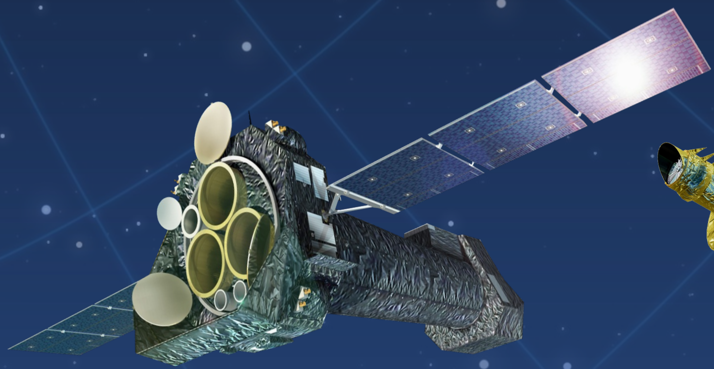
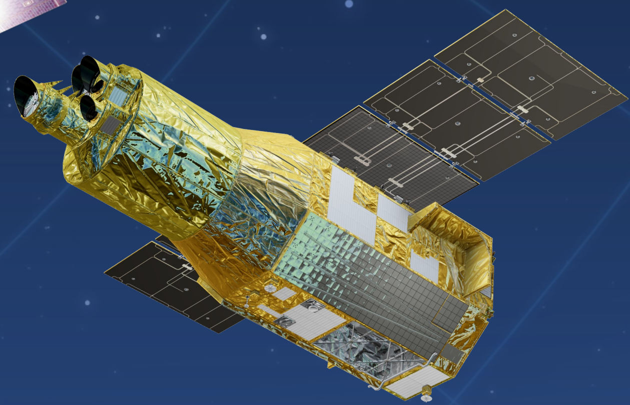
HYPERSPECTRAL DATA **FUSION** AND **SOURCE SEPARATION** FOR **X-RAY ASTROPHYSICS**

IAU-IAA ASTROSTATISTICS AND ASTROINFORMATICS SEMINAR

JULIA LASCAR, JÉRÔME BOBIN, FABIO ACERO

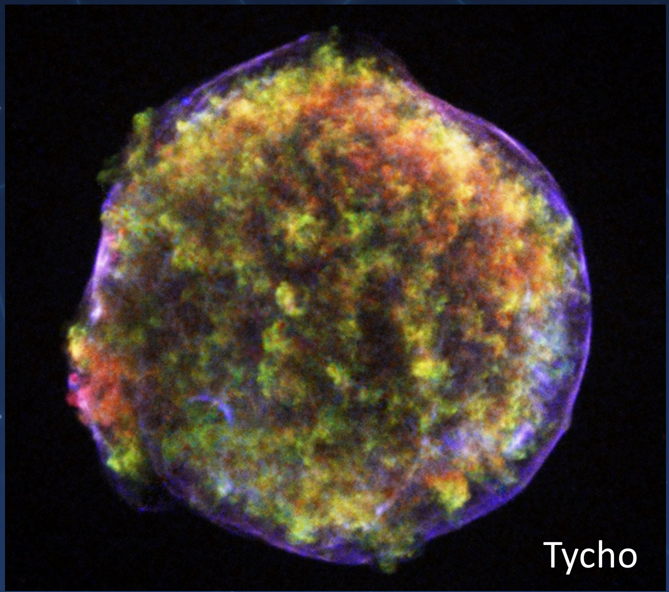
X-RAY ASTROPHYSICS



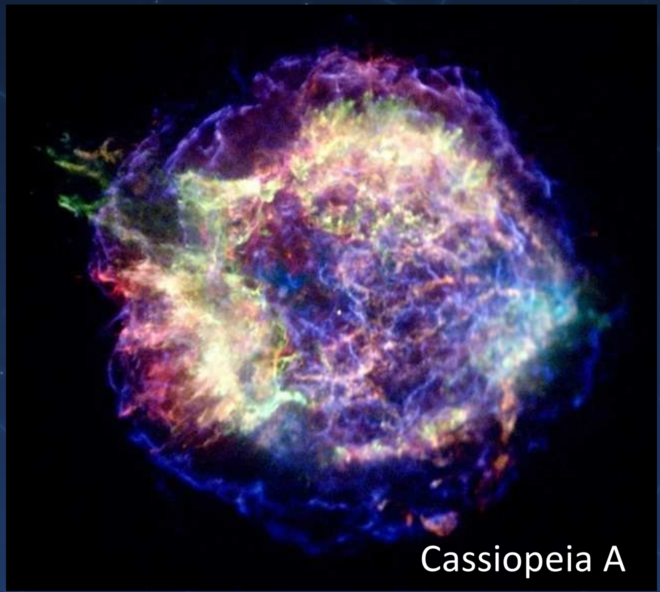


CONTEXT

- Supernova Remnants: hundreds of years after a stellar explosion



Type Ia (binary star collapse)



Type II (core collapse)

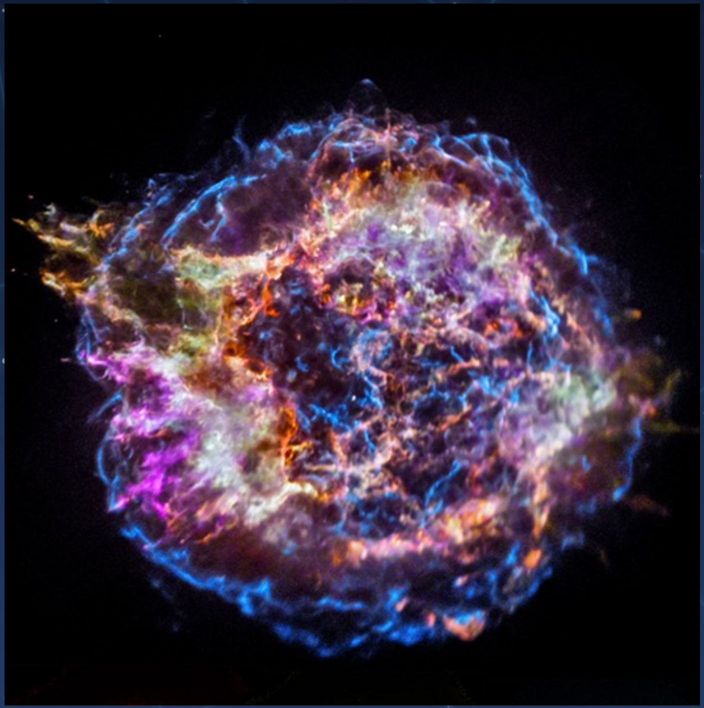
CASSIOPEIA A SUPERNOVA REMNANT

- **Silicon thermal emission**
- Ejecta from the original explosion

- **Iron thermal emission**

- **Synchrotron non-thermal emission**
- Shock wave accelerating particles

CASSIOPEIA A SUPERNOVA REMNANT



GOALS:

- Separate the components individually
- Map out their physical properties
- Element abundance, temperature, velocity…

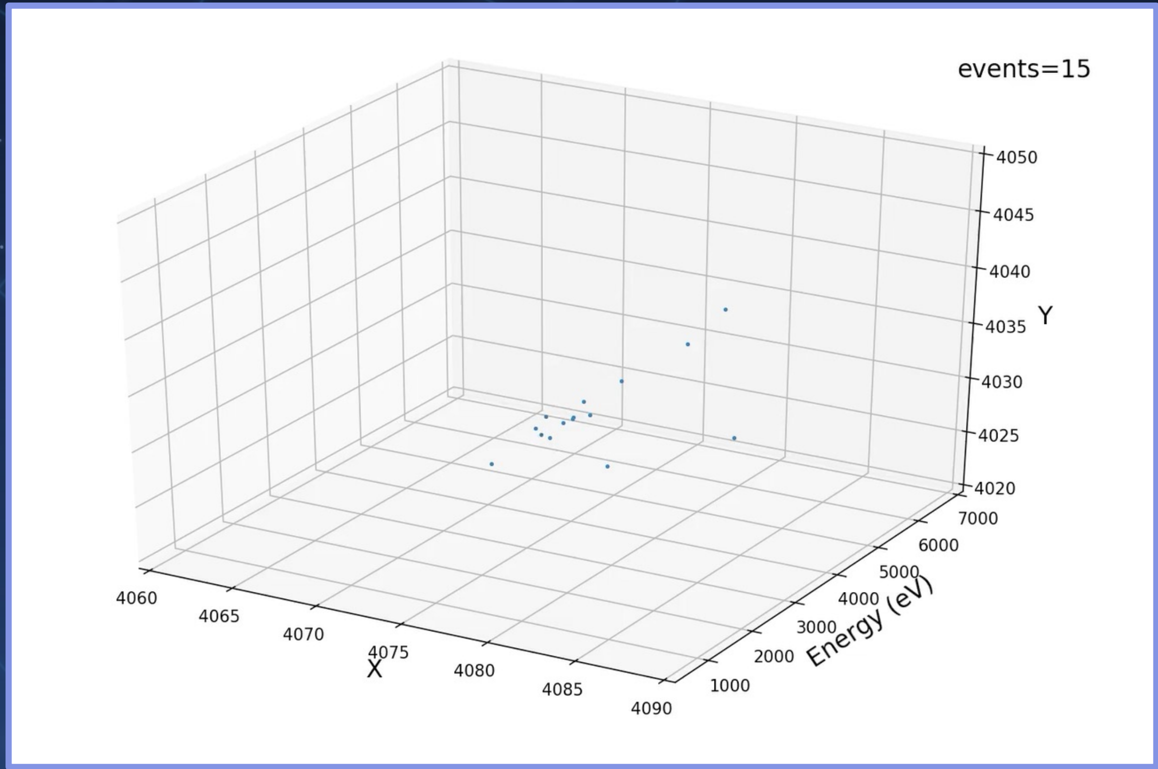
→ Constrain explosion models of supernova

→ **Better understanding of stellar evolution**

X-RAY SPECTRO-IMAGER DATA ACQUISITION

Chandra Acis

Pulsar B1259 observation



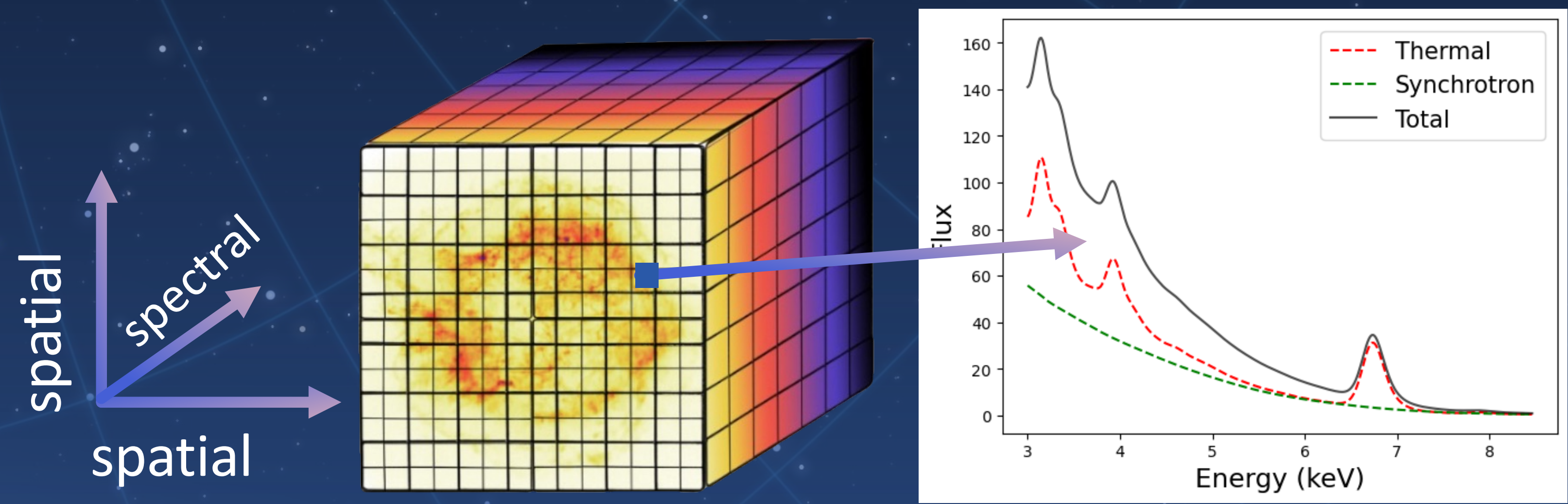
- Count statistics

→ Poisson distribution

Julia Lascar | julia.lascar@cea.fr | https://github.com/JMLascar/

HYPERSPECTRAL IMAGES

- Hyperspectral images: 2 spatial dimensions + 1 energy dimension
- For each pixel, a spectrum
- Entangled physical components



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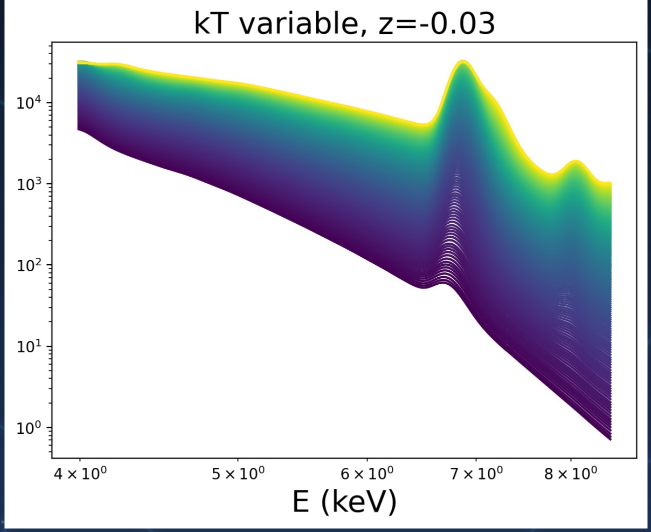
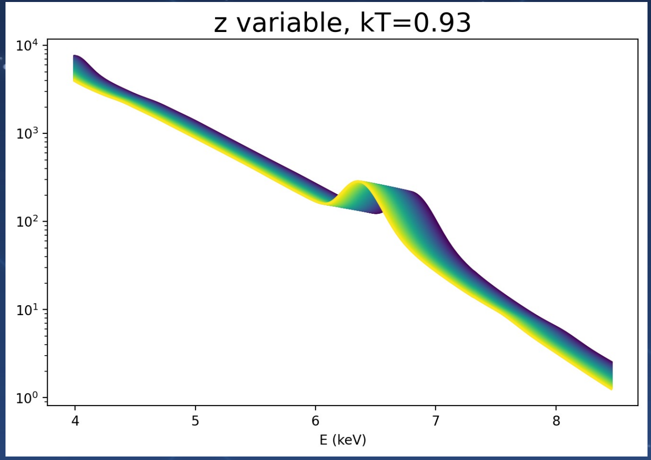
CHALLENGES IN X-RAY ASTROPHYSICS

