Astronomical Laser Frequency Combs for fundamental physics and cosmology

Pushing boundaries on precision and accuracy

Dinko Milaković, Spectral Fidelity conference, Firenze 2023

Scientific projects and measurables

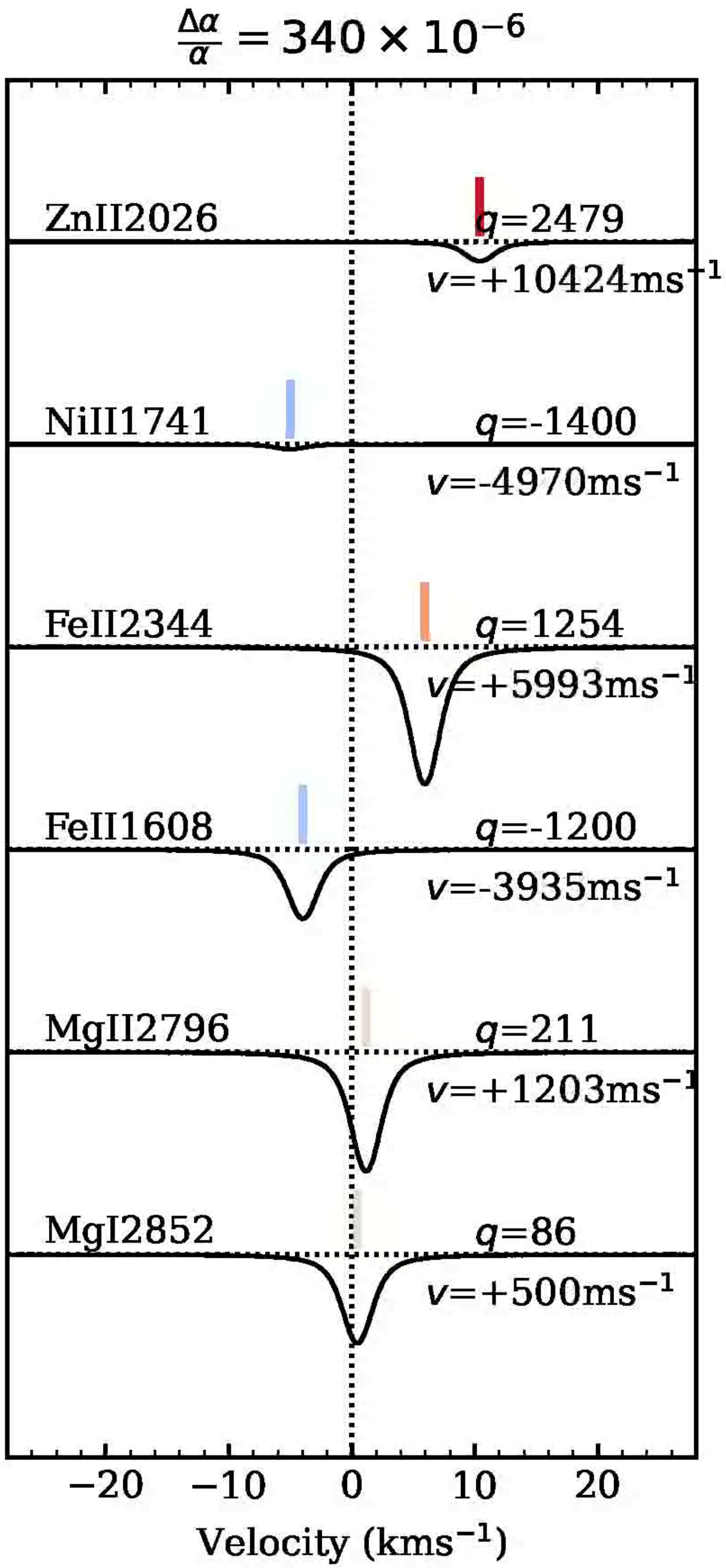
1. **Studies of exoplanets**
   - Measurable: the collective radial velocity of an ensemble of stellar absorption features. Shifts are measured between observations taken at different times (cadence ≲years).
2. **Measurements of fundamental constants**
   - Measurable: a set of relative shifts for an ensemble of absorption lines. Shifts are different for each atomic species considered but are correlated. Shifts are calculated within a single (sometimes coadded) spectrum.
3. **Redshift drift**
   - Measurable: the change in the radial velocity (acceleration) of an absorption feature. Shifts are a function of the line's cosmological redshift and are measured from observations taken at different times (cadence ≲ decades).

The effect of varying alpha

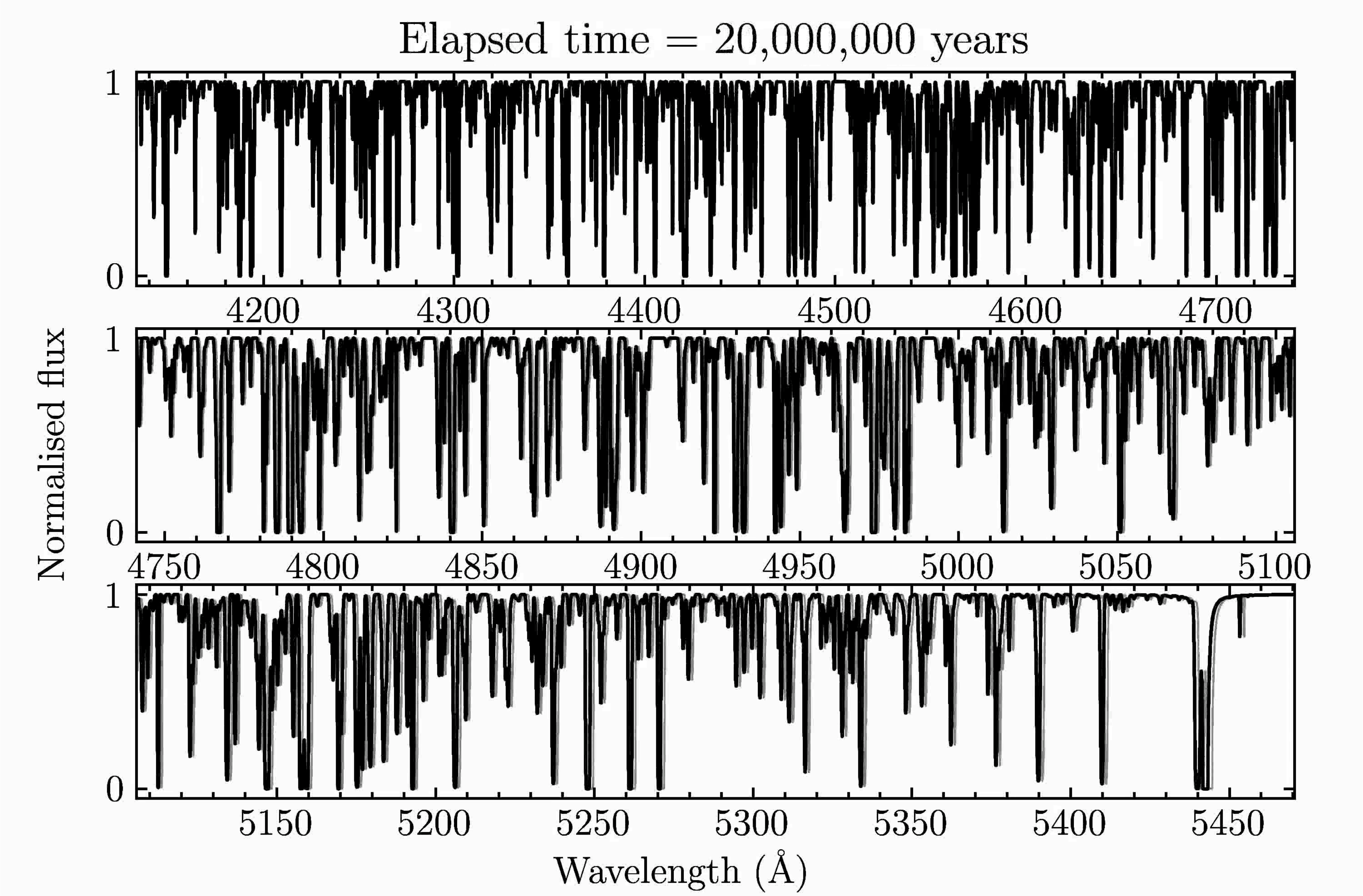
Wavelength shifts, velocity shifts, and change in α are related by:

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta v}{c} \propto q\frac{\Delta\alpha}{\alpha}$$

The broad range in q coefficients means that shift directions and amplitudes are very different for different transitions

