Imaging & Spectroscopy with the JWST

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Imaging & Spectroscopy with the JWST

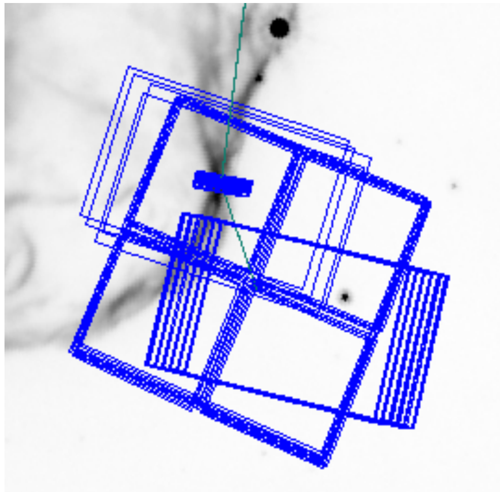
- JWST : unique combination of imaging and spectroscopic facilities
- Very different fields of view

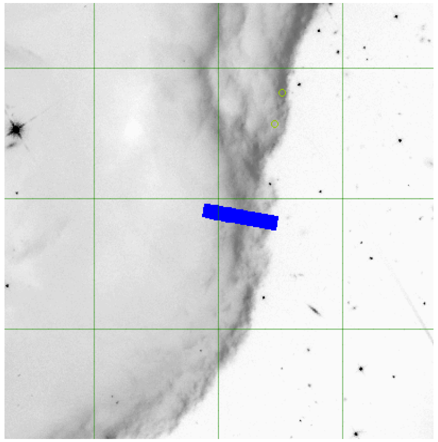
MIRI imager : 75'' X 113'', 9 filters

NIRCAM 2.2' X 2.2', 29 filters

MIRI MRS : 3.9'' to 7.7'

NIRSPEC IFU : 3'' X 3 '



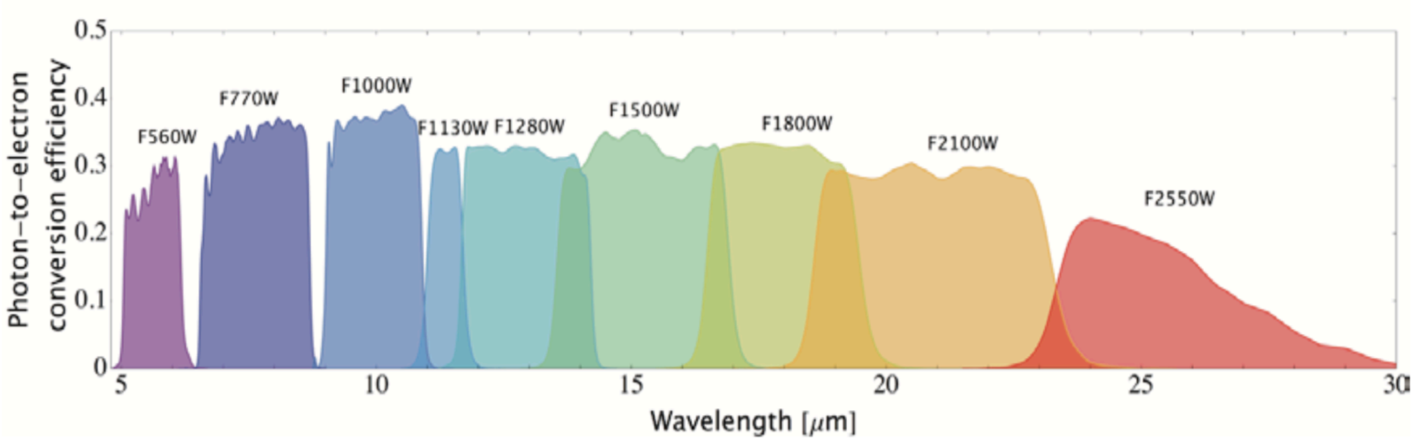


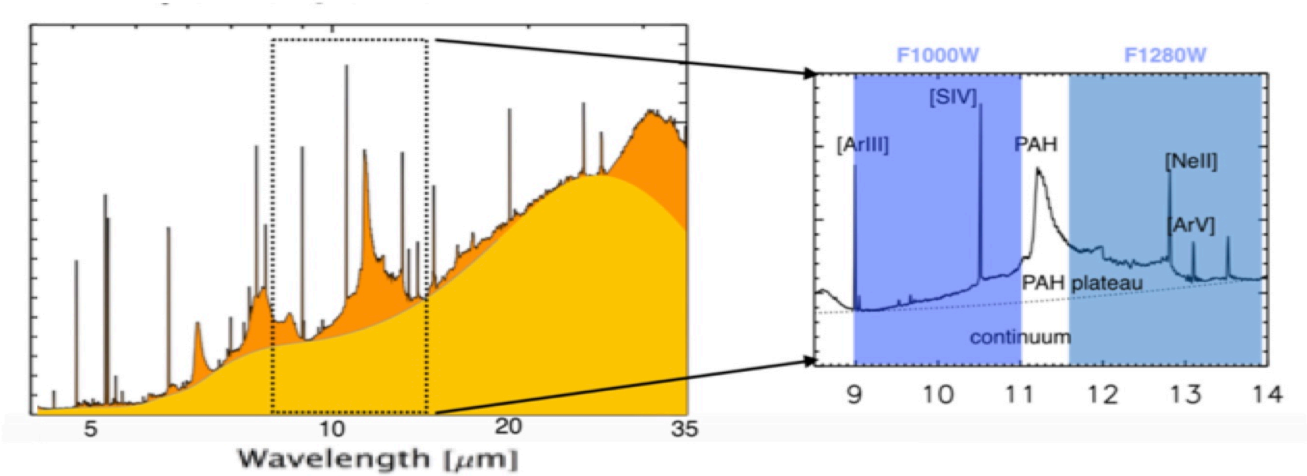
- The spectroscopy needs long observing times
  - to reach high sensitivity
  - to cover extended fields

Spectroscopy with the JWST

Instrument	Type	Wavelength (microns)	Spectral resolution	Field of view
NIRISS	slitless	1.0-2.5	~150	2.2′ x 2.2′
NIRCam	slitless	2.4-5.0	~2000	2.2′ x 2.2′ (TBC)
NIRSpec	MOS	0.6-5.0	100/1000/2700	9 square arcmin.
NIRSpec	IFU	0.6-5.0	100/1000/2700	3″ x 3″
MIRI	IFU	5.0-28.8	2000-3500	>3″ x >3.9″
NIRSpec	SLIT	0.6-5.0	100/1000/2700	Single object
MIRI	SLIT	5.0-10.0	60-140	Single object
NIRISS	Aperture	0.6-5.0	100/1000/2700	Single object
NIRSpec	Aperture	0.6-2.5	700	Single object

MIRI imaging , 9 filters





- The spectroscopy is mandatory, but very expensive
  - How to recover spectroscopic information from broad-band images ?
  - How to combine spectroscopic and imaging data ?
  - How to opimize the observing strategy and the data analysis ?

Soumis à l'ANR: LabCom IAS – ACRI-ST Innovative Laboratory for Space Spectroscopy

- 2019-2022 (période financée par l'ANR) et au-delà

- Adossé au Centre d'expertise MIRI → Apport de la spectroscopie (MIRI MRS)

  Expertise ACRI-ST: Spectroscopie infrarouge (Jeronimo Bernard-Salas)

- Actuellement 3 WPs:

  1. Développements méthodologiques et algorithmiques pour tirer la meilleure information spectroscopique des images et des spectres de MIRI

     Theses: Amine Hadj-Youcef (2015-2018), Ralph Abi Rizk (2018-2021)

  2. Simulations des observations MIRI MRS, et pipelines

  3. Développements logiciels pour la corrélation croisée imagerie-spectroscopie

PhD Defense :

Reconstruction spatio-spectrale à partir de données multispectrales basse résolution. Application à l'instrument infrarouge moyen du Télescope spatial James Webb (JWST)

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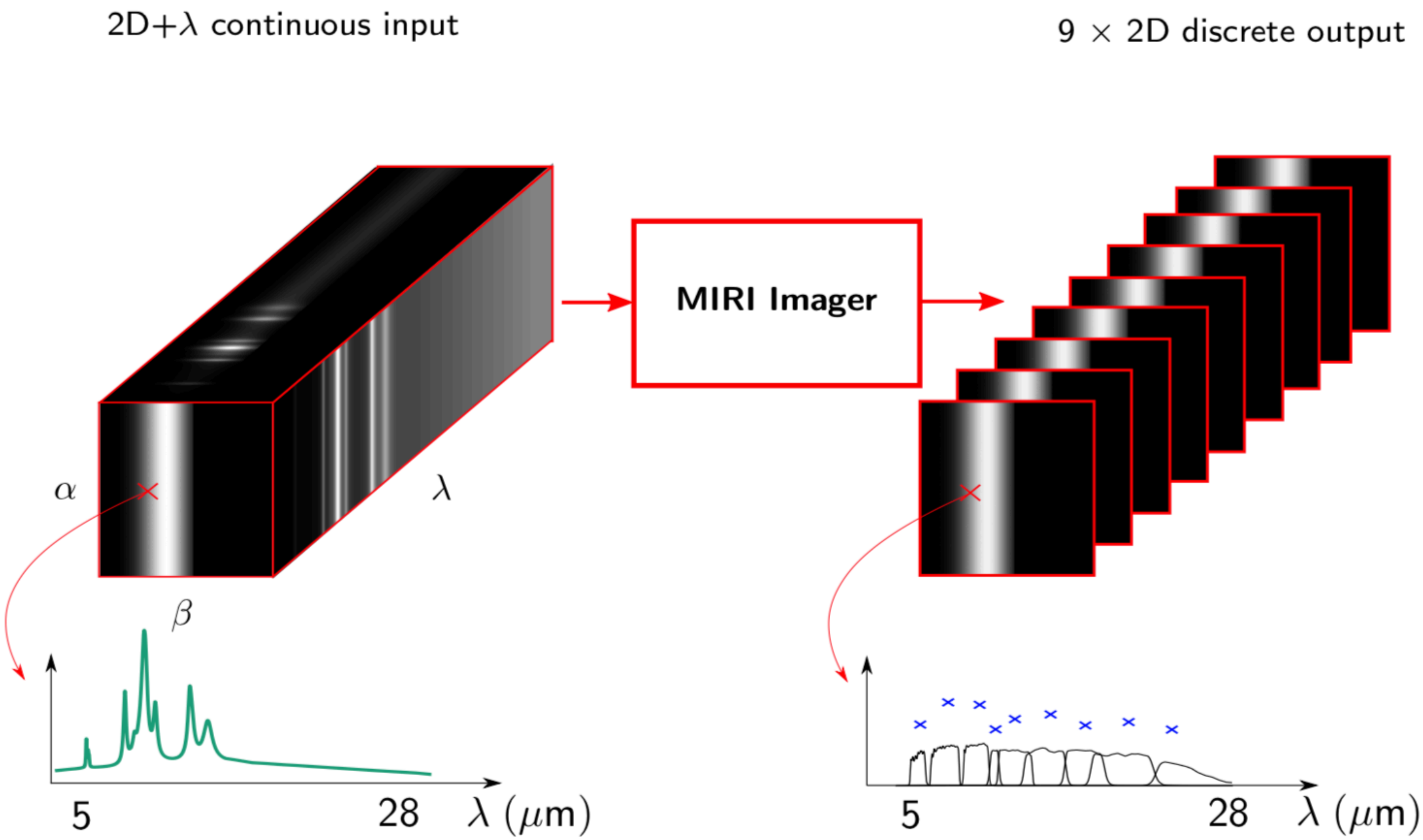
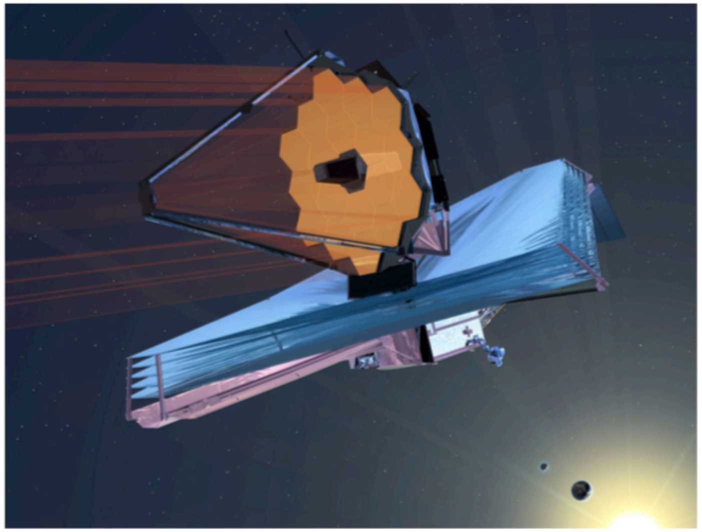
September 27, 2018