- Poisson Noise
- Low signal/noise ratio, noise variabilities
- High spectral variability
- Non analytical physical model

--> Need tools that account for these specific challenges

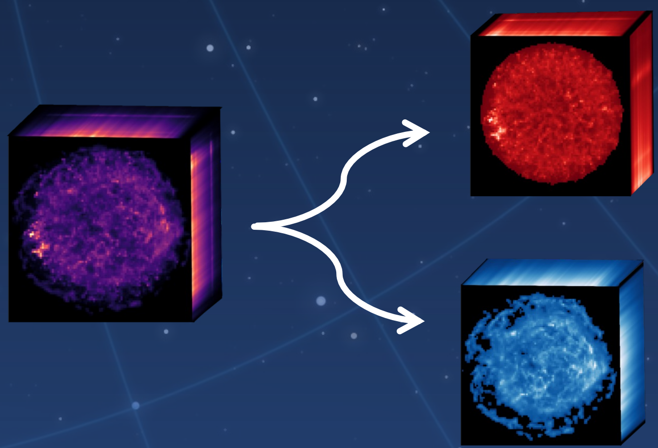




NEW GENERATION TOOLS FOR X-RAY ASTROPHYSICS

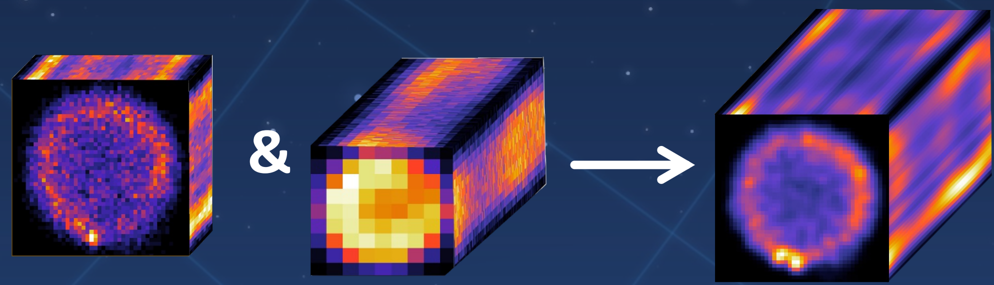
Source Unmixing

Separating untangled sources

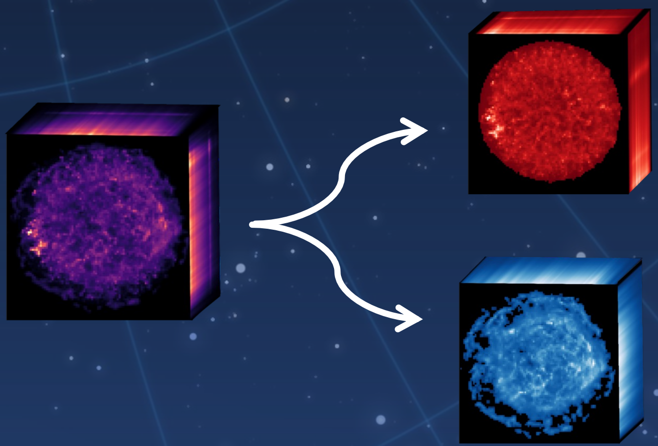


Hyperspectral fusion

Combining data from two generations of instrument



SOURCE SEPARATION WITH SPECTRAL VARIABILITIES



SUSHI

SEMI-BLIND UNMIXING WITH SPARSITY FOR HYPERSPECTRAL IMAGES

HOW TO UNMIX?

Local 1D fit

Pros:

- Account for **spectral diversity**
- Can produce **physical parameter mapping**

Cons:

- No neighbourhood information → Poor performance on low-signal pixels

(Lovisari et al. (2024), Mayer et al. (2023), and Sasaki et al. (2022), and many more.)

Matrix Factorization

Pros:

- Takes into account **neighbourhood information**

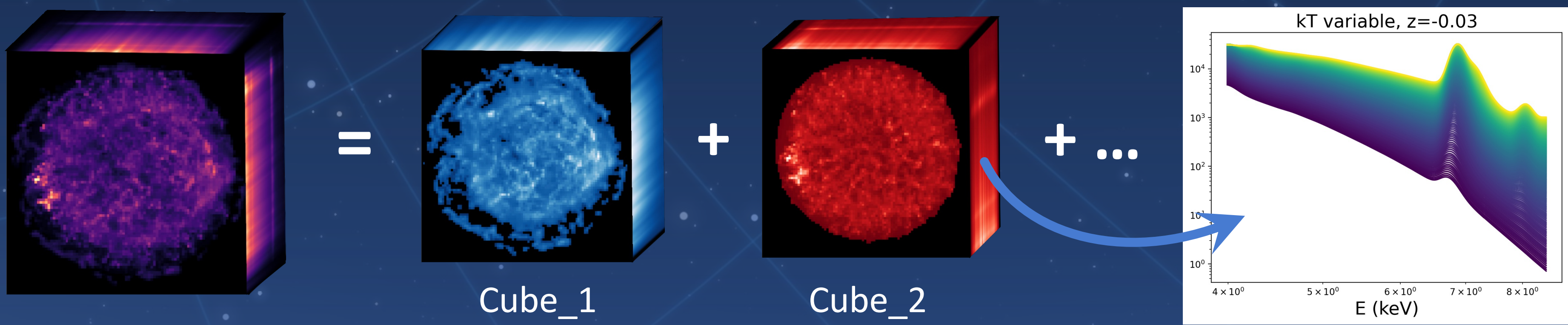
Cons:

- No spectral diversity
- Cannot produce parameter maps

(See Feng et al. (2022) for review)

Matrix Factorization:

More realistic model includes spatial variability:



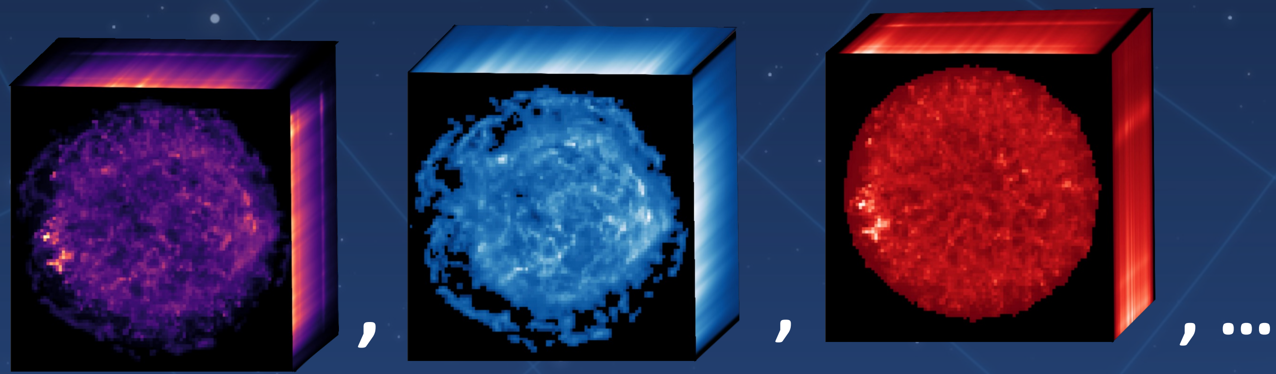
SUSHI: AN OVERVIEW

→ **Plug a learnt model for spectral variation**

→ **Applies a spatial regularisation on the parameters map of the learnt model**

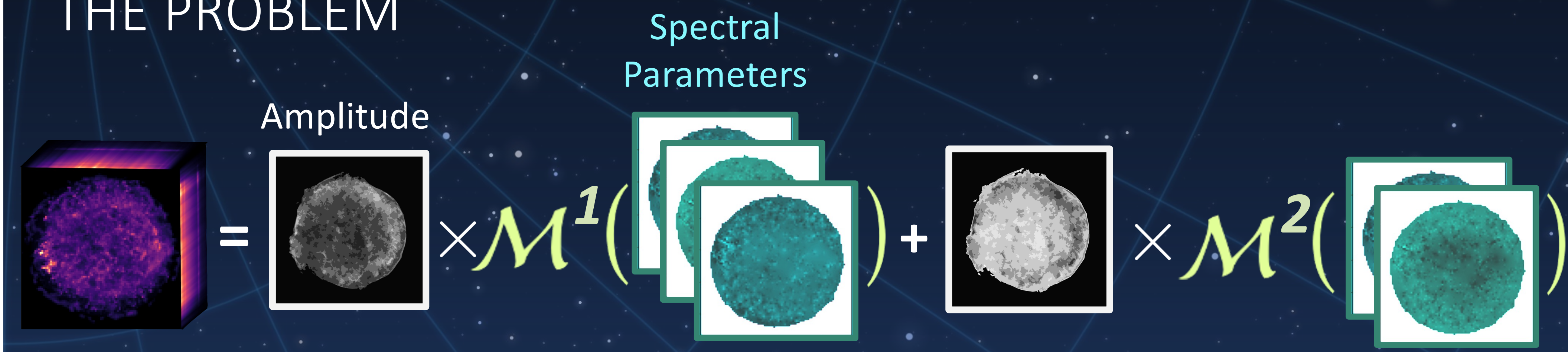
→ **Obtains, for each component, a cube that varies spatially and spectrally.**

SUSHI output



Denoised total, Component 1, Component 2, ...

THE PROBLEM



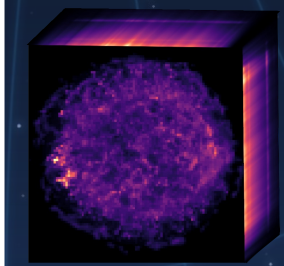
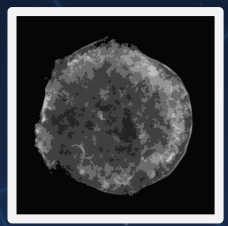
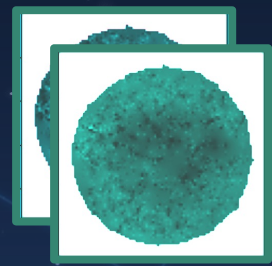
$$A,\ \theta = \underset{A,\ \theta}{\operatorname{argmin}} \sum_{c}^{n_C} \mathcal{L}\left(A^c \mathcal{M}^c(\theta^c)\right) + \rho\varphi(\theta^c)$$

Data fidelity **Spectral Model** **Spectral Parameters** **Spatial Reg**

THE PROBLEM

Spectral Parameters

Amplitude

 =  $\times \mathcal{M}^1($  $)$ +  $\times \mathcal{M}^2($  $)$

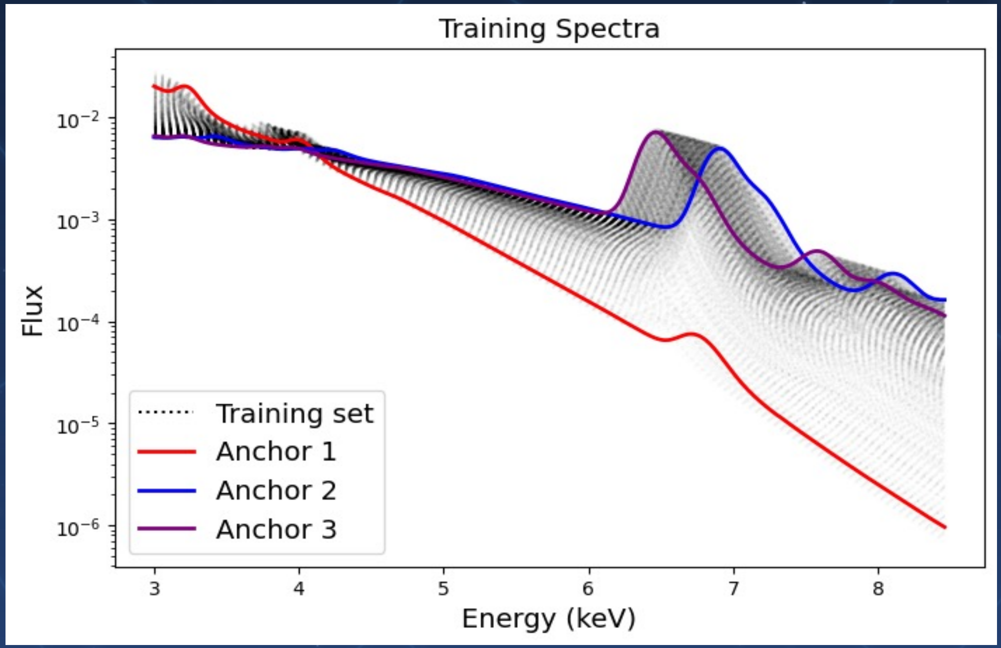
$$A,\, \theta = \underset{A,\, \theta}{\mathrm{argmin}} \sum_{c}^{n_C} \mathcal{L}\Big(A^c \mathcal{M}^c(\theta^c)\Big) + \rho\varphi(\theta^c)$$

Spectral Model → **Needs to be differentiable!**

LEARNT MODEL:
INTERPOLATORY AUTO ENCODER (IAE)