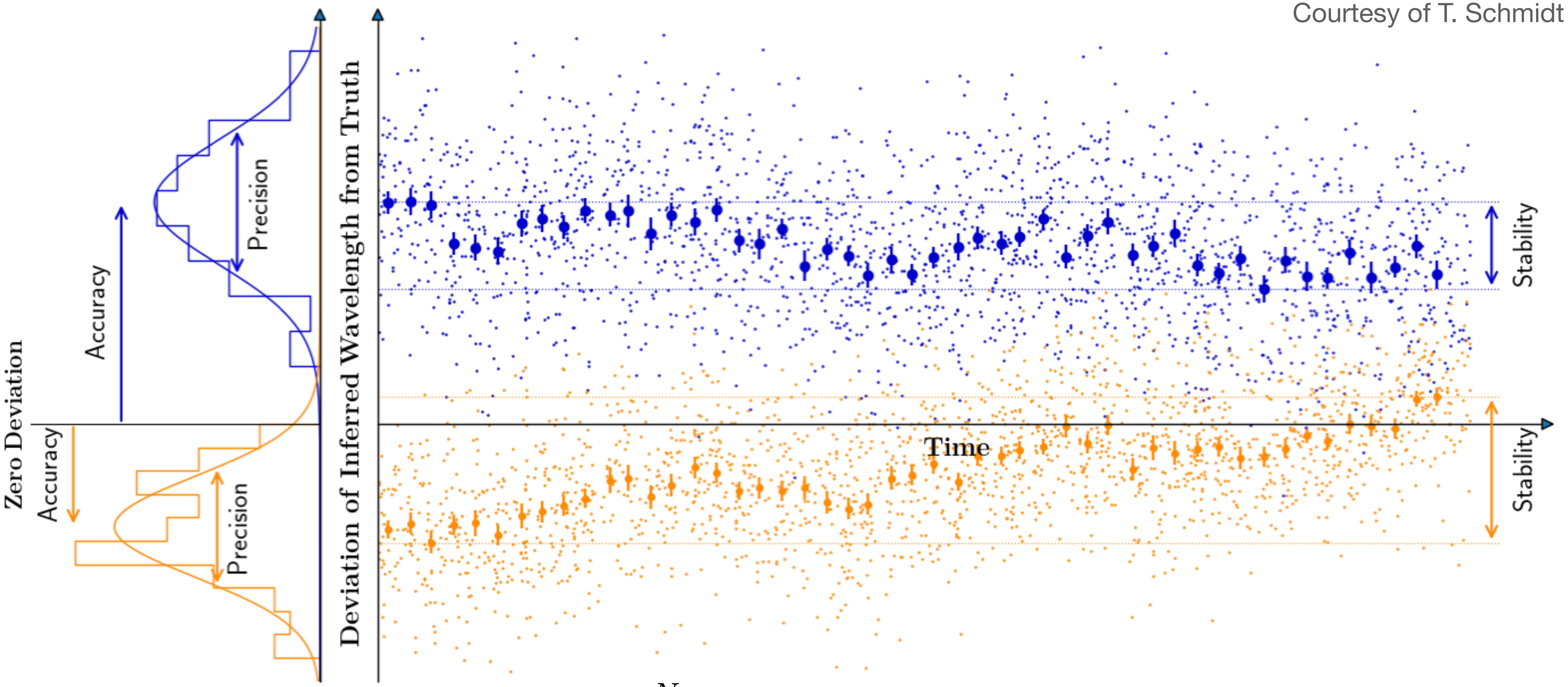


Simulation in ΛCDM



$$\frac{\mathrm{d}z_{|\chi}}{\mathrm{d}t_{obs}} = [1 + z_{|\chi}(t_{obs})]H(t_{obs}) - H(t_{em})$$

Defining accuracy, precision, and stability



$$\lambda = \mathcal{N}(\mu, \sigma^2)$$

$$\mu = \frac{1}{N}\sum_{i=0}^{N} \lambda_i$$

$$\sigma^2 = \frac{1}{N-1}\sum_{i=0}^{N}(\lambda_i - \mu)^2$$

$$\text{accuracy}, a = \mu - \lambda_{true}$$

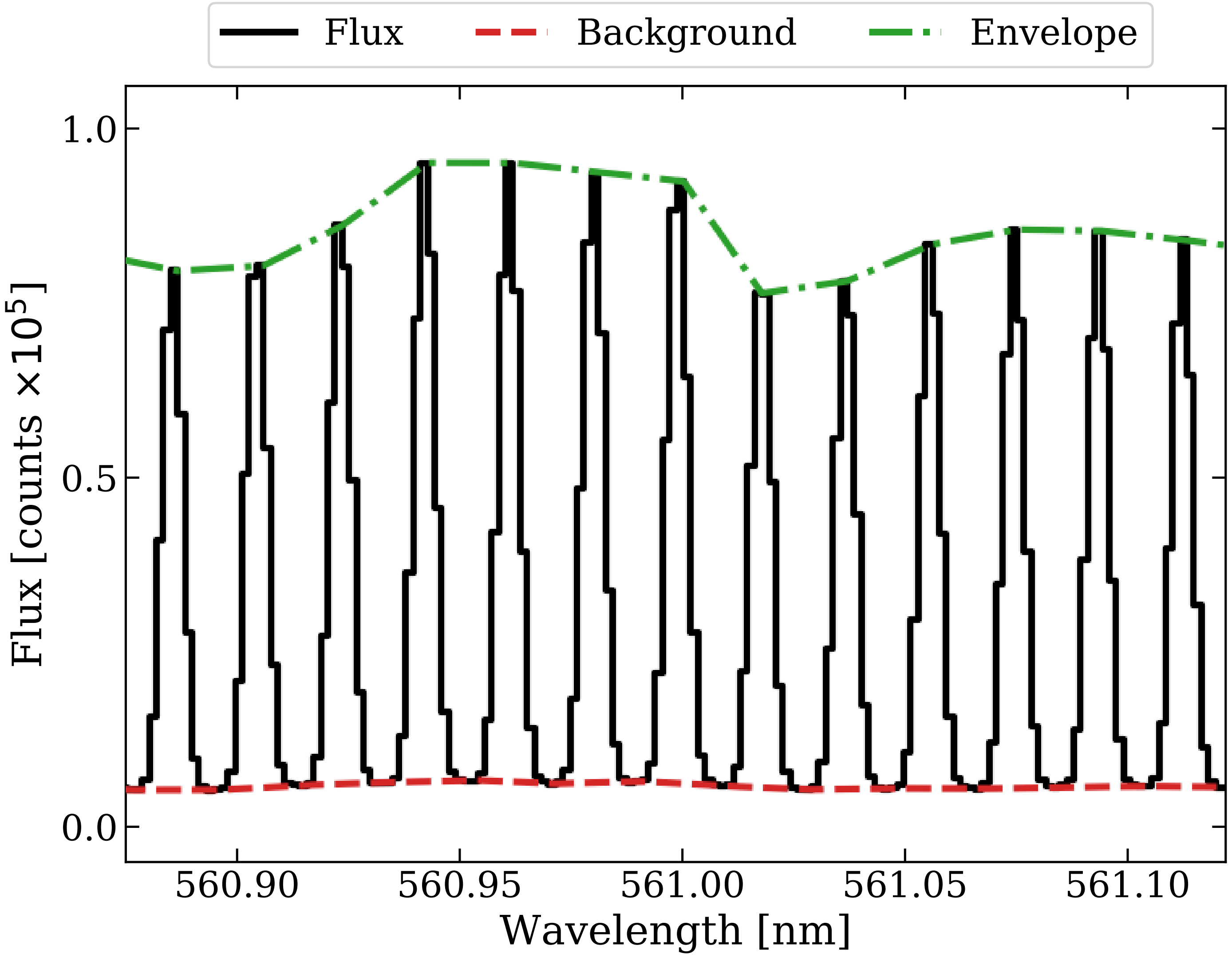
$$\text{precision}, p = \sigma$$

$$\text{stability}, s = \langle a(t) - a(t_0)\rangle_{\text{RMS}}$$

Technical requirements imposed by the science cases

	EXOPLANETS	**FUNDAMENTAL CONSTANTS**	**REDSHIFT DRIFT**
Expected signal	0.1 ms^{-1}/year, periodic	5-30 ms^{-1} relative between lines	0.003 ms^{-1}/year, linear with time
	Over 1000s of lines	For a single line	Over 100s/1000s of lines
Precision (ms^{-1})	0.02	<5	0.01
Accuracy (ms^{-1})	?	<1	?
Instrument stability (ms^{-1}/year)	0.02	1	0.02

Laser Frequency Combs



Frequency of each line given by

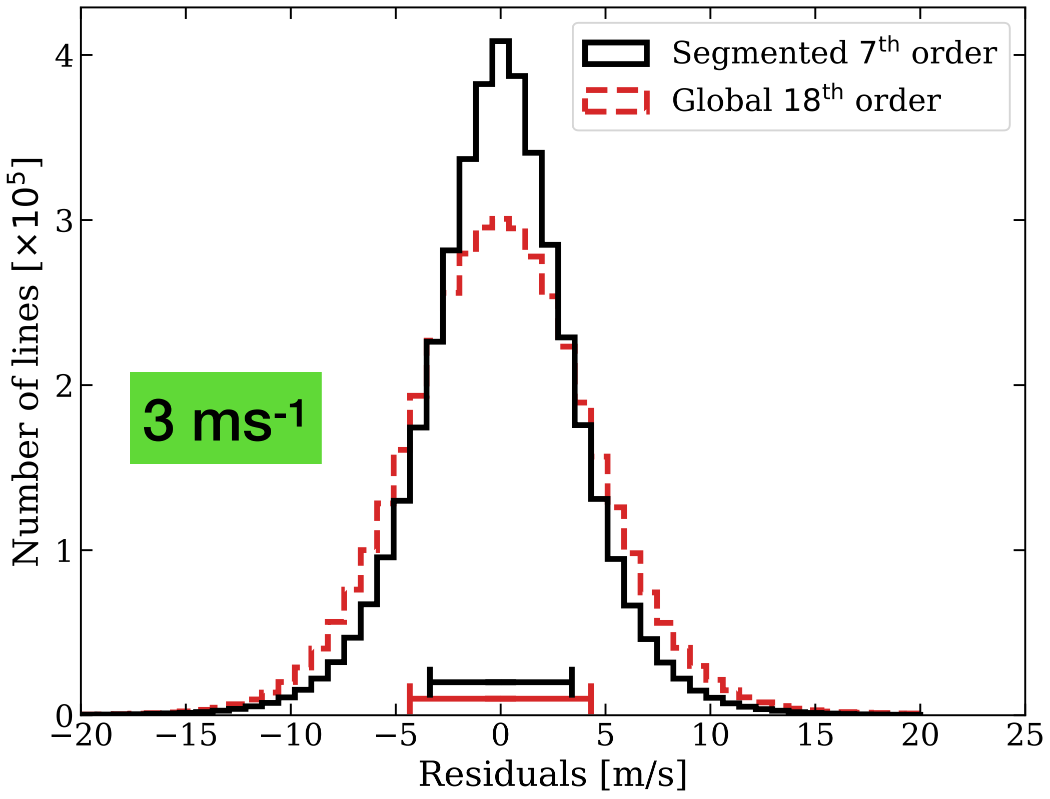
$$f_n = f_0 + n \times f_r$$
$$\lambda_n = c/f_n$$

and known with accuracy 10^{-12}
(<mms^{-1} in velocity units)