Data Acquisition

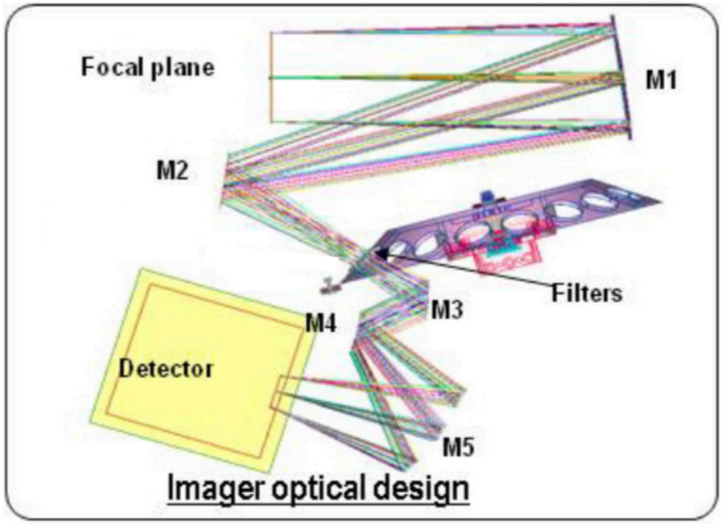


. Courtesy to Nathalie Ysard

MIRI optical design [Bouchet *et al.* 2015]



$\Longrightarrow$



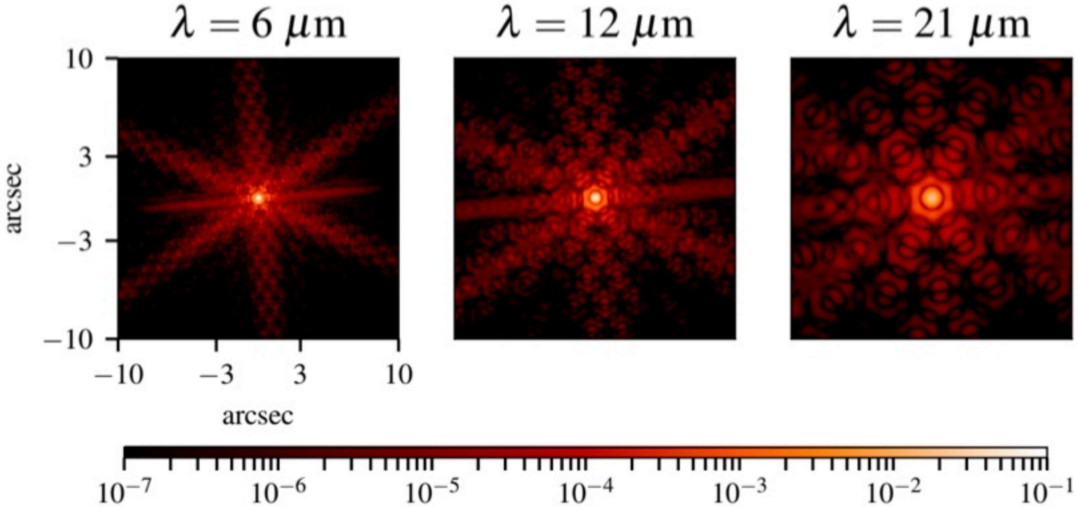
Proposed Instrument Model

2D+λ Object ϕ → [Optics → Filter → Detector] → 2D Data $y^{(p)}$

Optics: h — PSF

Filter, Detector: ω_p — Spectral response of band p

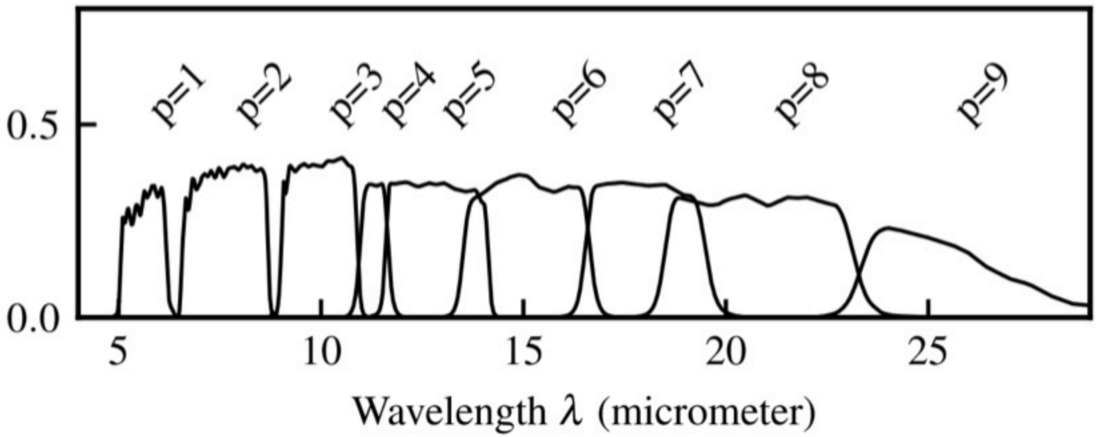
Spectral Variations of the PSF : h



- *WebbPSF* (STScI) [Perrin *et al.* 2014].

⇒ Spatial resolution of the data change according to λ

Nine Spectral Responses of the MIRI Imager : ω_p



- ω_p : Filter transmission × Quantum efficiency

⇒ Broad responses + Correlation between the data

Complete Equation of the Model

For the band p and the pixel (i, j)

$$y_{i,j}^{(p)} = \int_{\mathbb{R}_+} \omega_p(\lambda) \times \left(\iint_{\Omega_{\text{pix}}} \left(\iint_{\mathbb{R}^2} \phi(\alpha', \beta', \lambda)\, h(\alpha - \alpha', \beta - \beta', \lambda) d\alpha' d\beta' \right) b_{\text{samp}}(\alpha - \alpha_i, \beta - \beta_j) d\alpha d\beta \right) d\lambda + n_{i,j}^{(p)}$$

where $p = 1, \ldots, P, i = 1, \ldots, N_i, j = 1, \ldots, N_j$

N_i, N_j	**Numbers of rows and columns**	ω_p	**Spectral response** of the band p
P	**Number of spectral bands**	b_{samp}	**Spatial integration function** over Ω_{pix}
h	Spatial response **PSF**	$n^{(p)}$	**Additive noise**

Hypothesis

- Photon noise neglected
- All issues related to the detector are corrected

Forward Model

Instrument model + object model

$$\boldsymbol{y}^{(p)} = \sum_{m=1}^{N_\lambda} \boldsymbol{H}^{p,m}\, \boldsymbol{x}^{(m)} + \boldsymbol{n}^{(p)}, \qquad \text{for the band } p$$

with

$$H^{p,m}_{i,j;k,l} = \iint_{\Omega_{\text{pix}}} \left(\left(\int_{\mathbb{R}_+} \omega_p(\lambda) h(\alpha, \beta, \lambda) b^m_{\text{spec}}(\lambda) d\lambda \right) \underset{\alpha,\beta}{*} b_{\text{spat}}(\alpha - \alpha_k, \beta - \beta_l) \right) b_{\text{samp}}(\alpha - \alpha_i, \beta - \beta_j) d\alpha d\beta$$

Joint processing of all multispectral data $\Rightarrow$ Under-determined problem ($N_\lambda > P$)

$$\underbrace{\begin{pmatrix} \boldsymbol{y}^{(1)} \\ \boldsymbol{y}^{(2)} \\ \vdots \\ \boldsymbol{y}^{(P)} \end{pmatrix}}_{\boldsymbol{y}} = \underbrace{\begin{pmatrix} \boldsymbol{H}^{1,1} & \boldsymbol{H}^{1,2} & \cdots & \boldsymbol{H}^{1,N_\lambda} \\ \boldsymbol{H}^{2,1} & \boldsymbol{H}^{2,2} & \cdots & \boldsymbol{H}^{2,N_\lambda} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{H}^{P,1} & \boldsymbol{H}^{P,2} & \cdots & \boldsymbol{H}^{P,N_\lambda} \end{pmatrix}}_{\boldsymbol{H}} \underbrace{\begin{pmatrix} \boldsymbol{x}^{(1)} \\ \boldsymbol{x}^{(2)} \\ \vdots \\ \boldsymbol{x}^{(N_\lambda)} \end{pmatrix}}_{\boldsymbol{x}} + \underbrace{\begin{pmatrix} \boldsymbol{n}^{(1)} \\ \boldsymbol{n}^{(2)} \\ \vdots \\ \boldsymbol{n}^{(P)} \end{pmatrix}}_{\boldsymbol{n}}$$

$$\boldsymbol{y} = \boldsymbol{H}\,\boldsymbol{x} + \boldsymbol{n}$$

Reconstruction : Regularized Least-Squares Method

Convex Minimization

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\text{argmin}} \ \mathcal{J}(\boldsymbol{x})$$

Need to add regularization terms in order to stabilize the solution

with

$$\mathcal{J}(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}\|_2^2 + \{\mu_{\text{spat}}\mathcal{R}_{\text{spat}}(\boldsymbol{x}) \ + \ \mu_{\text{spec}}\mathcal{R}_{\text{spec}}(\boldsymbol{x})\}$$

$$\mathcal{R}_{\text{spat}}(\boldsymbol{x}) = \sum_{m=1}^{N_\lambda}\left(\sum_{k=1}^{N_k}\sum_{l=1}^{N_l}\left(\left(x_{k+1,l}^{(m)} - x_{k,l}^{(m)}\right)^2 + \left(x_{k,l+1}^{(m)} - x_{k,l}^{(m)}\right)^2\right)\right) = \|\boldsymbol{D}_{\text{spat}}\boldsymbol{x}\|_2^2$$

$$\mathcal{R}_{\text{spec}}(\boldsymbol{x}) = \sum_{k=1}^{N_k}\sum_{l=1}^{N_l}\left(\sum_{m=1}^{N_\lambda}\left(x_{k,l}^{(m+1)} - x_{k,l}^{(m)}\right)^2\right) = \|\boldsymbol{D}_{\text{spec}}\boldsymbol{x}\|_2^2$$

$\boldsymbol{D}_{\text{spat}}$ and $\boldsymbol{D}_{\text{spec}}$ are 2D and 1D finite difference operator.