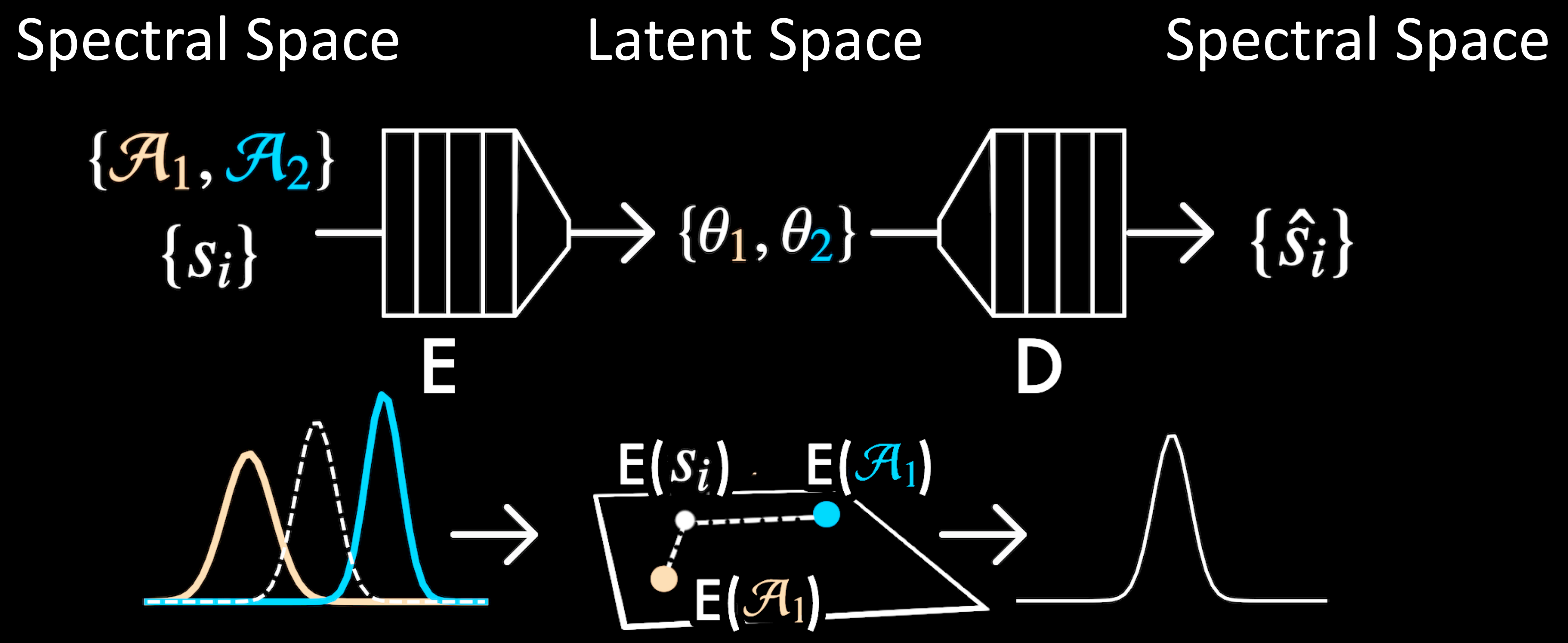
Bobin, J., Gertosio, R., Thiam, C., Bobin C. 2021.

- Learn to interpolate between anchor points

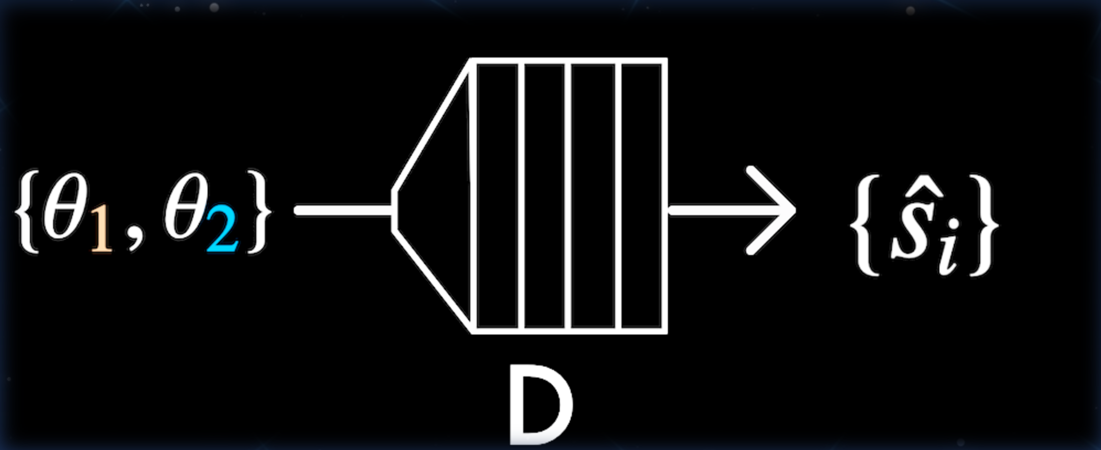


LEARNT MODEL:

INTERPOLATORY AUTO ENCODER (IAE)



THE DECODER AS A GENERATIVE MODEL



- D is differentiable
- Not costly to call upon

- Latent parameters vary smoothly with physical parameters

→ Spatial regularization makes sense

SPATIAL REGULARIZATION OF LATENT PARAMETERS

- Undecimated Isotropic Wavelet Transform: Starlet Transform (useful in astro)
- Minimize L1 norm

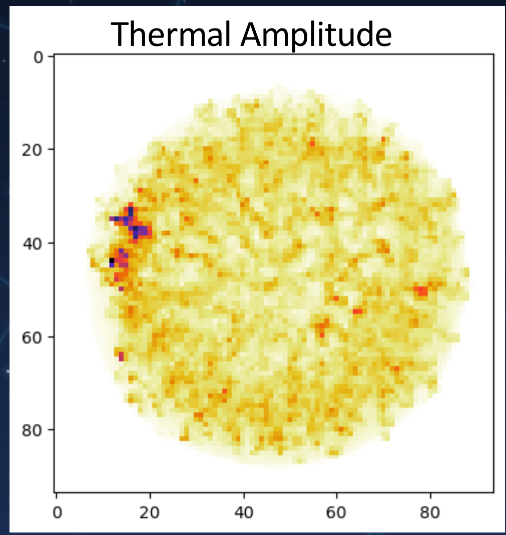
$$A,\, \theta = \underset{A,\,\theta}{\operatorname{argmin}} \sum_{c}^{n_C} \underbrace{\mathcal{L}}_{\text{Likelihood}}\Big(A^c \underbrace{\mathcal{M}^c}_{\text{Learnt Model}}(\underbrace{\theta^c}_{\text{Latent Parameters}})\Big) + \underbrace{\rho \|\mathcal{W}(\theta^c)\|_1}_{\text{Spatial Reg}}$$

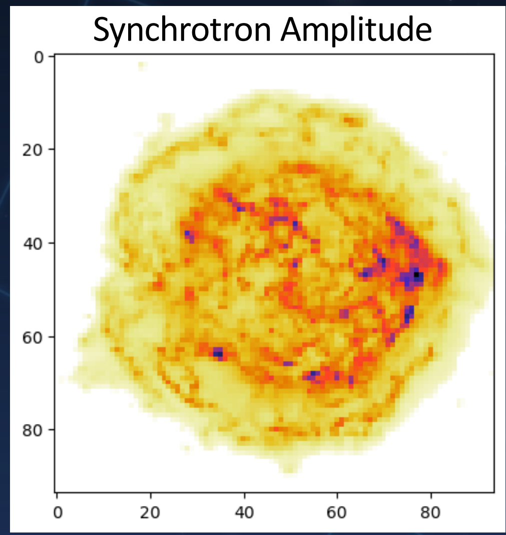
- Proximal Alternating Linearized Minimization (PALM, Bolte 2014)

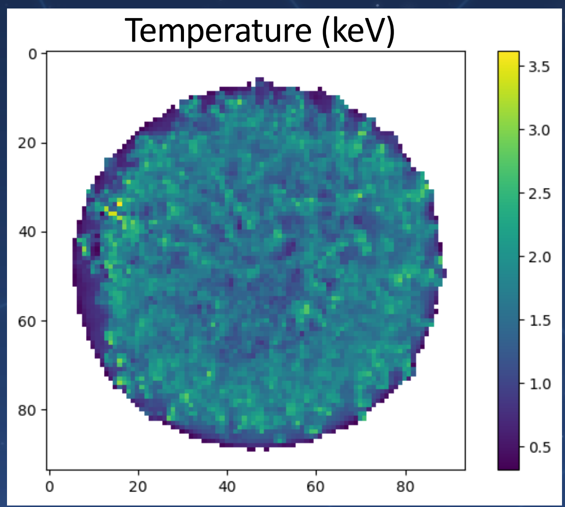
SUSHI RESULTS

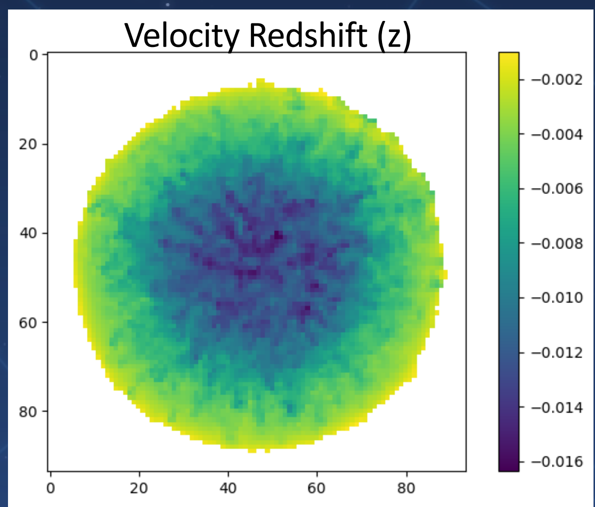
SIMULATED TOY MODEL

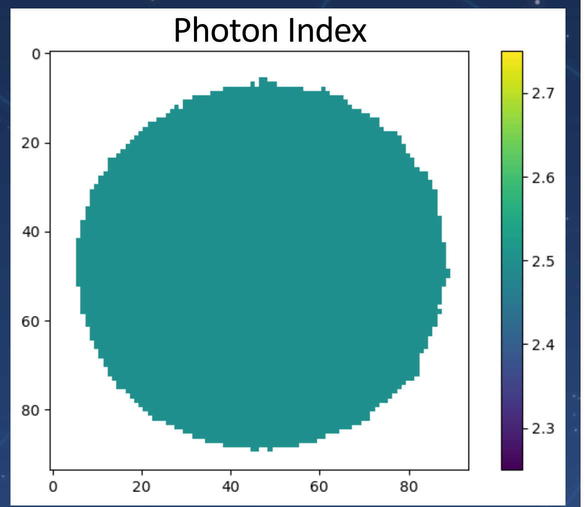
- from real images + numerical simulations of CasA
- Thermal Component: Varying redshift, temperature
- Synchrotron Component: Constant Photon Index







