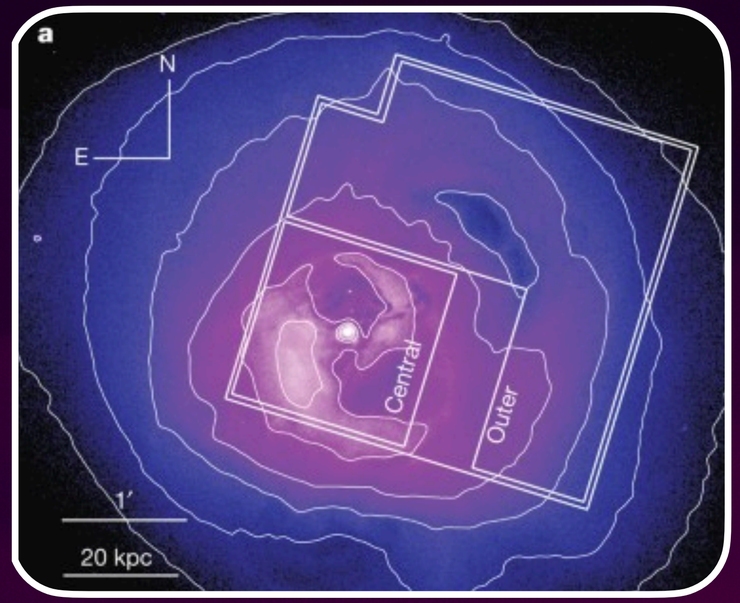
jaxspec : a pure Python, GPU ready and Bayesian framework for X-ray spectral fitting

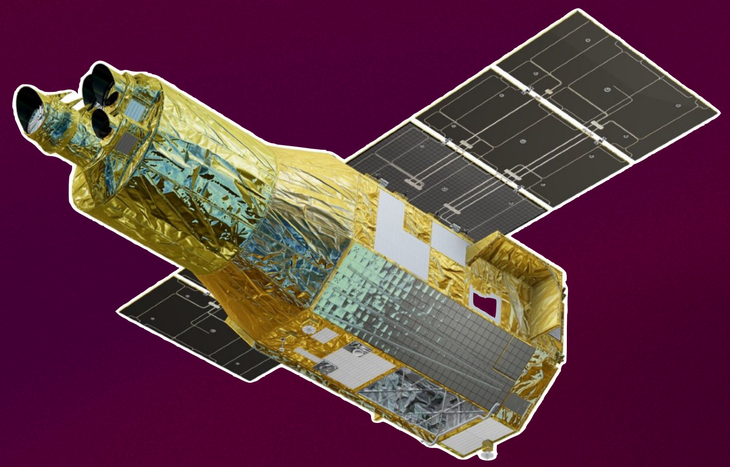
Simon Dupourqué,
On behalf of the jaxspec development team
D. Barret, C. Diez,, S. Guillot, E. Quintin
Many thanks to A. Molin, F. Castellani and X. Astiasarain for their contributions