Solution of the Problem : $\mathcal{J}$ is differentiable and strictly convex

$$\hat{\boldsymbol{x}} = \underbrace{\left(\boldsymbol{H}^T\boldsymbol{H} + \mu_{\text{spat}} \ \boldsymbol{D}_{\text{spat}}^T\boldsymbol{D}_{\text{spat}} + \mu_{\text{spec}} \ \boldsymbol{D}_{\text{spec}}^T\boldsymbol{D}_{\text{spec}}\right)}_{\boldsymbol{Q}}^{-1}\boldsymbol{H}^T\boldsymbol{y}$$

- $\boldsymbol{Q} \in \mathbb{R}^{N_\lambda N_k N_l \ \times \ N_\lambda N_k N_l}$ is a high-dimensional block-matrix.
- $\text{Size}(\boldsymbol{Q}) = 3932160 \times 3932160$ (~ 123 Terabit !) : $(N_k = N_l = 256, N_\lambda = 60)$

Proposed Algorithms

Algorithm 1 : Conjugated Gradient

Input : $\boldsymbol{H}, \boldsymbol{y}, \boldsymbol{Q}$,
$\hat{\boldsymbol{x}}_0 = \boldsymbol{0}, \boldsymbol{r}_0 = \boldsymbol{d}_0 = \boldsymbol{H}^T\boldsymbol{y} - \boldsymbol{Q}\hat{\boldsymbol{x}}_0$

for $n = 0 : N_{iter}$ **do**

Optimal step parameter
$a_n \leftarrow \frac{\boldsymbol{r}_n^T \boldsymbol{r}_n}{\boldsymbol{d}_n^T \boldsymbol{Q} \boldsymbol{d}_n}$

Computation of the next iteration
$\hat{\boldsymbol{x}}_{n+1} \leftarrow \hat{\boldsymbol{x}}_n - a_n\, \boldsymbol{d}_n$

Conjugate directions
$\boldsymbol{r}_{n+1} \leftarrow \boldsymbol{r}_n + a_n \boldsymbol{Q} \boldsymbol{d}_n$
$b_n \leftarrow \frac{\boldsymbol{r}_{n+1}^T \boldsymbol{r}_{n+1}}{\boldsymbol{r}_n^T \boldsymbol{r}_n}$
$\boldsymbol{d}_{n+1} \leftarrow \boldsymbol{r}_{n+1} + b_{n+1} \boldsymbol{d}_n$

return $\hat{\boldsymbol{x}}$

$\Rightarrow$ An approximate solution

$\Rightarrow$ Time consuming

Algorithm 2 : Multichannel Discrete Fourier Transform

Input : $\boldsymbol{H}, \boldsymbol{D}, \boldsymbol{C}, \boldsymbol{y}, \mu_{\text{spat}}, \mu_{\text{spec}}$

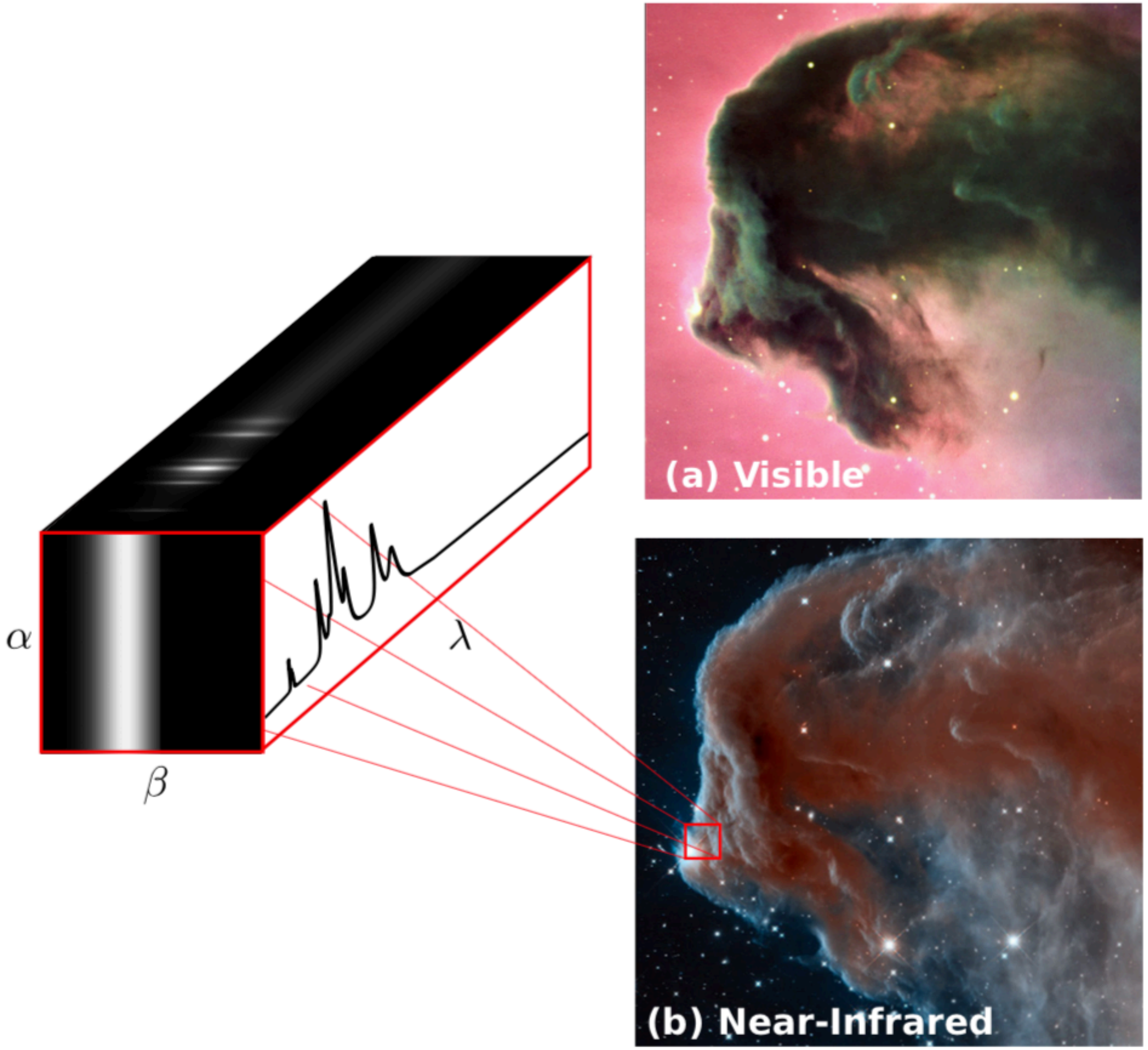
Compute the Hessian matrix
$\boldsymbol{Q} = \boldsymbol{H}^T \boldsymbol{H} + \mu_{\text{spat}} \boldsymbol{D}_{\text{spat}}^T \boldsymbol{D}_{\text{spat}} + \mu_{\text{spec}} \boldsymbol{D}_{\text{spec}}^T \boldsymbol{D}_{\text{spec}}$

Block diagonalization
$\boldsymbol{\Lambda_Q} \leftarrow \left\{ \boldsymbol{F} \boldsymbol{Q}^{i,j} \boldsymbol{F}^\dagger \right\}_{i,j=1}^{N_\lambda}$
$\boldsymbol{\Lambda_H} \leftarrow \left\{ \boldsymbol{F} \boldsymbol{H}^{i,j} \boldsymbol{F}^\dagger \right\}_{i,j=1}^{P,N_\lambda}$

Inversion of $\boldsymbol{\Lambda_Q}$
$N_\lambda, N_\lambda, N_k, N_l = \text{size}(\boldsymbol{\Lambda_Q})$
for $k = 0 : N_k$ **do**
  for $l = 0 : N_l$ **do**
    $\boldsymbol{R} = \boldsymbol{\Lambda_Q}[:, :, k, l]$
    $\boldsymbol{\Lambda_Q^{inv}}[:, :, k, l] = \boldsymbol{R}^{-1}$

Compute the solution
$\hat{\boldsymbol{x}} \leftarrow \overline{\boldsymbol{F}}^\dagger\, \boldsymbol{\Lambda_Q^{inv}} \boldsymbol{\Lambda_H^\dagger} \overline{\boldsymbol{F}}\, \boldsymbol{y}$
return $\hat{\boldsymbol{x}}$

Original spatio-spectral object

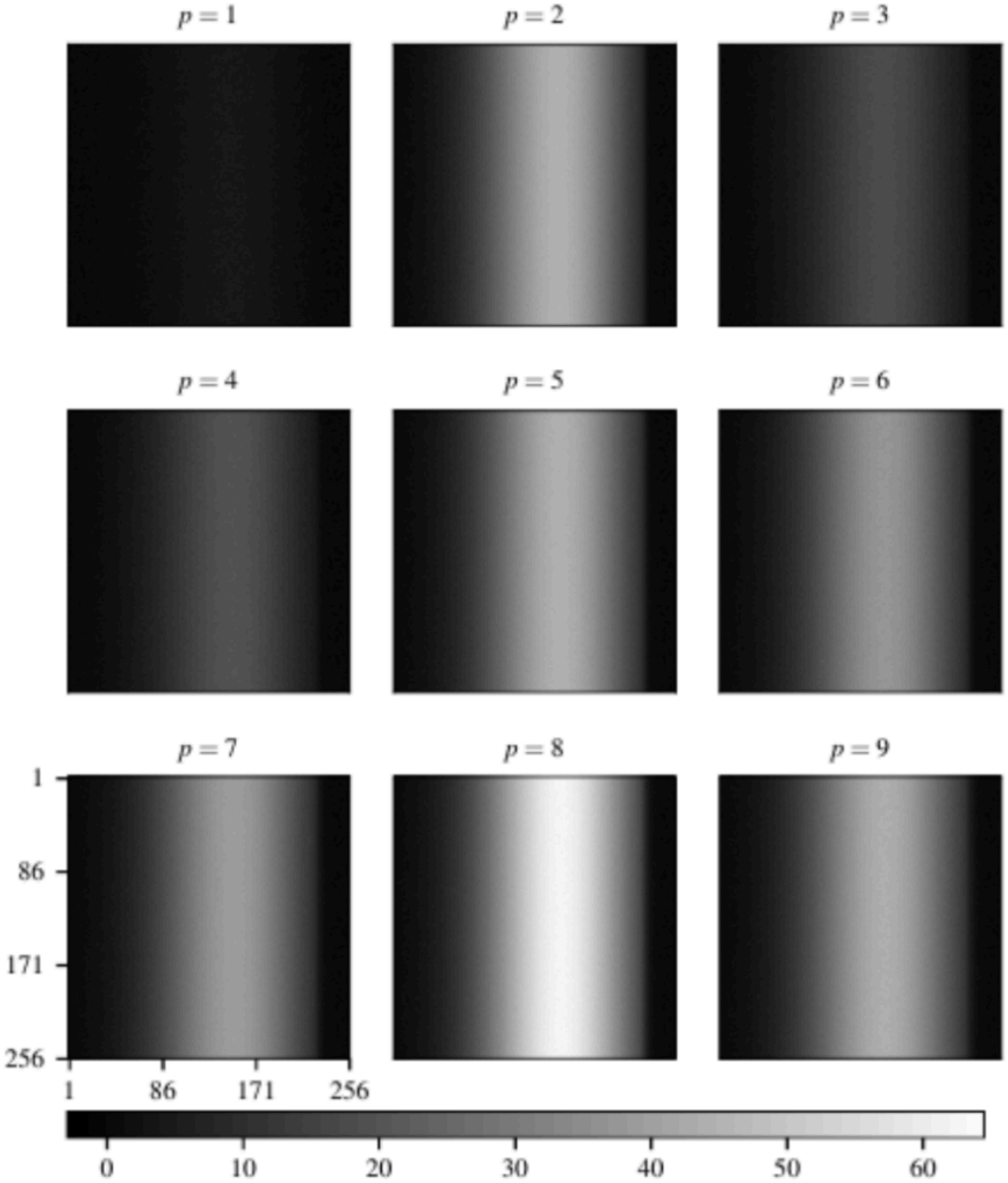


HorseHead nebula

- Size : $1000 \times 256 \times 256$

. Courtesy to Nathalie Ysard

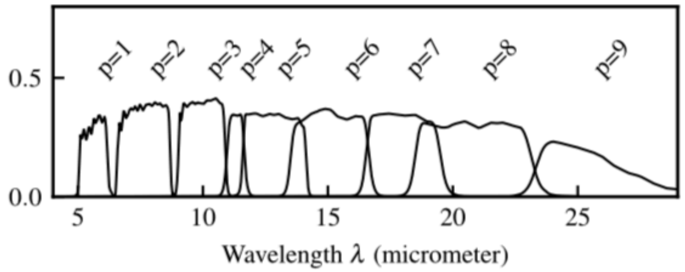
Simulation Results of the Multispectral Data