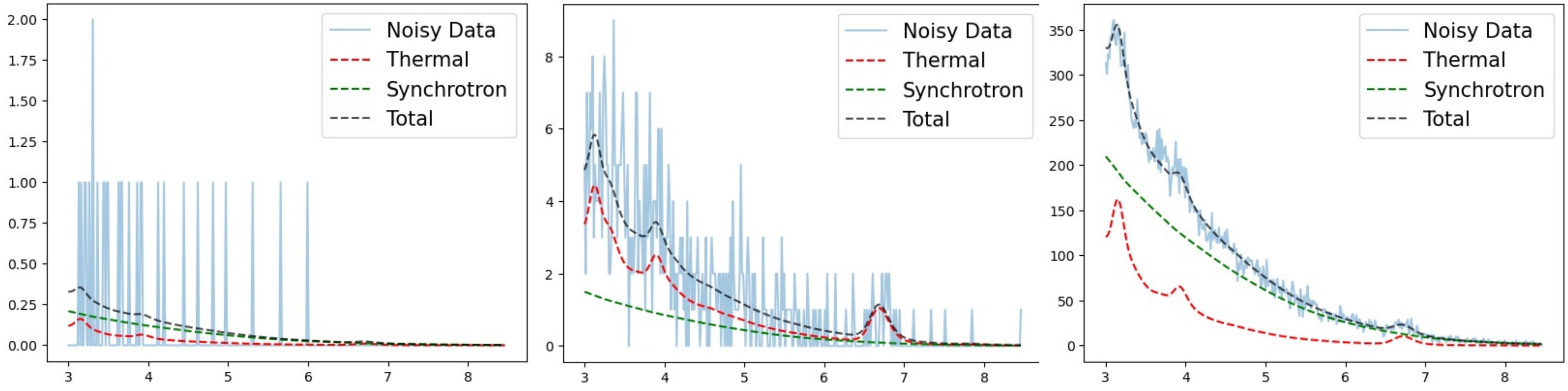




EXAMPLE OF SPECTRA FROM INDIVIDUAL PIXELS

- Varying levels of noise / count statistics

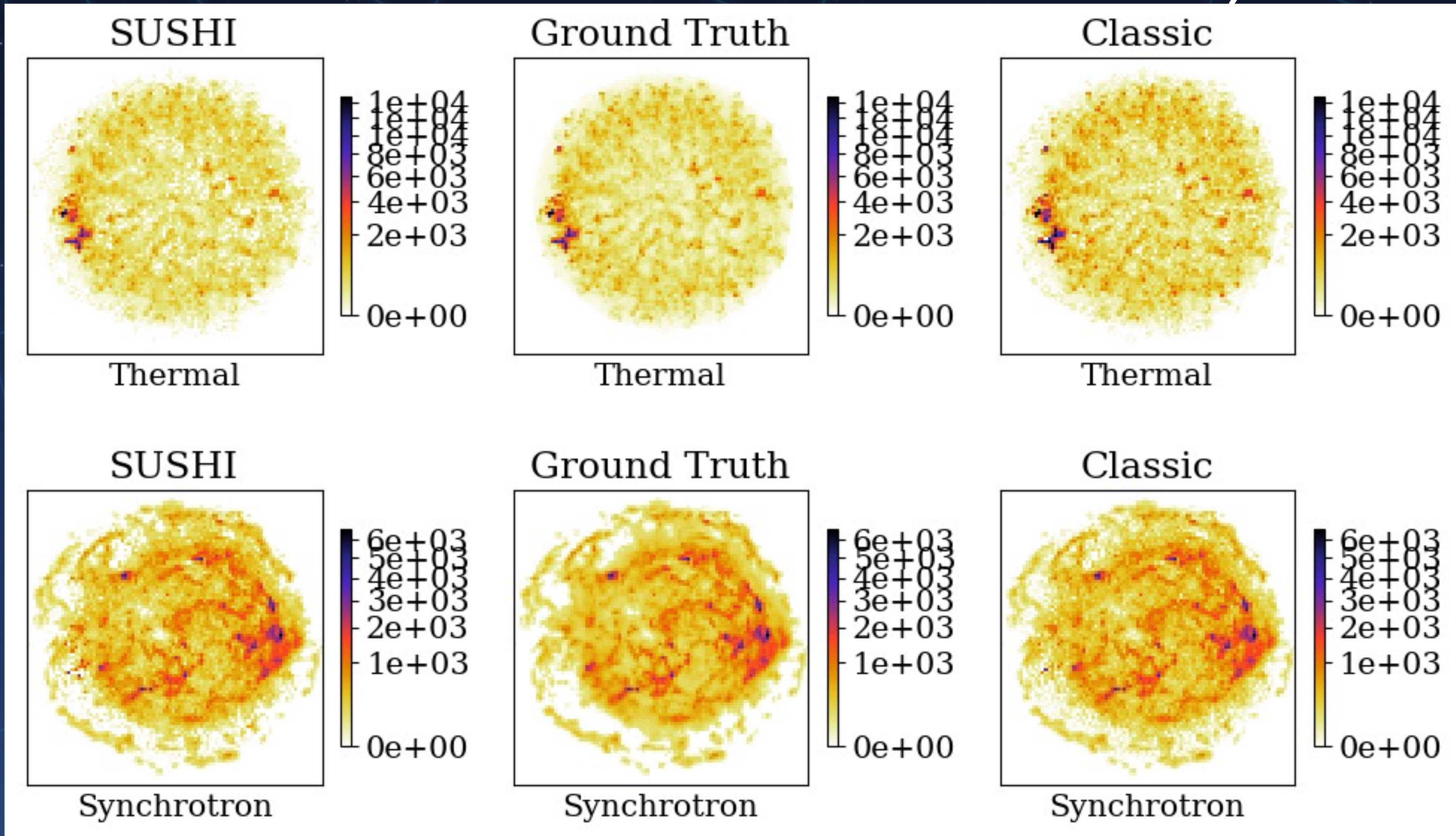
Flux



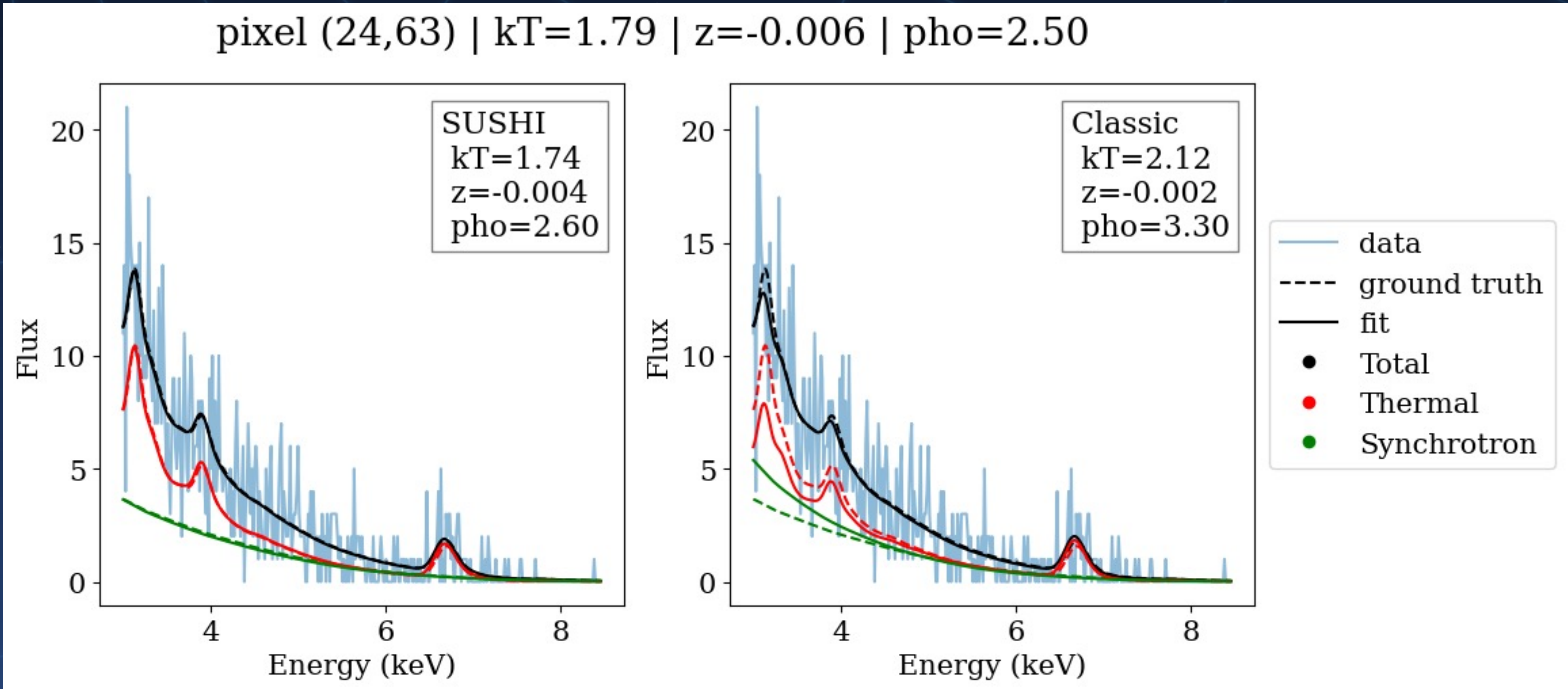
Energy (keV)

