

High-resolution spectroscopy for exoplanet characterisation

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What did we learn from yesterday's session?

Studying exoplanet atmospheres is useful to understand their nature, formation, evolution, and habitability

High-resolution spectroscopy:

Amplifies signals through cross correlation

Robustly identifies species

Filters out stationary spectral components (telluric lines)

Measure masses and inclination of non-transiting planets

A couple of dozen hot Jupiters have atoms and/or molecules detected at high spectral resolution

Open questions for this lecture:

Can the method be applied on large scale?

What's the effect of the stellar spectrum?

How do we assess the statistical significance of the cross correlation signals?

From demonstration to comparative exo-planetology

How can we increase the S/N of the cross correlation function?

$$\left. \frac{S}{N} \right|_{\text{CCF}} \propto \frac{N_{\gamma, P}}{\sqrt{N_{\gamma, \star}}} \sqrt{n_{\text{lines}}}$$

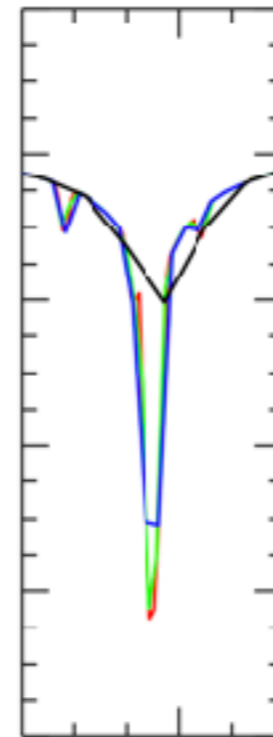
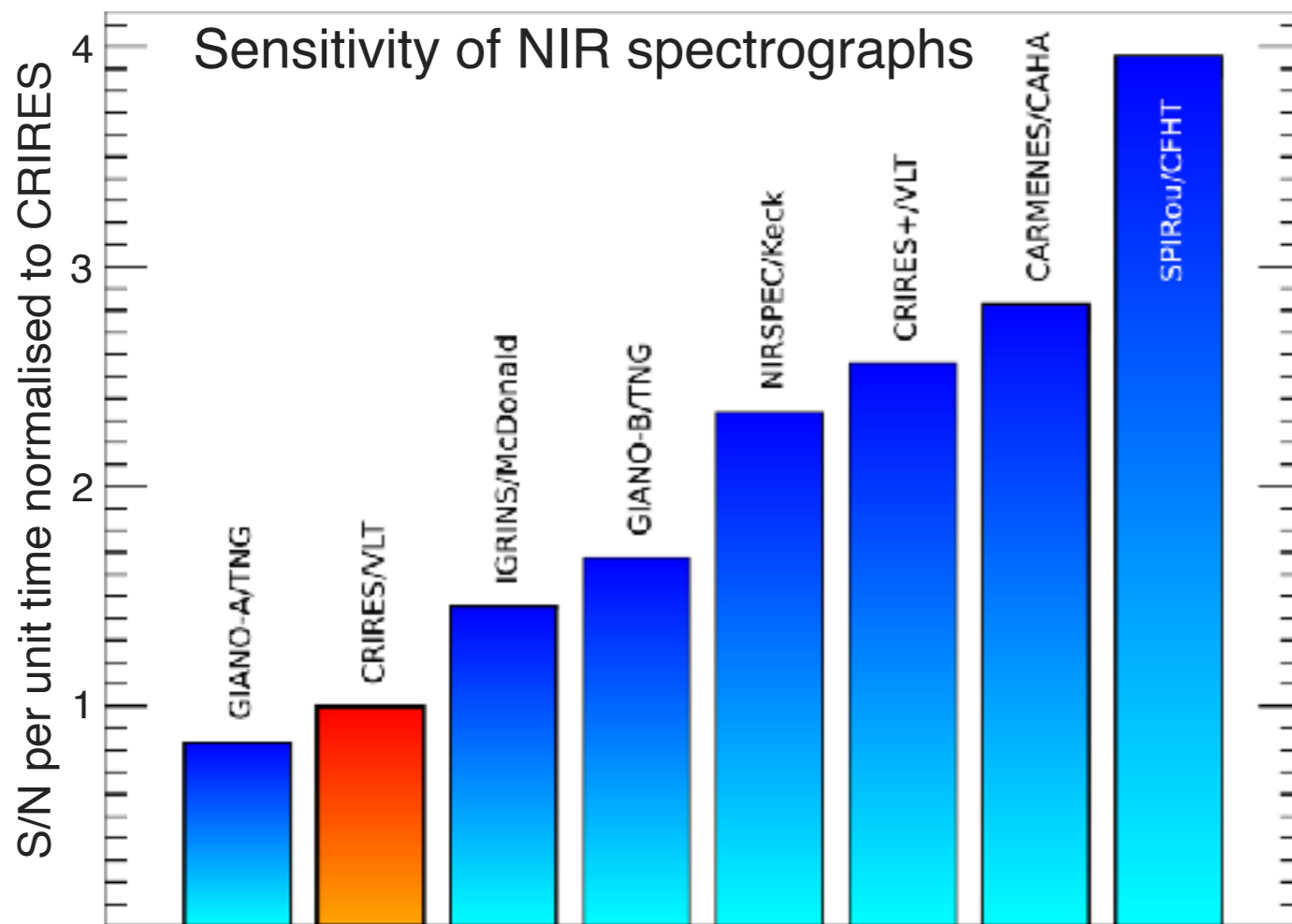
n_{lines}
spectral range of the instrument

N_{γ}
telescope size
instrument efficiency
brighter stars

$N_{\gamma, P}$
spectral resolution

*Example: O₂ line
around 760.45 nm
at $R=10^5$ (black), 3×10^5
(blue), 5×10^5 (green), and
 10^6 (red)*

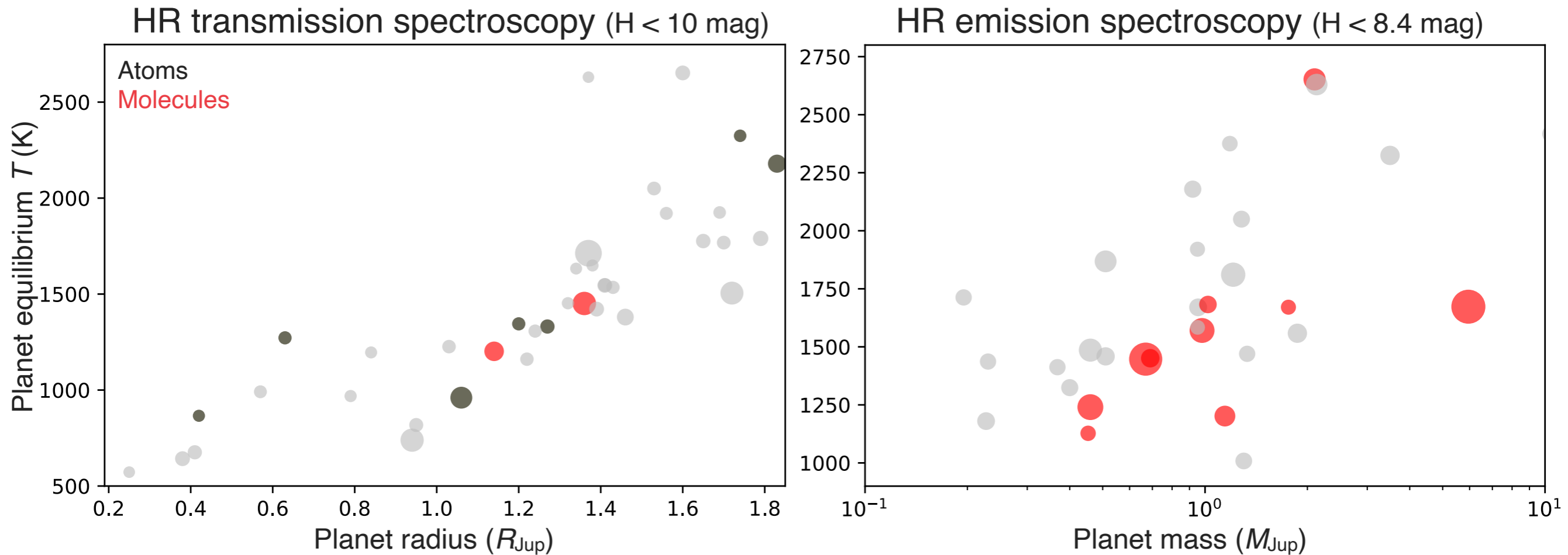
from Lopez-Morales+19



Modern spectrographs can compensate **smaller apertures**
with **increased spectral range** and **efficiency**

From demonstration to comparative exo-planetology

Only a small fraction of the current detectable sample has been observed



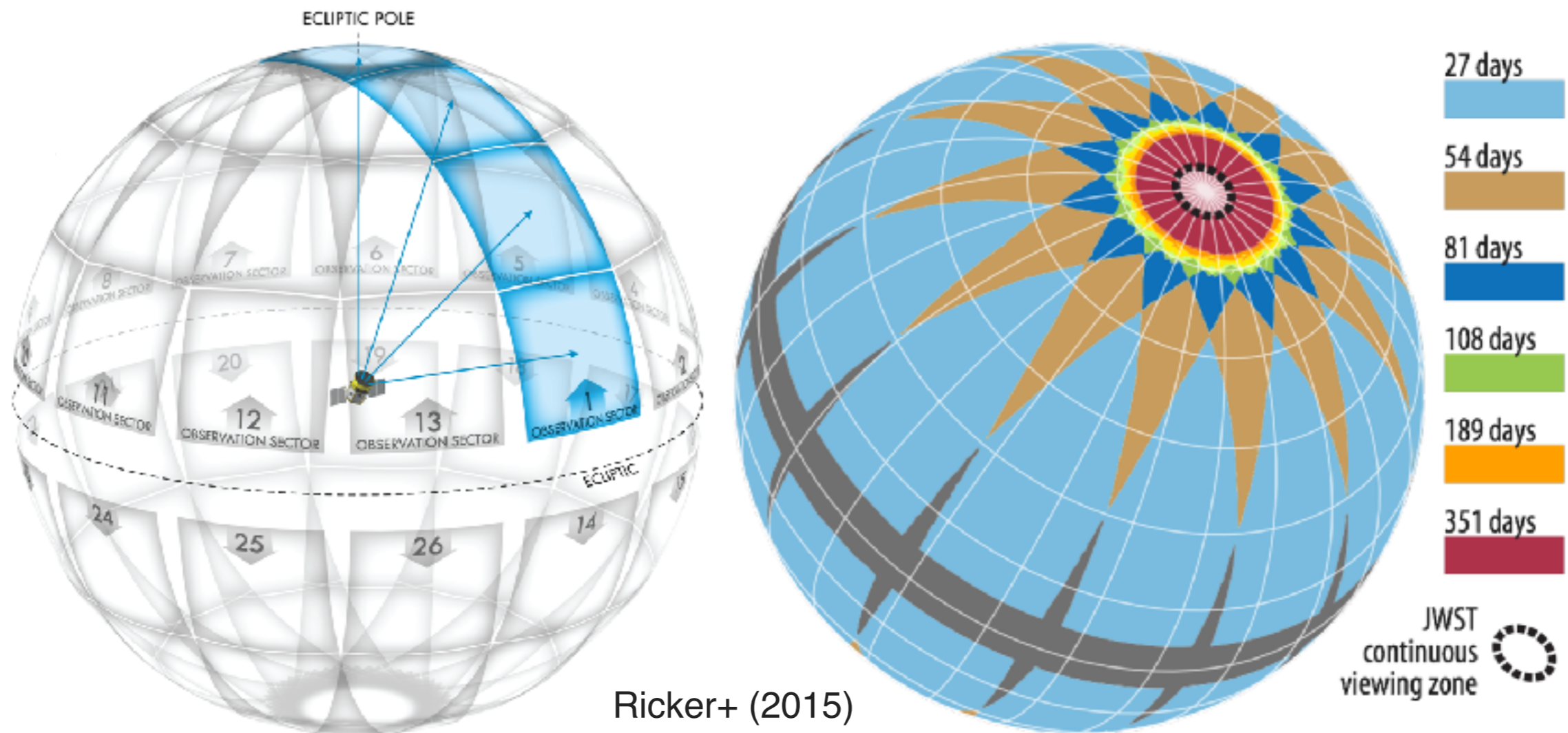
30-40 exoplanets (transiting and non-transiting) within reach of current facilities

Sensitivity range: from warm Neptunes to ultra-hot Jupiters

Current sample: most of the measurements still focussed on Jupiter/Saturn-size planets

The TESS mission: small(er) planets around bright stars

Small ($4 \times 10\text{cm}$) telescope on a 2:1 lunar resonance orbit, 2yrs+ mission



Optimised to find small planets ($< 4 R_{\oplus}$) around bright stars

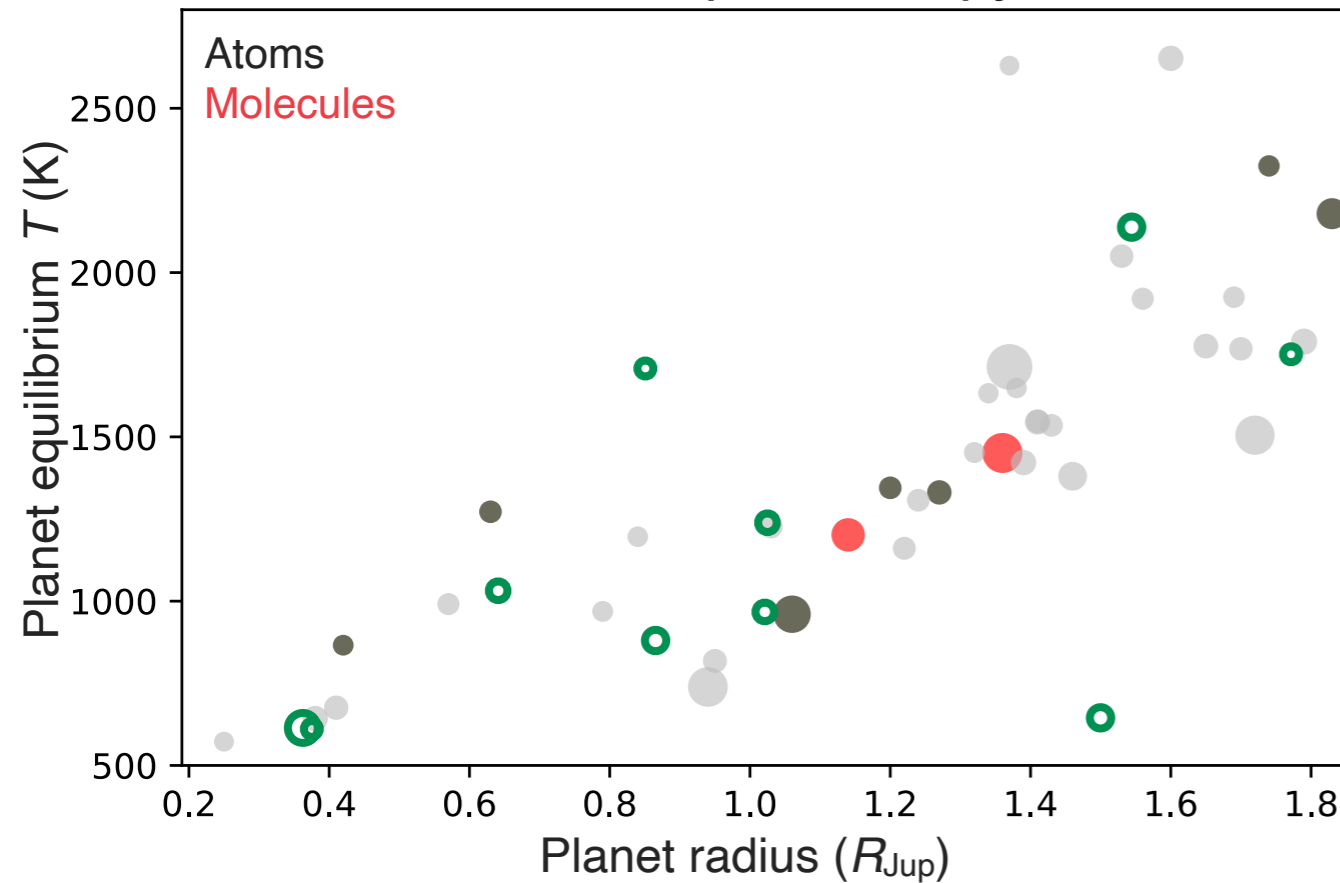
Launched in April 2018, primary mission completed in Aug 2020
Extended mission ongoing (half-way through)

3,300+ candidates (excl. false positives), 156 confirmed

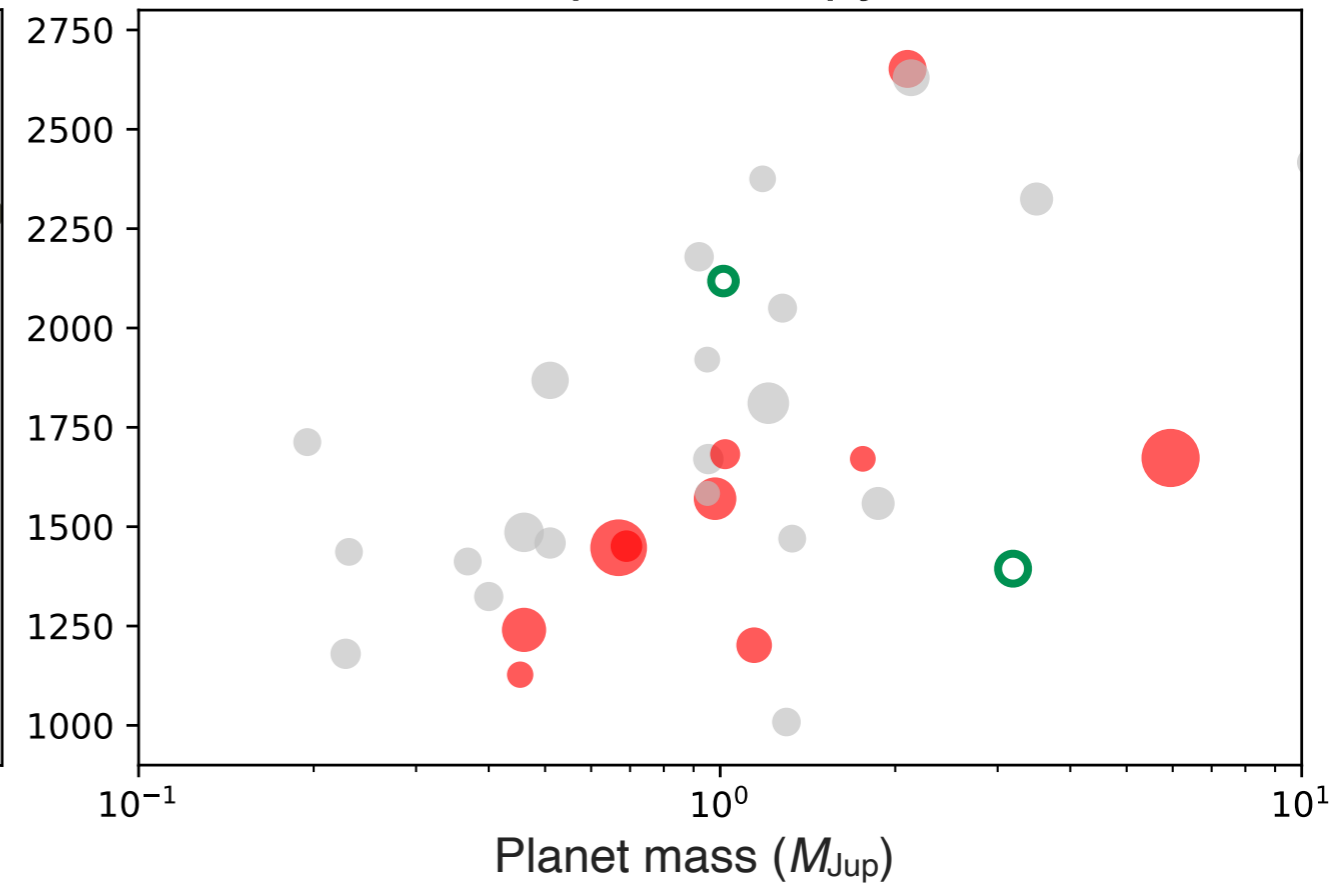
From demonstration to comparative exo-planetology

On paper there should be a few dozen TESS planets already observable

HR transmission spectroscopy ($H < 10$ mag)



HR emission spectroscopy ($H < 8.4$ mag)