HorseHead nebula

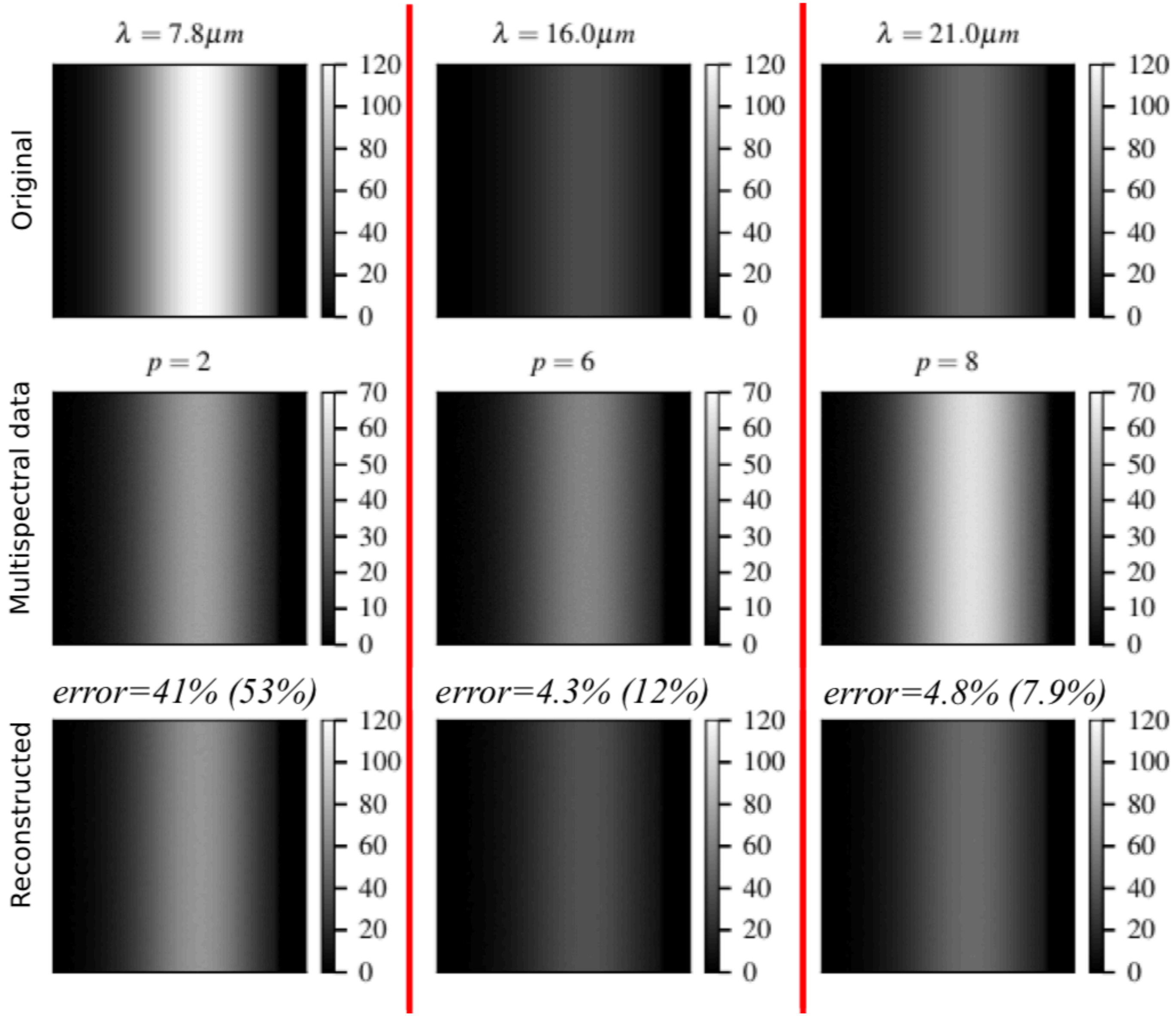
- JWST/MIRI Imager
- **9** × **256** × **256** pixels
- SNR = **30** dB white Gaussian noise

$$\mathrm{SNR} = 10\log_{10}\left(\frac{\frac{1}{N}\|\boldsymbol{y}\|_2^2}{\sigma_n^2}\right)$$



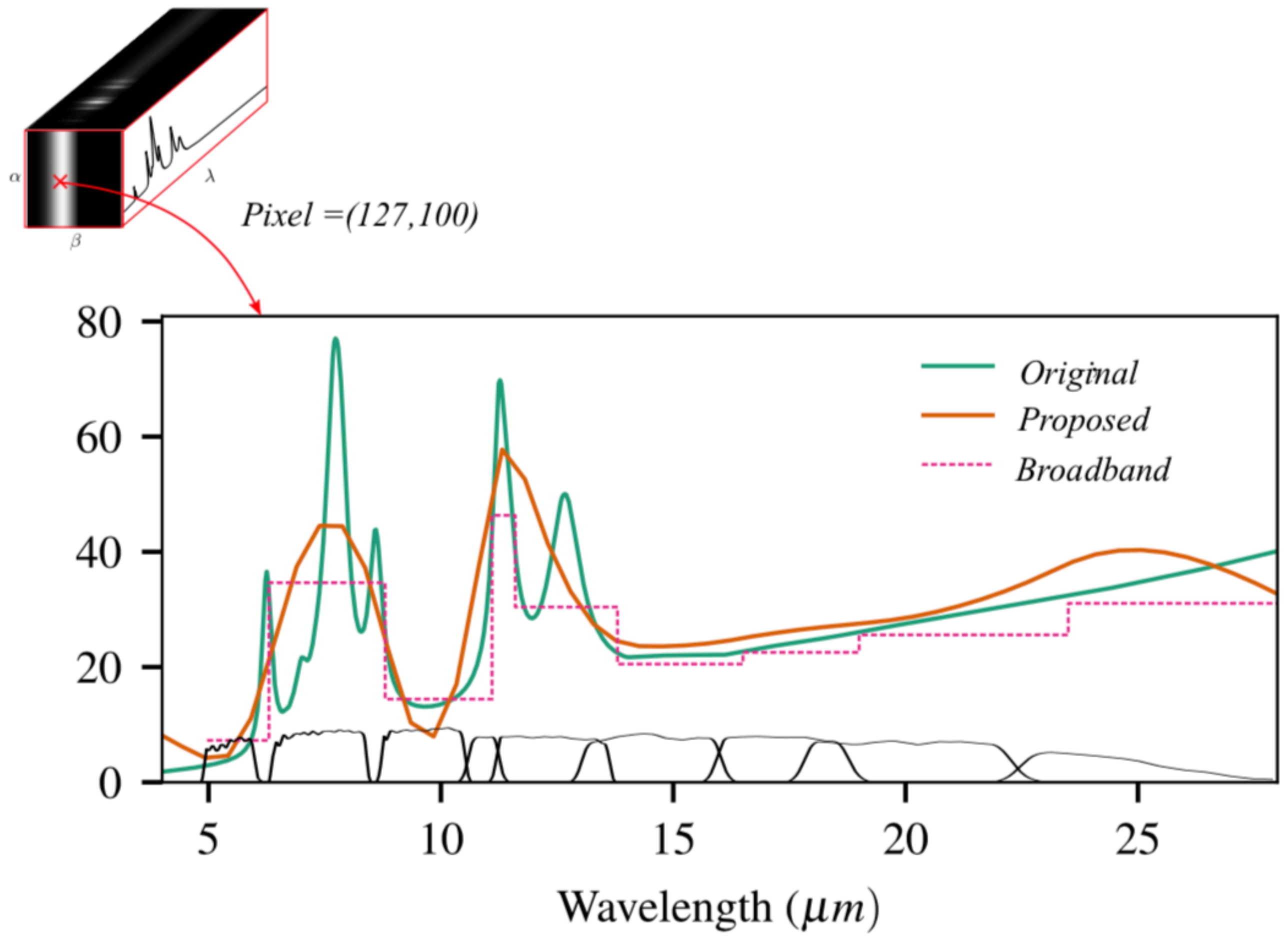
Reconstruction Results

Spatial distribution : [Hadj-Youcef *et al.* 2018]



Reconstruction Results

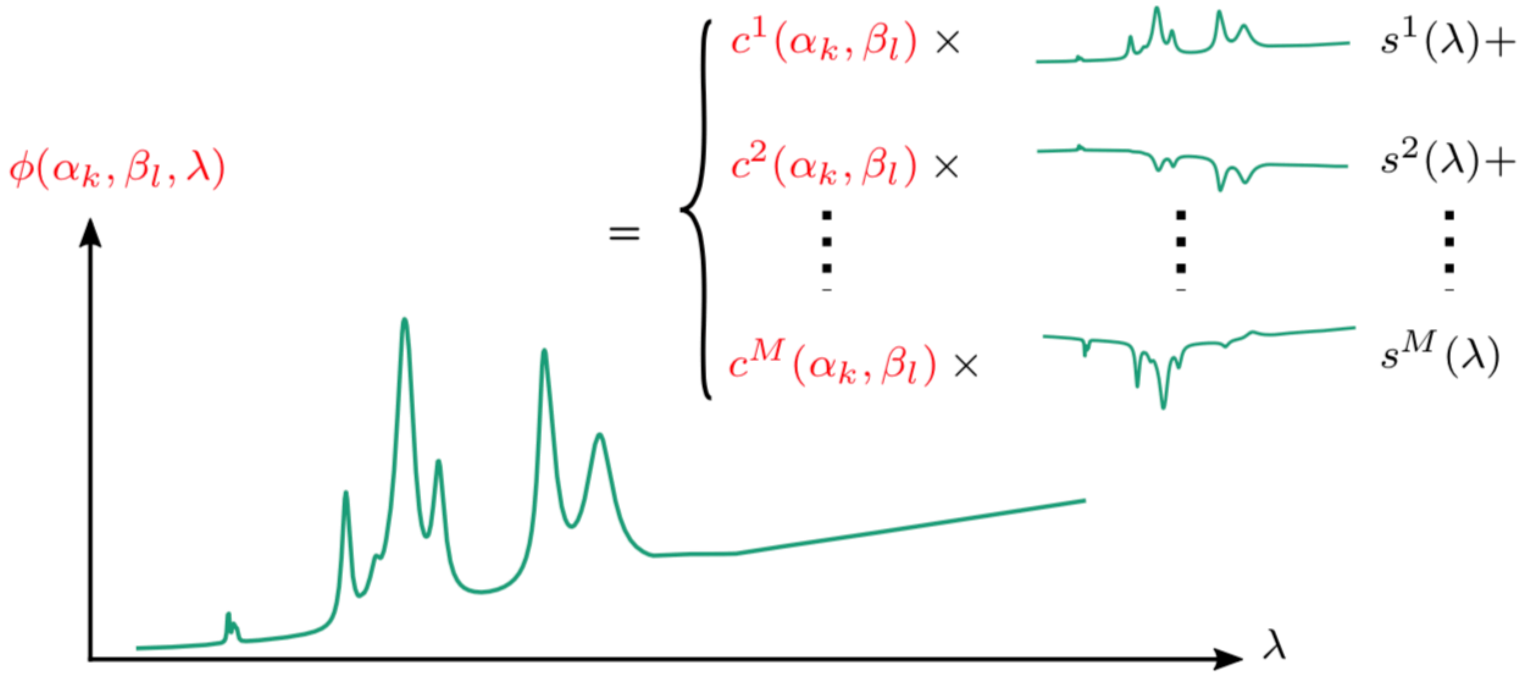
Spectral distribution : [Hadj-Youcef *et al.* 2018]



N_{λ}= 60

Object Representation : Linear Mixing Model [Adams *et al.* 1986]

For a single spatial position (α_k, β_l)



Object Model

$$\phi(\alpha, \beta, \lambda) = \sum_{m=1}^{M} \overbrace{\left(\sum_{k=1}^{N_k} \sum_{l=1}^{N_l} x_{k,l}^m \, b_{\mathrm{rec}}(\alpha - \alpha_k, \beta - \beta_l) \right)}^{c^m(\alpha_k, \beta_l)} s^m(\lambda)$$

x	Mixture coefficient
s	Spectral component
M	number of components
b_{rec}	Decomposition function

Only M numbers to be computed for each pixel

Forward Model

Instrument model + object model

$$y_{i,j}^{(p)} = \sum_{m=1}^{M} \left(\sum_{k=1}^{N_k} \sum_{l=1}^{N_l} H_{i,j;k,l}^{p,m} \, x_{k,l}^{m} \right) + n_{i,j}^{(p)}, \qquad \text{for band } p, \text{ pixel } i,j$$

with

$$H_{i,j;k,l}^{p,m} = \iint_{\Omega_{\text{pix}}} \left(\left(\int_{\mathbb{R}_+} \omega_p(\lambda) h(\alpha, \beta, \lambda) s^m(\lambda) d\lambda \right) \underset{\alpha,\beta}{*} b_{\text{rec}}(\alpha - \alpha_k, \beta - \beta_l) \right) b_{\text{samp}}(\alpha - \alpha_i, \beta - \beta_j) d\alpha d\beta$$