Examining λ-calibration residuals*

*the instrumental profiles were assumed to be Gaussian but they are not

HARPS LFC Milaković et al. 2020



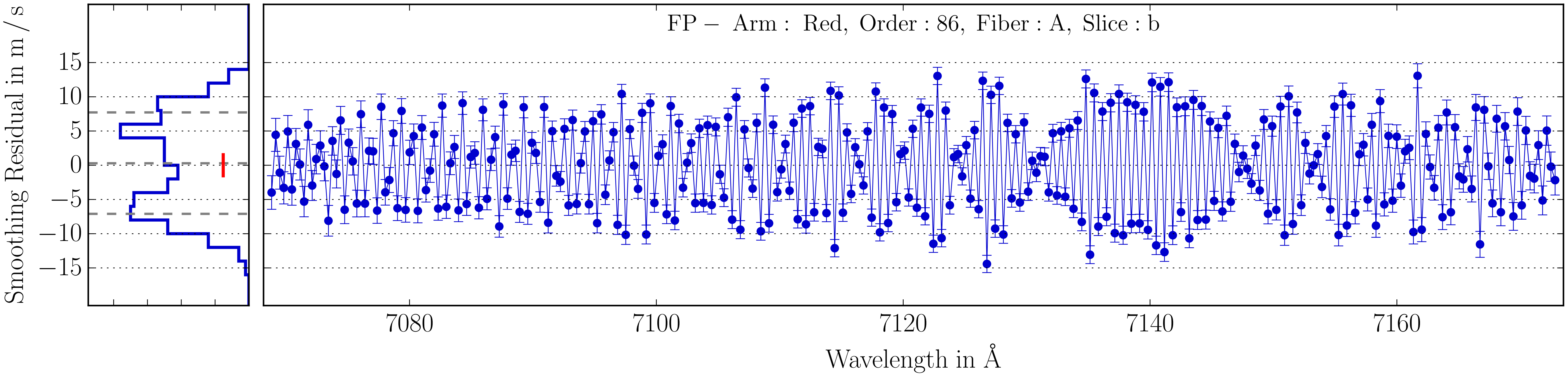
3 ms-1

RMS scatter of the calibration line centres around the best-fit wavelength solution →

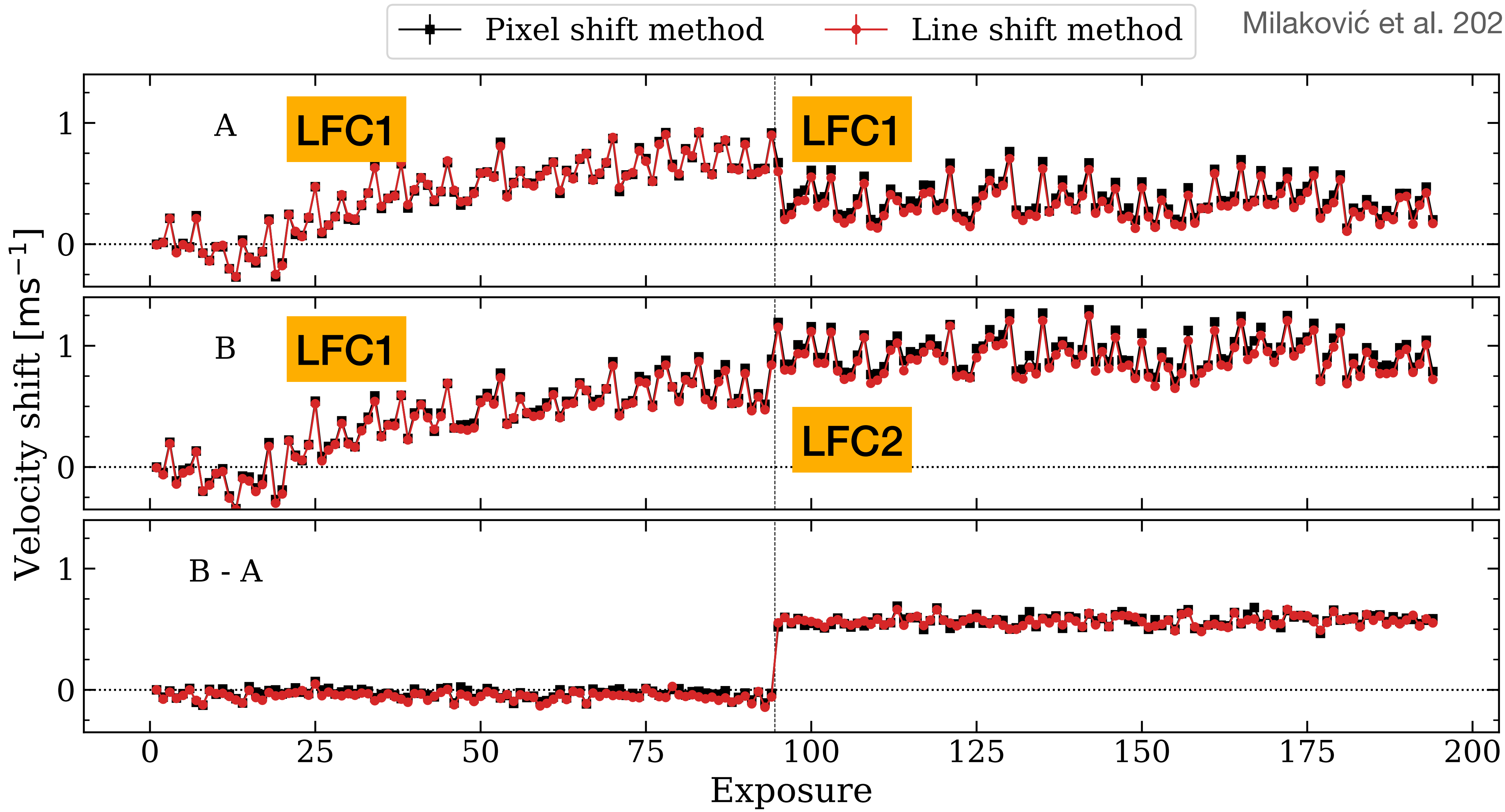
↓

6 ms-1

ESPRESSO FP but a very similar pattern for LFC Schmidt et al. 2021



A worrying result from a comparison of two LFCs



Milaković et al. 2020

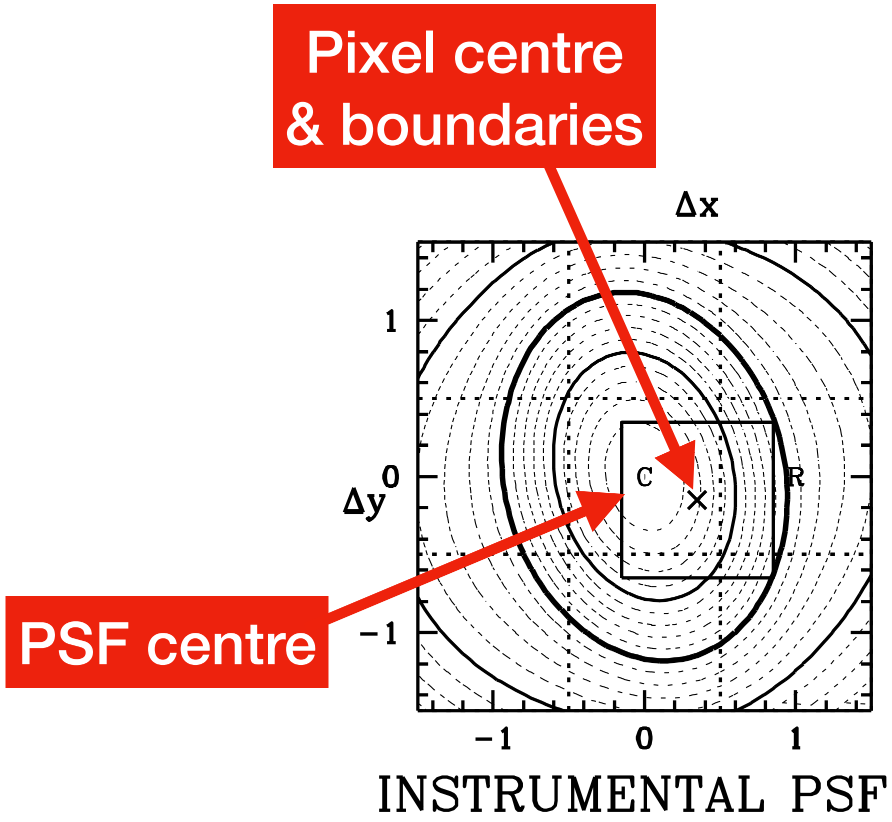
Approximately 50 cms^{-1} difference in the instrumental zero-point

The reason for the effect is unknown (partly flux-dependent).
The interpretation is that the zero-point cannot be measured with accuracy better than 50 cms^{-1} even when LFCs are used

Would have gone unnoticed if two LFCs were not used simultaneously!