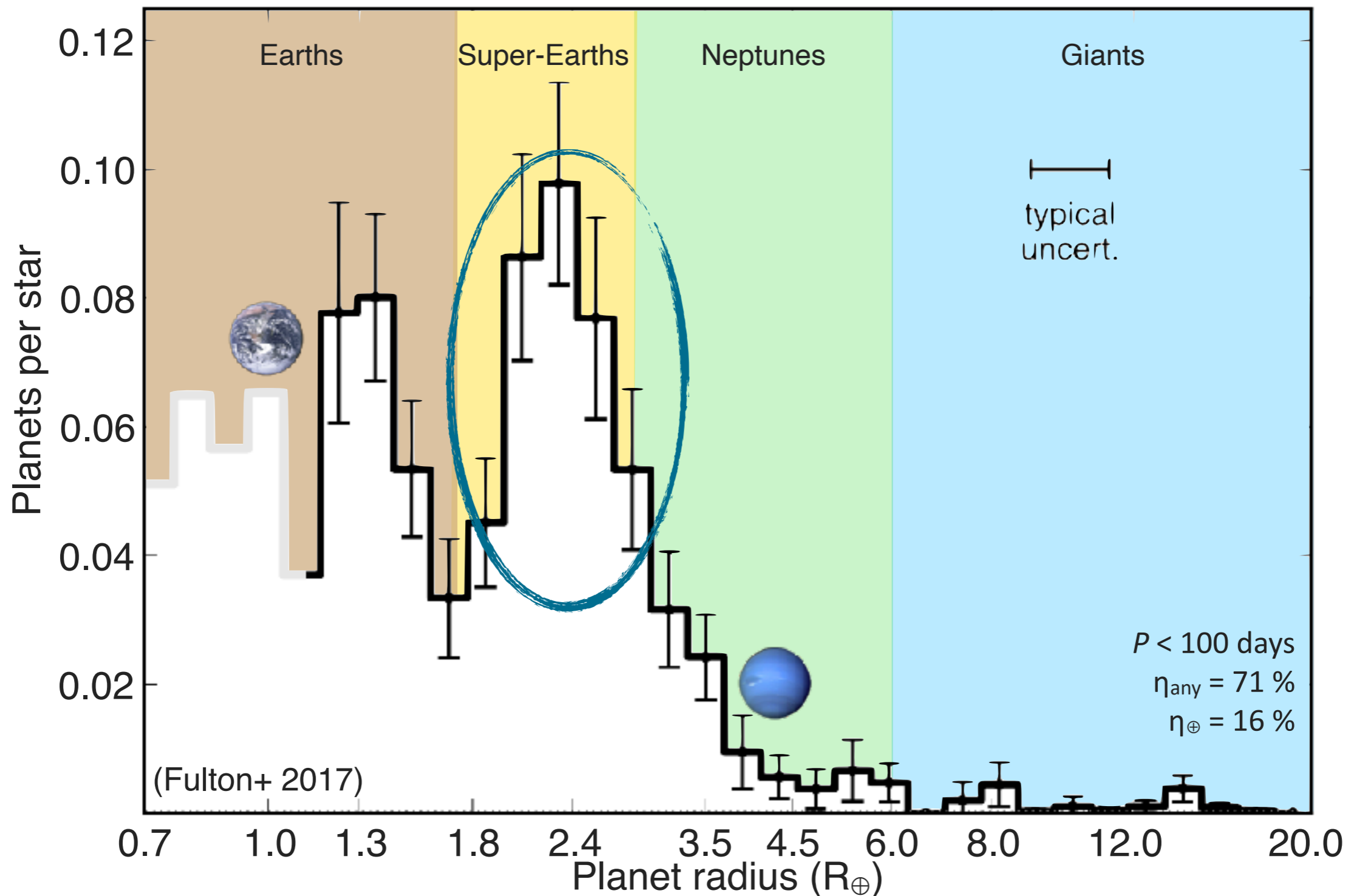


Confirmation of TESS planets focusses on rocky exoplanets
or planets in the evaporation valley

No significant change to the current observable sample yet

The most common exoplanets are not giants

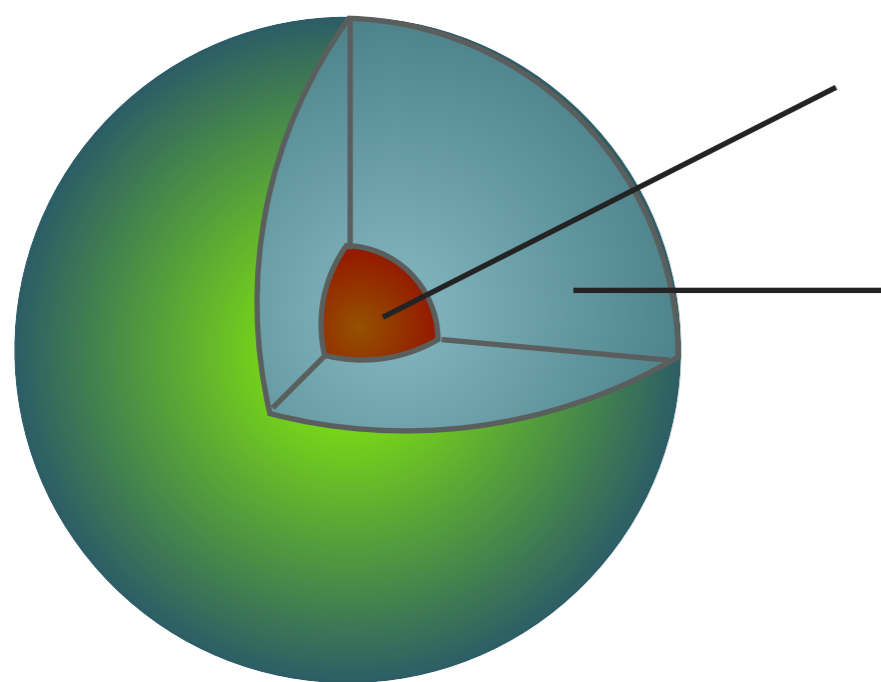
Statistics from *Kepler* detections of transiting planets around FGK stars



The most common planets have **no analogues** in the solar system
(their size is intermediate between Earth and Neptune)

Determining the nature of exoplanets

Intrinsic degeneracy between interior and envelope mass and composition



Small, dense core
(iron & silicates)

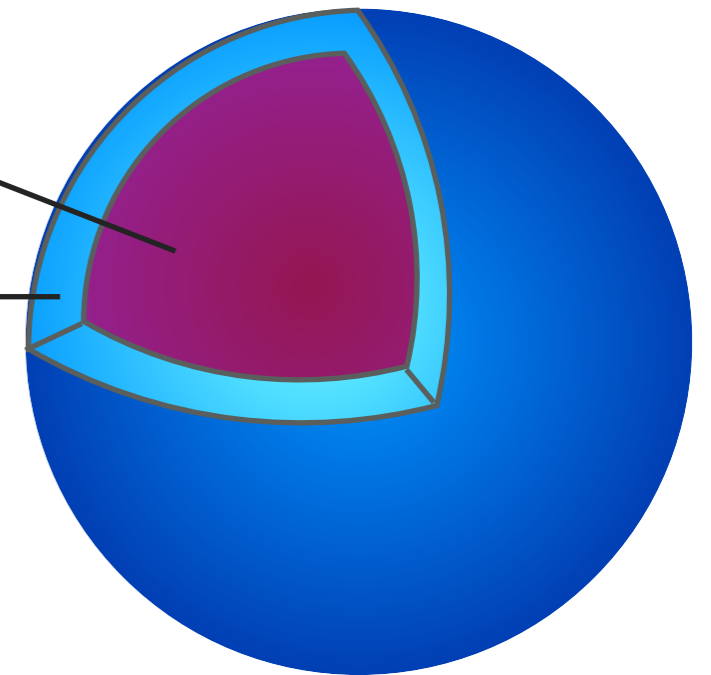
Extended atmosphere
(Hydrogen)

Super-Earths
Scaled-up versions
of rocky planets

Mini-Neptunes
Scaled-down versions
of giant gas planets

Big, light core
(mostly water ice)

Thin atmosphere
No H₂
H₂O [+ CO₂ etc.]

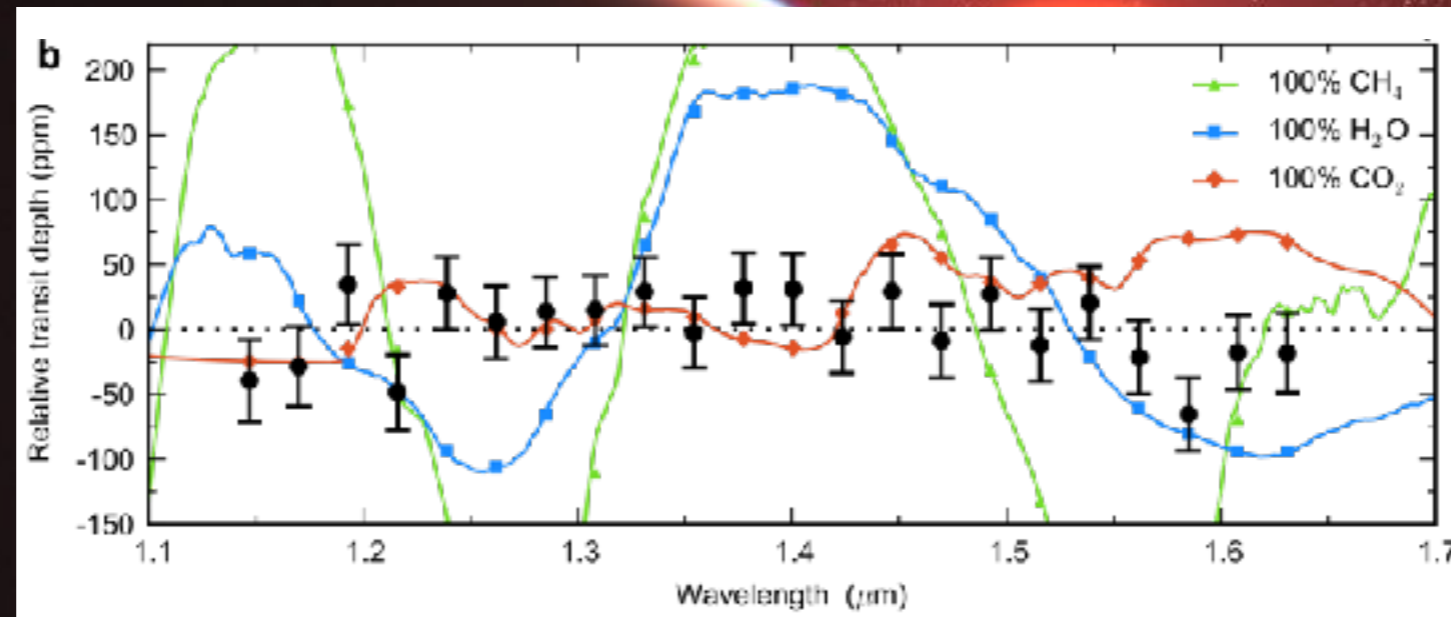


Studies of **exoplanet atmospheres** can solve the degeneracies

The cloudy atmosphere of GJ 1214 b

6.5× Earth mass, 2.7× Earth radius orbiting a small M-dwarf star
Planet temperature is 400-550 K

Nearly 100 hours of HST and 13 transits show a spectrum consistent with a flat line



Kreidberg+ 14

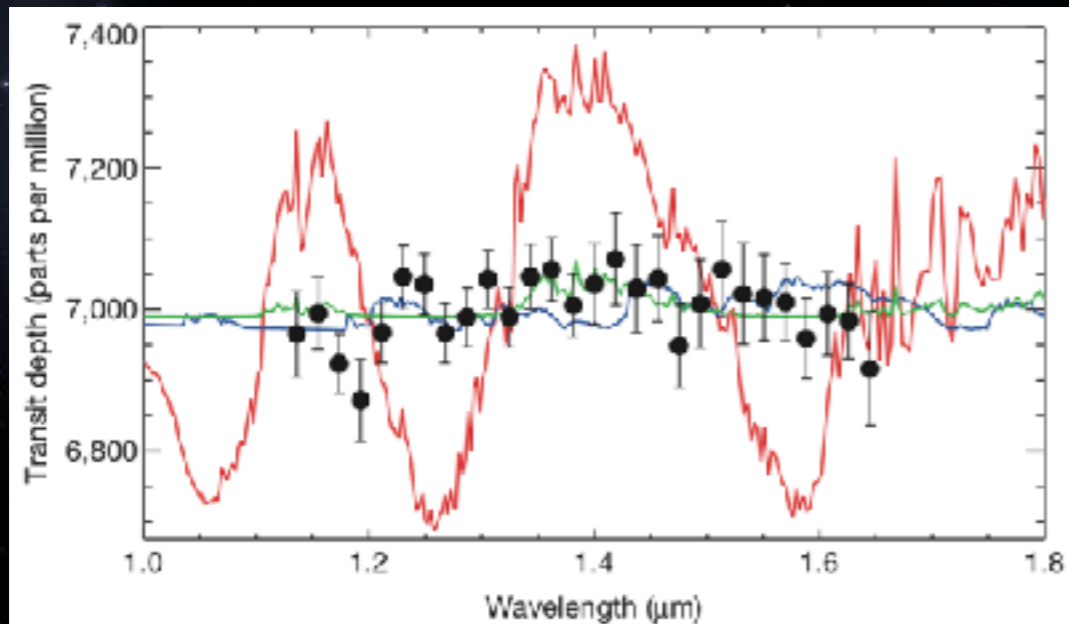
Density is 1.87 g cm^{-3} : too low to be lacking an atmosphere
Too big for a pure-water atmosphere: must have significant H_2

Most likely explanation is a high-altitude thick cloud layer equalising the planet radius regardless of wavelength

2.2x Earth mass, 4.2x Earth radius orbiting a small M-dwarf star
Planet temperature is 400-550 K

HST transit spectroscopy also sees a relatively flat spectrum
The data alone is not excluding a pure-water atmosphere due to lower precision

Knutson+14

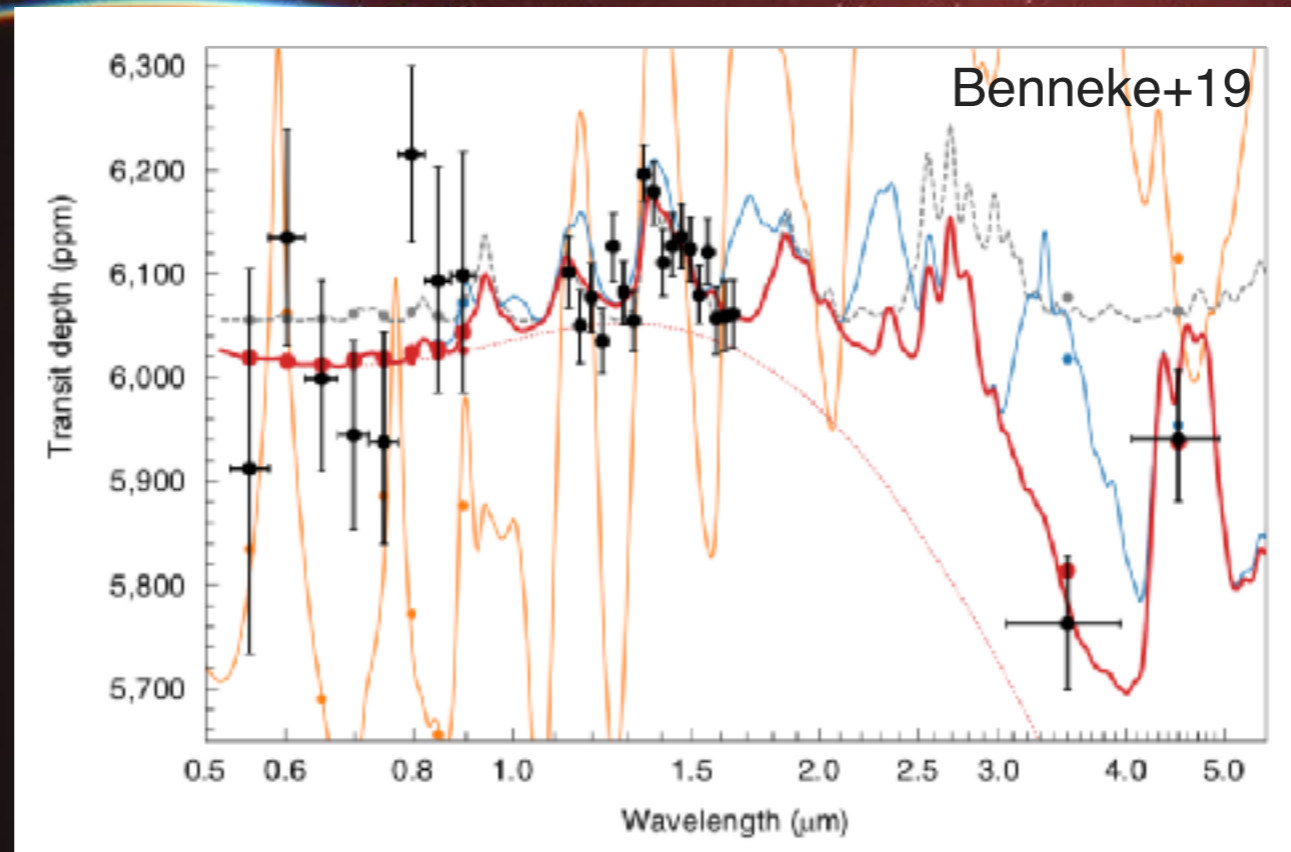


Massive H₂ evaporation has been measured
The planet has an extended hydrogen envelope

Peeking above the clouds: the Neptune-size GJ 3470 b

14× Earth mass, 4.6× Earth radius orbiting a small M-dwarf star

Much less telescope time: data cannot exclude a water world, but we have seen H₂



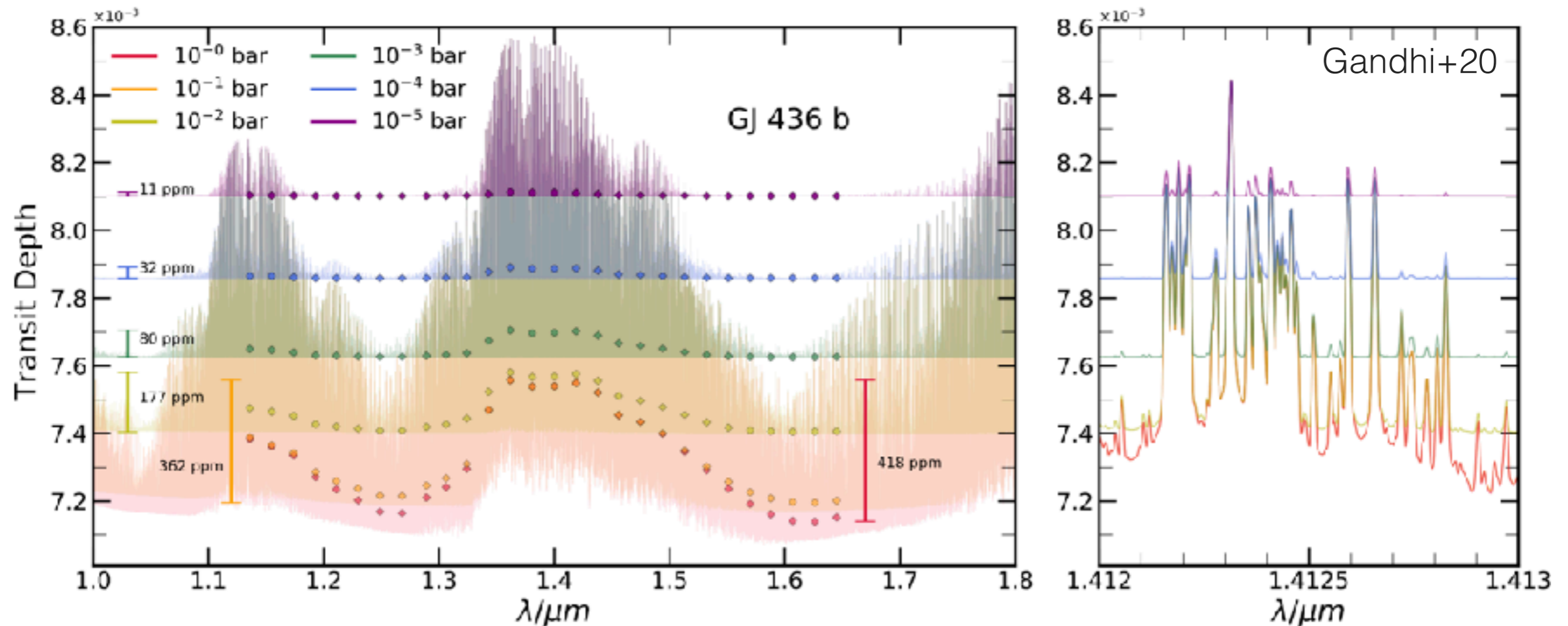
Density is 0.80 g cm^{-3} : too low to be lacking an atmosphere

Massive H₂ evaporation has been measured
The planet has an extended hydrogen envelope

Benneke+19: Mie scattering from $\sim 0.6 \mu\text{m}$ particles - opacity “drop-off” around $2\text{-}3 \mu\text{m}$

