for now
 - Need deep observations of bright sources (> 1 millions counts)
 - Can only differentiate if structured emission (not ~gaussian blobs)

Perspectives

- **Perspective :**
 - Deep learning for a learnt representation of spectral shapes,
==> mapping physical parameters at pixel level
 - Component separation with spatial variation (e.g. synchrotron + varying redshift component)
- **Athena :**
 - new tools are needed to fully exploits the wealth of data
 - => benchmark of new tools on realistic simulations
 - Side note for Athena Redesign : for extended sources HD imaging is needed for HR spectra to reduce confusion.

Archival data & future high spectral resolution instrument are gold mines.
Need to explore next generation analysis tools.



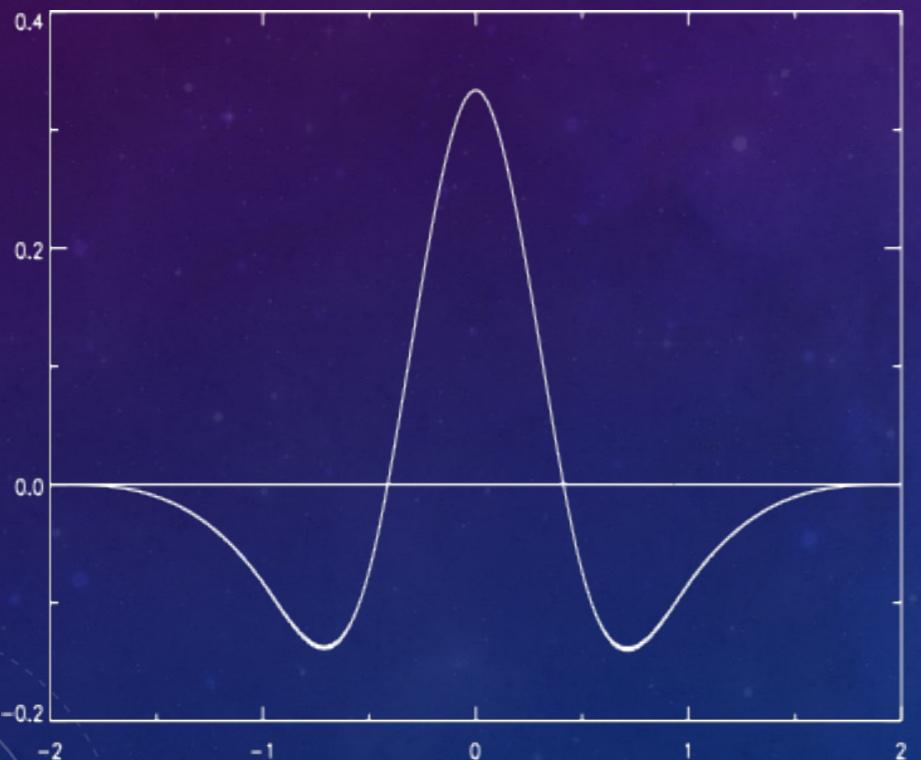
Back up slides

The starlet transform

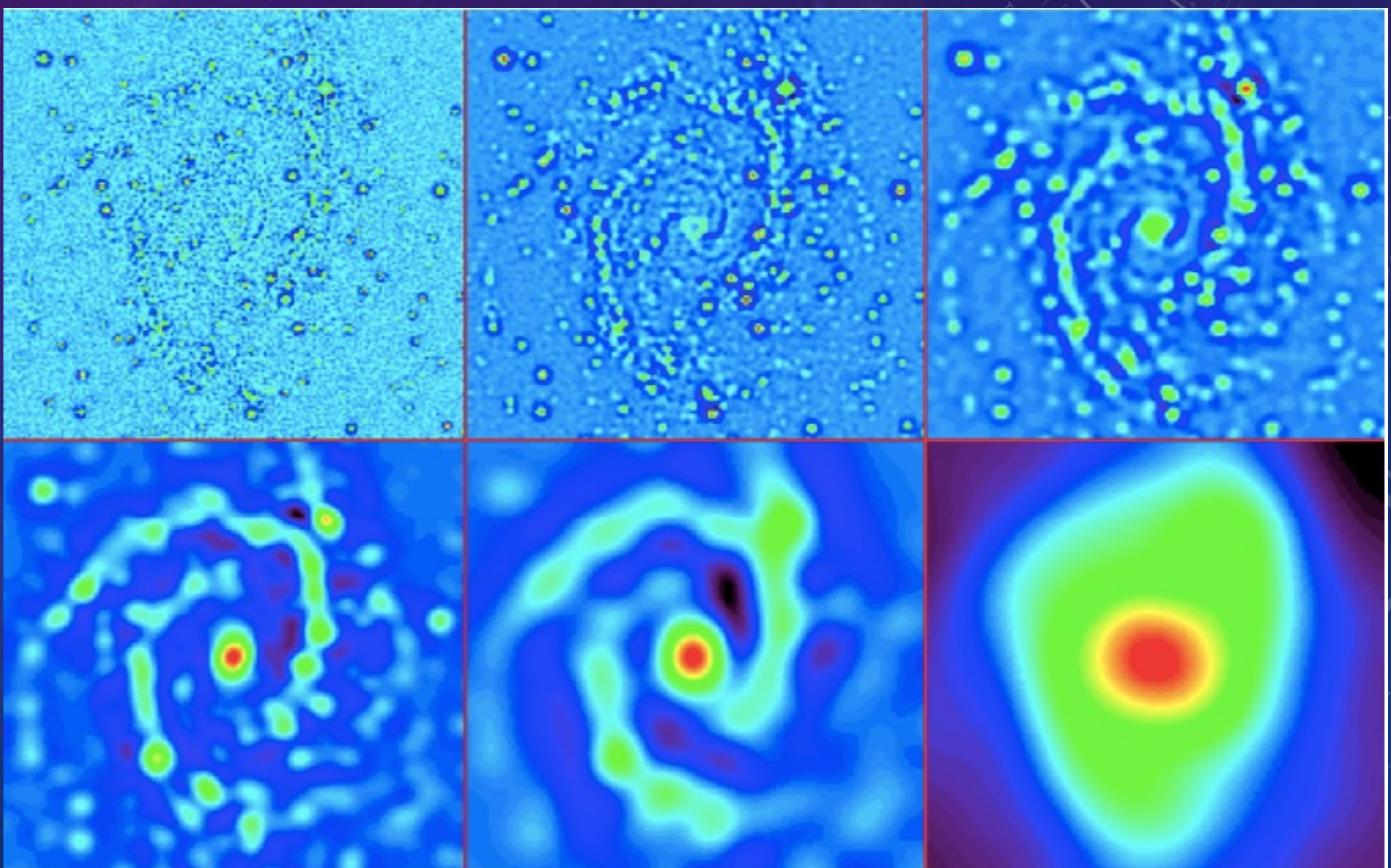
STARLET TRANSFORM

- Isotropic undecimated wavelet transform
- B3-spline for the scaling function

$$X = c_J + \sum_i^J w_i$$



the wavelet



from Starck [2011]

