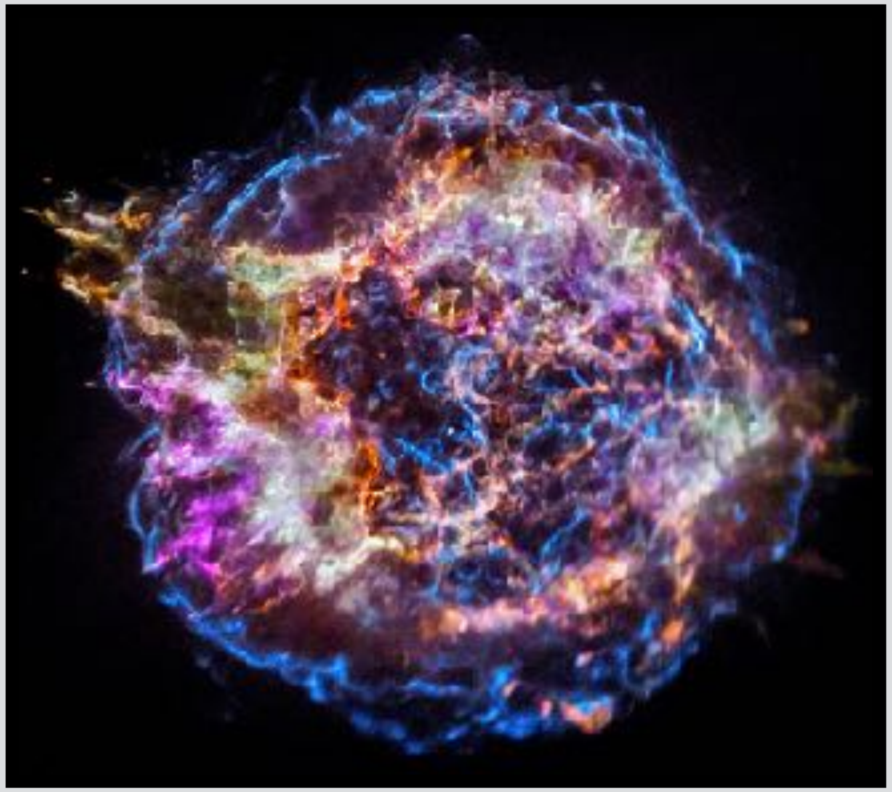
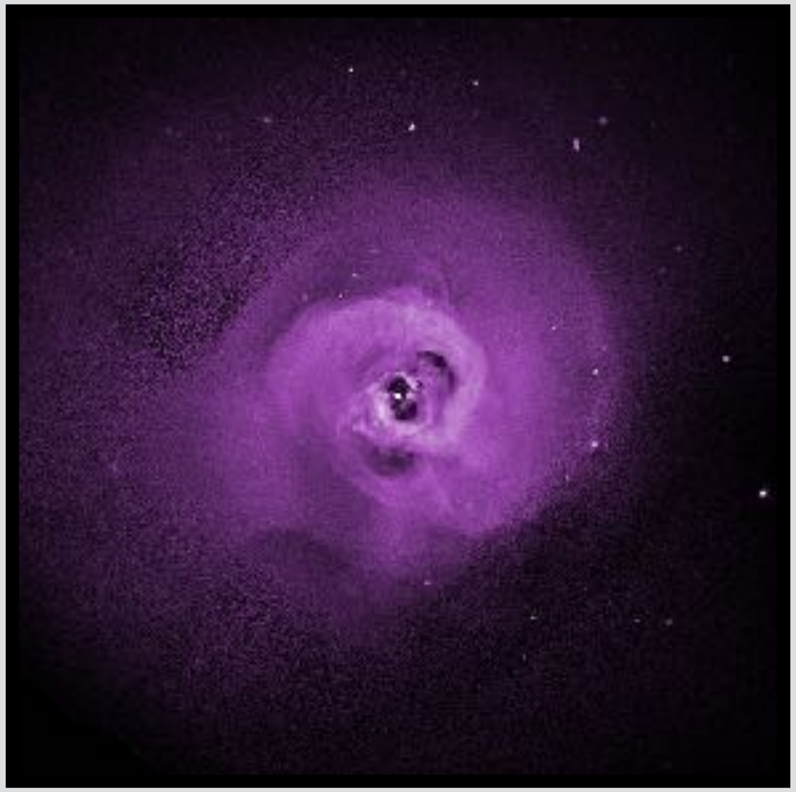
Introduction and application of a new blind source separation method for extended sources in X-ray astronomy

Galactic center



Cassiopeia A supernova remnant



Perseus galaxy cluster

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Summary

An introduction to SNRs

Methodology :

- Introduction of wavelets and GMCA
- Tests on toy models => Picquenot et al. (2019)
- Introduction of pGMCA => Bobin J., El Hamzaoui I., Picquenot A., Acero F. (2020)
- Error bars

Applications :

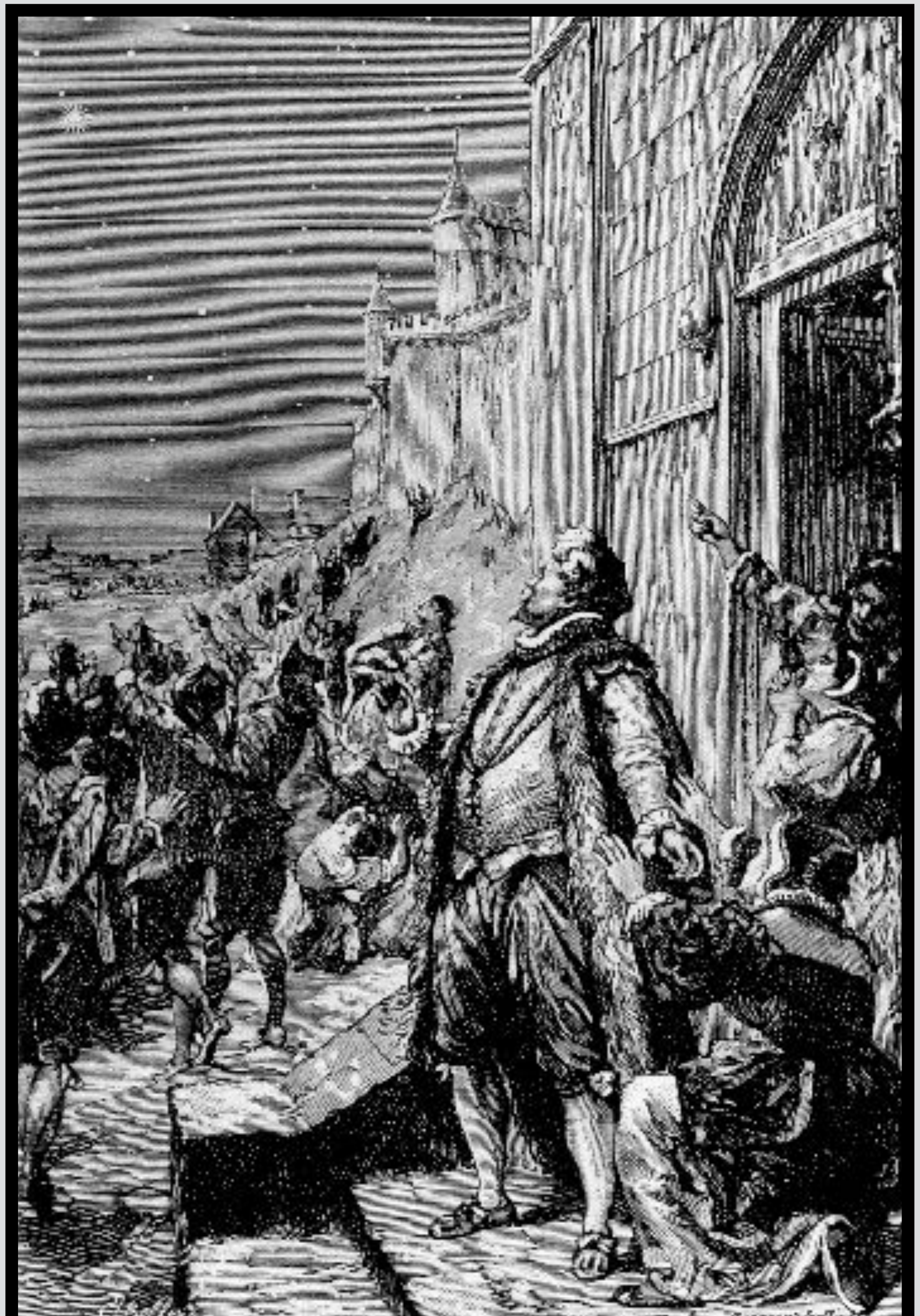
- Asymmetries in Cassiopeia A => Picquenot et al. (2021)
- Synchrotron rim widths in Cassiopeia A

Conclusion and perspectives

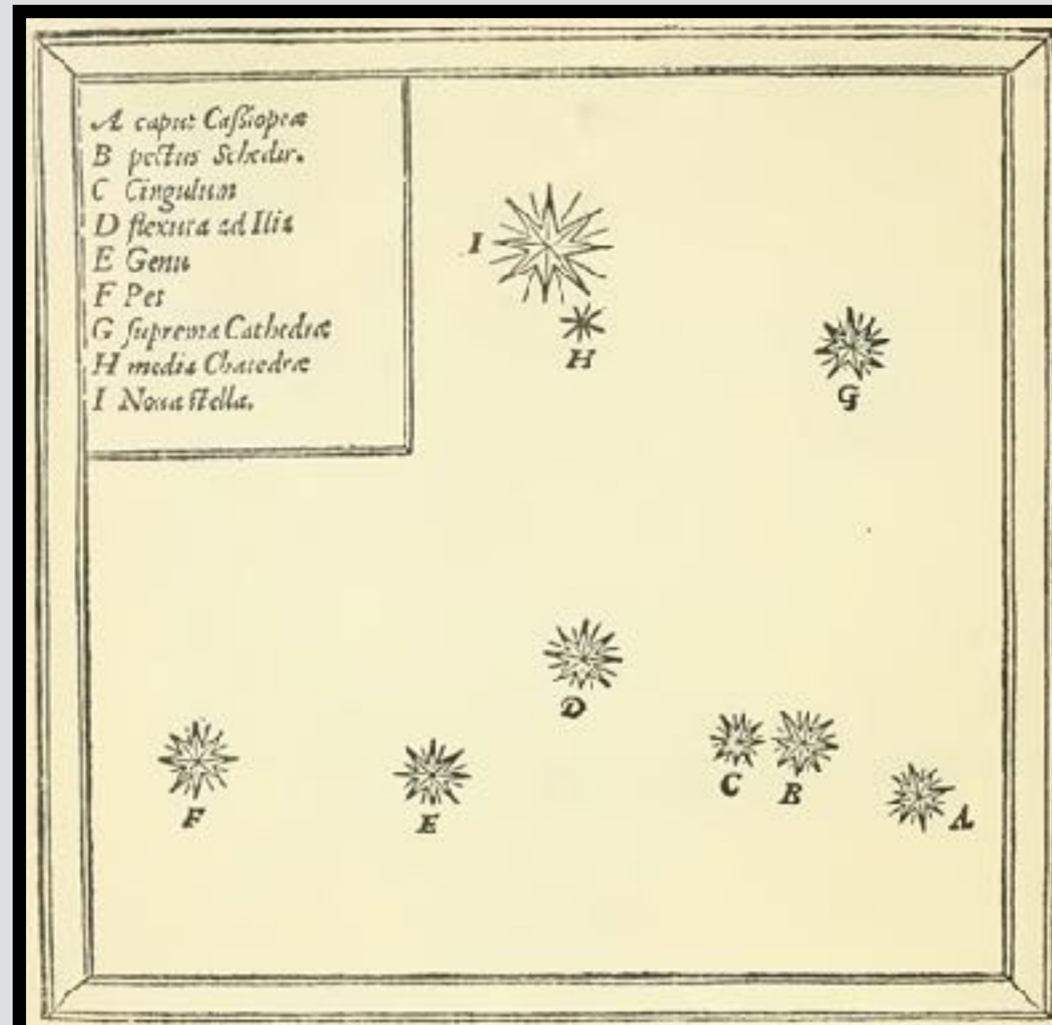
Introduction

Nova Stella

« Last night of all,
When yond same star that's westward from the pole
Had made his course to illume that part of heaven »



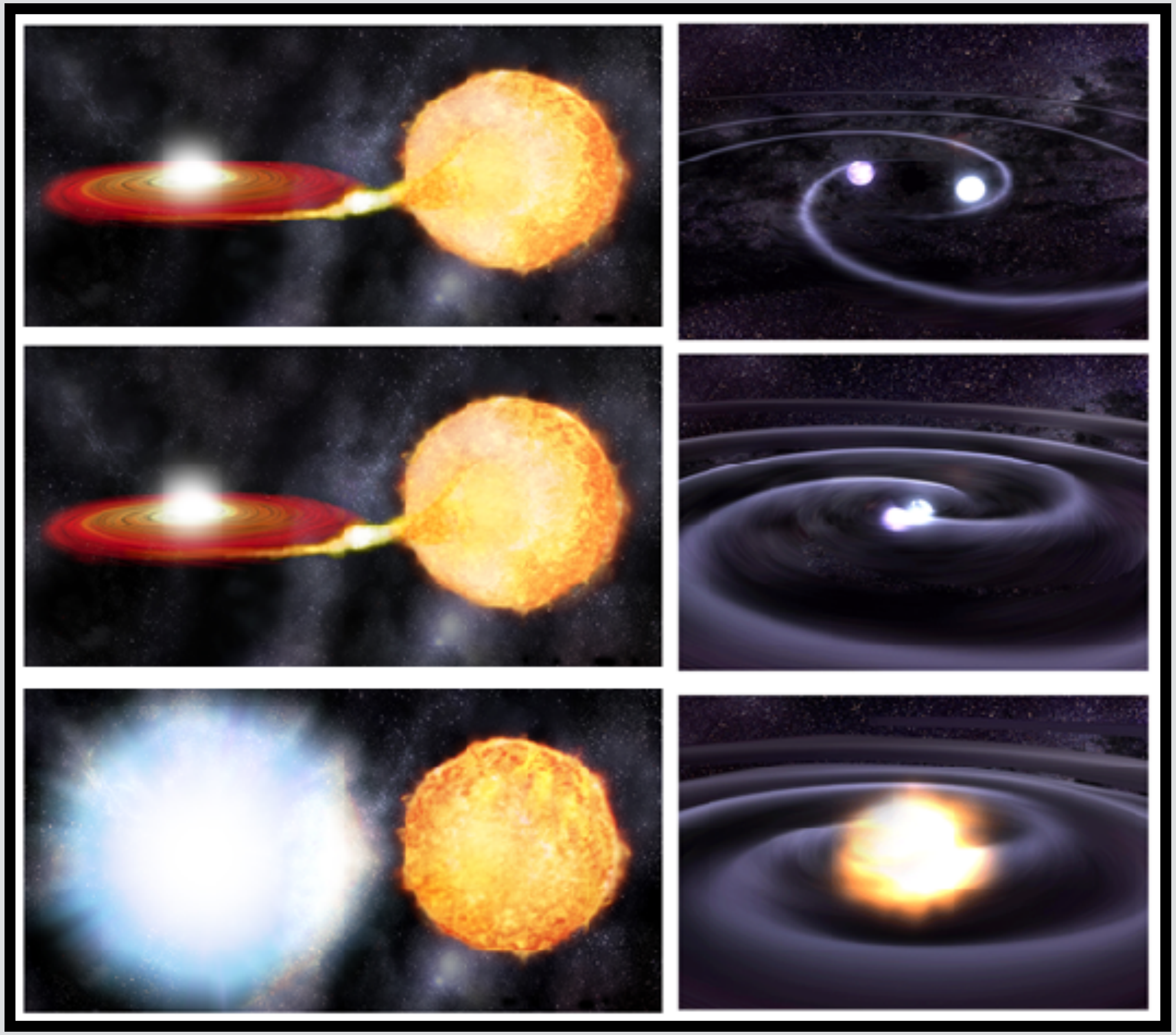
—Shakespeare's *Hamlet*, Act 1 Scene 1



Map of the sky from Tycho Brahe's *De nova stella*

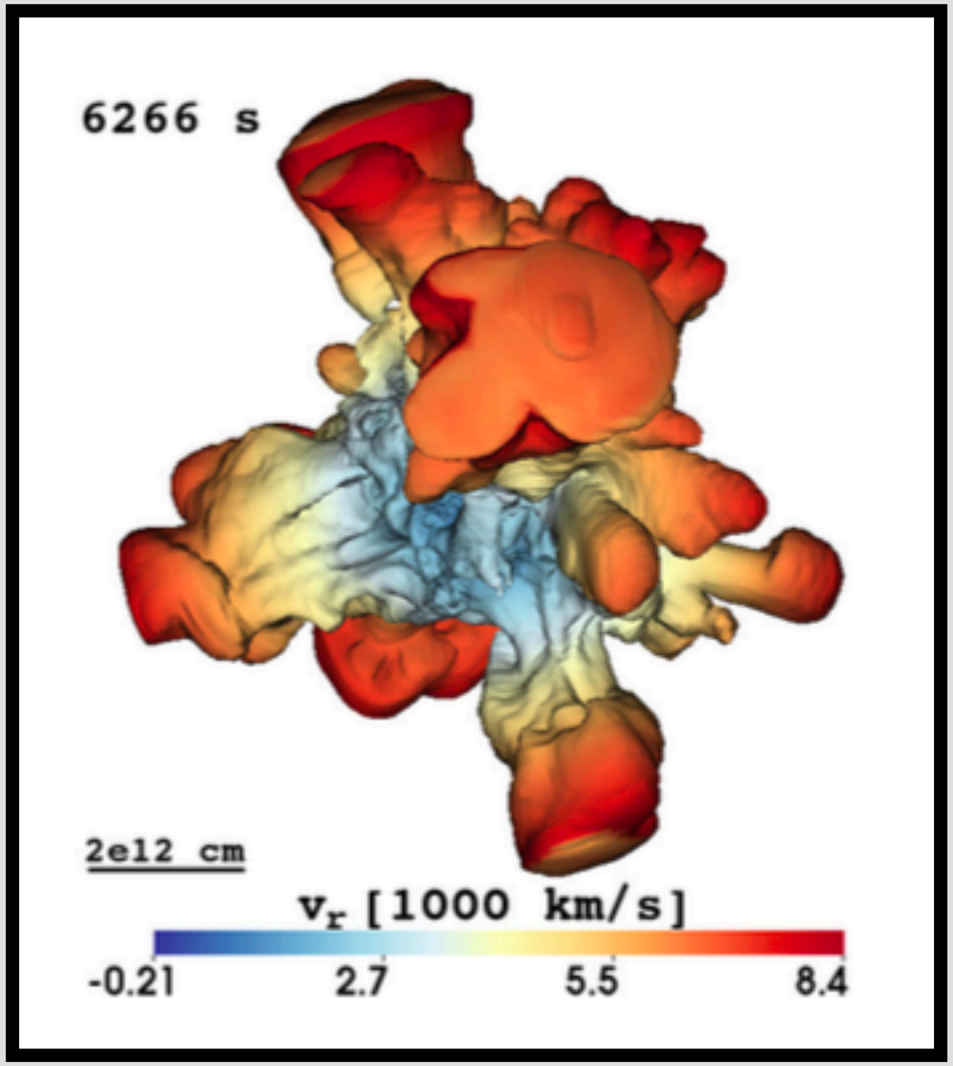
Supernovae types

Thermonuclear (Type Ia)



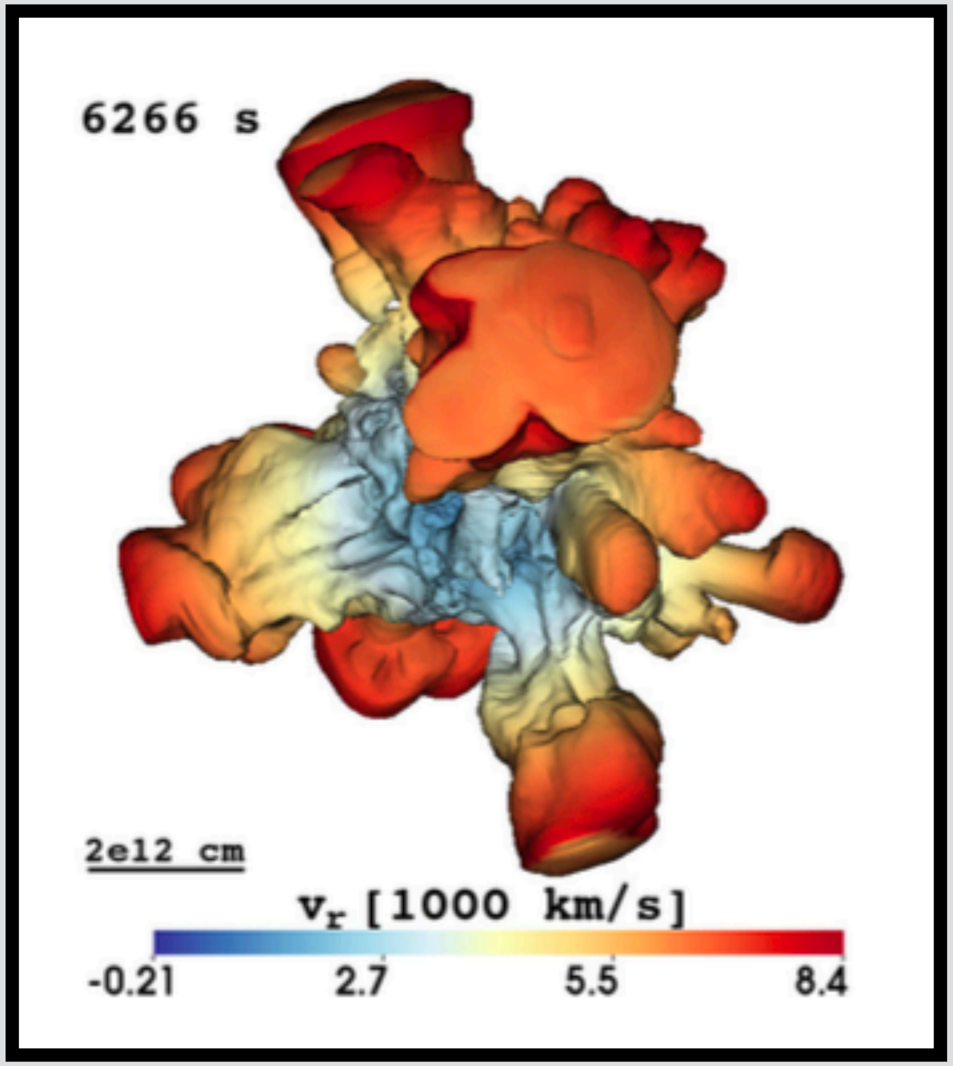
Single/double degenerate scenarii (white dwarves)

Core Collapse



Simulation, from
Wongwathanarat et al. (2015)

Core Collapse Supernovae



Simulation, from
Wongwathanarat et al. (2015)

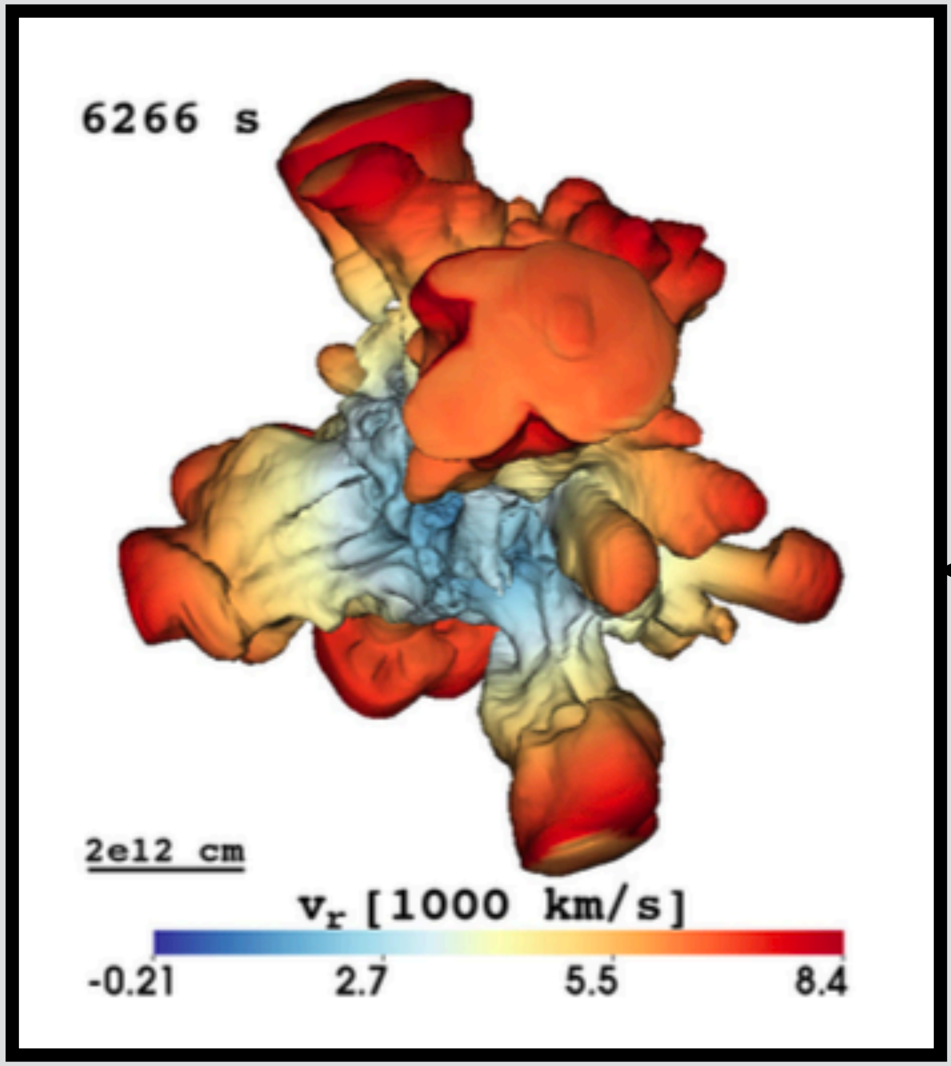
- Nuclear fusion does not counter gravity anymore : core collapse
- Shock revival by neutrino heating (boosted by instabilities) Janka+2012
- Outer layers are ejected
- Asymmetries induce the neutron star kick Nordhaus+2012

Janka and Mueller 1994

Asymmetries in the explosion proved necessary in the simulations.

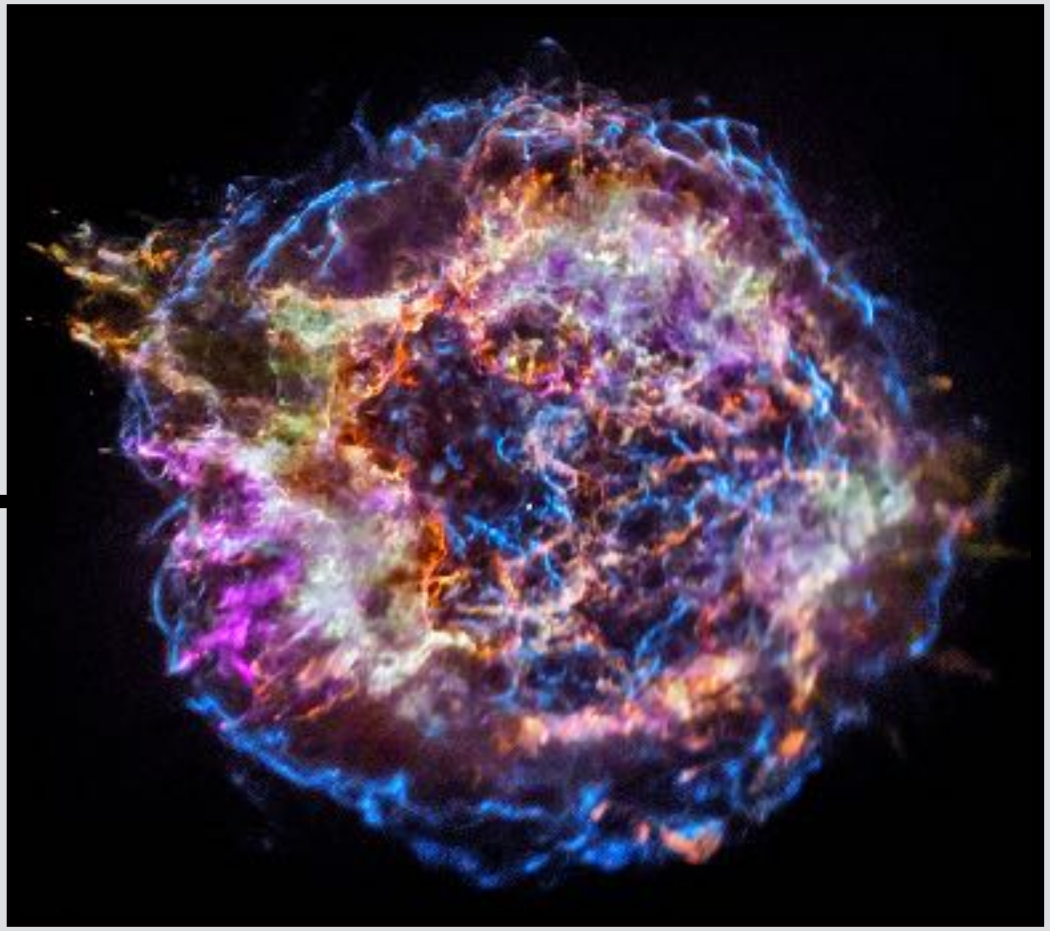
Linking the remnant to the supernova

t = 6266 seconds



Simulation, from
Wongwathanarat et al. (2015)

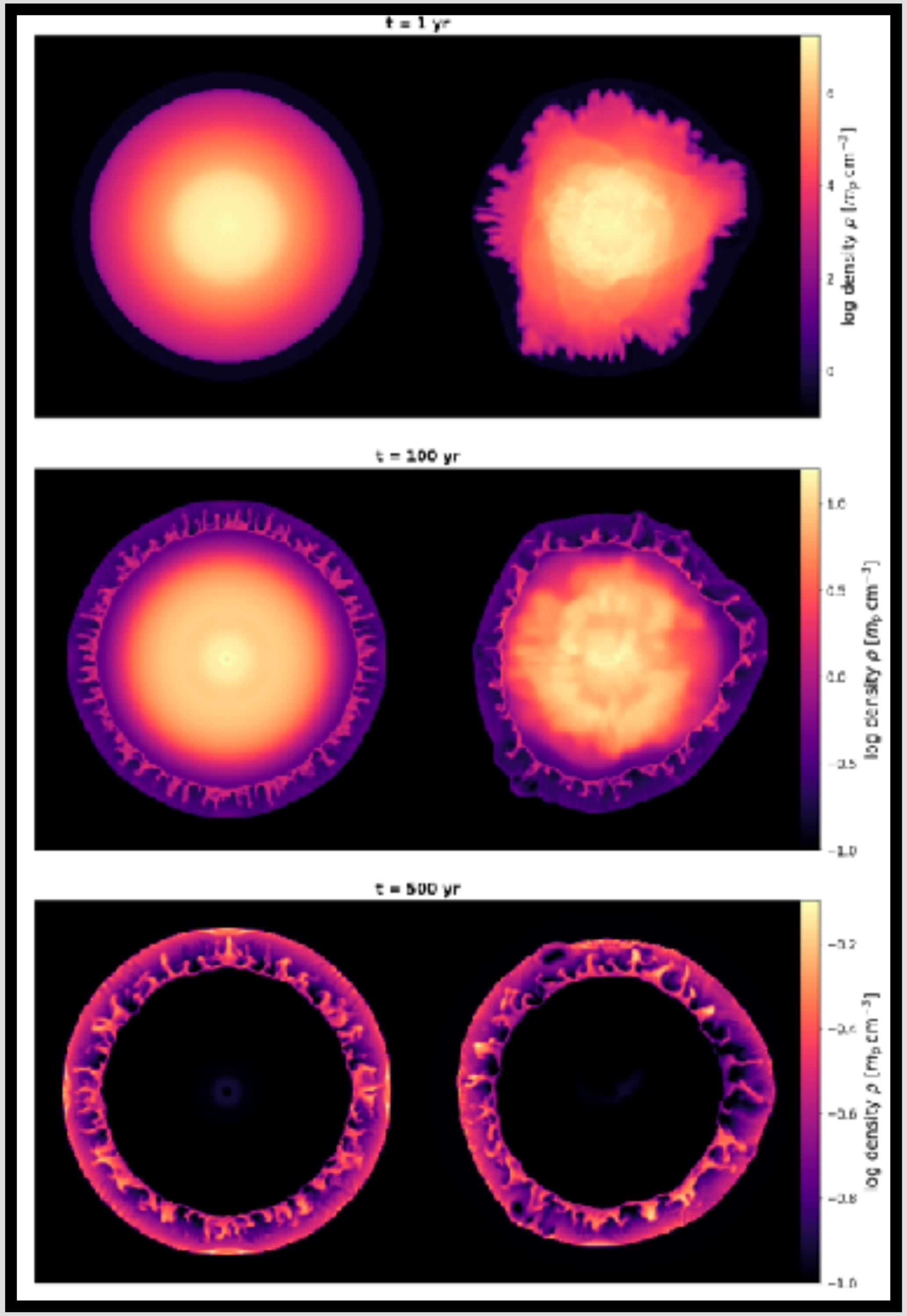
t = 340 years



Cassiopeia A seen by *Chandra*

What can the remnant ejecta tell us about the initial asymmetry ?