AMPLITUDE MAP COMPARISONS

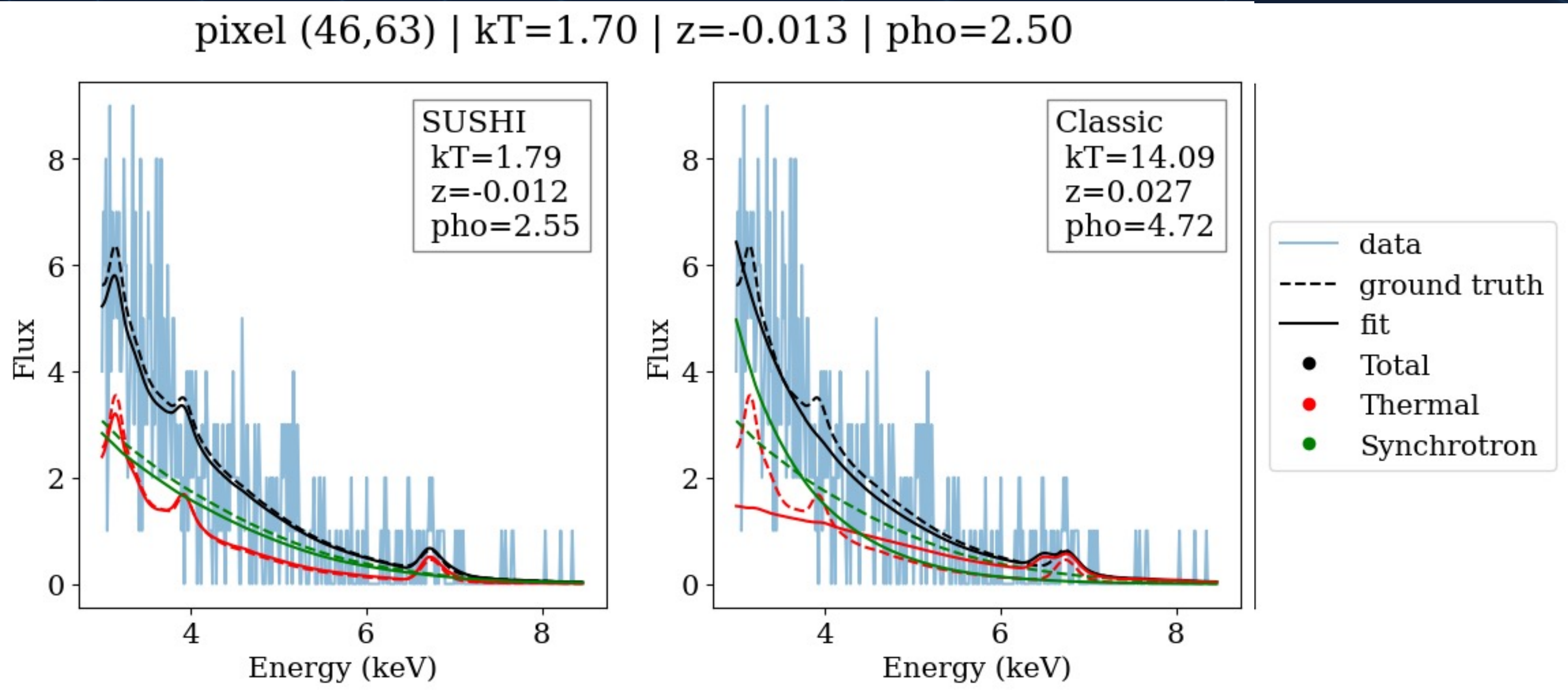
Fit 1D pixel-per-pixel

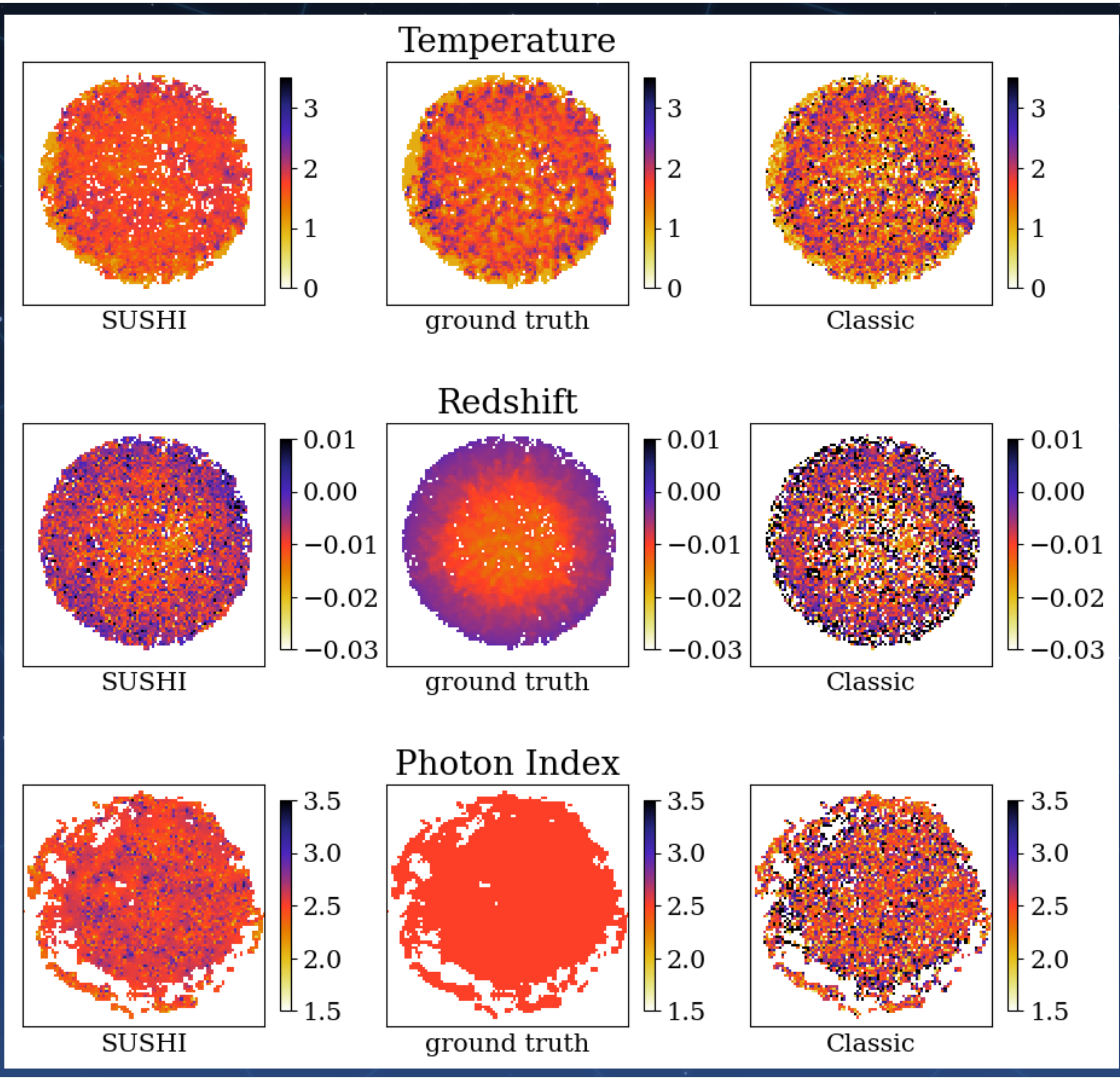


INDIVIDUAL PIXEL COMPARISONS



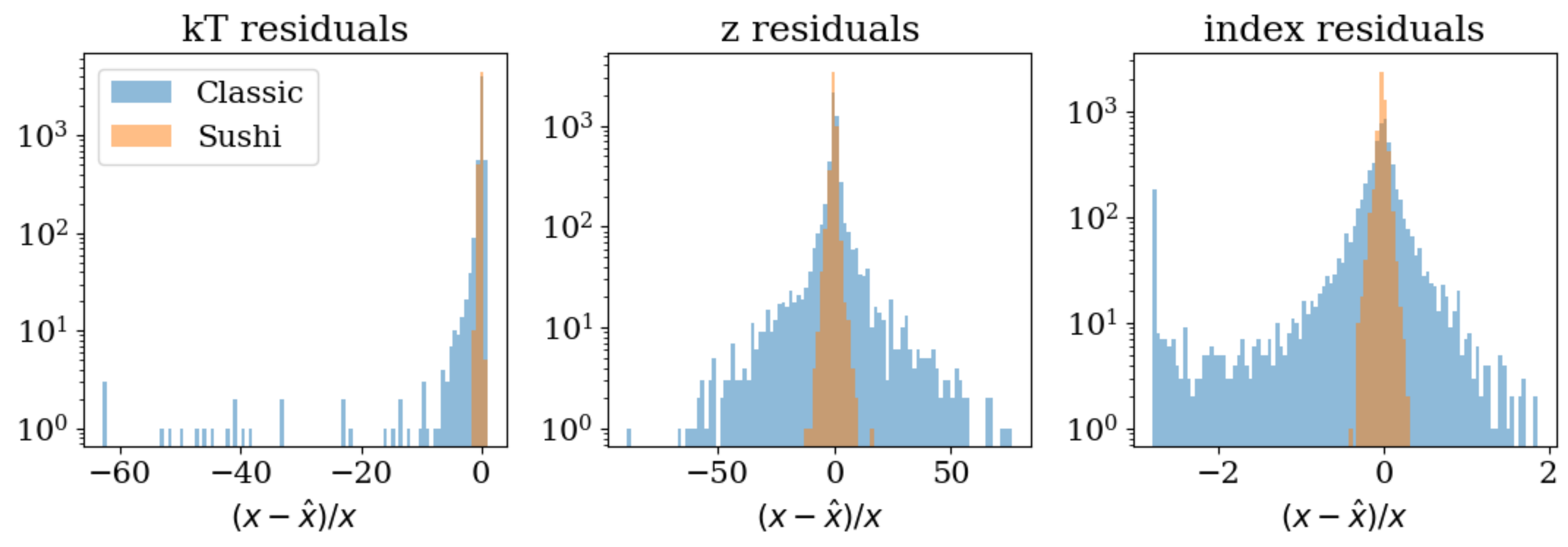
INDIVIDUAL PIXEL COMPARISONS





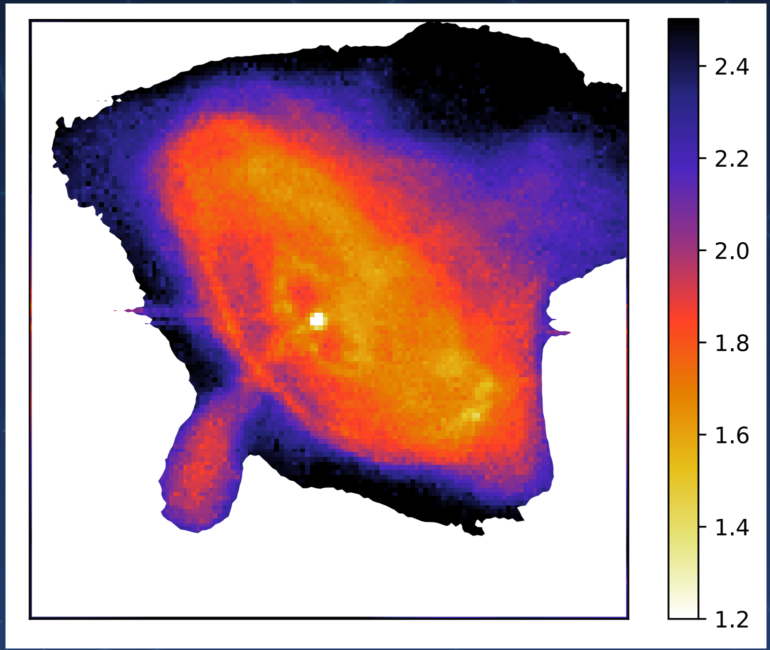
Temperature
3
2
1
0
SUSHI
ground truth
Classic
Redshift
0.01
0.00
−0.01
−0.02
−0.03
SUSHI
ground truth
Classic
Photon Index
3.5
3.0
2.5
2.0
1.5
SUSHI
ground truth
Classic

PARAMETER RESIDUALS HISTOGRAMS

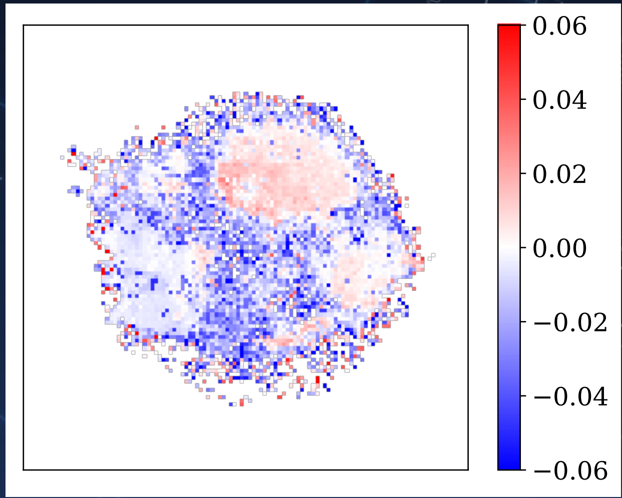


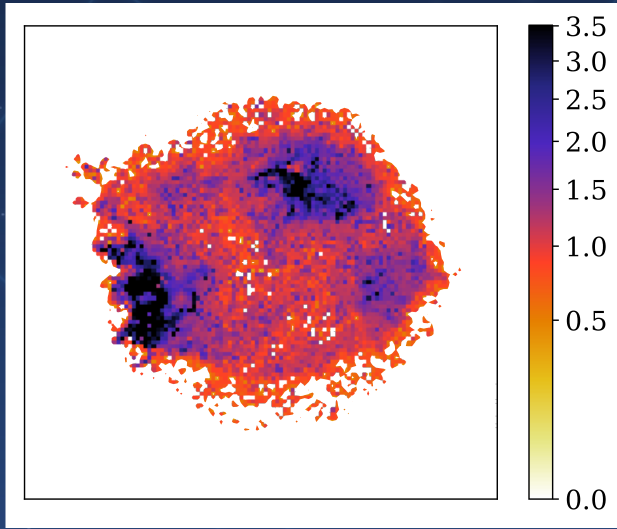
REAL DATA RESULTS

Crab Nebula Photon Index Map:



Cassiopeia A: z and kT maps





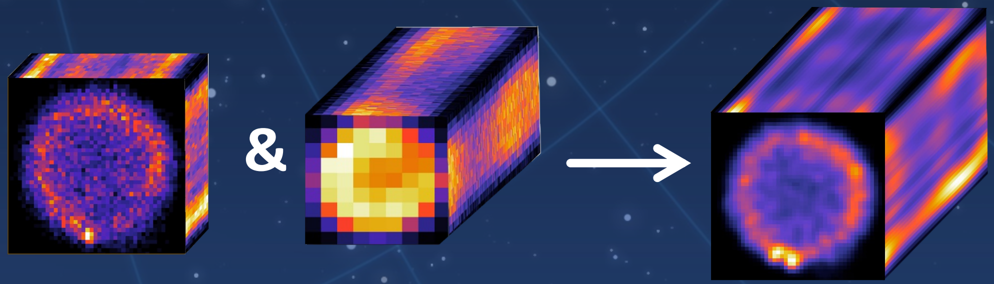
SUSHI SUMMARY

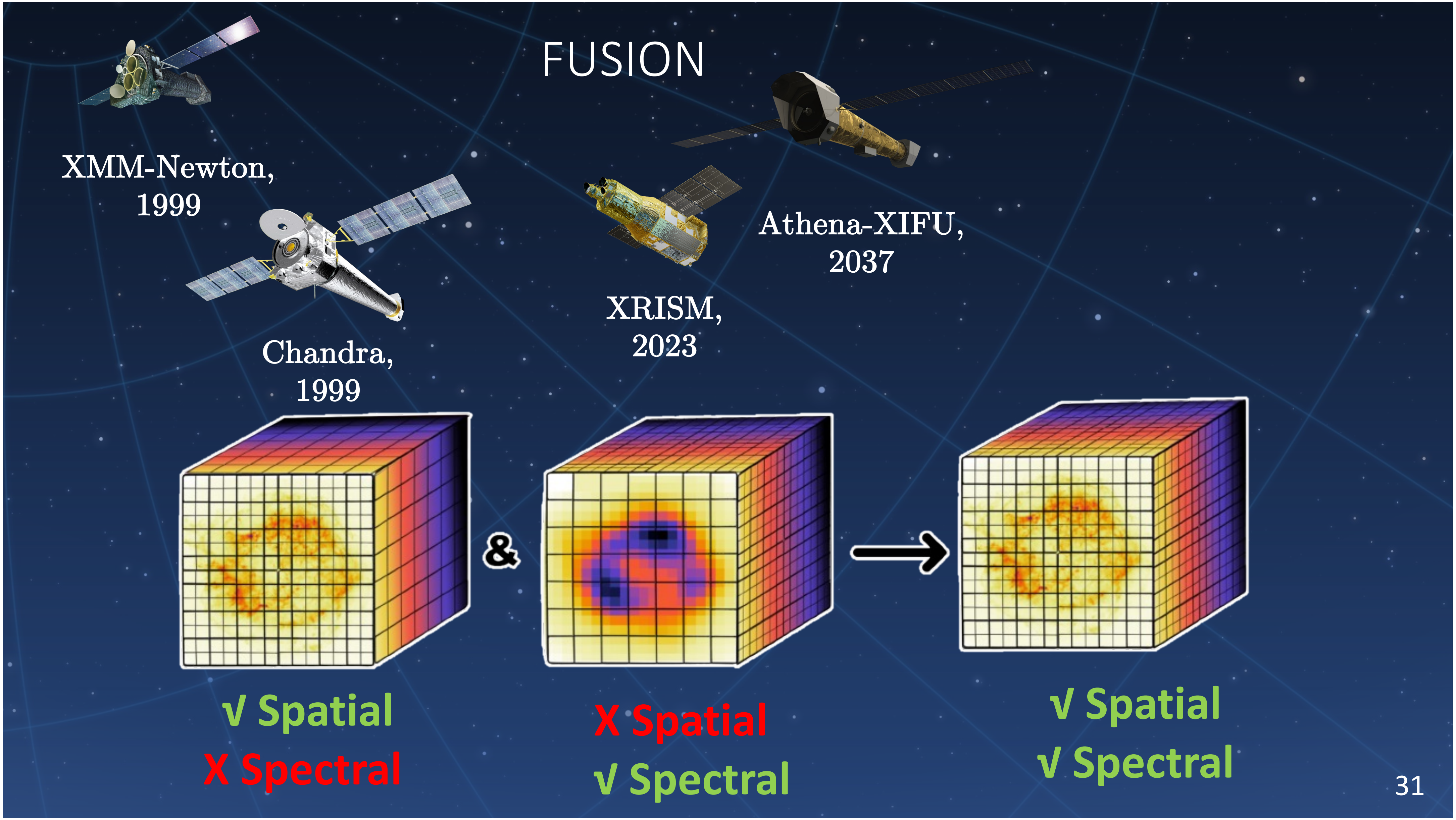
- **SUSHI** is a method to unmix hyperspectral images with spectral variations based on a physical model (one for each endmember).
  - As a surrogate model, SUSHI uses the decoder of an Interpolatory Auto-Encoder.
  - It applies a spatial sparsity regularization on the surrogate model's parameter maps.
- General framework applicable to hyperspectral images with spectral variabilities where a spectral model can be learnt.

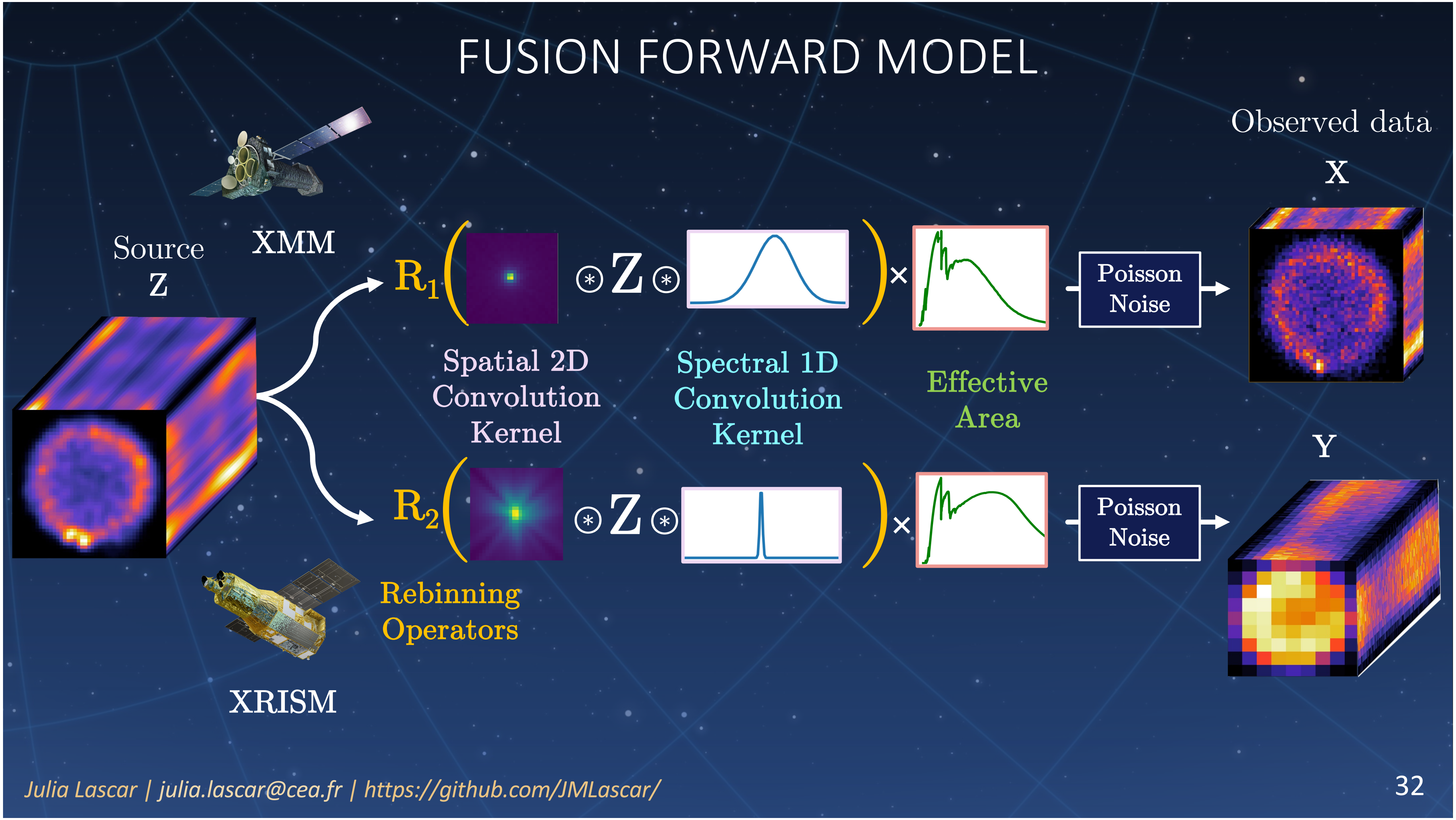
https://github.com/JMLascar/SUSHI

HYPERSPECTRAL IMAGE FUSION VIA REGULARIZED DECONVOLUTION

HI-FRED




FUSION
XMM-Newton, 1999
Chandra, 1999
XRISM, 2023
Athena-XIFU, 2037
&
√ Spatial
X Spectral
X Spatial
√ Spectral
√ Spatial
√ Spectral
31



FUSION FORWARD MODEL
Observed data
X
Source
Z
XMM
R_1
$\circledast$ Z $\circledast$
×
Poisson Noise
Spatial 2D Convolution Kernel
Spectral 1D Convolution Kernel
Effective Area
Y
R_2
$\circledast$ Z $\circledast$
×
Poisson Noise
Rebinning Operators
XRISM
Julia Lascar | julia.lascar@cea.fr | https://github.com/JMLascar/
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ESTIMATOR

$$\hat{Z} = \arg\min_{Z \geq 0} \mathcal{L}_P\left(X \mid Z_X\right) + \mathcal{L}_P\left(Y \mid Z_Y\right) + \varphi(Z),$$