1. Reminders on X-ray spectral fitting

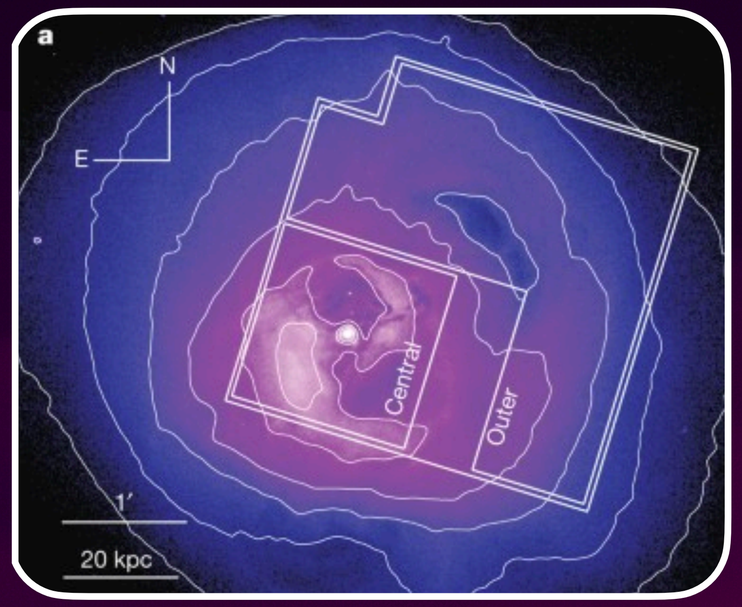
X-ray source



X-ray instrument

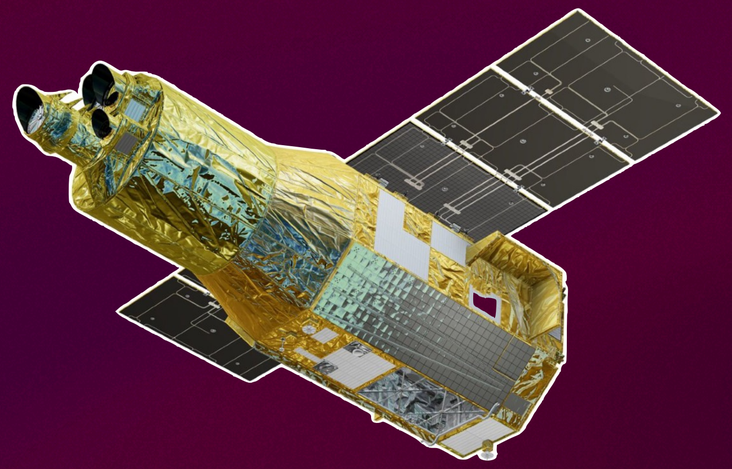


X-ray source

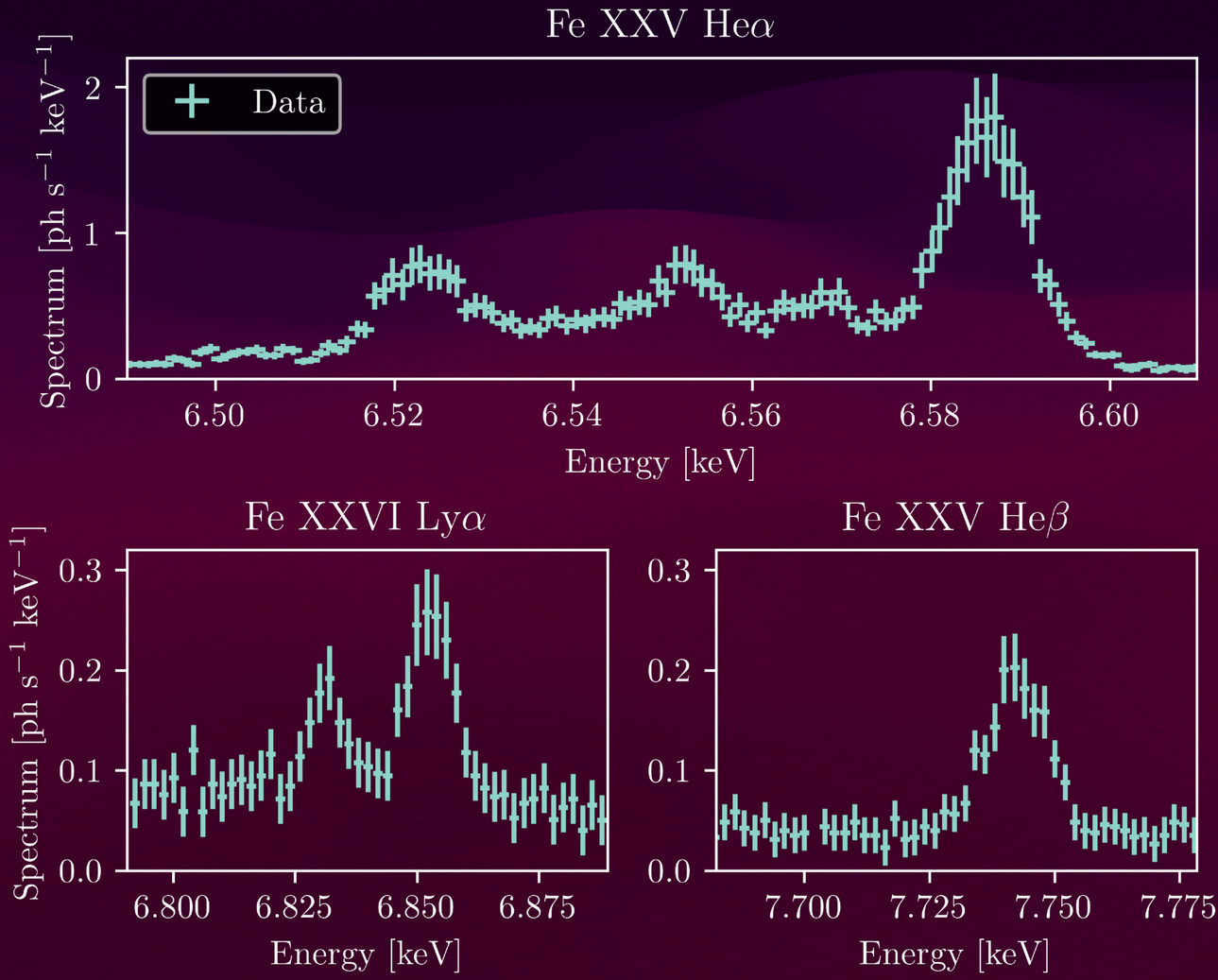


Observation

X-ray instrument

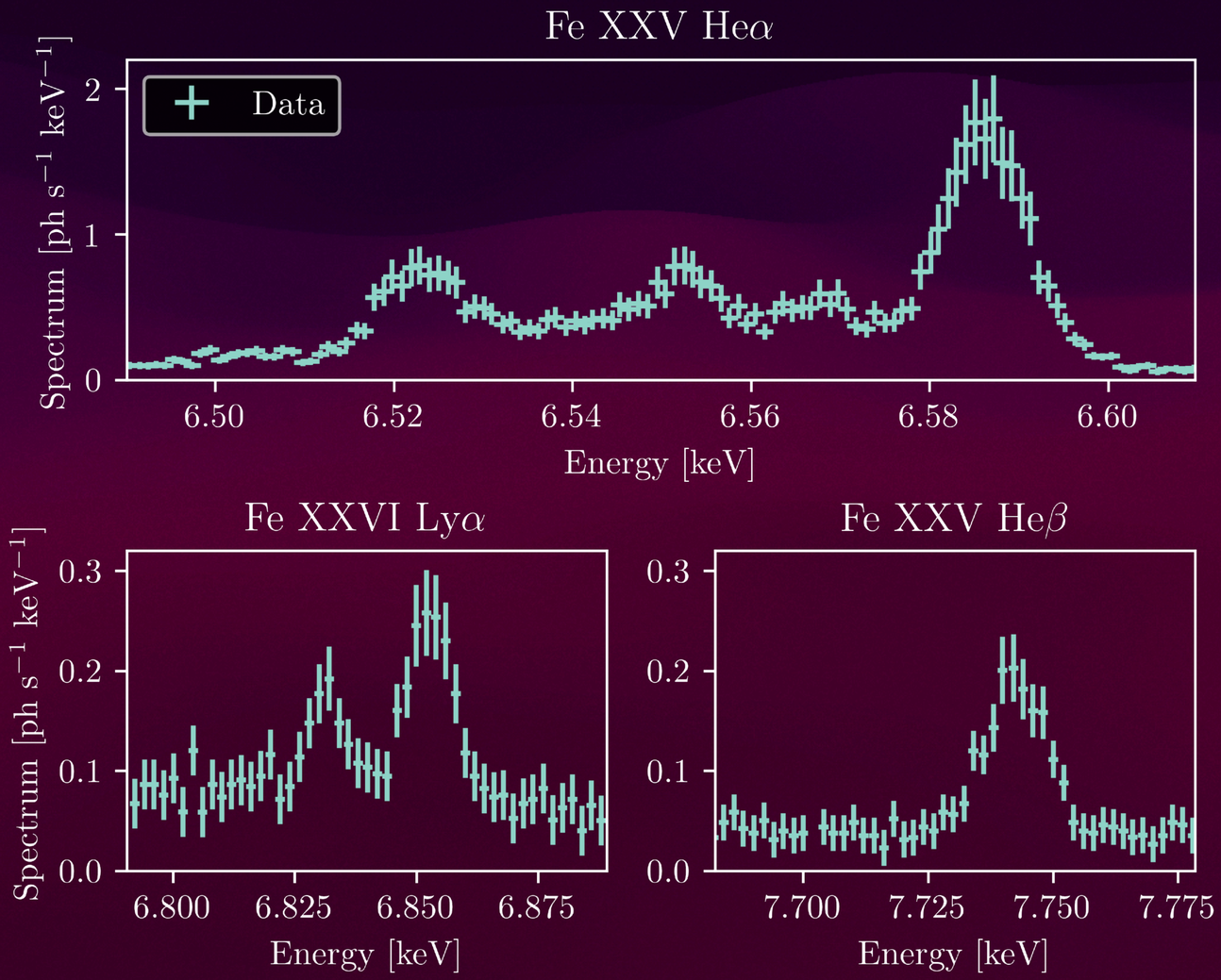


X-ray spectrum



Adapted from the Hitomi collaboration papers

X-ray spectrum

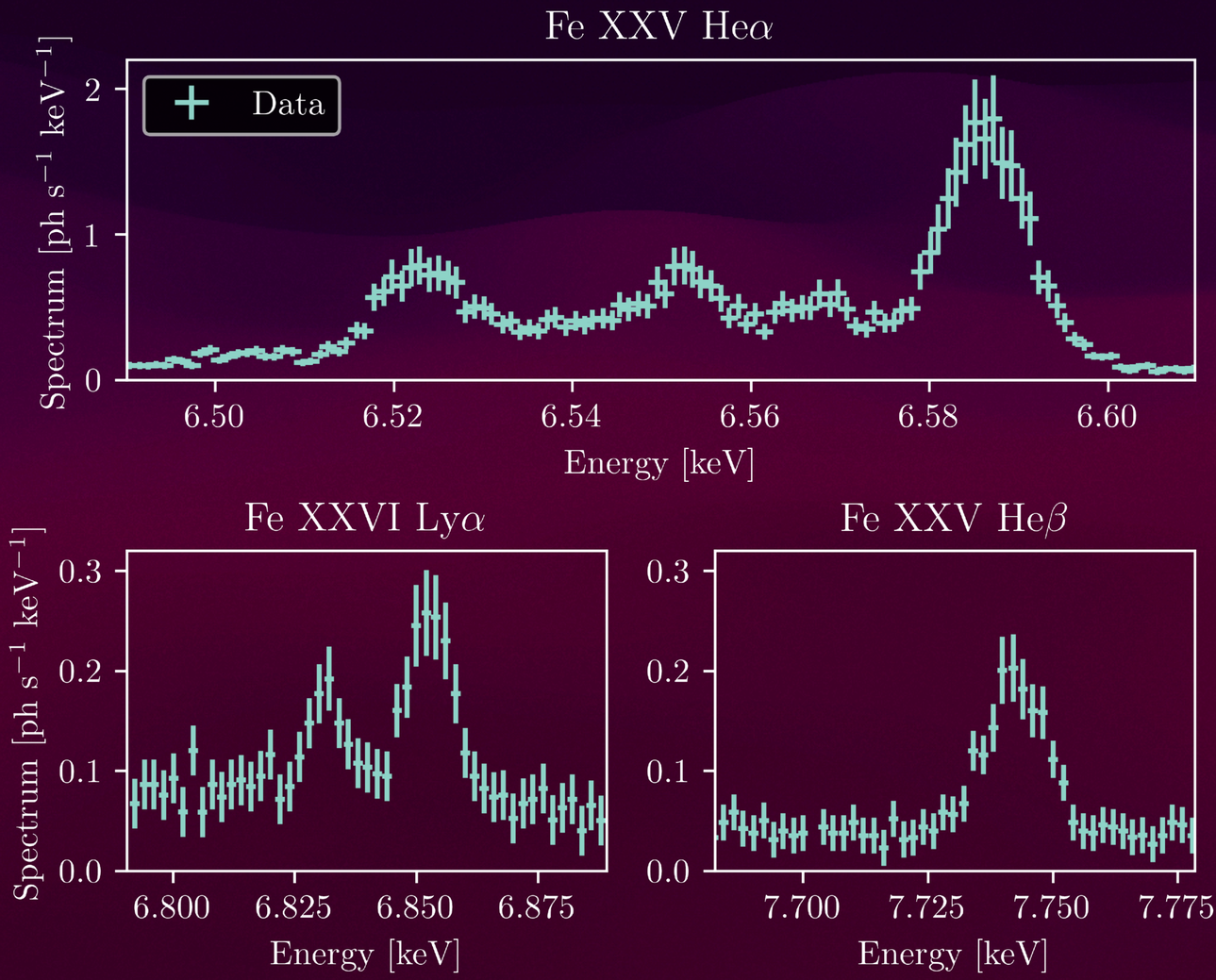


Adapted from the Hitomi collaboration papers

1. Define a spectral model
2. Determine the best parameters
3. Interpret with physical knowledge
4. Publish your results to *Nature*