Seeing above the clouds at high spectral resolution

H₂O transmission spectrum of a hot Neptune across the NIR spectral range



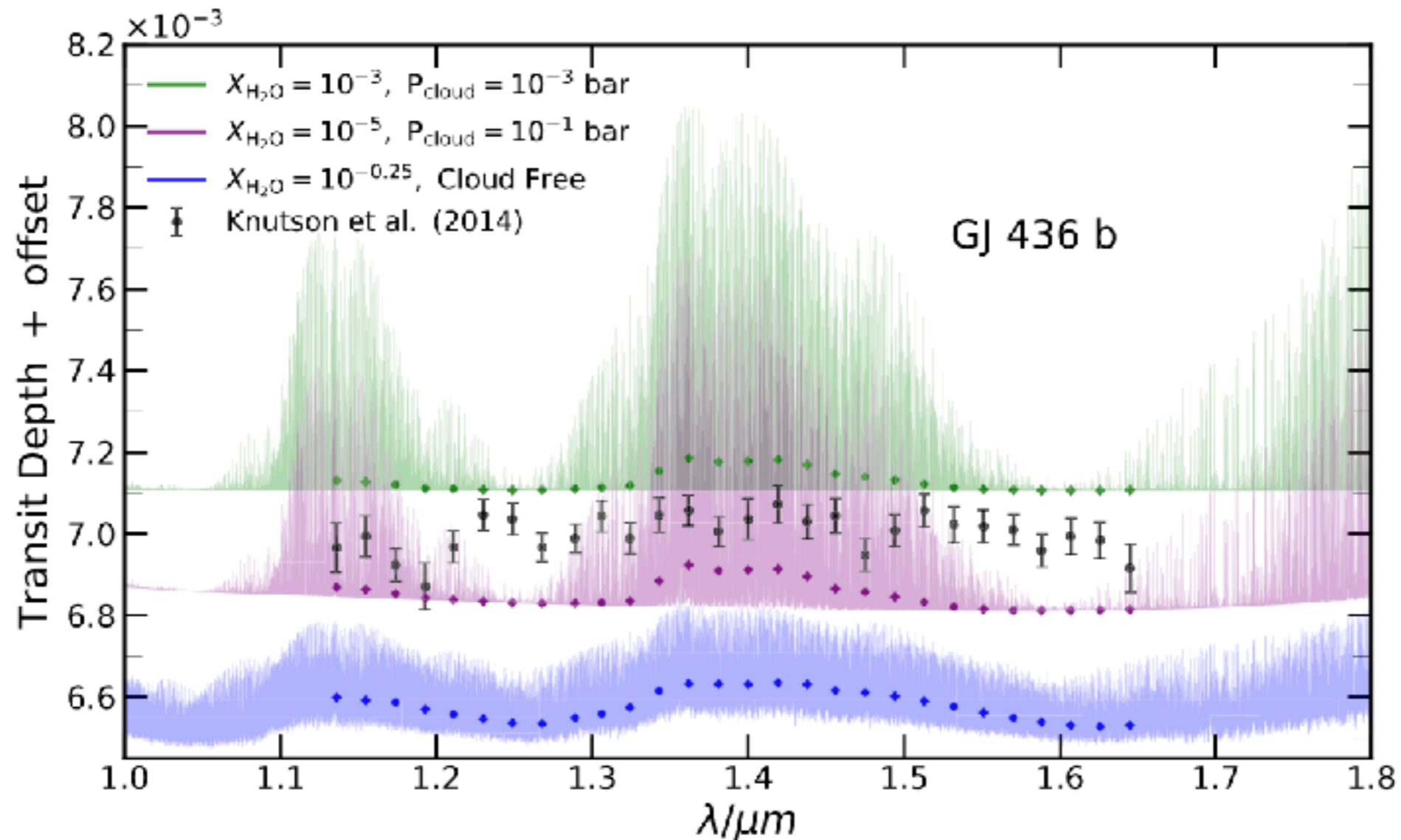
High-altitude cloud deck (0.1-1 mbar) completely mutes “weak” water lines
Peaks of H₂O band still form above the clouds

Observations at **low spectral resolution** produce flat spectra for clouds top ≤ 1 mbar
At **high spectral resolution** there is still residual spectrum above the clouds

(see Gandhi+20, Hood+20)

Solving the cloud-metallicity degeneracy

H₂O transmission spectrum of a hot Neptune across the NIR spectral range

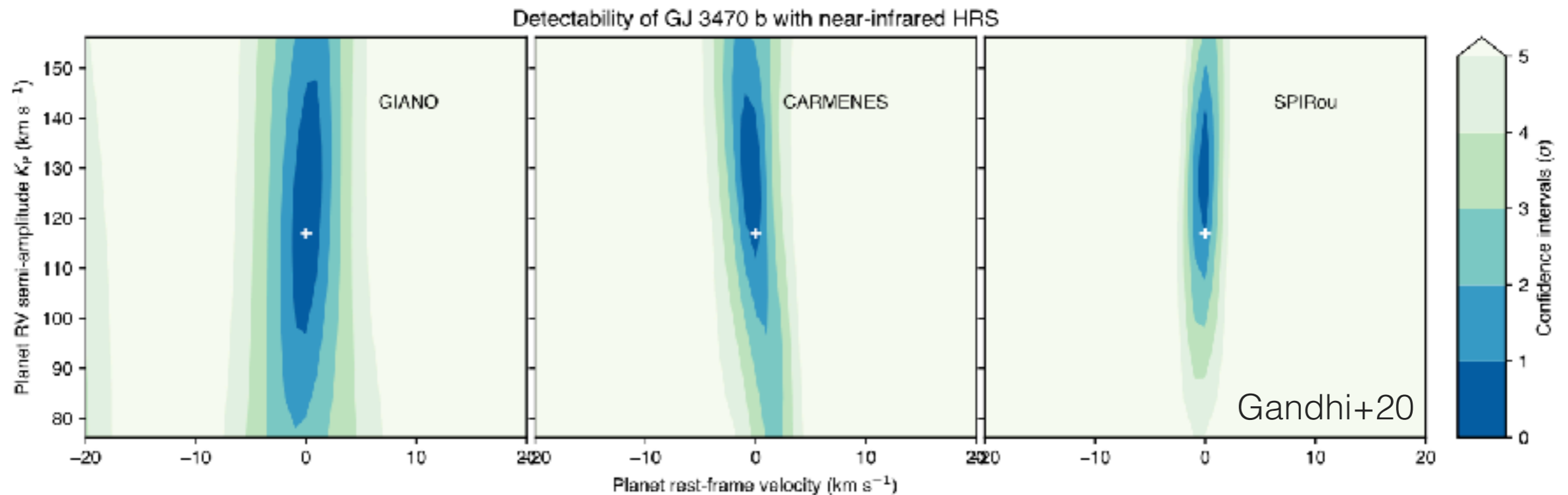
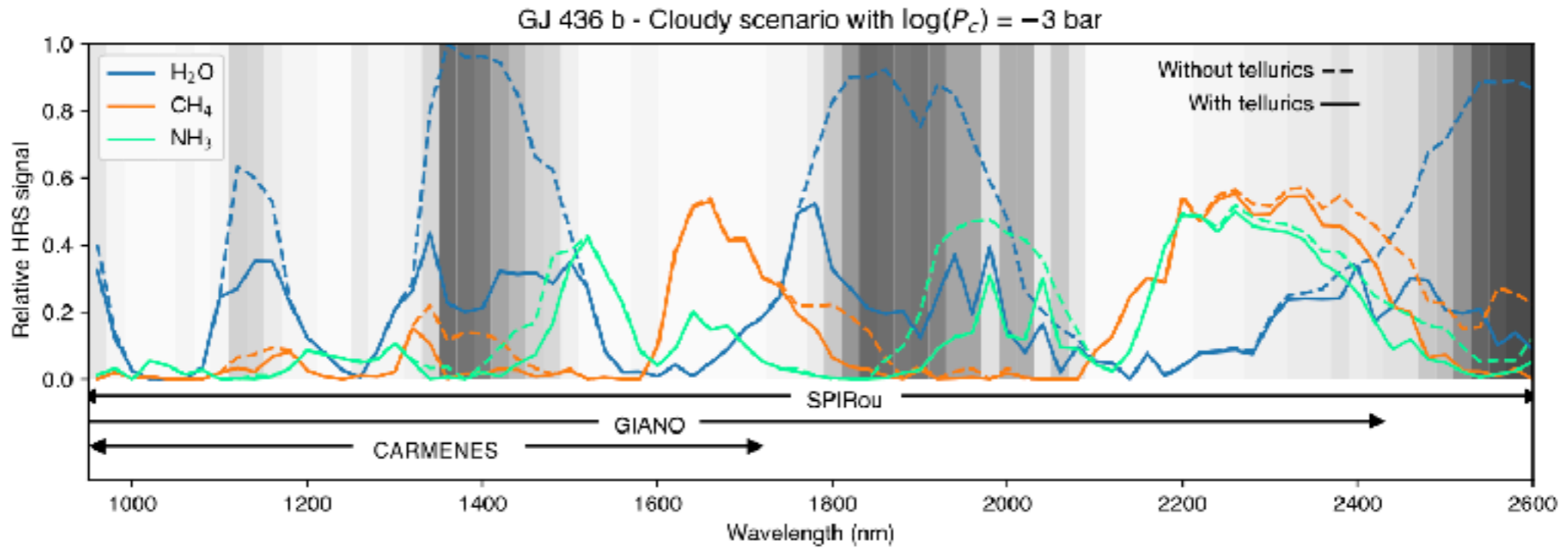


Cloud decks extending to high altitudes are degenerate with **high metallicity** (= high mean molecular weight) at low spectral resolution

High metallicity and high clouds both contribute to mute the spectral features

Simulating observations with HR spectrographs

Need to account for telluric absorption cancelling some of the advantages of HRS



8 hrs of observations (~ 4 transit) sufficient to confidently detect the Benneke+19 scenario

Estimating significance and error bars

S/N versus statistical significance

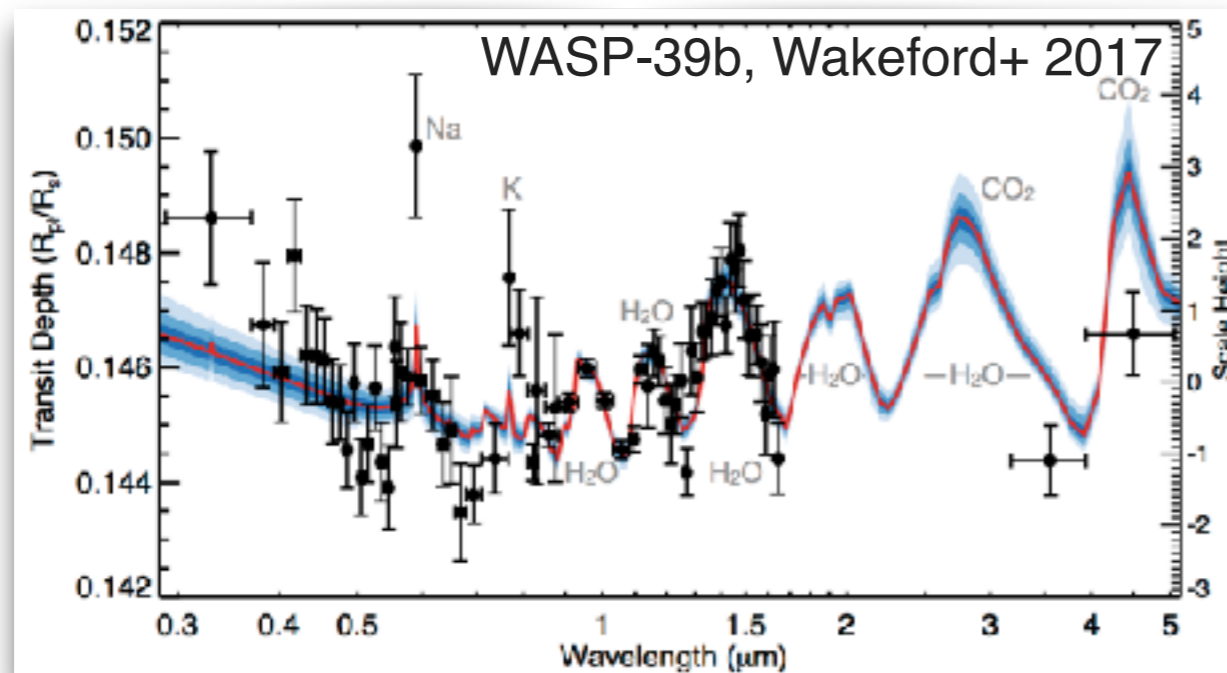
Injection and retrieval of models

Bayesian retrievals via MonteCarlo

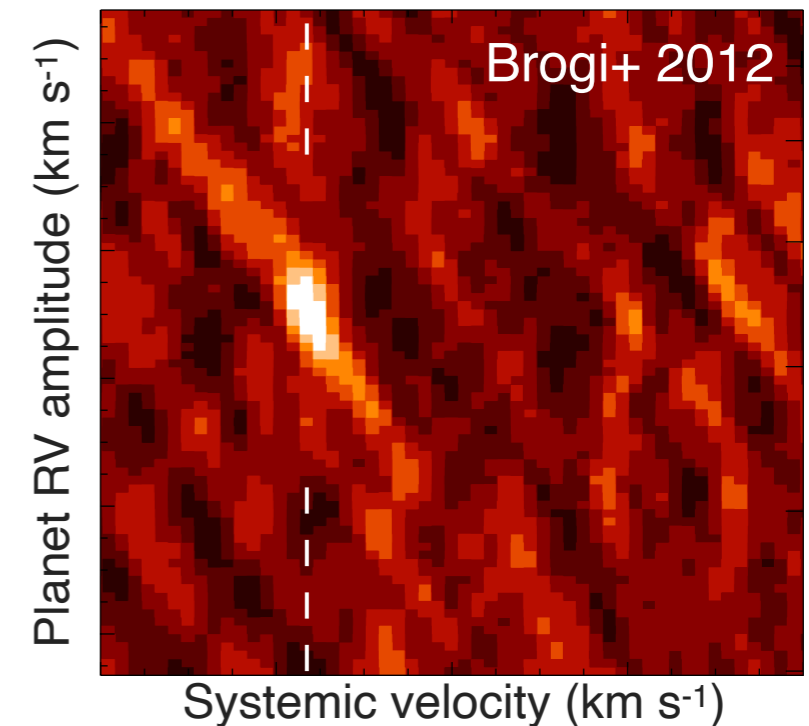
From detecting to measuring: detection significance

Quantifying the “goodness of fit” of a model is not (yet) possible at high-res

Low-res spectroscopy



High-res spectroscopy



Low-res spectroscopy recovers an actual **spectrum**

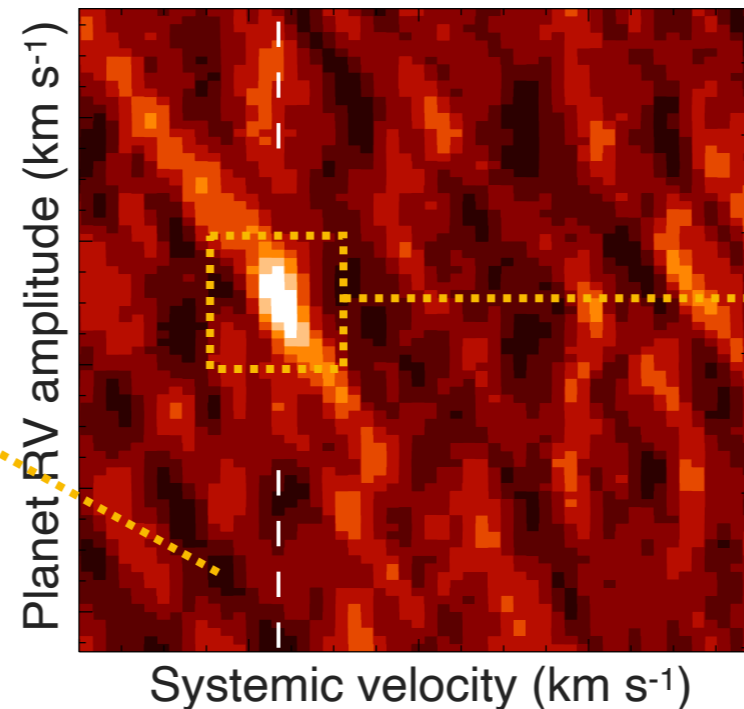
Models can be matched to observations via chi-square fitting (also in a Bayesian way)

High-resolution spectroscopy measures a **level of correlation**

***How do we even quantify significance?
How do we “select” models?***

S/N as a proxy for detection significance

Noise: the standard deviation of all the other cross correlation values



Signal: the peak value of the total cross correlation

$$S/N = \text{Peak CC} / \text{stdev}(\text{CC})$$

Immediate and intuitive quantity to compute

Some of the “noise” is actually auto-correlation / aliasing signal

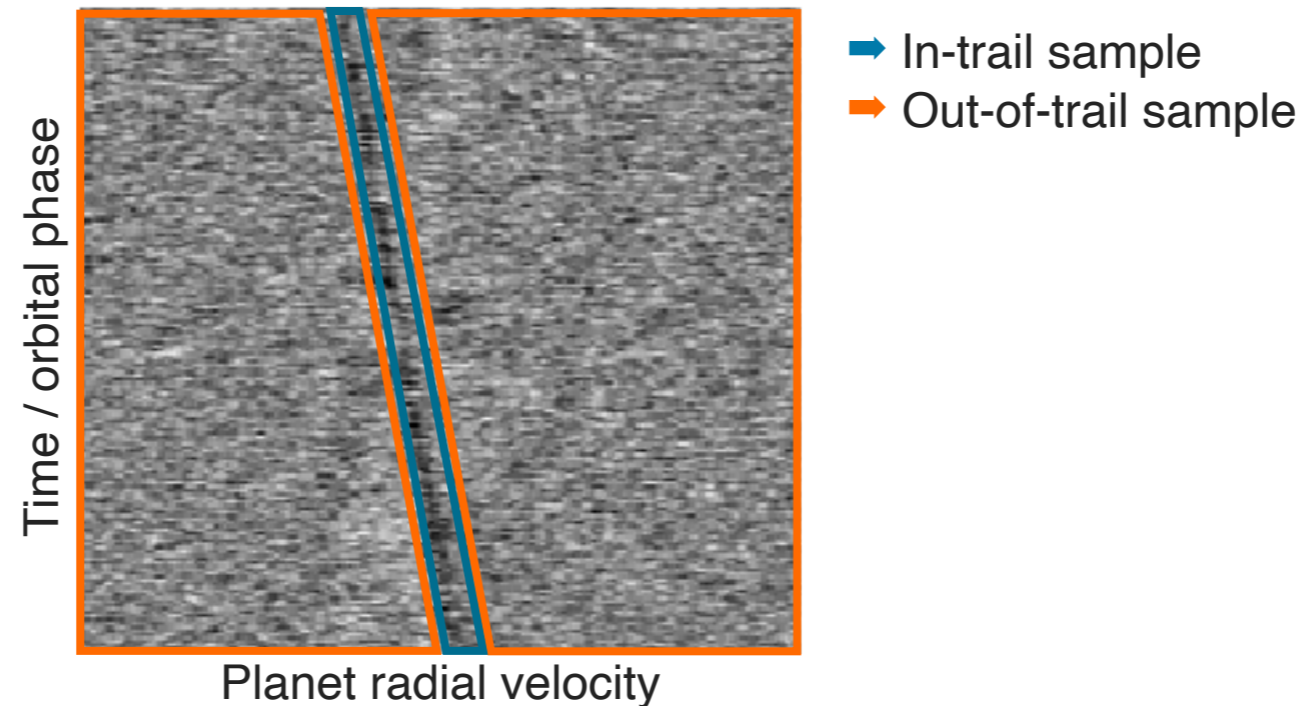
Some (V_{sys}, K_P) values will have increased noise due e.g. to residual telluric or stellar lines

At low SNR peaks can arise by just noise fluctuations

Error bars are usually defined by (V_{sys}, K_P) values corresponding to $(S/N)_{\text{max}} - 1$

Detection significance from statistical tests on the CCFs

Testing the means of the in-trail and out of trail cross-correlation values



Null hypothesis H_0 : in-trail and out-of-trail sample have the same mean

Welch t-test (data samples can have \neq size and variance) used to reject H_0
p-value \Rightarrow detection significance σ

Hp #1: the cross correlation values follow a Gaussian distribution (usually true)

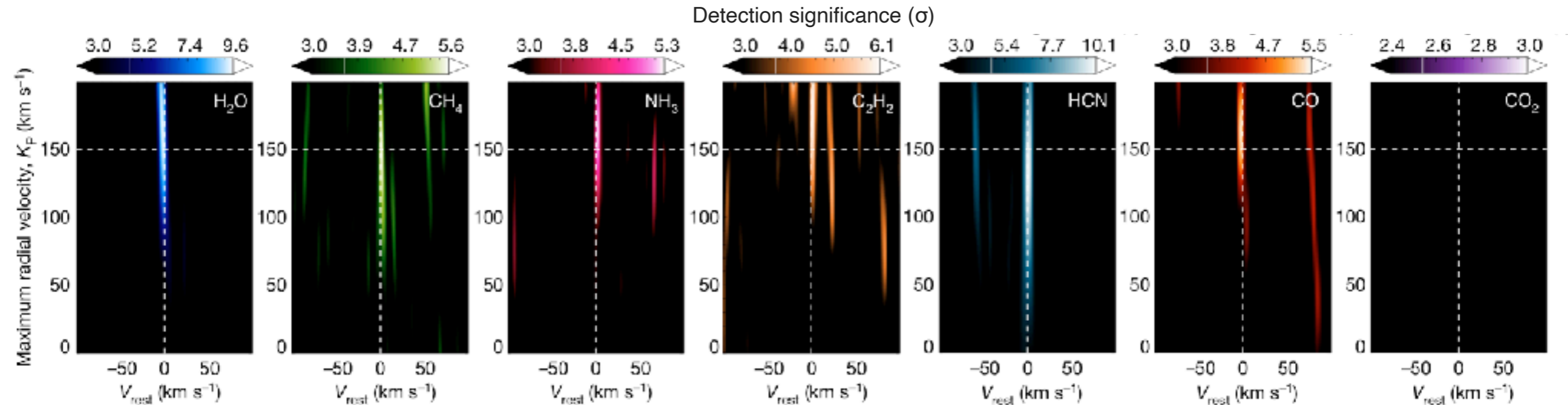
Hp #2: the cross correlation values are independent (depends on RV sampling)