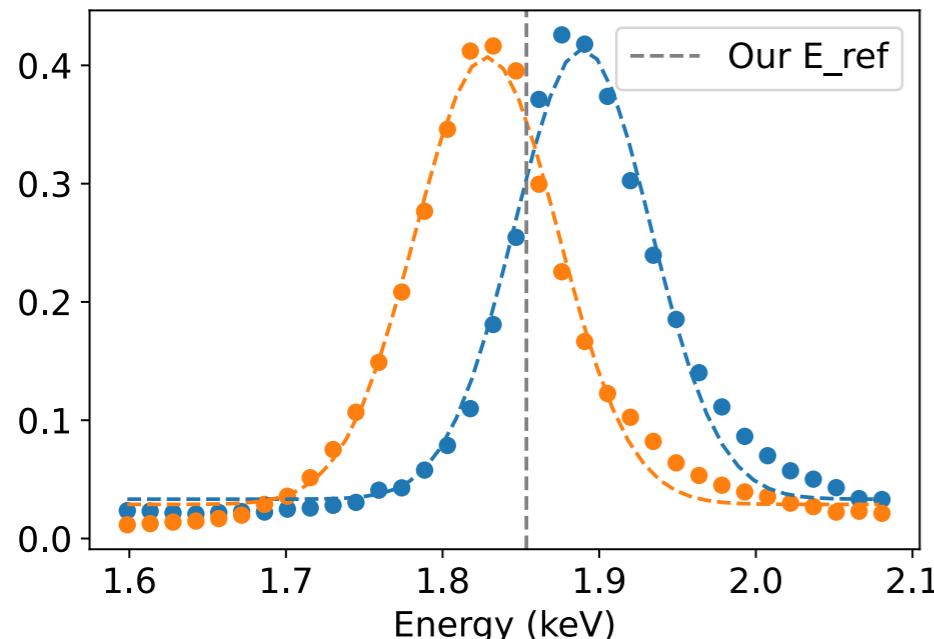
From Red/Blue maps to centroid energy maps

Method to obtain Ec map

1) We use GMCA's definition to "reconstruct" the spectrum in each pixel (i,j)

$$\text{Spectrum}_{i,j} = \sum_{\text{Component } k} \text{Image}_{GMCA,k,i,j} \text{Spectrum}_{GMCA,k}$$

2) We fit the GMCA spectrum with a gaussian.
We obtain an analytical expression of these spectra and so, of the spectrum in each pixel.



3) To find the maximum of the silicon line Ec in the spectrum of each pixel, we must solve this equation :

$$\frac{d \text{Spectrum}_{i,j} (E_c)}{dE} = 0$$

4) And an analytical proxy of the solution is :

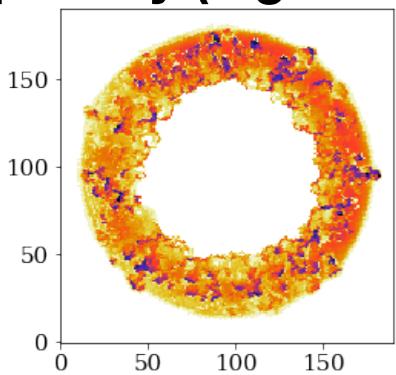
fit parameters from GMCA's spectrum red and blueshifted

$$E_c = \frac{\text{Image}_{ij,r} \frac{\alpha_r}{\sigma_r^2} E_{r,\text{mean}} + \text{Image}_{ij,b} \frac{\alpha_b}{\sigma_b^2} E_{b,\text{mean}}}{\text{Image}_{ij,r} \frac{\alpha_r}{\sigma_r^2} + \text{Image}_{ij,b} \frac{\alpha_b}{\sigma_b^2}}$$

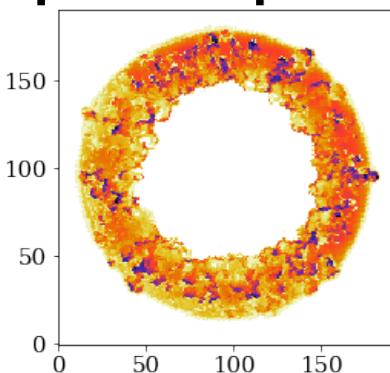
Diagram illustrating the calculation of the centroid energy E_c . The equation shows E_c as a weighted average of red (r) and blueshifted (b) images, where the weights are proportional to the ratio of the red and blueshifted image amplitudes to their respective standard deviations squared. Red arrows point to the terms involving the red image, and blue arrows point to the terms involving the blueshifted image.