Reduction

X-ray spectrum



Adapted from the Hitomi collaboration papers

For the Perseus cluster spectrum

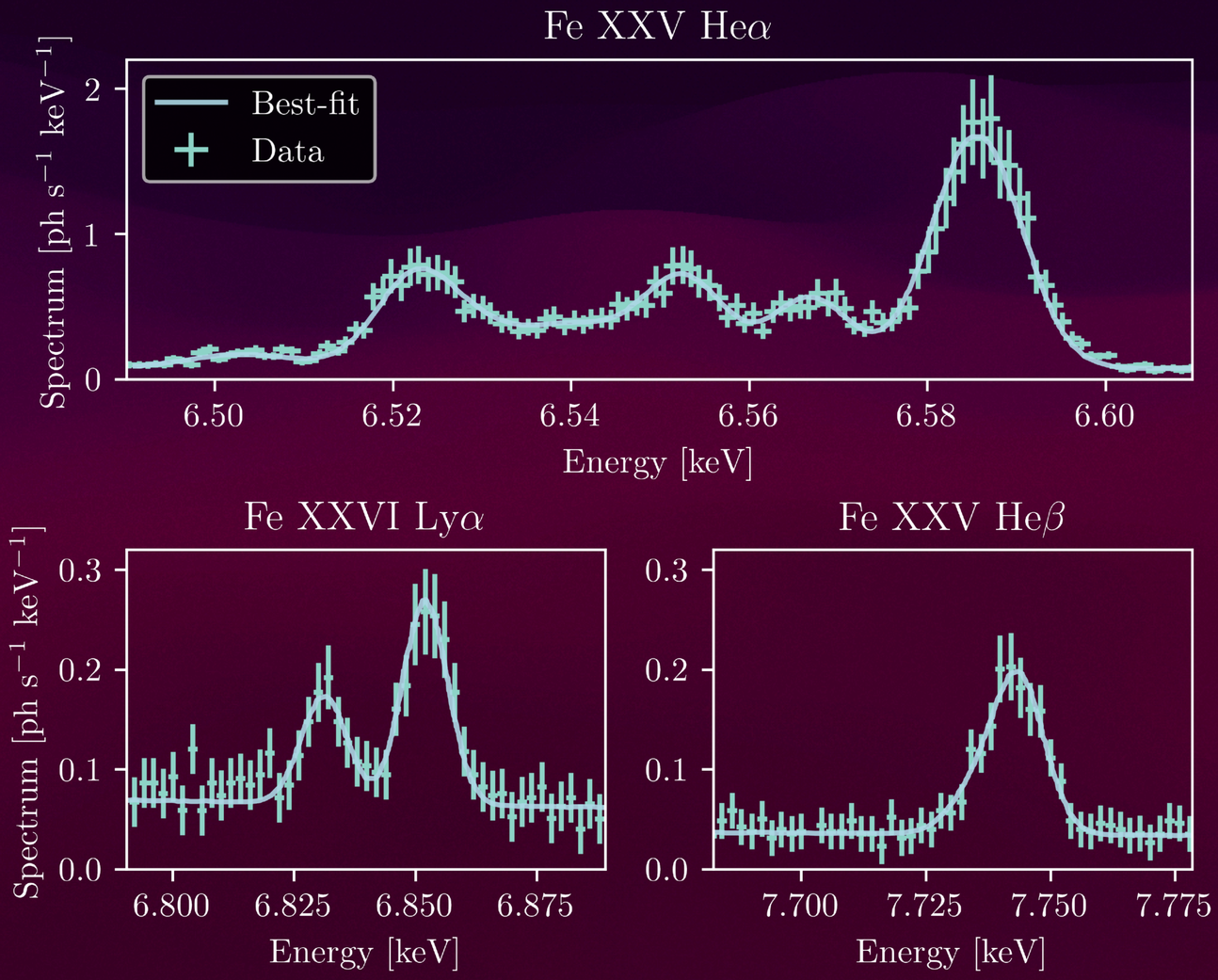
1. Gaussian emission lines for Iron complexes

2. Determine the centroid shift and broadening

3. Line of sight bulk and turbulent motions (~160 km/s) of the intracluster medium

4. The quiescent intracluster medium in the core of the Perseus cluster, Hitomi Collaboration, *Nature* **volume 535**, pages 117–121 (2016)

X-ray spectrum

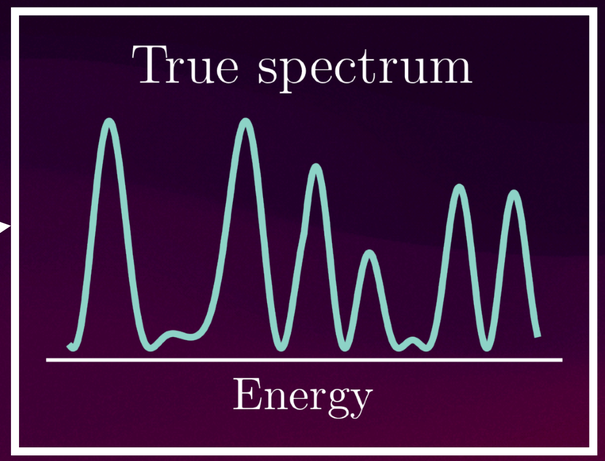


How to determine the best parameters of a given model ?

Parameters θ
for the model

How to determine the best parameters of a given model ?

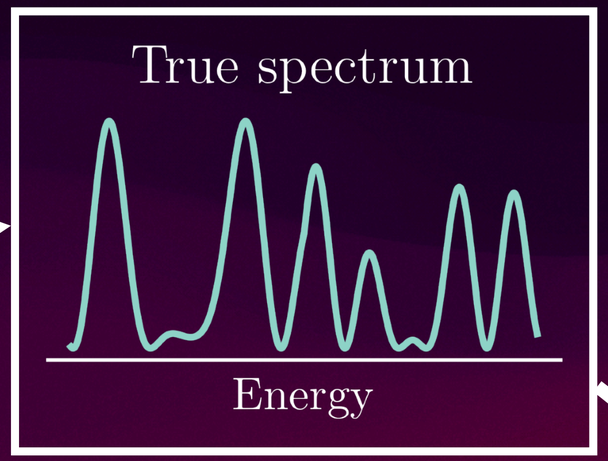
Evaluate the model at multiple energies



Parameters θ for the model

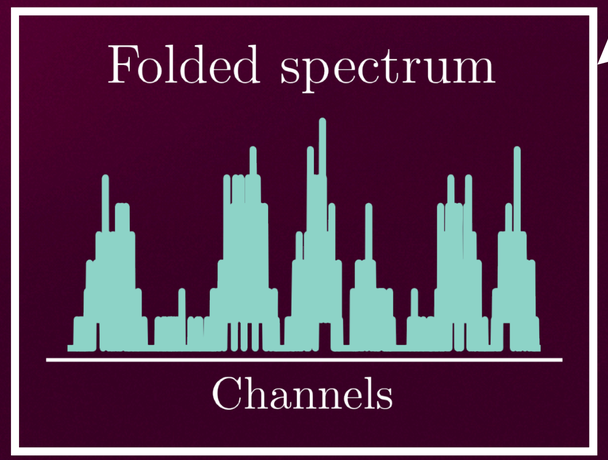
How to determine the best parameters of a given model ?