Dependence on the “width” of the in-trail sample (at least 1 FWHM)

n- σ error bars can correctly be determined as $\sigma_{\max} - n$

Five carbon- and nitrogen-bearing species in a hot giant planet's atmosphere

P. Giacobbe, M. Brogi, S. Gandhi et al., *Nature* **592**, 205-208 (2021)



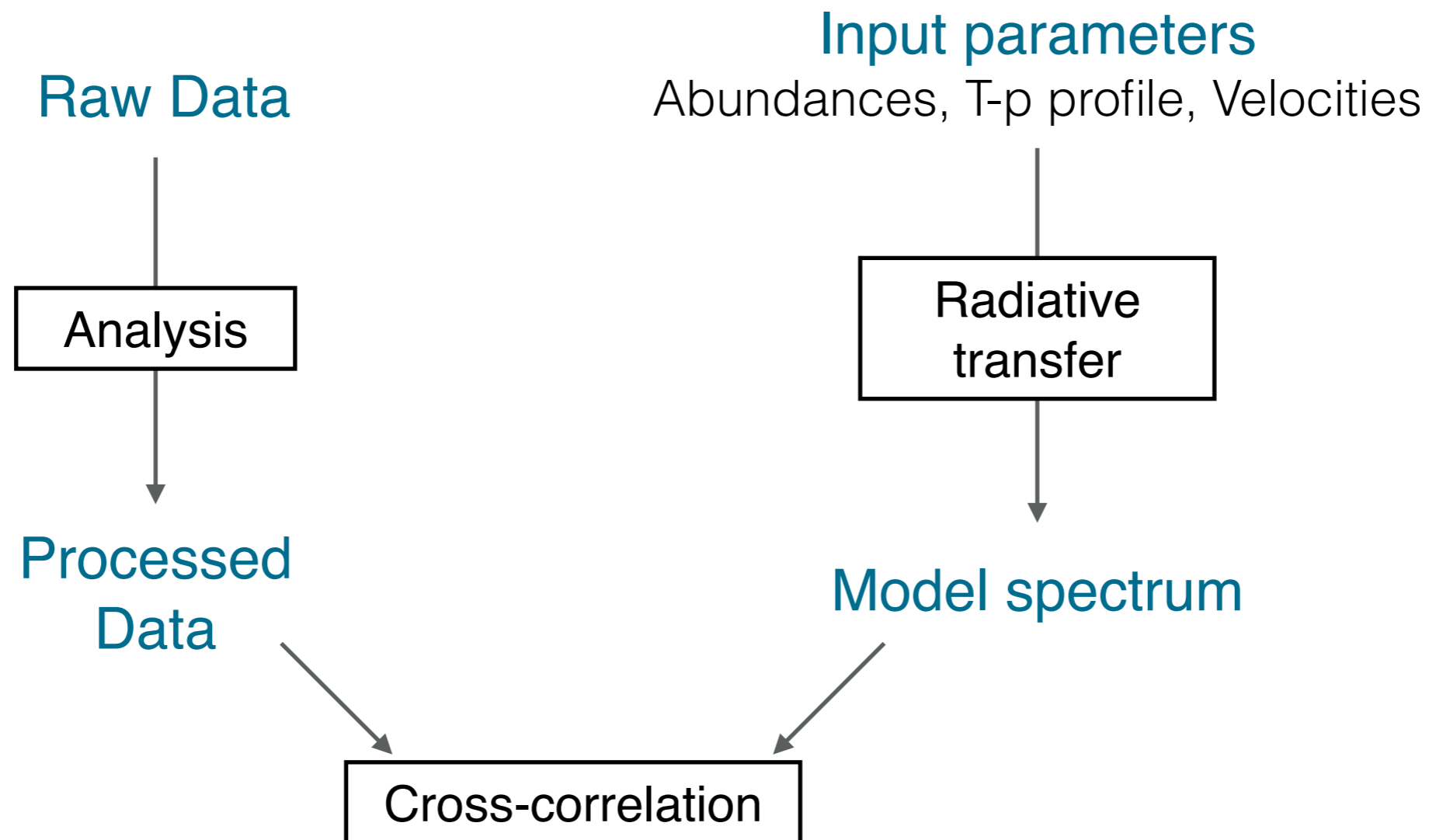
4 transits of hot Jupiter HD 209458b (1,500K) \Rightarrow H_2O + 5 species simultaneously detected



What does it mean for the atmosphere of HD 209548 b?

Need to move *beyond detecting* and towards *measuring*
(We will see this in the next lecture!)

From detecting to measuring: our checklist

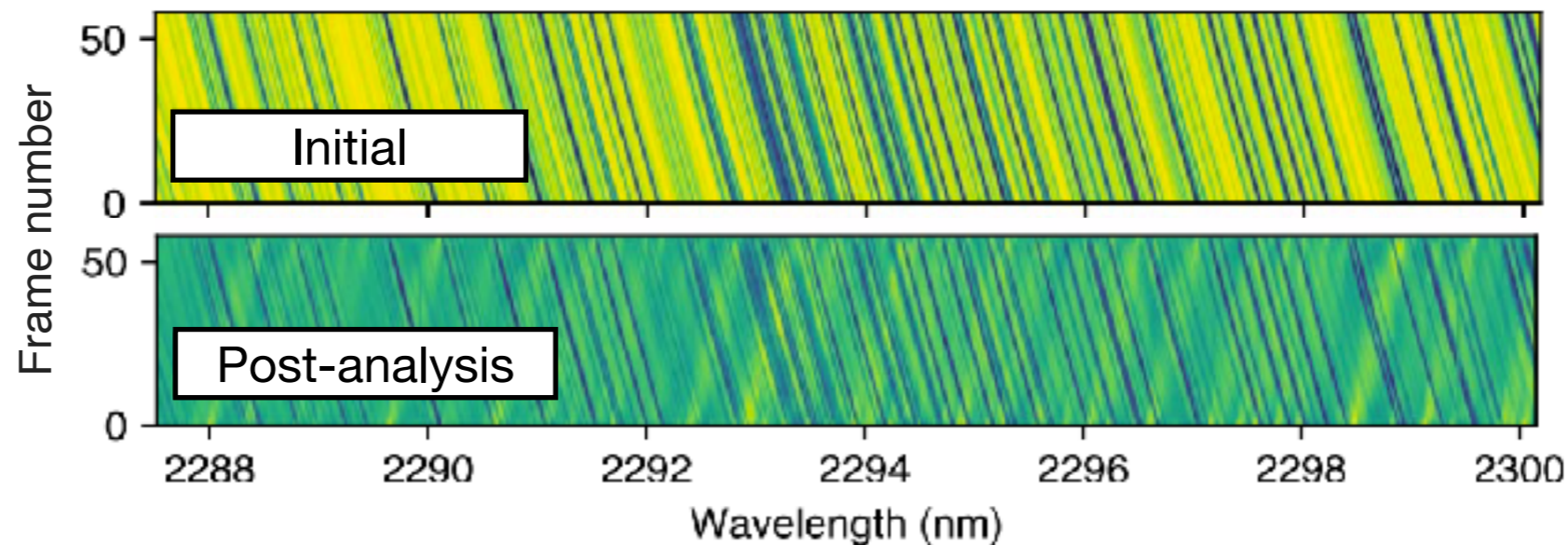


- Need to:**
- account for any biases of the analysis
 - understand what's the information content at high-res
 - design a method to select the best model within a grid
 - explore the whole parameter space to understand degeneracies

The data analysis is not completely harmless

The removal of telluric and stellar lines affects exoplanet lines

Shown by Brogi & Line (2019) on simulated data - easy to see in the noiseless case



Different telluric removal techniques show different biases
(e.g. airmass de-trending, PCA, Sysrem)

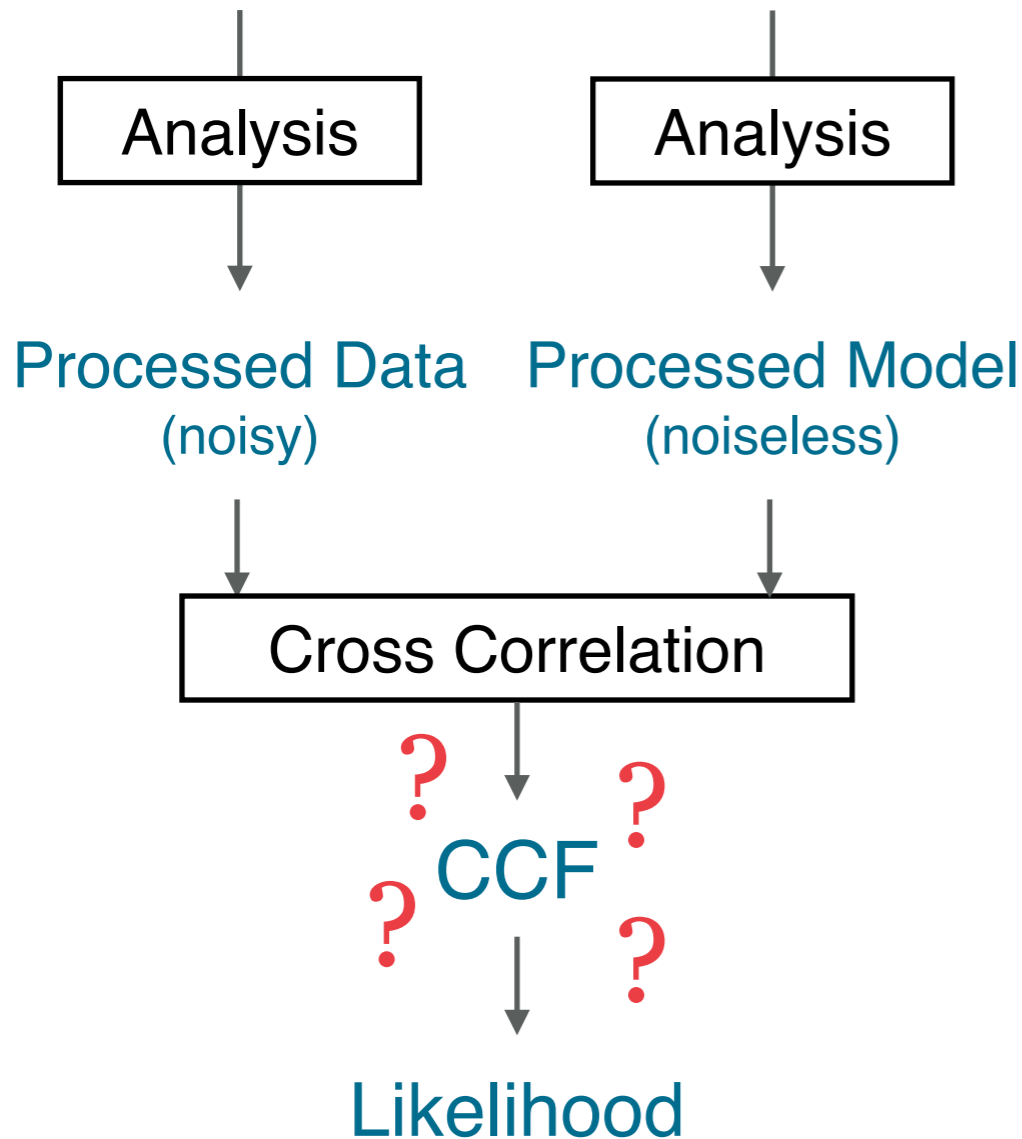
Altered shape & depth of spectral lines \Rightarrow biased abundances and T

Model reprocessing is **unavoidable** to obtain **unbiased measurements** from HRCCS

Model reprocessing: an unavoidable step

The model planet spectrum is **injected** in the data or a **synthetic sequence** is created

Observed Data Modelled Data ← Model spectrum



Can we translate cross correlation into a statistically meaningful quantity (a likelihood)?

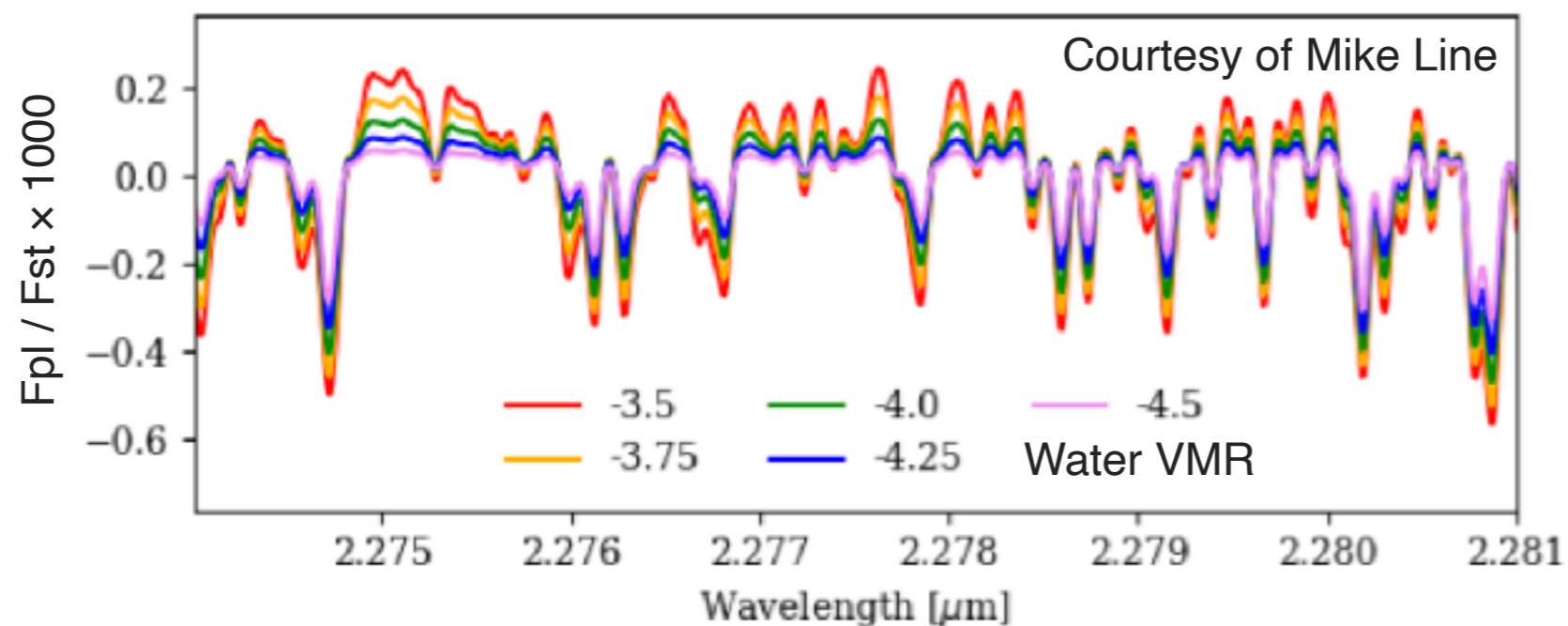
What is the information content in high-res data?

High-res data is normalised to remove stellar & telluric spectrum
(loss of absolute level of continuum in both emission and transmission)

No actual “spectrum” is visible
(no ground truth - consequences for goodness of fit)

Data is still expressed in units of stellar spectrum
(absolute line-to-line and line-to-continuum depths can still be recovered)

Line ratios and line shape change with absolute abundances and temperatures



HRCCS can measure absolute and relative abundances with the right framework

Building a likelihood function for high-res data

Brogi & Line (2019), but also Zucker (2003) and Gibson et al. (2020)

We would like to:

- use the match in line position
- distinguish between +ve and -ve correlation
- use information about line shape and amplitude

$$\log(L) = -\frac{N}{2} \log [s_f^2 - 2R(s) + s_g^2].$$

Length of array

Data Variance Cross-covariance Model Variance

Cross correlation

$$C(s) = \frac{R(s)}{\sqrt{s_f^2 s_g^2}}.$$

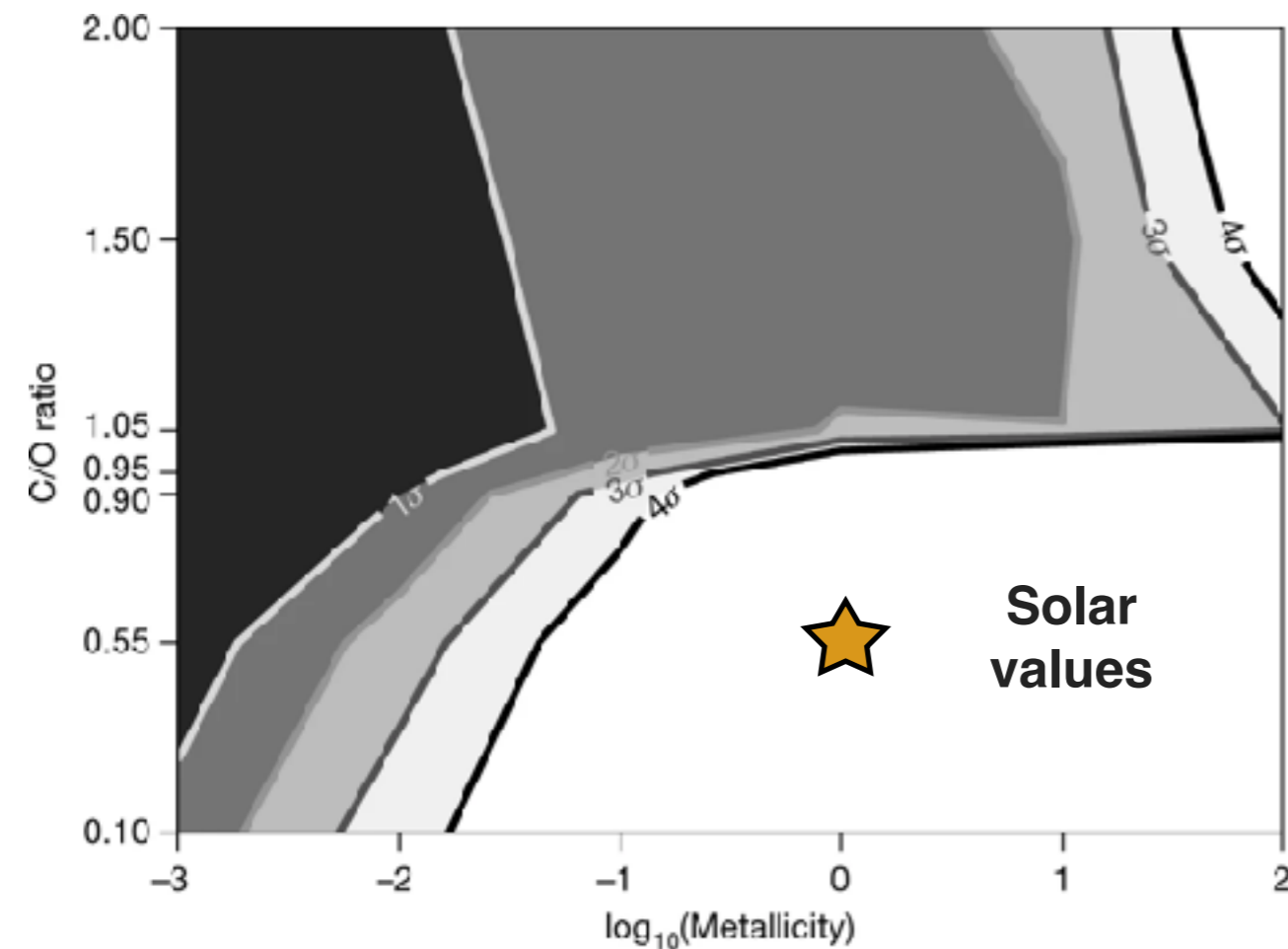
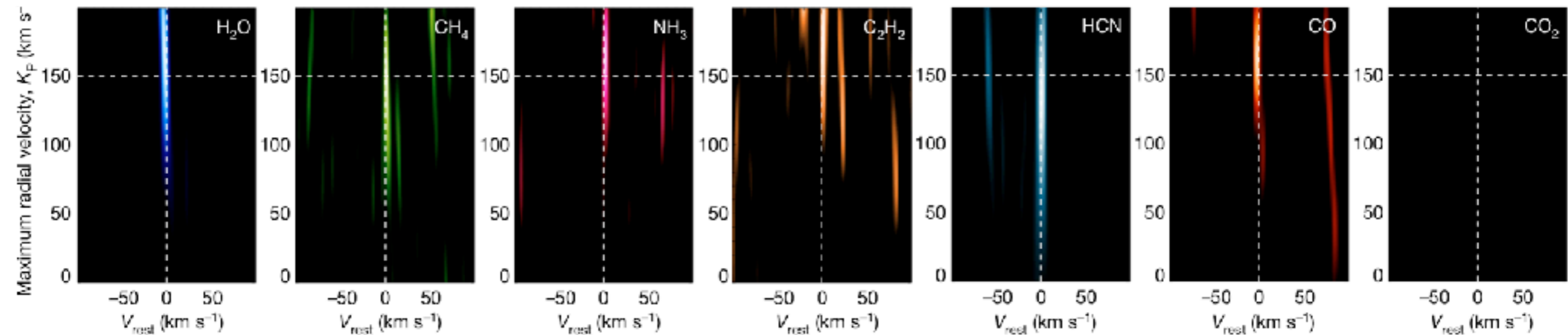
logL contains the **model** and **data variances** s^2
(it accounts for the amplitude of lines)

logL contains the **cross covariance** R
(not normalised - accounts for amplitude of lines)
(penalises anti-correlation - accounts for emission/absorption)

Model selection through likelihood-ratio tests

Exploring a grid of equilibrium models by varying metallicity and C/O

Giacobbe, Brogi, Gandhi et al., *Nature* (2021)