Instrumental profile modelling: HARPS

The instrumental profile



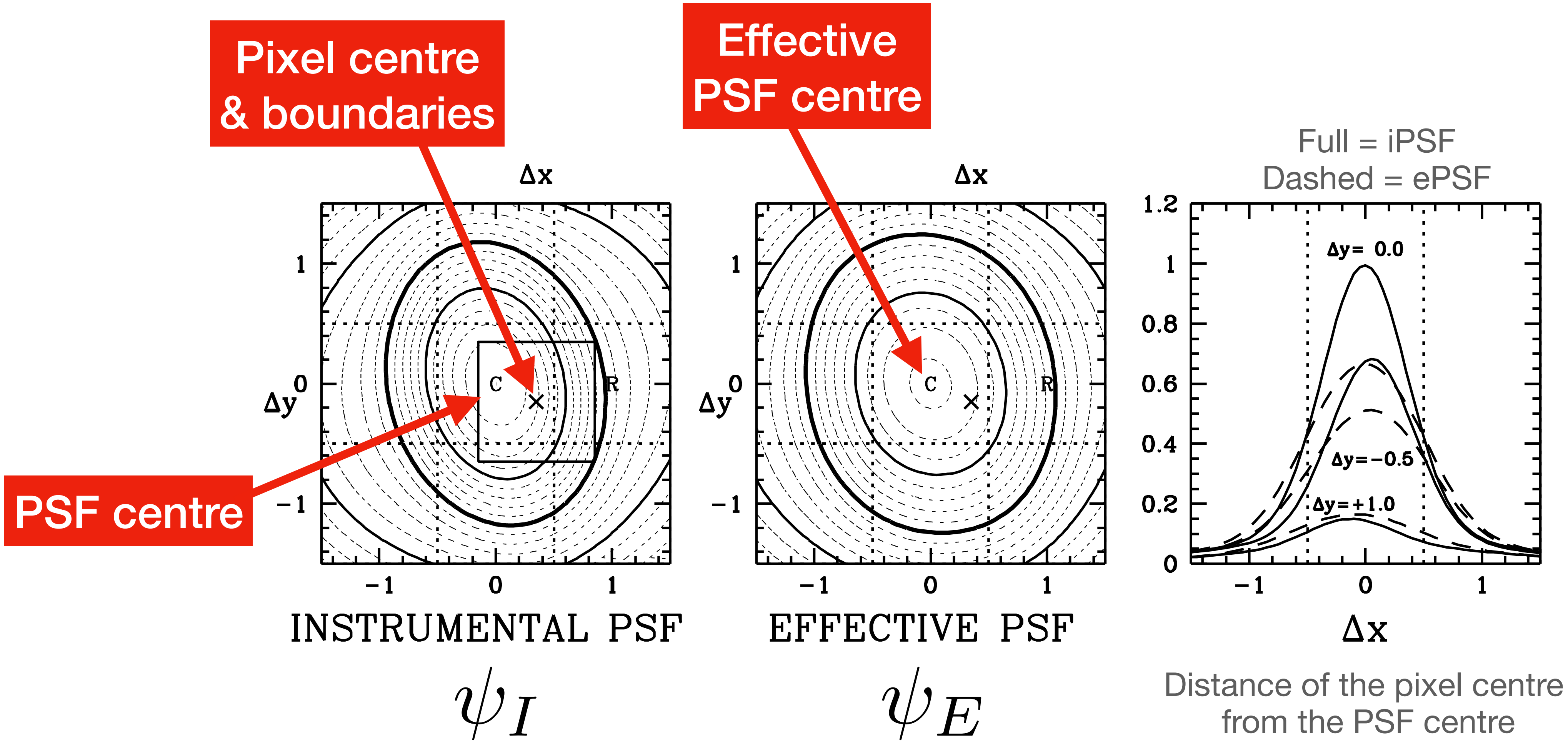
Pixel centre & boundaries

PSF centre

ψ_I

Figure 3 from Anderson & King 2000

The instrumental profile



Pixel centre & boundaries

Effective PSF centre

PSF centre

Full = iPSF
Dashed = ePSF

Distance of the pixel centre from the PSF centre

Figure 3 from Anderson & King 2000

$$\psi_E(\Delta x, \Delta y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathcal{R}(-x, -y) \psi_I(\Delta x - x, \Delta y - y)\, \mathrm{d}x \mathrm{d}y$$

The math and the advantages of the effective IP

Anderson & King 2000

The value of the effective PSF is the integral
of the instrumental PSF over a pixel centred at the some location

$$\psi_E(\Delta x, \Delta y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \underset{\uparrow}{\mathcal{R}}(-x, -y)\psi_I(\Delta x - x, \Delta y - y)\,\mathrm{d}x\mathrm{d}y$$

Intra-pixel response function

The observed flux in a pixel centred at i from a line source located at x$_*$

$$F_{ij} = \underset{\uparrow}{f_*}\psi_E(i - \underset{\nwarrow}{x_*}, j - y_*) + \underset{\nwarrow}{B_{ij}}$$

Source brightness   Source position   Background

The functional form of the effective IP can be estimated from

$$\hat{\psi}(\Delta x, \Delta y) = \frac{F_{ij} - B_{ij}}{f_*}$$

If x_*, y_*, f_*, B_{ij} are known

Advantages

1. No integration is required, simply evaluate the effective IP at the pixel centre
2. No need to know the true instrumental profile (it is never directly observable in any case)
3. Naturally takes into account the unknown intra-pixel response function

The effective IP for 1d

The value of the effective PSF is the integral
of the instrumental PSF over a pixel centred at the some location

$$\psi_E(\Delta x, \Delta y) = \int_{-\infty}^{+\infty} \cancel{\int_{-\infty}^{+\infty}} \mathcal{R}(-x, \cancel{-y})\,\psi_I(\Delta x - x, \cancel{\Delta y - y})\,\mathrm{d}x\cancel{\mathrm{d}y}$$

Intra-pixel response function

The observed flux in a pixel centred at i from a line source located at x_*

$$F_{i\cancel{j}} = f_*\psi_E(i - x_*, \cancel{j - y_*}) + B_{i\cancel{j}}$$

Source brightness Source position Background

The functional form of the effective IP can be estimated from

$$\hat{\psi}(\Delta x, \cancel{\Delta y}) = \frac{F_{i\cancel{j}} - B_{i\cancel{j}}}{f_*}$$

If $x_*, \cancel{y_*}, f_*, B_{i\cancel{j}}$ are known

Advantages

1. No integration is required, simply evaluate the effective IP at the pixel centre
2. No need to know the true instrumental profile (it is never directly observable in any case)
3. Naturally takes into account the unknown intra-pixel response function

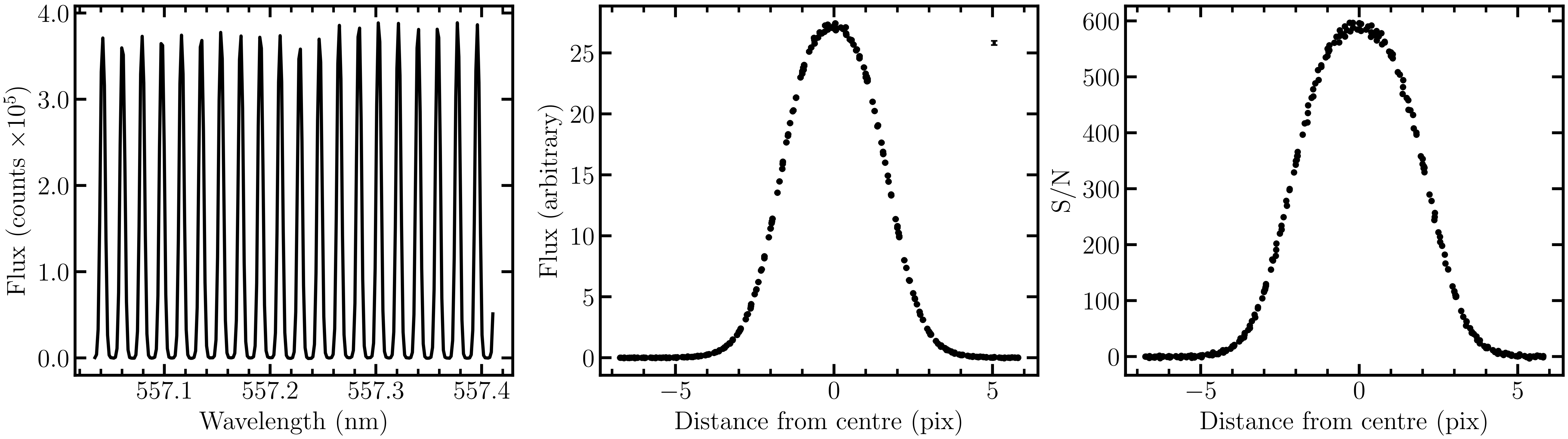
Gaussian IP approximation

$$I(x; A, \mu, \sigma) = \frac{A}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right].$$

$$x_* = \mu$$

$$f_* = A\sigma\sqrt{2\pi}$$

I divided each echelle order into 16 segments (256 pixels)
and stacked the normalised lines on top of their Gaussian centres



Echelle order 50, segment 10/16

Gaussian Process: getting the most likely IP

Given pairs of data points {x,y} with noise ϵ, find the most likely function f(x)=y+ϵ

Function f(x) is sampled from a multivariate normal distribution

$$p(\mathbf{f}) = \mathcal{N}\left(\mathbf{m}, \mathbf{K}\right),$$

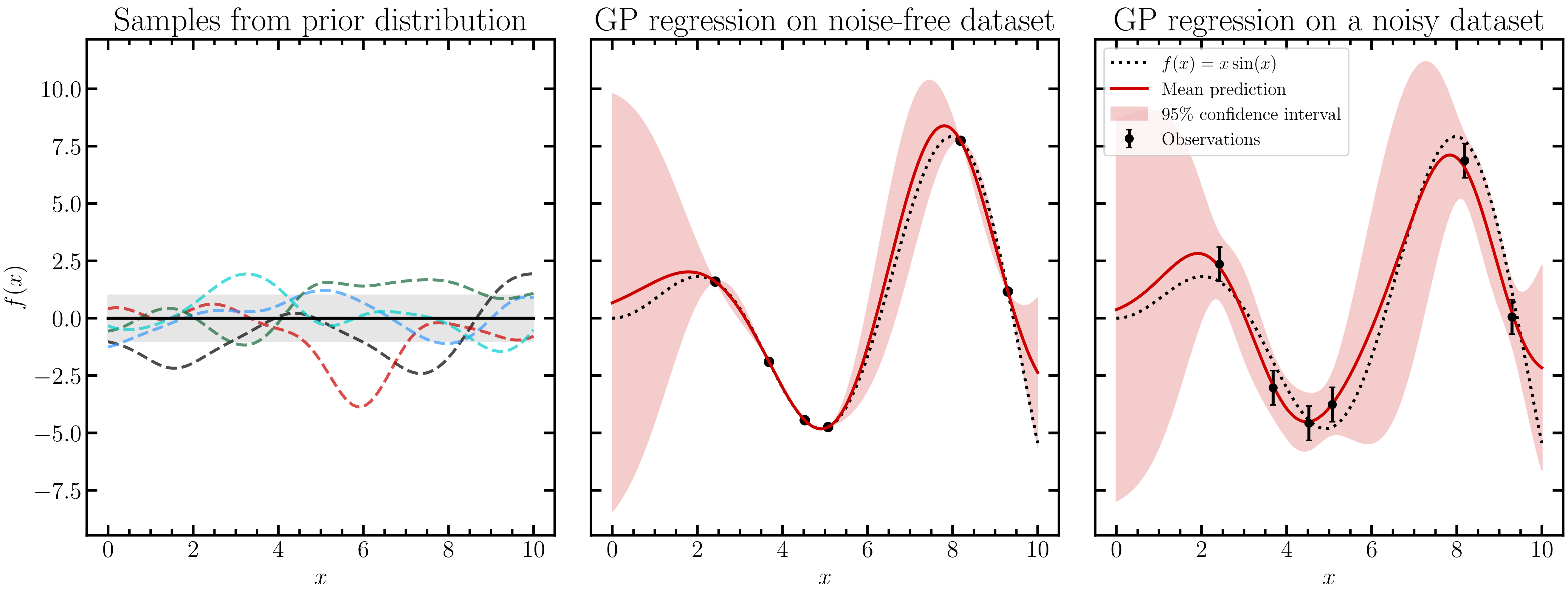
where

$$m_i = m(x_i; \theta),$$ is the mean function

$$K_{ij} = k(x_i, x_j; \phi)$$ is the covariance matrix

Likelihood of the data as a function of hyperparameters

$$\mathcal{L}(\theta, \psi) = \mathcal{N}(\mathbf{y}; \mathbf{m}, \mathbf{K} + \mathrm{diag}(\{\sigma_i\}))$$