Evaluate the model at multiple energies

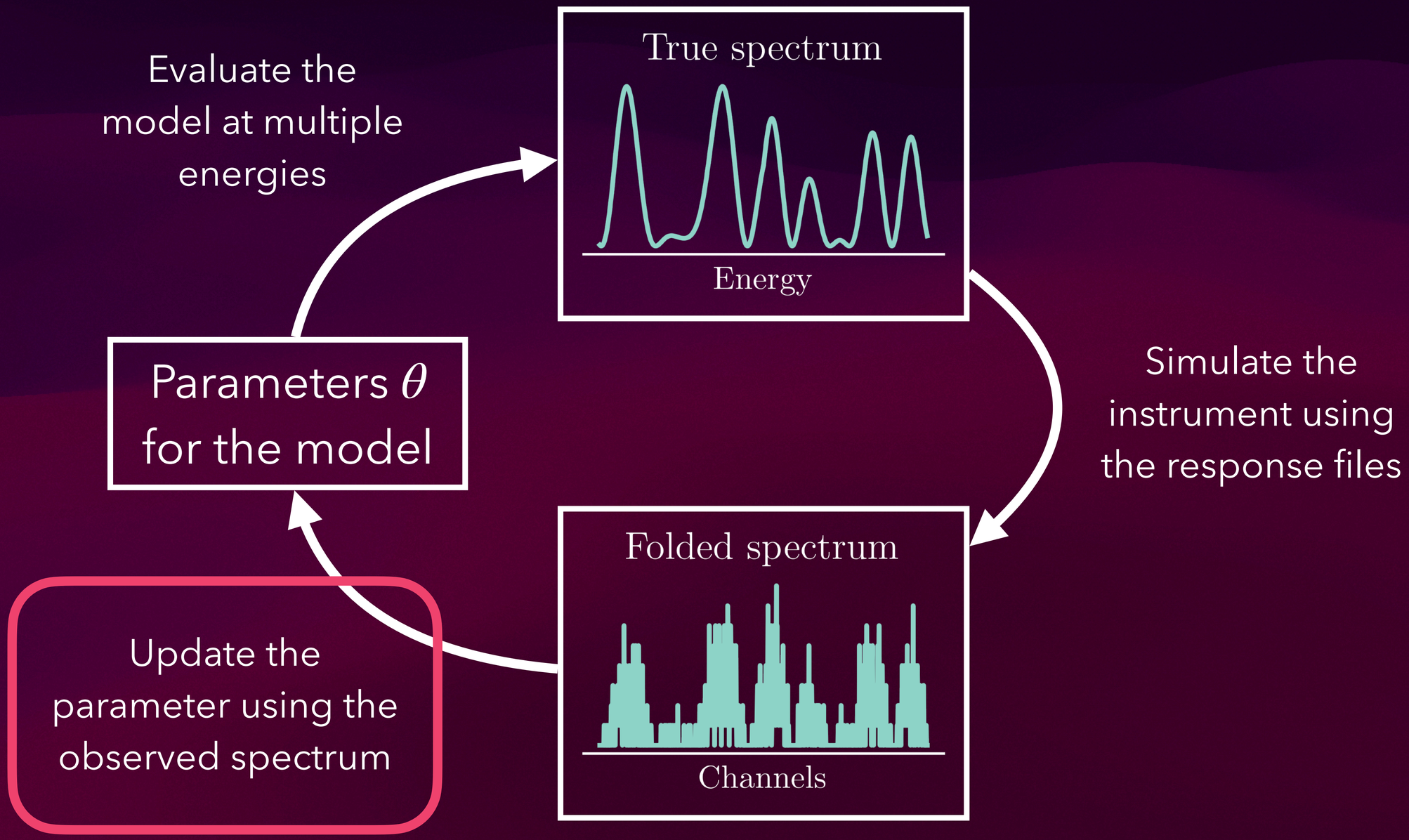


Parameters θ for the model

Simulate the instrument using the response files



How to determine the best parameters of a given model ?



Fit statistic minimization		Posterior distribution estimation	
Pros	**Cons**	**Pros**	**Cons**
Fast inference	Prone to local minima 😱	Improbed robustness against local	Utterly slow
Analytical expressions	Inaccurate approx. of the parameters	Exact distribution of the parameters	Harder formalism

Fit on XSPEC
χ^2 approaches

BXA
MCMC on XSPEC

The ecosystem of X-ray spectral fitting

SPEX (1996)

ISIS (2000)

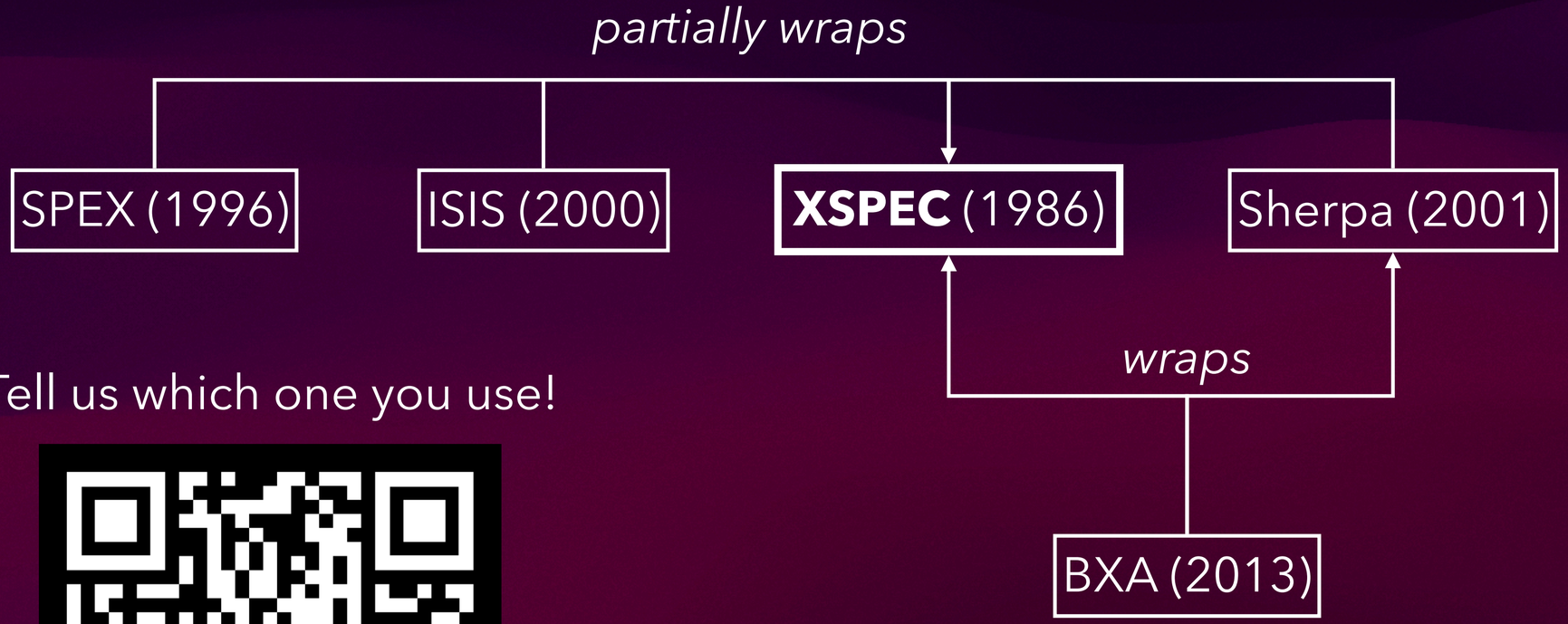
XSPEC (1986)

Sherpa (2001)

Tell us which one you use!

BXA (2013)

The ecosystem of X-ray spectral fitting



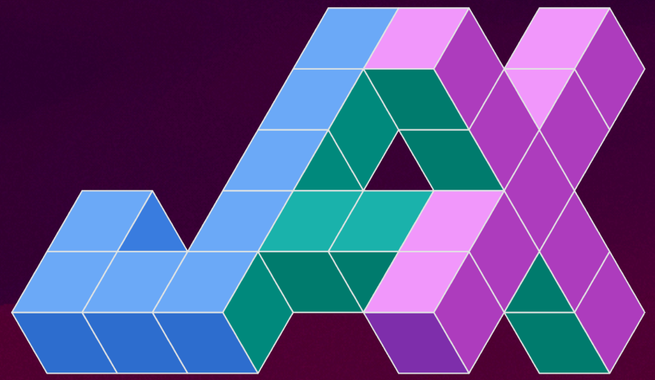
Tell us which one you use!