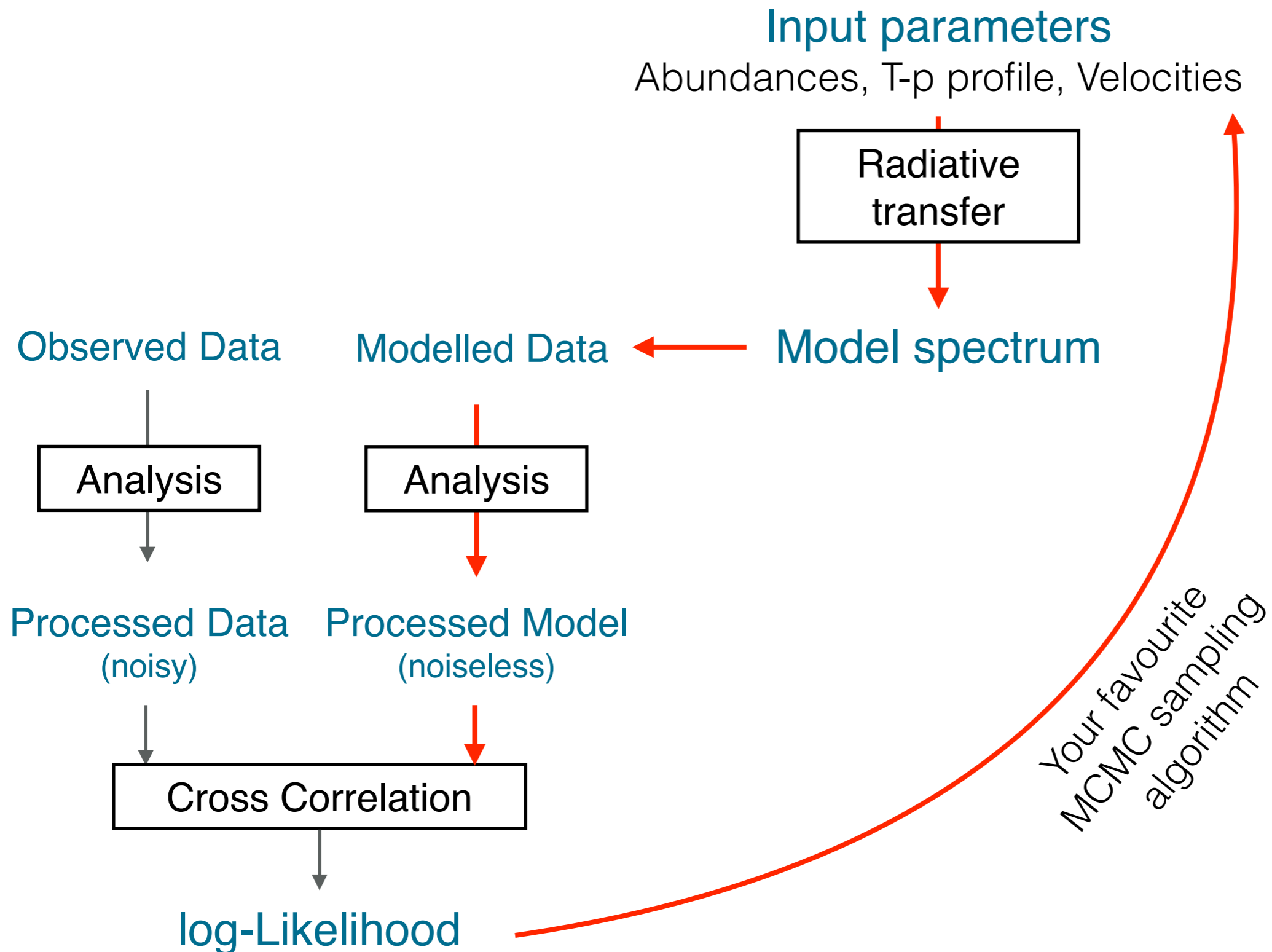
Addition of clouds (with LR parameters)
highly favoured (17 sigma)

Disequilibrium chemistry disfavoured

**HD 209458b formed beyond the snow line and
subsequently migrated w/o accreting ice
planetesimals**

Running a Bayesian retrieval on HR data

Letting the data “inform” model selection to explore full parameter space

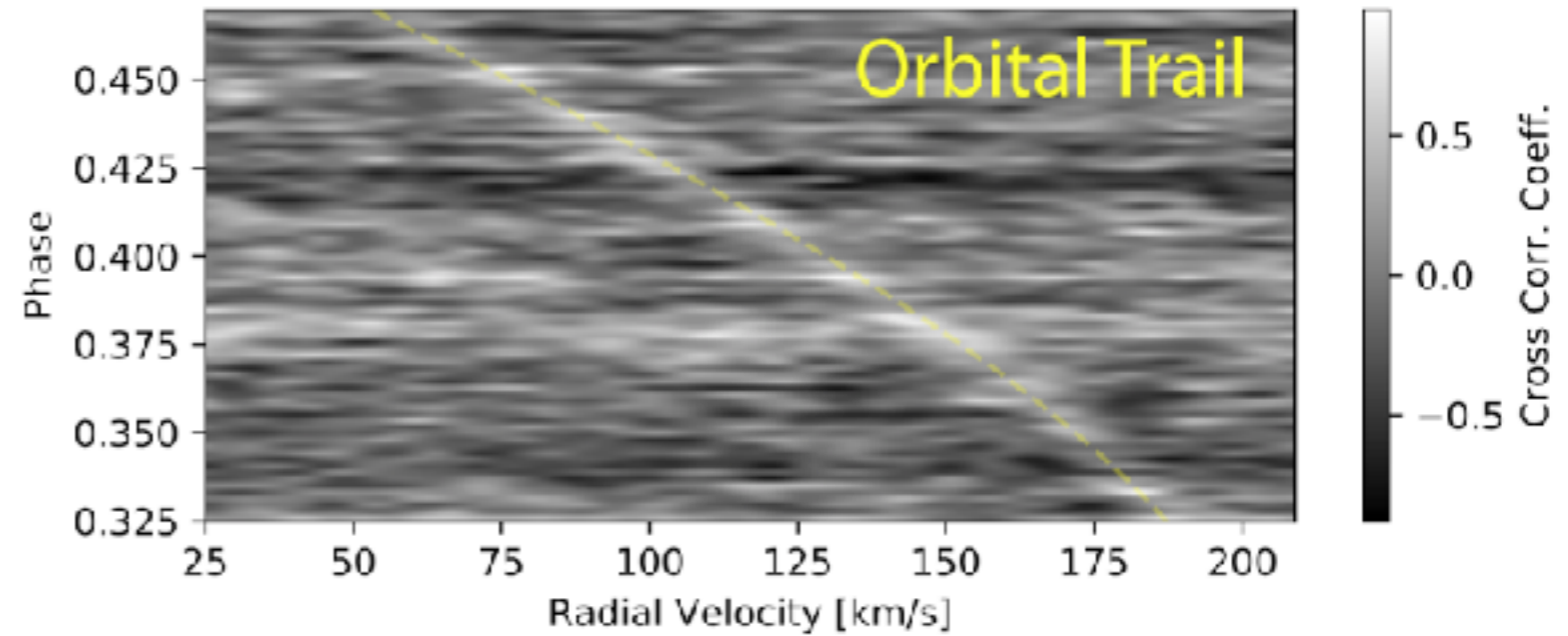


The emission spectrum of WASP-77 A b

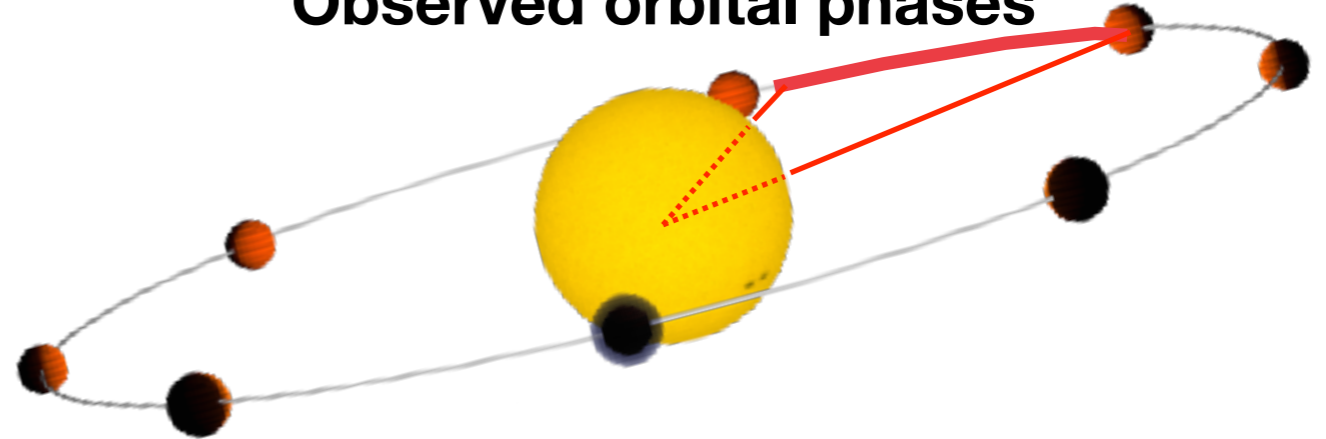
Line, Brogi, Gandhi et al., *Nature*, accepted (coming soon!)



IGRINS@Gemini-S (8.1m)



Observed orbital phases



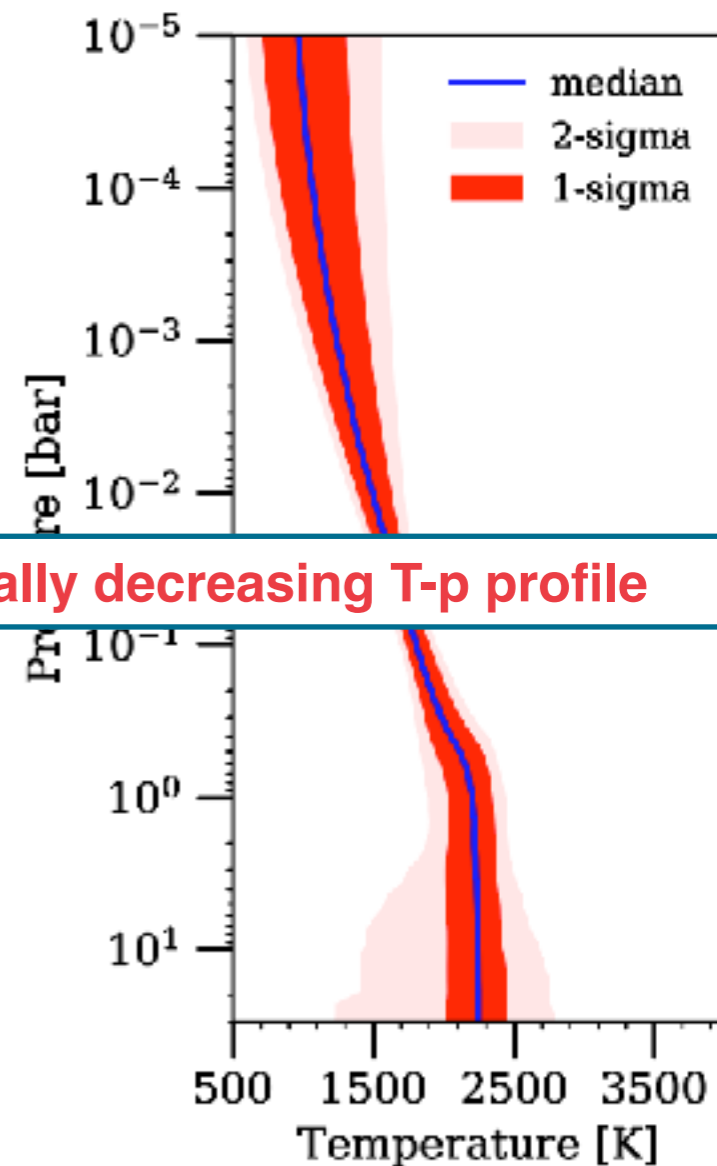
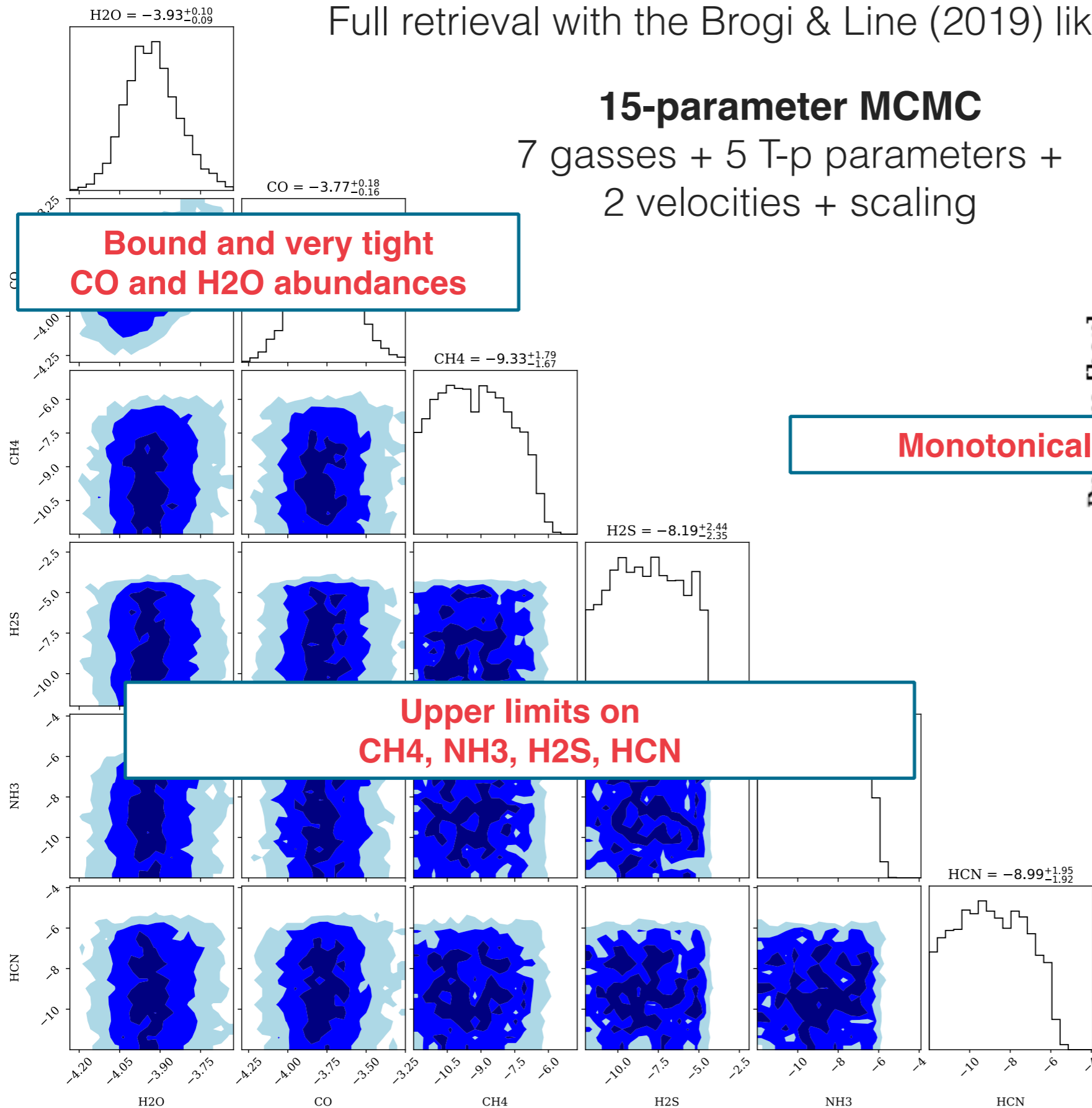
R~45,000
1.45 - 2.45 μm simultaneously
Silicon immersion grating
(keeping the instrument compact)

Achieving “solar system” precisions in the chemistry

Full retrieval with the Brogi & Line (2019) likelihood

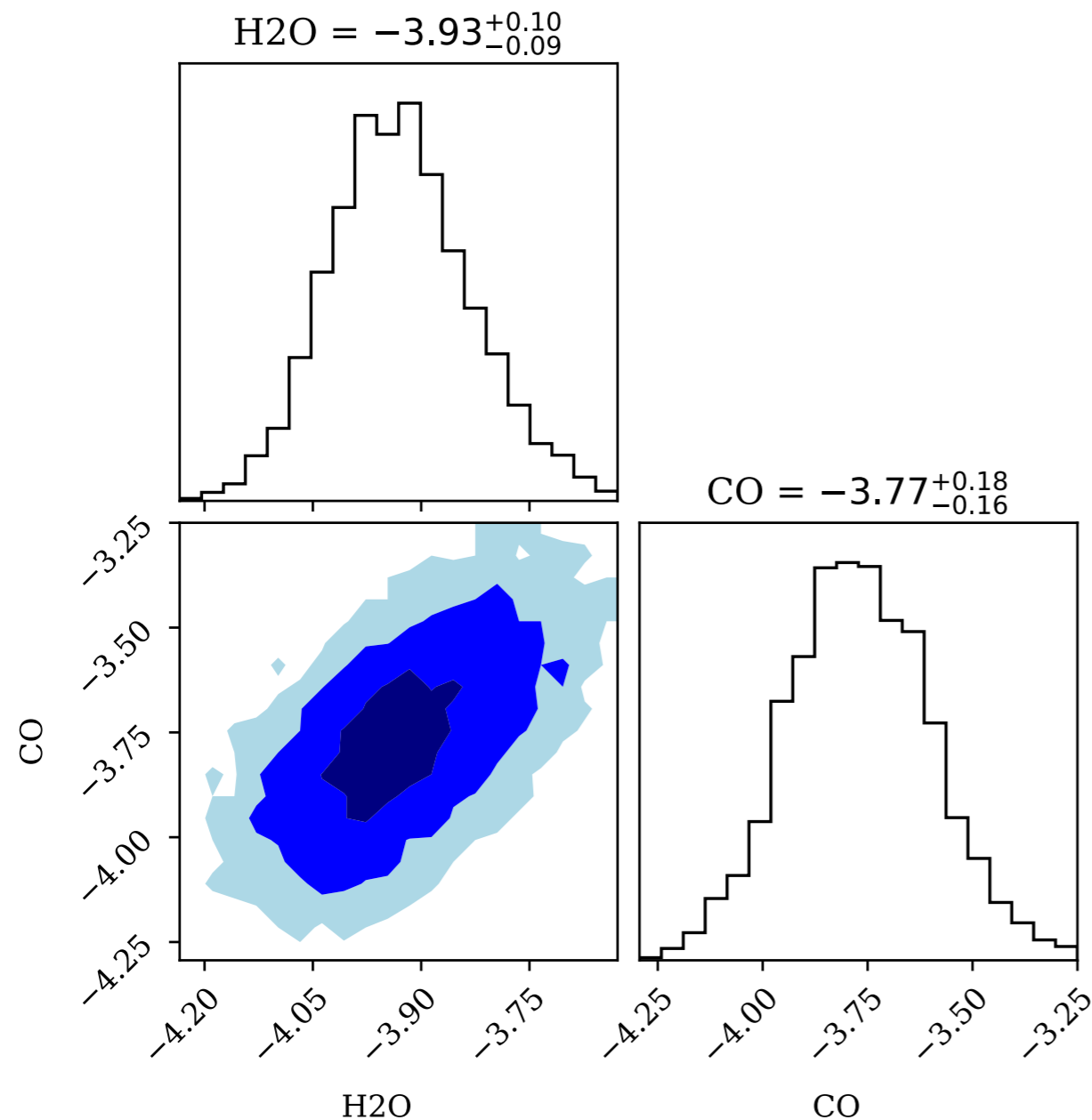
15-parameter MCMC

7 gasses + 5 T-p parameters +
2 velocities + scaling



Achieving JWST precisions in the chemistry

0.1-0.2 dex precision in **absolute abundance** for H₂O and CO



Validated independently with
2 retrieval frameworks
CHIMERA (Line)
GENESIS/HyDRA-H (Gandhi)

Accuracy tested by changing:
Data processing
T-p parametrisation
Choice of line lists

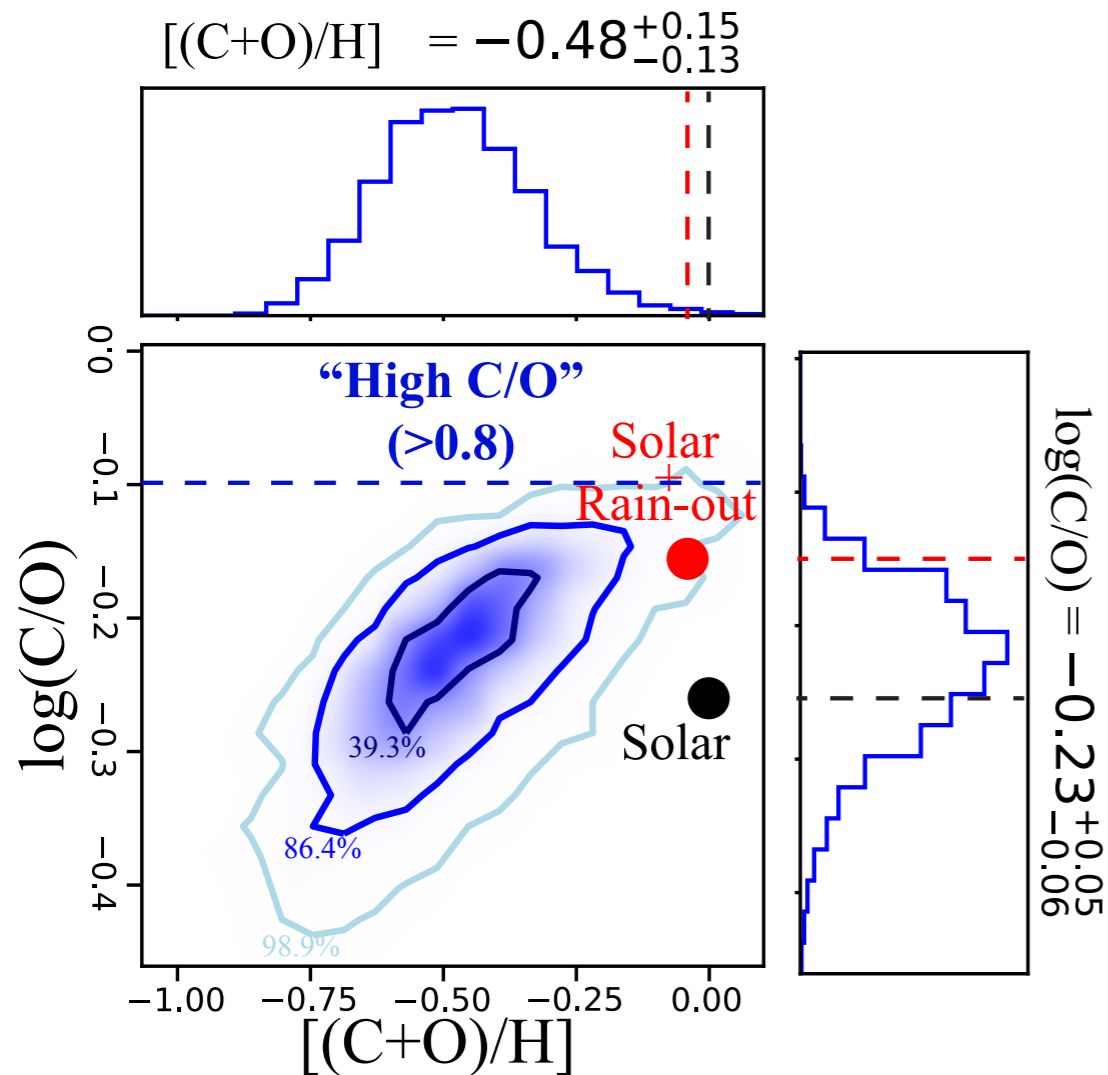
Computationally intensive
1 model evaluation =
5-10s on a single CPU core
(GPU+parallel computing)

What can we do with such precision?