Plots produced using code from https://scikit-learn.org/stable/auto_examples/gaussian_process/plot_gpr_noisy_targets.html

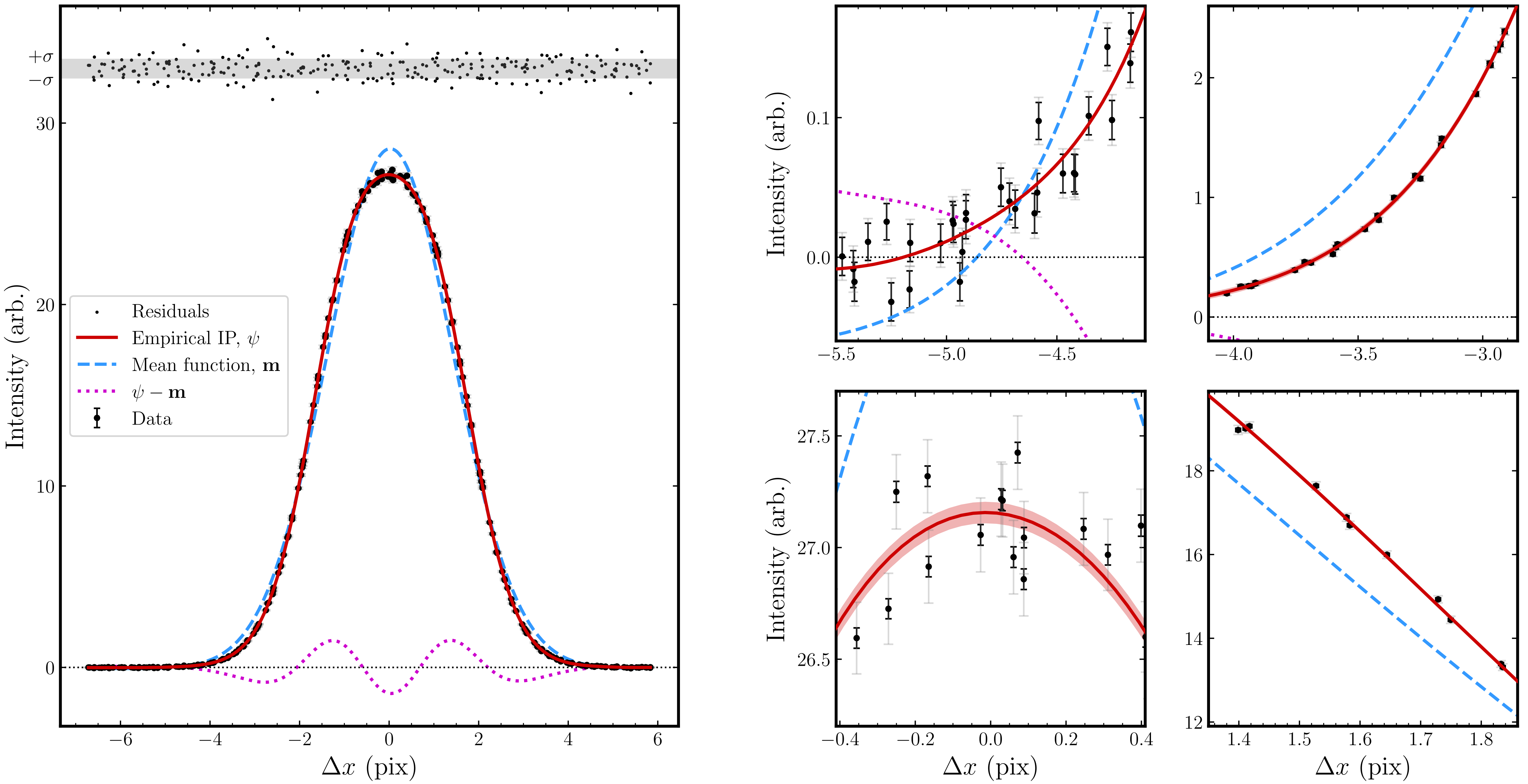
IP model for a single segment

Mean function

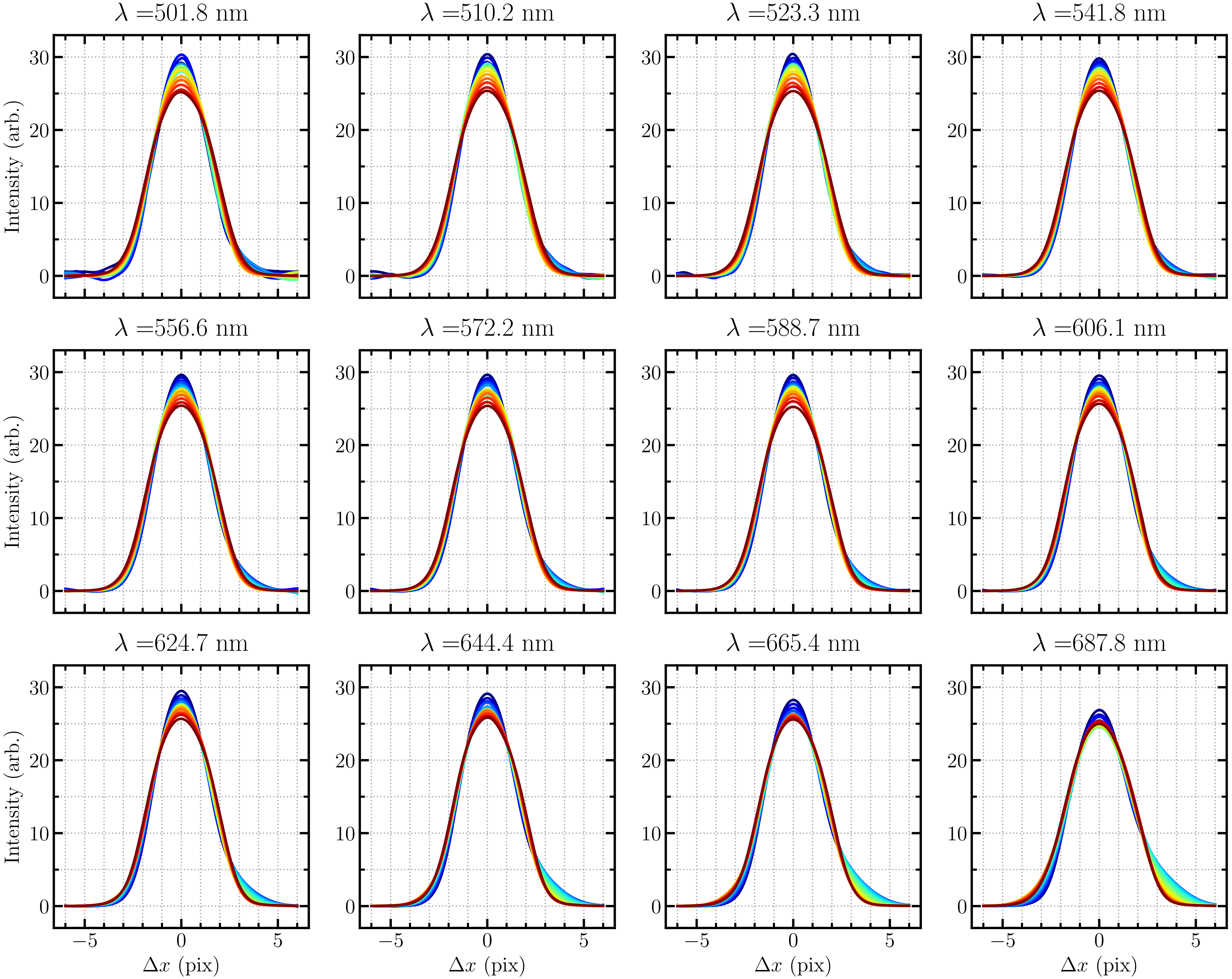
$$m(x;\theta) = \underline{A}\,\mathcal{N}(x;\underline{\mu},\underline{\sigma}) + \underline{y_0}$$

Covariance matrix

$$k_{\mathrm{SE}}(x_i, x_j;\phi) = \underline{a}^2 \exp\left(-\frac{|x_i - x_j|^2}{2\underline{l}^2}\right)$$