GMCA's image red and blueshifted

Simulation hydro quantity (e.g. density)



Post-processing for plasma quantities

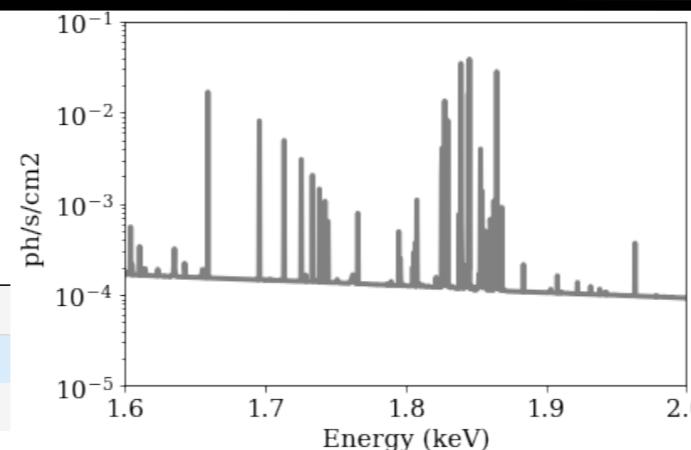


Using spectral package as Xspec or SPEX

From simulation to observation :

Plasma spectral properties

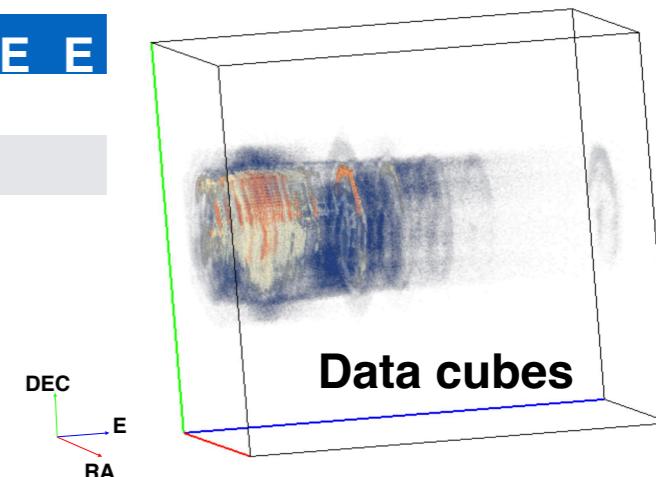
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kT	<input checked="" type="checkbox"/>	1.0
H	<input type="checkbox"/>	1.0
He	<input type="checkbox"/>	1.0
C	<input type="checkbox"/>	1.0
N	<input type="checkbox"/>	1.0
O	<input type="checkbox"/>	1.0
Ne	<input type="checkbox"/>	1.0
Mg	<input type="checkbox"/>	1.0
Si	<input type="checkbox"/>	1.0
S	<input type="checkbox"/>	1.0
Ar	<input type="checkbox"/>	1.0
Ca	<input type="checkbox"/>	1.0
Fe	<input type="checkbox"/>	1.0
Ni	<input type="checkbox"/>	1.0
Tau	<input checked="" type="checkbox"/>	1000000000000.0
redshift	<input type="checkbox"/>	0.0
norm	<input checked="" type="checkbox"/>	1.0