Joint processing of all multispectral data → Over-determined system

$$\underbrace{\begin{pmatrix} \boldsymbol{y}^{(1)} \\ \boldsymbol{y}^{(2)} \\ \boldsymbol{y}^{(3)} \\ \vdots \\ \boldsymbol{y}^{(P)} \end{pmatrix}}_{\boldsymbol{y}} = \underbrace{\begin{pmatrix} \boldsymbol{H}^{1,1} & \boldsymbol{H}^{1,2} & \cdots & \boldsymbol{H}^{1,M} \\ \boldsymbol{H}^{2,1} & \boldsymbol{H}^{2,2} & \cdots & \boldsymbol{H}^{2,M} \\ \boldsymbol{H}^{3,1} & \boldsymbol{H}^{3,2} & \cdots & \boldsymbol{H}^{3,M} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{H}^{P,1} & \boldsymbol{H}^{P,2} & \cdots & \boldsymbol{H}^{P,M} \end{pmatrix}}_{\boldsymbol{H}} \underbrace{\begin{pmatrix} \boldsymbol{x}^{1} \\ \boldsymbol{x}^{2} \\ \vdots \\ \boldsymbol{x}^{M} \end{pmatrix}}_{\boldsymbol{x}} + \underbrace{\begin{pmatrix} \boldsymbol{n}^{(1)} \\ \boldsymbol{n}^{(2)} \\ \boldsymbol{n}^{(3)} \\ \vdots \\ \boldsymbol{n}^{(P)} \end{pmatrix}}_{\boldsymbol{n}}$$

$$\boldsymbol{y} = \boldsymbol{H}\,\boldsymbol{x} + \boldsymbol{n}$$

Reconstruction : Estimation of the Mixture Coefficients

Convex Minimization

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\text{argmin}} \left\{ \mathcal{J}(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}\|_2^2 + \mu\, \mathcal{R}(\boldsymbol{x}) \right\}$$

where the multichannel regularization is

$$\mathcal{R}(\boldsymbol{x}) = \sum_{m=1}^{M} \left(\sum_{k=1}^{N_k} \sum_{l=1}^{N_l} \varphi\left(x_{k+1,l}^{m} - x_{k,l}^{m}\right) + \sum_{k=1}^{N_k} \sum_{l=1}^{N_l} \varphi\left(x_{k,l+1}^{m} - x_{k,l}^{m}\right) \right)$$

Only spatial regularization

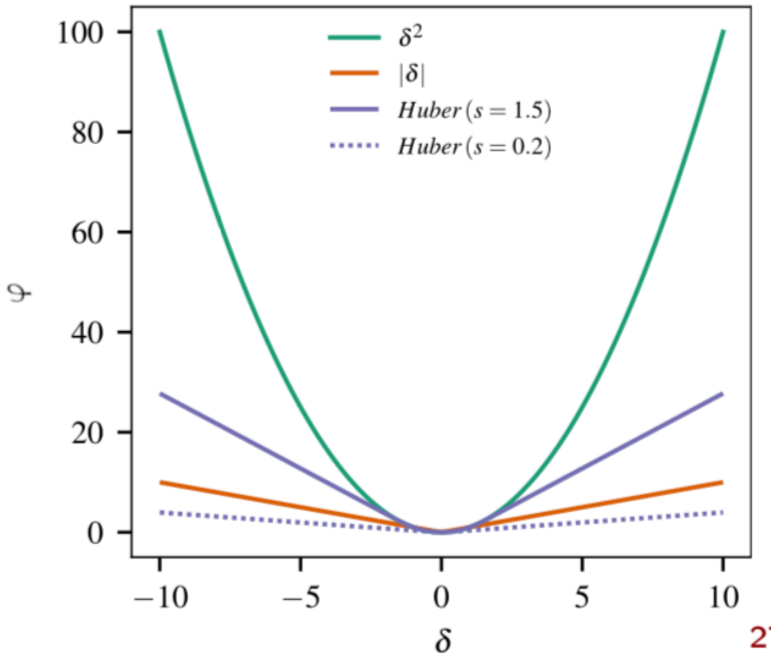
Regularization functions

1) Quadratic function (l_2) : $\varphi(\delta) = \delta^2$

2) Huber function (l_2/l_1) :

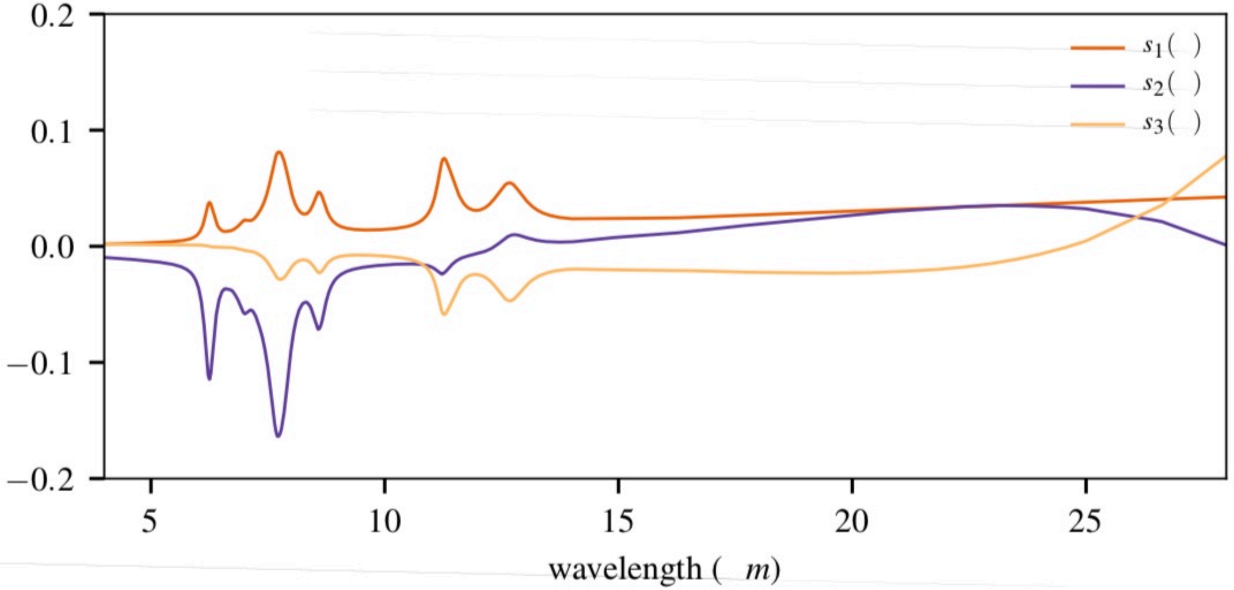
$$\varphi(\delta) = \begin{cases} \delta^2 & \text{if } |\delta| < s \\ 2s|\delta| - s^2 & \text{otherwise} \end{cases}$$

s : Threshold parameter



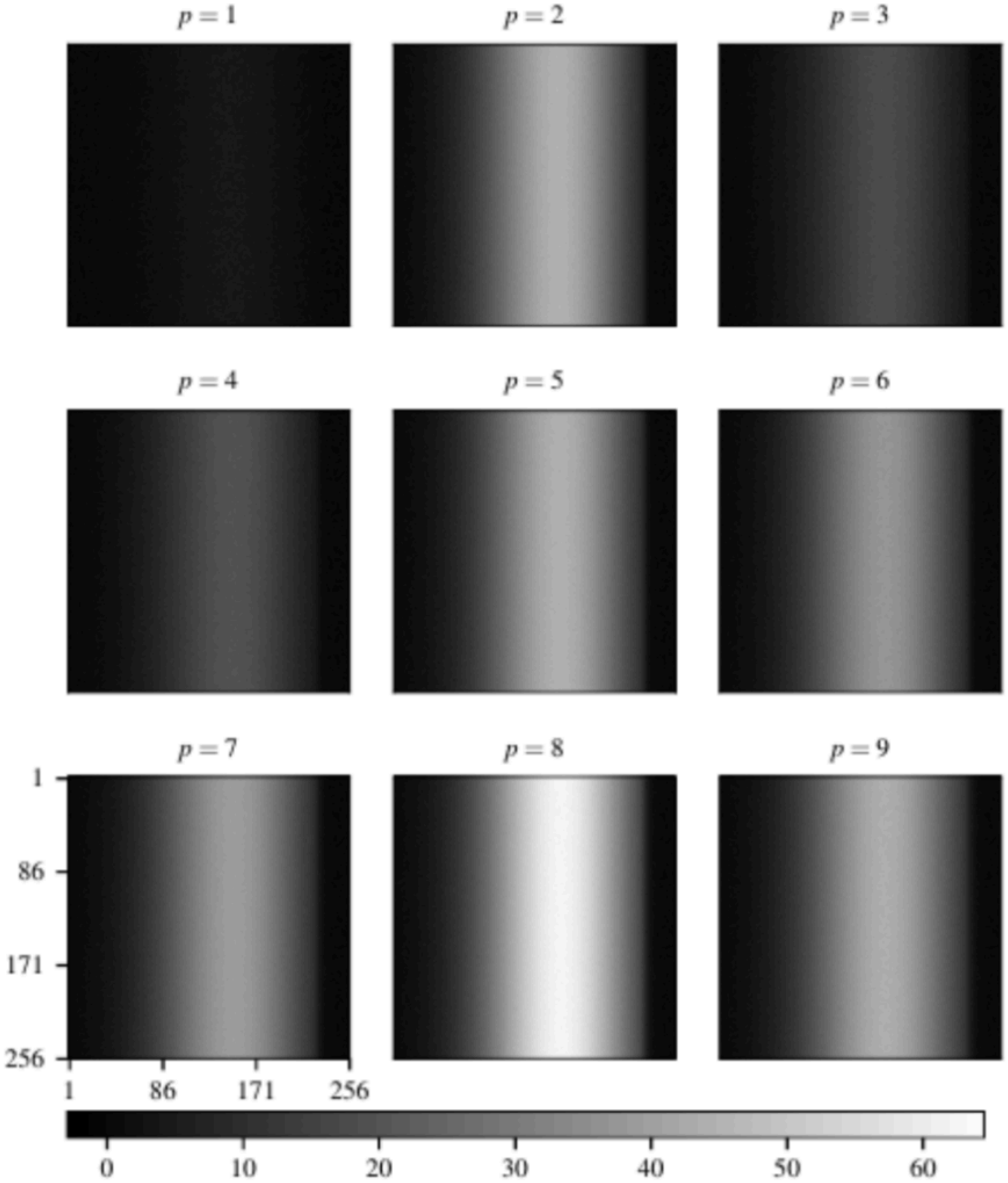
Original Spatio-Spectral Object :

Horsehead Nebula ($M = 3$)



Spectral component are extracted using the **Principal Component Analysis** (PCA) method.