Spectral Response

Rebinning

$$Z_X = (t_X Z \odot A_X)\mathcal{S}_X \mathcal{R}_L$$

$$Z_Y = \mathcal{R}_{MN}\mathcal{B}_Y(t_Y Z \odot A_Y),$$

$$\left(\mathcal{B}_Y Z\right)_k = B_Y \circledast Z_k$$

$$\left(Z\mathcal{S}_X\right)_{ij} = Z_{ij} \circledast S_X,$$

Spatial Response

Effective Area

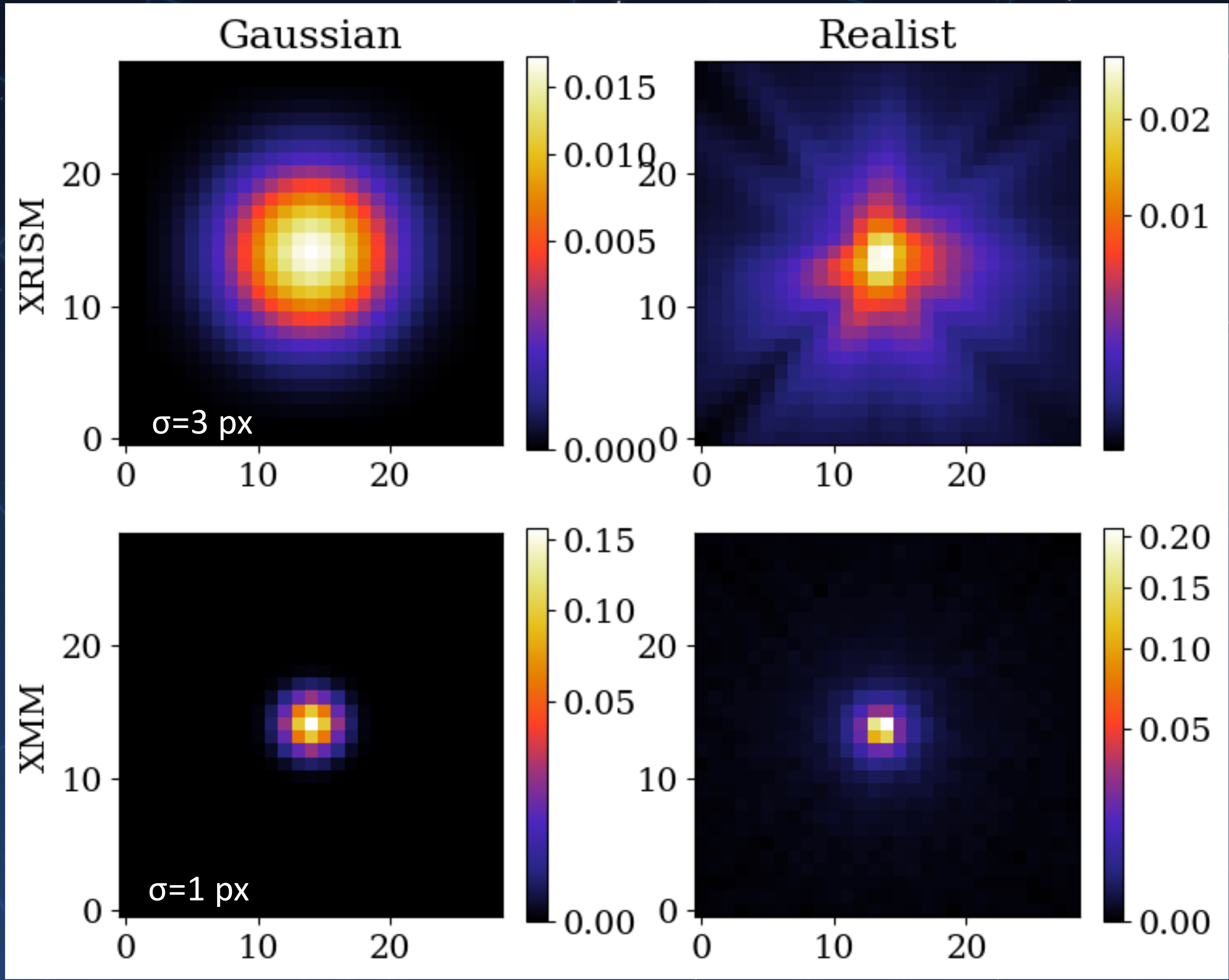
OPTIMIZATION

$$\hat{Z} = \underset{Z \geq 0}{\arg\min}\, \mathcal{L}_P\left(X \mid Z_X\right) + \mathcal{L}_P\left(Y \mid Z_Y\right) + \varphi(Z),$$

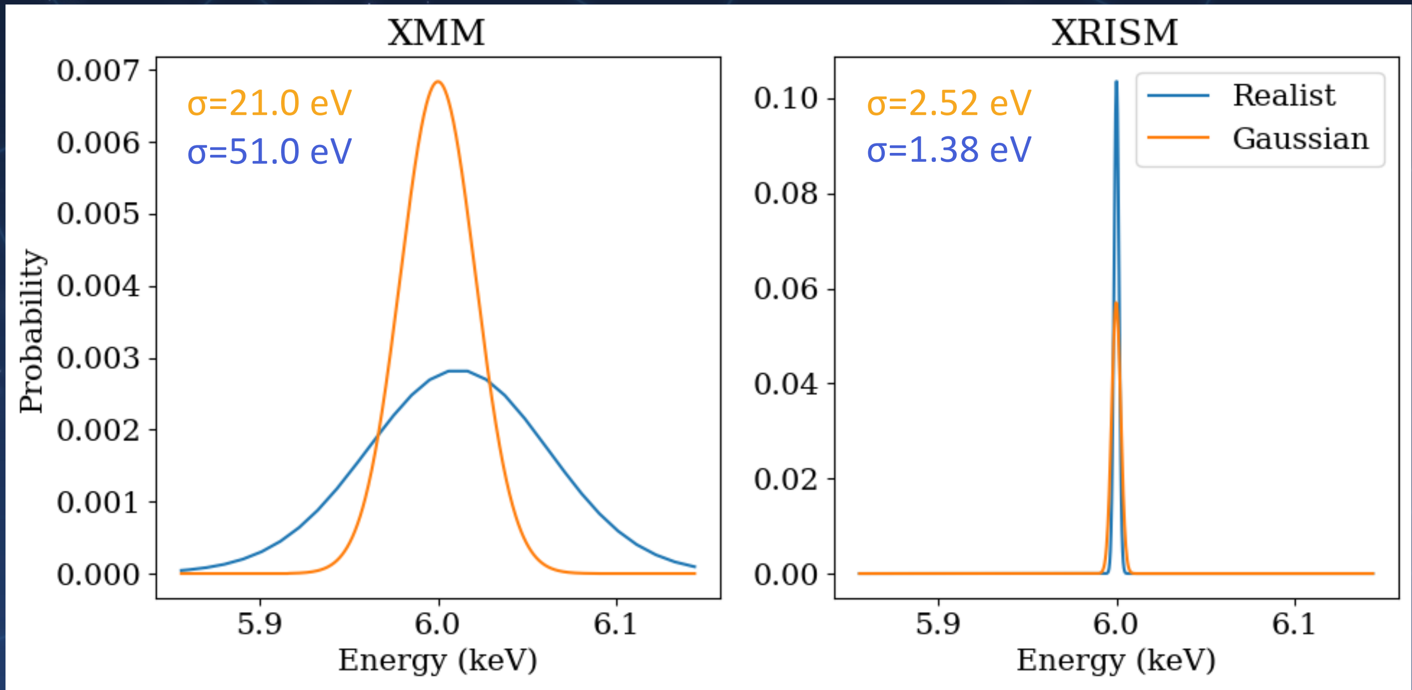
- Negative log likelihood Poisson
- Most of the cost function is differentiable (except $\varphi(Z)$)
  - Proximal Gradient Descent / ISTA
- Convolutions done in Fourier space to save time