Linking the remnant to the supernova



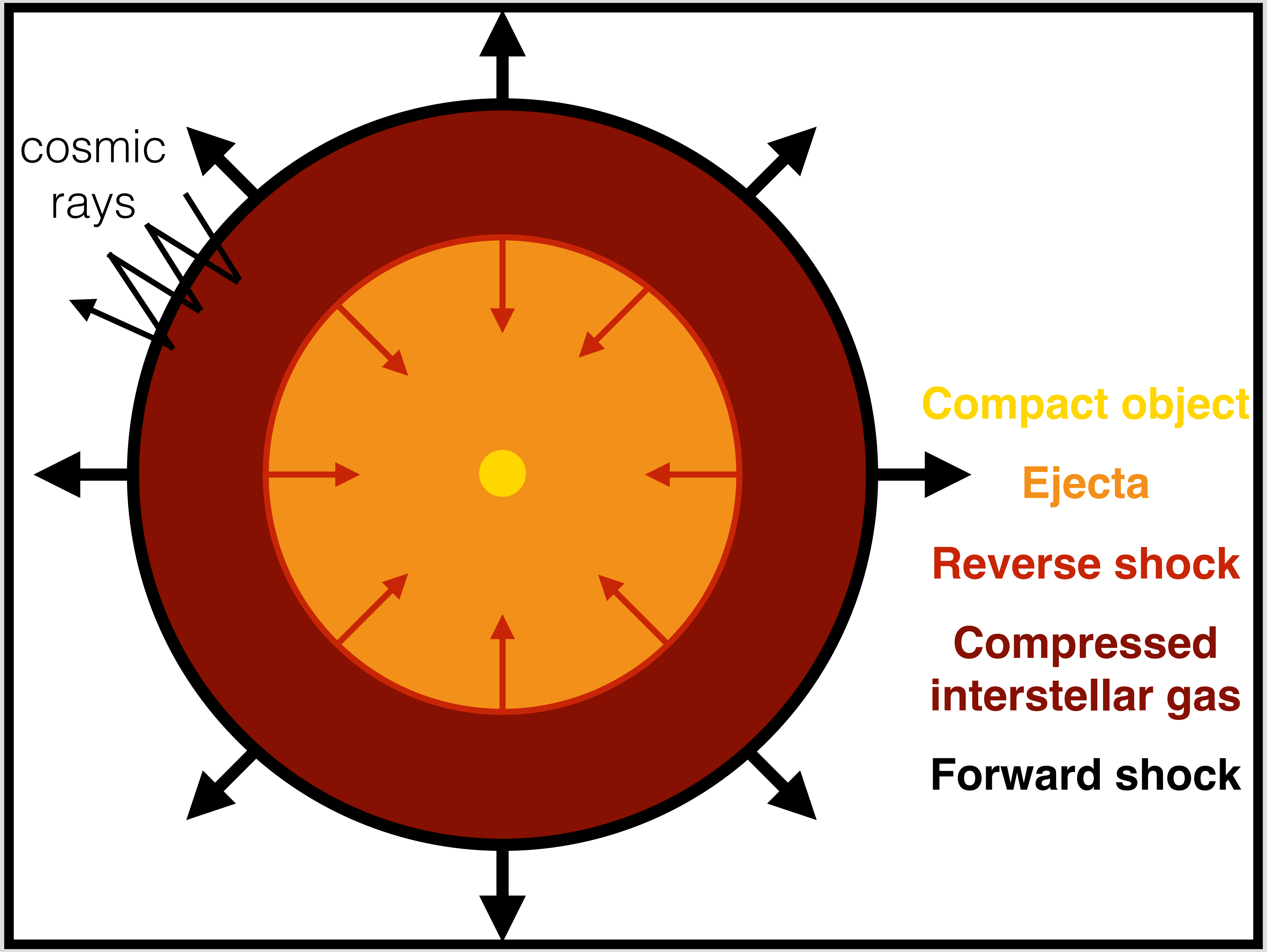
t = 1 year

t = 100 years

t = 500 years

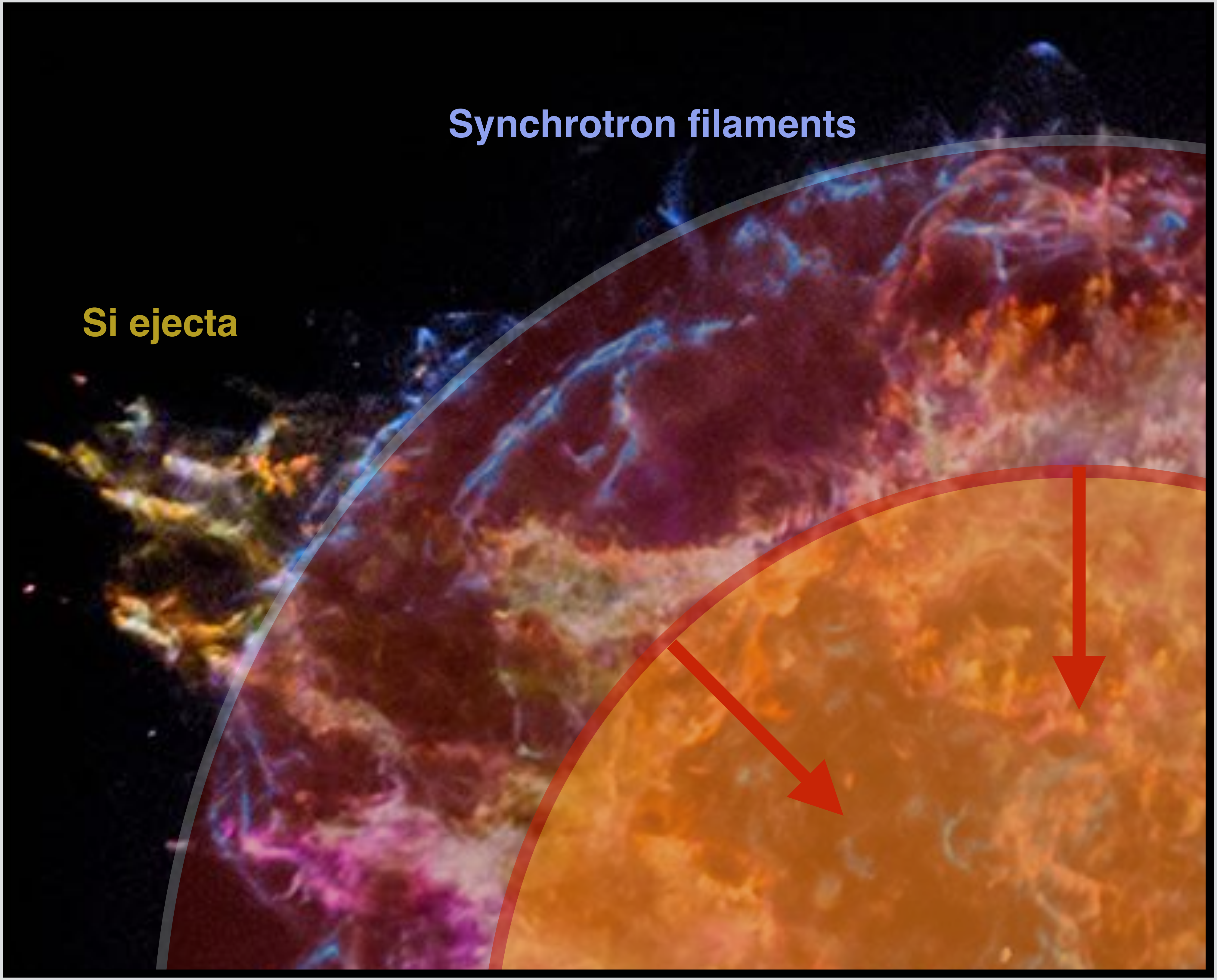
Simulation about the evolution of a type Ia SNR from Ferrand et al. (2019). A similar work was done in Orlando et al. (2016) for CC SNR

Schematic supernova remnant

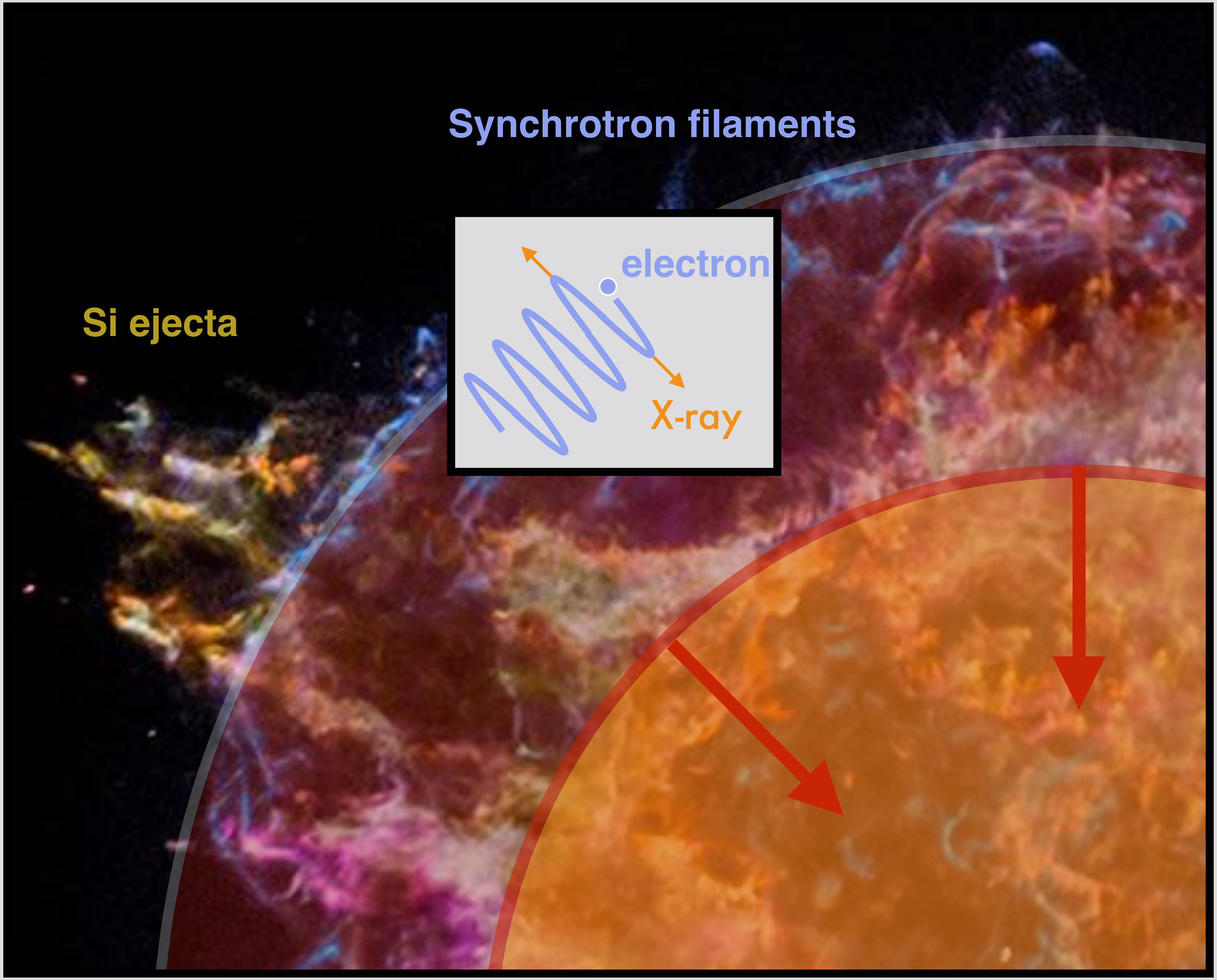


Ejecta can trace the explosion mechanisms.

Real supernova remnant



Real supernova remnant



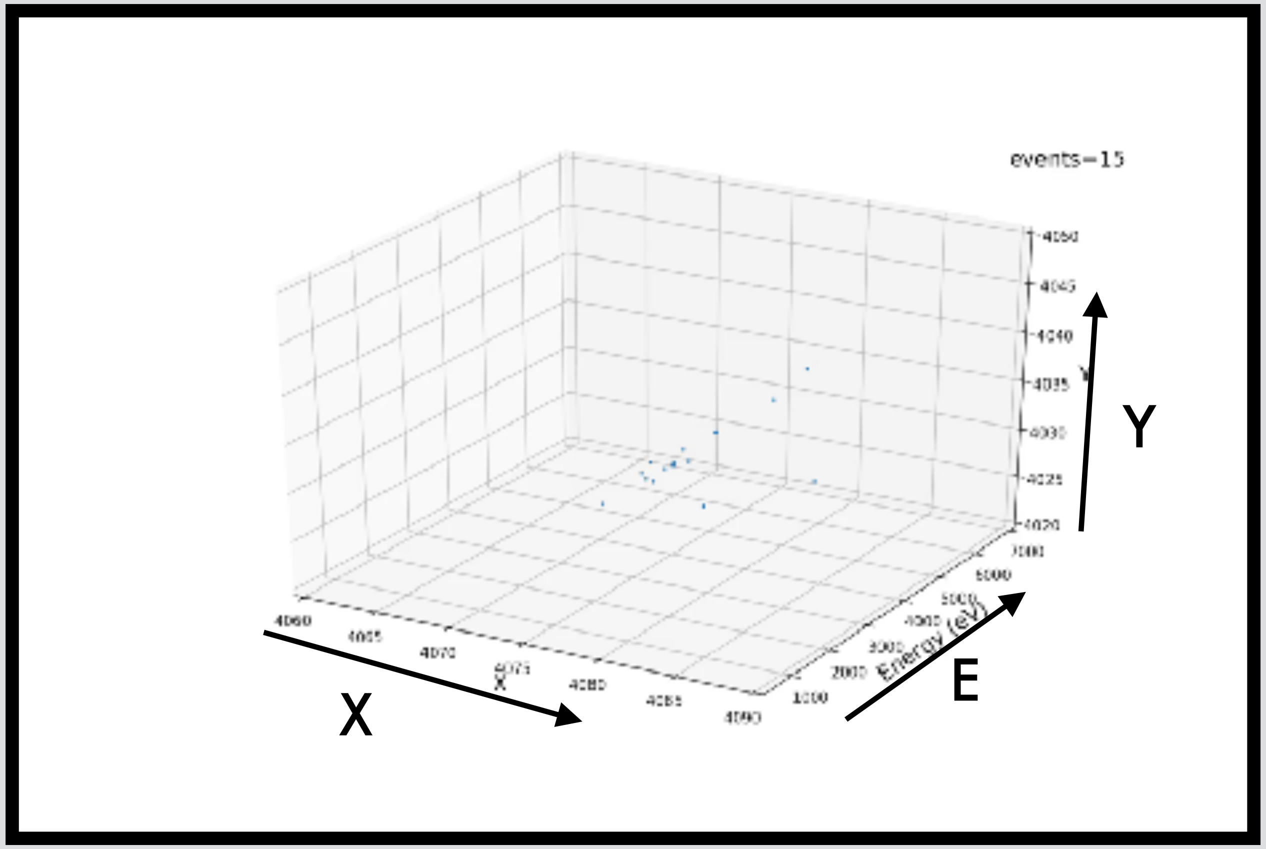
Spectro-imaging instruments

Chandra ACIS

spatial : 0.5 arcsec ; spectral : 150 eV

XMM-Newton EPIC

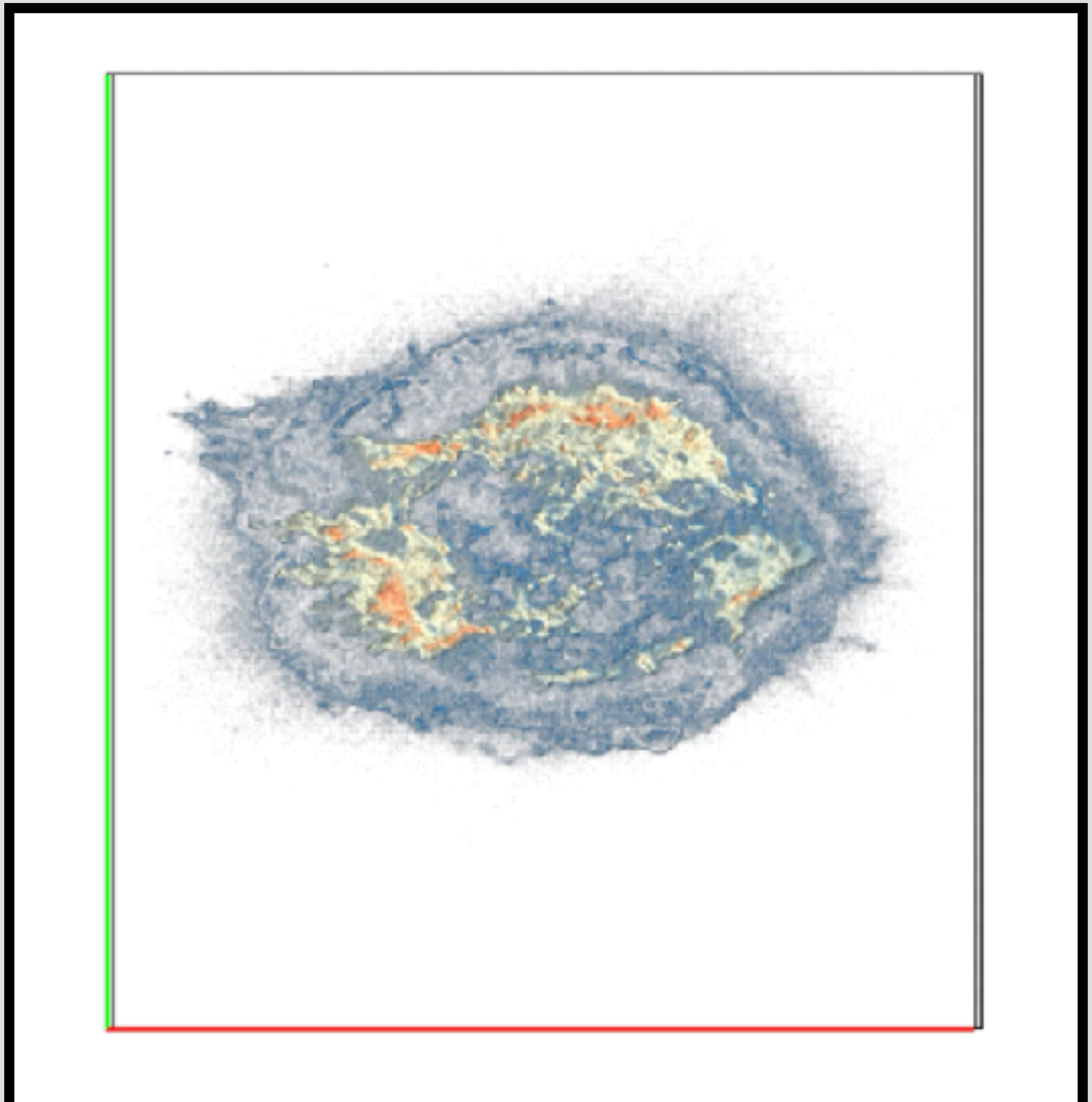
spatial : 6 arcsec ; spectral : 150 eV

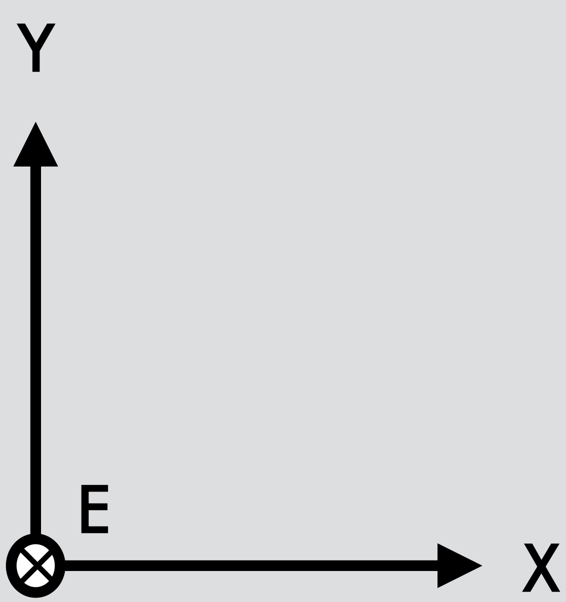


For each photon, the instruments detect (x,y,E,t).

Supernova Remnants in X-rays

Cas A data cube (x,y,E)



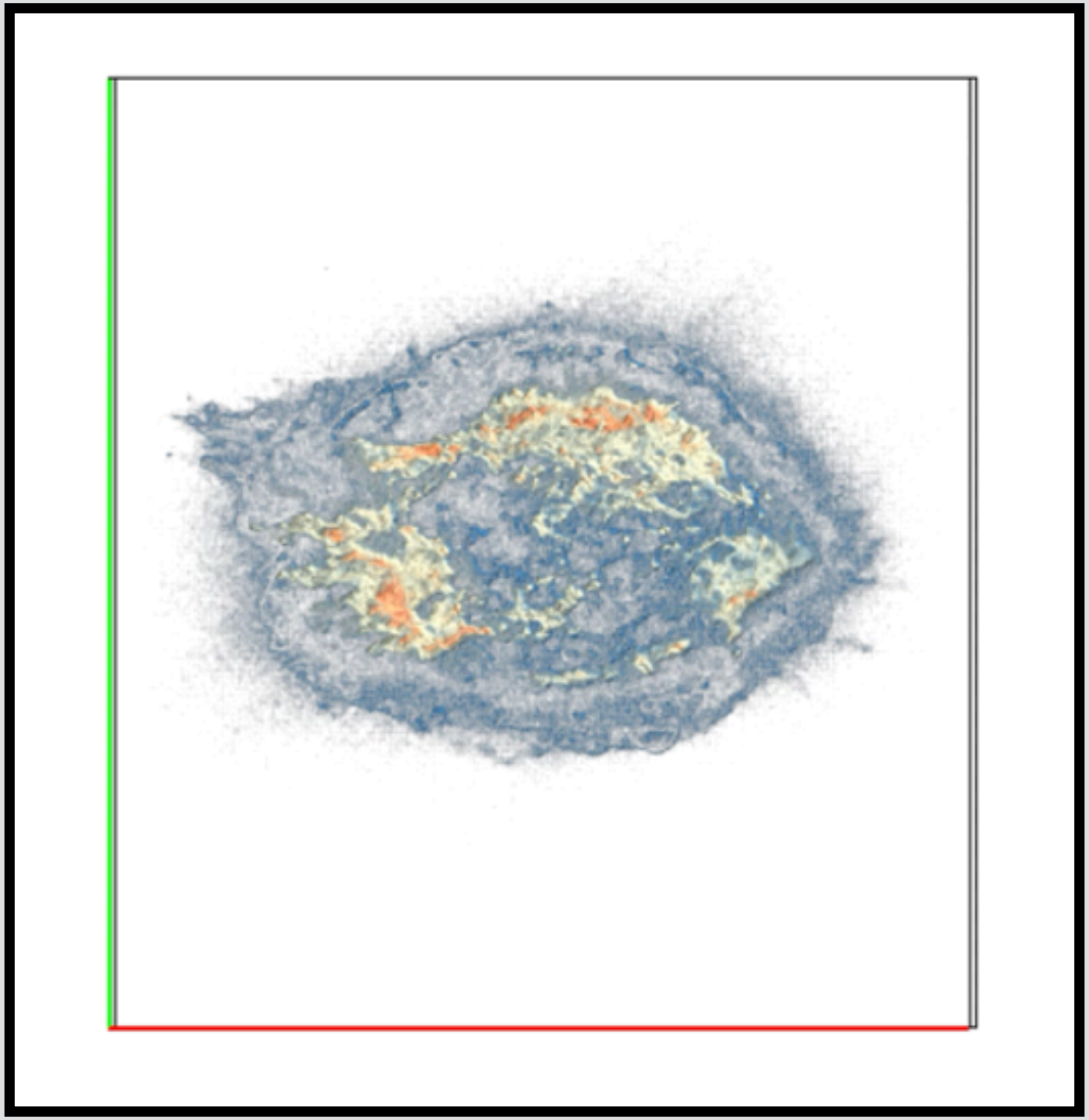


Chandra data (1Ms, 2004), visualized with vaex

Colors show flux density

Supernova Remnants in X-rays

Cas A data cube (x,y,E)



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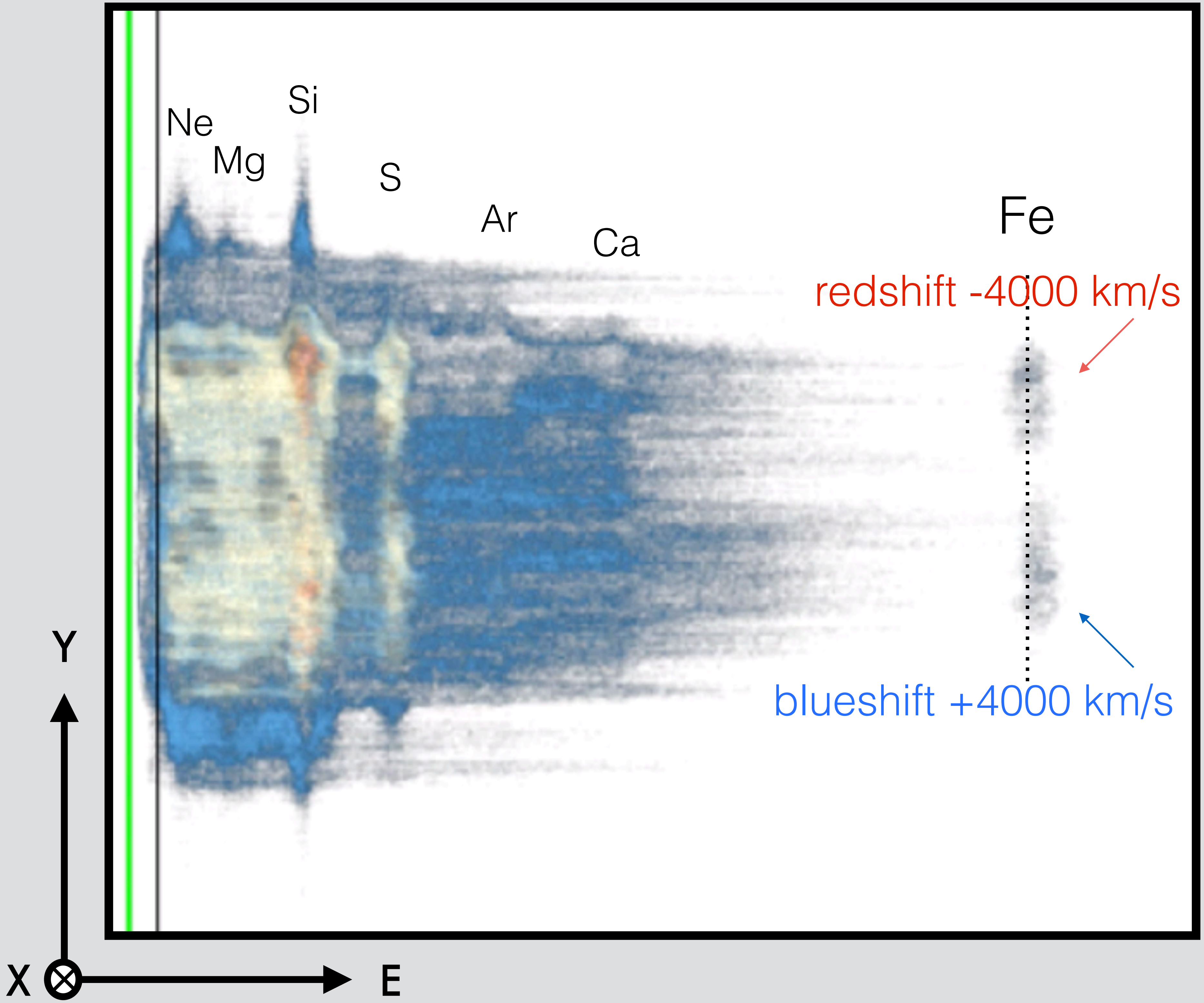
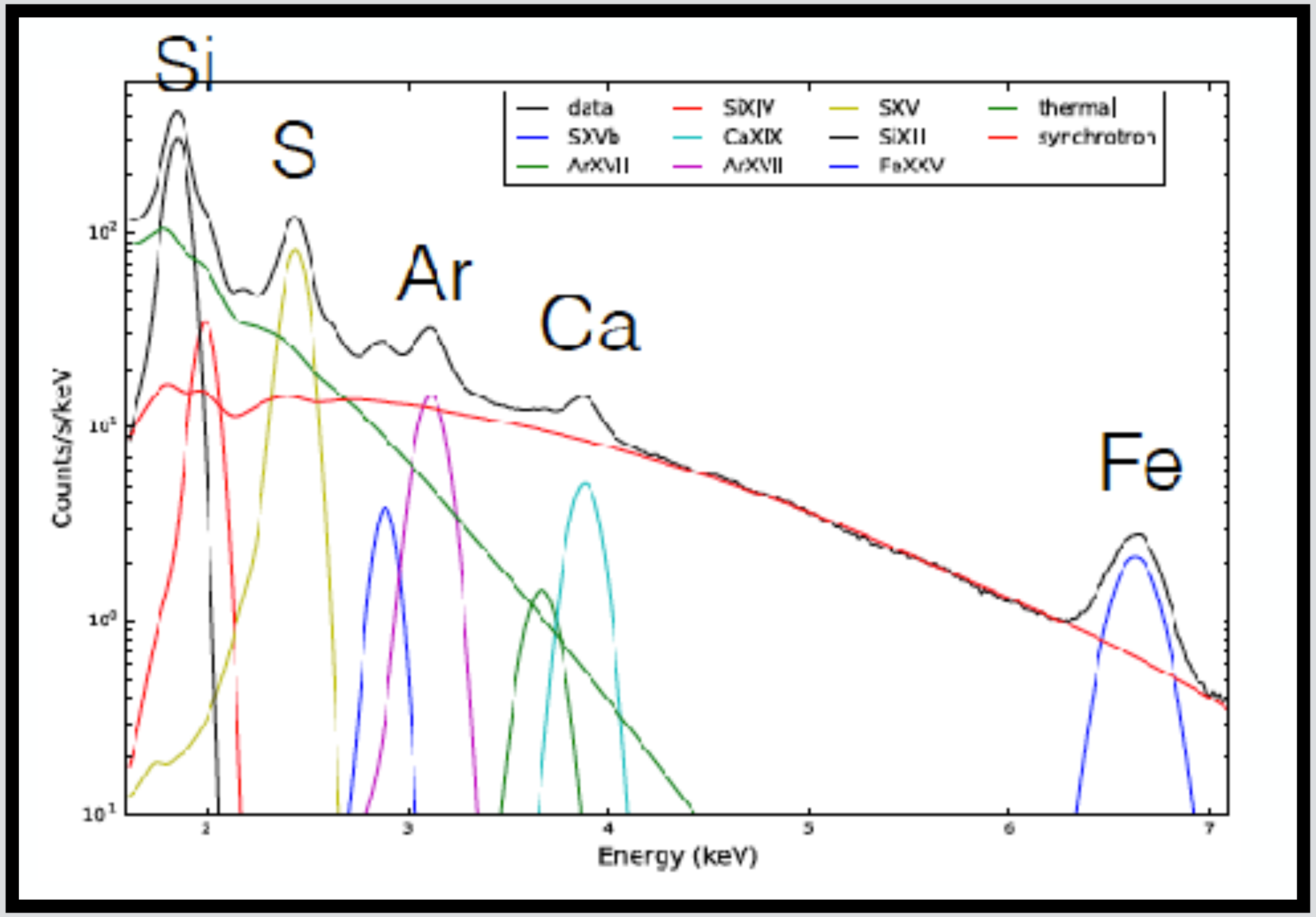
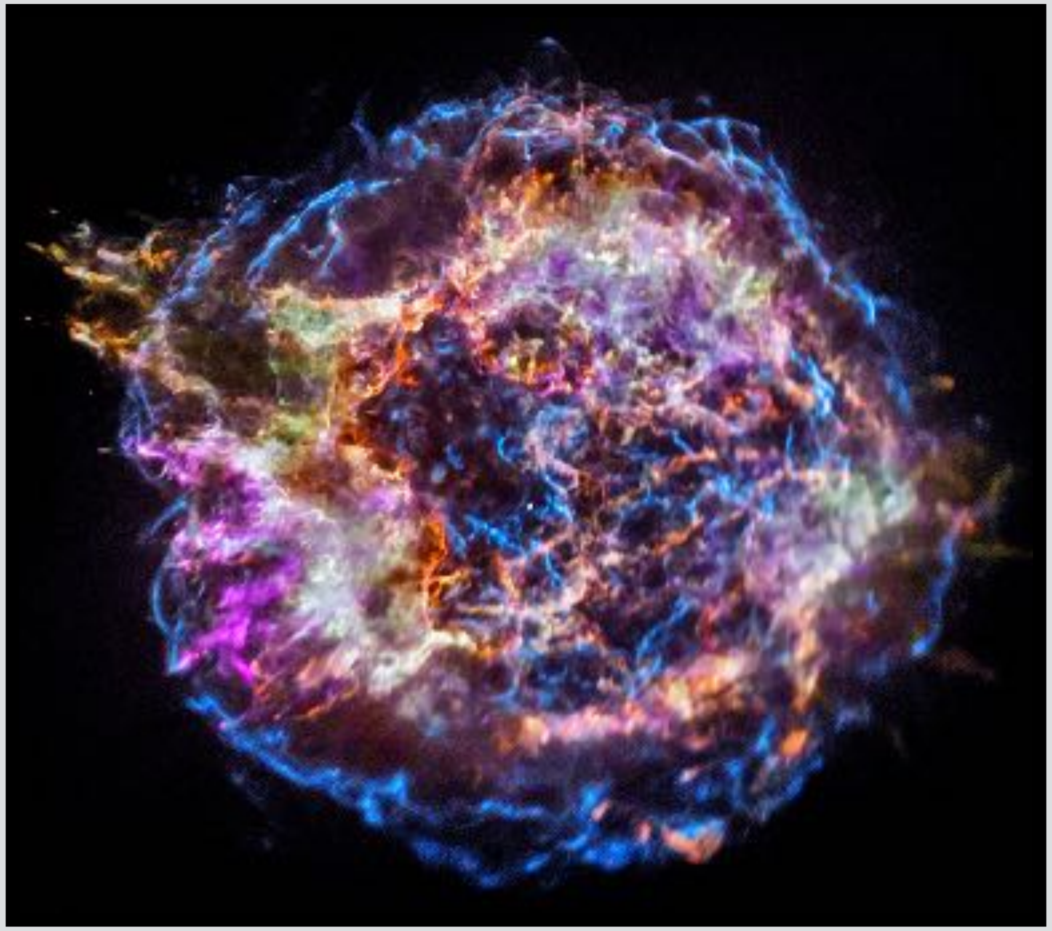
Chandra data (1Ms, 2004), visualized with vaex

Supernova Remnants in X-rays



Supernova Remnants in X-rays



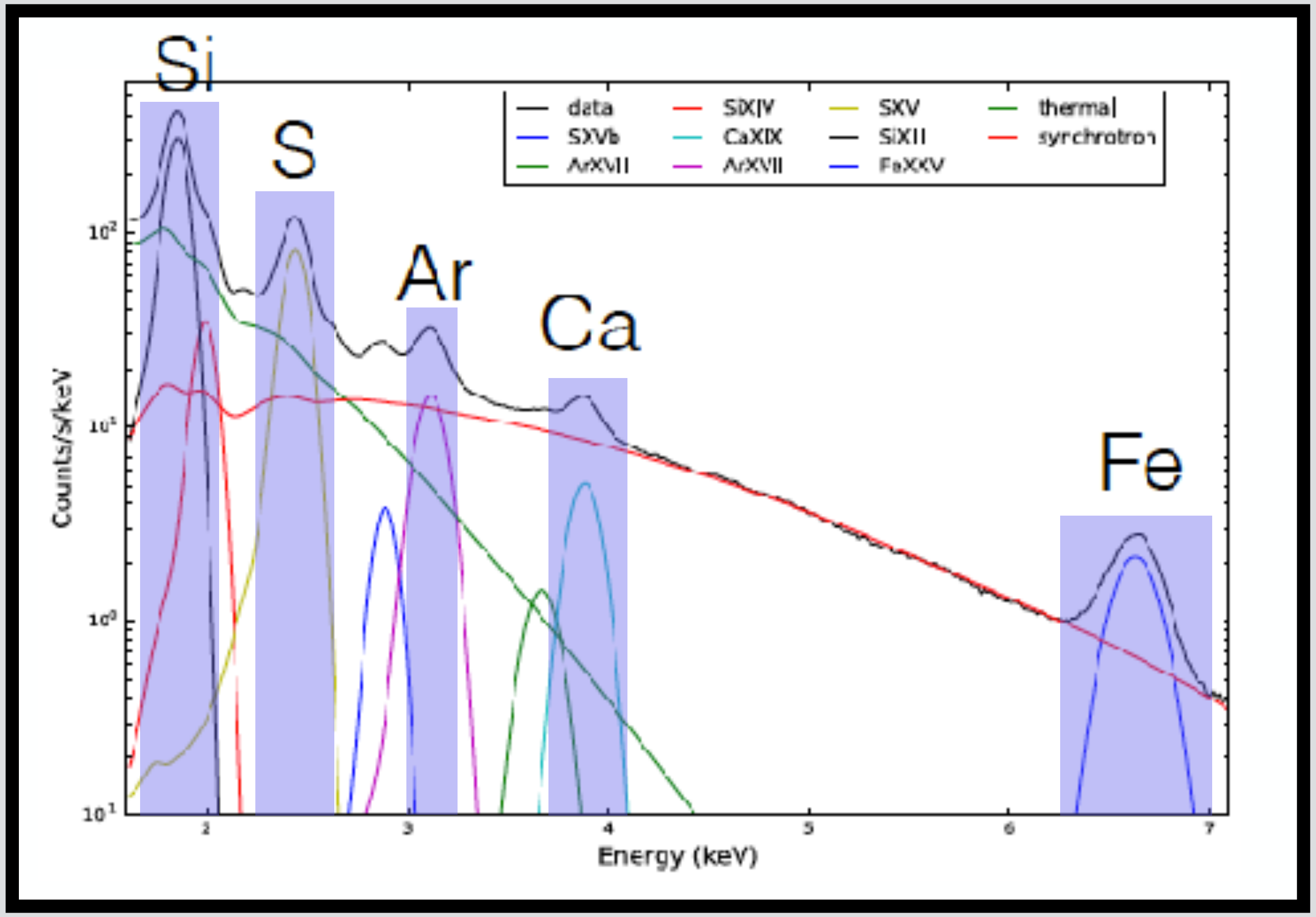


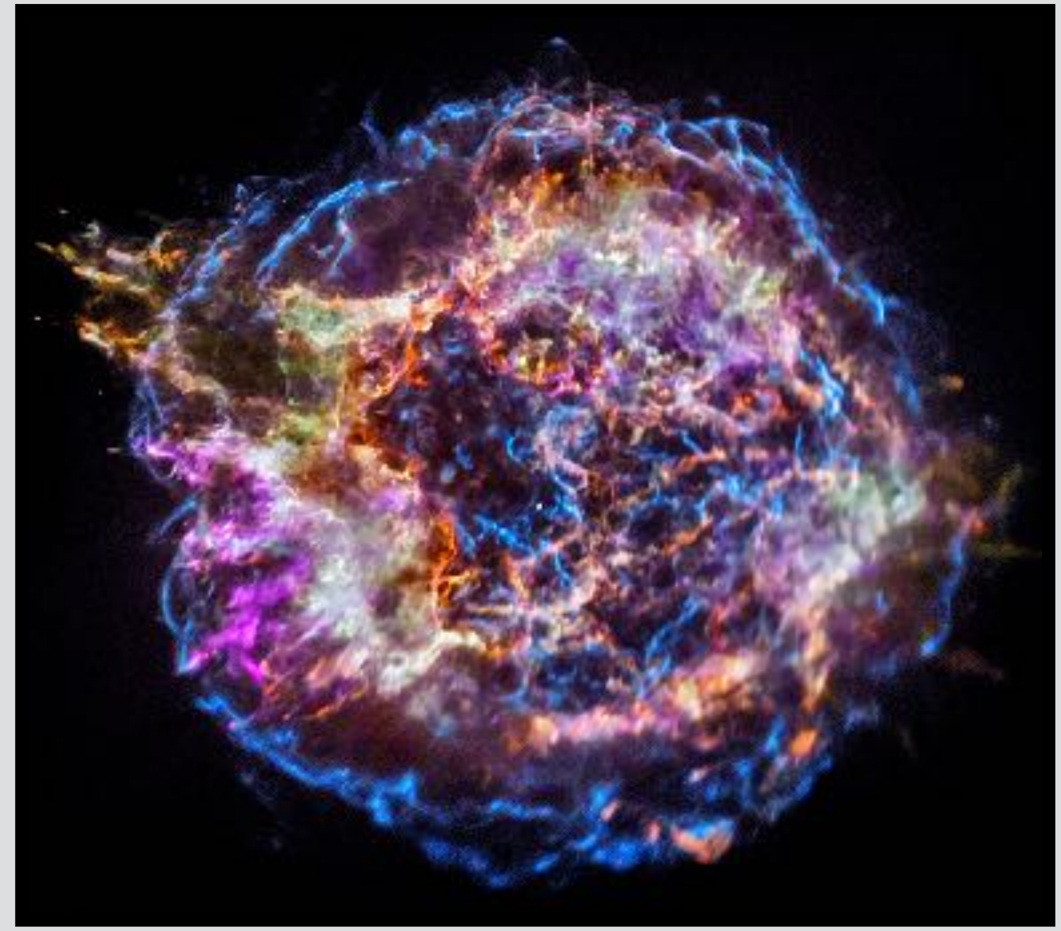
- Thermal emission : continuum + line emission
- Synchrotron emission continuum

How can we obtain distinct maps of the ejecta and synchrotron distributions ?