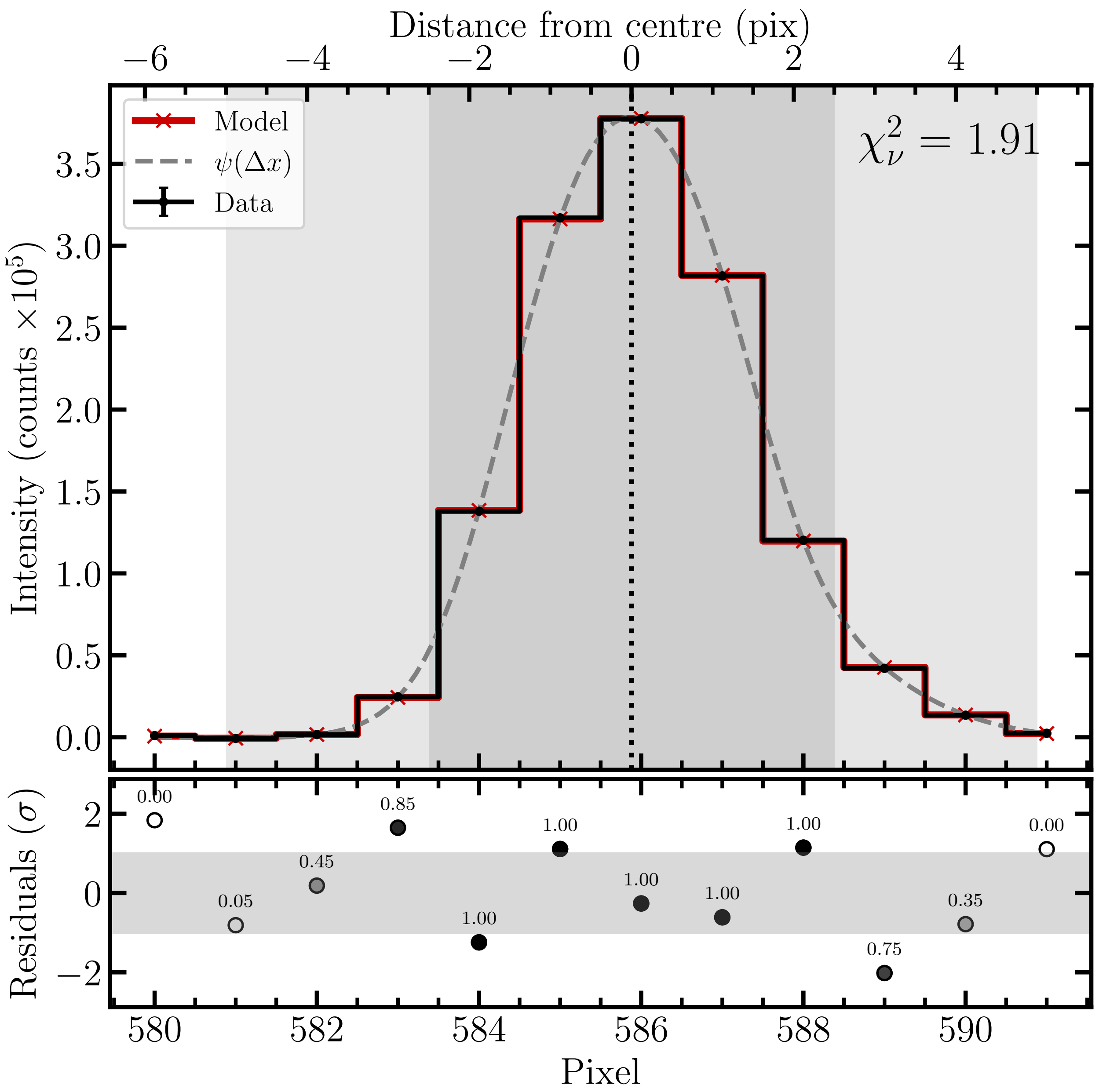
HARPS IP in pixel space



Fit comparison for a single LFC line

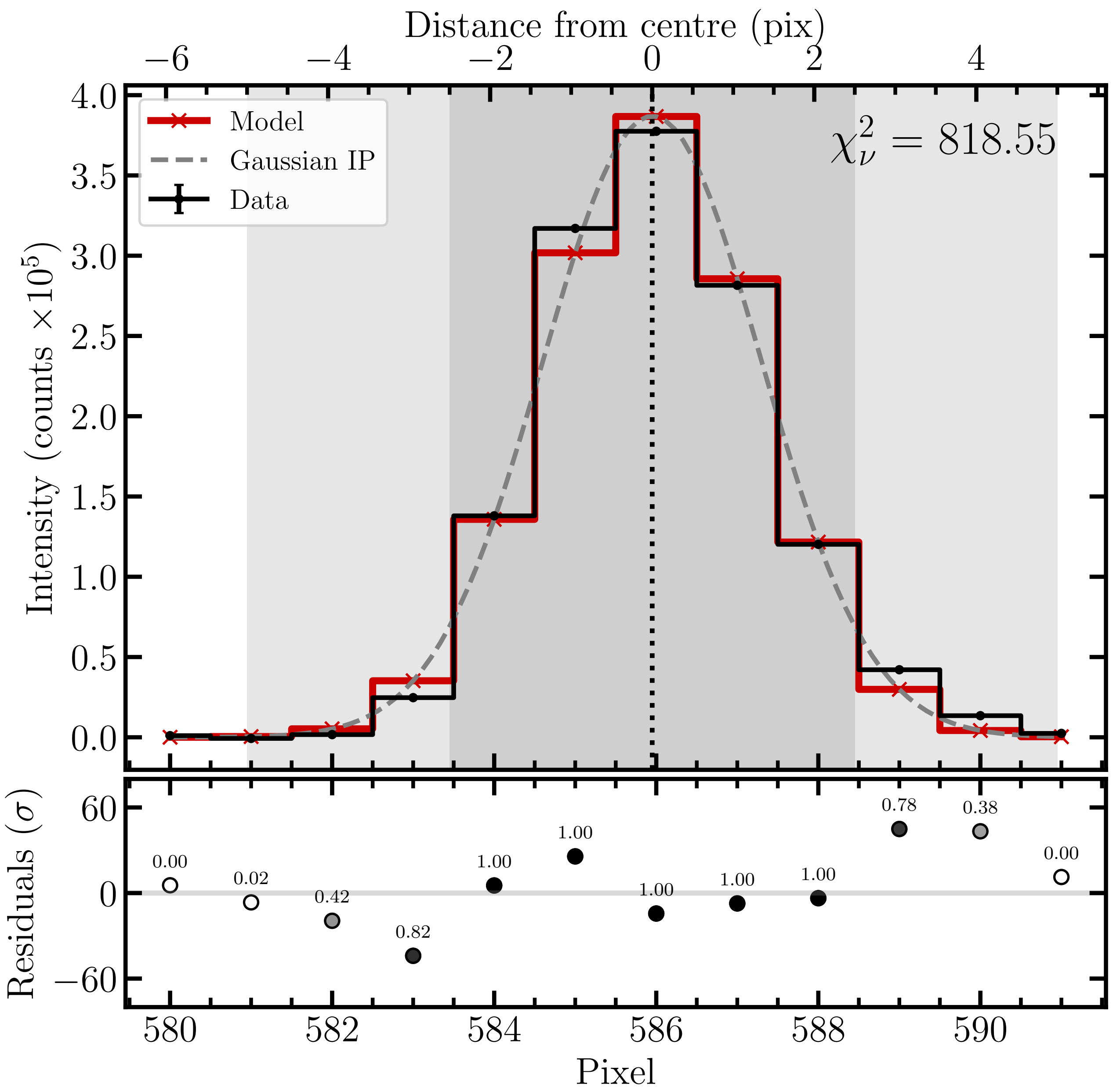
Empirical HARPS IP

$$I(x) = \underline{A}_* \psi\left(\underline{\omega}(x - \underline{x}_*)\right)$$



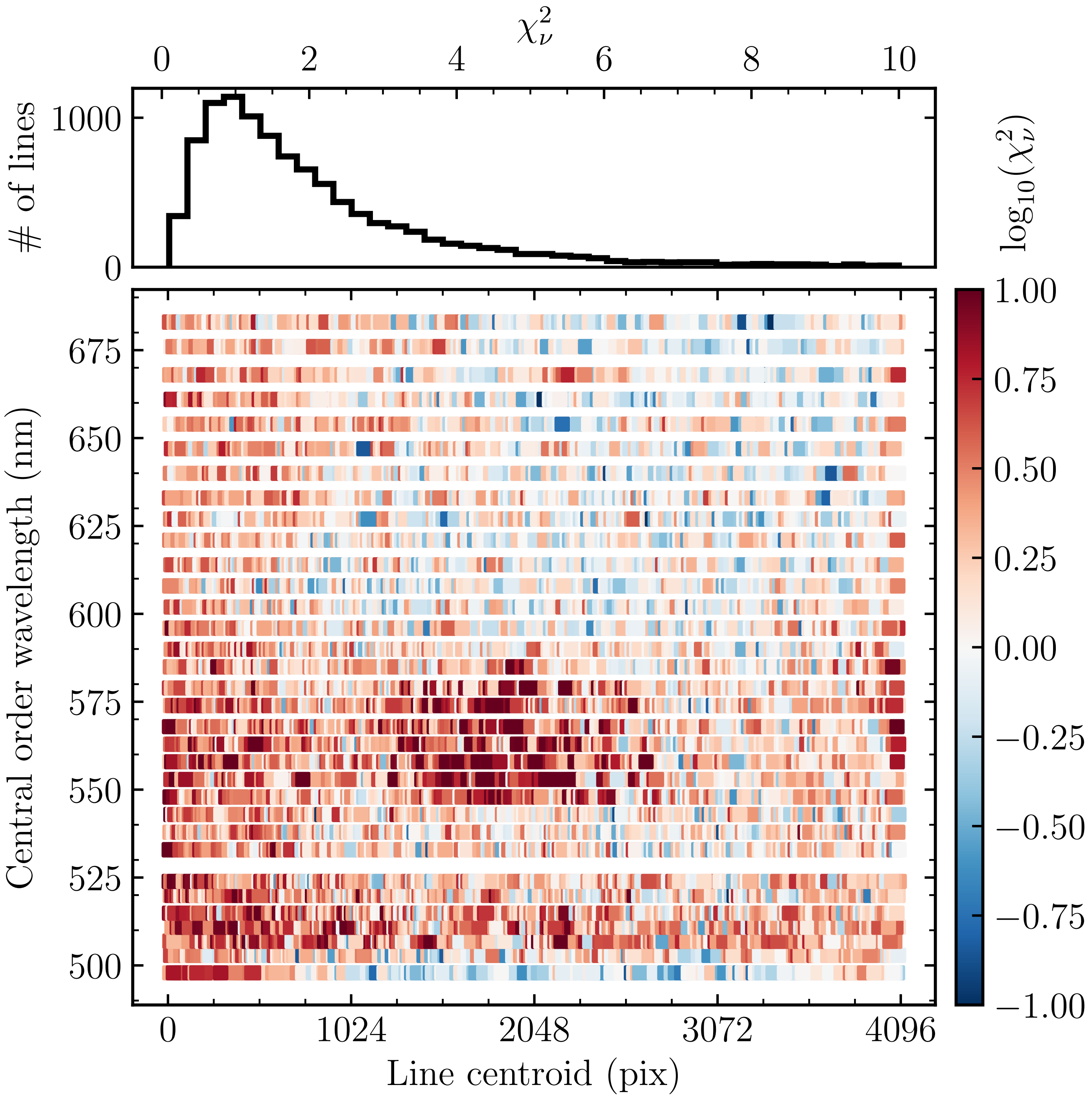
Gaussian IP

$$I(x) = \frac{\underline{A}}{\underline{\sigma}\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x - \underline{\mu}}{\sigma}\right)^2\right]$$