FUSION RESULTS

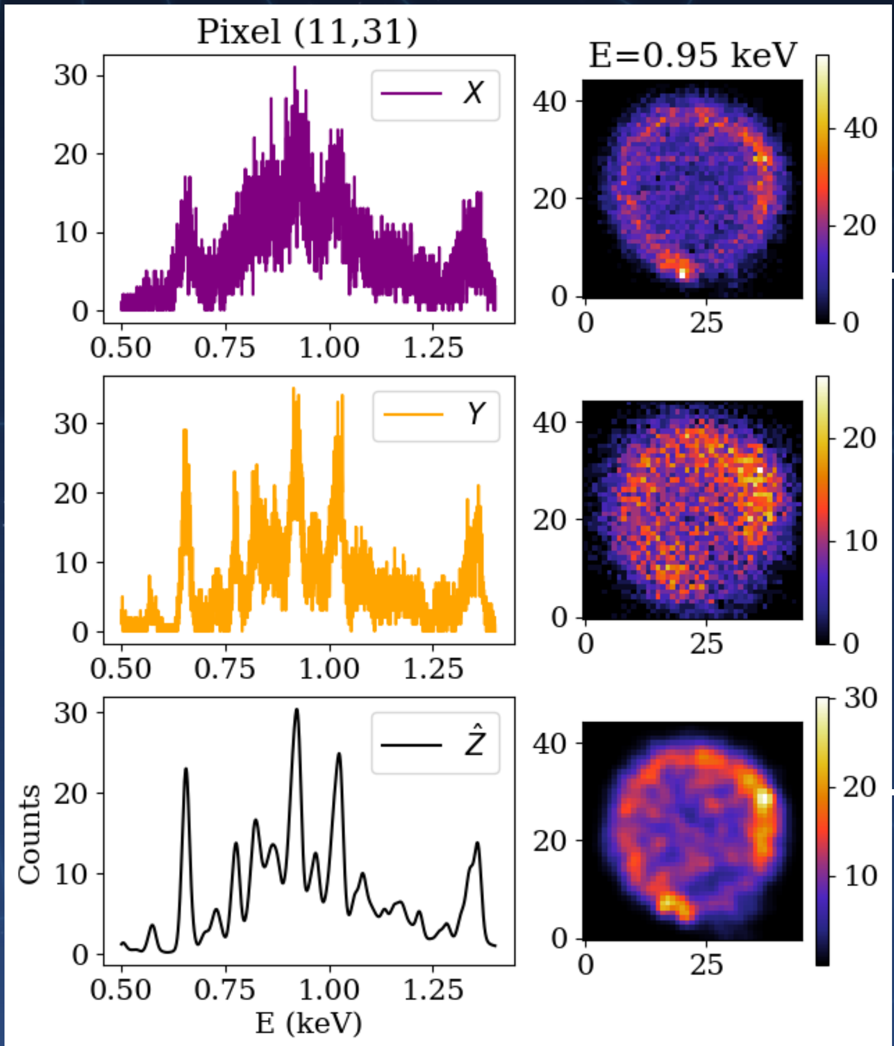
SPATIAL RESPONSES

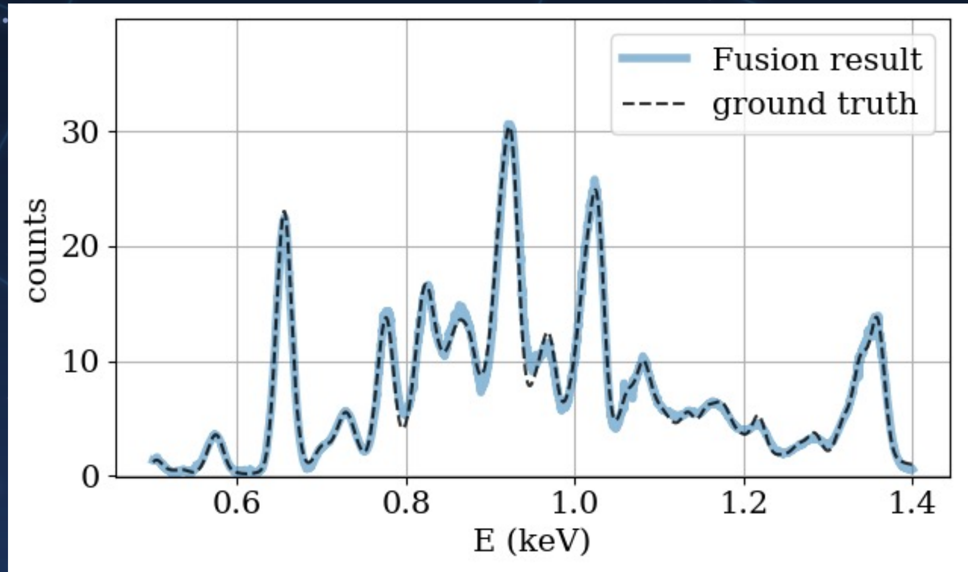


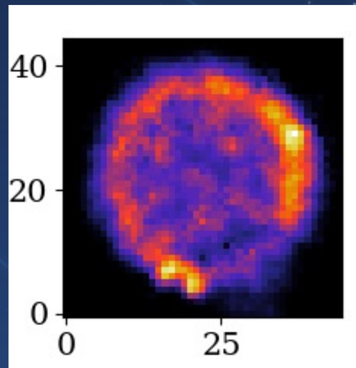
SPECTRAL RESPONSES



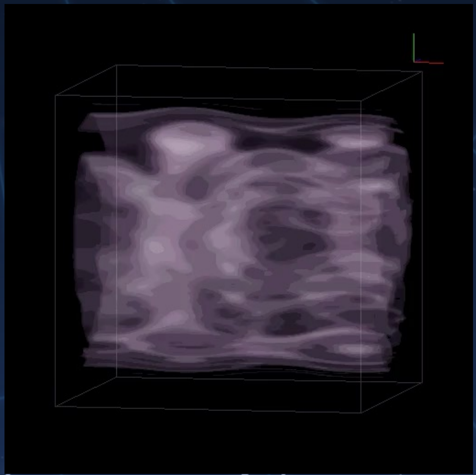
RESULT: GAUSSIAN

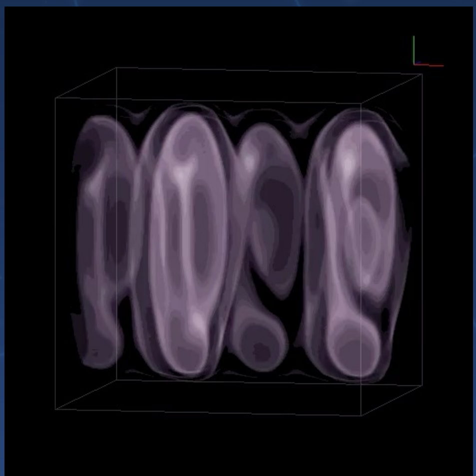




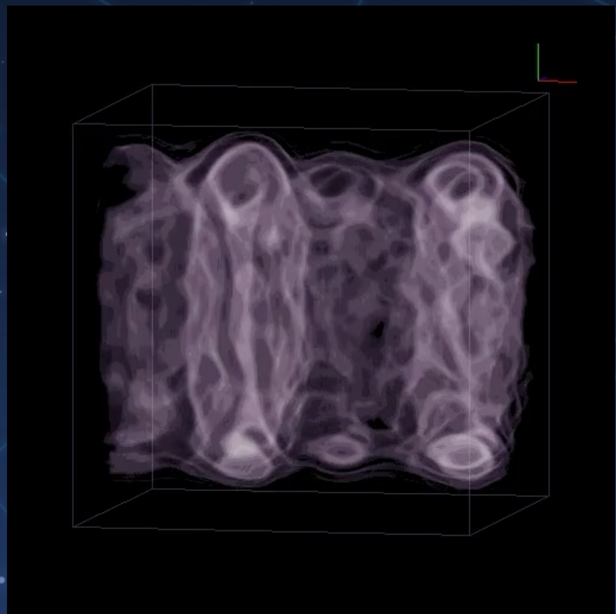


INPUT

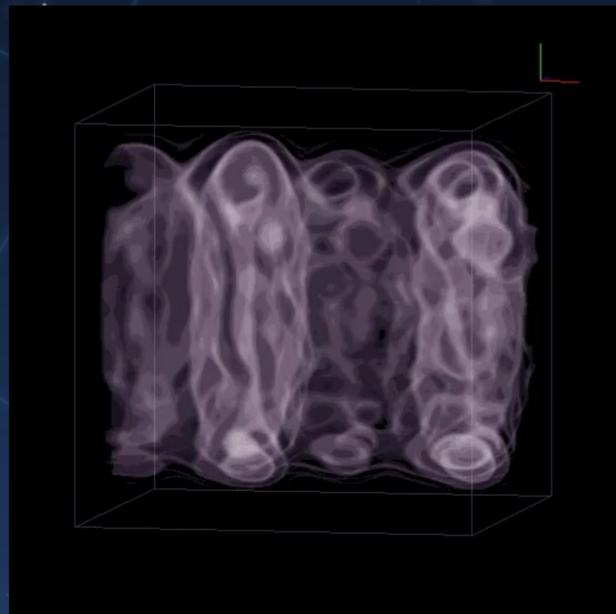




RESULT

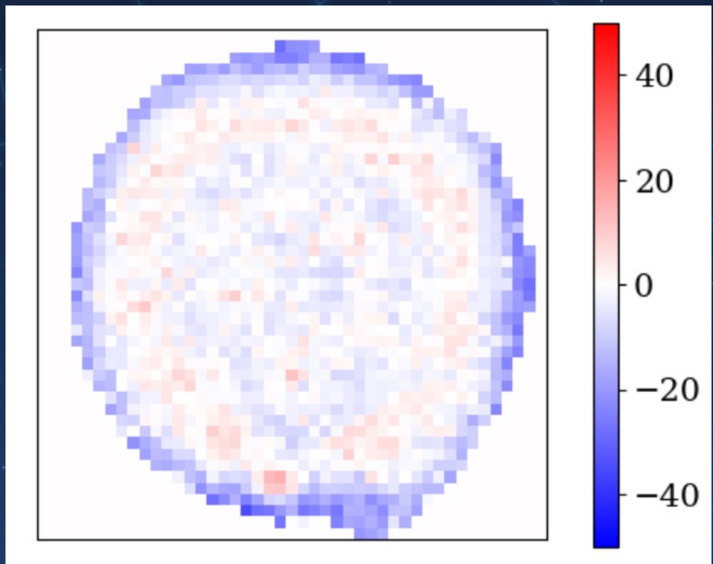


GROUND TRUTH

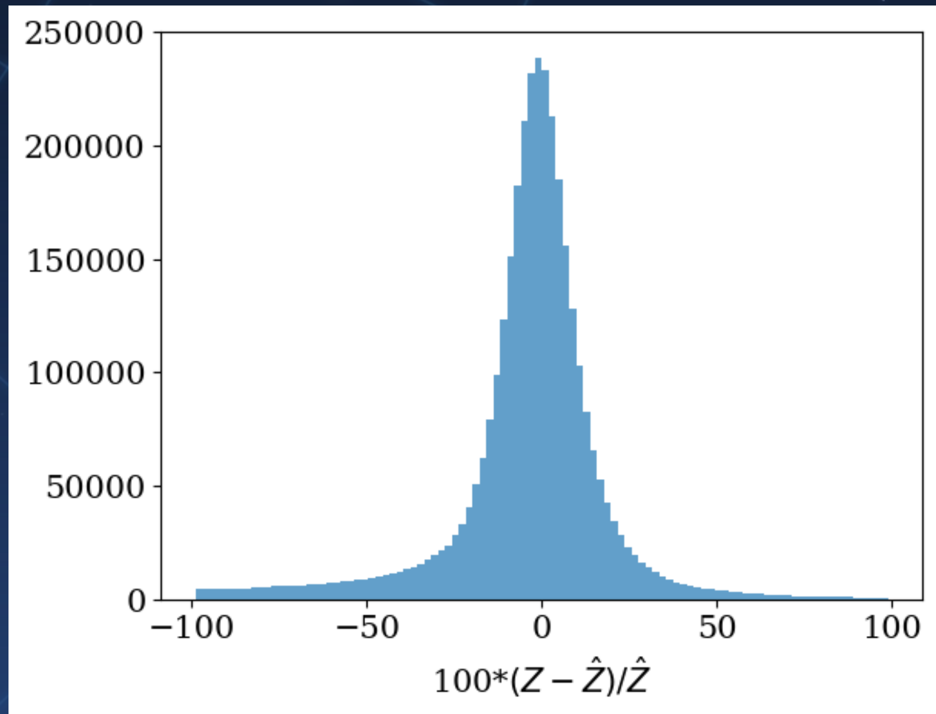


GAUSSIAN MODEL

GAUSSIAN MODEL: RELATIVE ERROR (%)