2. What is jaxspec ?

Work in progress

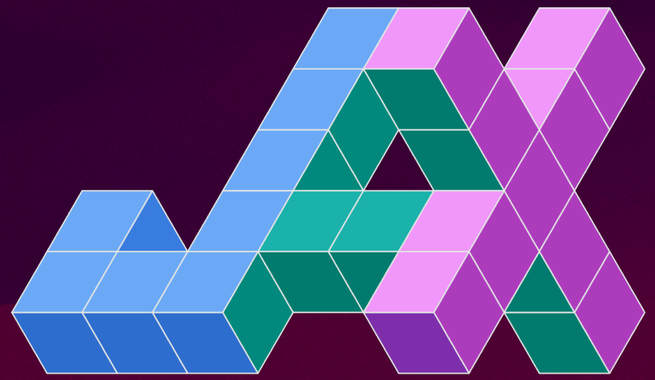
jaxspec is a library for high performance X-ray spectral fitting

Based on JAX



jaxspec is a library for high performance X-ray spectral fitting

Based on JAX

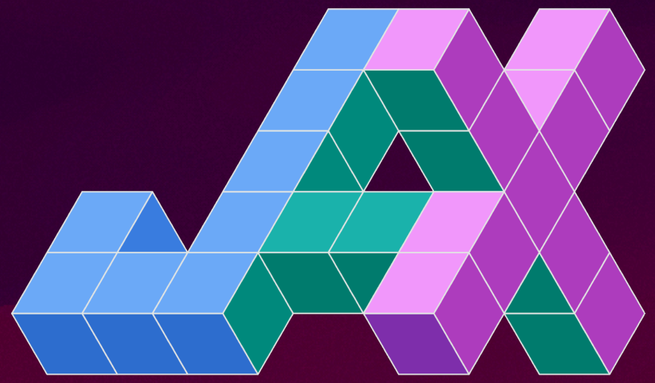


→

Just in time compilation
Automatic differentiation
Accelerators (GPUs, TPUs)

jaxspec is a library for high performance X-ray spectral fitting

Based on JAX



→

Just in time compilation
Automatic differentiation
Accelerators (GPUs, TPUs)

XRISM

Paves the way for powerful samplers and new approaches to X-ray spectral fitting for next & current X-ray spectra

E.G. Hamiltonian Monte Carlo (HMC), No U-Turn Sampler (NUTS), Stochastic Variational Inference (SVI)

jaxspec is a library for high performance X-ray spectral fitting

Task

Get the posterior distribution of an absorbed power law + blackbody model on fake spectra

```
tbabs*(blackbodyrad + powerlaw)
```

- MCMC : run several chains until convergence is achieved ($\hat{R} < 1.01$)
- Nested sampling : run until termination criterion is validated

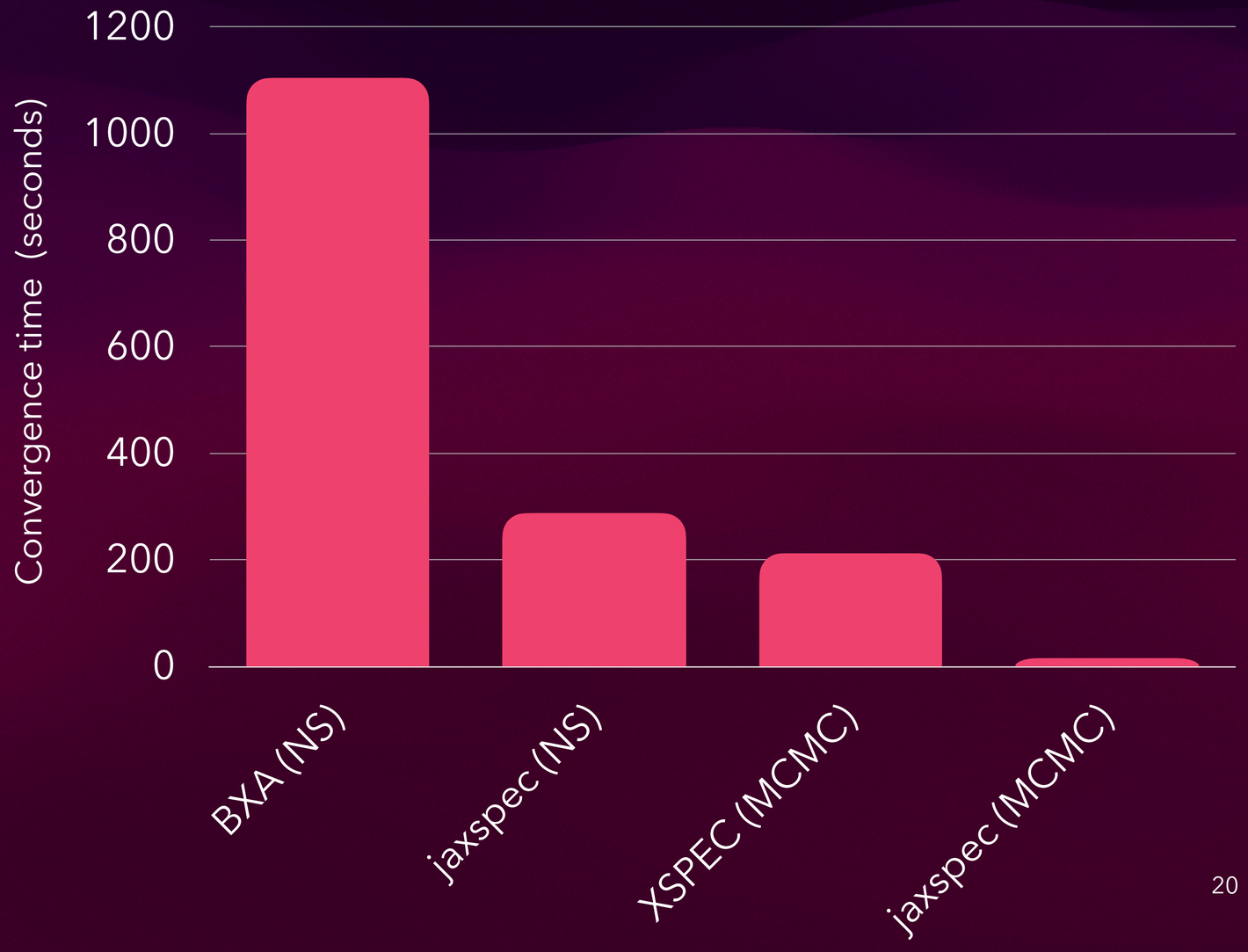
jaxspec is a library for high performance X-ray spectral fitting

Task

Get the posterior distribution of an absorbed power law + blackbody model on fake spectra

```
tbabs*(blackbodyrad + powerlaw)
```

- MCMC : run several chains until convergence is achieved ($\hat{R} < 1.01$)
- Nested sampling : run until termination criterion is validated



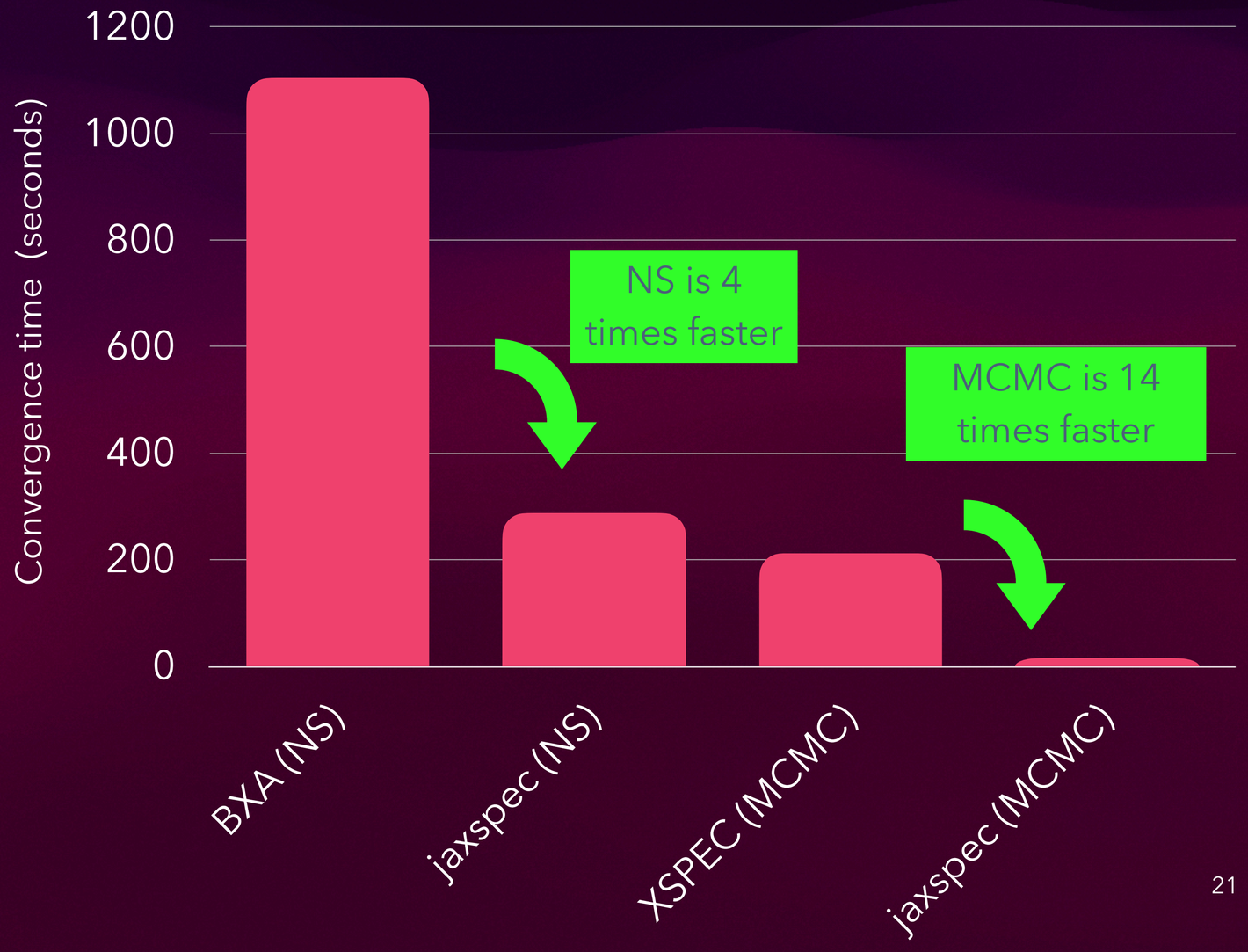
jaxspec is a library for high performance X-ray spectral fitting