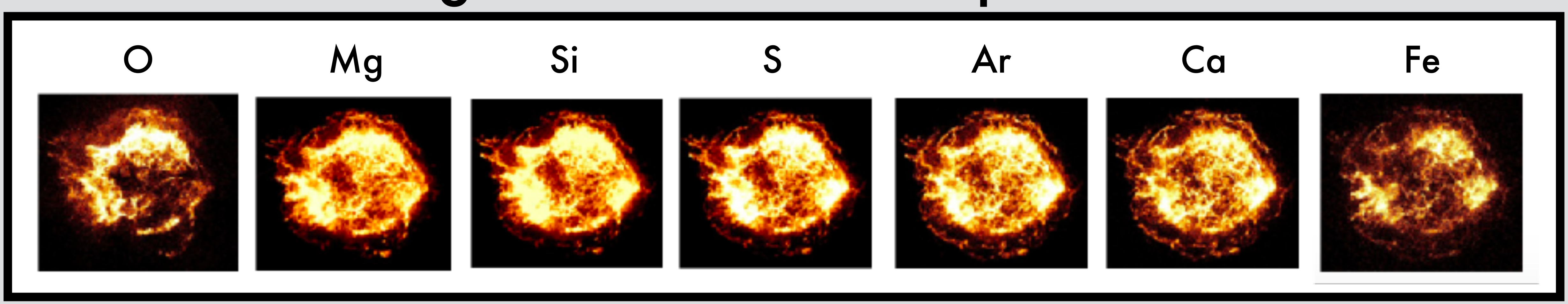
Part I : Methodology

Traditional Analysis Methods





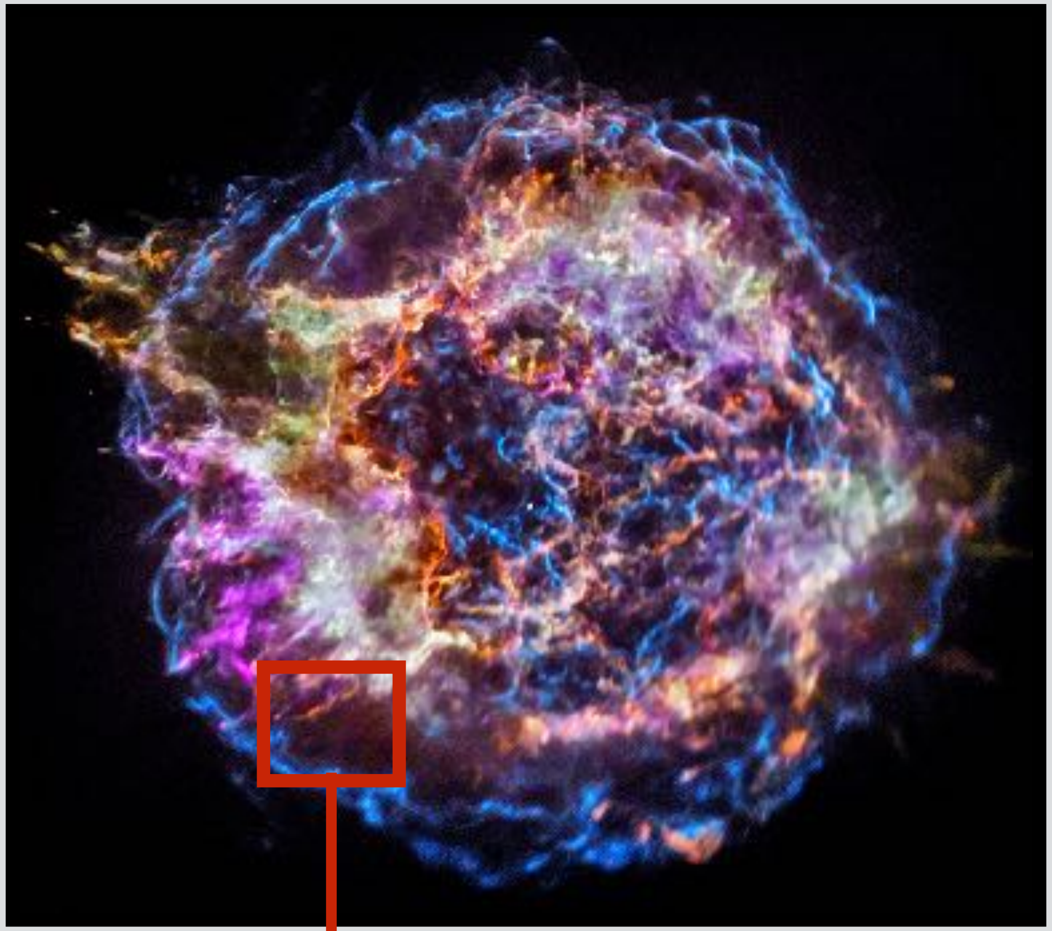
Integration around the peaks :



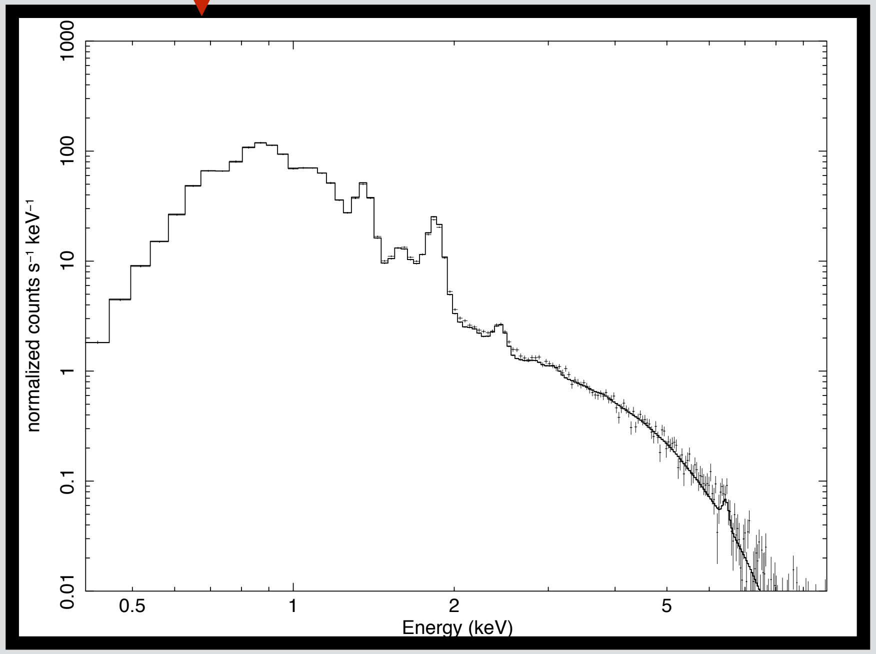
From Lopez et al. (2011)

Traditional Analysis Methods

Spectra are retrieved from small regions for fitting in *Xspec* (spectral modeling package), without leveraging Chandra's great spatial resolution.

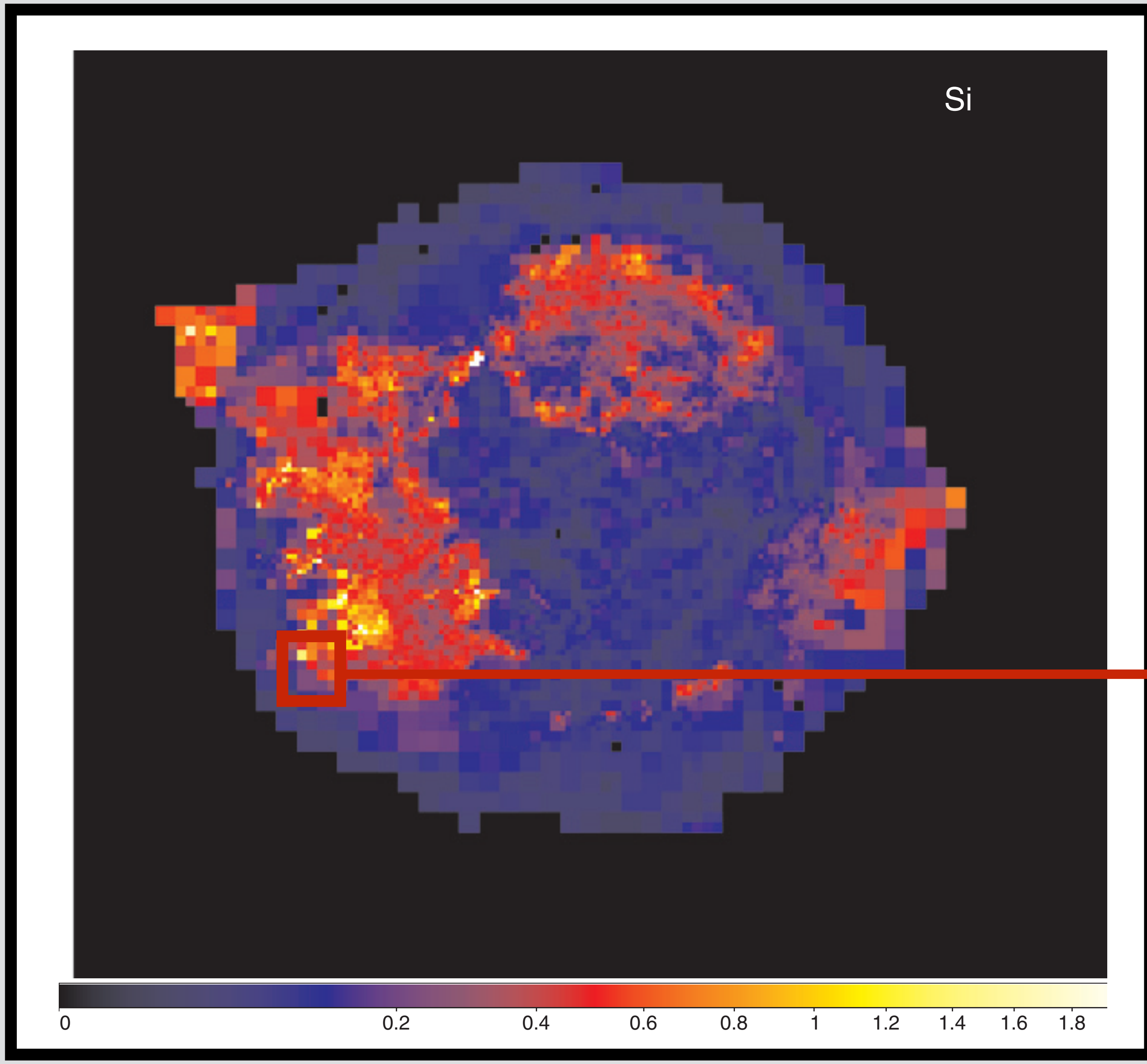


2D, then 1D



Abundances, temperature, nH... Many free parameters for each component in *Xspec*.

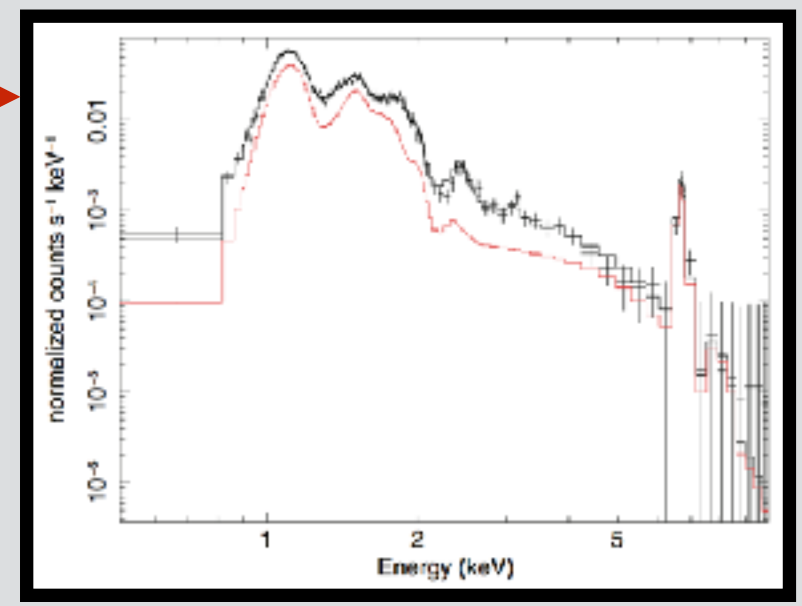
Traditional Analysis Methods



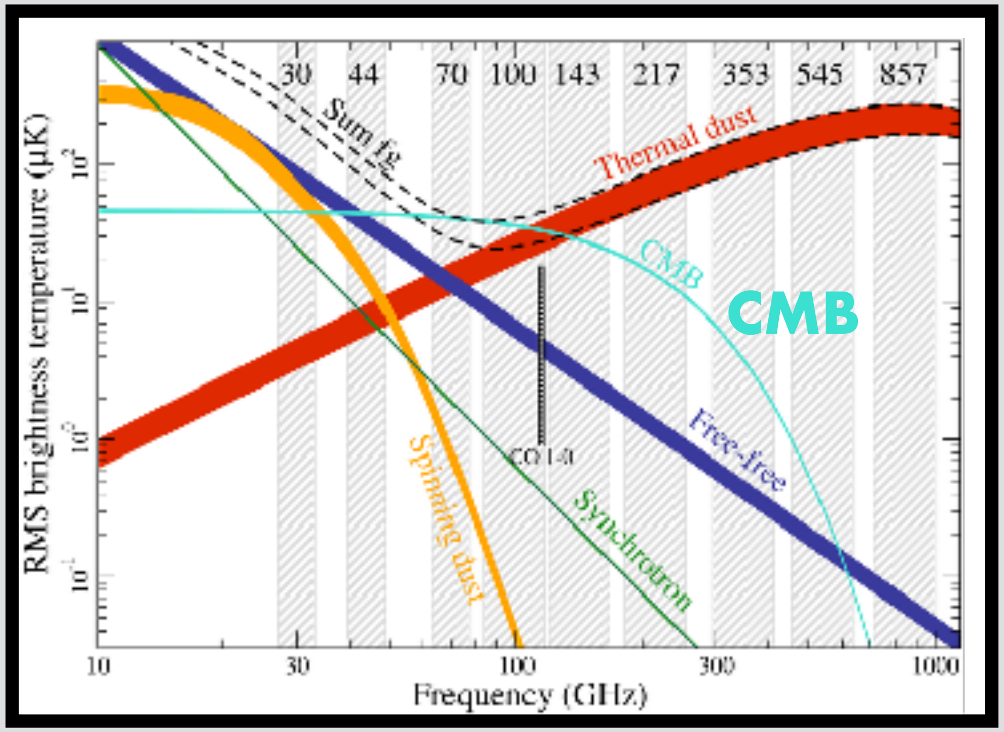
Si abundancy, Cassiopeia A, Hwang et al., 2012

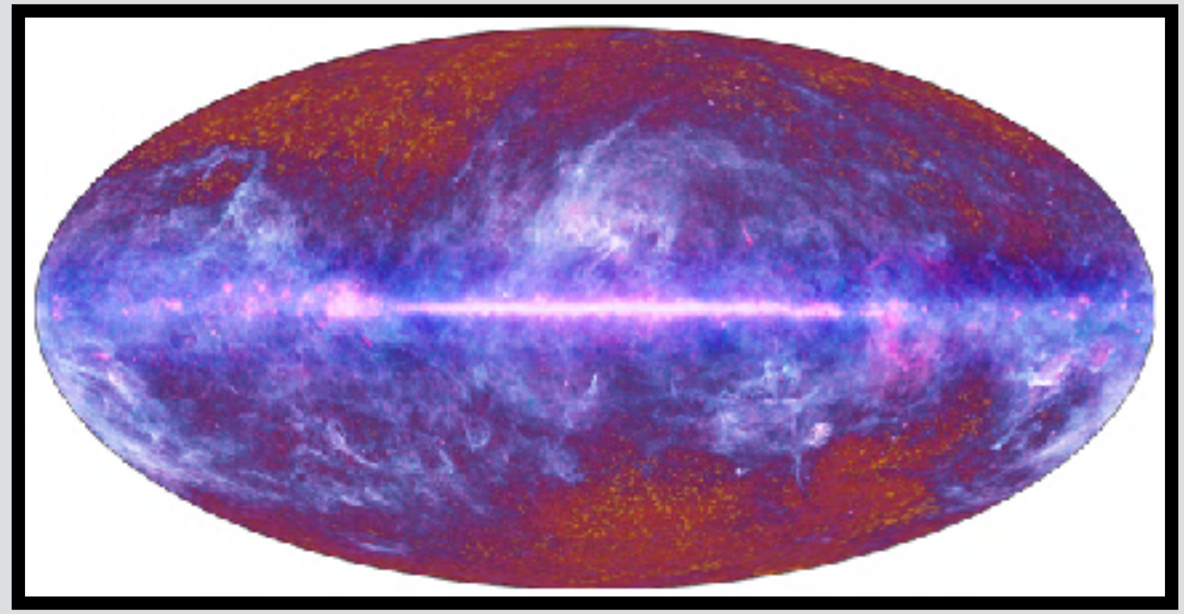
The region definition impacts the spectra.

Adaptative tiling (Voronoï) : defining cells thanks to surface brightness.

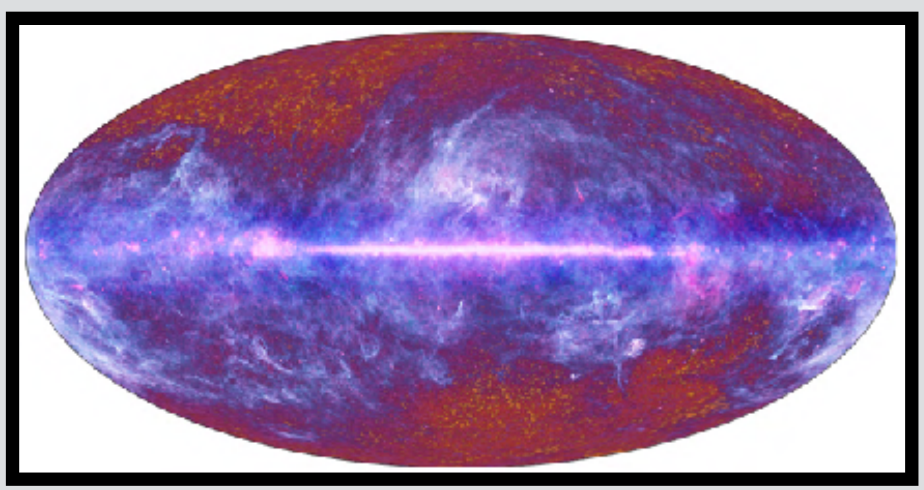


Analogy with the CMB

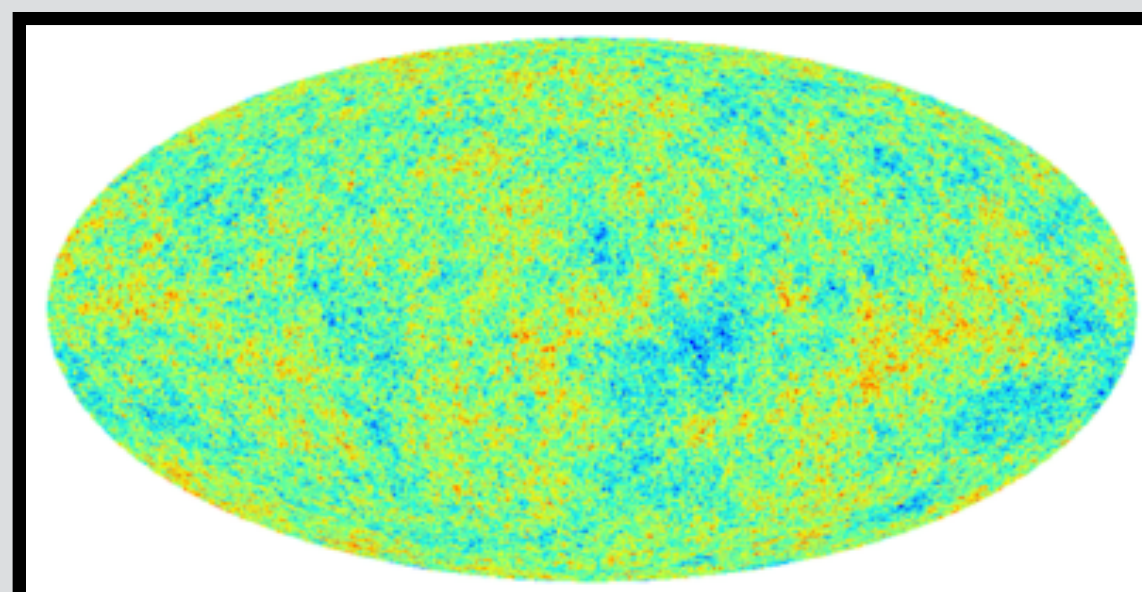




Planck survey of the sky



extraction →

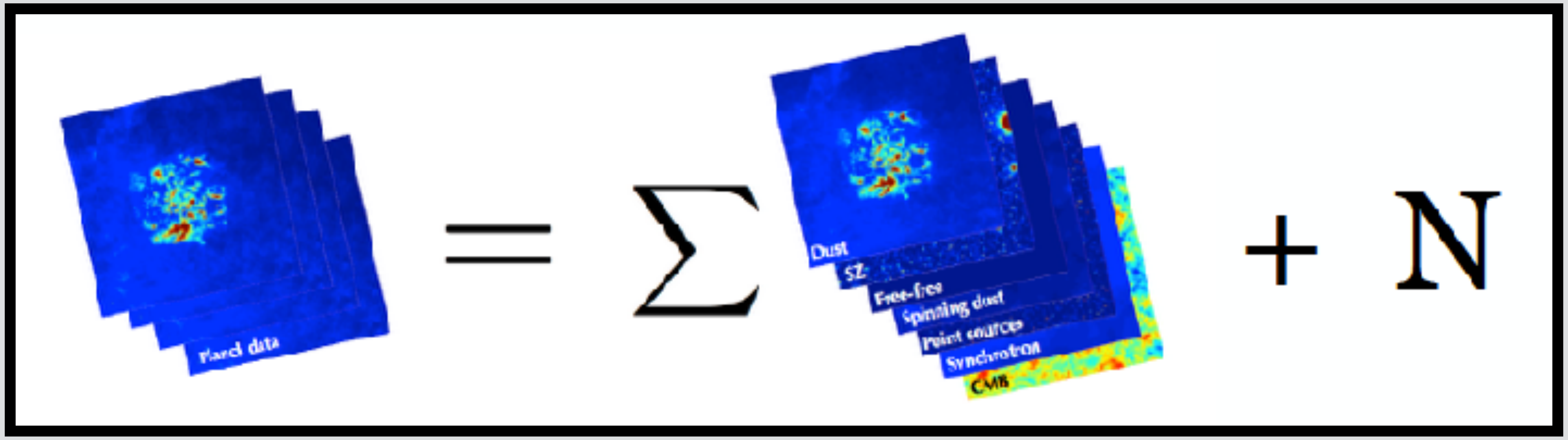


CMB

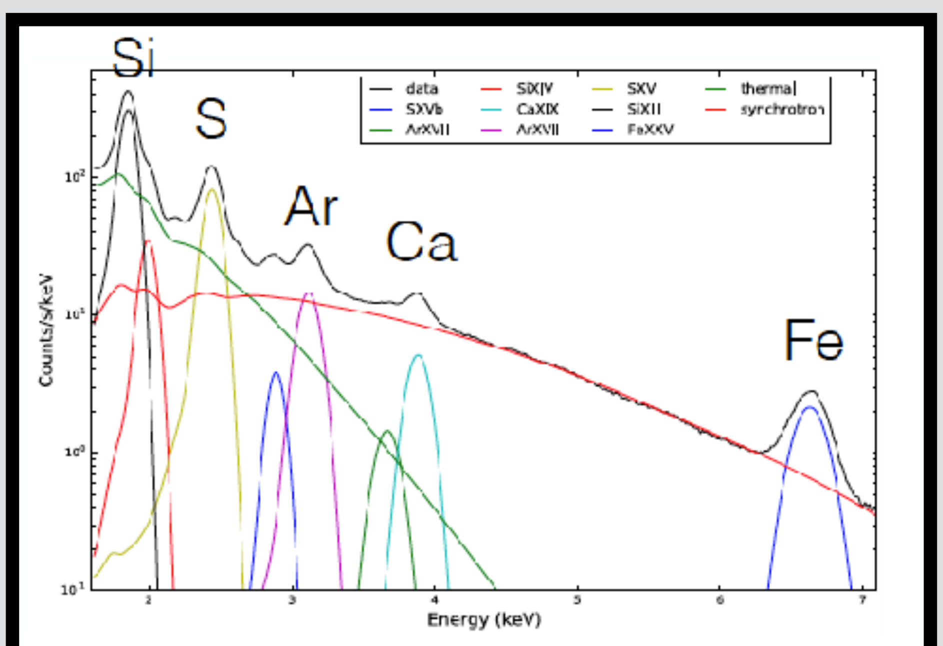
GMCA

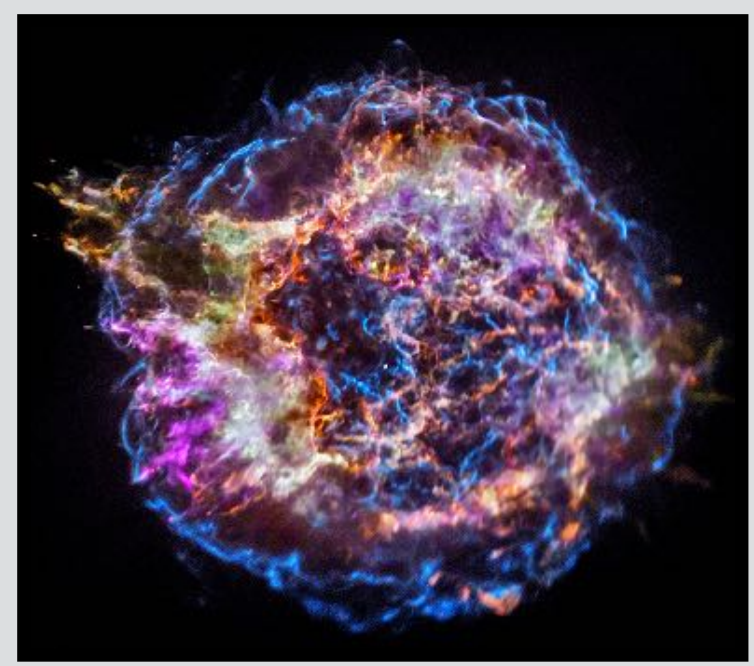
Generalized Morphological Components Analysis

(Bobin et al. 2016)



Blind Source Separation (BSS) algorithm retrieving entangled components from a data set



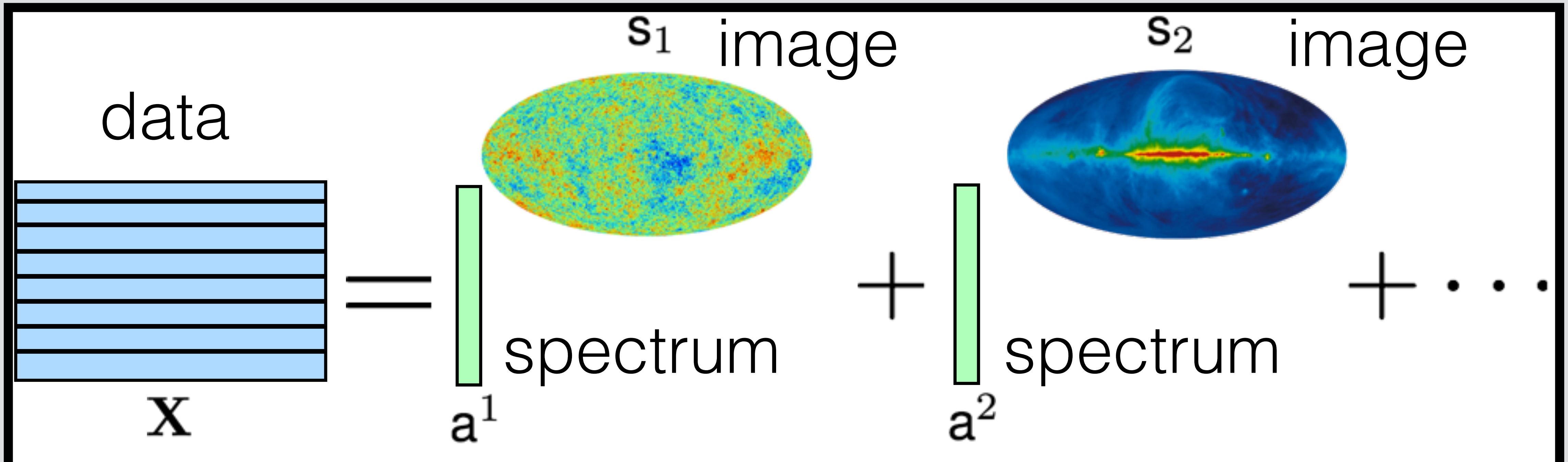


GMCA

Generalized Morphological Components Analysis (Bobin et al. 2016)

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

Blind Source Separation algorithm : The aim is to retrieve n images (x,y) and spectra (E) from the initial (E,x,y) data set without prior instrumental or physical knowledge.



GMCA

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

n is user defined

Without any information on A and S,
this problem is ill-posed (infinite number of solutions).

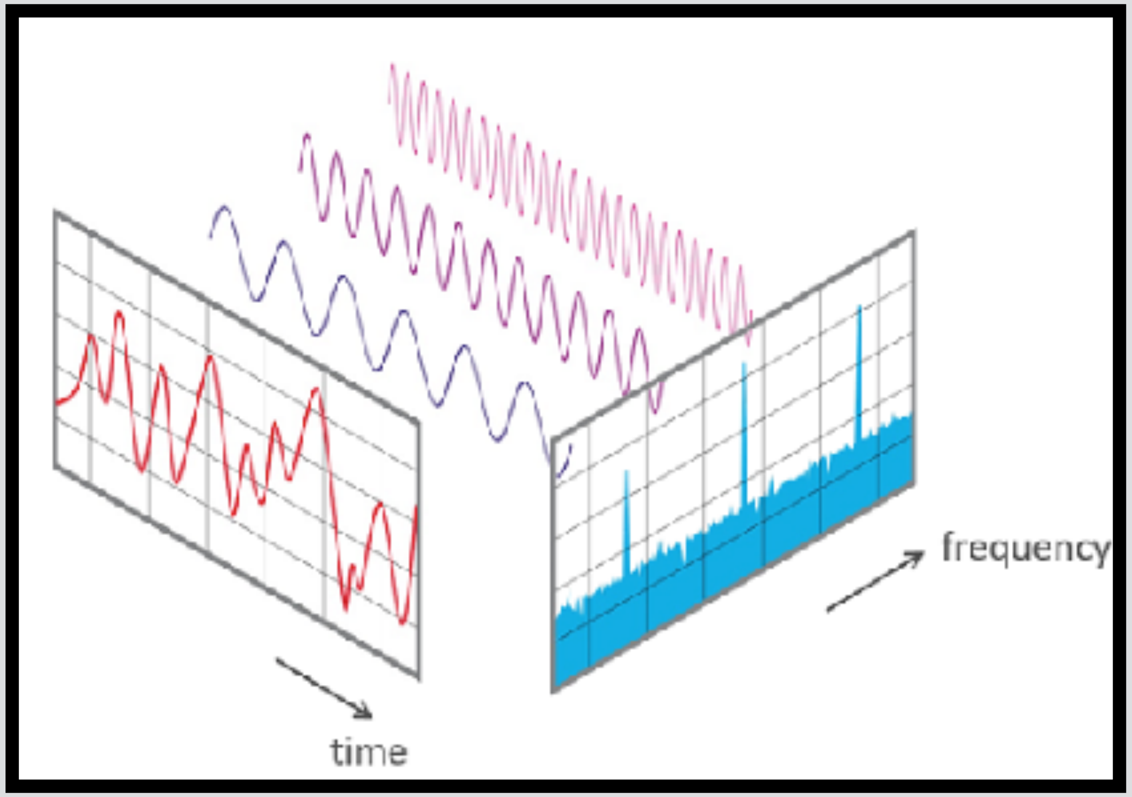
$$\min_{A,S} \|X - AS\|_F^2$$

We need a constraint : sparsity

GMCA

Finding a sparse representation :

Analogy with 1-D :



The Fourier transform allows to describe periodic signals with only a few non zero coefficients.

It makes the different components easier to disentangle by diminishing the overlapping.

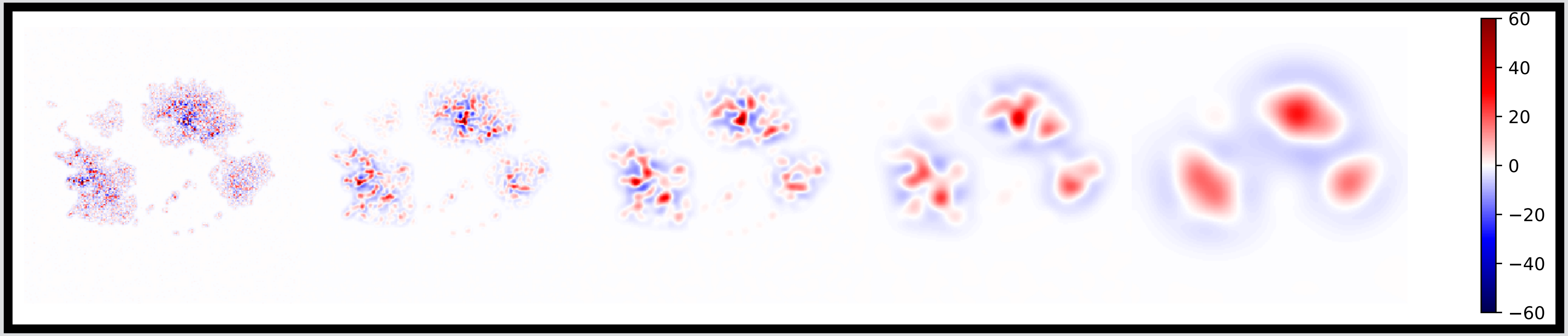
The concept of sparsity

In 2-D :

Wavelet transforms give sparse representations of images. In particular, *Starlets* are well adapted for astrophysical images.