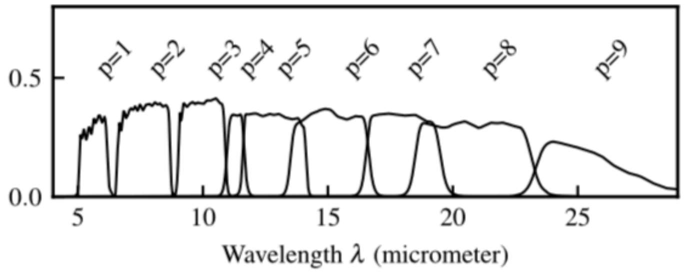
Simulation Results of the Multispectral Data



HorseHead nebula

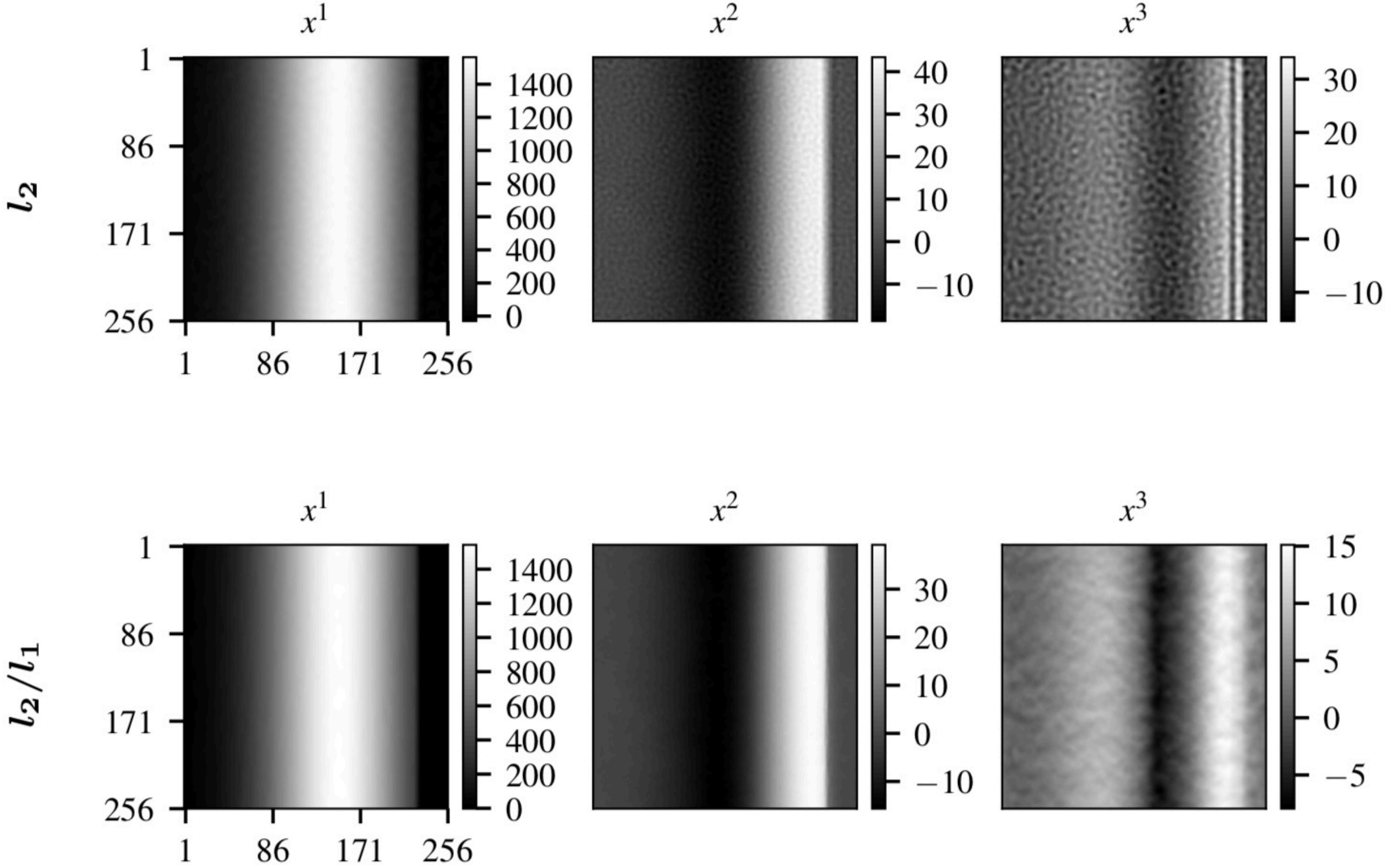
- JWST/MIRI Imager
- **9** × **256** × **256** pixels
- SNR = **30** dB white Gaussian noise

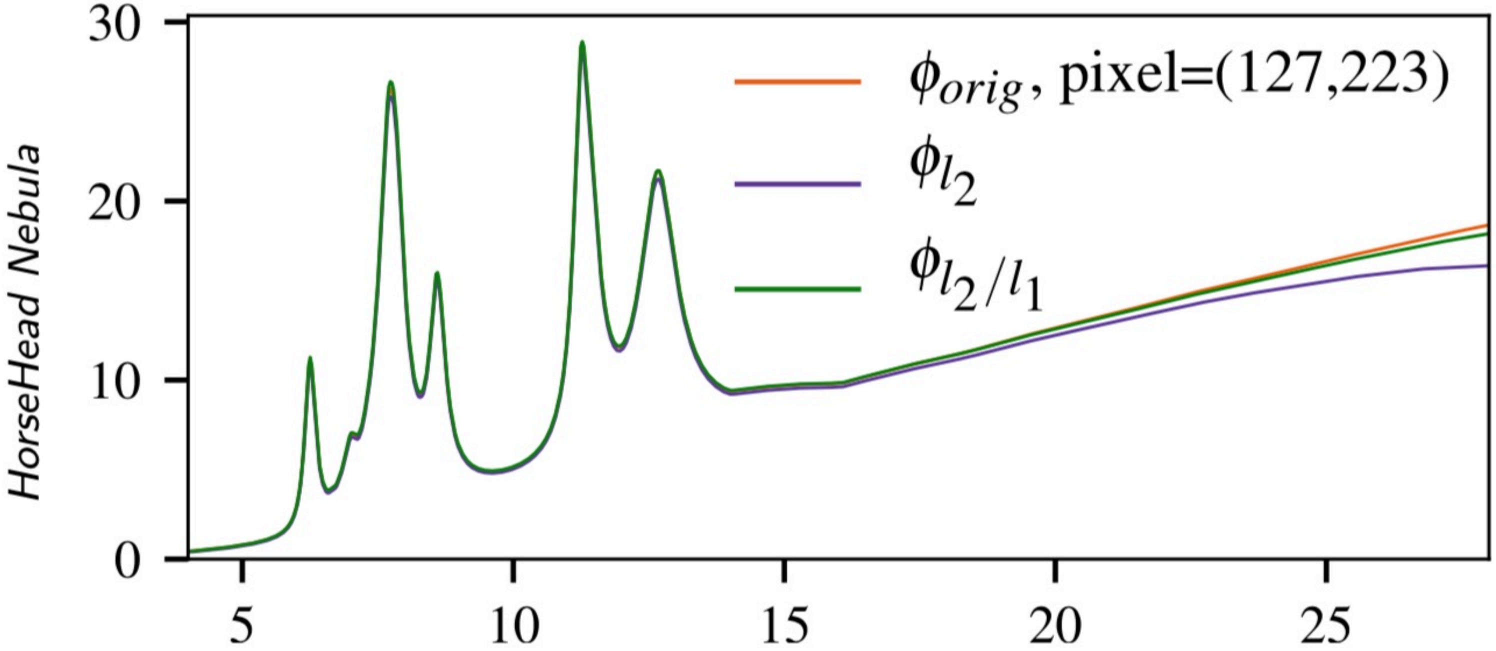
$$\mathrm{SNR} = 10\log_{10}\left(\frac{\frac{1}{N}\|\boldsymbol{y}\|_2^2}{\sigma_n^2}\right)$$



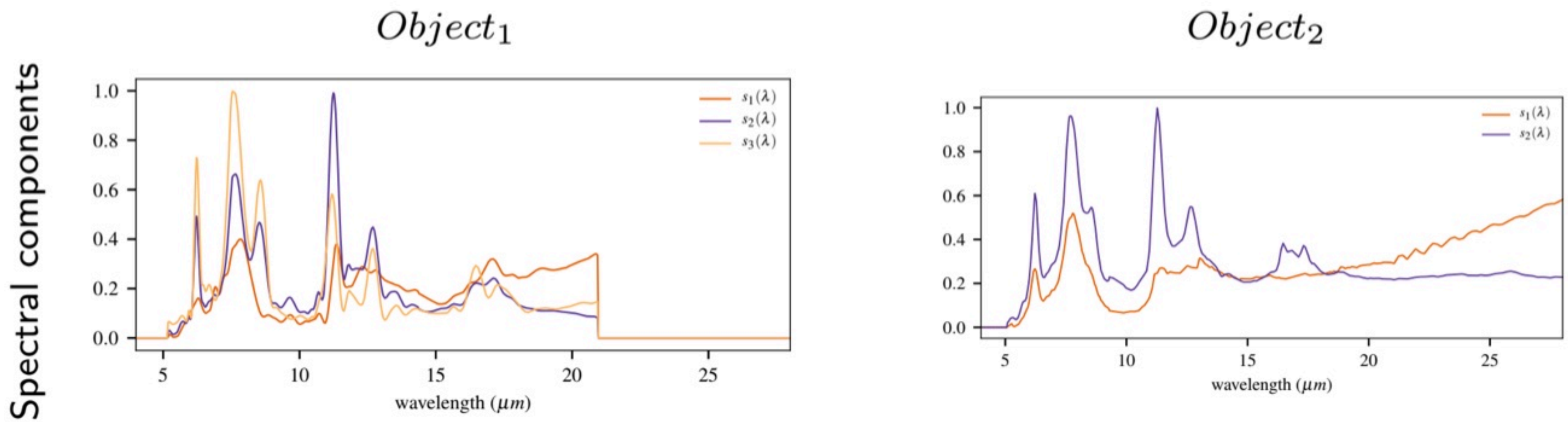
Estimated Mixture Coefficients

HorseHead

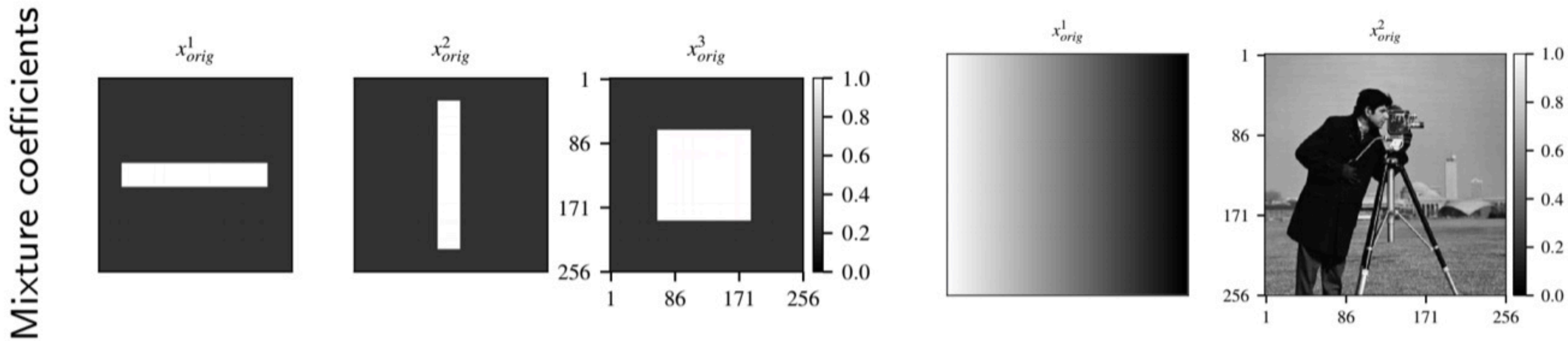



HorseHead Nebula
ϕ_{orig}, pixel=(127,223)
ϕ_{l_2}
ϕ_{l_2/l_1}
0
10
20
30
5
10
15
20
25