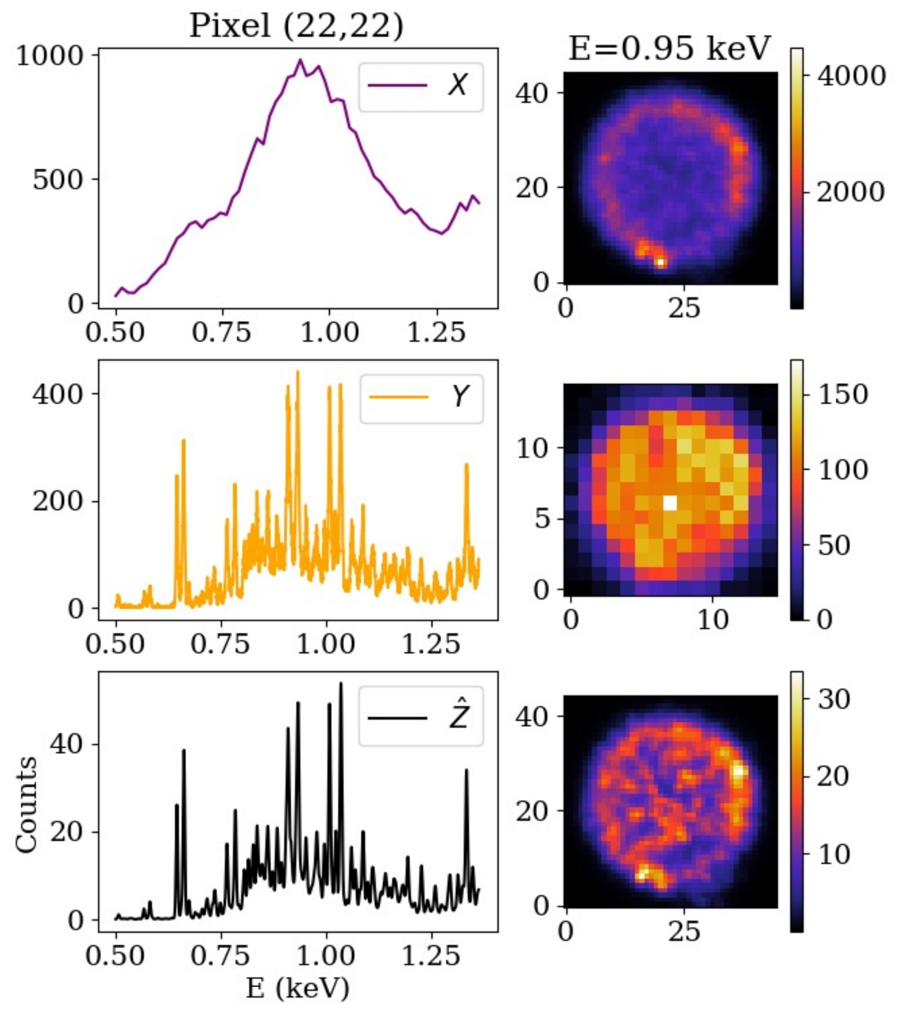


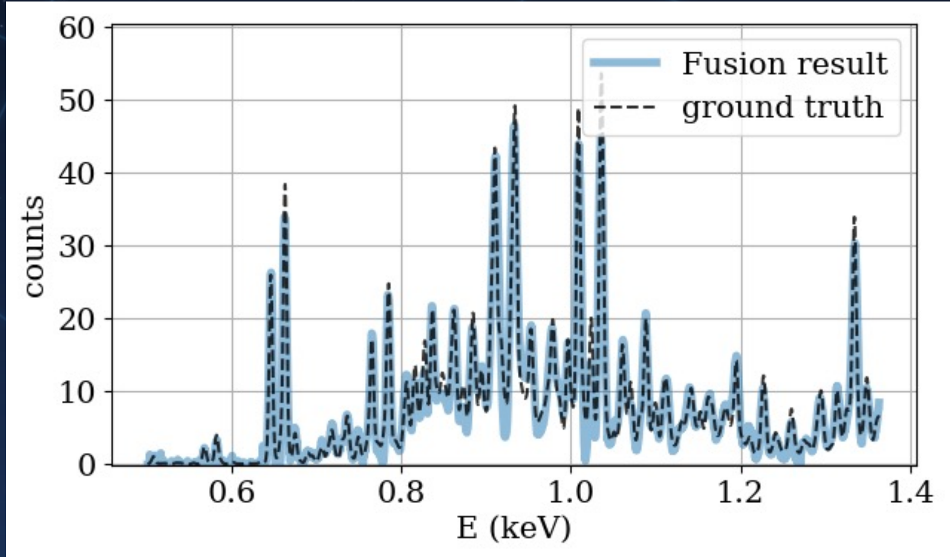
Mean error per pixel

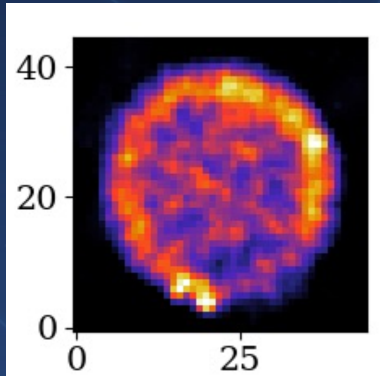


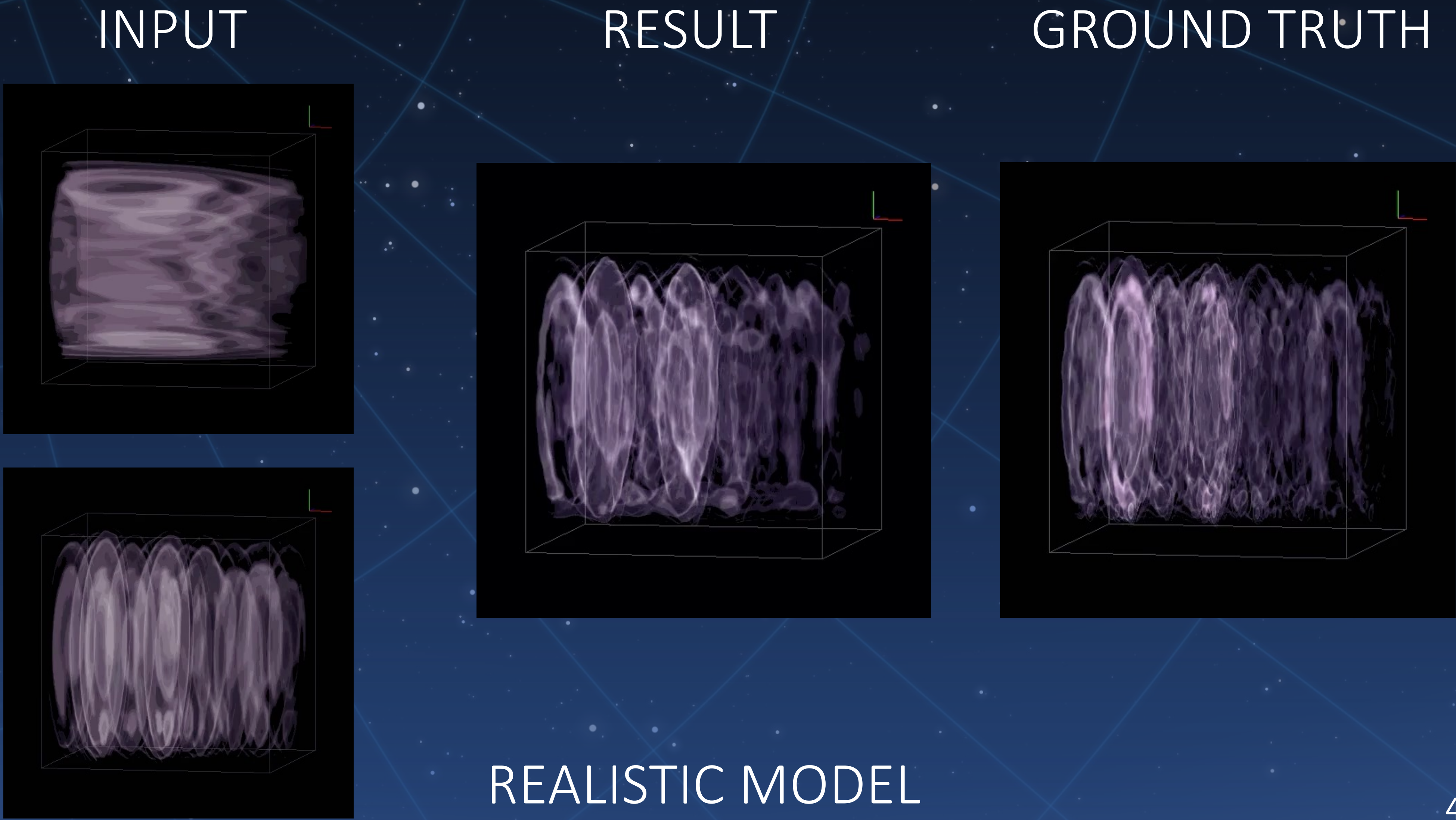
Error per voxel

RESULT: REALISTIC



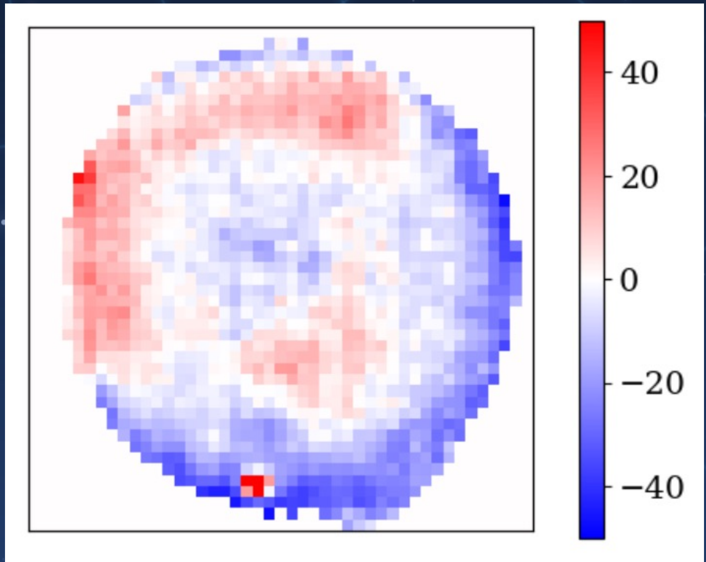




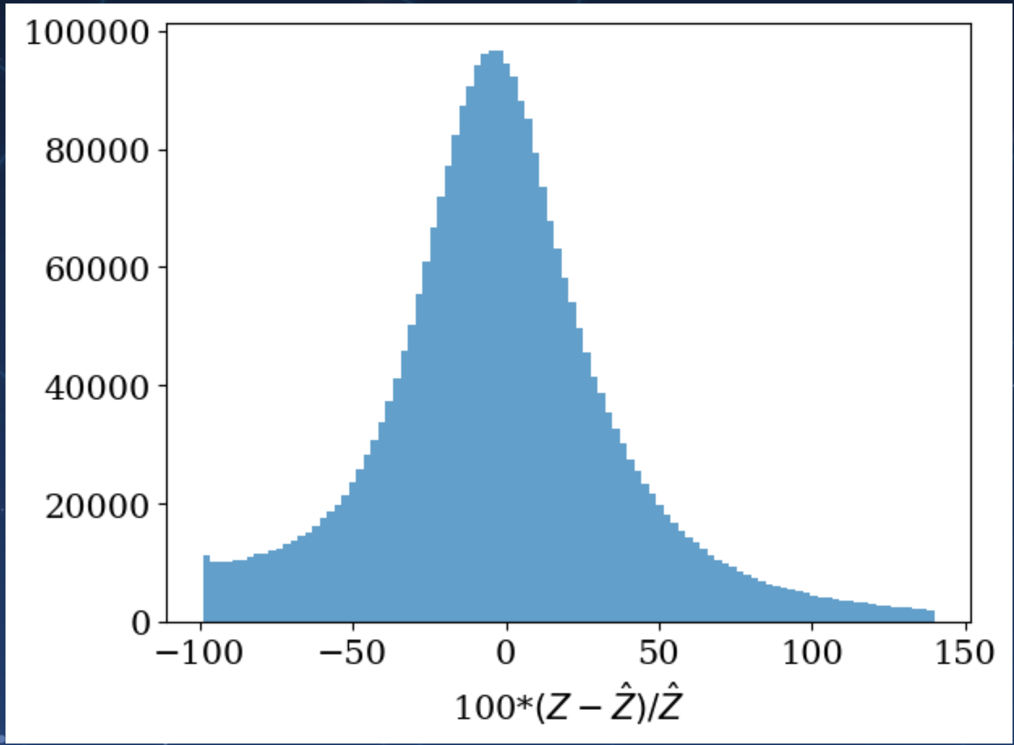


REALISTIC MODEL

REALISTIC MODEL: RELATIVE ERROR (%)



Mean error per pixel



Error per voxel

FUSION SUMMARY

- Propose a new algorithm for **hyperspectral fusion** adapted to X-ray imaging
- Compared **different regularizations** (e.g. low rank), which helped the algorithm go faster but introduced spectral distortion
- Need a method that reduces dimension, preserves variabilities

  → **include physical information**

https://github.com/JMLascar/HIFReD_fusion

FUTURE WORK

- **FUSION + SOURCE SEPARATION**
  - Will have the acceleration obtained by dimension reduction
  - Including physical information
  - Perform source separation and fusion at the same time

CONCLUSION

- **X-ray hyperspectral images** are complex to analyse because of Poisson noise and high spectral variability
- **SUSHI** is a method to unmix hyperspectral images with **spectral variations** based on a physical model (one for each endmember).
- **HIFReD** is a **fusion method**, which combines two hyperspectral images to obtain the **best spatial and spectral resolutions**
- Looking for post-docs for fall 2025

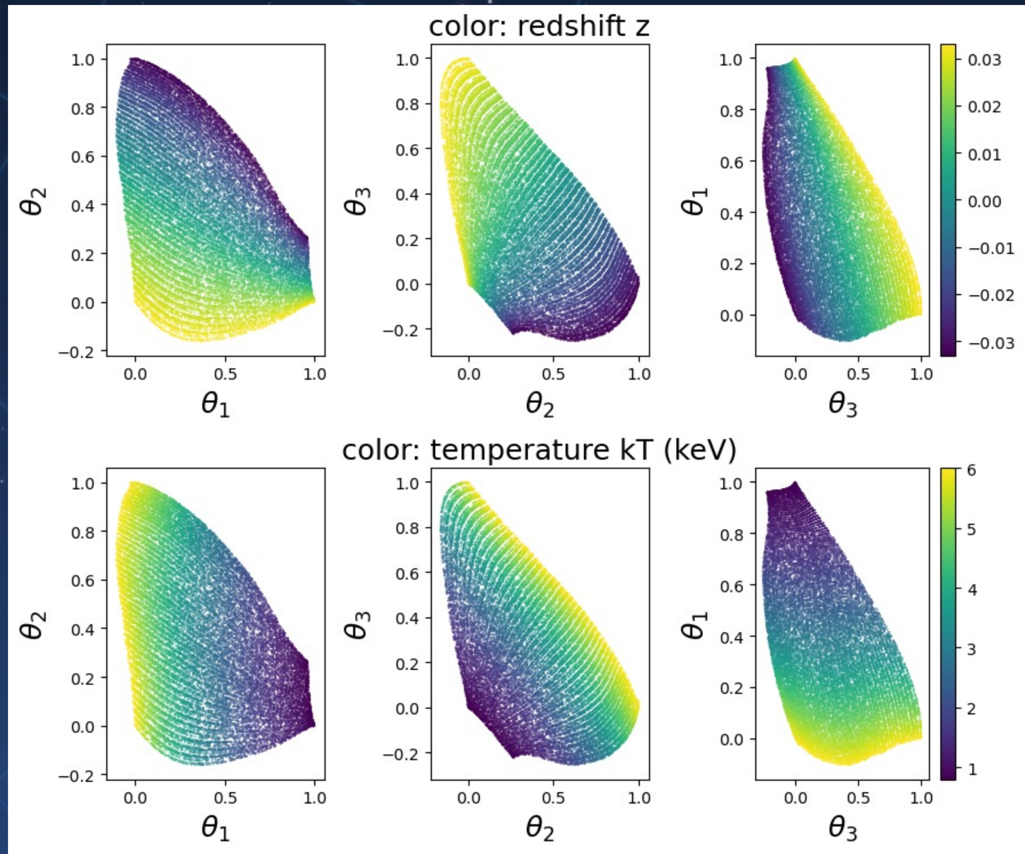
julia.lascar@cea.fr | **Articles:**

EXTRA SLIDES

DECODER FUNCTION AS A GENERATIVE MODEL

- D is differentiable
- Not costly to call upon
- Keeps a notion of neighborhood

→ spatial regularization makes sense



ALGORITHM OUTLINE

- Until stopping criterion:
  - For each component C :
    - 1. Update latent parameters for C, keep all else fixed
      - **Gradient descent** for the latent parameters
      - **Soft thresholding in wavelet domain** of the parameter maps
    - 2. Update Amplitude for C, keep all else fixed
      - **Gradient descent** for the Amplitude

STATE OF THE ART

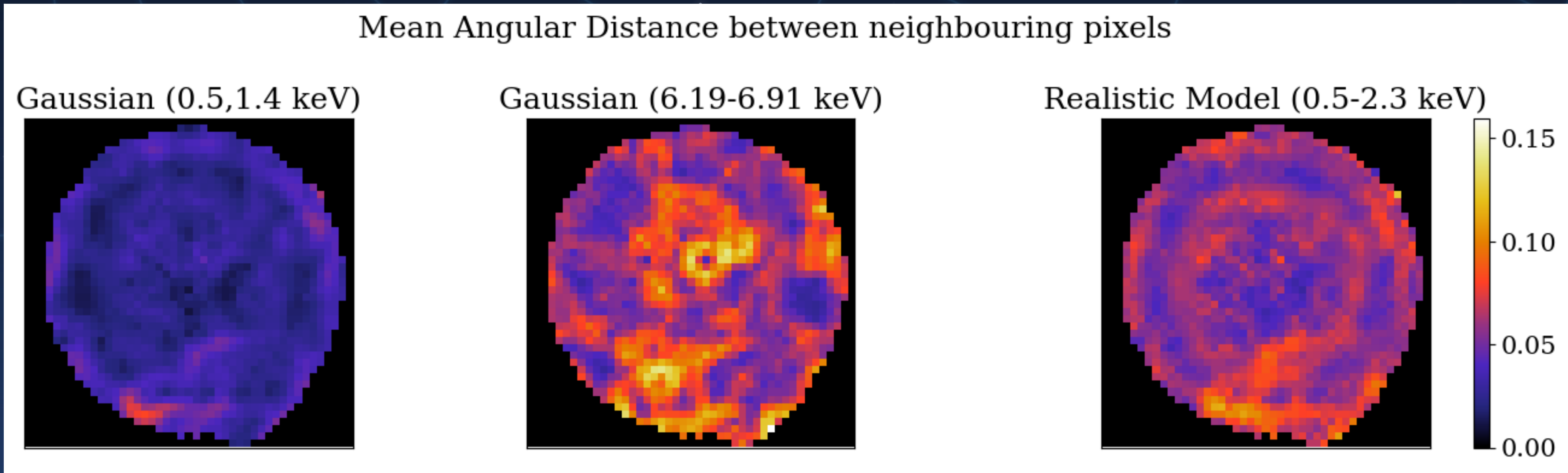
- First, panchromatic / multi-spectral, then multispectral / hyper-spectral
- Subspace projection
  - Unmixing*, e.g. Yokoya et al., 2012, Prévost et al. 2022*
  - Low rank approximation*, e.g. Simões et al., 2015*
- Spatial Regularization
  - TV, sparse dictionary (*Wei et al., 2015*), deep learning (*Uezato et al., 2020*)
- **Astrophysics, mainly for JWST:**
  - *Guilloteau et al. 2020*, low rank approximation with Sobolev regularization
  - *Pineau et al., 2023*, exact solution for fusion with unmixing

REGULARIZATION

- Three methods:
  - l1 norm of Wavelet 2D-1D coefficients
  - Low rank Approximation (using PCA) with Sobolev Regularization

    (inspired by Guilloteau 2020 work on JWST)
  - Low rank Approximation with 2D Wavelet Regularization

SPECTRAL VARIABILITY OF EACH MODEL



$$\theta(Z_k) = \sum_{Z_{k'} \in \mathcal{N}} \arccos\left(\frac{< Z_k, Z_{k'} >}{\sqrt{(\|Z_k\|_2^2 * \|Z_{k'}\|_2^2)}}\right)/\mathrm{card}(\mathcal{N}),$$

SUMMARY

ASAM: Moyenne de Carte d'angle spectral, PSNR: Pic Rapport Signal sur Bruit,
acSSIM: moyenne complémentaire de l'indice de similarité structurelle

Gaussian 1 keV

	regularizer	PSNR	ASAM	acSSIM
0	W2D1D	21.357812	0.570574	0.016970
1	LRS	20.968931	0.556864	0.011182
2	LRW2D	21.011660	0.559537	0.012045

Gaussian 6 keV

	regularizer	PSNR	ASAM	acSSIM
0	W2D1D	18.666015	0.598740	0.005083
1	LRS	14.155266	0.599992	0.010619
2	LRW2D	16.566201	0.609229	0.010068

Gaussian with Rebinning 1 keV

	regularizer	PSNR	ASAM	acSSIM
0	W2D1D	14.681063	0.602940	0.043332
1	LRS	14.302753	0.609036	0.044248
2	LRW2D	13.849244	0.617097	0.051285

Realistic 1 keV

	regularizer	PSNR	ASAM	acSSIM
0	W2D1D	11.479859	0.665938	0.020218
1	LRS	10.076144	0.654854	0.031135
2	LRW2D	11.464761	0.669527	0.024311

FUTURE WORK

- FUSION + SOURCE SEPARATION
  - Will have the acceleration obtained by dimension reduction
  - Including physical information
  - Performs source separation and fusion at the same time

$$Z_X(\theta) = (t_X \sum_c \mathcal{M}^c(\theta^c) \odot A_X)\mathcal{S}_X$$

$$Z_Y(\theta) = \mathcal{B}_Y(t_Y \sum_c \mathcal{M}^c(\theta^c) \odot A_Y)$$