Small scales

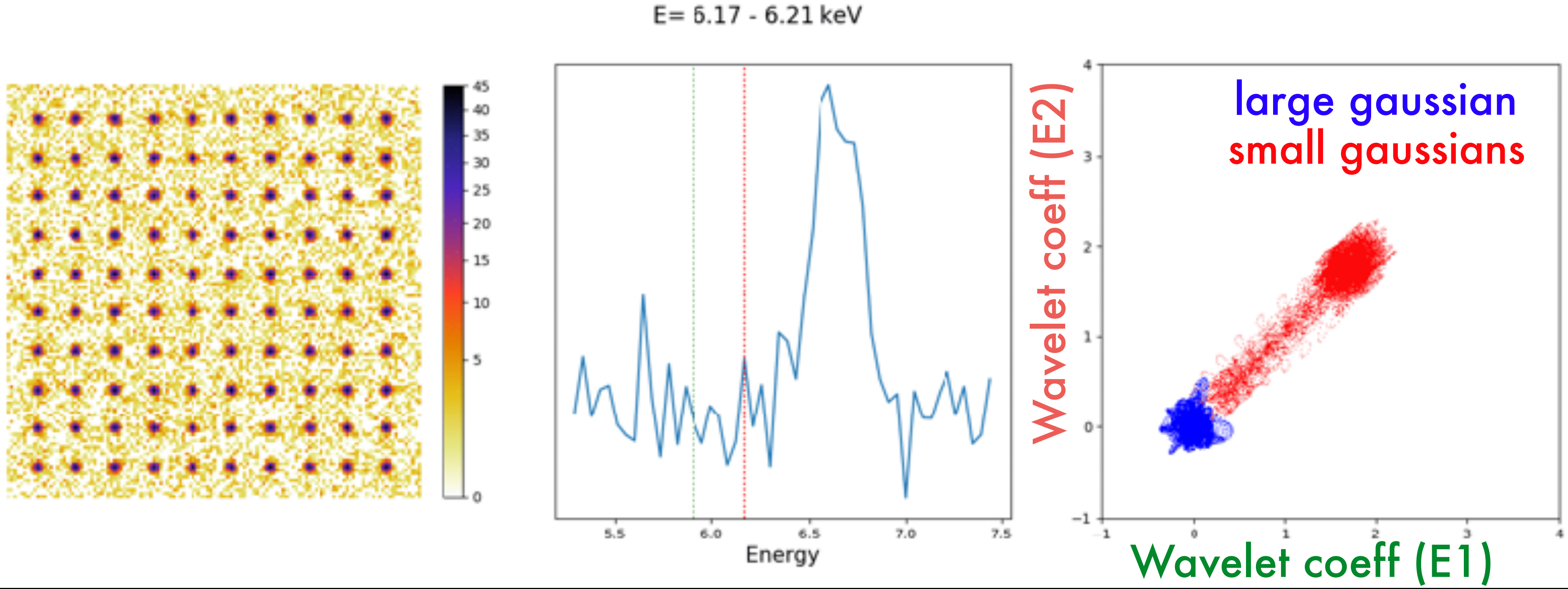
Large scales



Starlet transform of the Fe structure in Cassiopeia A

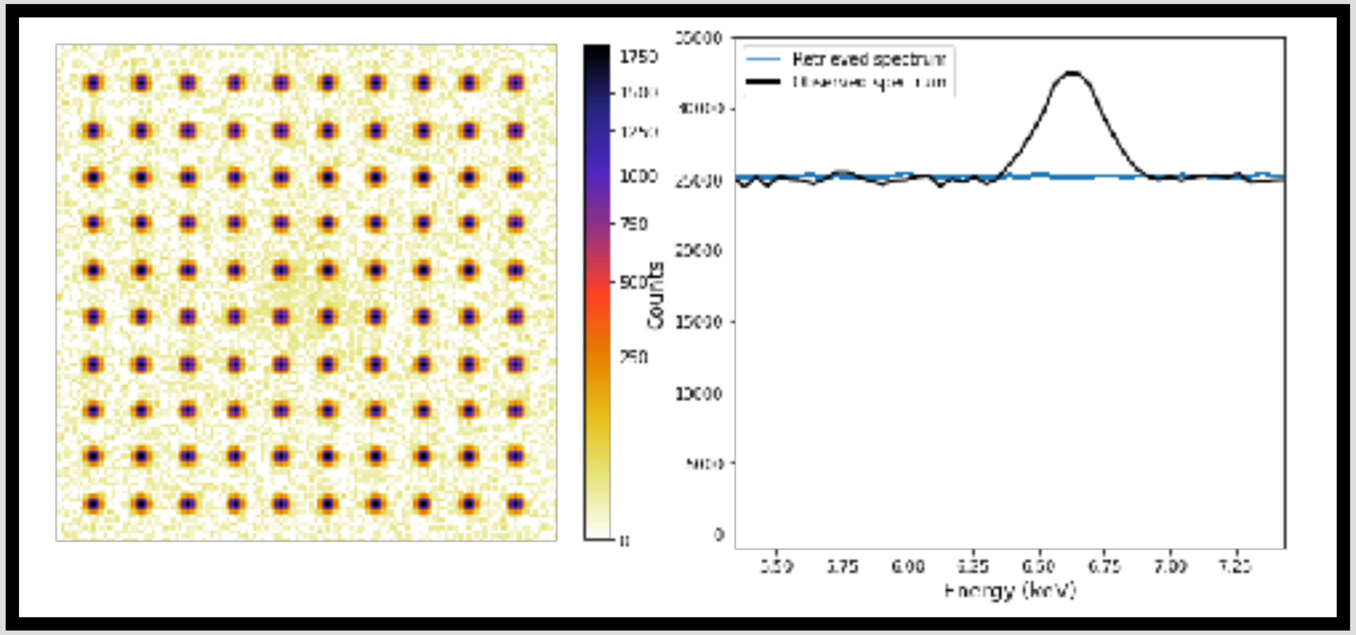
The concept of sparsity

In 2-D :

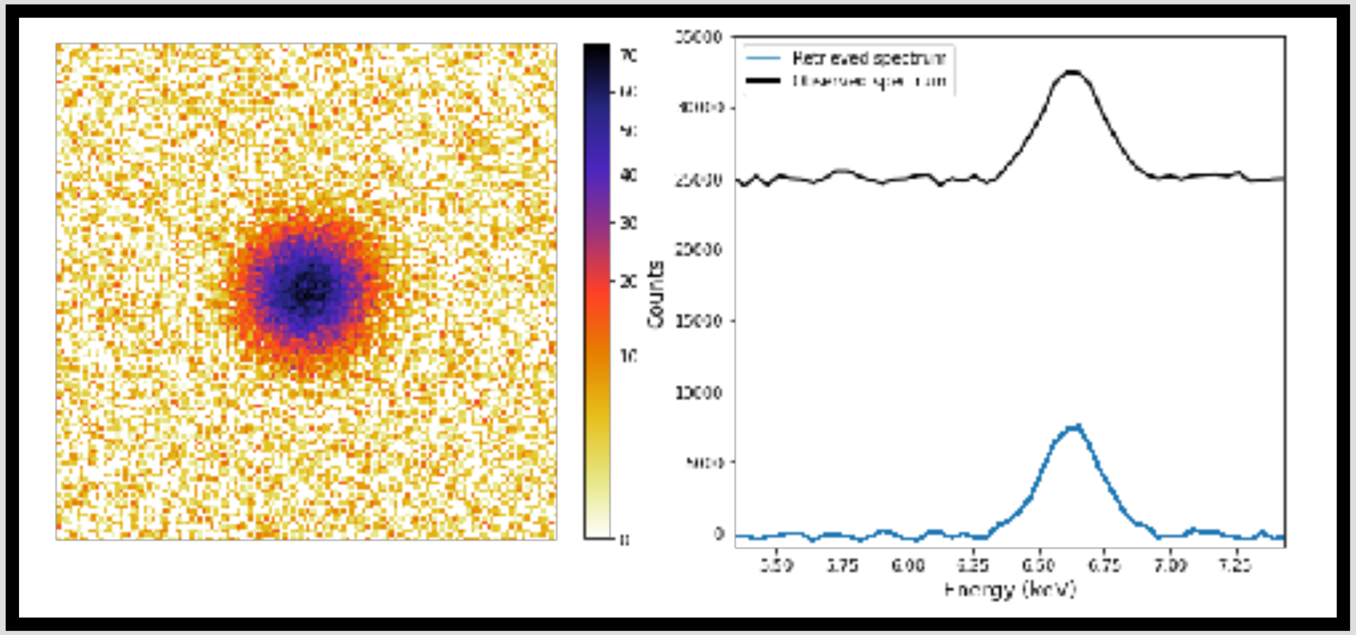


On the right, *Starlet* transform third scale coefficients of gaussians of different sizes

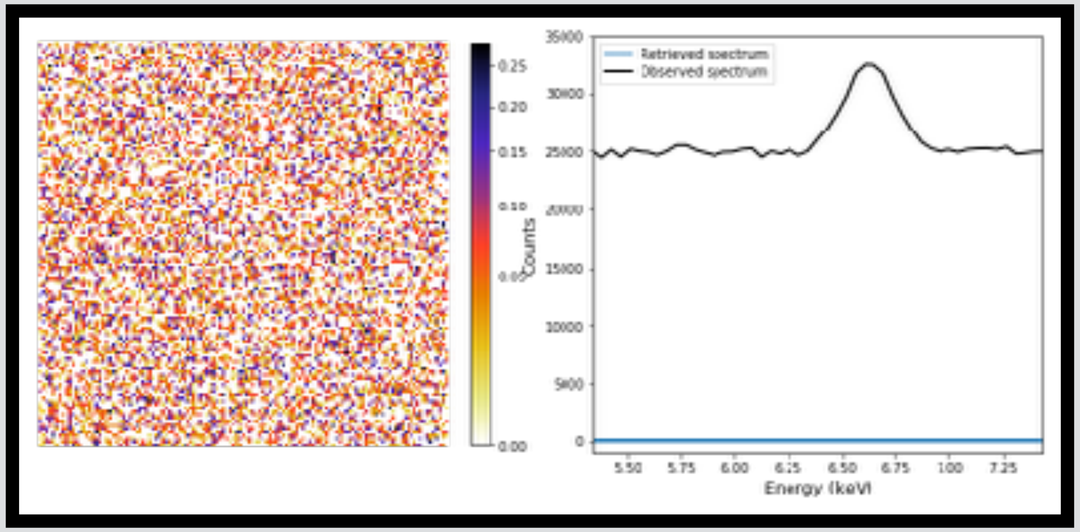
GMCA



A grid of small gaussians with a constant spectrum



A large gaussian with a gaussian spectrum



Noise

GMCA

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

Without any information on A and S,
this problem is ill-posed.

$$\min_{A,S} \| X - AS \|_F^2$$

GMCA

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

With a sparsity constraint term :

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

A constraint using morphological diversity.

GMCA

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

The algorithm is iterative, each iteration containing two steps :

– Step 1: Estimation of S for fixed A, by simultaneously minimizing $\|X - AS\|_F$ and the term enforcing sparsity in the Wavelet domain;
– Step 2: Estimation of A for fixed S by minimizing $\|X - AS\|_F$.

GMCA

Generalized Morphological Components Analysis (Bobin et al. 2016)

First hypothesis : linear decomposition

Second hypothesis : different components have different morphology

Third hypothesis : the noise is gaussian additive

GMCA

Generalized Morphological Components Analysis (Bobin et al. 2016)

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Is it appropriate for X-ray studies ?

GMCA on X-ray data

Generalized Morphological Components Analysis (Bobin et al. 2016)

First hypothesis : linear decomposition

=> Associates mean spectra to retrieved images : every pixel has the same spectrum. Consistent ?

Second hypothesis : different components have different morphology

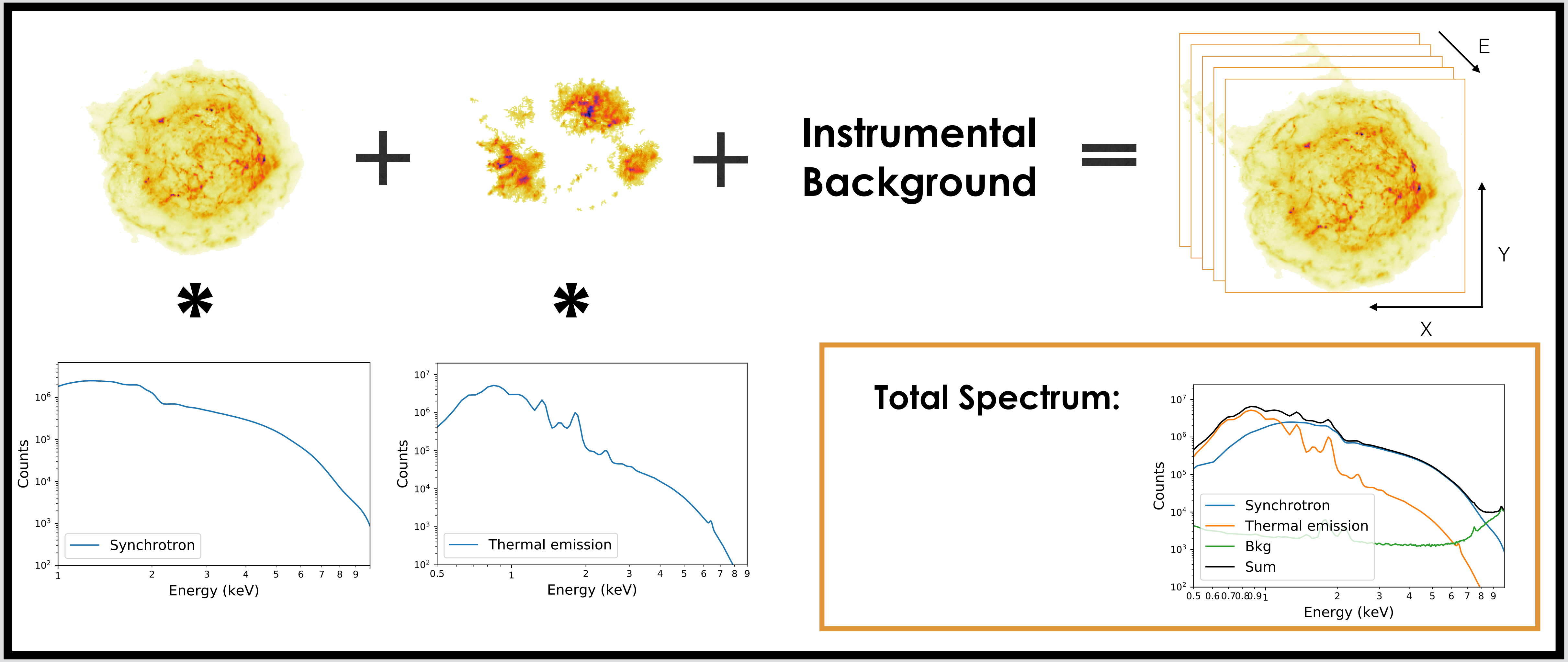
=> Yes for extended sources (filaments, clumps, knots...)

Third hypothesis : the noise is gaussian additive

=> No, the noise is Poissonian in X-rays

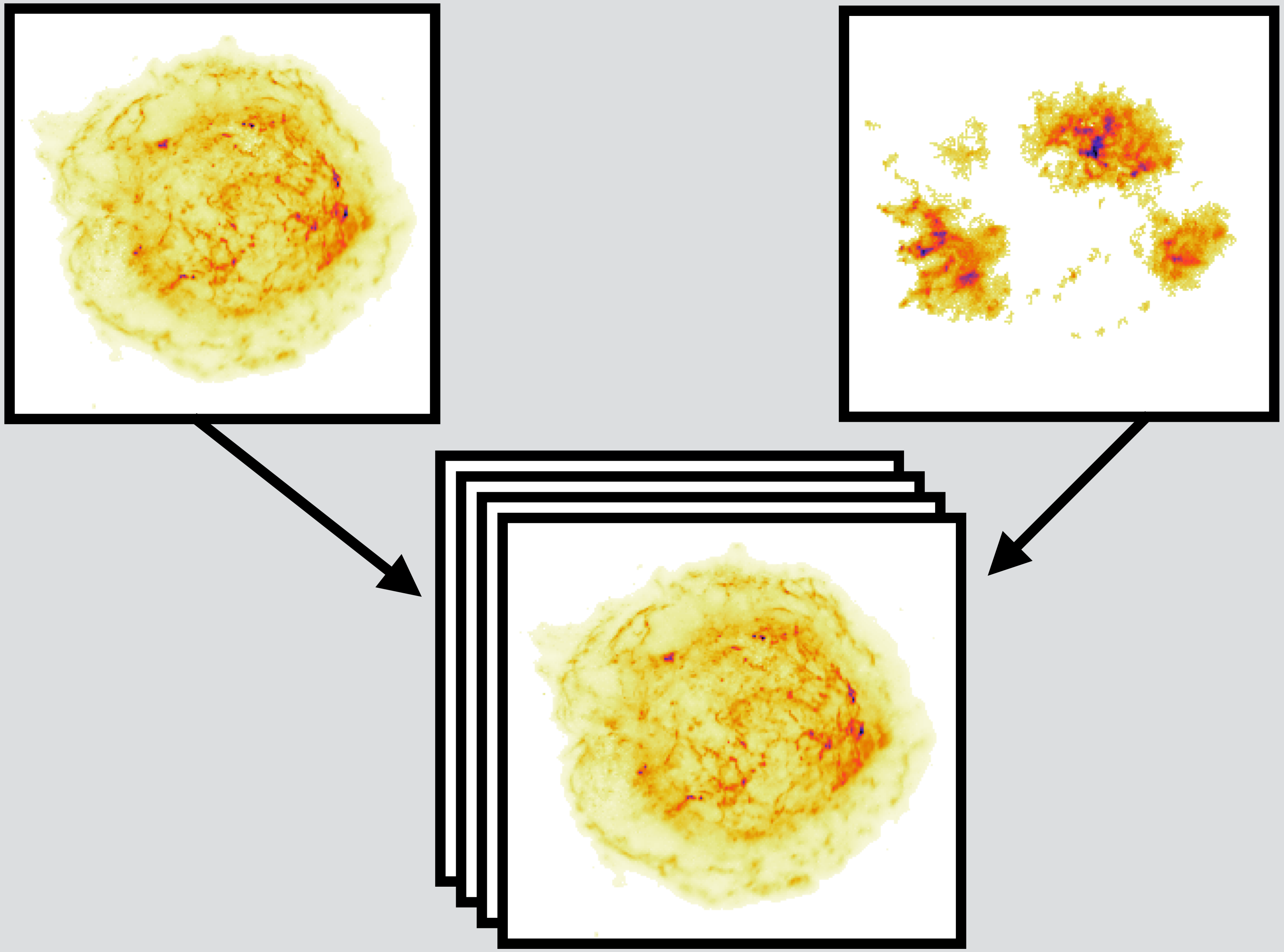
Test on toy models

Our two toy models have two components :



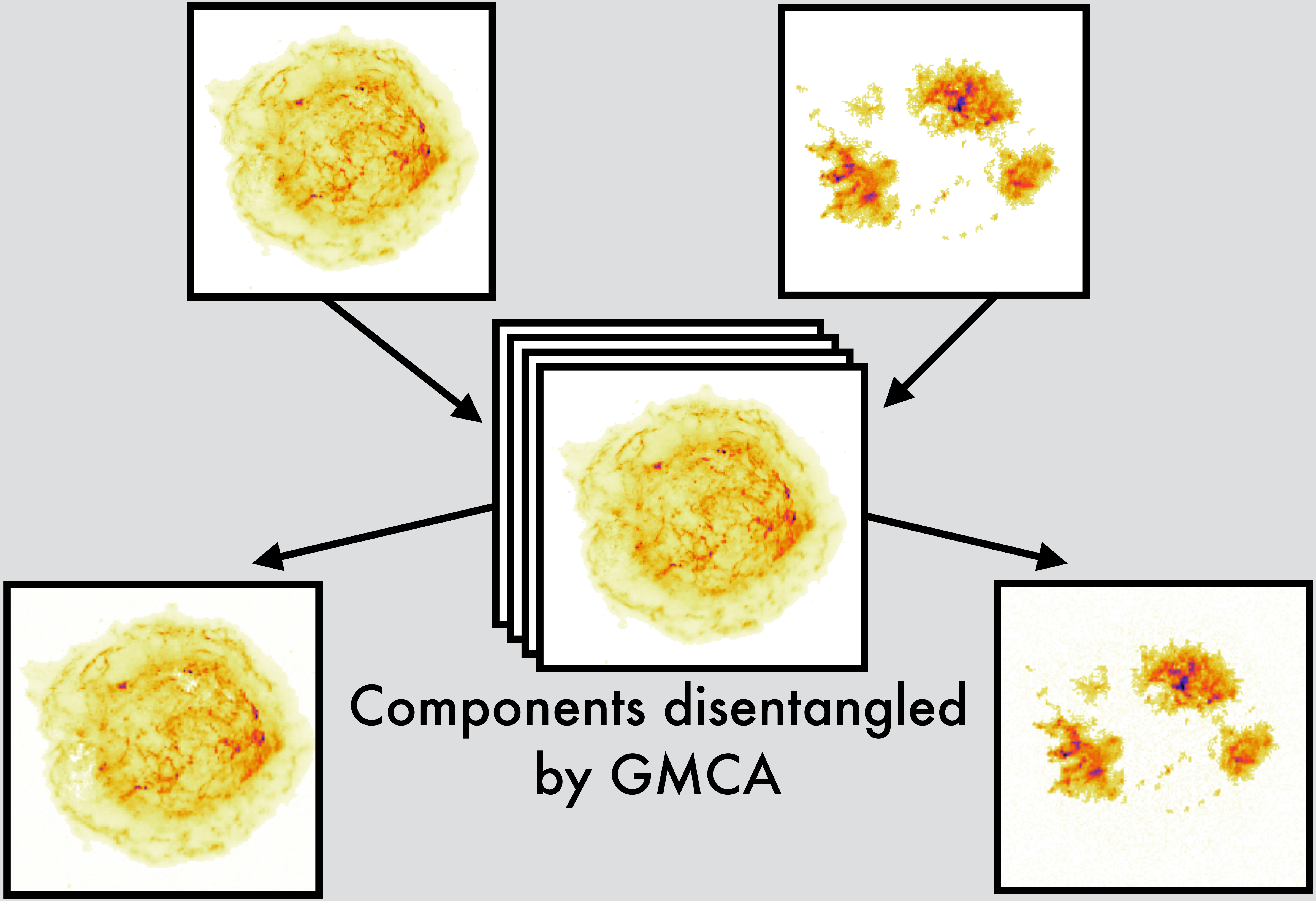
The first component is a synchrotron emission, the second one is either a thermal emission or a line emission. We generate Poisson noise.

Test on toy models

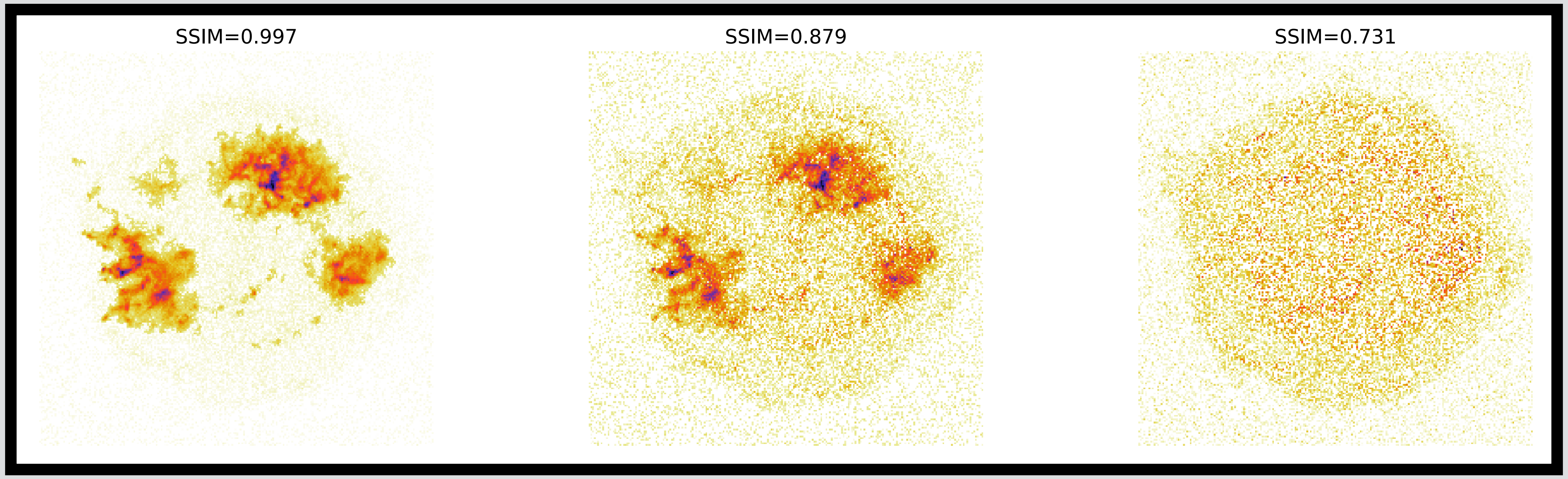


Both components are entangled in our toy model

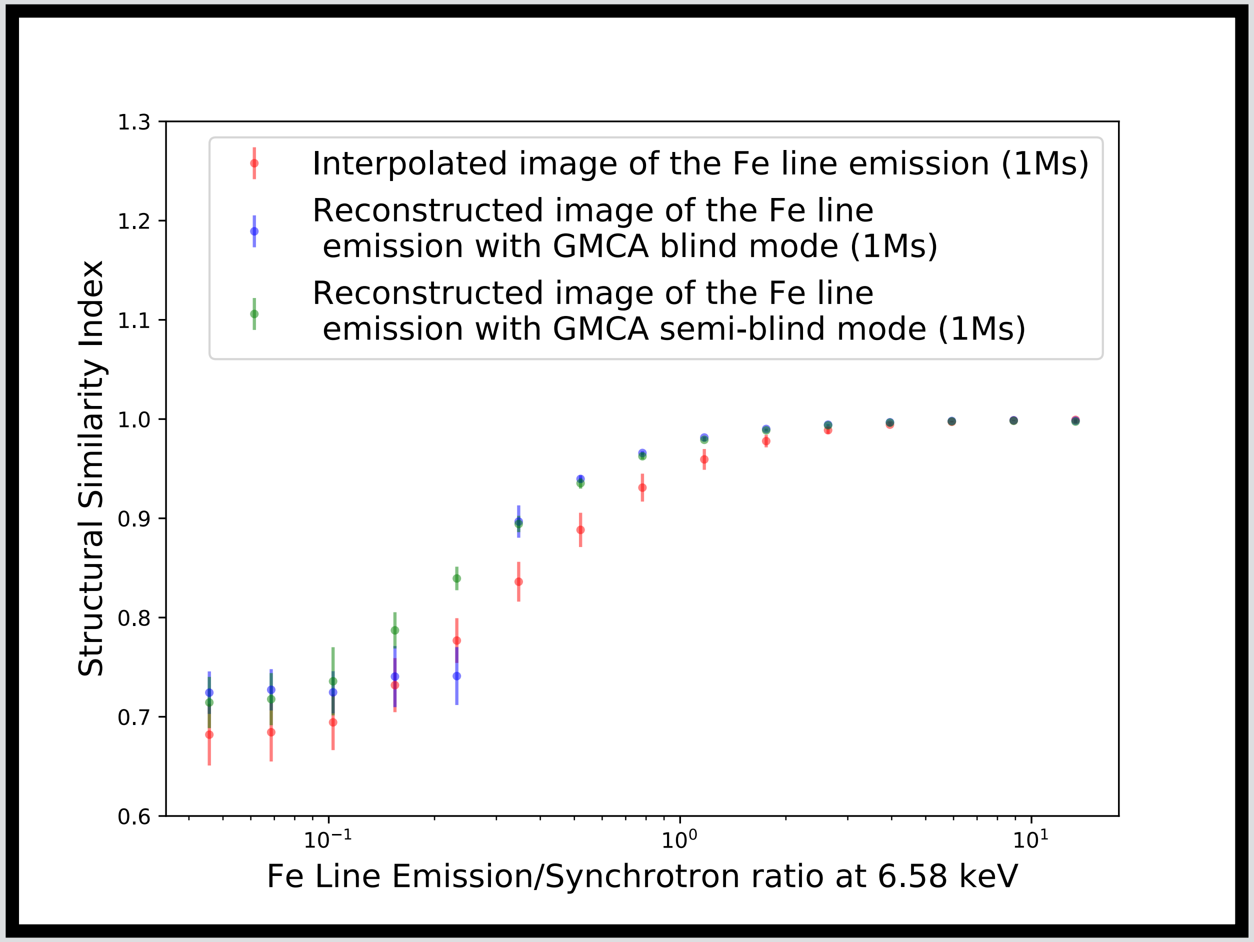
Test on toy models

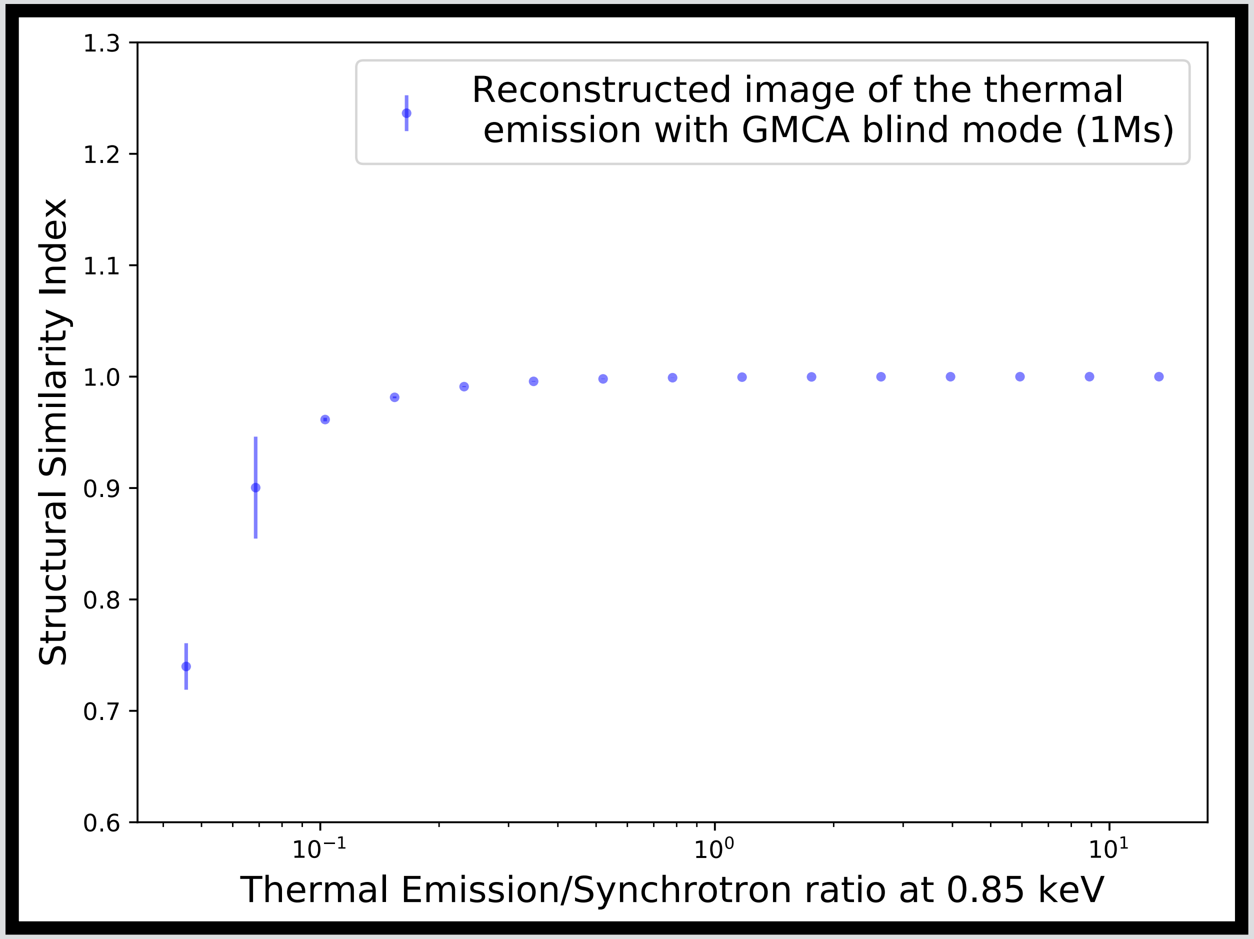


Reconstructed image accuracy



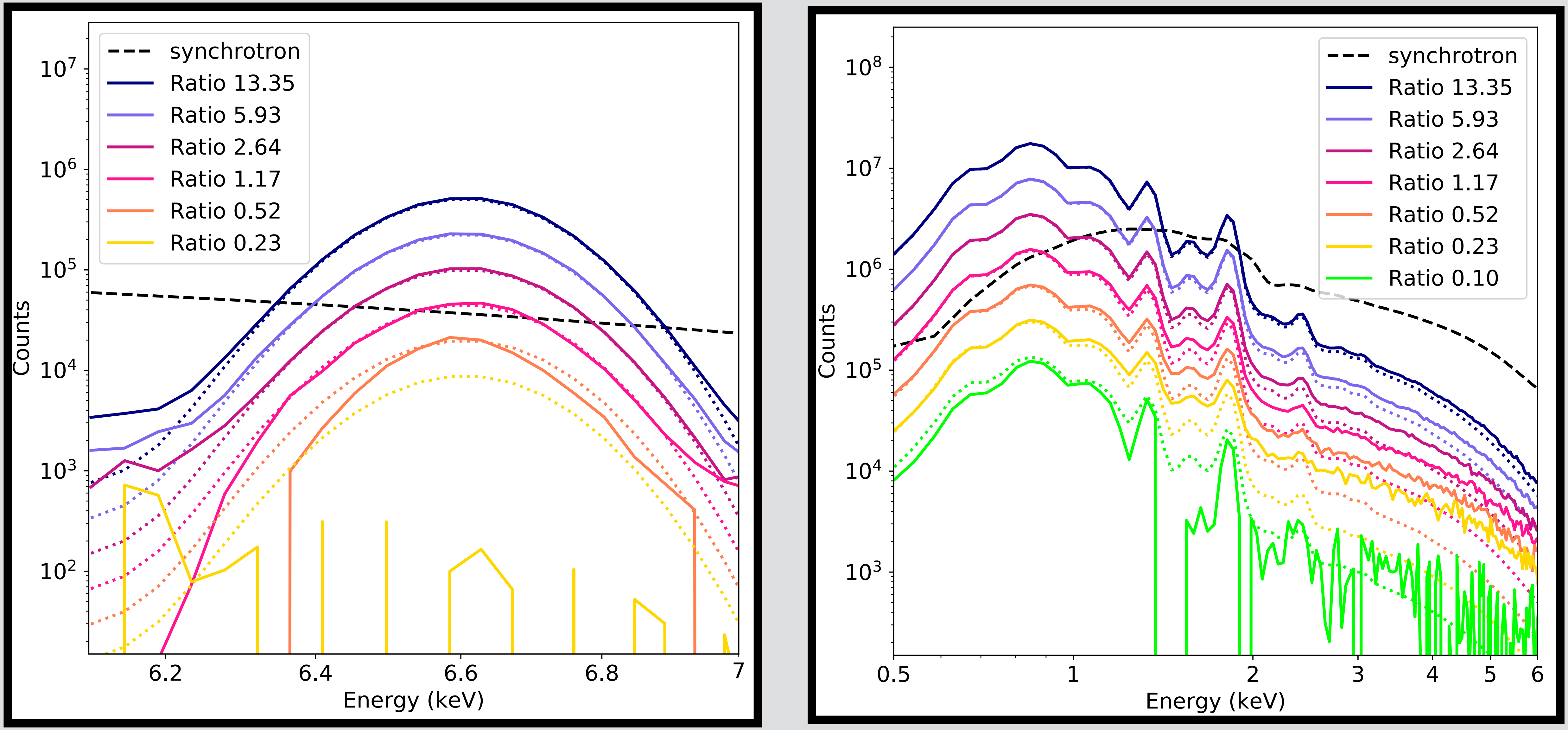
Examples of Structural similarity index (SSIM) coefficients associated with the corresponding images





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

Spectral accuracy



Spectra of second component retrieved by GMCA in both toy models

Dashed lines : theoretical models. On the right, we can see important deviations in high energy from the model.