Synthetic Spatio-Spectral Objects : $1000 \times 256 \times 256$

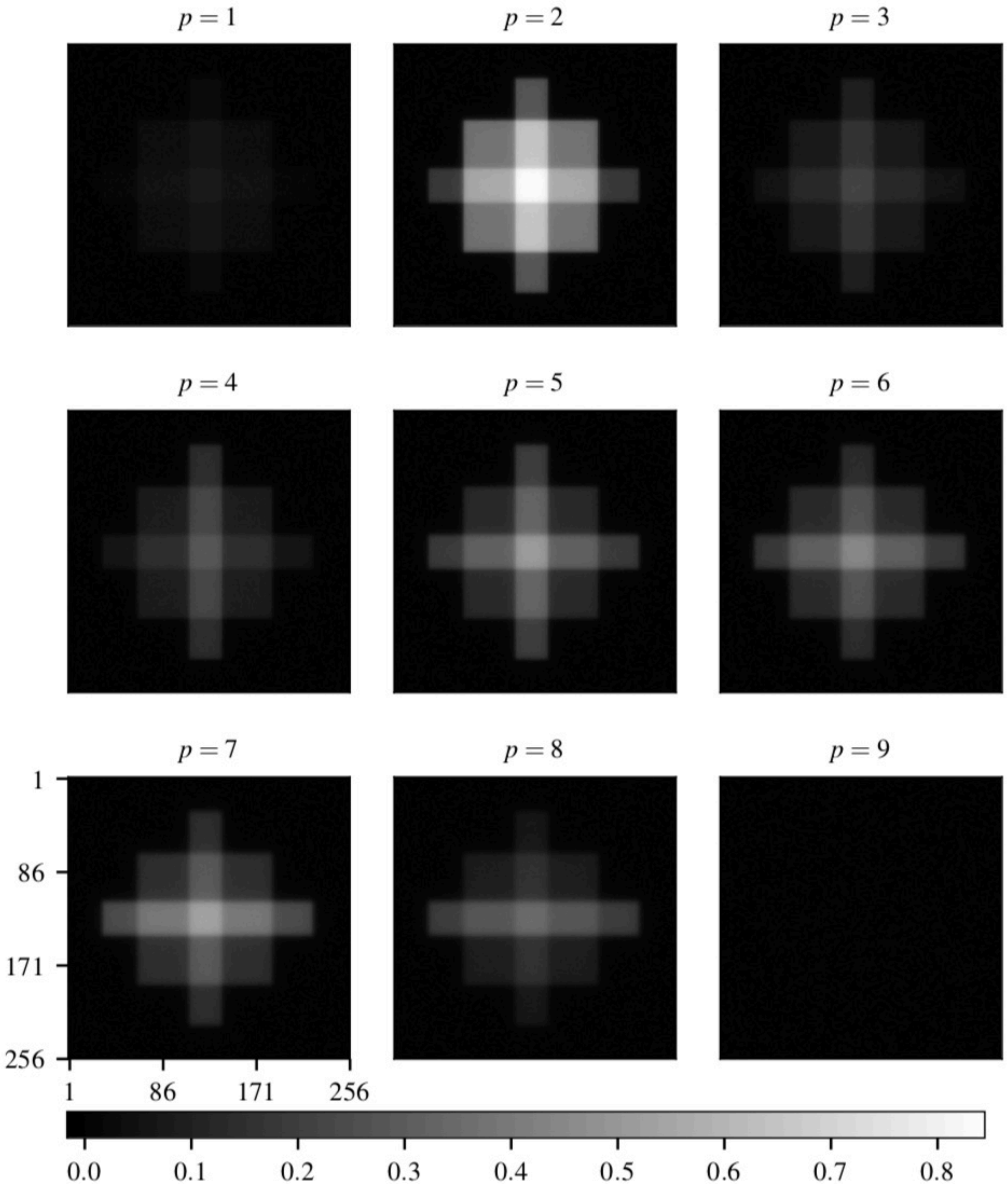


R around 100



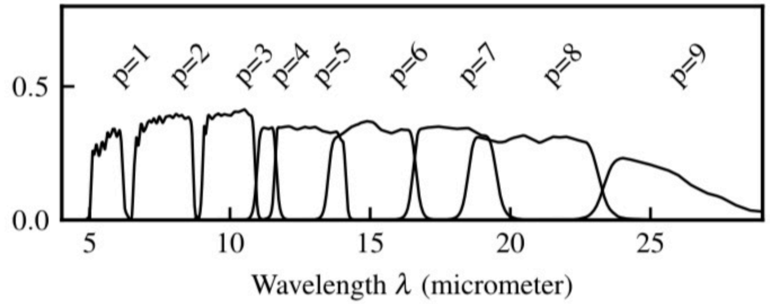
. Spectra extracted from real data observed by the Spitzer Telescope [Berne *et al.* 2007]

Simulation of Multispectral Data



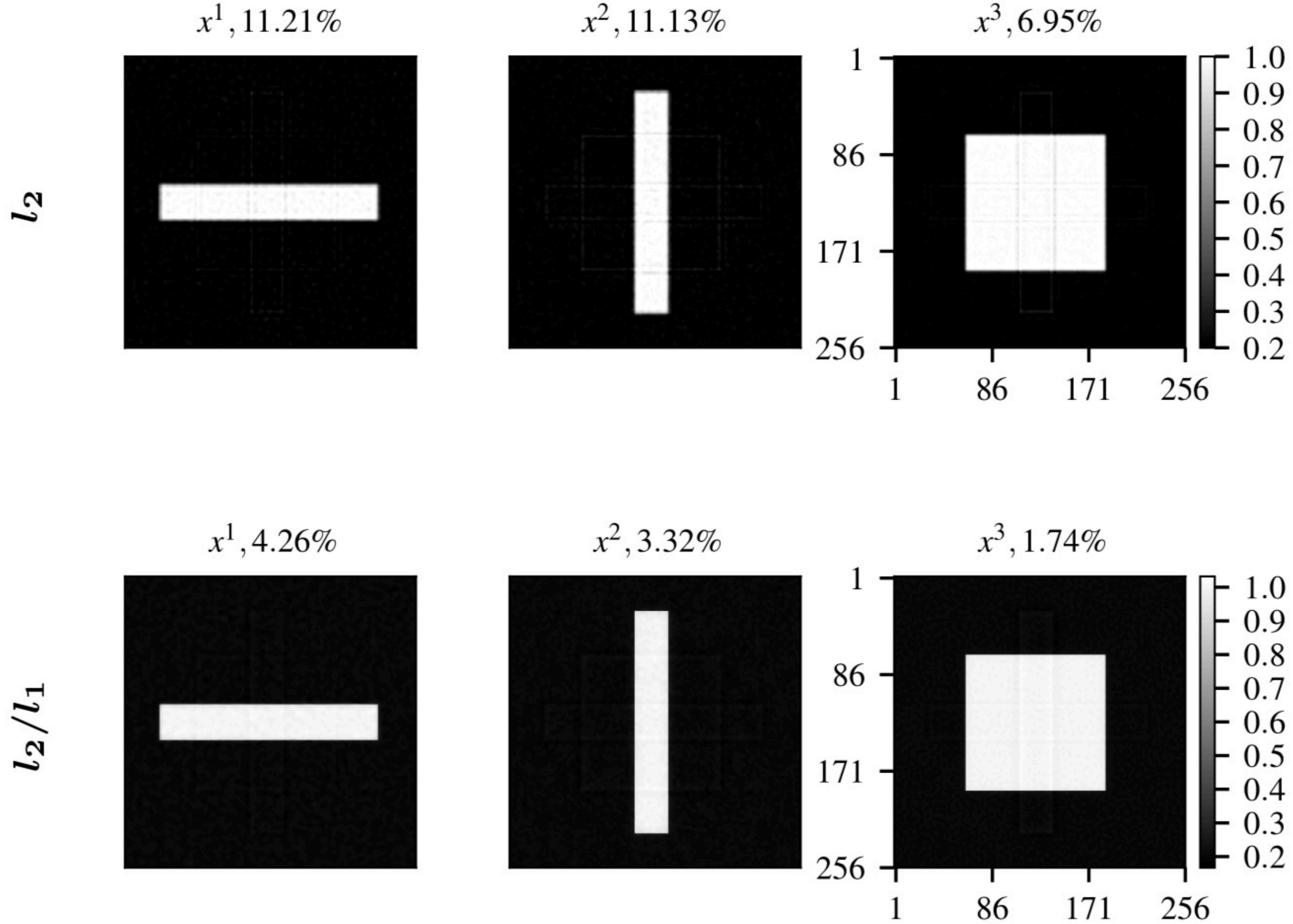
$Object_1$

- JWST/MIRI Imager
- $9 \times 256 \times 256$ pixels
- $\mathrm{SNR} = 30$ dB white Gaussian noise