Task

Get the posterior distribution of an absorbed power law + blackbody model on fake spectra

```
tbabs*(blackbodyrad + powerlaw)
```

- MCMC : run several chains until convergence is achieved ($\hat{R} < 1.01$)
- Nested sampling : run until termination criterion is validated



jaxspec is a library for high performance X-ray spectral fitting

Task

Generate fake spectra with a given instrumental response and observational setup

`fakeit`

Generate 100 realisations of an absorbed blackbody spectrum using EPIC/PN response

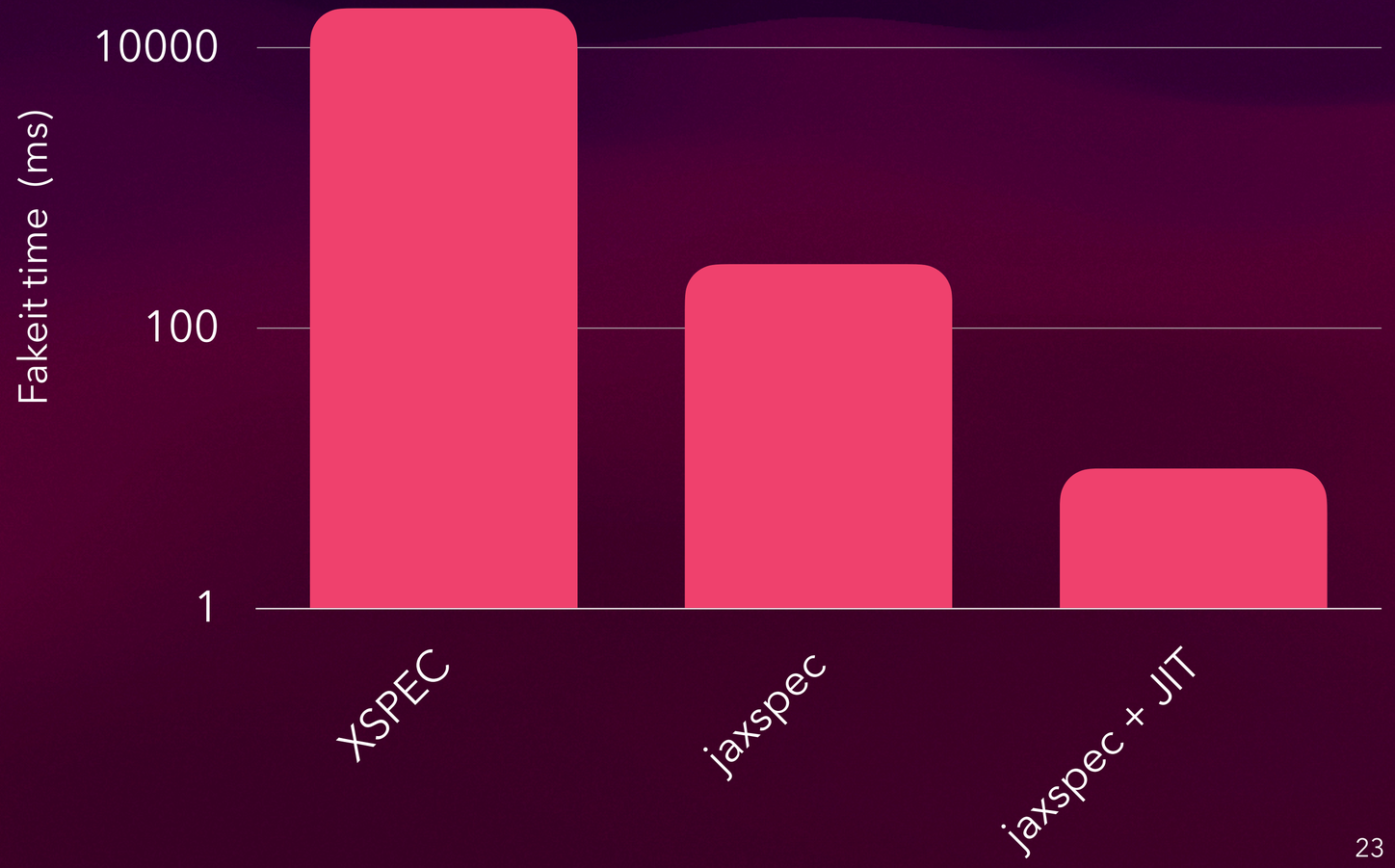
jaxspec is a library for high performance X-ray spectral fitting

Task

Generate fake spectra with a given instrumental response and observational setup

`fakeit`

Generate 100 realisations of an absorbed blackbody spectrum using EPIC/PN response



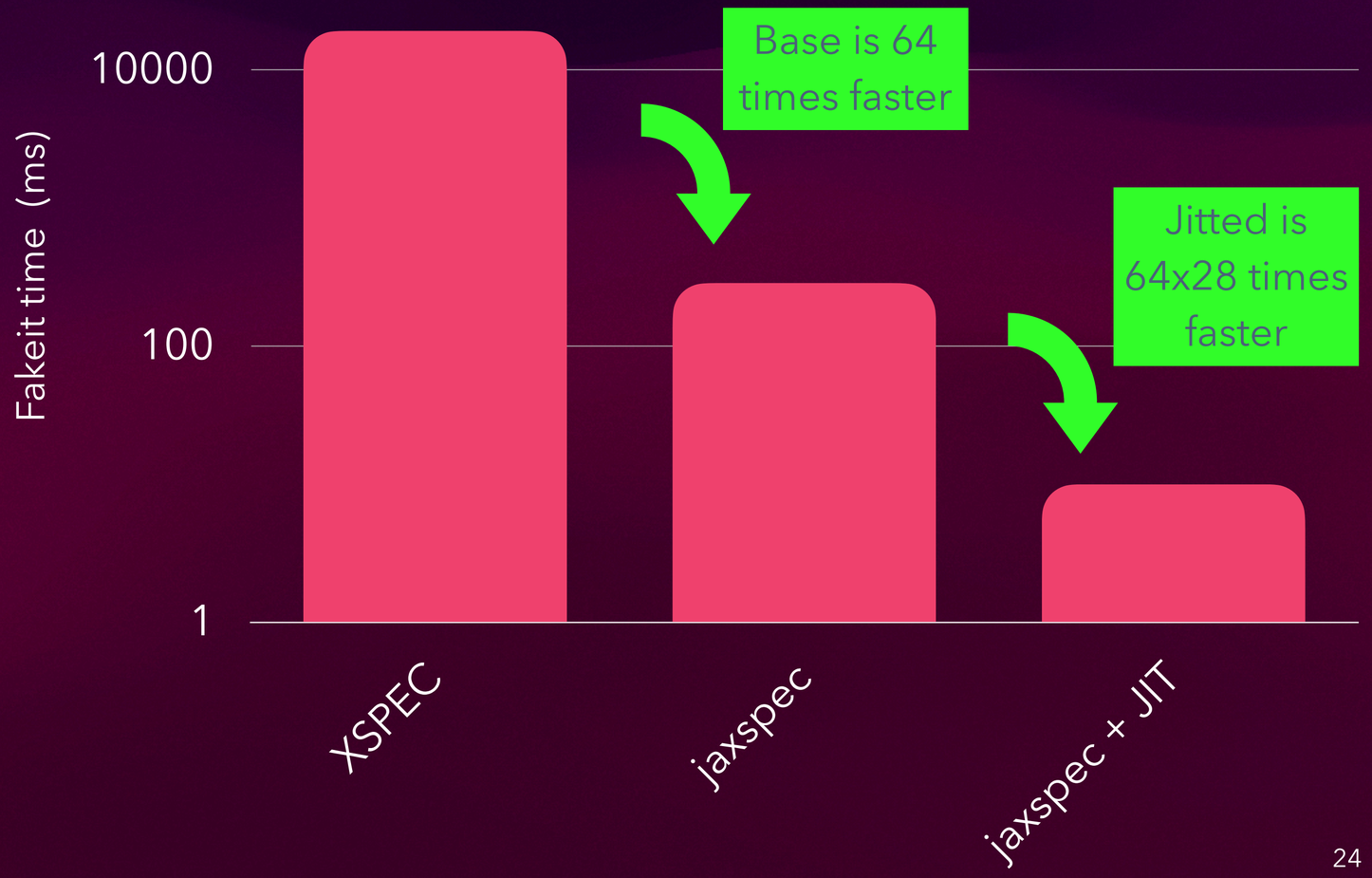
jaxspec is a library for high performance X-ray spectral fitting