Test on real data of Cas A

Ca line emission :

Integration on 3.75-3.95 keV

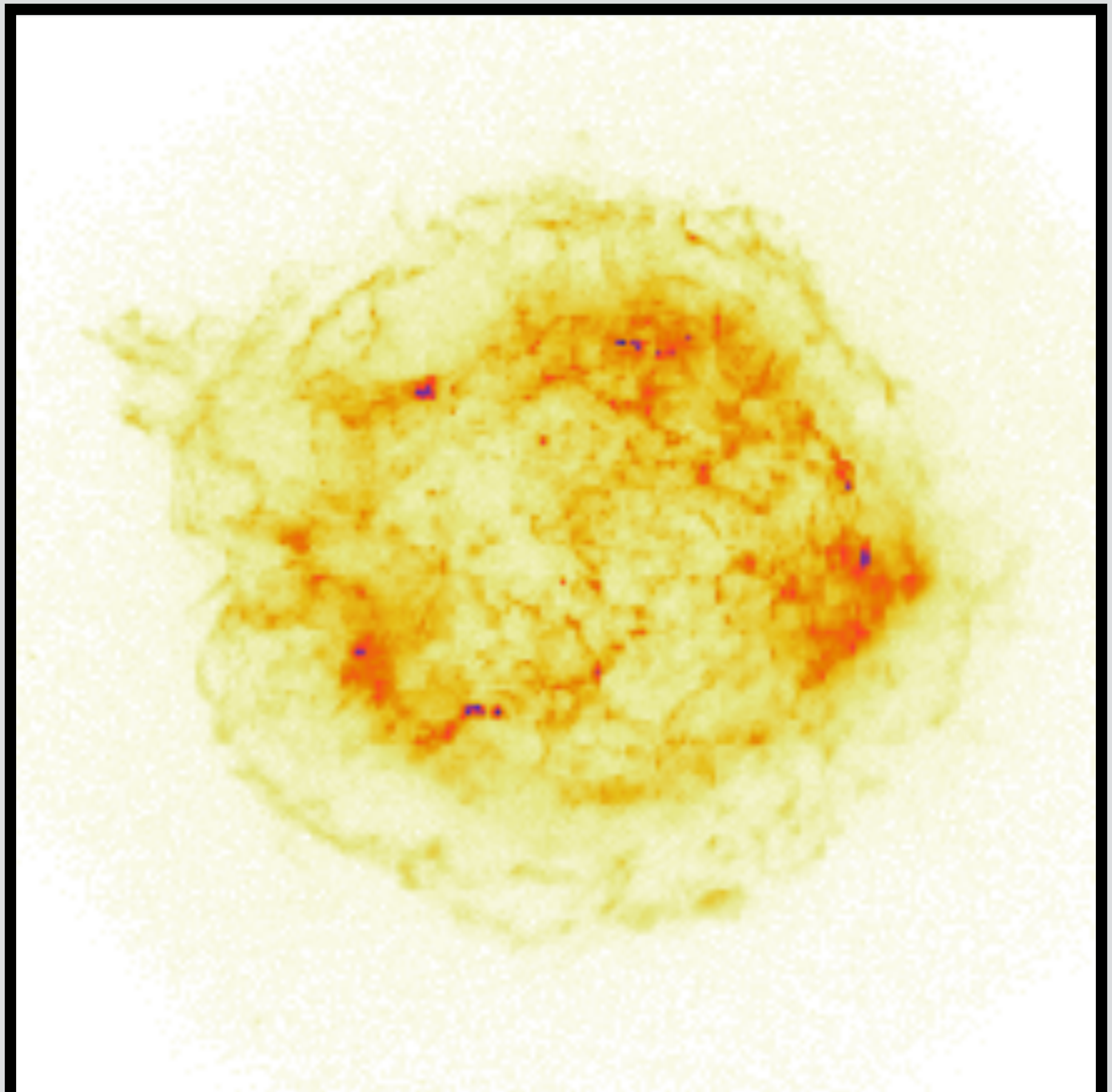


Image in square root scale

Test on real data of Cas A

Ca line emission :

GMCA on 3.6-4.1 keV

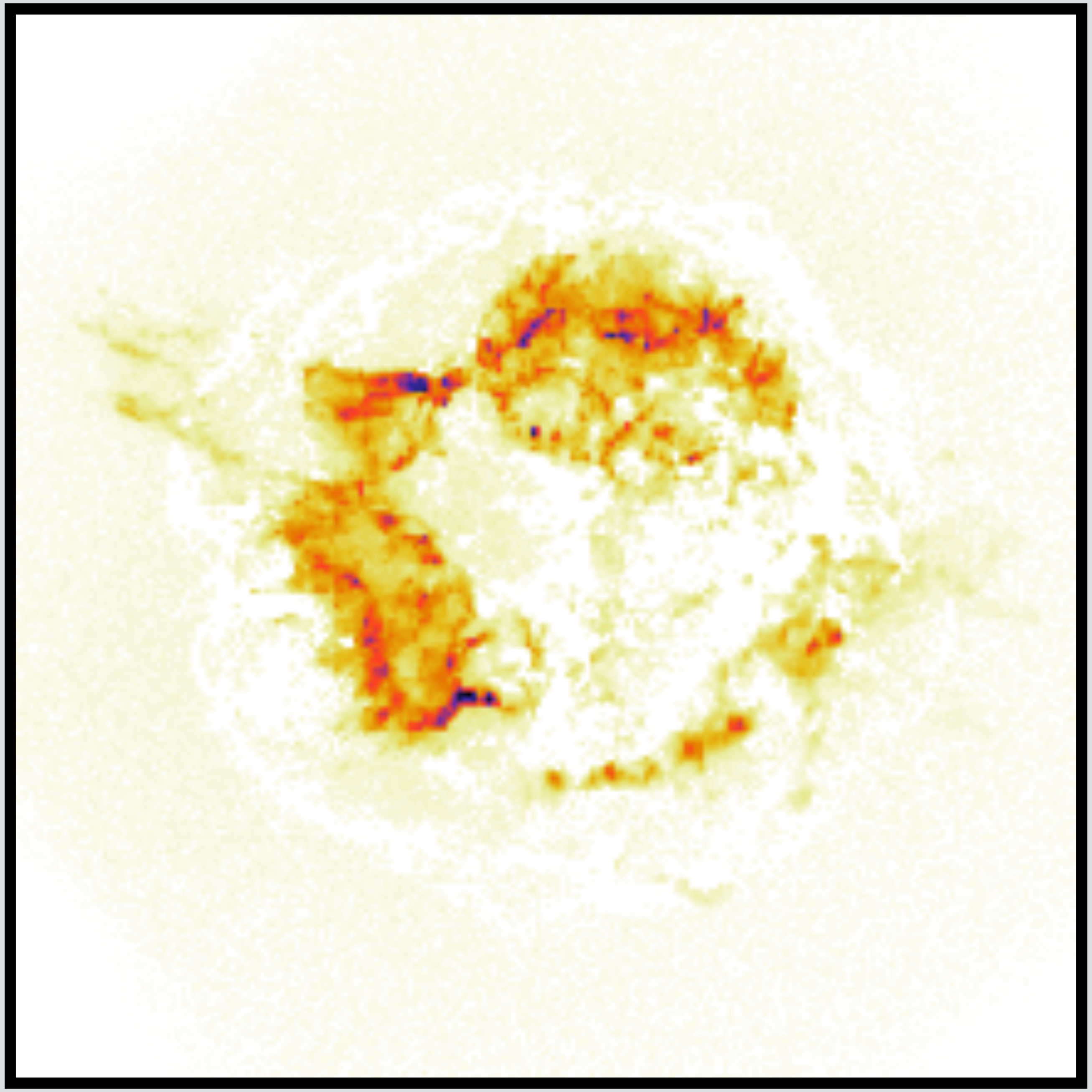
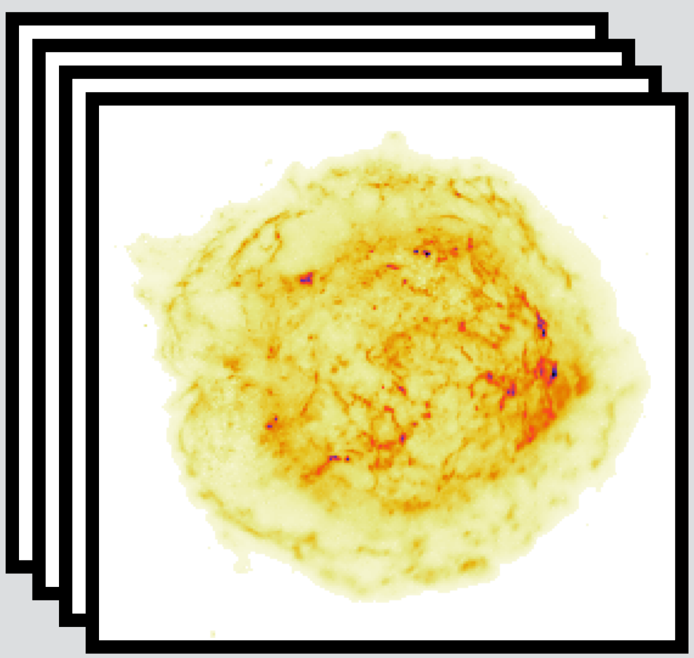


Image in square root scale

Application on real data of Cas A

Application to the data cube between 5 and 8 keV :

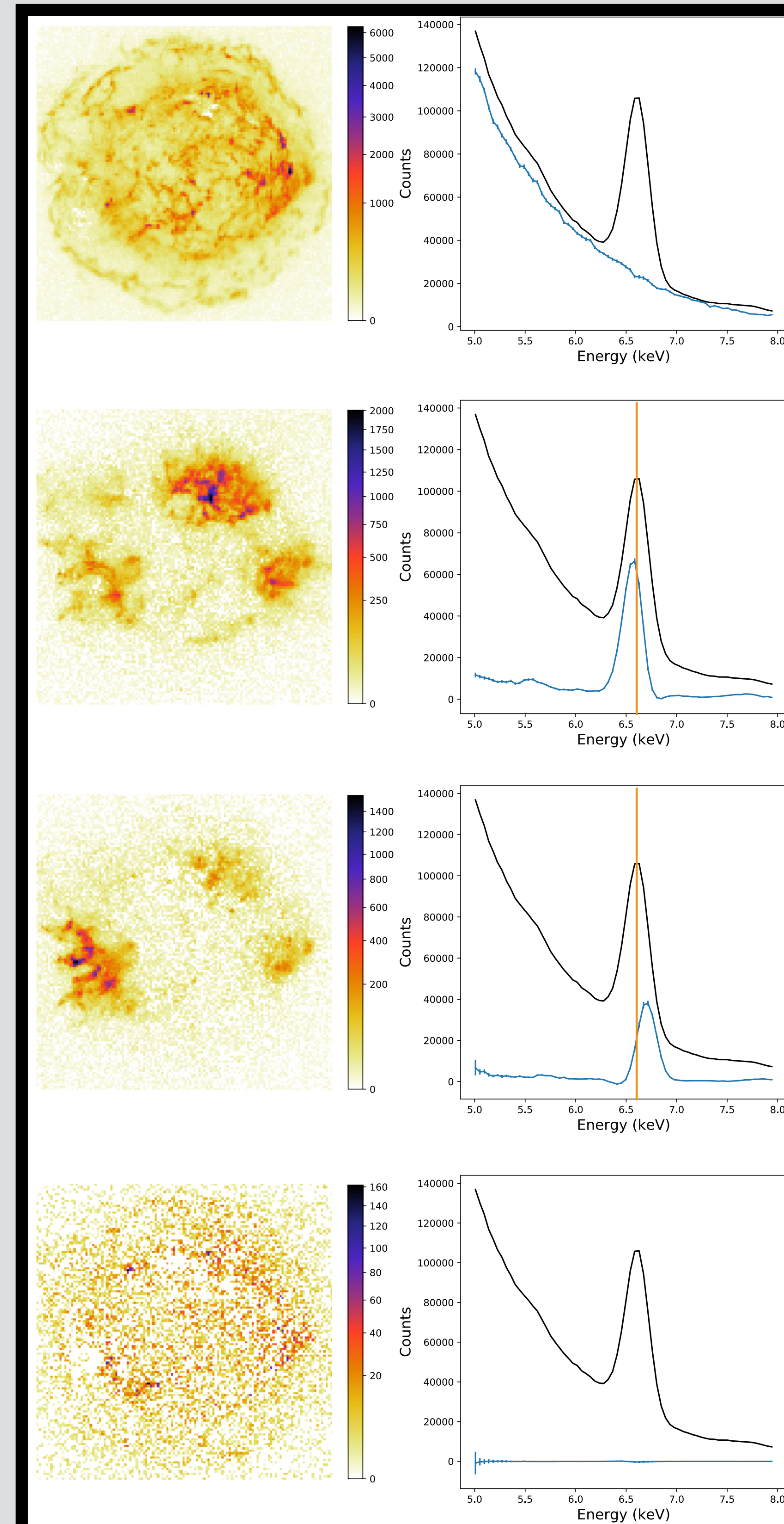


Synchrotron

Red-shifted Fe structure

Blue-shifted Fe structure

Noise



GMCA

Generalized Morphological Components Analysis (Bobin et al. 2016)

First hypothesis : linear decomposition

=> Associates mean spectra to retrieved images.
Consistent results !

Second hypothesis : different components have different morphology

=> Yes for extended sources (filaments, clumps, knots...)

Third hypothesis : the noise is gaussian additive

=> No, the noise is Poissonian in X-rays.
But the results are consistent nonetheless.

Akaike Information Criterion

How can we choose *n*, the number of components to retrieve ?

Akaike Information Criterion

How can we choose *n*, the number of components to retrieve ?

The algorithm being fast-running, the best solution is to try different values of *n*.

The minimum of the Akaike Information Criterion (AIC) can help to determine a good number of components :

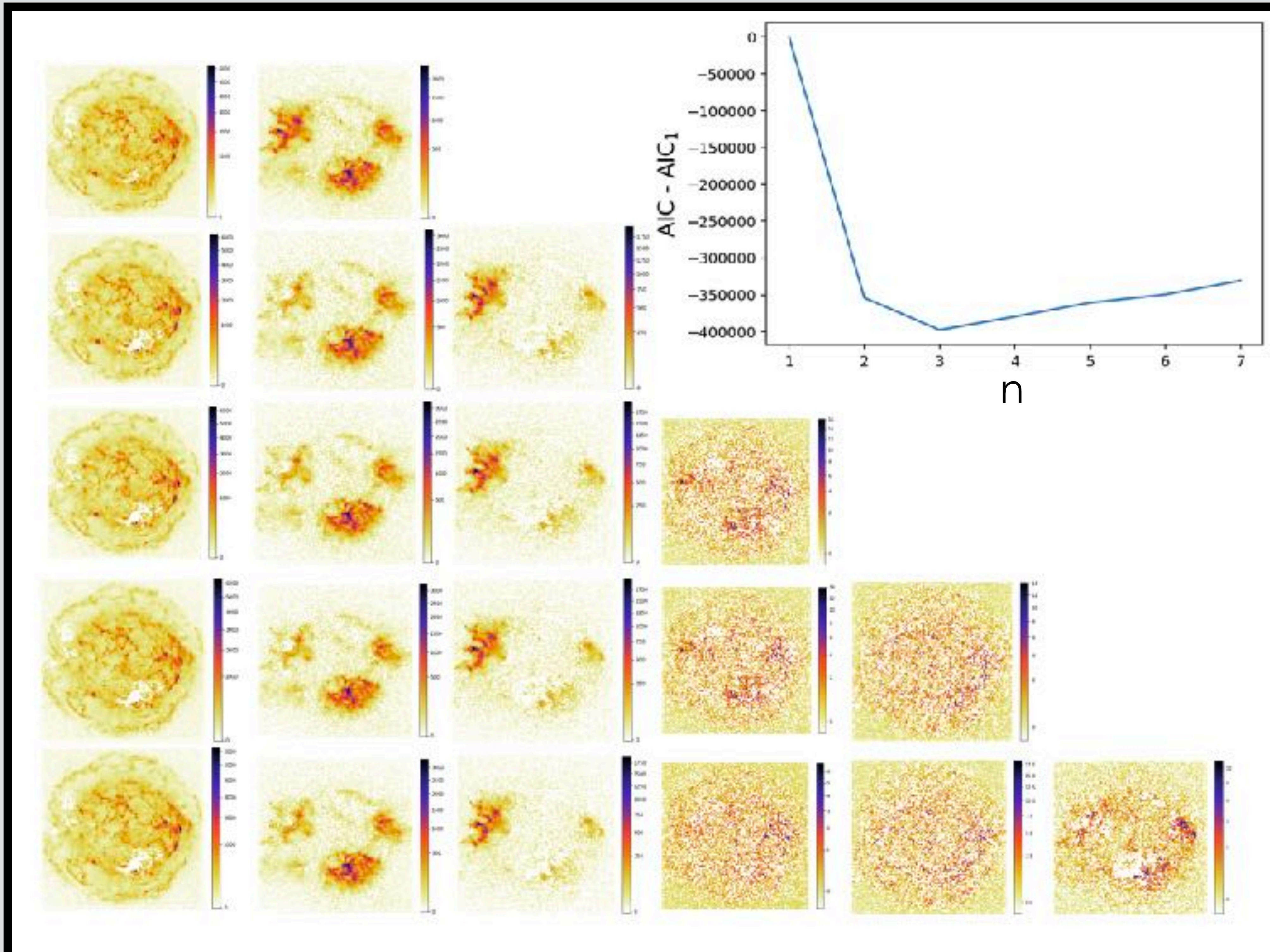
$$AIC = n \times C - 2\ln(L)$$

complexity of the model proportional to n

goodness of fit

Akaike Information Criterion

n



Components retrieved in the real data of Cas A depending on *n*, and the corresponding AIC

pGMCA

(Bobin J., El Hamzaoui I., Picquenot A., Acero F.)

A brand new version of GMCA has been developed during this thesis to take into account Poissonian noise.

The linear model $X = AS + N$ is replaced by the probability for a given sample to take the value $X[elem]$, given by the Poisson law :

$$\mathcal{P}(X[elem] | AS_{direct}[elem]) = \frac{e^{-AS_{direct}[elem]} AS_{direct}[elem]^{X[elem]}}{X[elem]!}$$

pGMCA

pGMCA needs every wavelet scale to reconstruct S in the pixel domain between each iteration in order to calculate the likelihood.

The $\min_{A,S} \|X - AS\|_F^2$ term is replaced by the

Poisson likelihood $\mathcal{L}(X, AS_{direct})$

The implementation is still iterative, but a preliminary GMCA is needed to make a first guess, as pGMCA is very sensitive to the initial conditions.

pGMCA

First hypothesis : linear decomposition

=> Associates mean spectra to retrieved images : every pixel has the same spectrum. Consistent results !

Second hypothesis : different components have different morphology

=> Yes for extended sources (filaments, clumps, knots...)

Now the Poissonian noise is properly handled !

Errorbars with real data

In order to fit the spectra with physical models, we need errorbars associated with the retrieved spectra.

Errorbars with real data

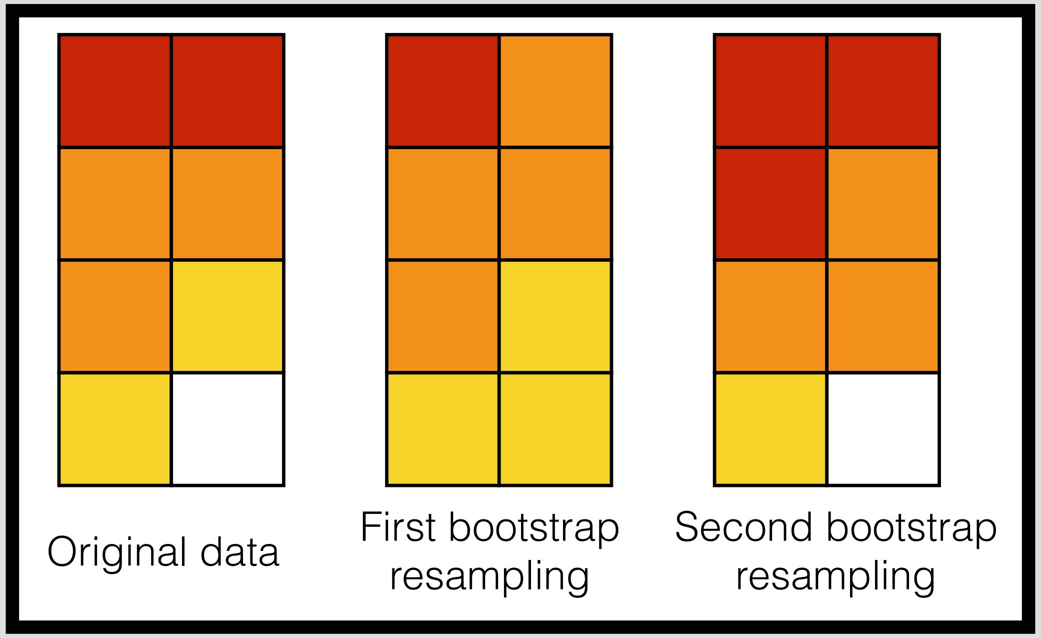
In order to fit the spectra with physical models, we need errorbars associated with the retrieved spectra.

However, the count distribution of the disentangled components are not of a Poissonian nature.

How can we obtain errorbars from a single dataset ?

Bootstrap

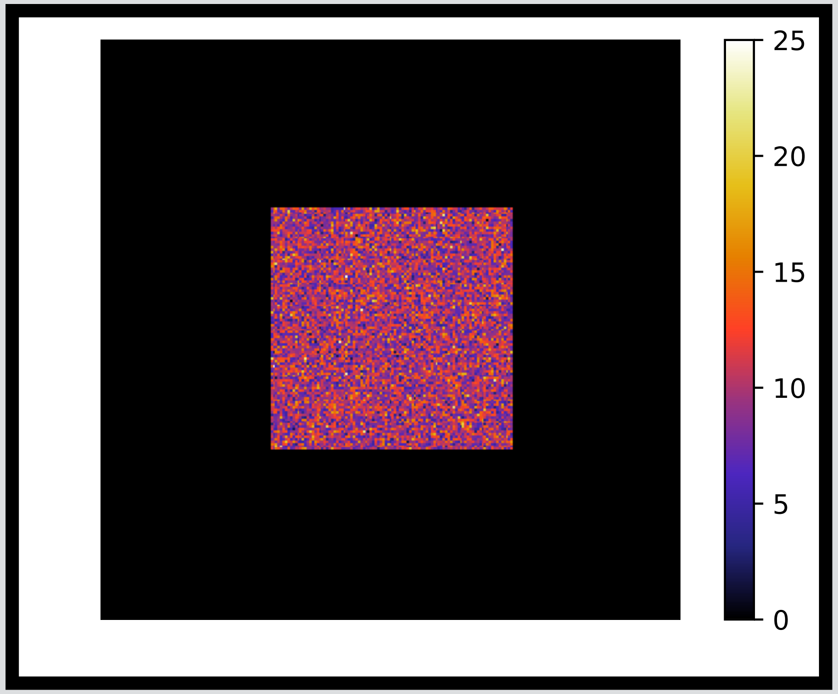
The Bootstrap is a statistical method consisting of a random sampling with replacement from a current set of data. In our case, the events are the detected photon characterized by the triplet (x,y,E).



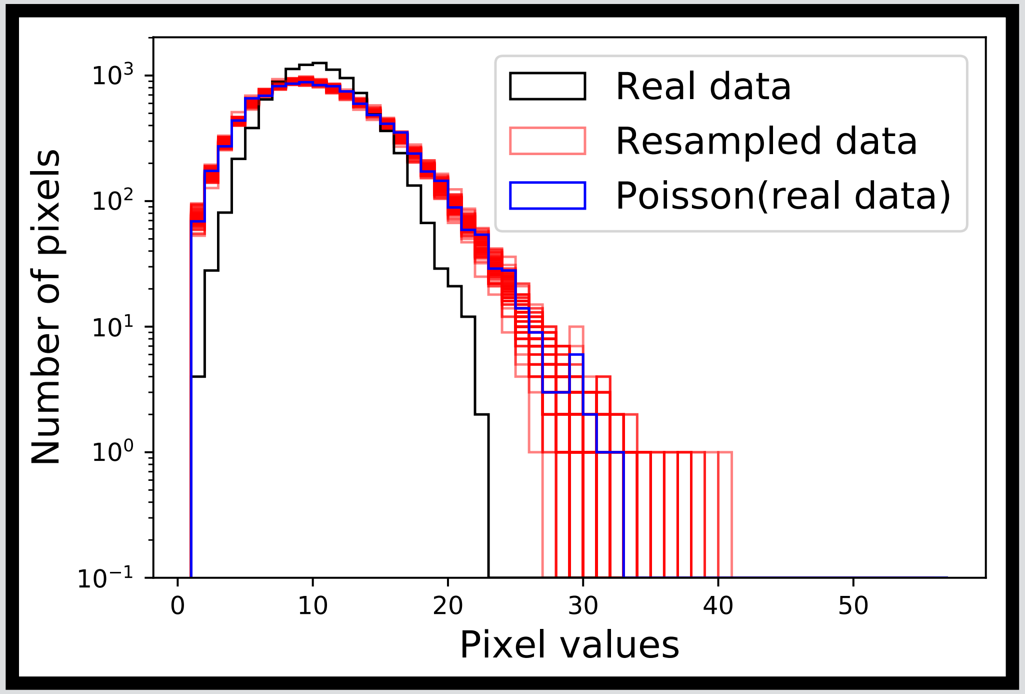
An example of Bootstrapping

Retrieving Error bars

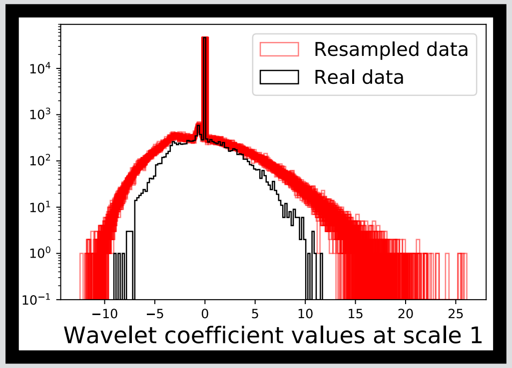
Applying bootstrap on a Poisson data set is exactly equivalent to adding Poisson noise to the Poisson data set :

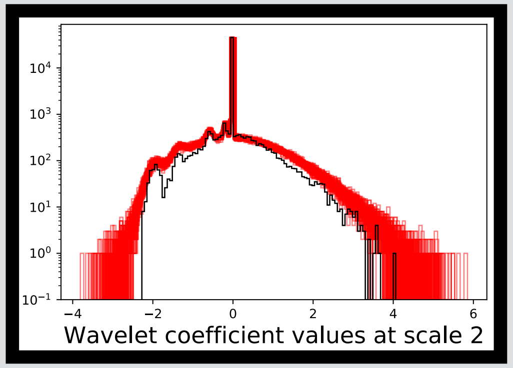


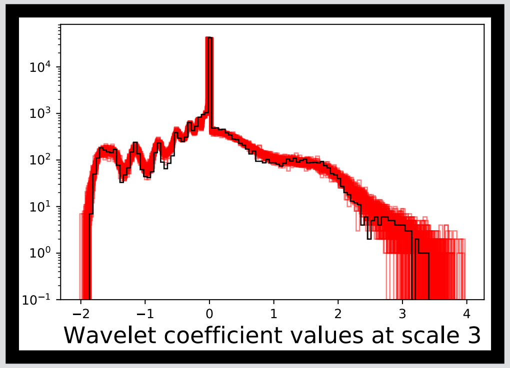
Real data = Poisson realization of the image of a square

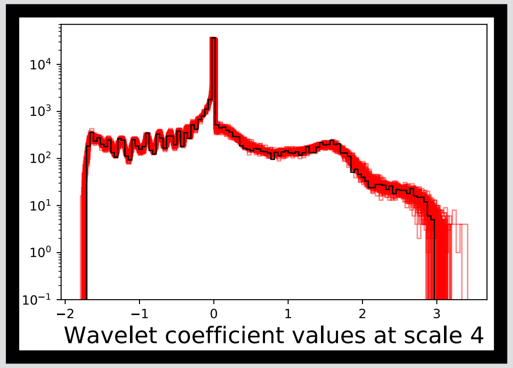


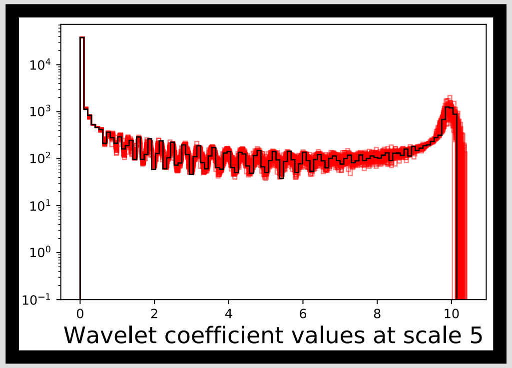
Associated histogram and resampled histogram







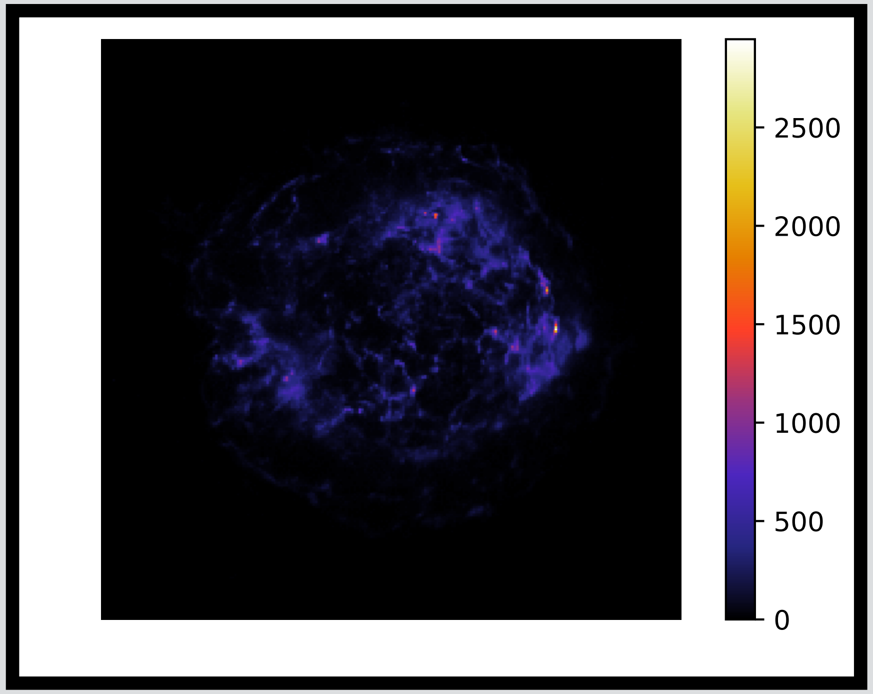




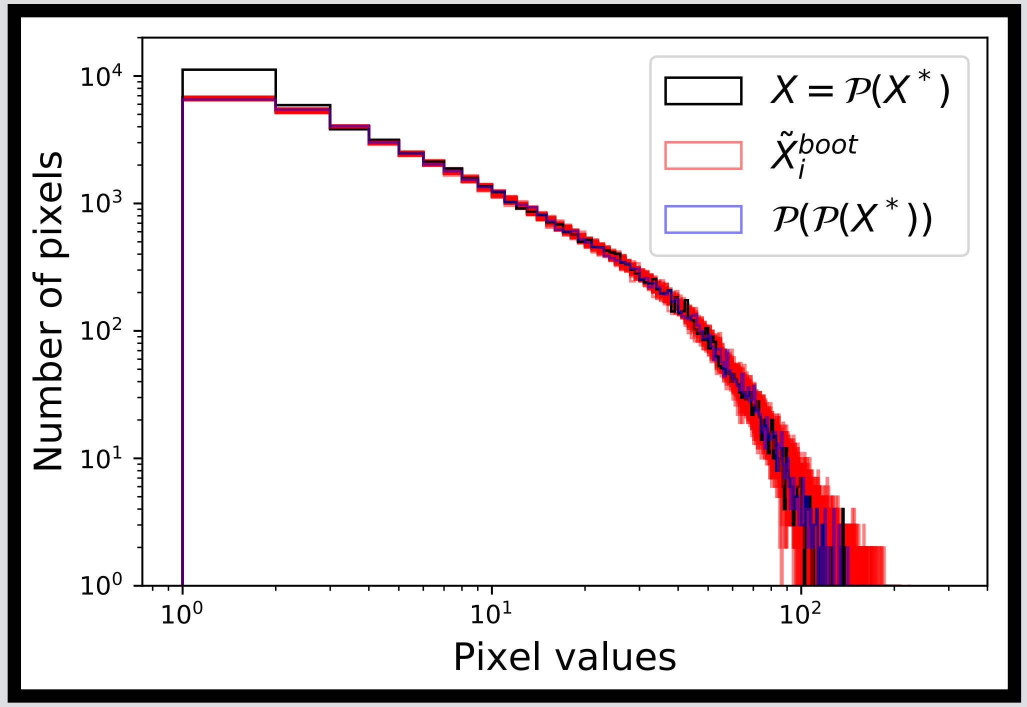
In wavelet scales

Retrieving Error bars

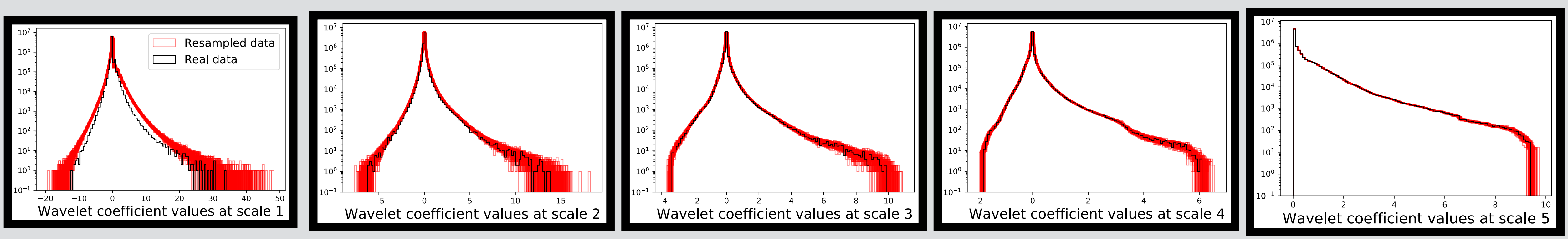
With a simulated image of Cassiopeia A :



Poisson realization of a simulated image of Cas A



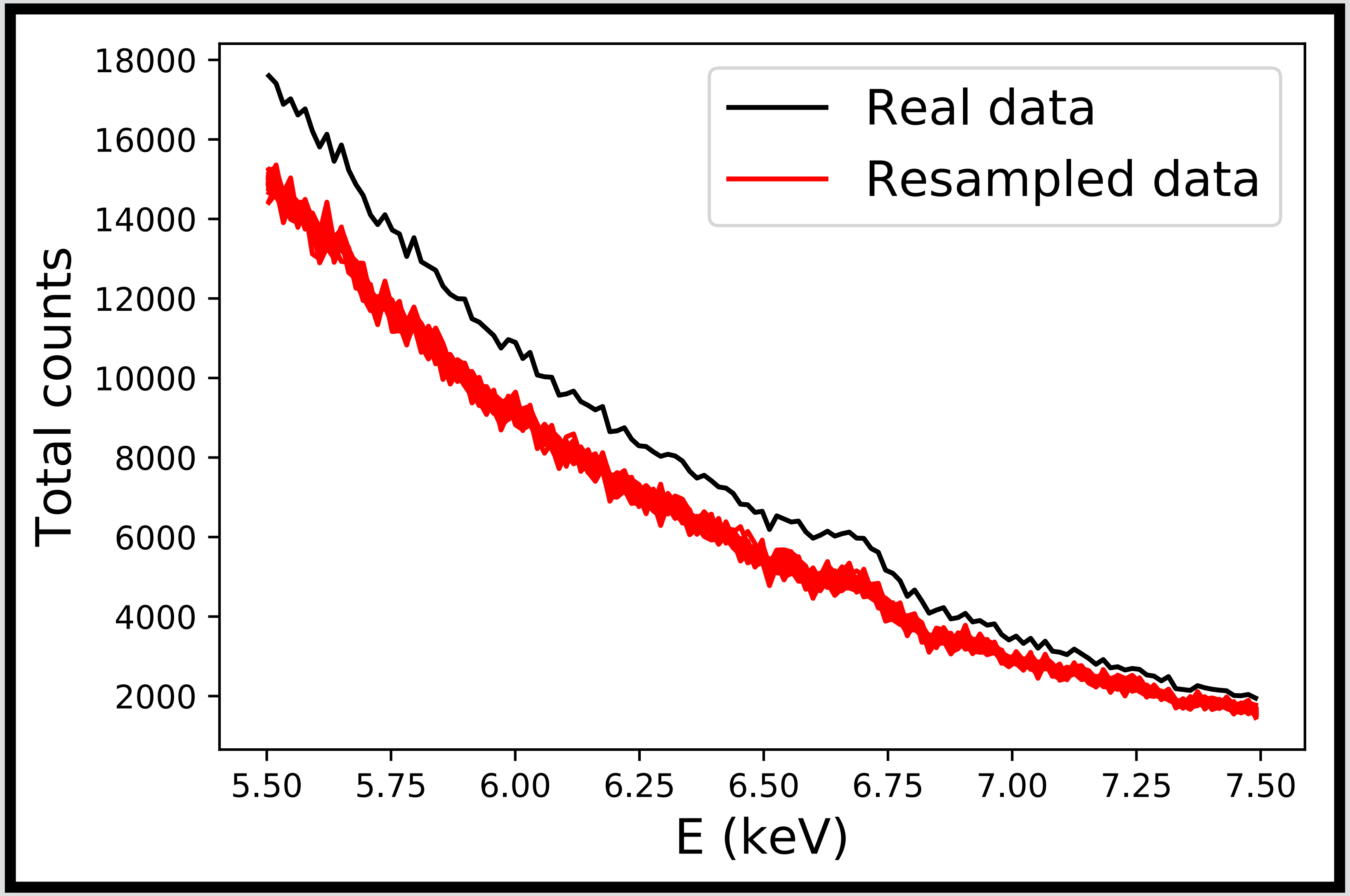
Associated histogram and resampled histogram



In wavelet scales

Retrieving Error bars

...which is reflected in the bias in the components retrieved by pGMCA on bootstrap resamplings



pGMCA is highly sensitive to the additional noise

Constrained bootstrap method

How can we develop a method giving an appropriate histogram ?

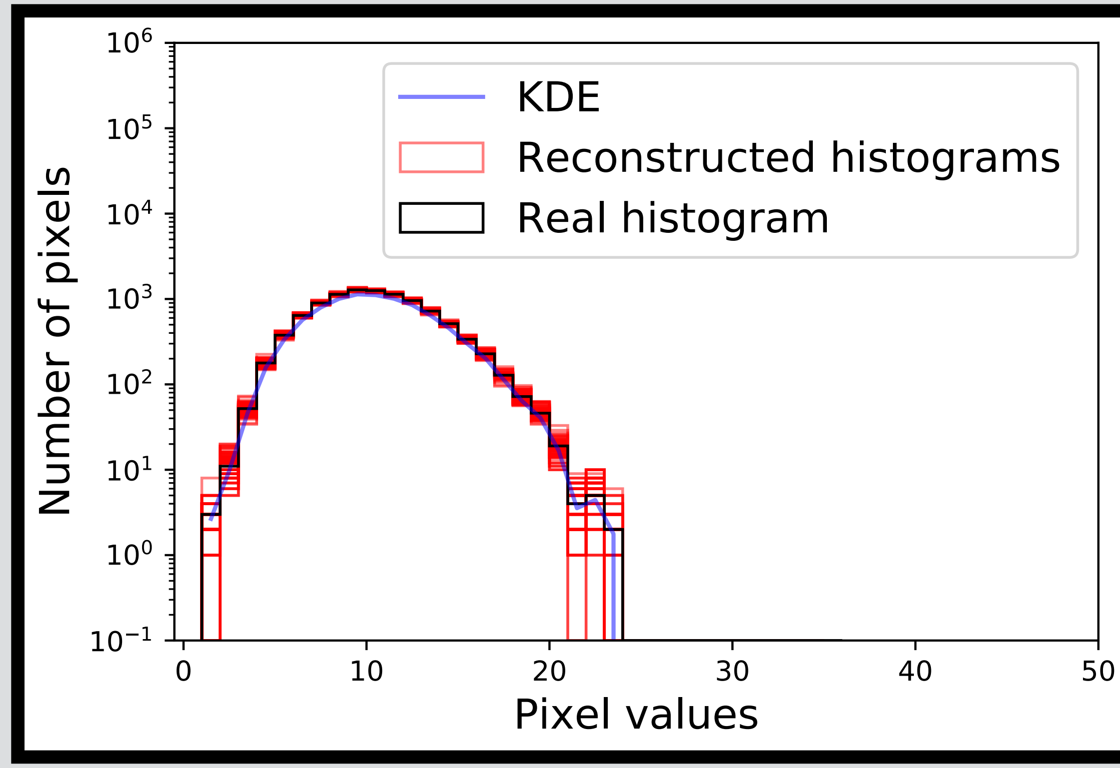
Constrained bootstrap method

How can we develop a method giving an appropriate histogram ?