Synthetic X-ray spectrum for each cell

SIXTE +Instrument configuration

Event list



Studying the projection effects and mixing

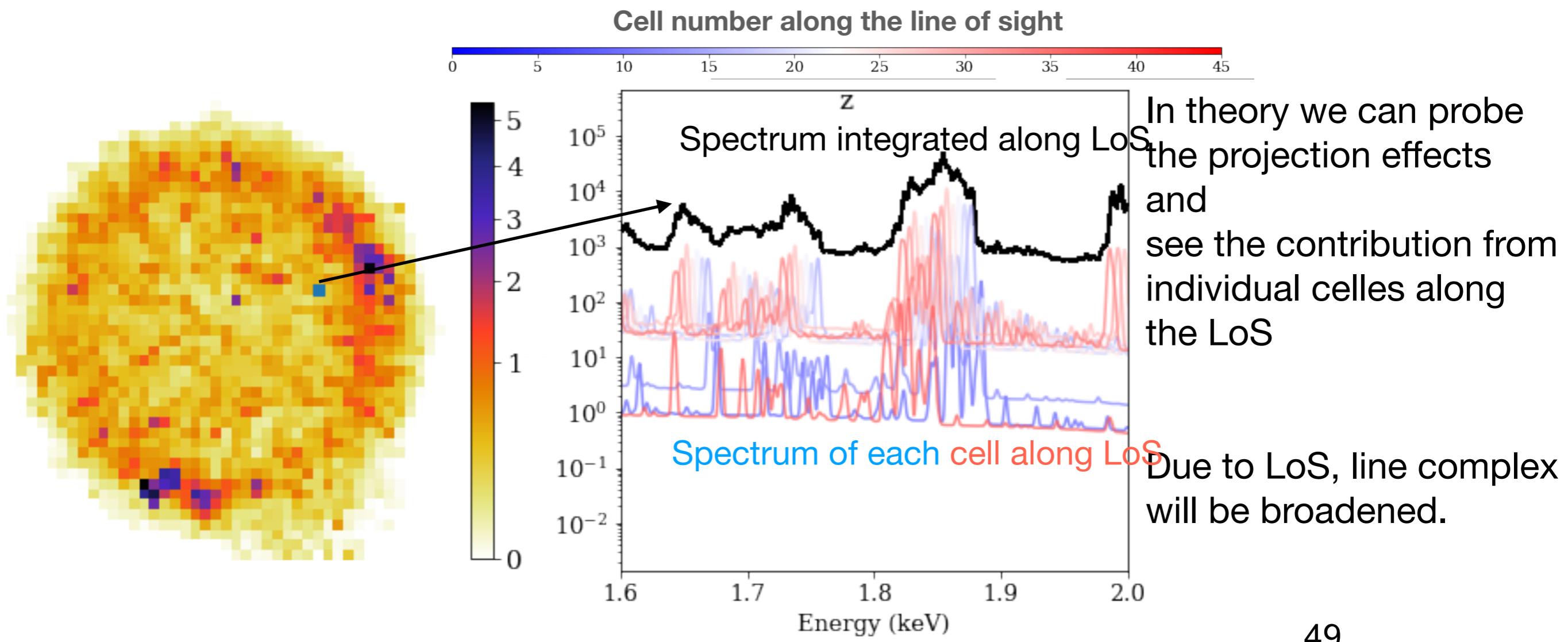