Task

Generate fake spectra with a given instrumental response and observational setup

`fakeit`

Generate 100 realisations of an absorbed blackbody spectrum using EPIC/PN response

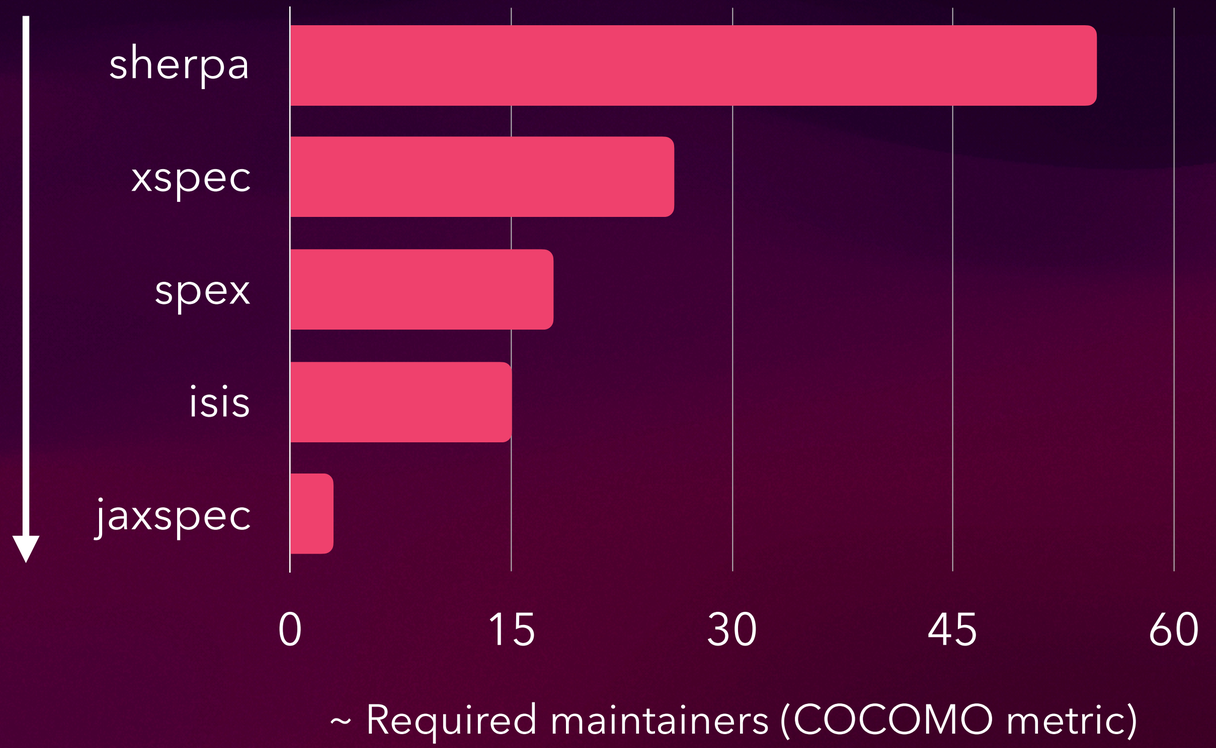


jaxspec is an open source software and community driven project

- Community driven
- Easy to install
- Easy to contribute
- Continuous integration

jaxspec is an open source software and community driven project

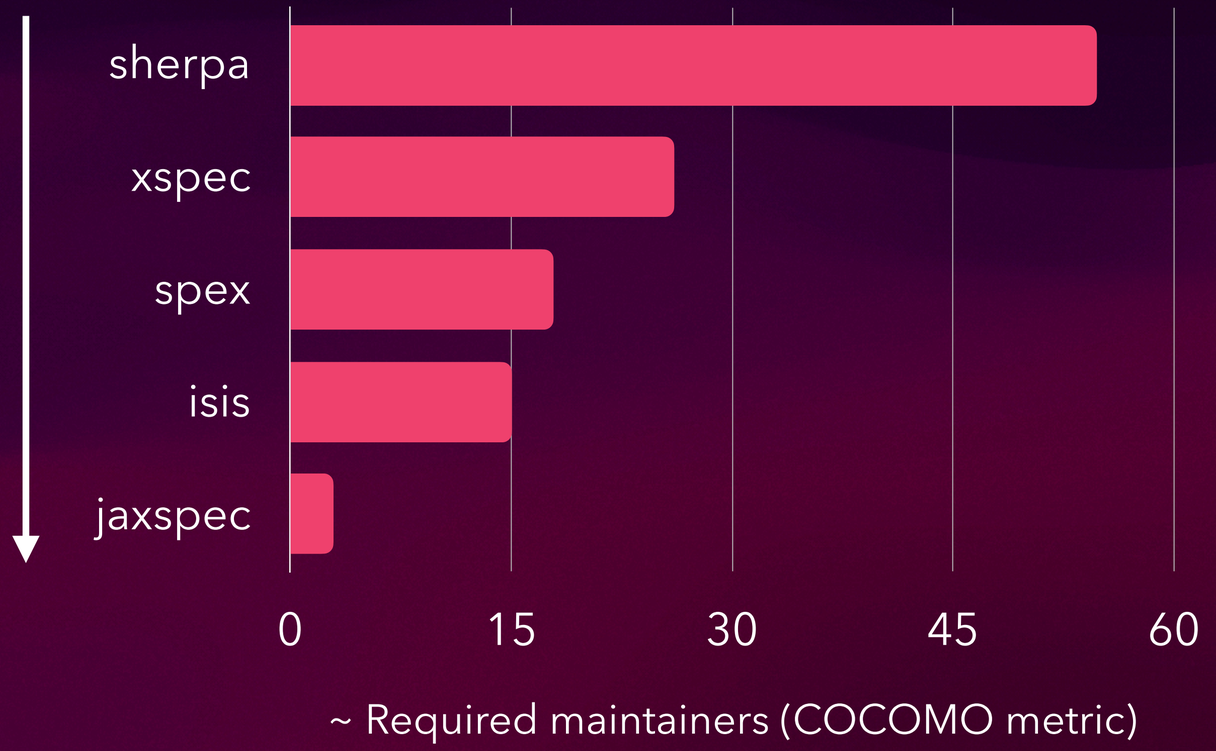
Low code complexity due to dependence on active libraries



- Community driven
- Easy to install
- Easy to contribute
- Continuous integration (automatic testing and documentation in place!)

jaxspec is an open source software and community driven project

Low code complexity due to dependence on active libraries



- Community driven
- Easy to install
- Easy to contribute
- Continuous integration, automatic testing and documentation in place

We want you to join and contribute to this project if you are interested!