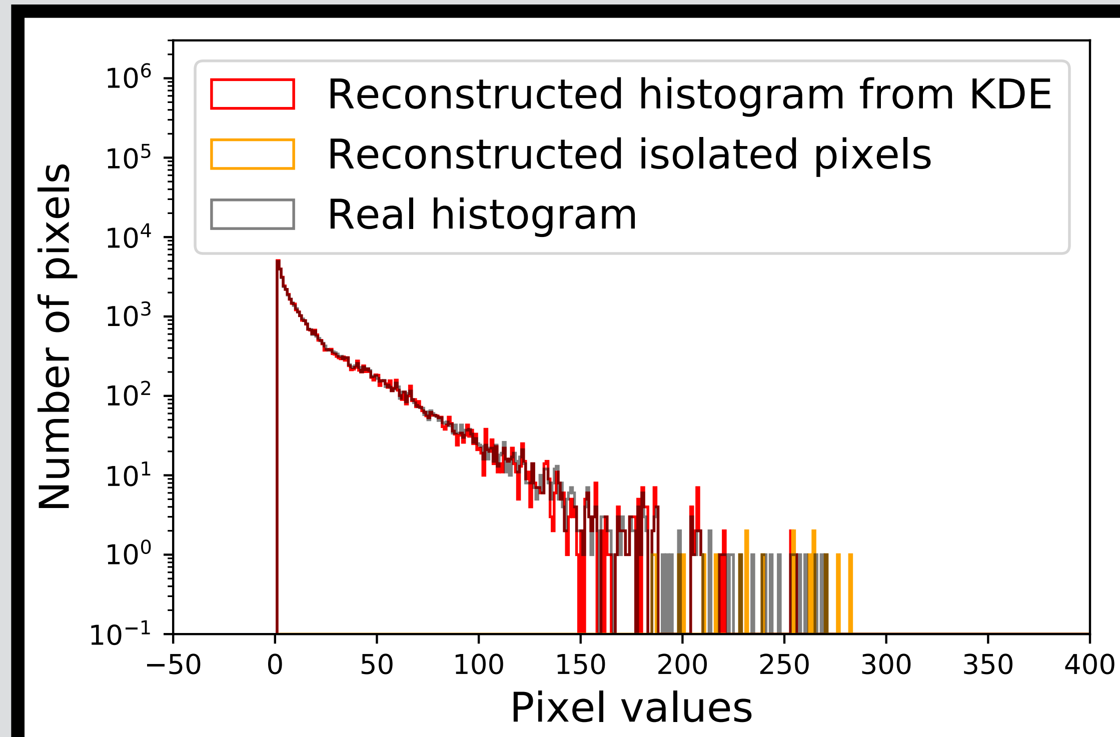
By working directly on the histogram, rather than on the individual events !

Constrained bootstrap method

Step 1 :Generating N histograms with a spread around the data mimicking that of a Monte-Carlo



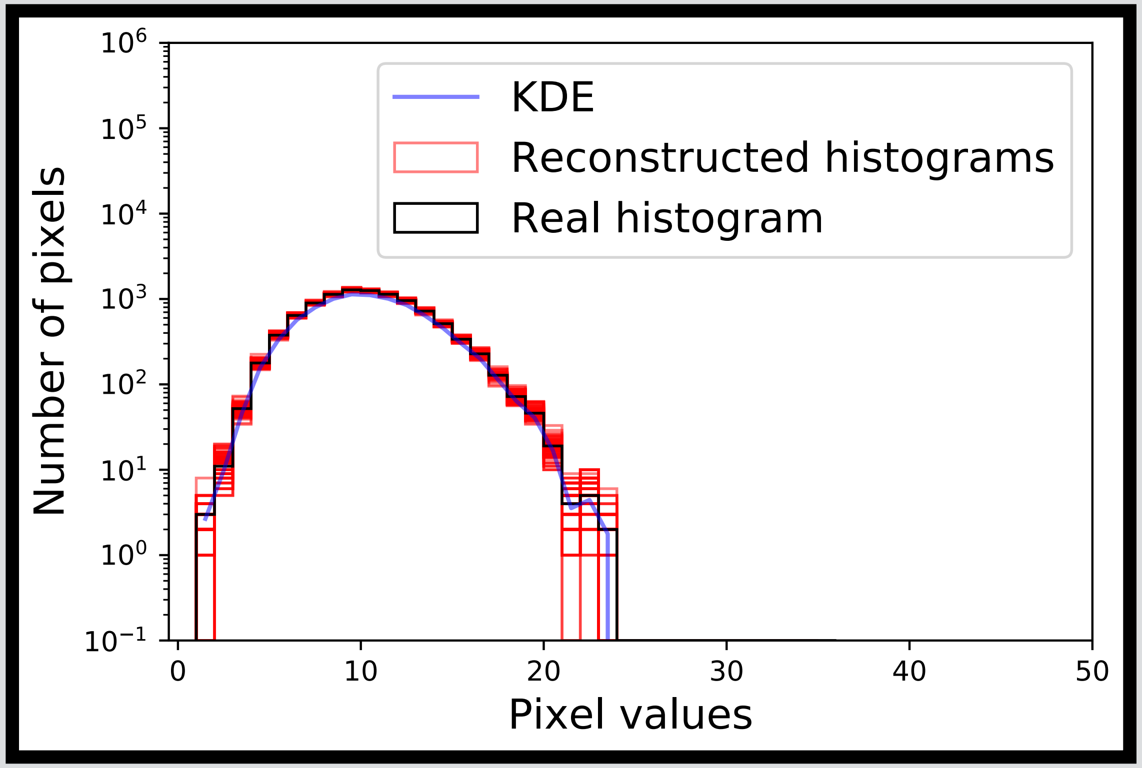
Square example



Simulated Cas A

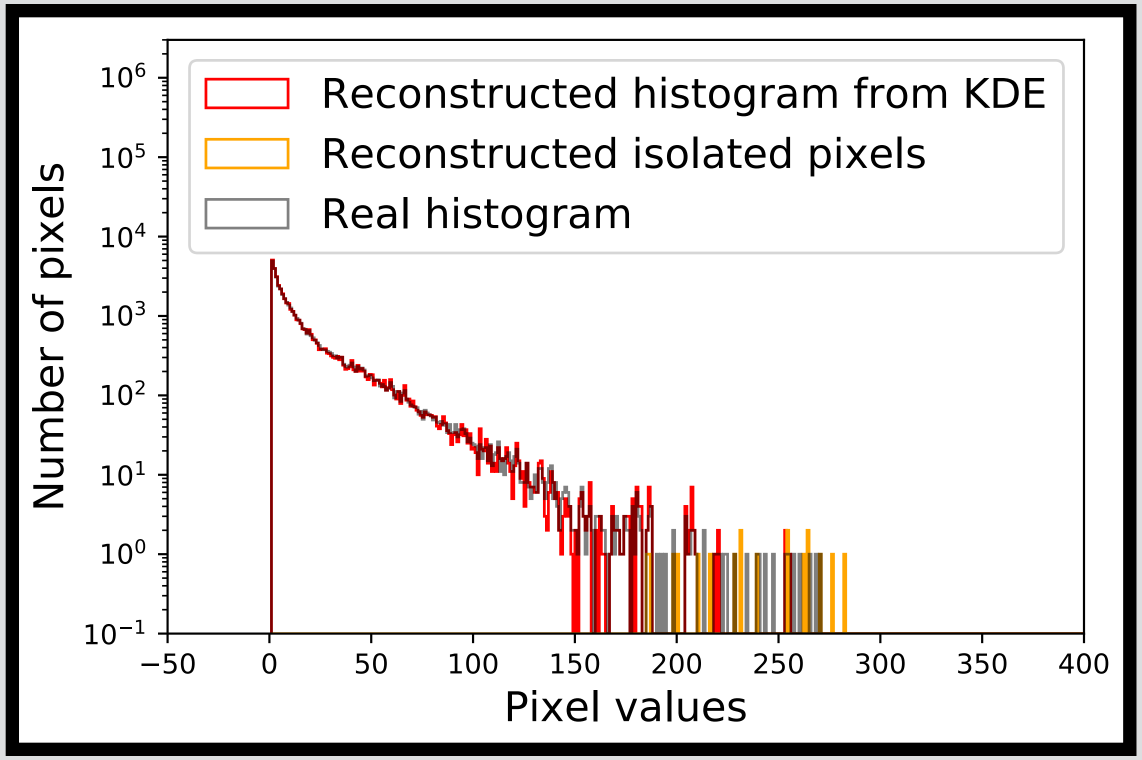
Constrained bootstrap method

<u>Step 1</u> :Generating N histograms with a spread around the data mimicking that of a Monte-Carlo



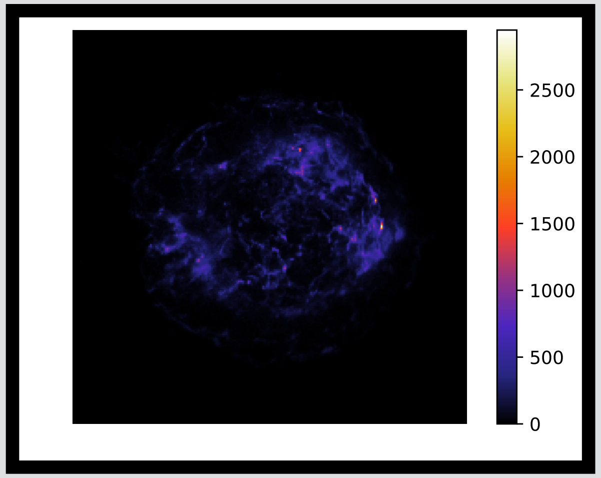
Square example

<u>Step 2</u> : Creating new images by imposing the new histograms on the original image

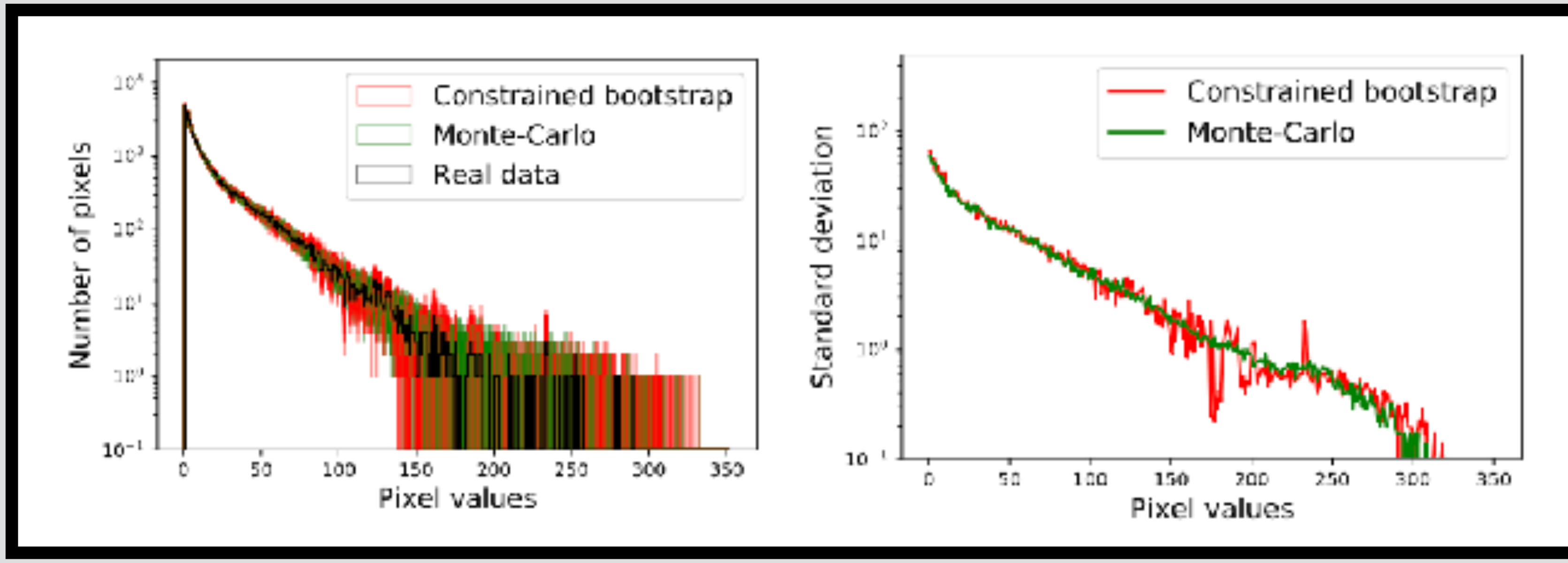


Simulated Cas A

Constrained bootstrap method



Simulated image of a Cas A



Histograms

Associated standard deviation

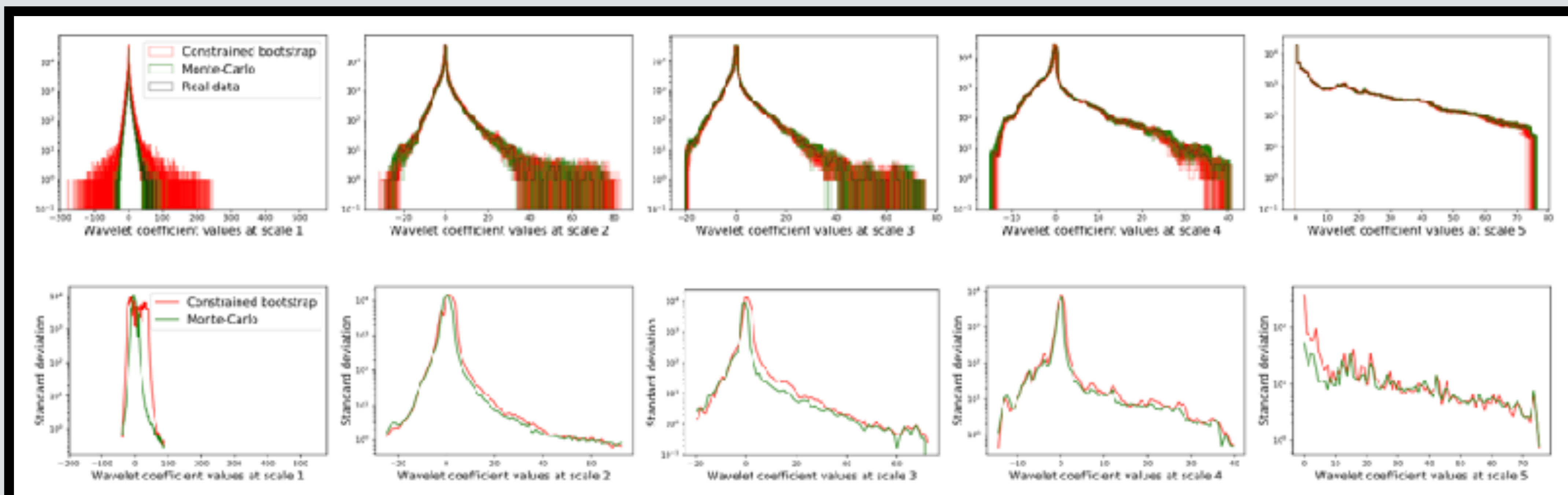
Black : Original data

Red : Resampled data

Green : Monte-Carlo

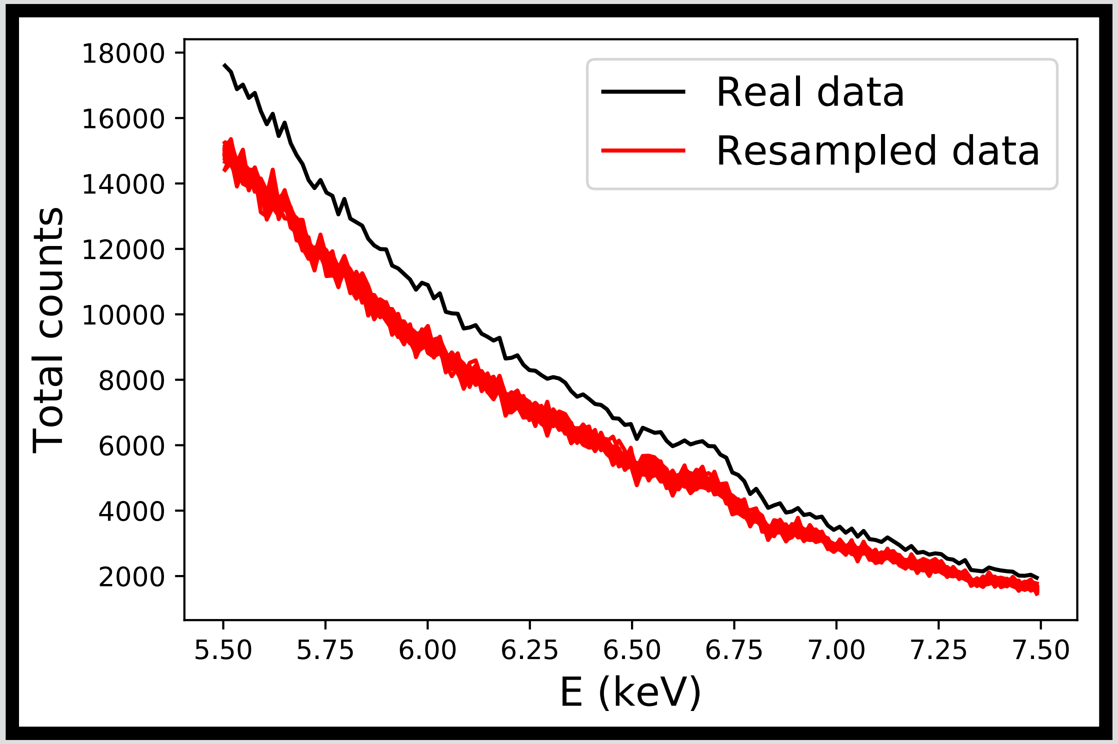
Wavelet scales

Standard deviation

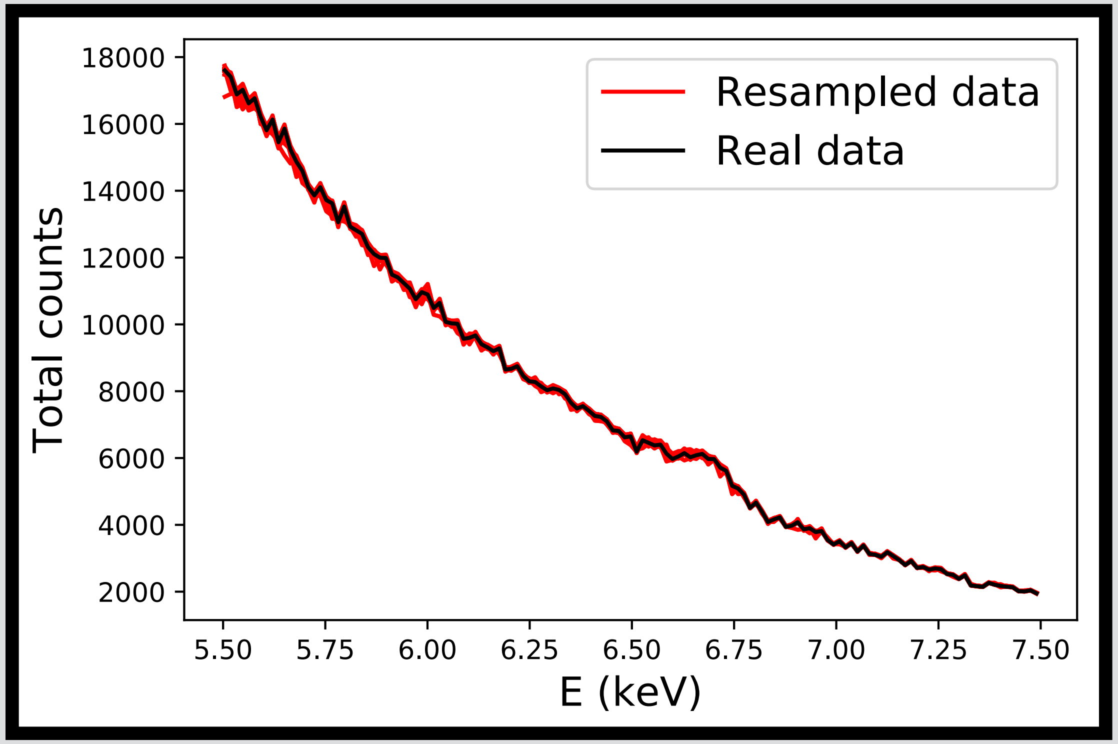


Constrained bootstrap method

The constrained bootstrap corrects the bias in the pGMCA results



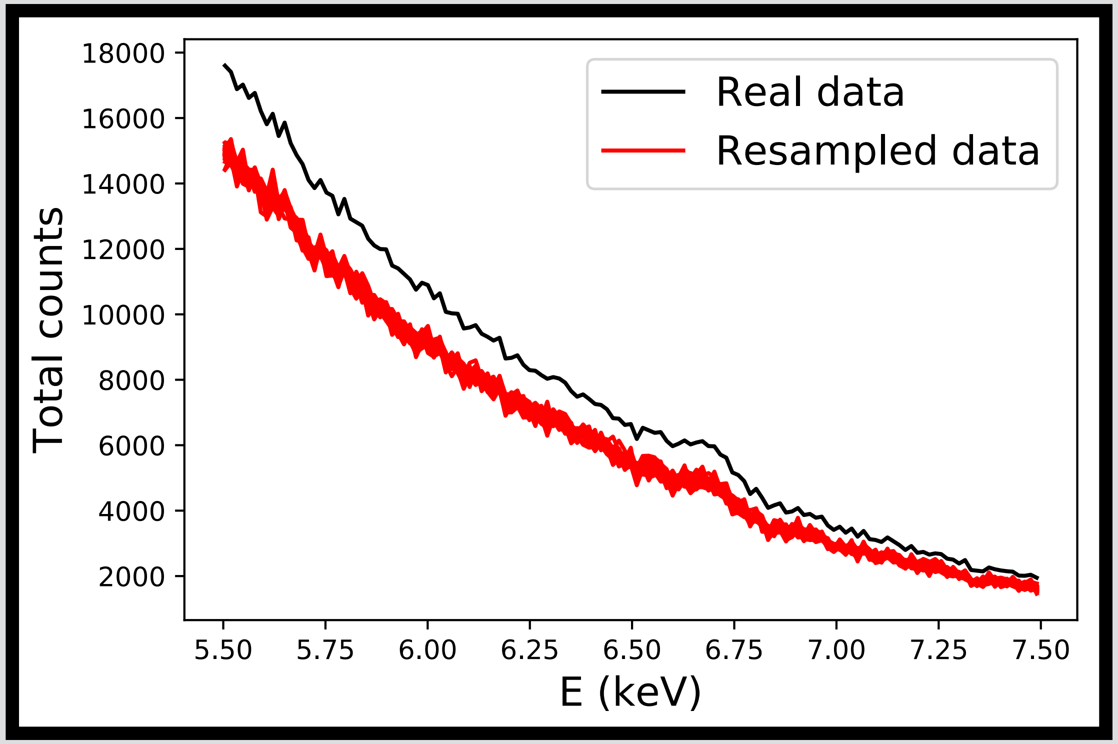
Classical bootstrap



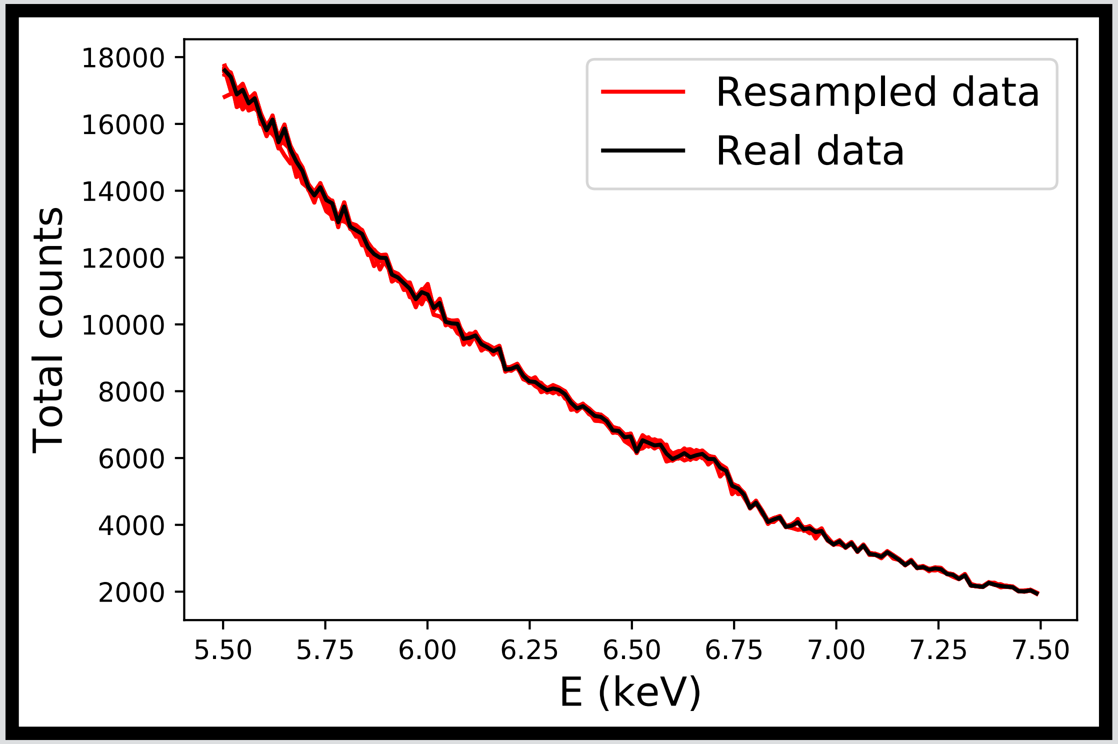
Constrained bootstrap

Constrained bootstrap method

The constrained bootstrap corrects the bias in the pGMCA results



Classical bootstrap



Constrained bootstrap

We removed the bias, but we do not control the variance

Constrained bootstrap method

Retrieving errorbars on Poissonian data sets for non-linear estimators is an open and general question.

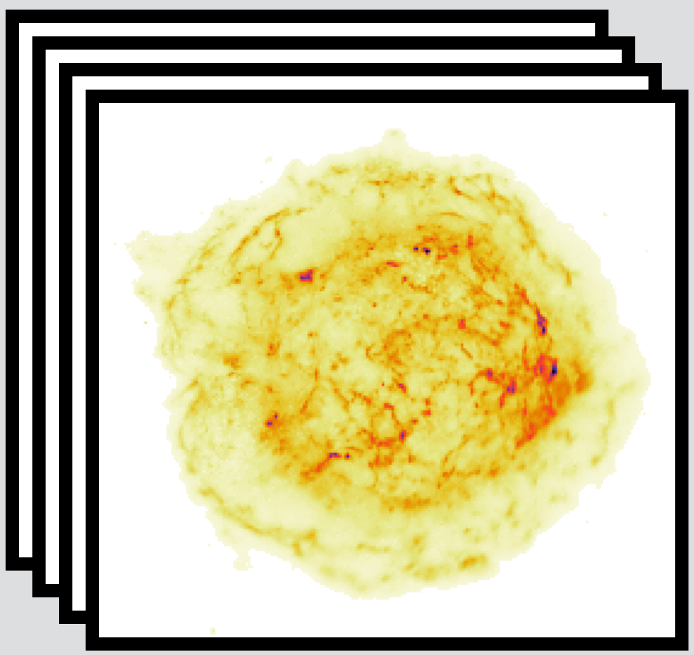
Our constrained bootstrap :

- gives unbiased results => test of robustness around initial conditions
- gives inconsistent spread => no physical significance

Part II : Applications

Asymmetries in Cassiopeia A

Our first application on real data :