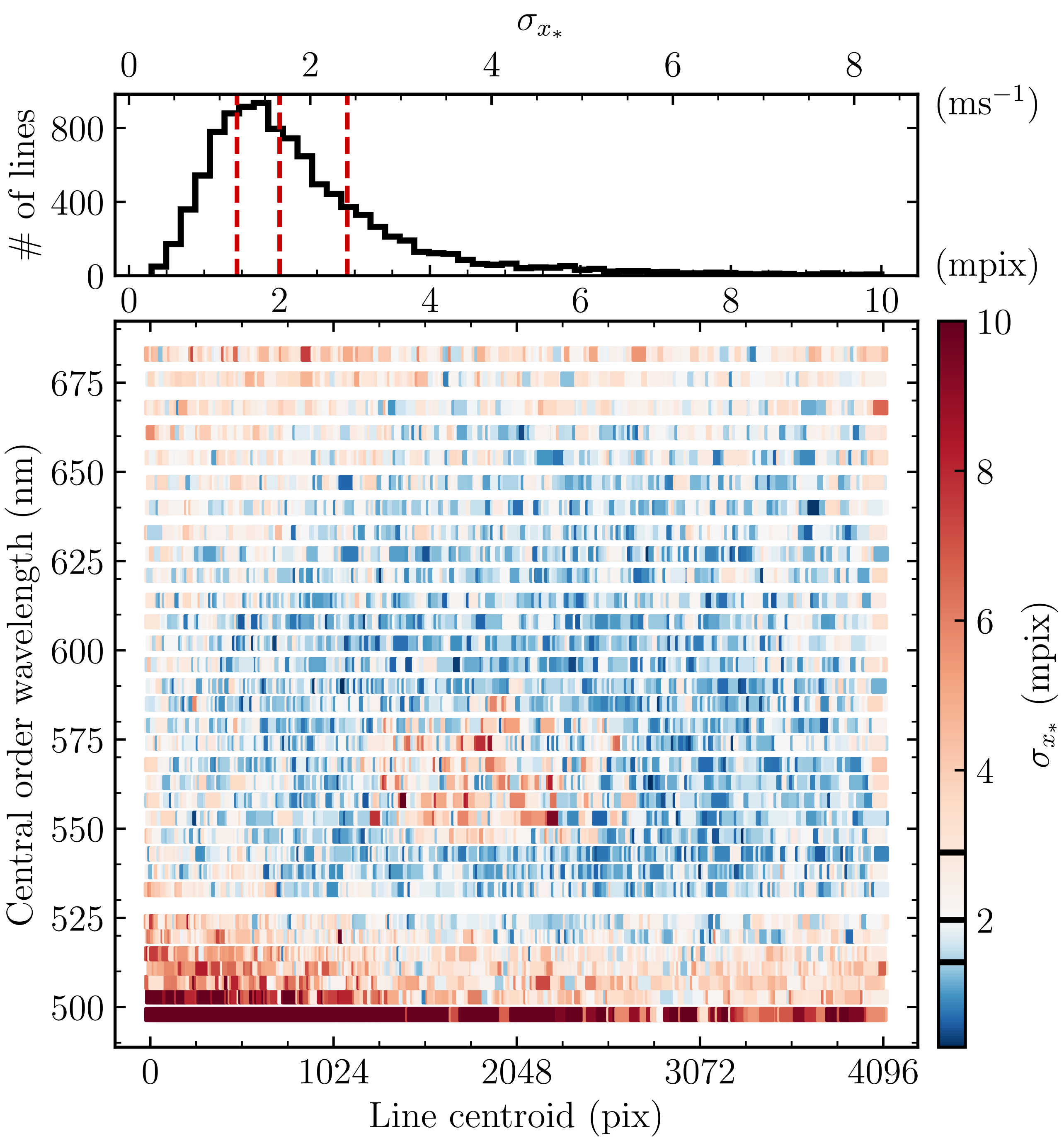
Fit quality is excellent everywhere

Colour is logarithm(!) of chi-squared
(a reasonably good fit everywhere)



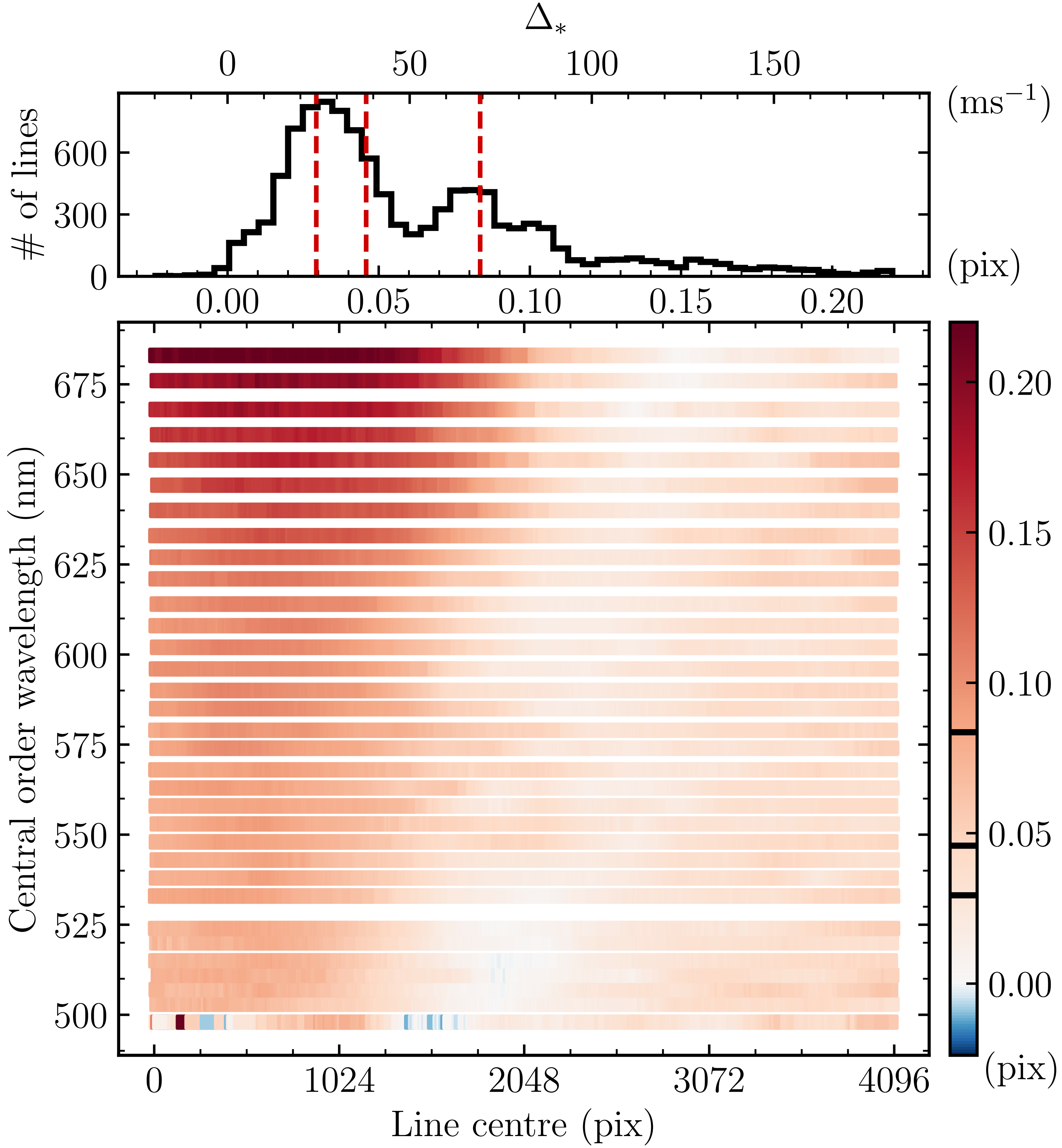
White colour set to $\chi^2_\nu = 1$

Colour is uncertainty on line positions
(consistent with photon noise limit)



White colour set to distribution median

Gaussian IP centres - empirical IP centres (astrocomb)

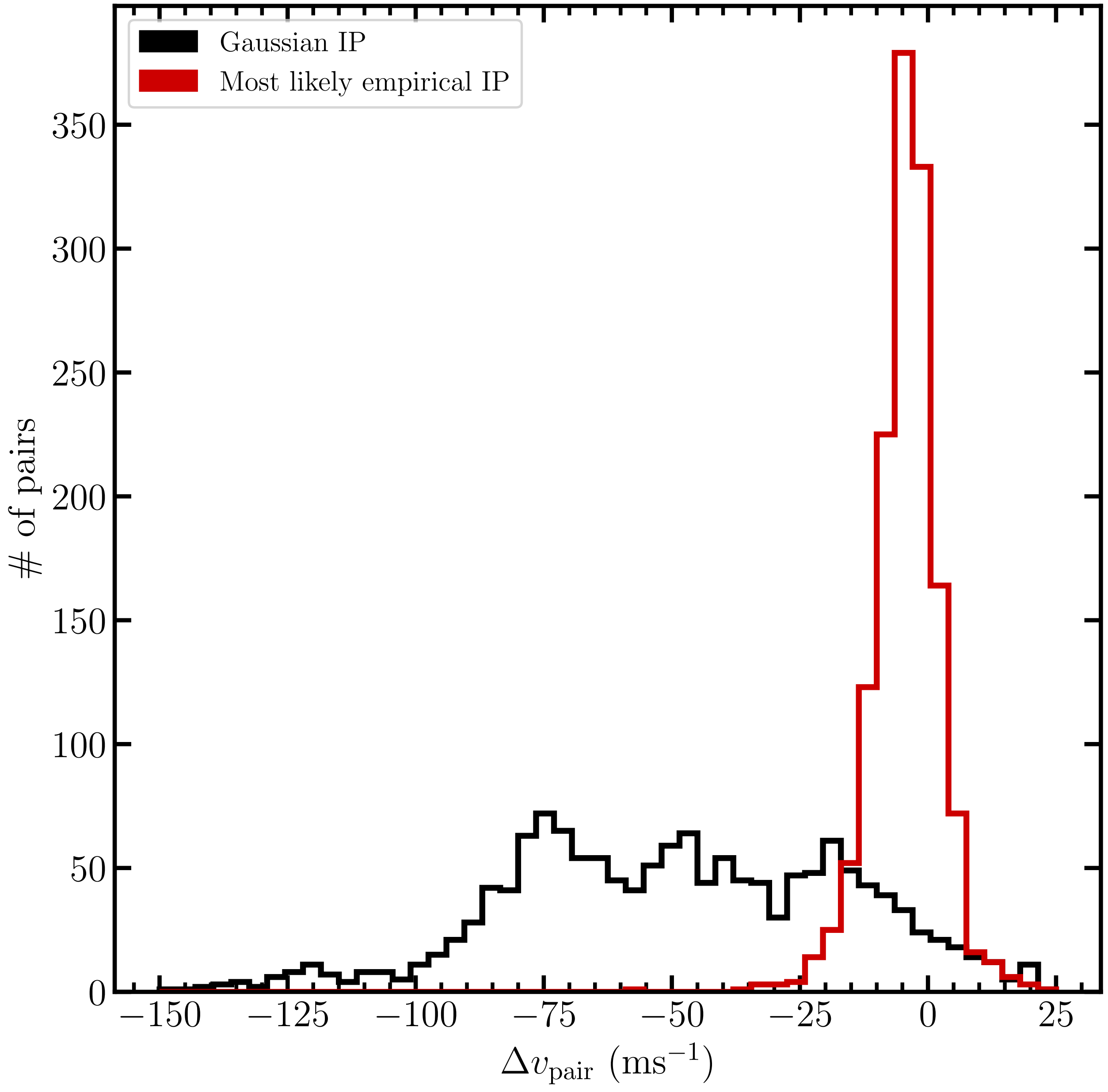


- Zero difference (white colour) rarely observed
- Differences up to 0.22 pix (approx 180 ms^{-1})
- Correlations across the detector