The repository will be available at the end of this presentation

SIXSA : enabling machine learning to fit X-ray spectra

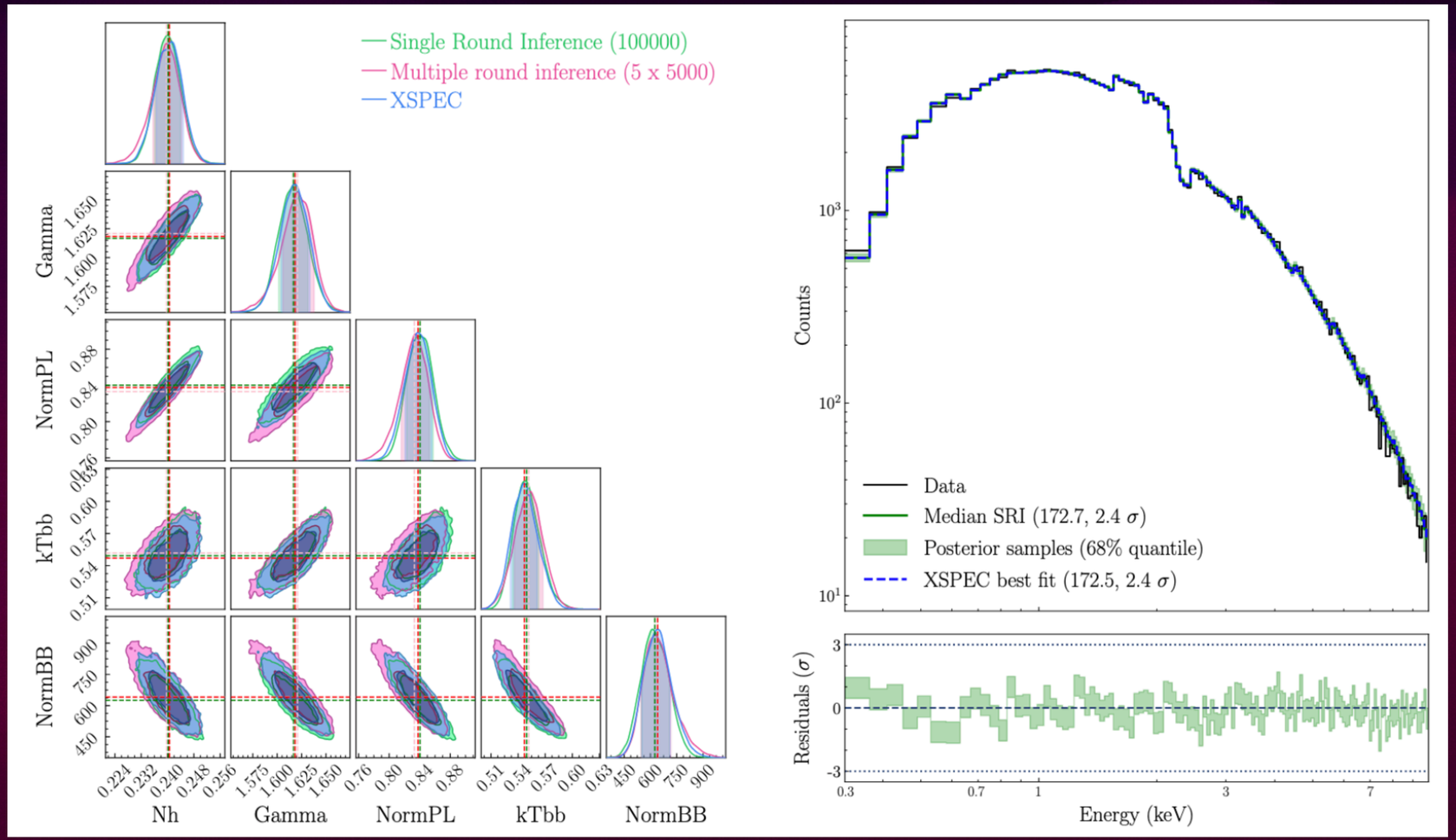
Simulation-based inference

Simulate X-ray spectra and train a neural network to learn the posterior distribution

SIXSA : enabling machine learning to fit X-ray spectra

Simulation-based inference

Simulate X-ray spectra and train a neural network to learn the posterior distribution



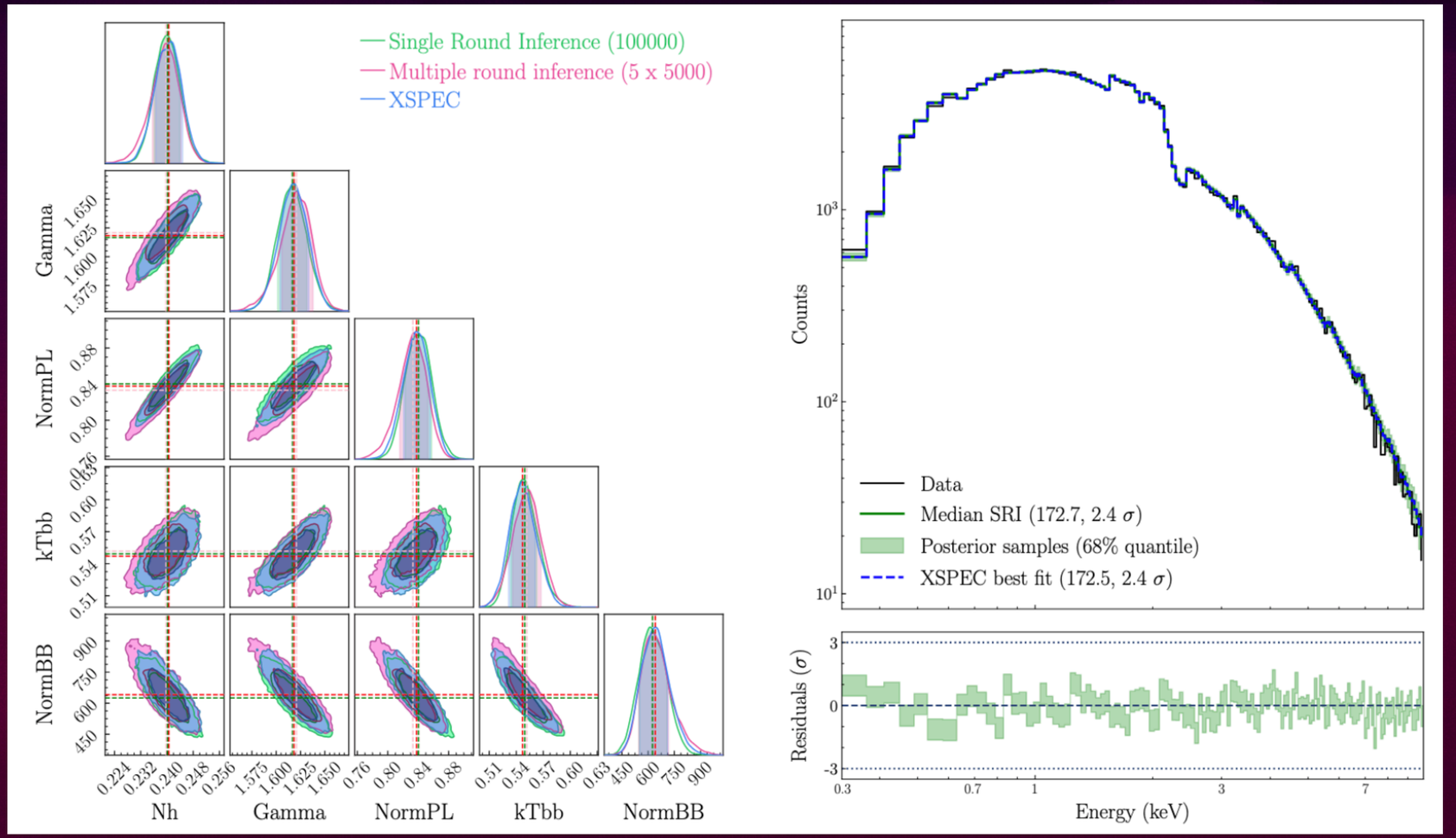
See Barret & Dupourqué (accepted in A&A, arxiv.2401.06061)

SIXSA : enabling machine learning to fit X-ray spectra

Simulation-based inference

Simulate X-ray spectra and train a neural network to learn the posterior distribution

- Tested both on simulated and observed data
- Resilient to local minima down to the Poisson regime
- Order of magnitude faster than traditional approaches, especially when working with hundreds of spectra



See Barret & Dupourqué (accepted in A&A, arxiv.2401.06061)

Check the repositories and star us!
We are awaiting your feedbacks

jaxspec

https://github.com/renecotyfanboy/jaxspec

Official release in ~ a month
(Dupourqué & al. to be sub.)

SIXSA

https://github.com/dbxifu/sixsa

Accepted in A&A
(Barret & Dupourqué 2024)

Thank you for your attention !