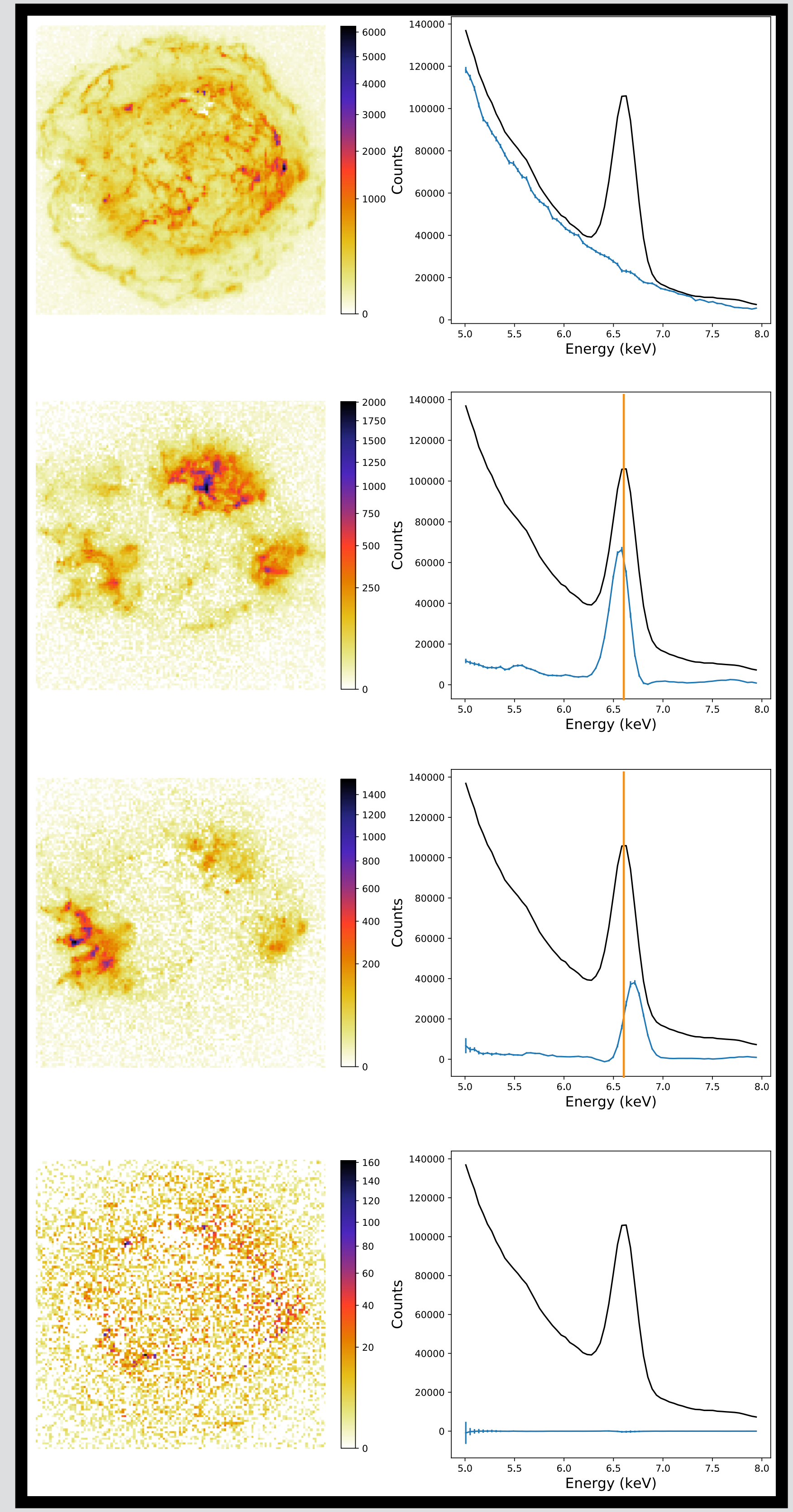


Synchrotron

Red-shifted Fe structure

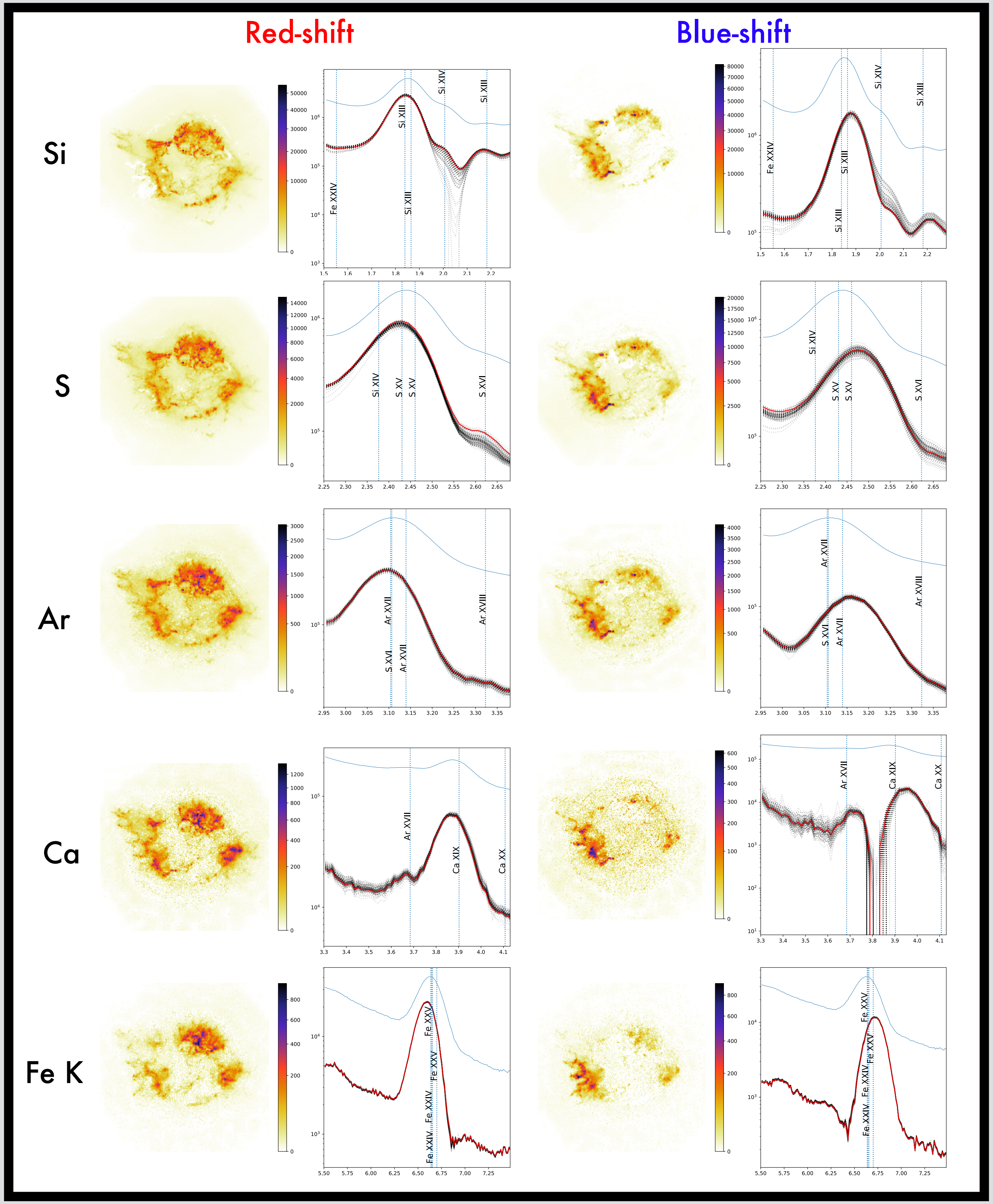
Blue-shifted Fe structure

Noise



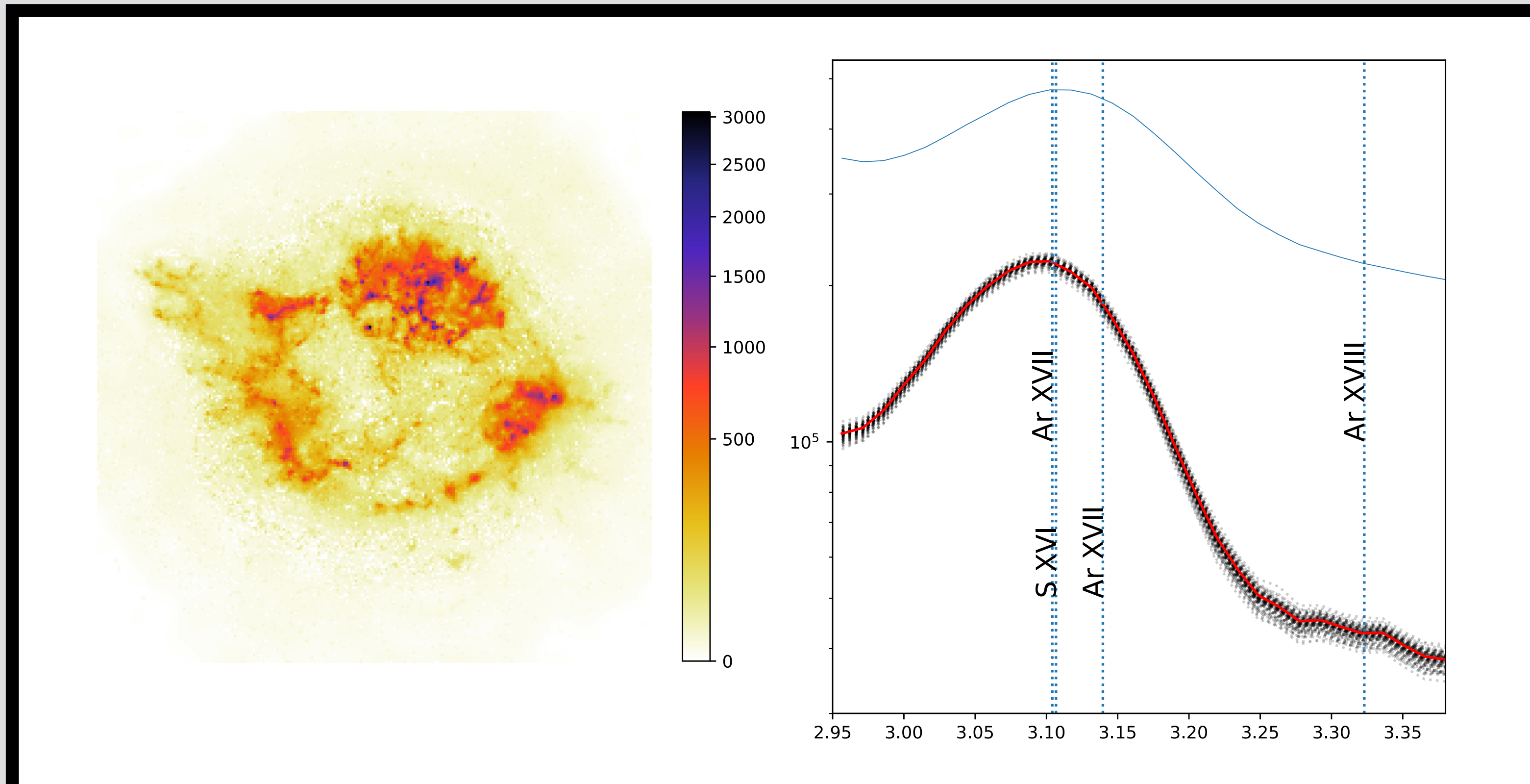
=> 3D reconstruction of the ejecta

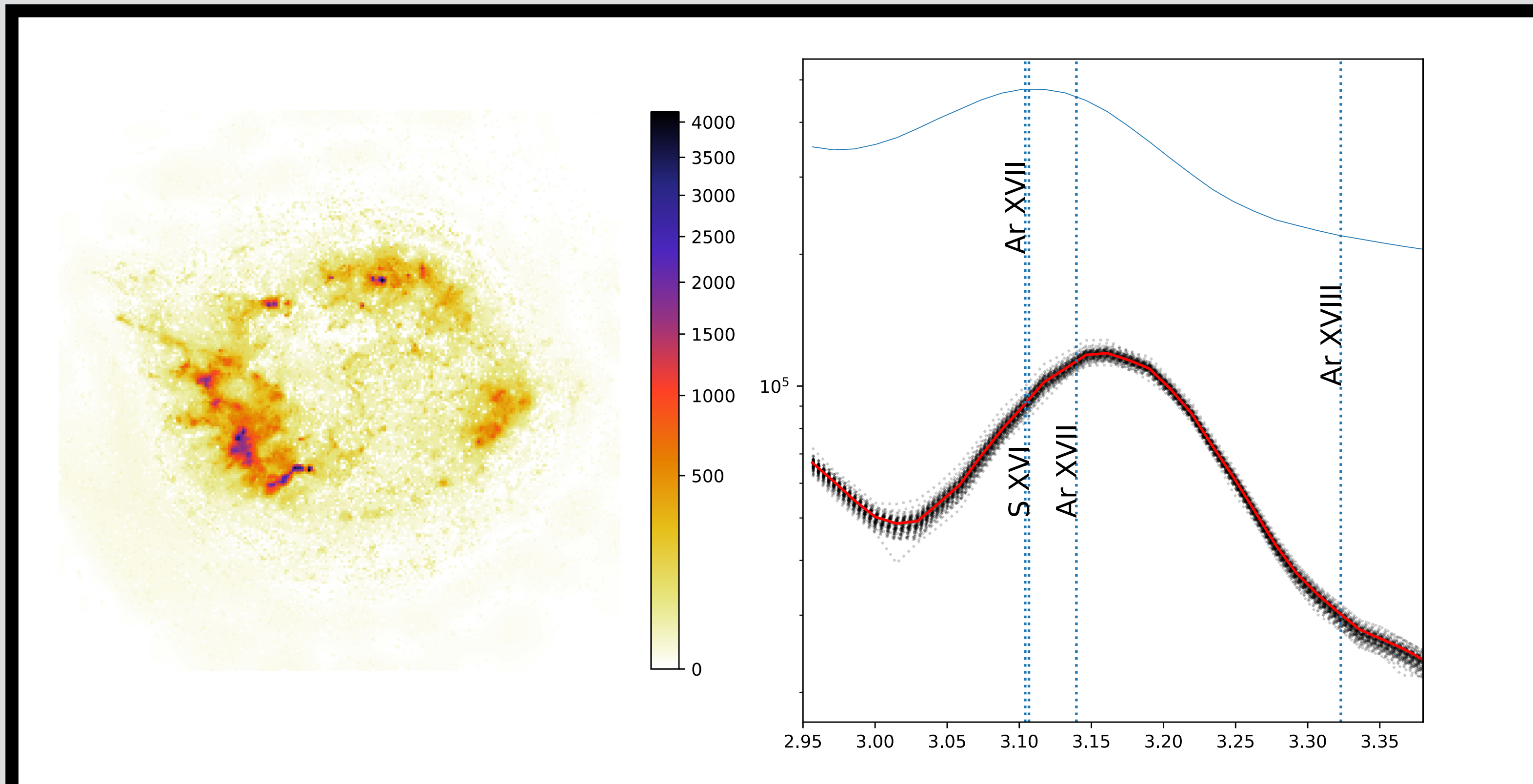
Velocity Asymmetries



Velocity Asymmetries

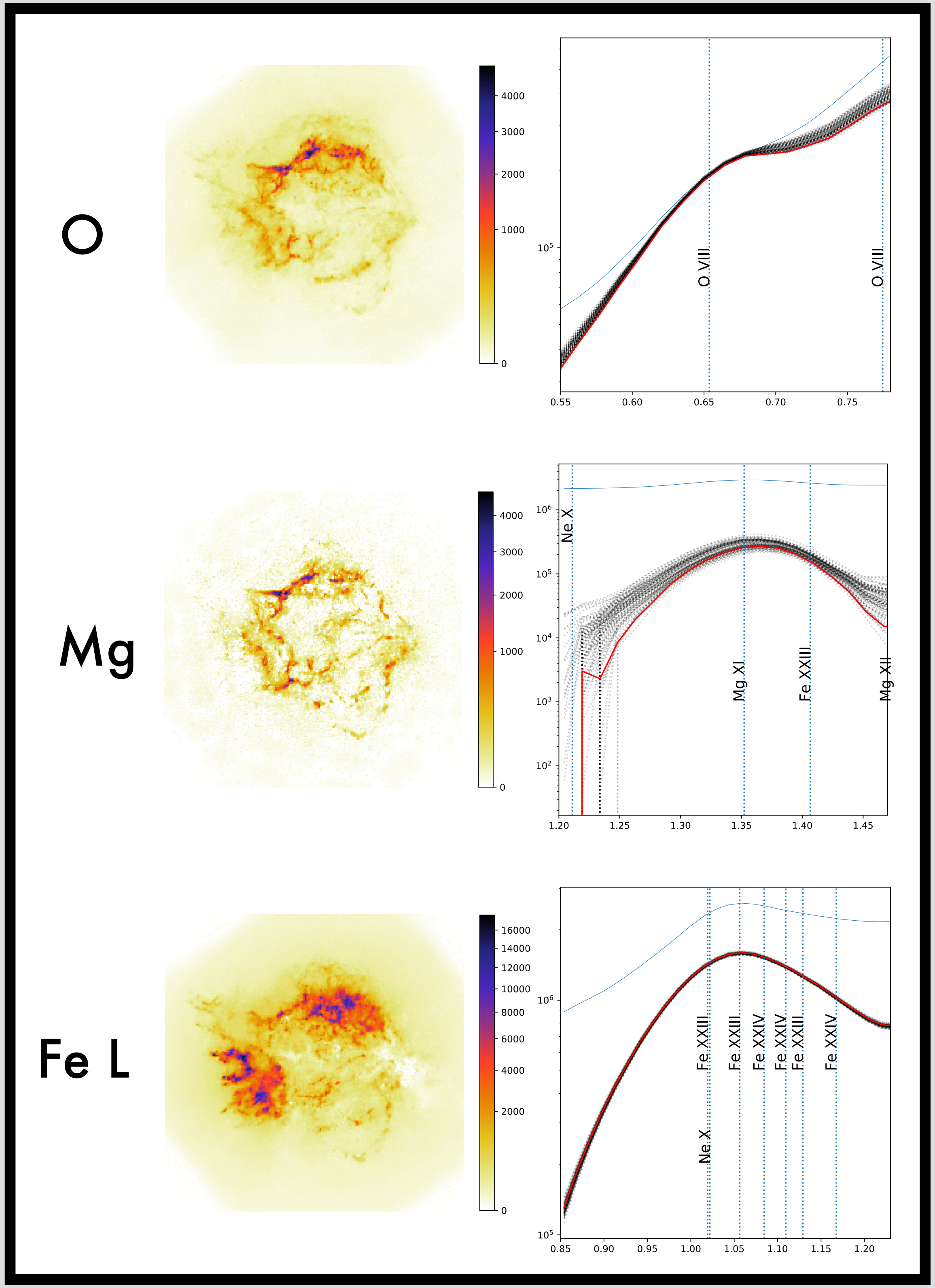
red-shifted Ar





blue-shifted Ar

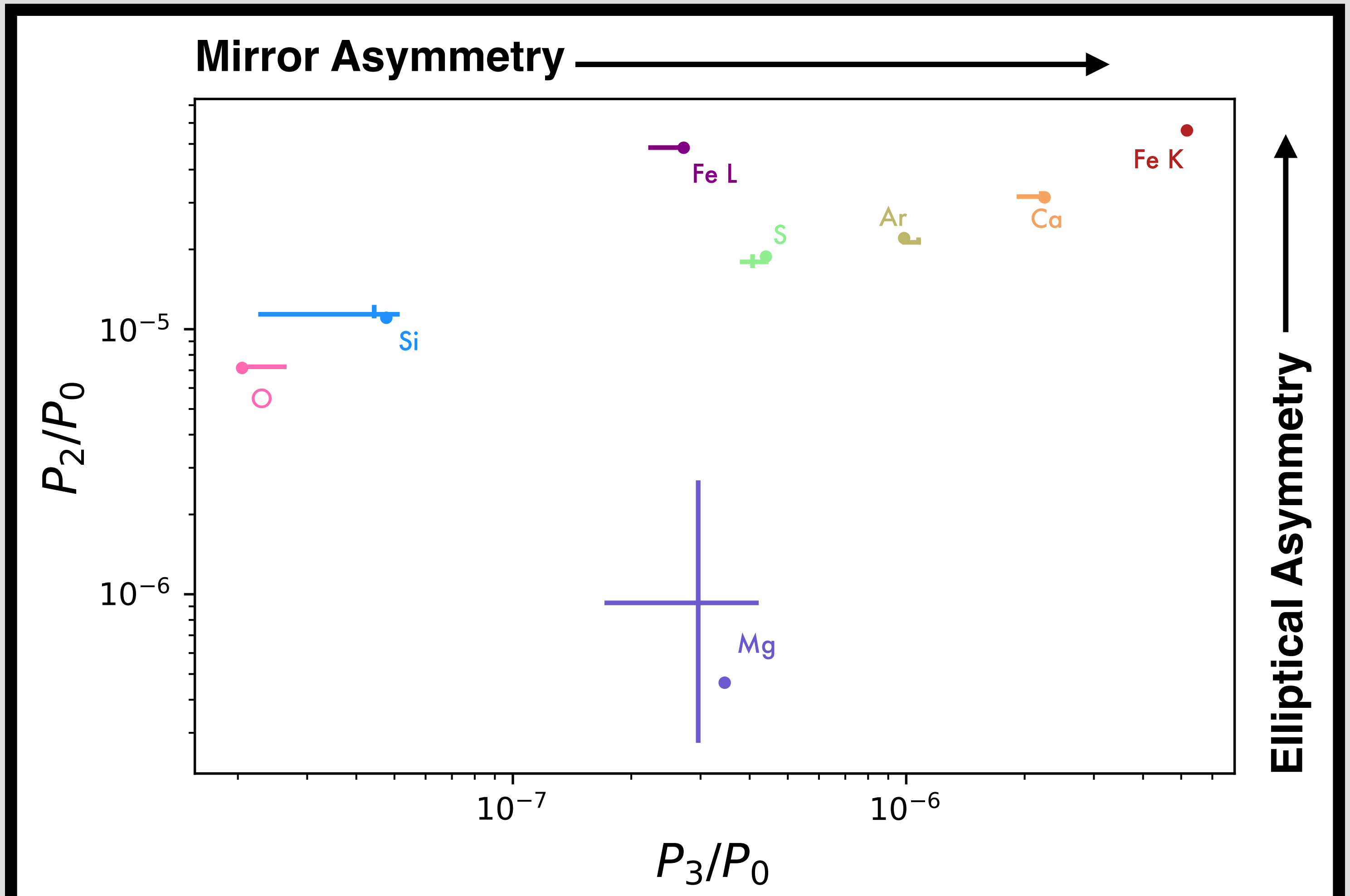
Lighter elements



Probing the Fe at different ionization states

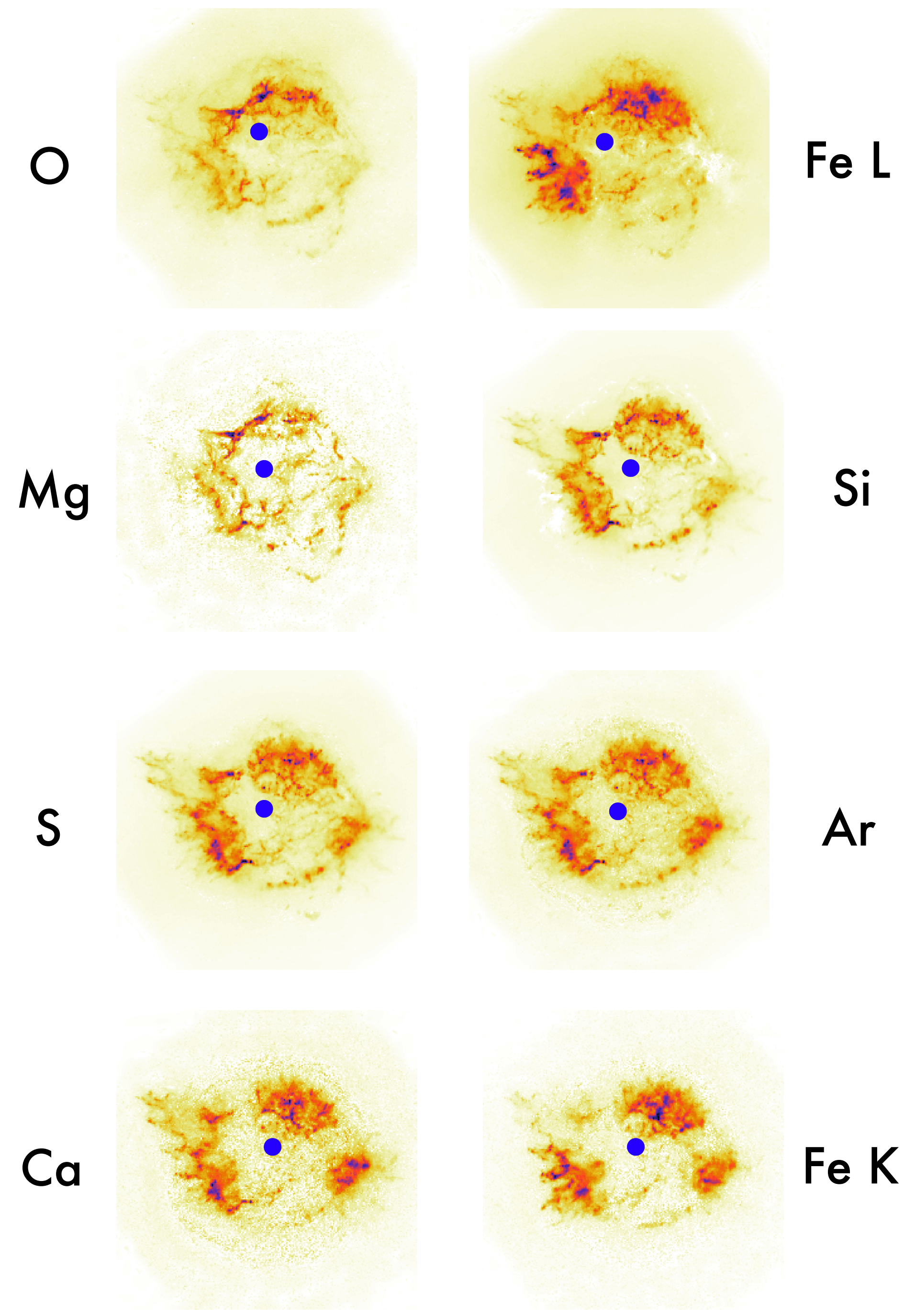
Morphological Asymmetries

The Power-Ratio method characterizes the distribution asymmetries of elements in Cas A.



PRM introduced by Buote et al. (1995) and for SNRs by Lopez et al. (2009)

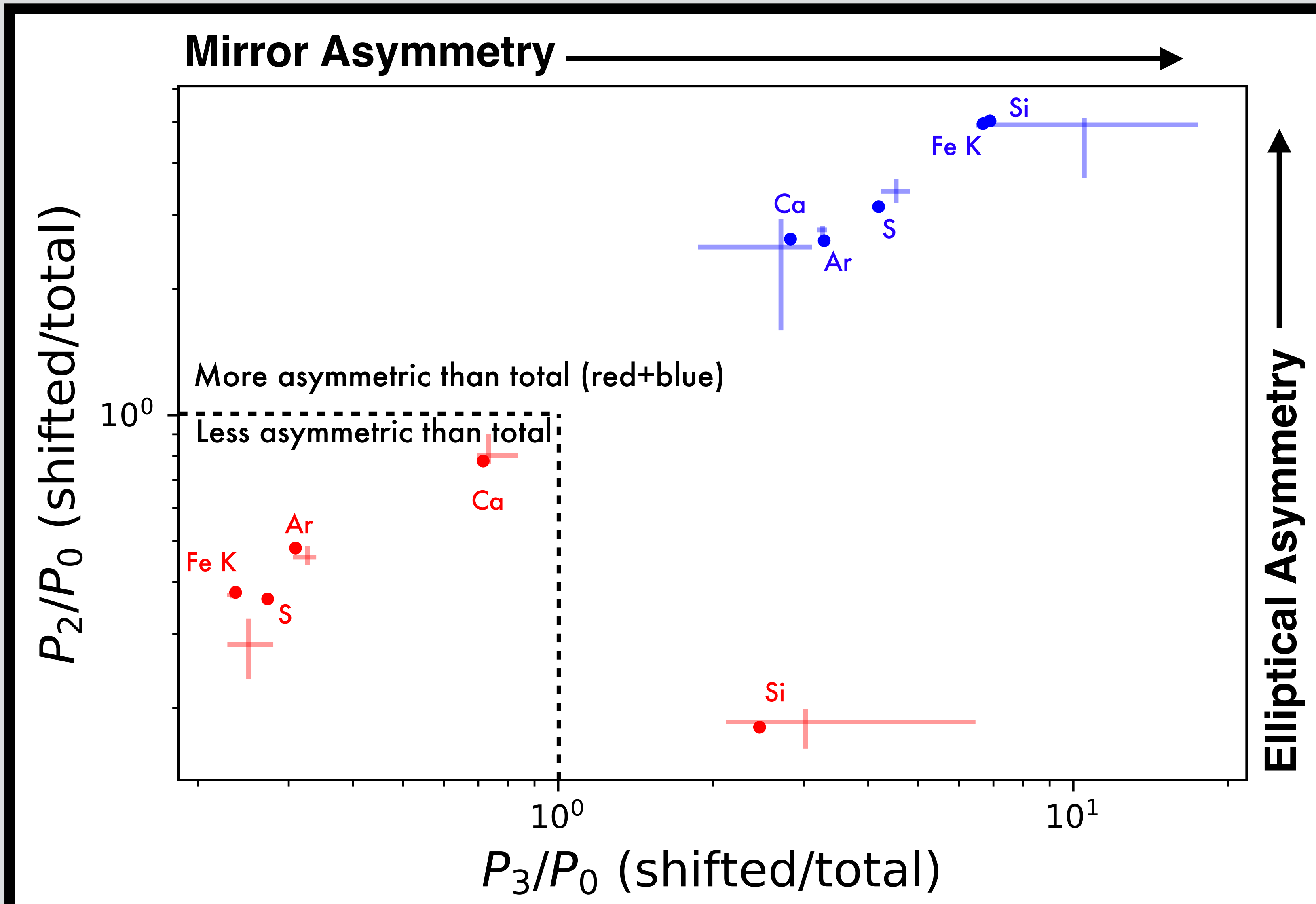
GMCA images (red+blue)

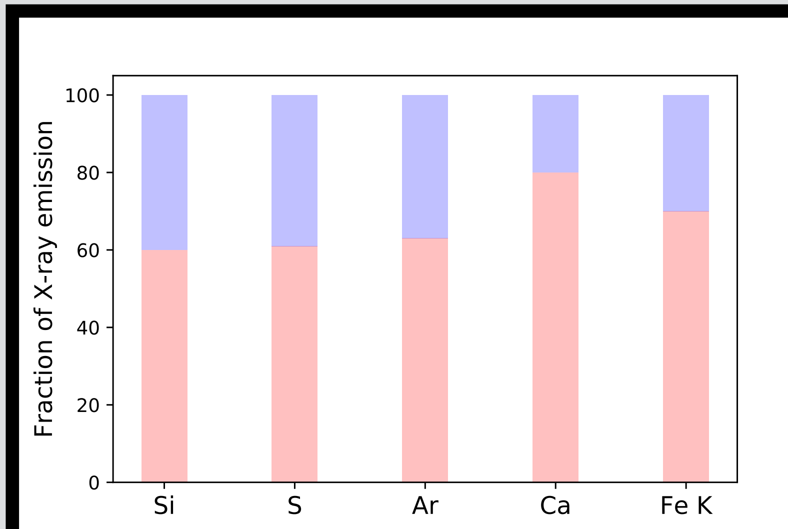


The blue dots are the centroids

Morphological Asymmetries

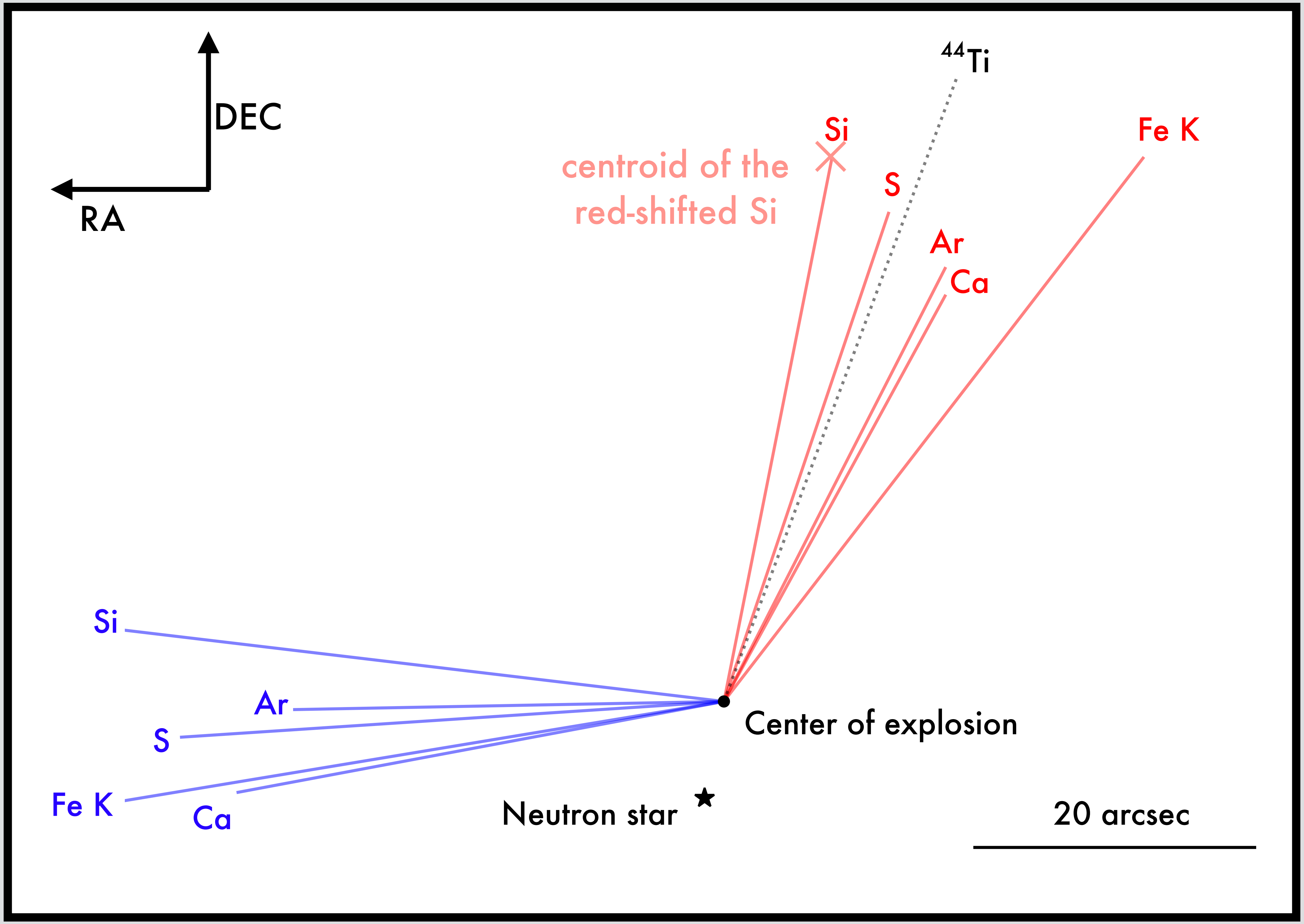
Distribution asymmetries in Blue or Red shifted components :





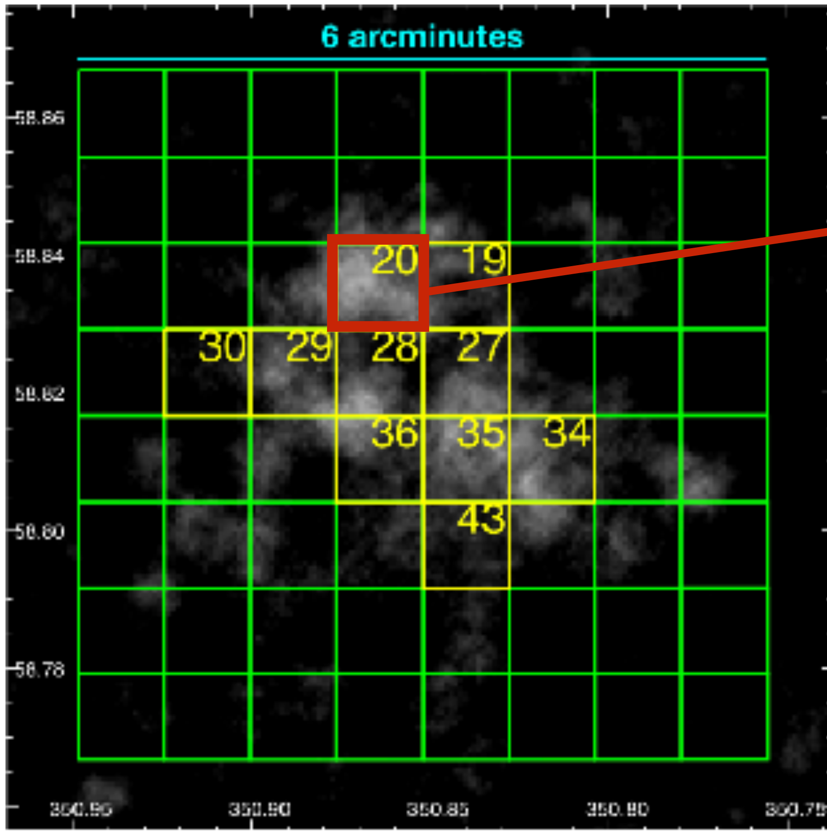
Relative fractions of red- and blue-shifted materials

Ejecta and neutron star



Directions of each red- and blue-shifted components
from the center of explosion.

Ejecta velocities



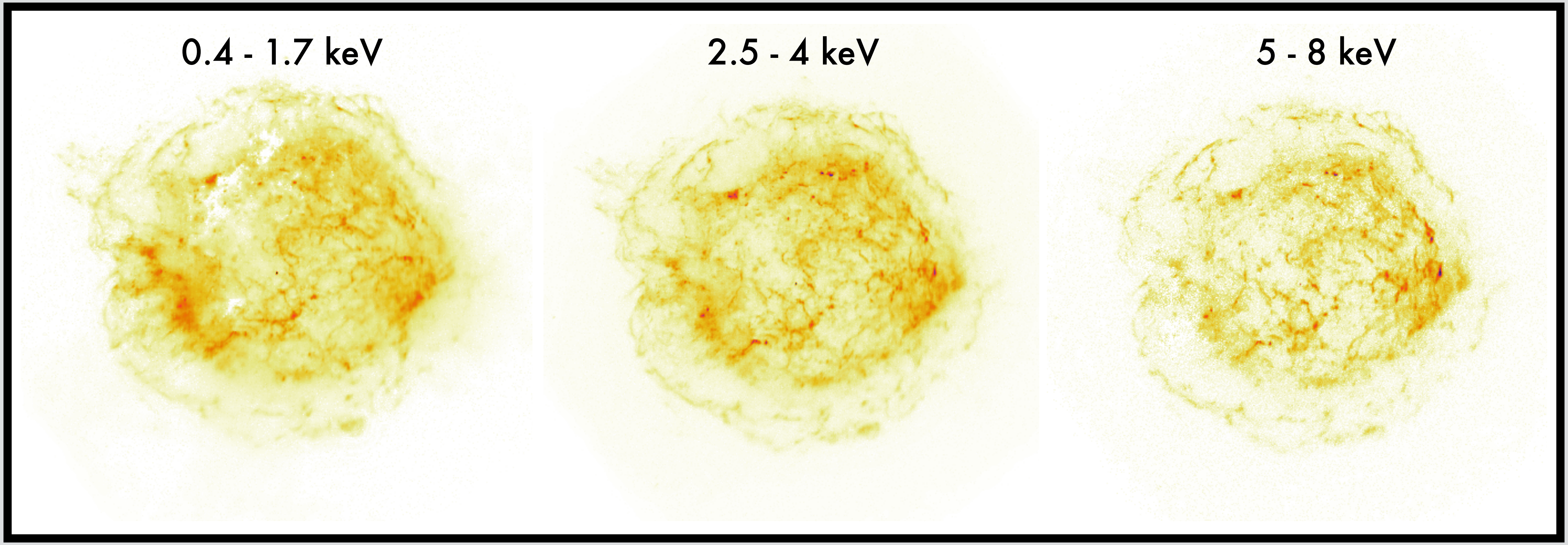
ID	Line of Sight[b]
19	2300 ± 1400
20a	3200 ± 500
20b	−7500 ± 1600
27	5700 ± 910
28	1400 ± 1400
29	230 ± 1300
30	410 ± 1700
34	4700 ± 590
35	2100 ± 730
36	1100 ± 770
43	3300 ± 500
Mean[c]	920 ± 510

From 44Ti *NuSTAR* study of Grefenstette et al. (2017).

Velocities retrieved by fitting gaussians : large calibration uncertainties not included

Line	ΔV km/s	V_{red} km/s	V_{blue} km/s
Si XIII	5787	804	4983
Si XIII*	5762	2081	3681
S XV	6092	2632	3460
Ar XVII	6684	2826	3858
Ca XIX	6684	1721	4963
Fe complex	5716	2768	2948

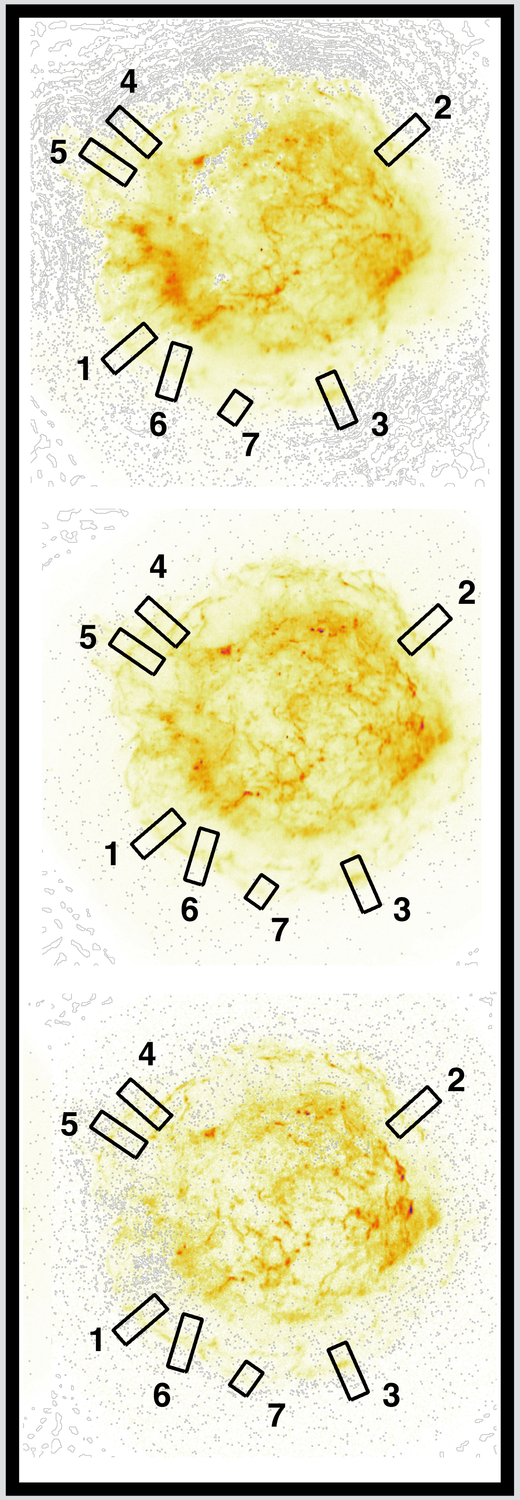
Synchrotron filaments

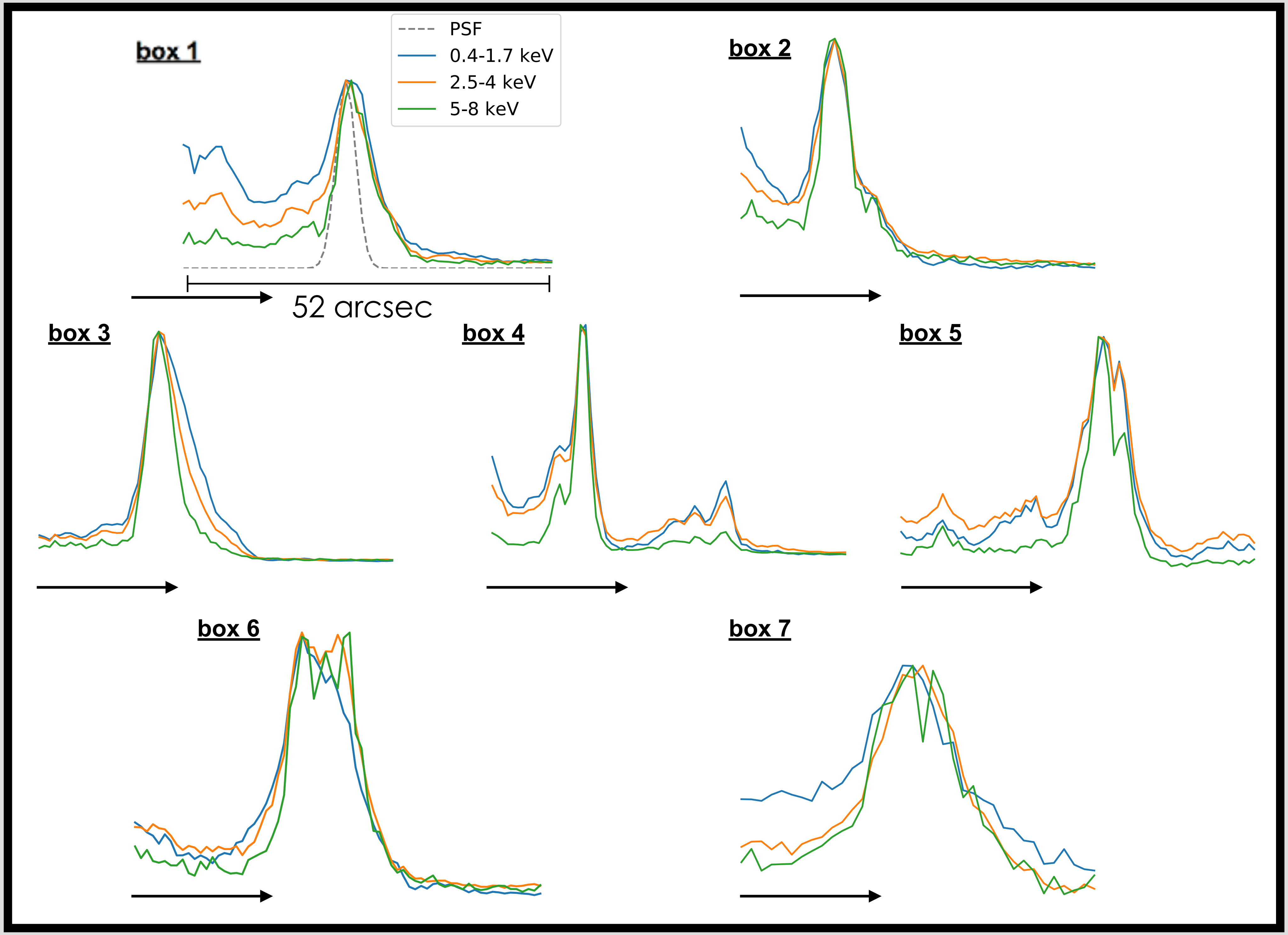


Two main models to account for the filaments :