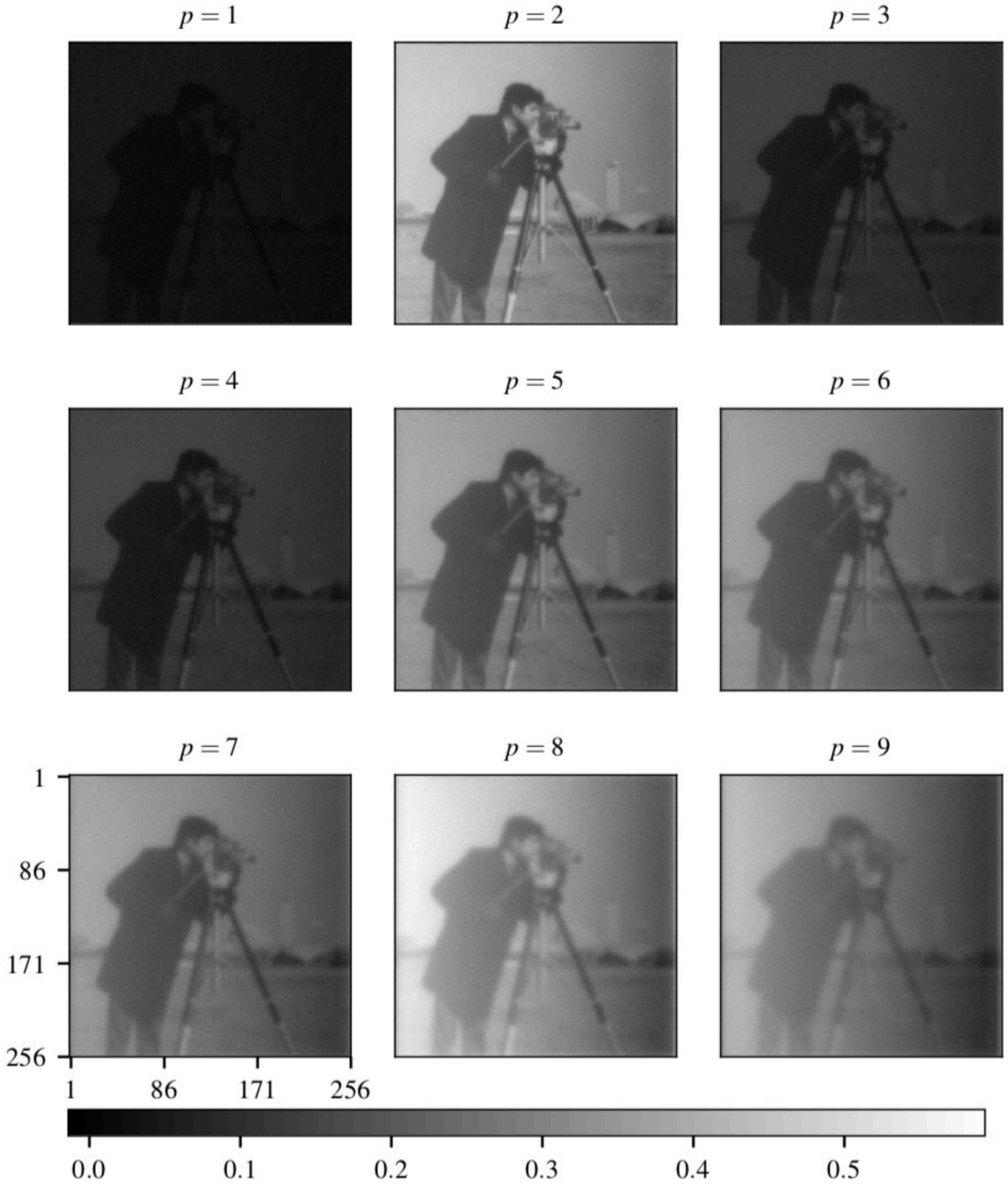


Estimated Mixture Coefficients

$Object_1$

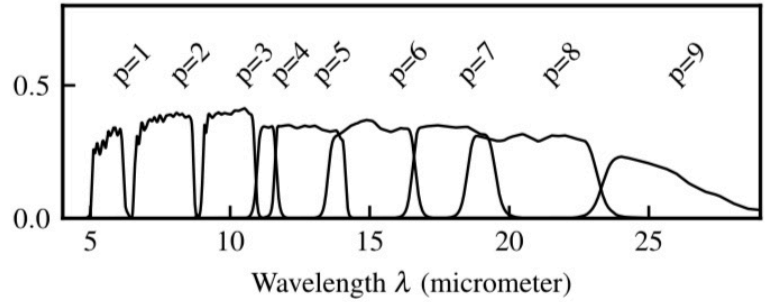


Simulation of Multispectral Data



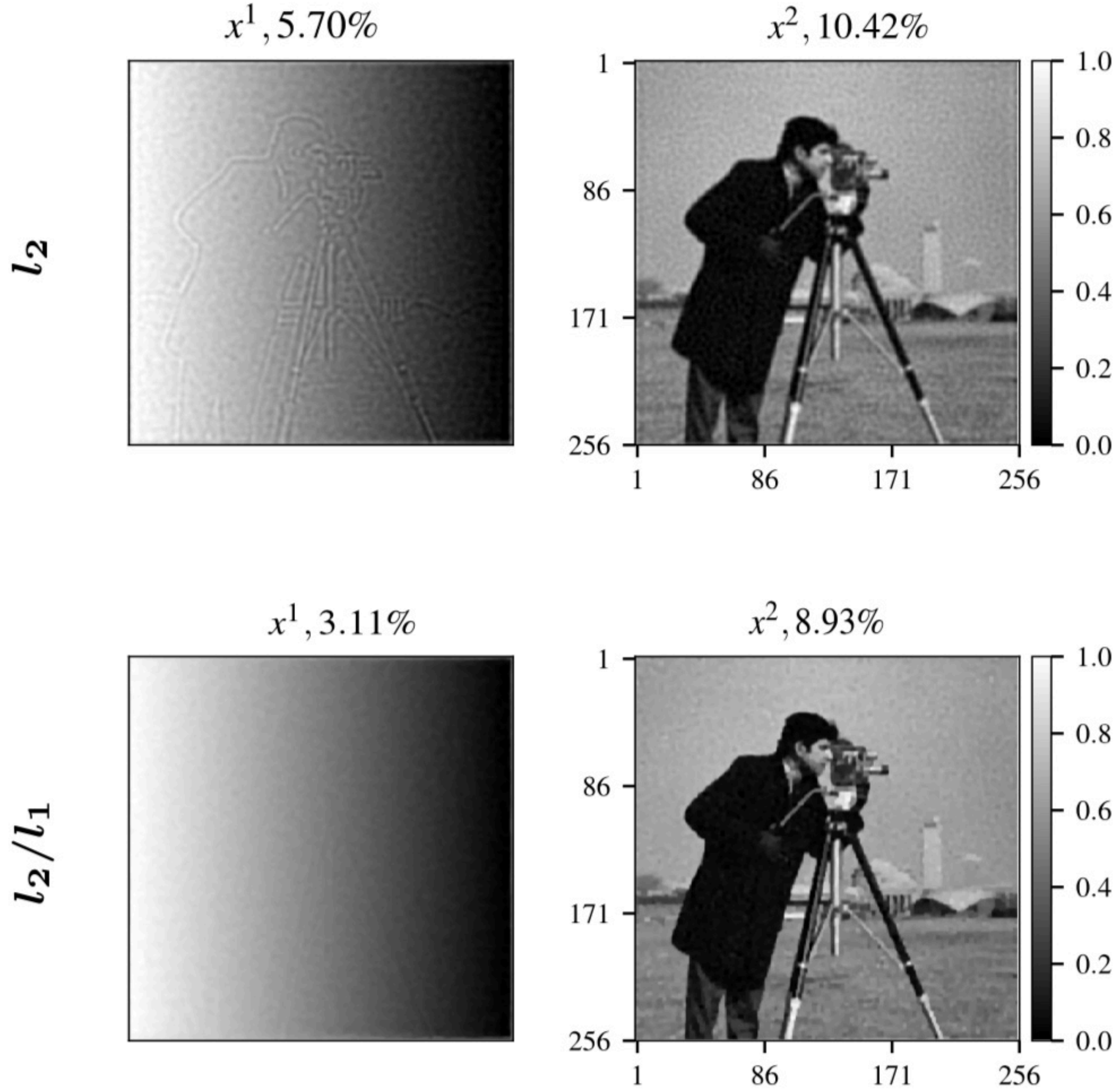
$Object_2$

- JWST/MIRI Imager
- $9 \times 256 \times 256$ pixels
- $\mathrm{SNR} = 30$ dB white Gaussian noise

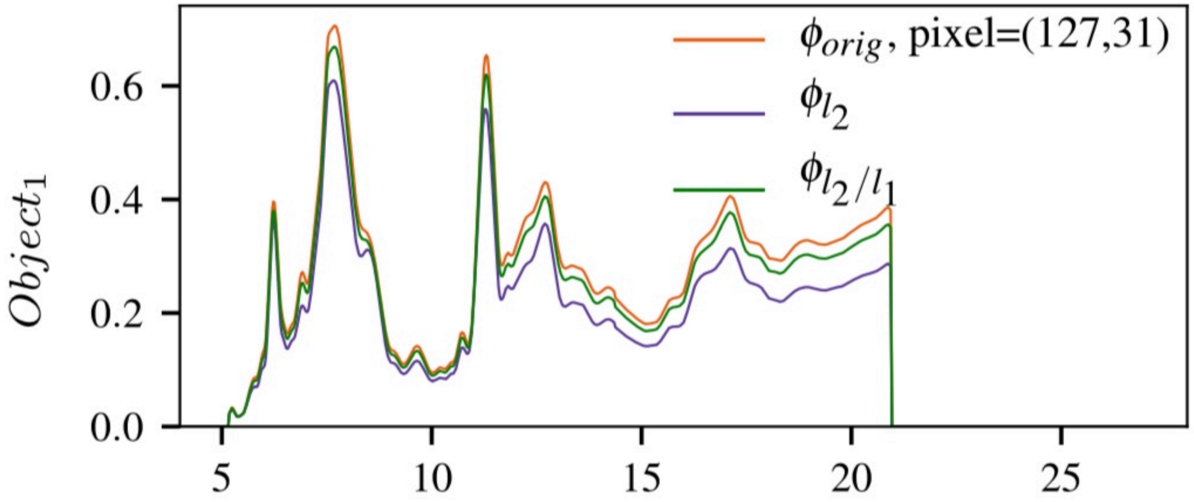


Estimated Mixture Coefficients

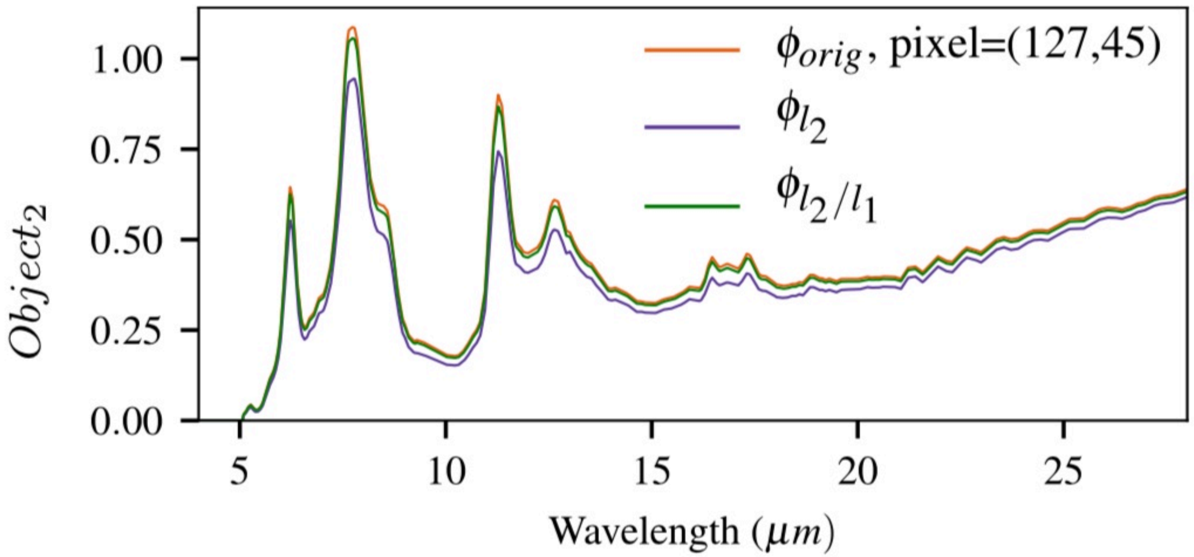
$Object_2$



Reconstruction Results

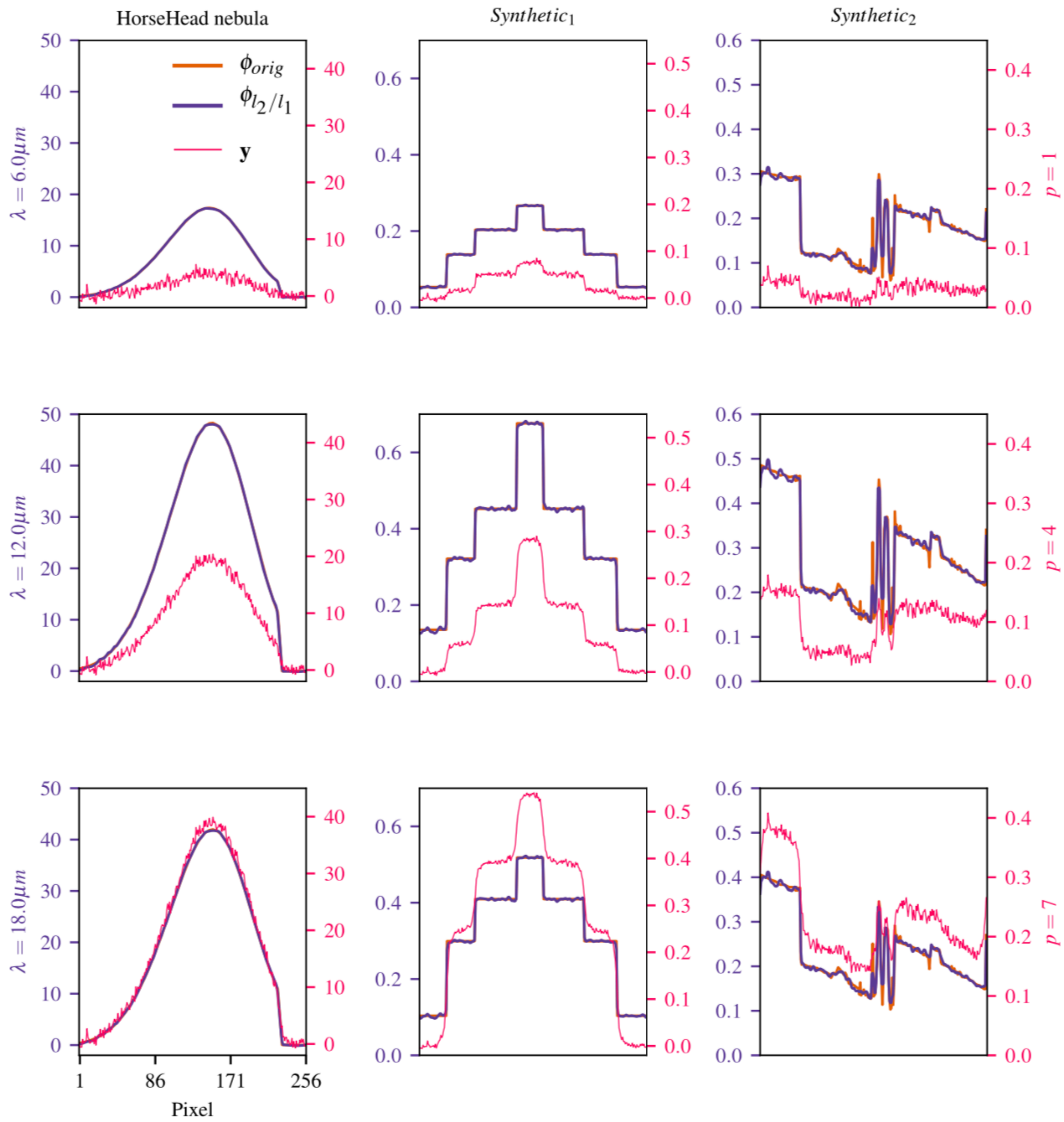


R around 100



L2-L1 results

→ Deconvolution
→ Denoising



Reconstruction Results

Spatio-Spectral Object	Regularization	Error (%)	Runtime (seconds)	N_{iter}
HorseHead Nebula	l_2	1.14	**1.36**	
	l_2/l_1	**0.66**	20.33	50
$Object_1$	l_2	5.29	**1.19**	
	l_2/l_1	**1.91**	19.98	50
$Object_2$	l_2	5.95	**0.97**	
	l_2/l_1	**4.91**	18.50	50

- Reconstructed spatio-spectral objects of size $\mathbf{1000} \times \mathbf{256} \times \mathbf{256}$.
- Relative error : $\mathrm{Error}(\%) = 100 \times \frac{\|\boldsymbol{x}_{orig} - \boldsymbol{x}_{rec}\|_2}{\|\boldsymbol{x}_{orig}\|_2}$

Influence of the Noise Level