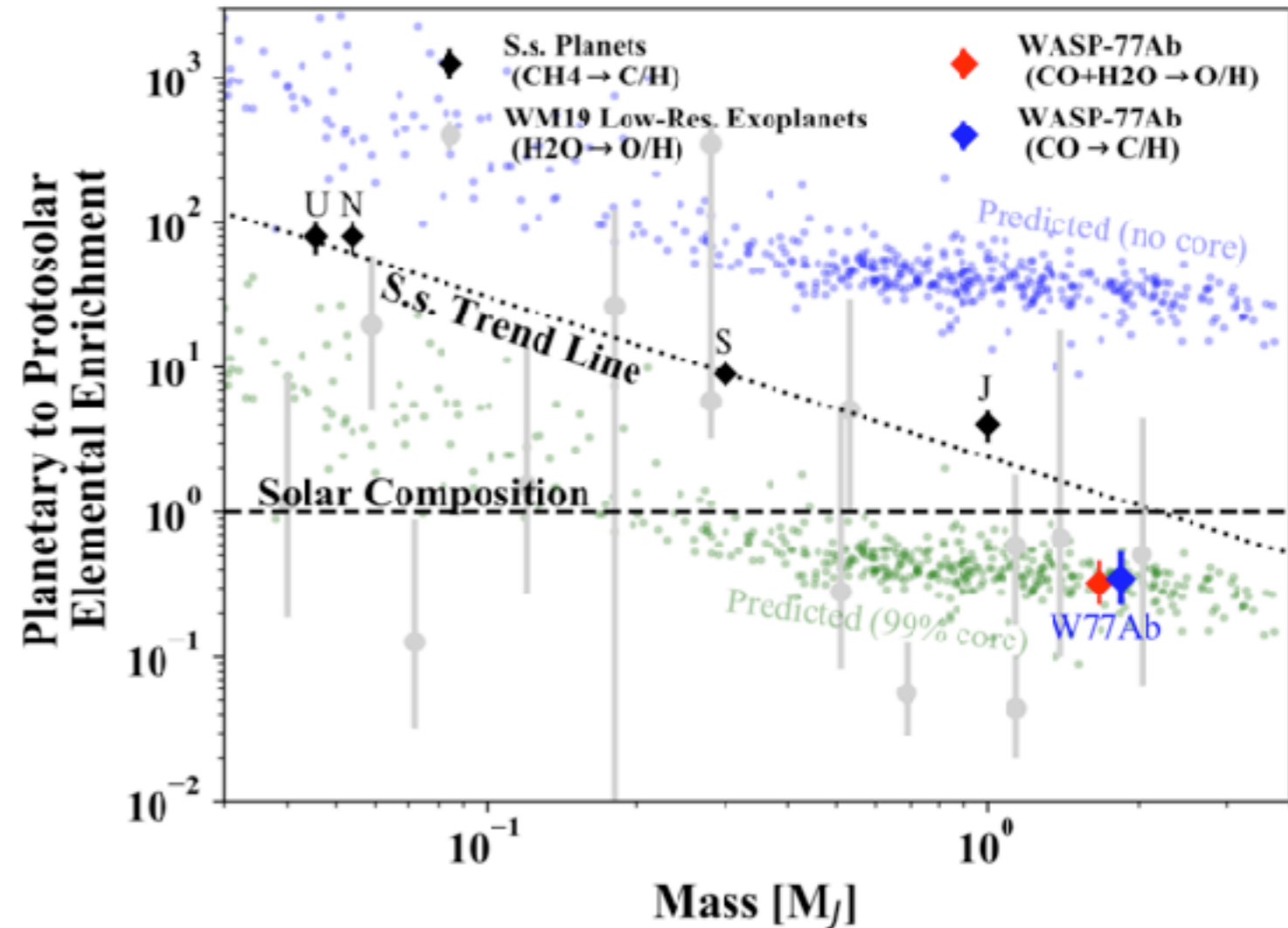
Constraints in the chemistry

WASP-77 A b has sub-solar metallicity but solar C/O

CO+H₂O ⇒ Metallicity, C/O



Mass-metallicity relation



C/O & metallicity of hot Jupiters can be connected to formation and early evolution scenarios

2021 has seen three measurements of C/O & metallicity (Giacobbe+21; Line+21; Pelletier+21)

The host star as a source of noise

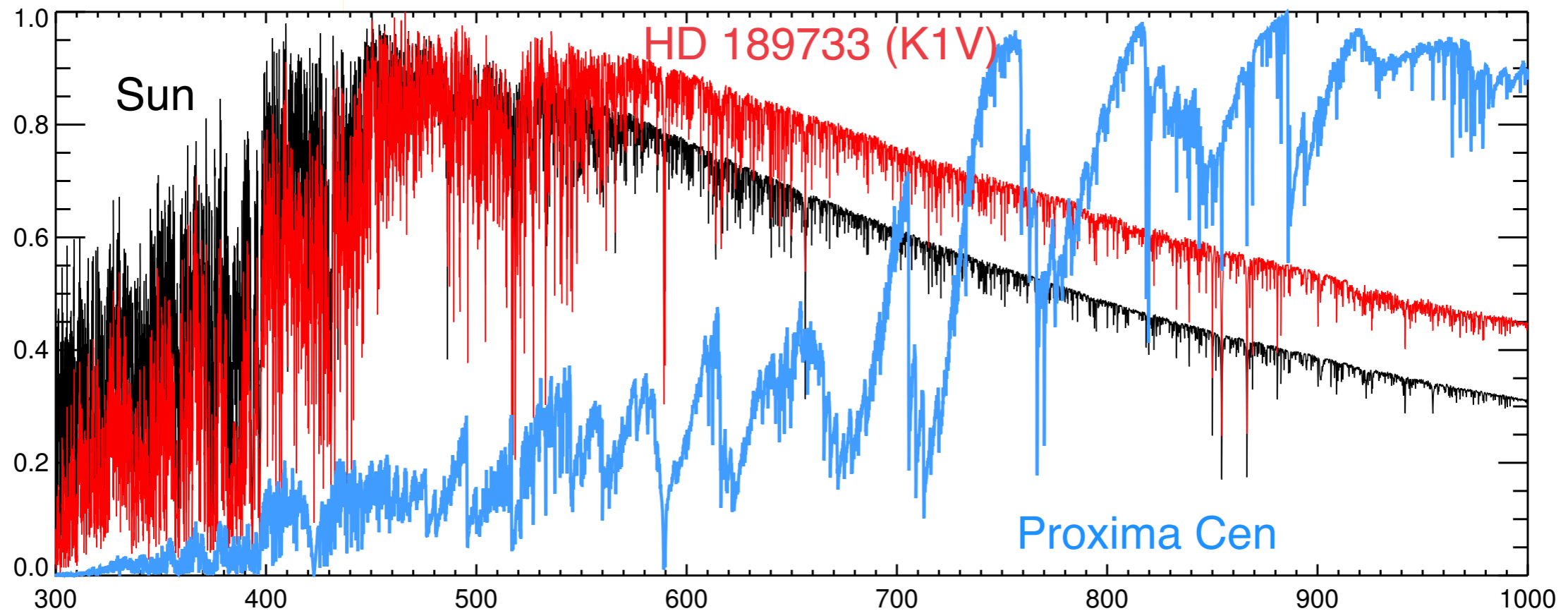
Influence on both emission and transmission spectra

Modelling and removal of the stellar spectrum

One example: rotation of giant exoplanets

Stars are not black bodies

Their spectra have an “envelope” (continuum) plus spectral lines



Spectral lines are formed by different atoms / molecules vs. temperature

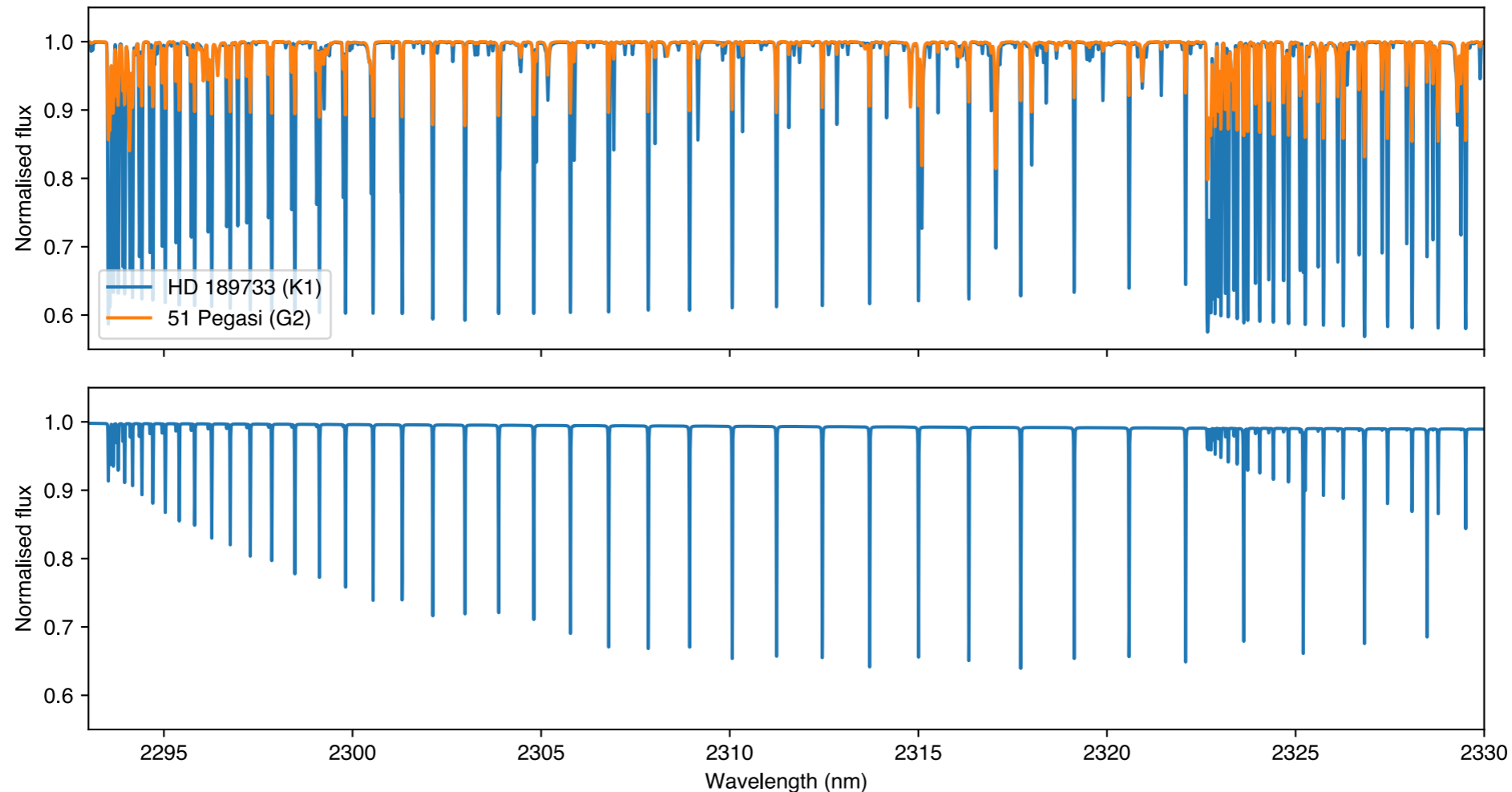
Spectral lines are formed at various depths, each characterised by T and ν

Spectral lines are formed at various points on a rotating stellar surface

We expect stellar spectra to be a “nuisance” for exoplanet detections

Stars and hot Jupiters can have “similar” spectra

Especially true for the CO spectrum at 2.3 μm



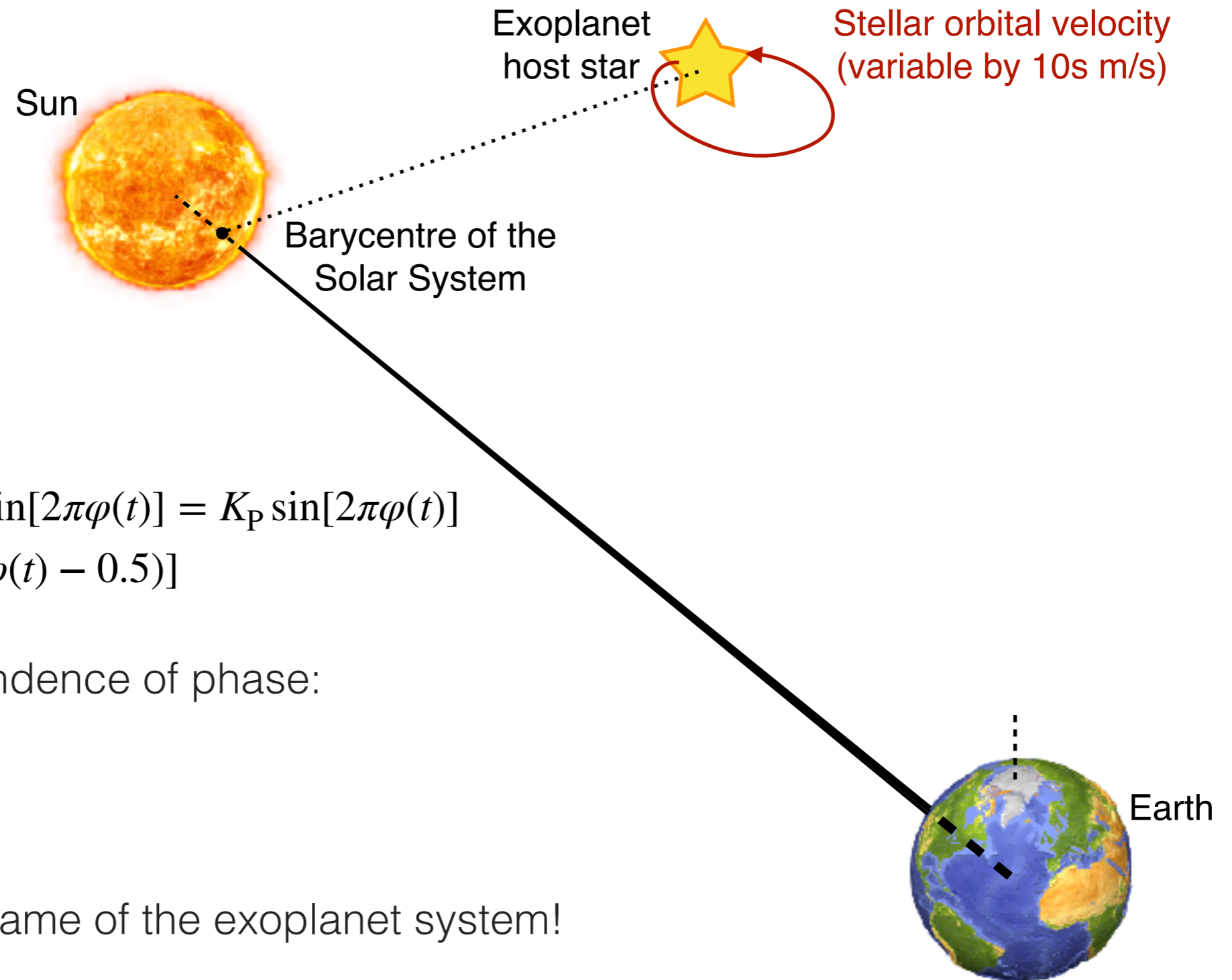
Stars of spectral type G or later exhibit strong CO lines, as hot Jupiters do!

Cooler stars (M-dwarfs) also have TiO and H₂O similarly to hot exoplanets

We expect stellar spectra to be a “nuisance” for exoplanet detections

Stars are not stationary sources of noise

If they were stationary, our data analysis techniques would suppress their spectra



From yesterday:

$$RV_P = V_{\text{orb}} \sin(i) \sin[2\pi\varphi(t)] = K_P \sin[2\pi\varphi(t)]$$

$$RV_{\star} = K_{\star} \sin[2\pi(\varphi(t) - 0.5)]$$

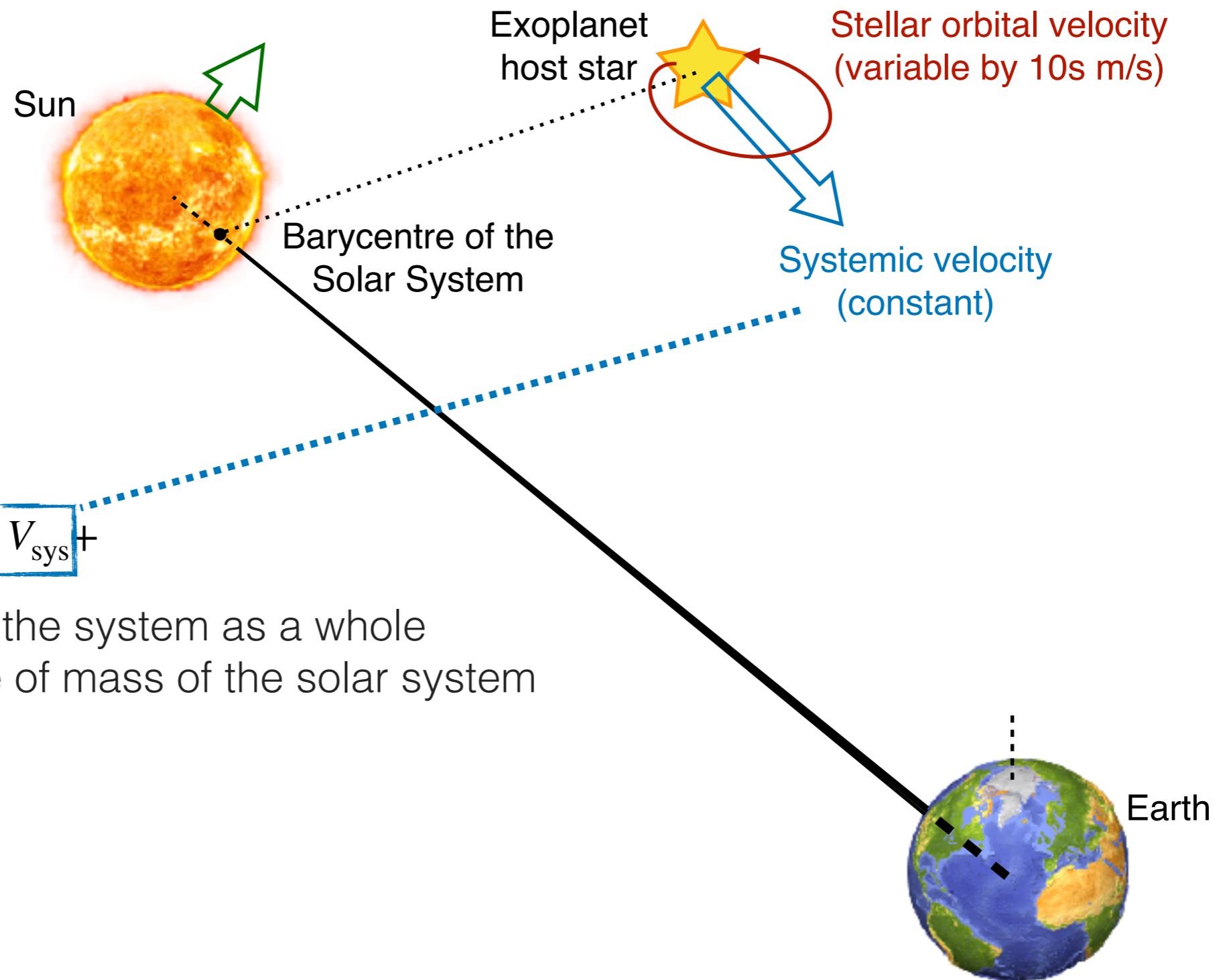
Explicit time dependence of phase:

$$\varphi(t) = \frac{t - T_0}{P_{\text{orb}}}$$

This is in the rest frame of the exoplanet system!