- Energy loss of the electrons. Energy dependent widths
- Damping of the magnetic field. No energy dependent widths

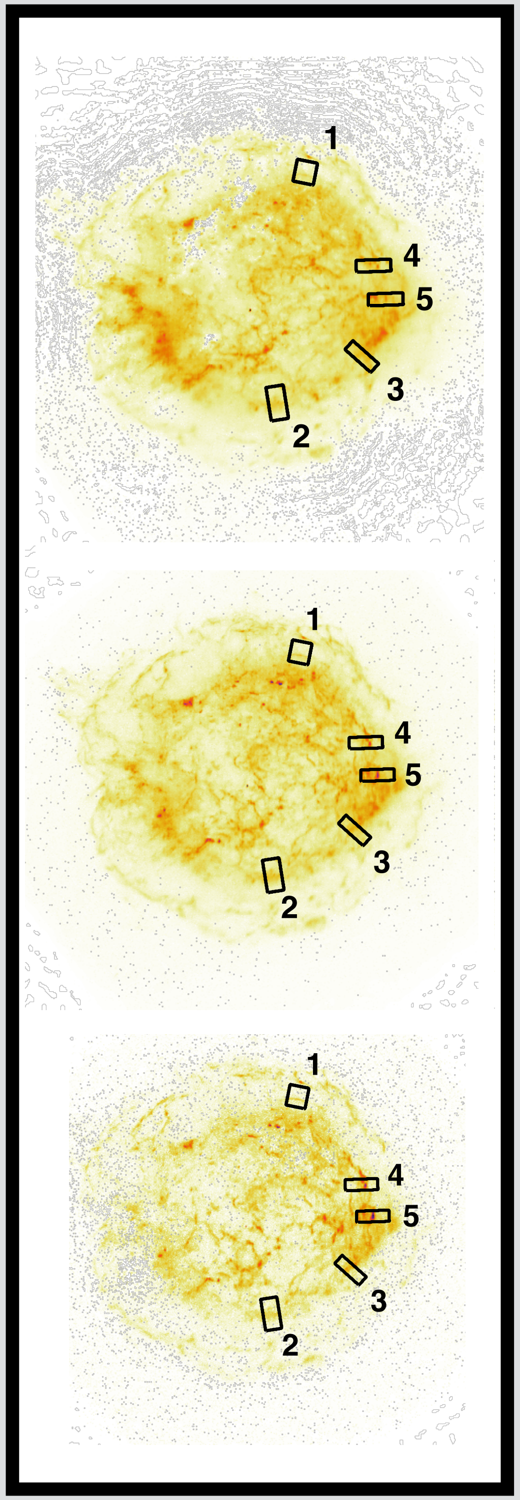
Synchrotron filaments in X-rays

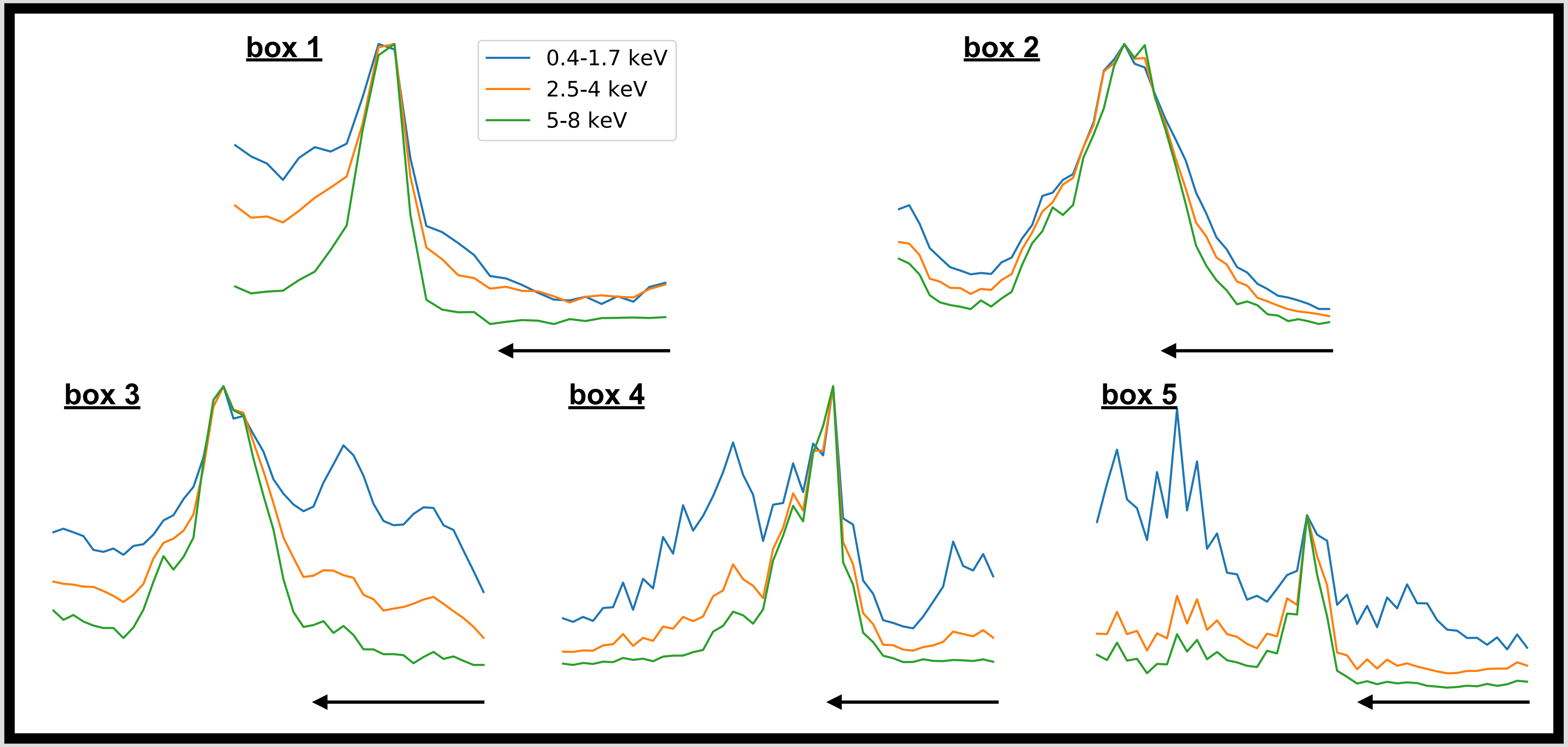




Profiles at the forward shock

Synchrotron filaments in X-rays





Profiles at the reverse shock

Conclusion and Perspectives

pGMCA

Generalized Morphological Components Analysis (Bobin et al. 2016)

First hypothesis : linear decomposition

=> Associates mean spectra to retrieved images : every pixel has the same spectrum. Consistent results, information on velocity asymmetries.

Second hypothesis : different components have different morphology

=> Without prior physical information, physically consistent components. No spurious artifacts.

=>The Poissonian noise is properly handled by pGMCA

pGMCA

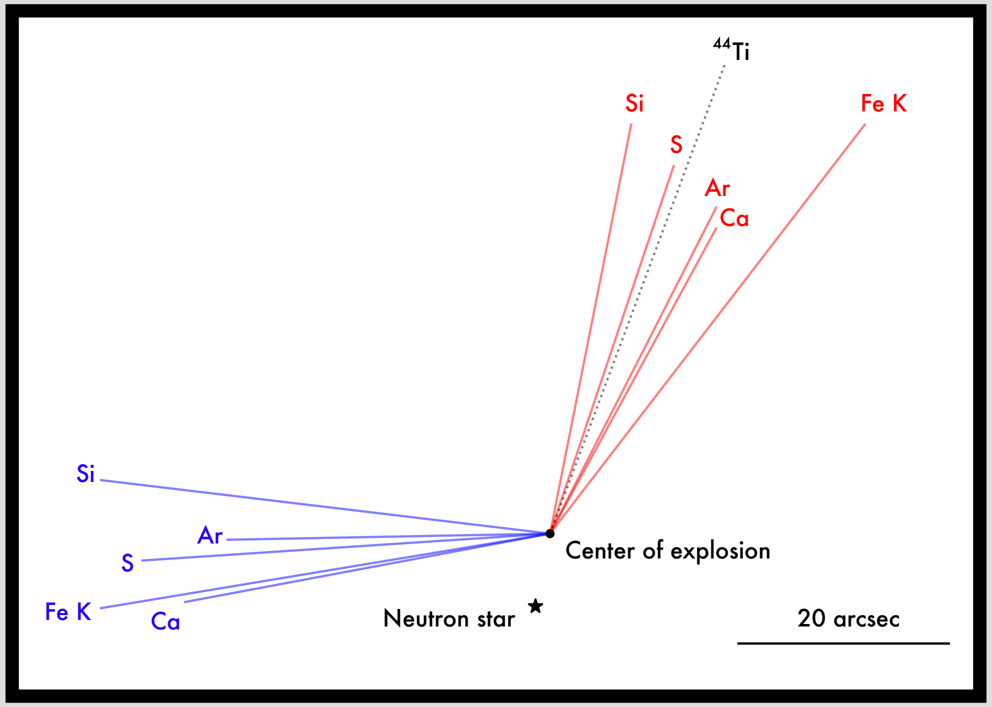
Generalized Morphological Components Analysis (Bobin et al. 2016)

=> The performances of the algorithms are very case-specific. They highly depend on the morphologies of the components to disentangle. Minimum count of roughly one million in total.

=> There is currently no way to retrieve physically significant error bars. Classical bootstrap introduces biases in the results. Our constrained bootstrap method is promising, as it gives unbiased results, but the spread cannot be trusted.

Cassiopeia A ejecta

- Application of pGMCA provided a 3D view of the distribution of individual elements.



- Most of the ejecta are red-shifted

=> Proof of an asymmetric explosion

- Bulk of the ejecta opposite to the neutron star

=> Neutron star kick possibly due to recoil

- Red and blue components are not diametrically opposed, disfavouring the idea of a jet/counter jet mechanism.

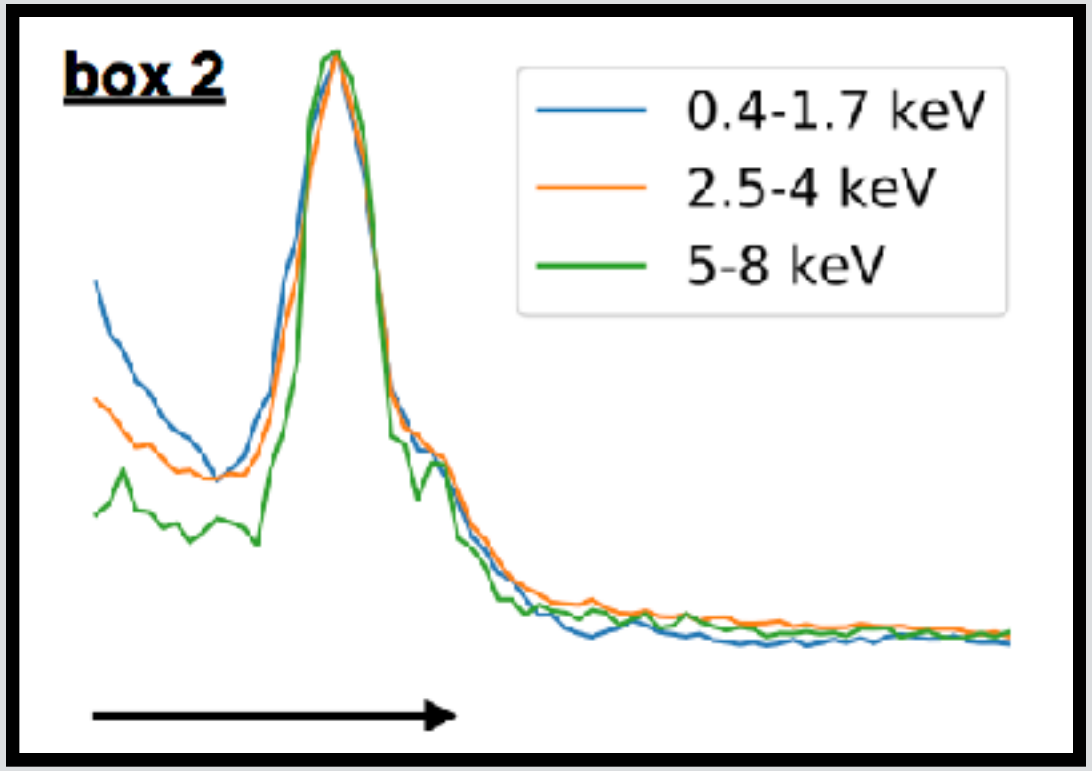
Cassiopeia A filaments

- Narrowing of the filaments with energy :

=> First detection in Cas A

=> Similar to SN1006 (Ressler et al., 2014)

=> Disfavours damping mechanism

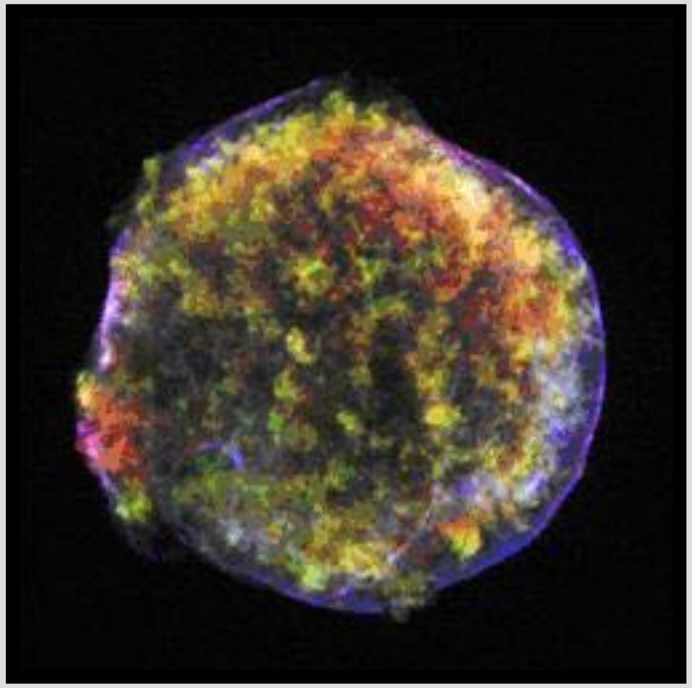


- The dependency in energy of the filaments widths will allow us to constrain the diffusion properties and testing the damping hypothesis.

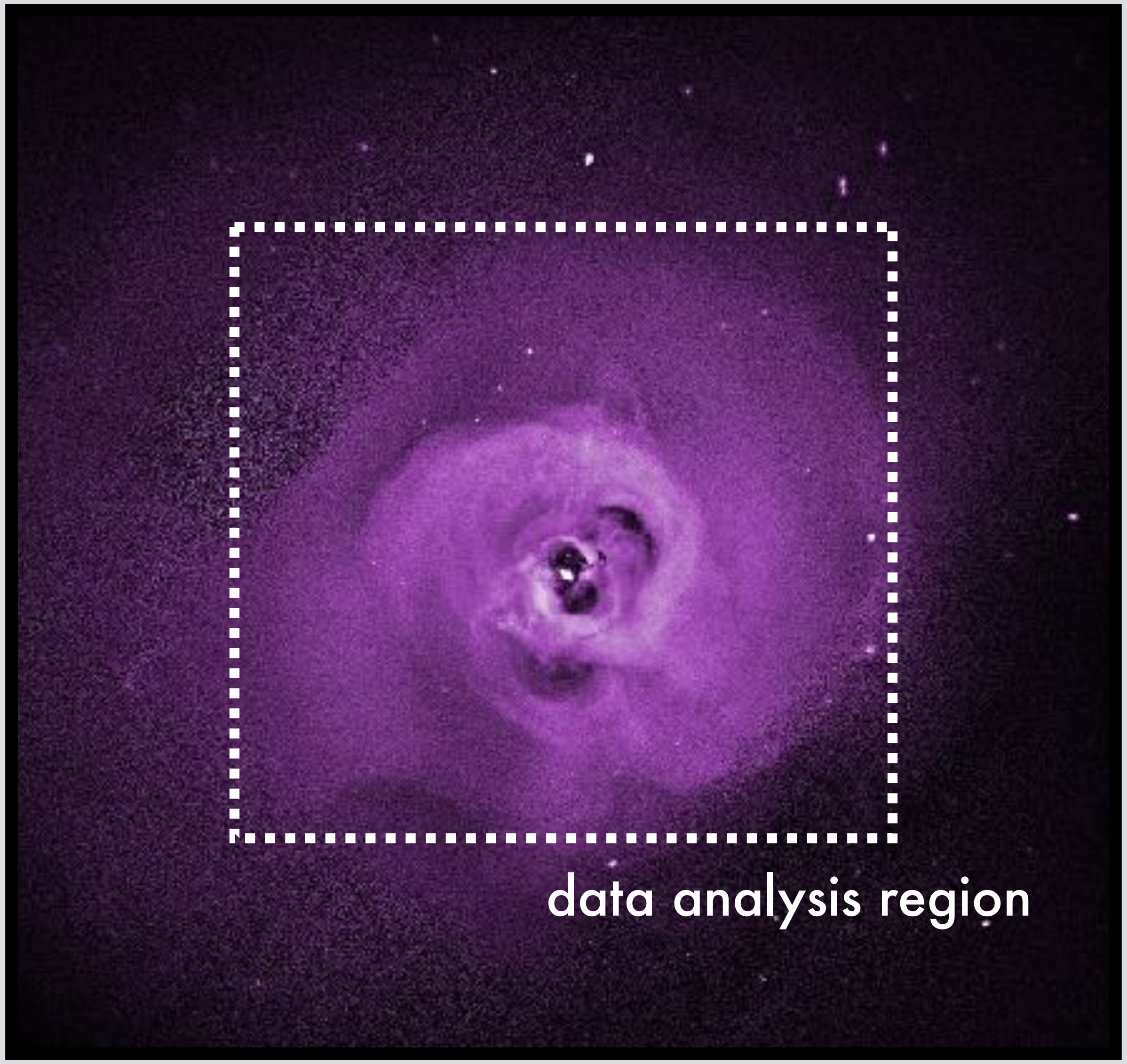
Perspectives

Constraining asymmetries on SNR population
Type Ia v. Core-Collapse

- 10 SNRs with more than 250 ks observations (Chandra+XMM)



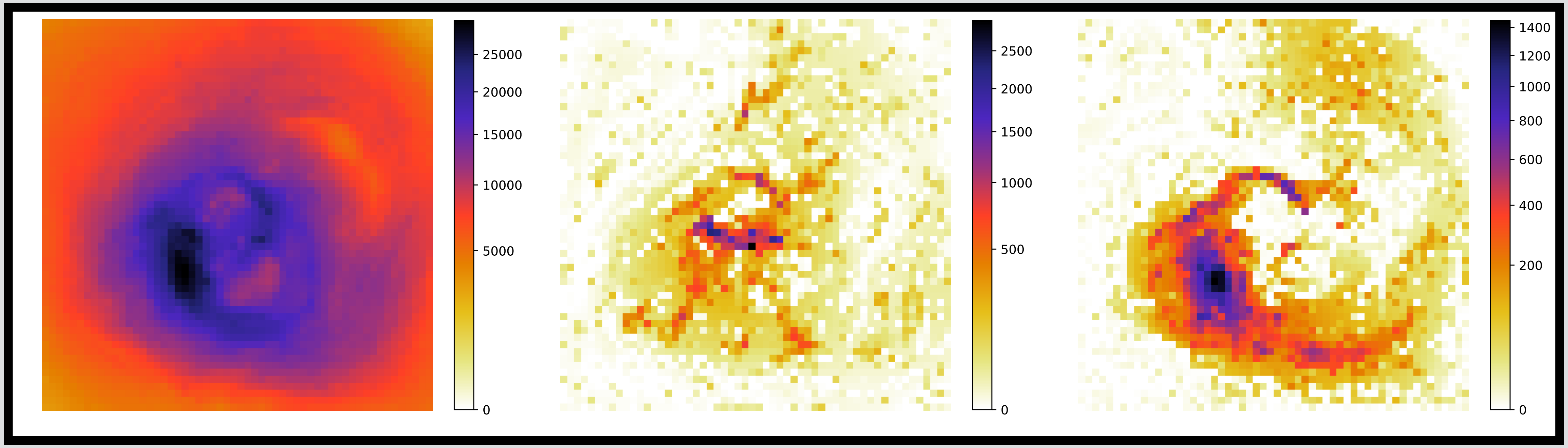
Perseus in X-rays



The Perseus galaxy cluster seen by *Chandra*

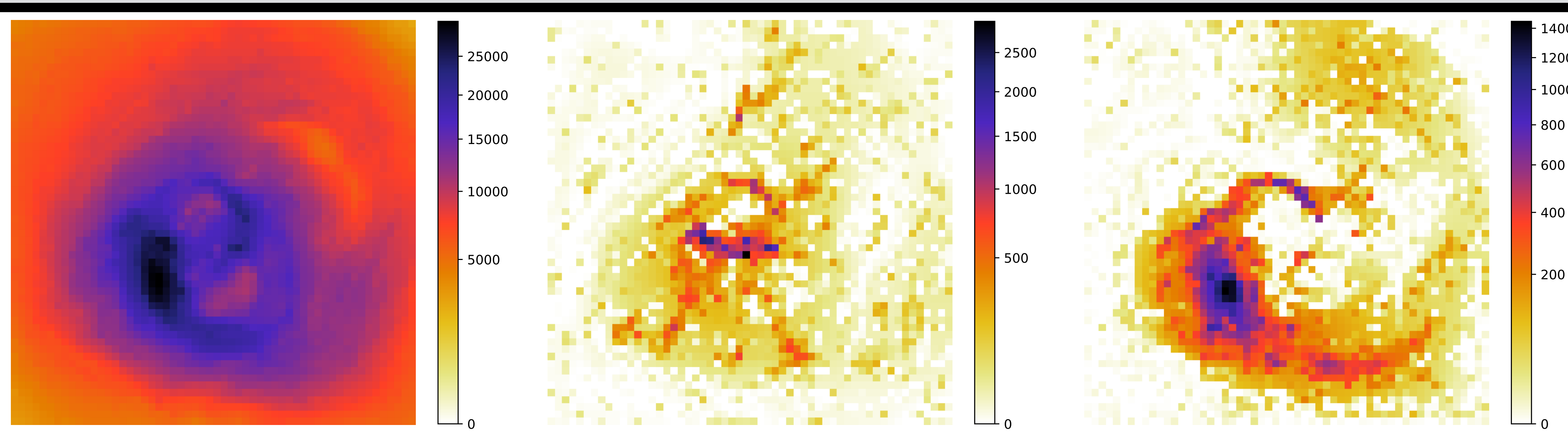
Perseus in X-rays

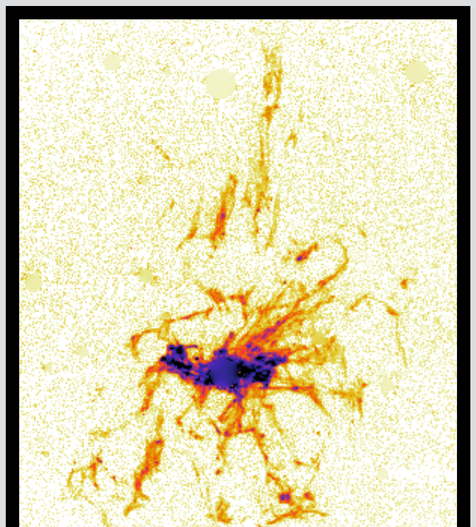
Application of pGMCA :



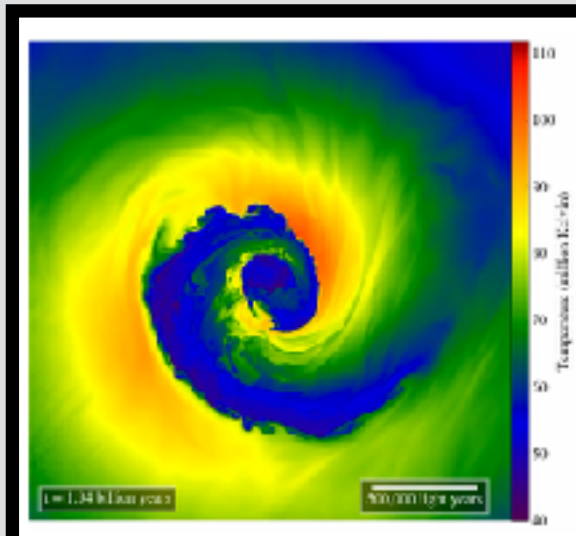
Perseus in X-rays

Application of pGMCA :





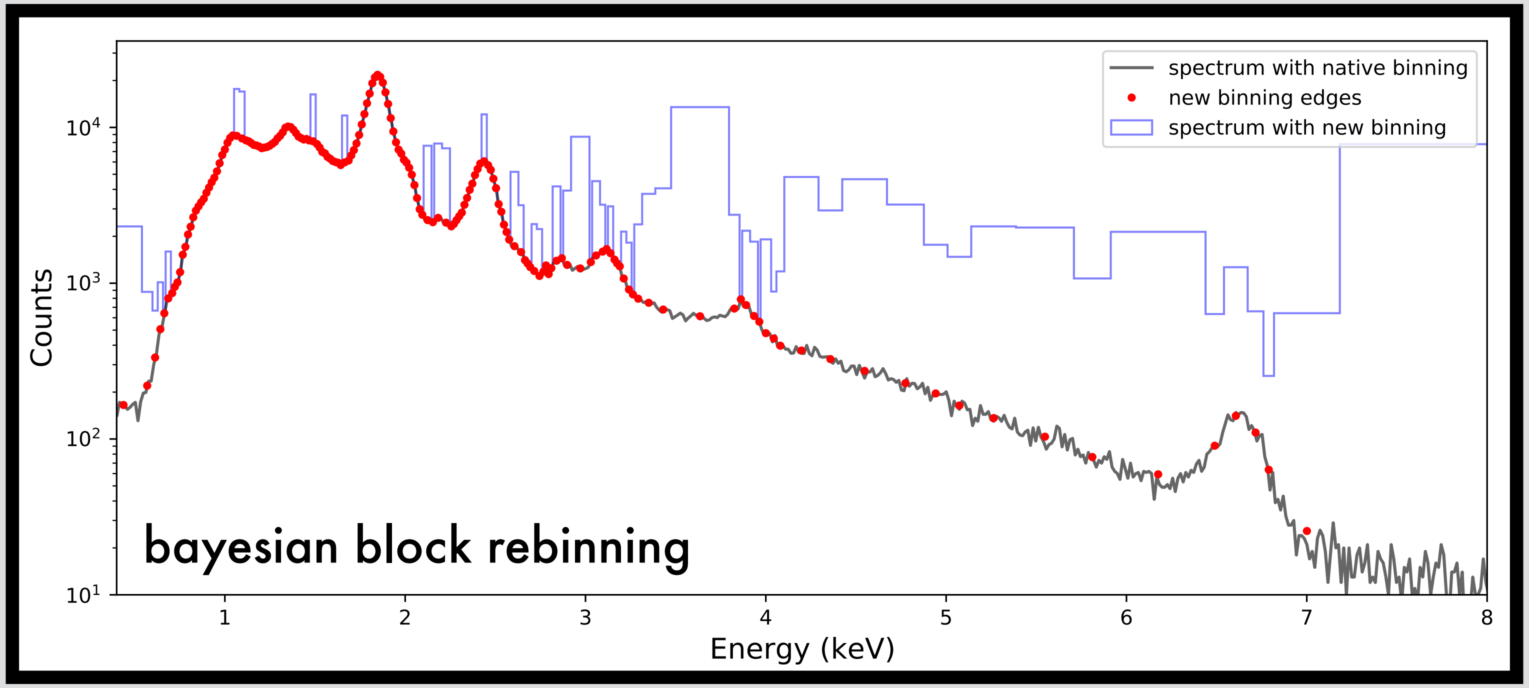
Optical data



Simulation ZuHone et al., 2018

Perspectives

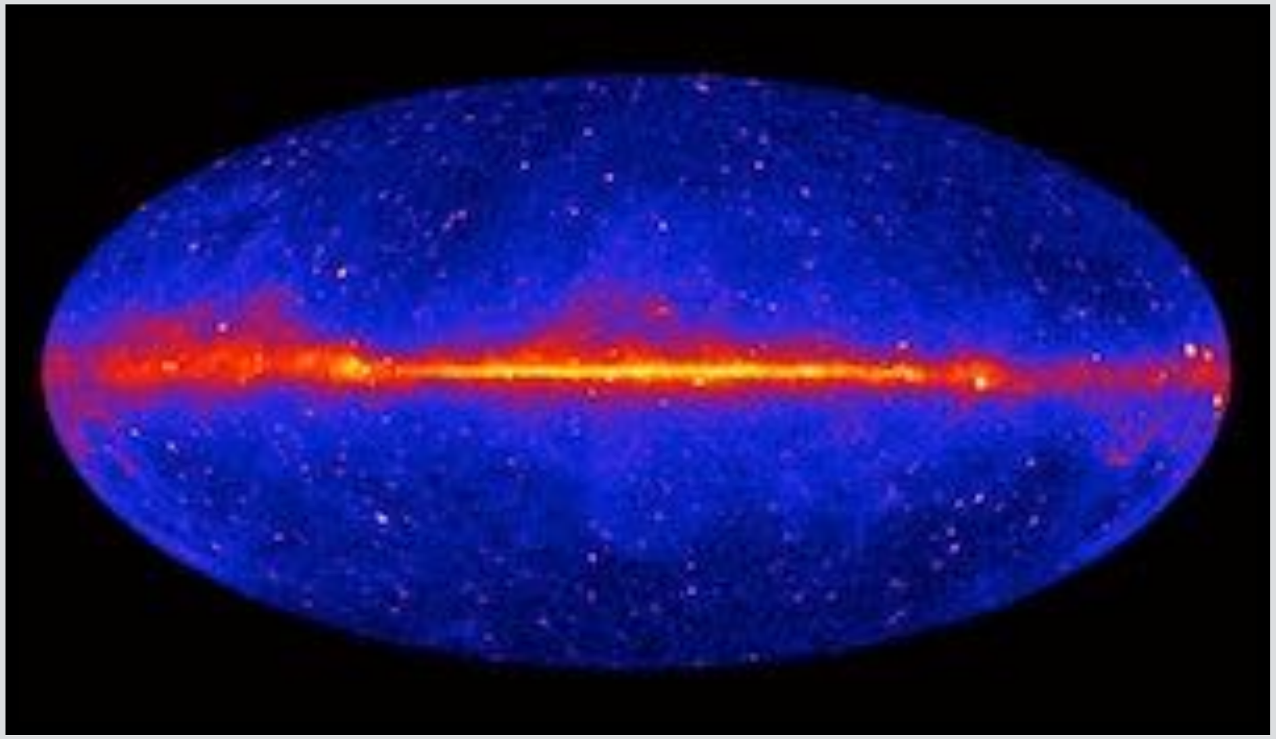
- Introduction of machine learning to constrain the spectral shapes of the components to retrieve (for example power laws or thermal models).
- Using adaptive binning to reduce the dynamic range between high and low energies.



Perspectives

- Taking into account mosaic observations (large SNRs, Magellanic clouds or galactic center)

- Taking into account the PSF. In X-rays, we can consider it constant, but it is energy dependent in CTA or *Fermi-LAT*.

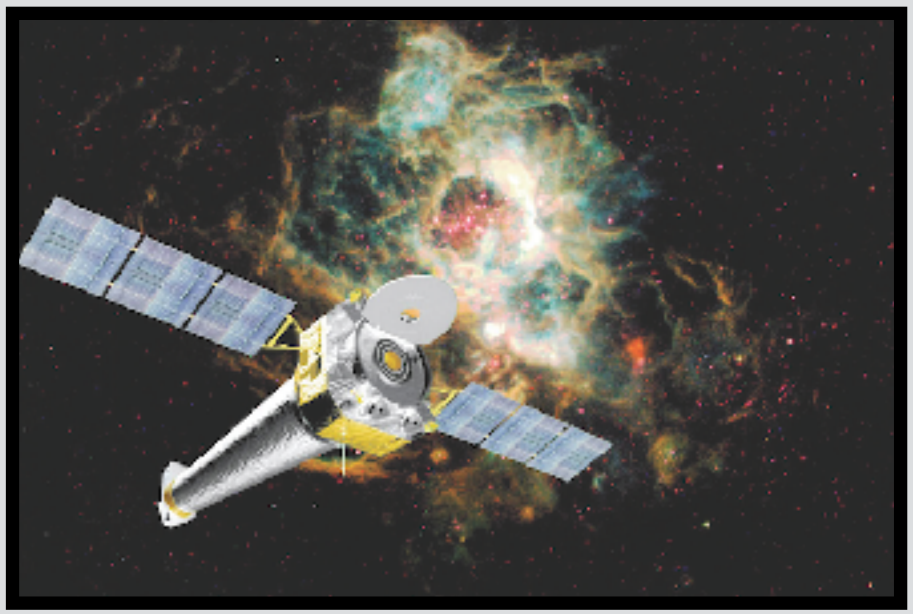


- Using data of a different type than (x,y,E) cubes. For example, transient or other temporally variable sources (x,y,t) could be studied with our method.

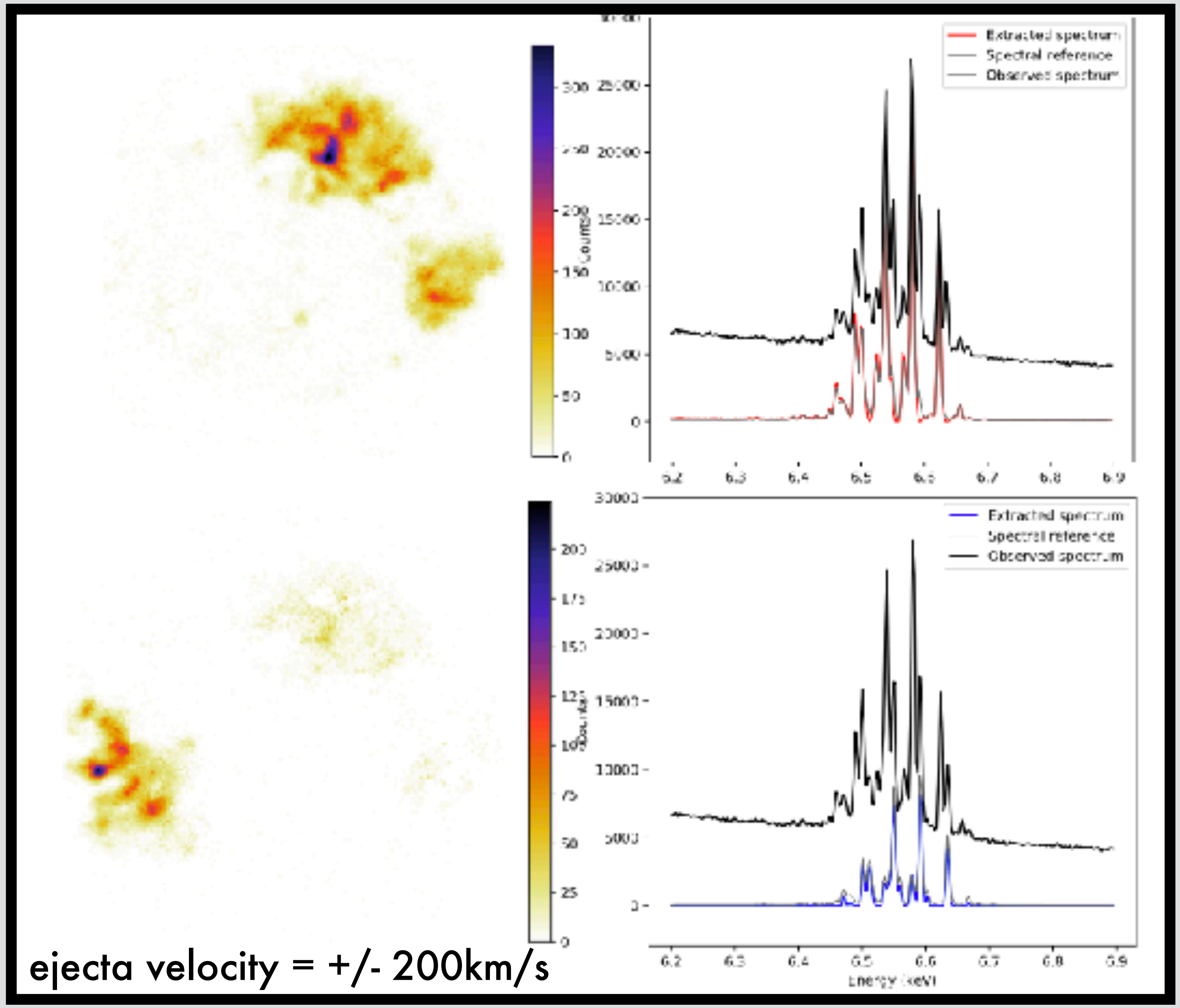
Perspectives

- On future instruments, such as *Lynx* or *Athena*'s X-IFU to exploit fully the amazing data it will gather.

Artist's impression



spatial : 5 arcsec ; spectral : 2.5 eV



GMCA on the Fe complex in simulations of X-IFU data

THE END