Measuring the wavelengths of lines in the spectral overlap regions

- 1440 LFC modes were observed twice
- Wavelength of each line was measured by fitting it using the empirical IP (IP in velocity space) in the λ-calibrated spectrum
- Velocity shift between two measured wavelengths

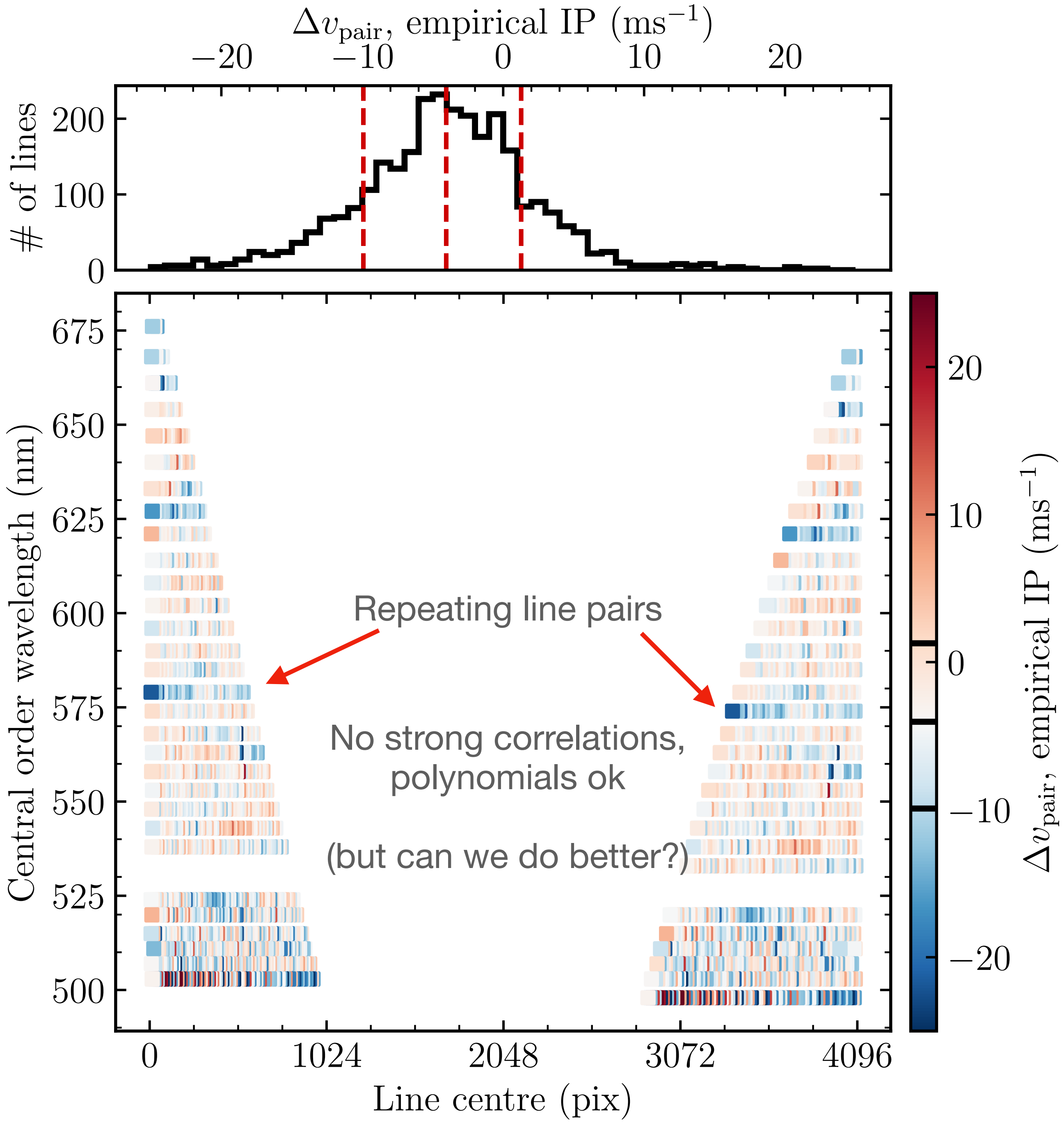
$$\frac{\Delta v_{\mathrm{pair}}}{c} = \frac{\lambda_{*,2} - \lambda_{*,1}}{\lambda_{\mathrm{LFC}}}$$



	Median v (ms^{-1})	RMS v (ms^{-1})	70% |v| (ms^{-1})
Empirical IP	-4.04	6.92	7.32
Gaussian IP	-49.28	32.43	69.20

Repeating line pair velocity shifts on the detector

Empirical HARPS IP

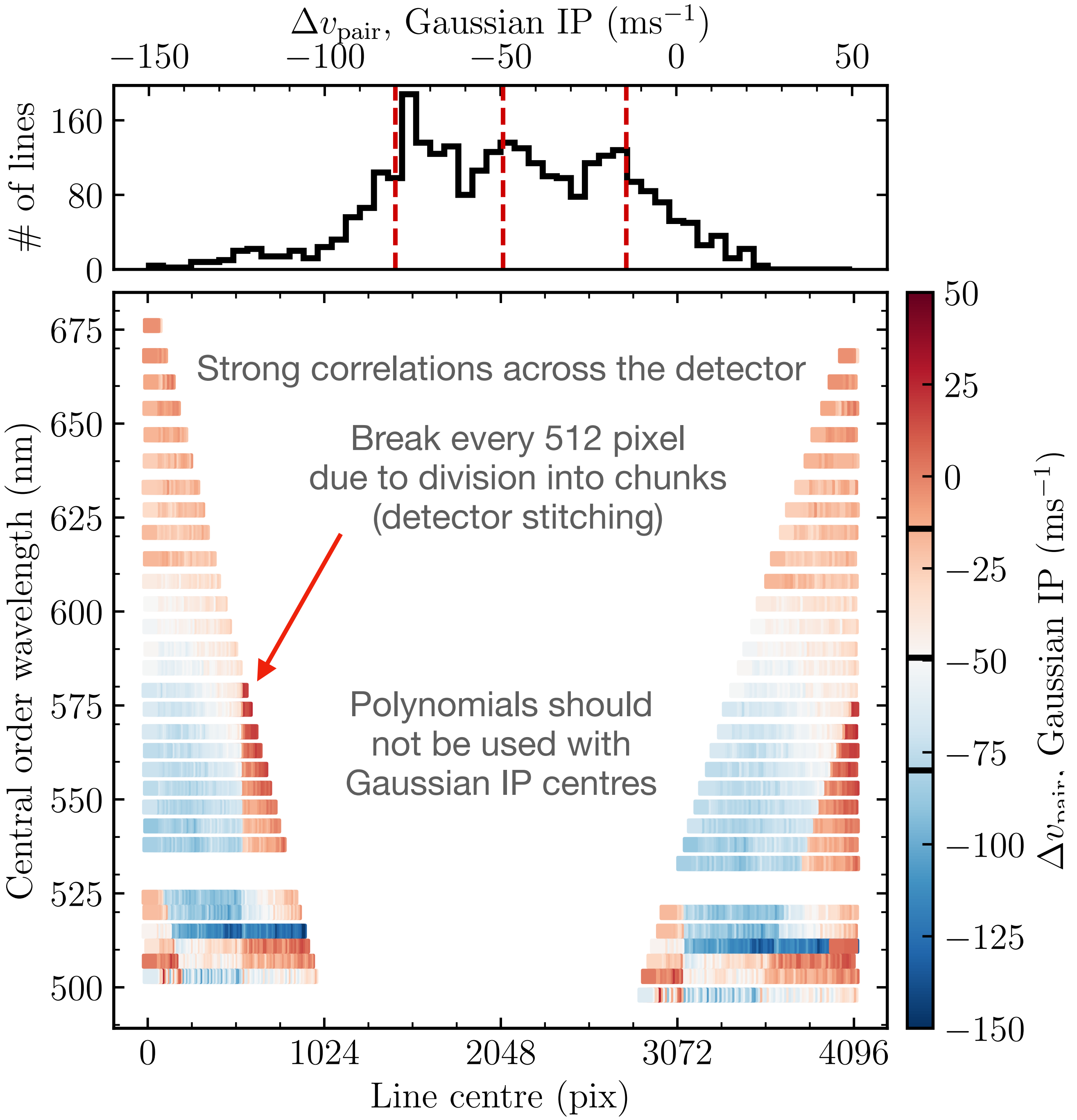


Repeating line pairs

No strong correlations, polynomials ok

(but can we do better?)

Gaussian IP



Strong correlations across the detector

Break every 512 pixel due to division into chunks (detector stitching)

Polynomials should not be used with Gaussian IP centres

Results

- The HARPS IP is asymmetric everywhere in the λ range of the astrocomb (in both fibres)
- The asymmetry varies quickly and strongly as a function of position on the detector (fibre B more asymmetric)
- Line centres measurements may differ up to 0.22 pix between Gaussian and empirical IP
- The average shift between the wavelength calibrations determined from Gaussian IP and empirical IP centres is -51 ms^{-1} but can be as large as -180 ms^{-1}
- If the empirical IPs are correct, and the wavelength calibration derived from them is accurate, using Gaussian IPs for line fitting and calibration introduces both short and long scale distortions in the HARPS wavelength scale as large as 180 ms^{-1}
- Accuracy for a single line is not better than 7 ms^{-1} even when empirical IPs are used

Open questions

- Should orders be merged given the shifts between the repeating lines?

- What parameters does the IP depend on (charge transfer, etc.)? Temporal evolution?

- How do we re-establish the zero-point of the instrument **accurately** to enable long term studies? Tunable combs!

- Redundancy? Two LFCs operated simultaneously? LFC+I_2 absorption cell?

- Should we go to 2D, avoiding spectral extraction altogether? E.g. forward modelling using ray-tracing models

- Next: neural networks to reconstruct the 2D IP as a function of relevant parameters