Stars are not stationary sources of noise

If they were stationary, our data analysis techniques would suppress their spectra

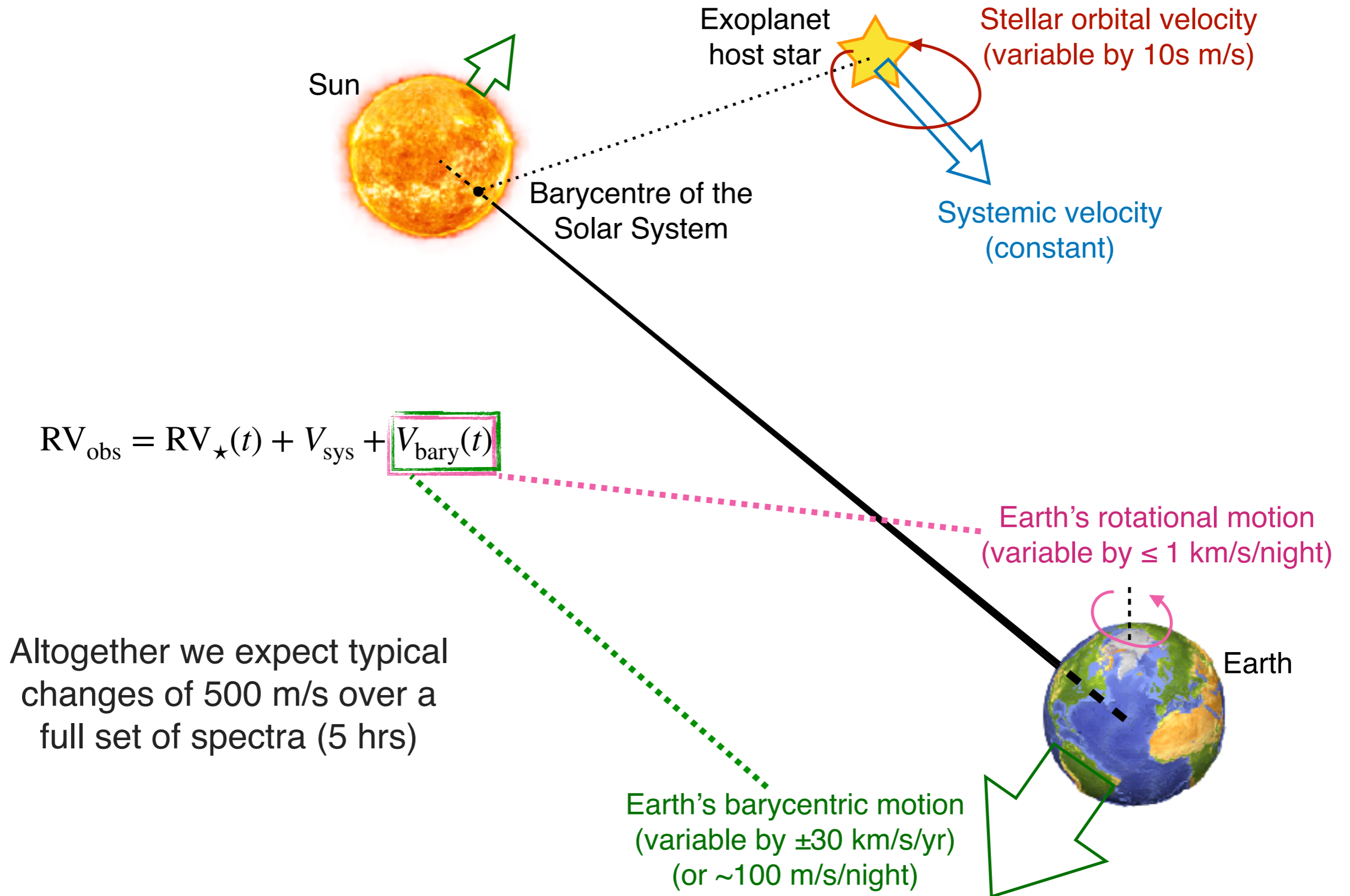


$$RV_{\text{obs}} = RV_{\star}(t) + V_{\text{sys}} +$$

Radial velocity of the system as a whole compared to the centre of mass of the solar system

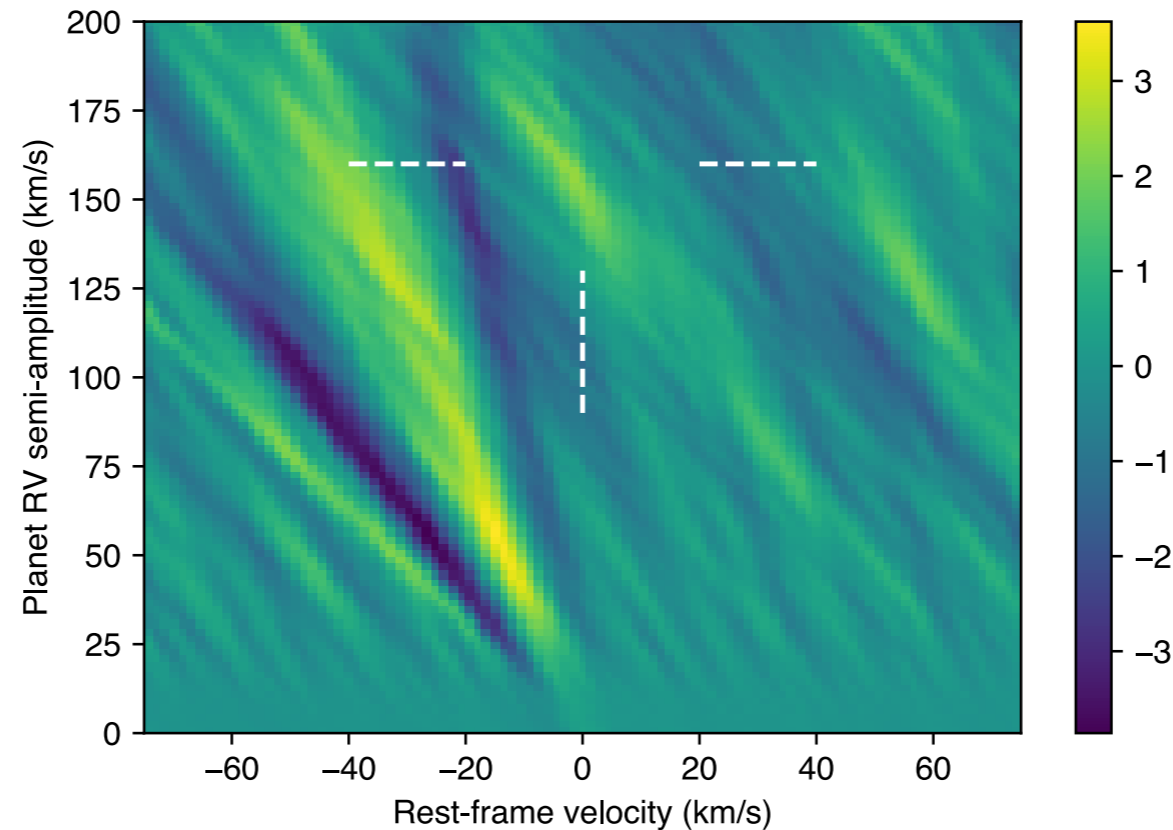
Stars are not stationary sources of noise

If they were stationary, our data analysis techniques would suppress their spectra



Stellar cross correlation noise in dayside spectroscopy

Case 1: Search for CO in the thermal spectrum of HD 189733 b (de Kok+13)
The star HD 189733 also has CO lines \Rightarrow contaminating signal



Where does stellar noise appear in the (V_{rest}, K_P) diagram?

The star moves with the system, so it should be at $V_{\text{rest}}=0$
It should also appear at $K_P \sim 0$ because its RV amplitude is < 1 km/s

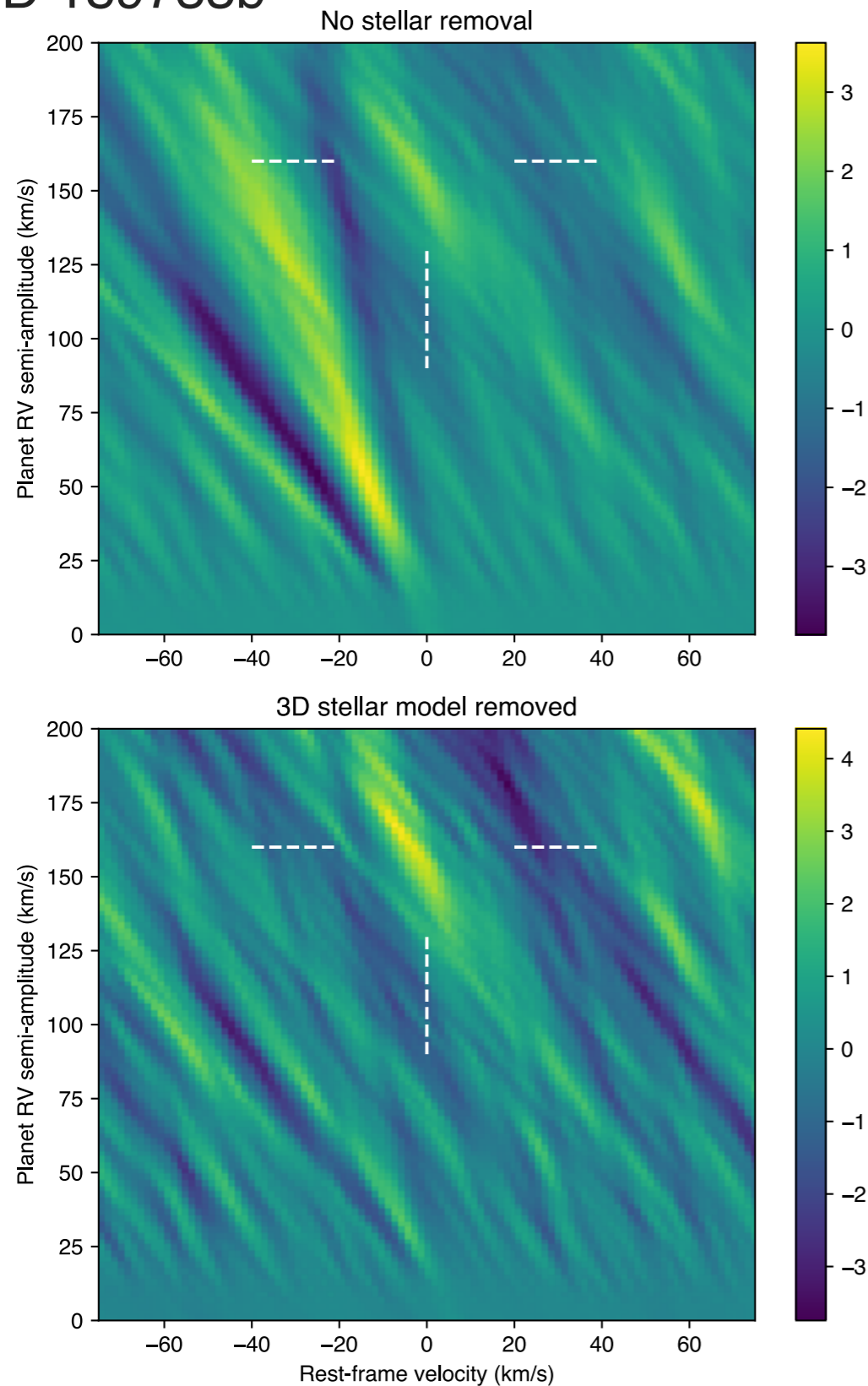
Very strong residuals and small change of the Earth's barycentric velocity
cause stellar residuals to propagate to $K_P \neq 0$ and peak at small K_P

Planet detection is not prevented but highly confused

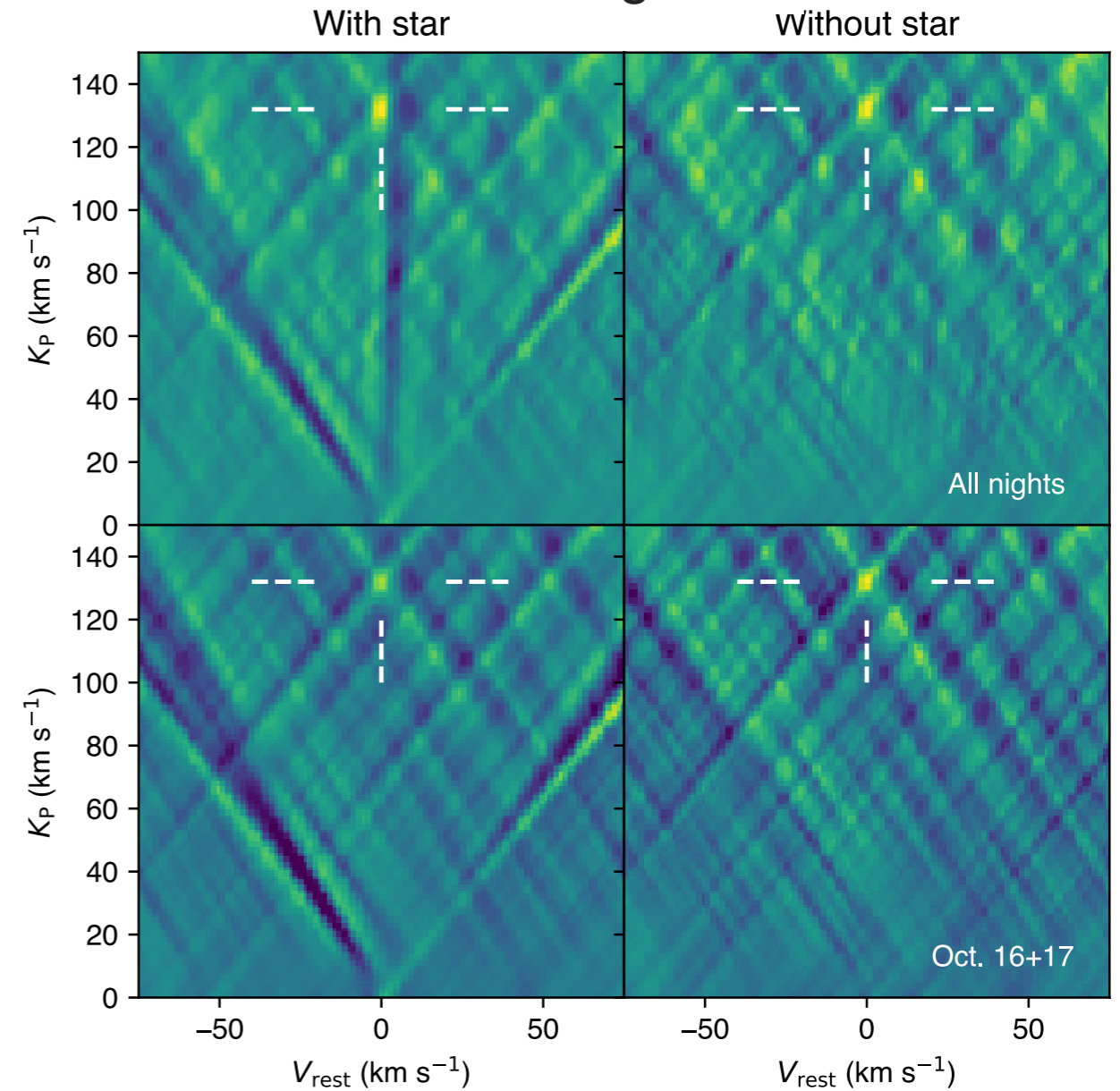
Applications to emission spectroscopy

Results from Chiavassa & Brogi (2019)

HD 189733b



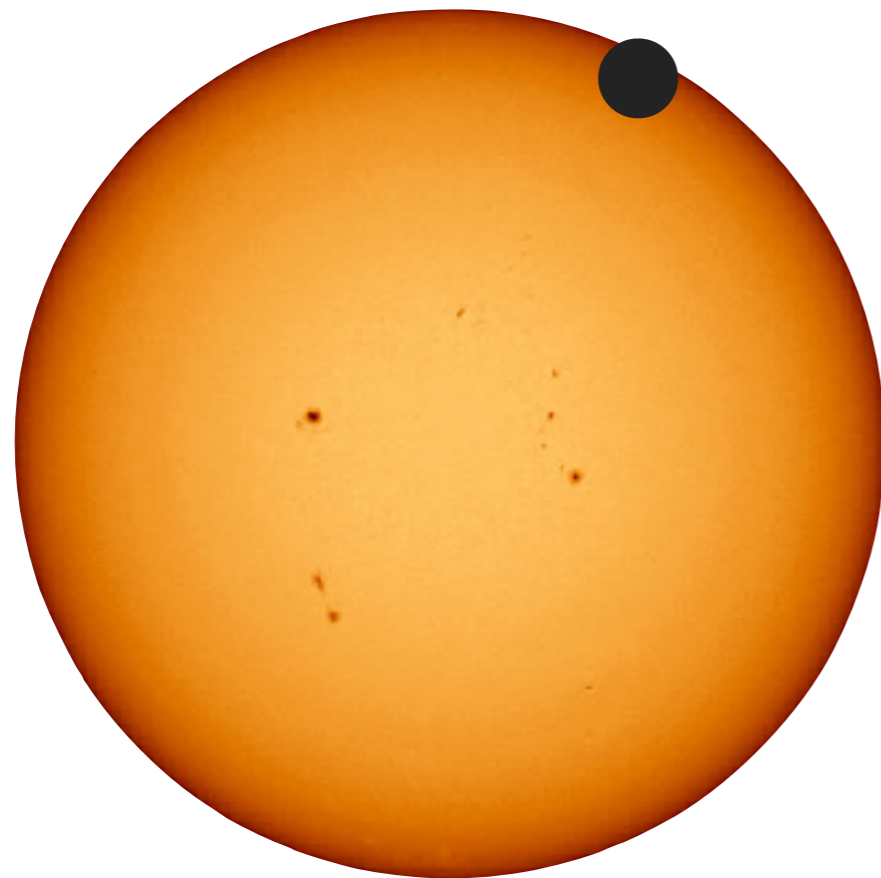
51 Pegasi b



Stellar spectra in emission spectroscopy
can be corrected with both 1D and 3D
stellar models

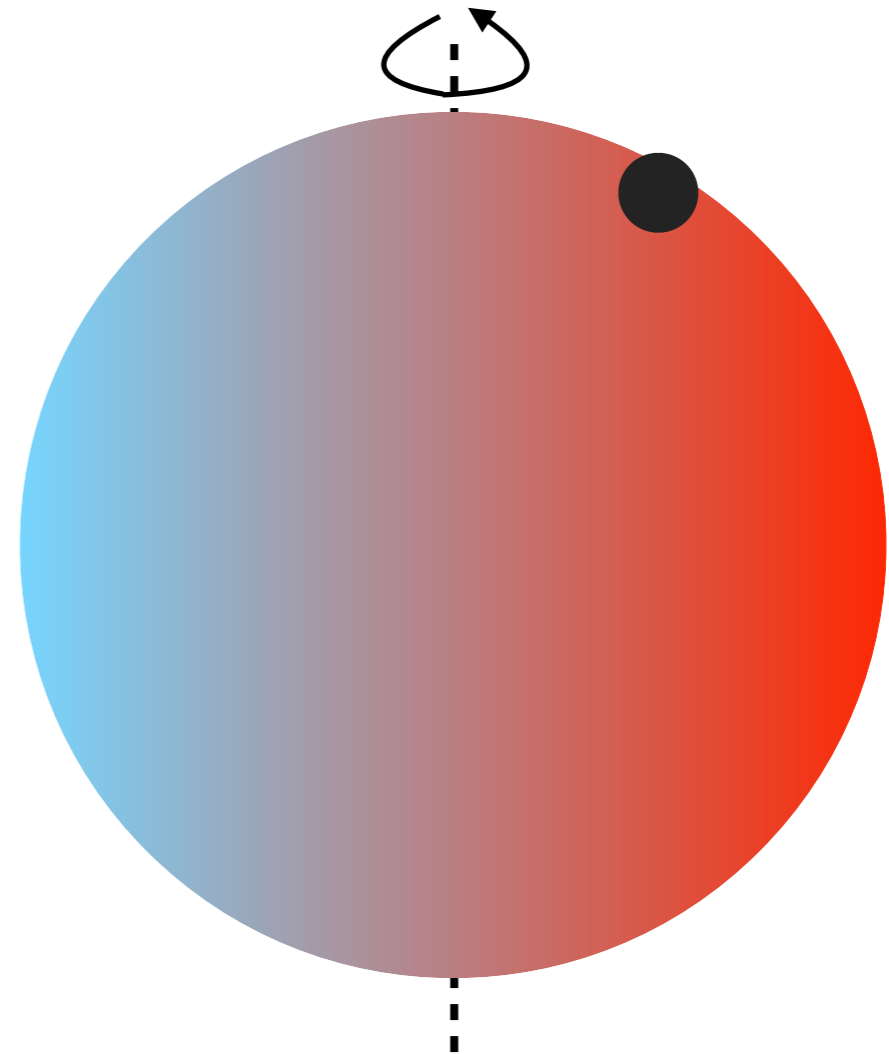
A transiting planet distorts the stellar spectrum

Stellar intensities vary according to distance from centre (limb darkening)
Stars are rotating with a spin-orbit angle that can be non-zero



Centre-to-limb variations

A transiting planet blocks regions of the stellar surface with different intensities