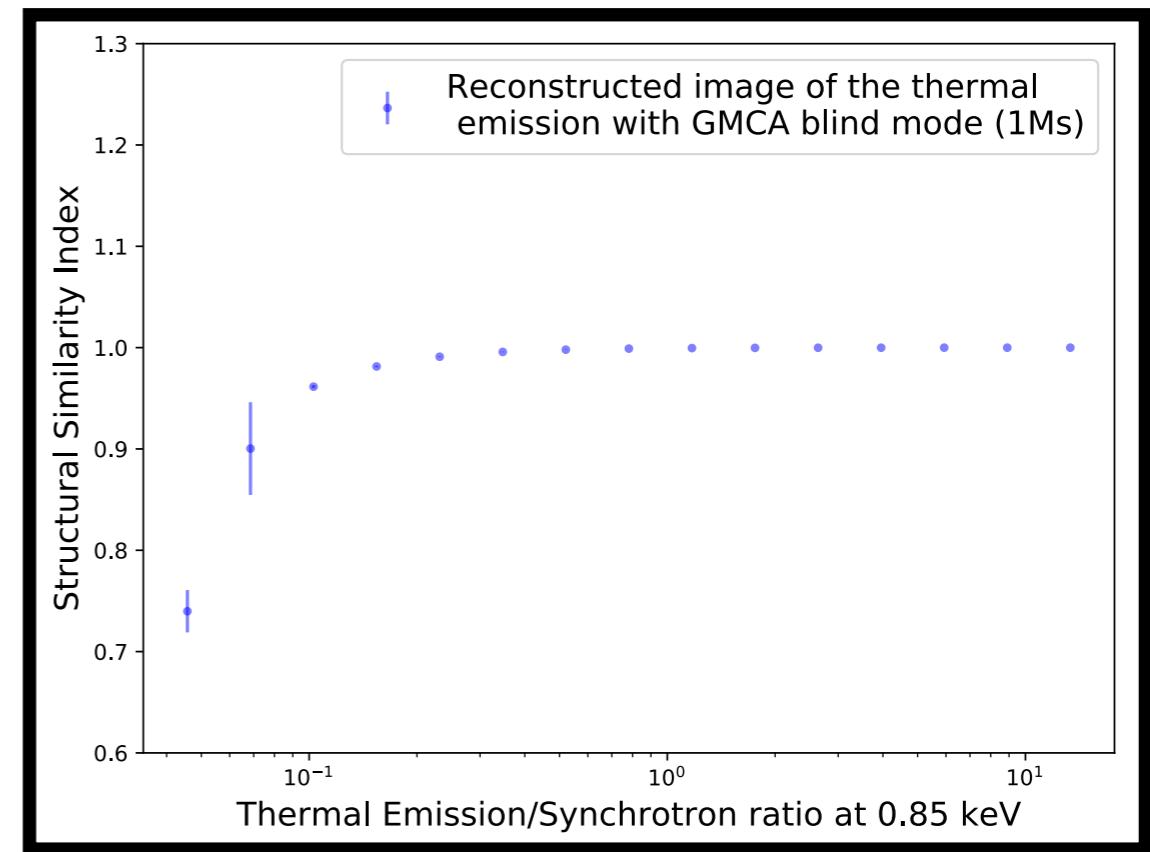
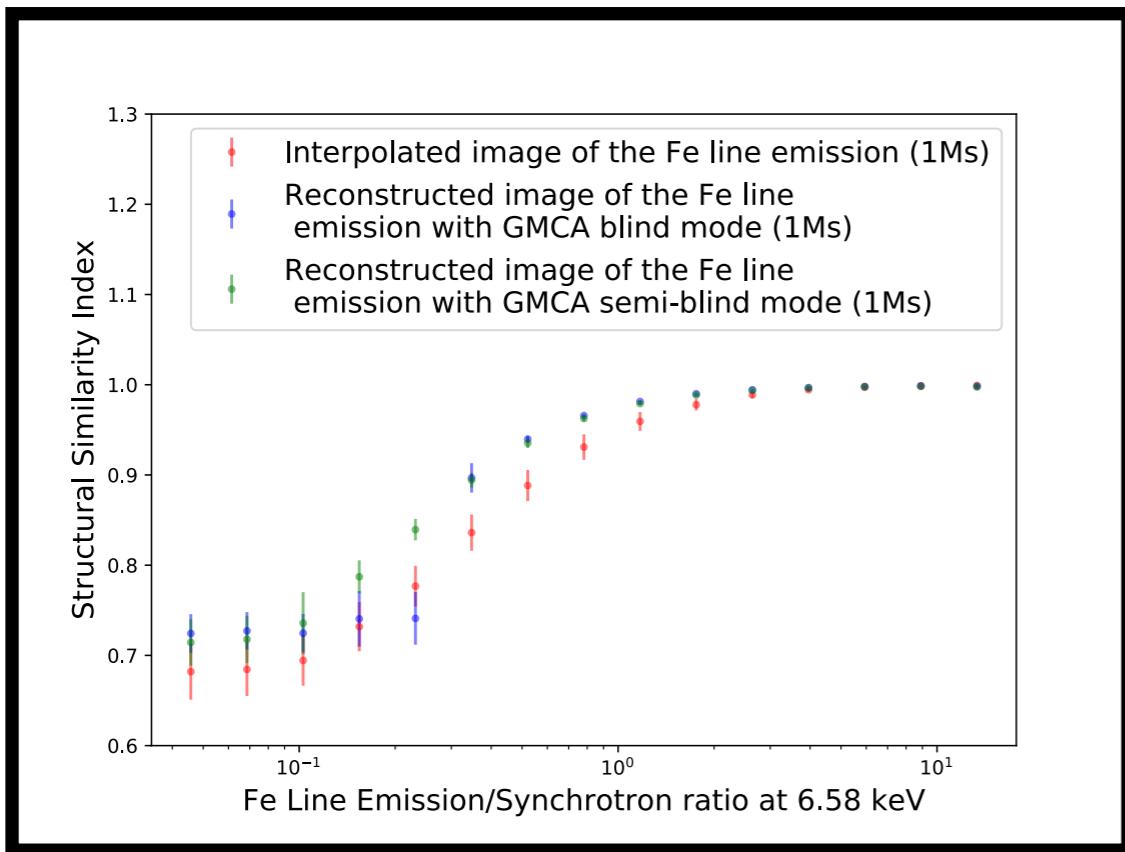
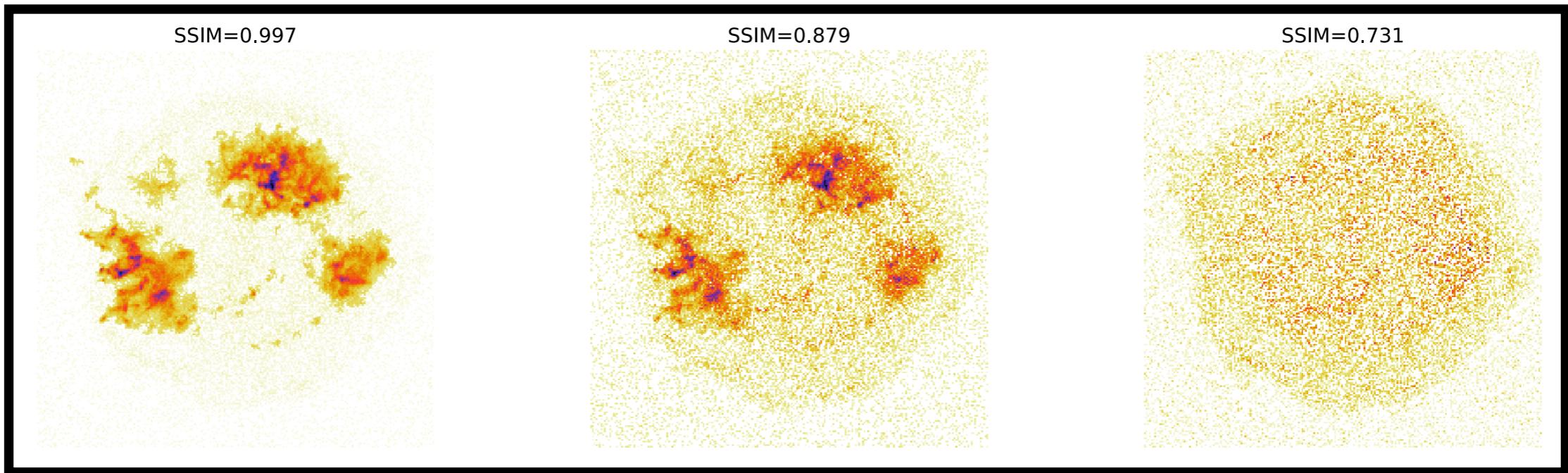


Image accuracy



SSIM coefficients of the images of the retrieved second component in both toy models



Examples of SSIM coefficients associated with the corresponding images