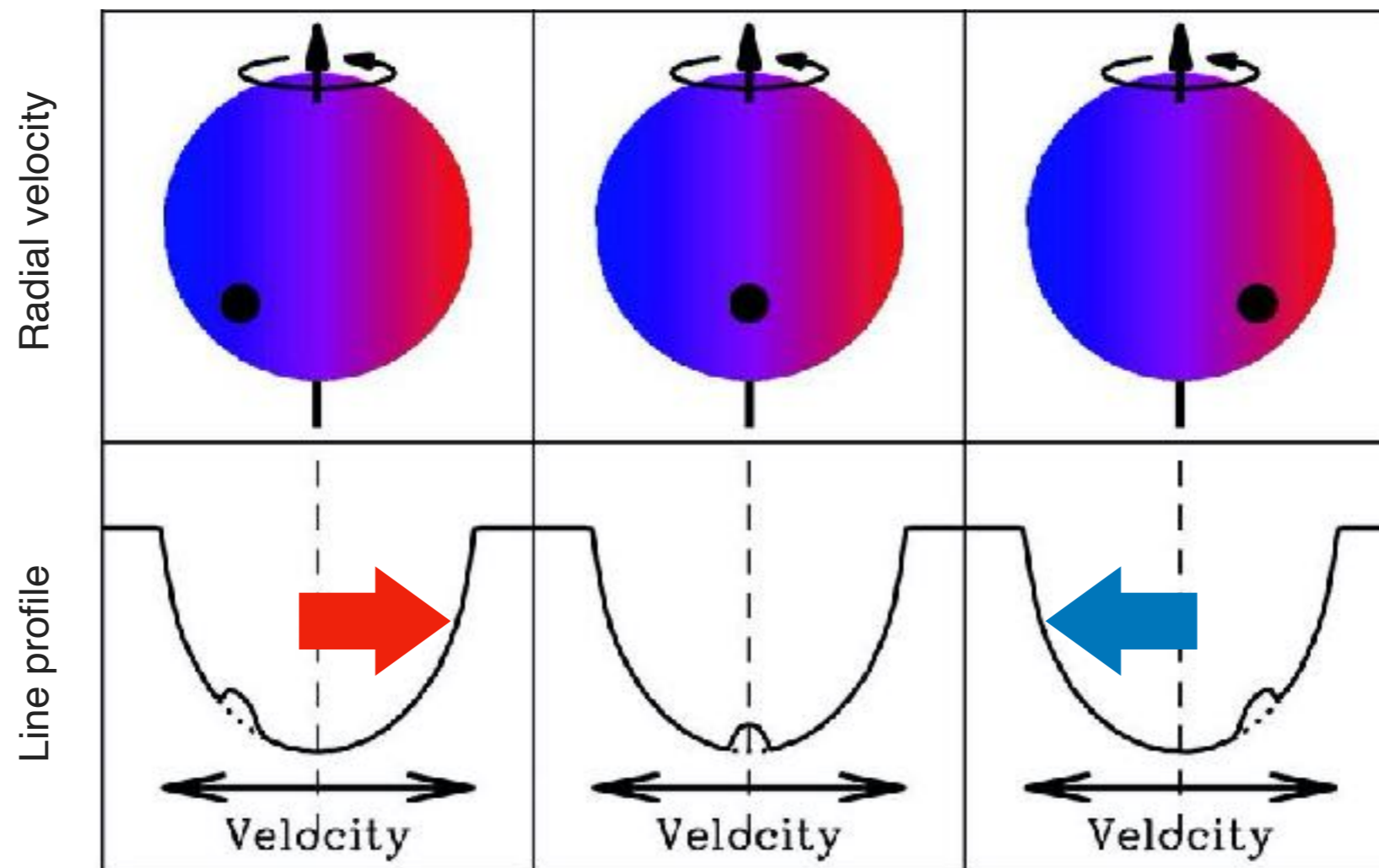
Rossiter-McLaughlin effect

A transiting planet blocks regions of the stellar surface with different rotation

If uncorrected, stellar residuals during transit can dominate the cross correlation signal

The Rossiter-McLaughlin effect

A transiting planet blocks a (changing) portion of a rotating star
The line profile gets distorted, and the CCF is also asymmetric



Adapted from
Gaudi & Winn 2007

Problem: stellar RVs are determined by fitting the CCF with a symmetric profile

Beginning of the transit

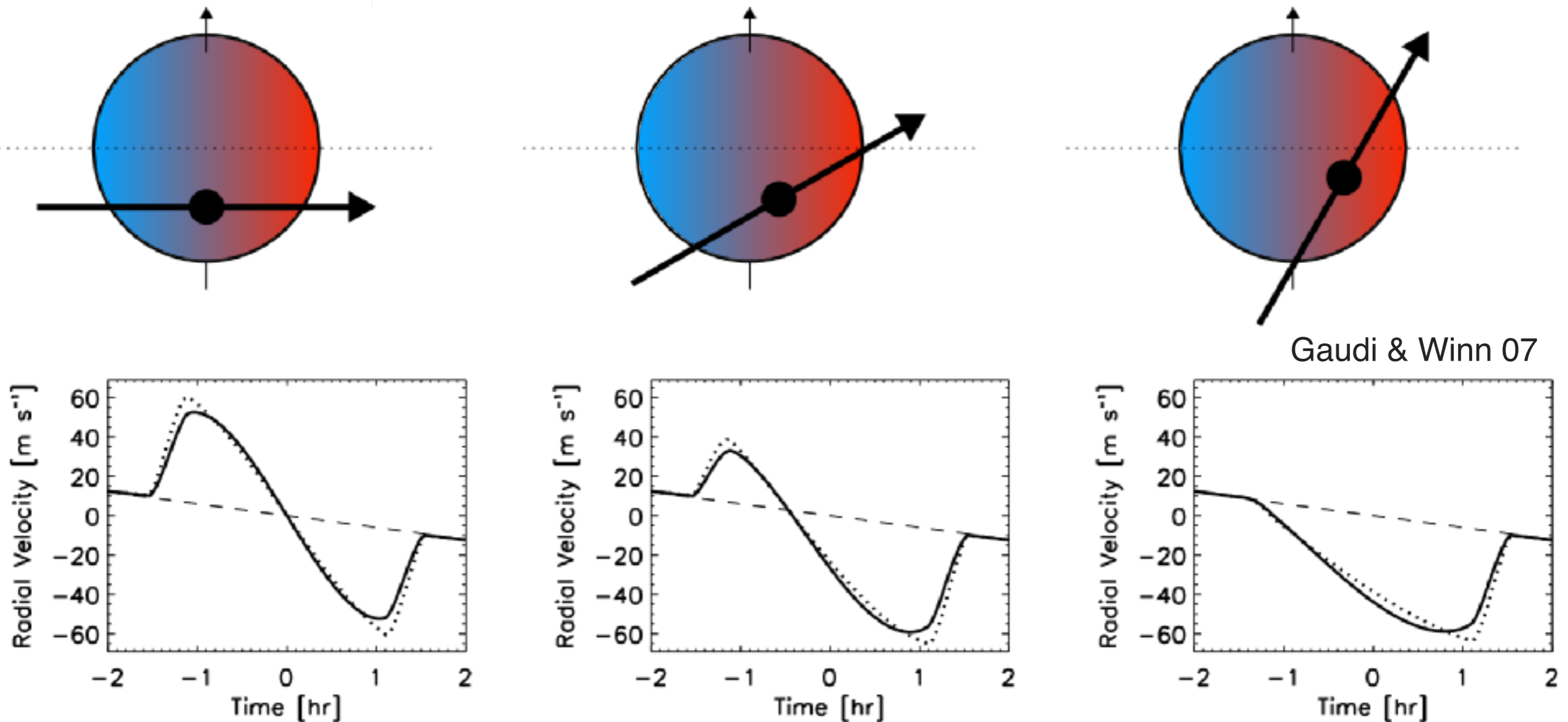
Blue-shifted part of the rotating disk is
blocked \Rightarrow red-shifted CCF

End of the transit

Red-shifted part of the rotating disk is
blocked \Rightarrow blue-shifted CCF

RM effect shifts centroid of cross correlation functions

Distorted line profiles are fitted with Gaussian profiles

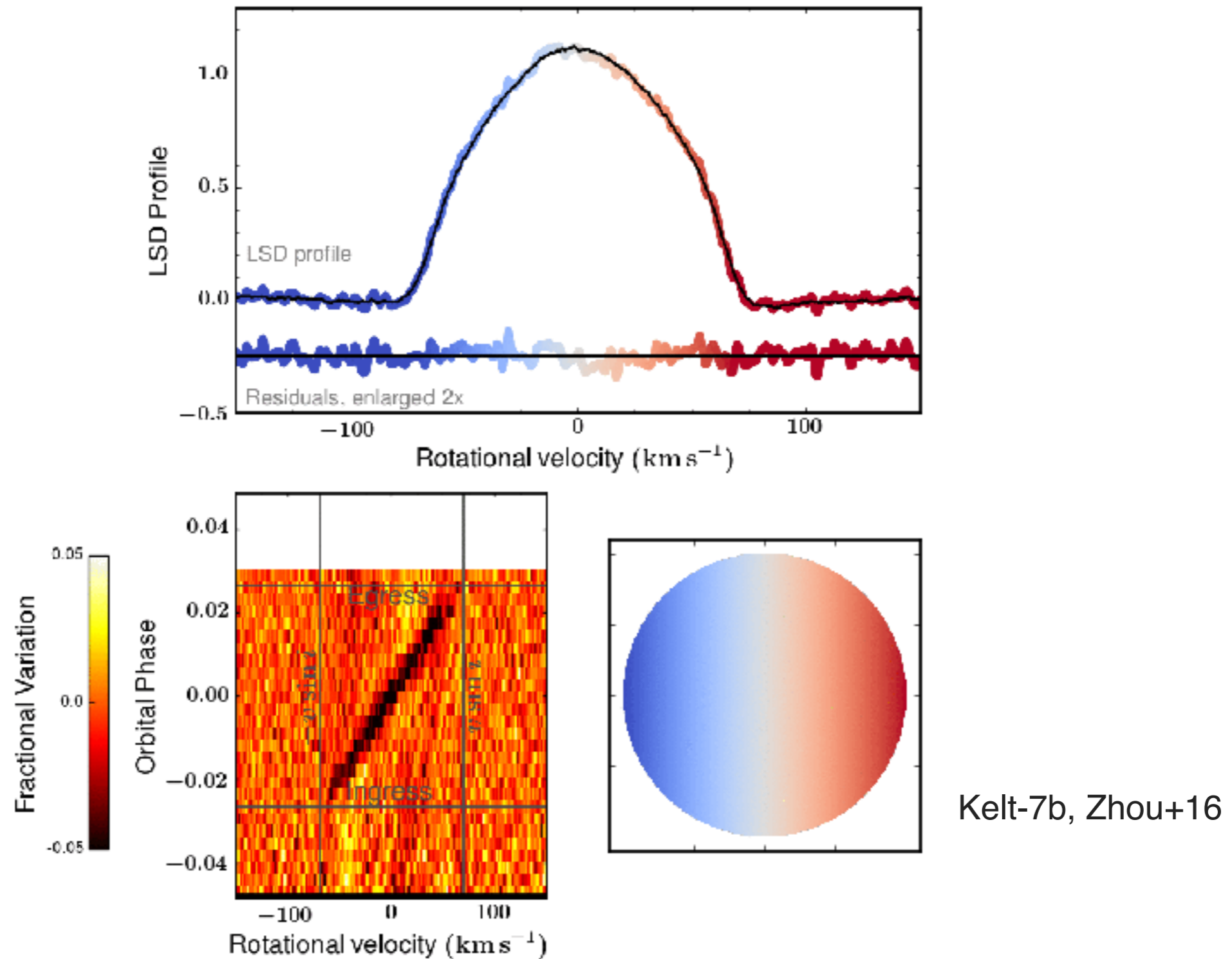


The shape of the RM effect can be used to estimate the angle between the orbit of the planet and the spin of the star: the spin-orbit angle

Smaller planets or highly misaligned planets can have very small RM effect

RM effect visualised through Doppler tomography

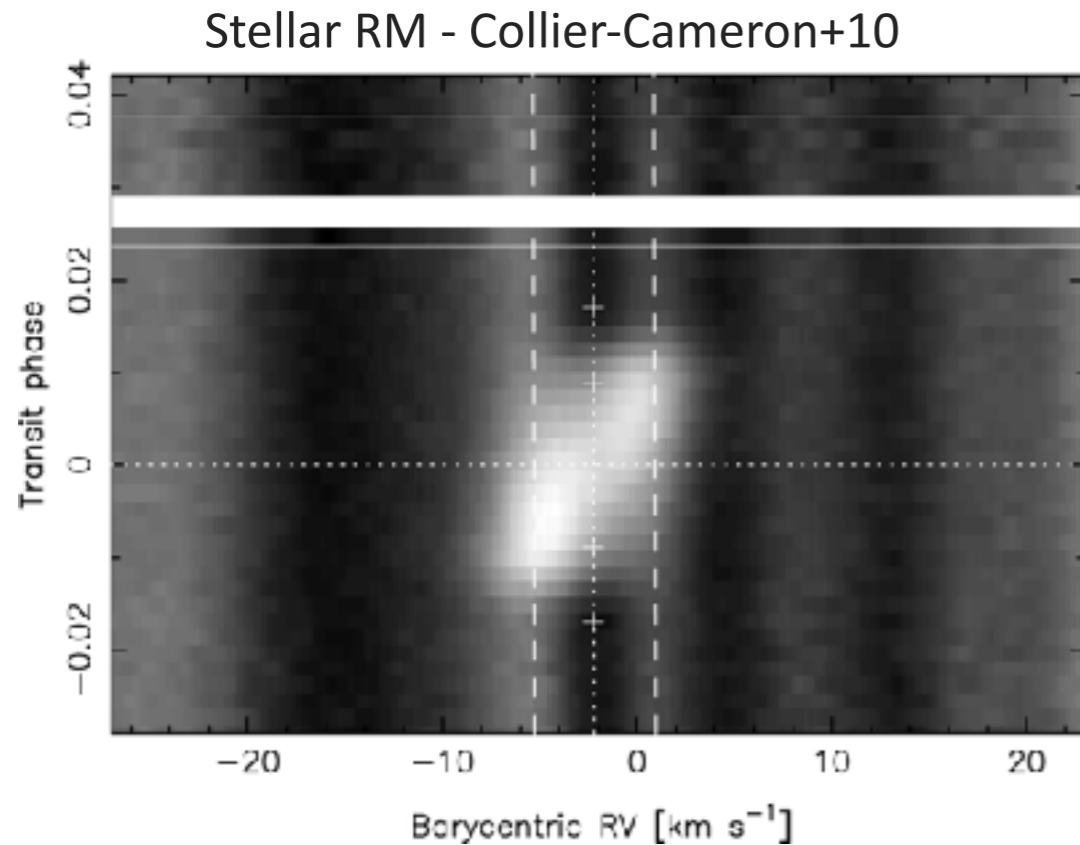
Requires dividing each CCF by the out-of-transit (symmetric) CCF



This allows us to see the planet shadow sweeping in radial velocity between $\pm v \sin i$

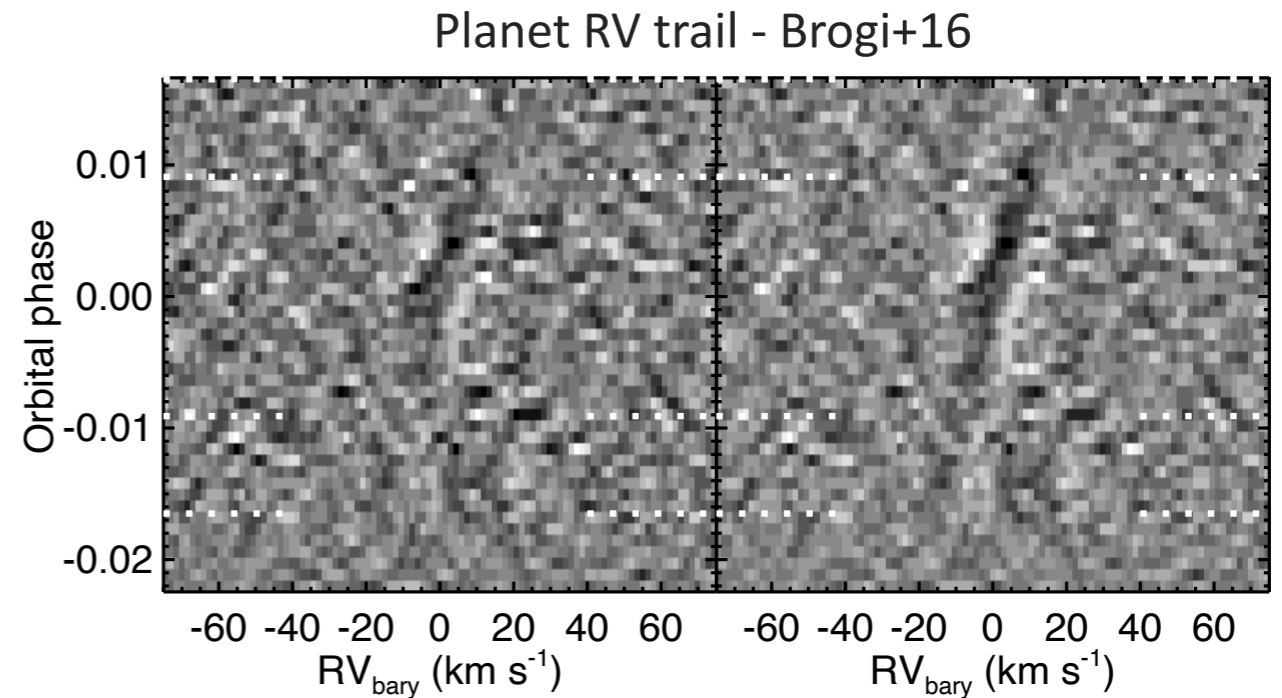
But wait... isn't that what the planet does too?

Yes, planet transmission spectra and planet shadows both sweep in RV during transit
Example: the transmission spectrum of HD 189733b



Stellar RM

Sweeping $\pm v \sin i = \pm 3.3 \text{ km/s}$



Planet signal

Changing by $\pm 16 \text{ km/s}$

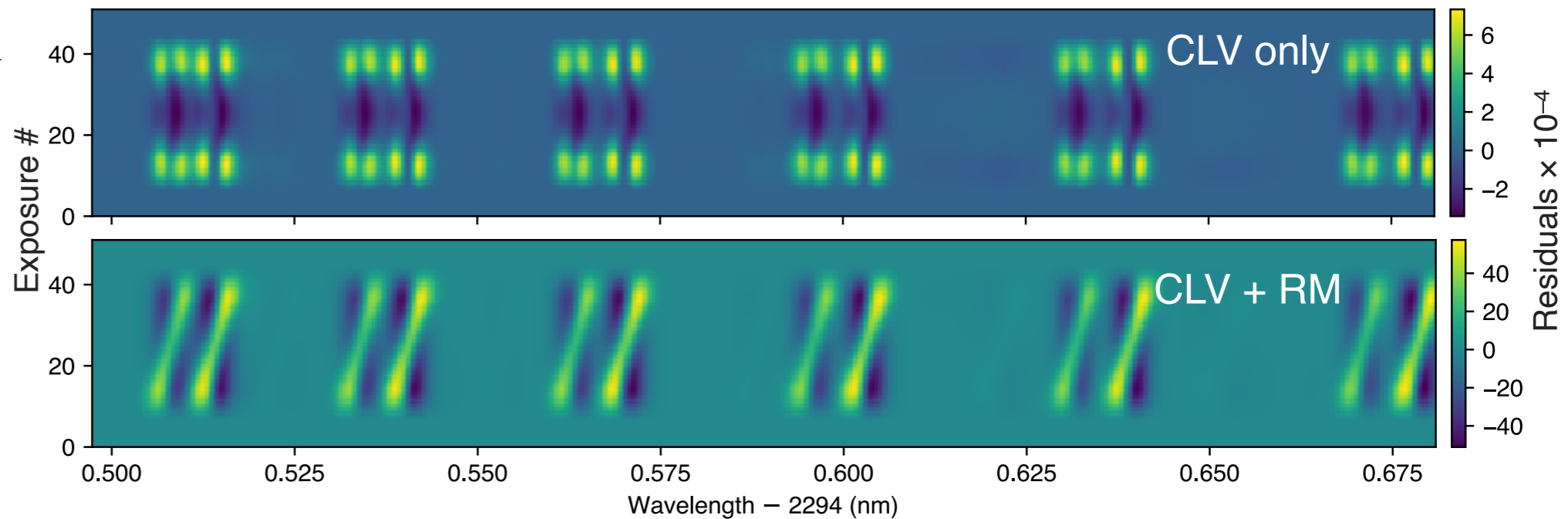
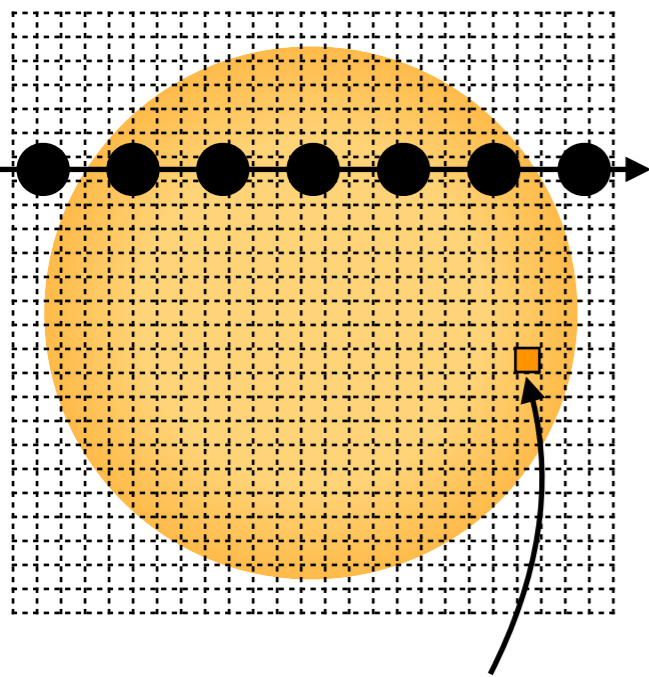
The stellar RM is \sim transit depth, the planet signature is 10-100 \times smaller!

Even if the slope of the RM effect is significantly different, it can still contaminate the planet signal due to its big amplitude!

Modelling the distorted stellar spectrum

see e.g. Chiavassa & Brogi 2019

Example: Doppler tomography of modelled CO stellar lines in HD 189733

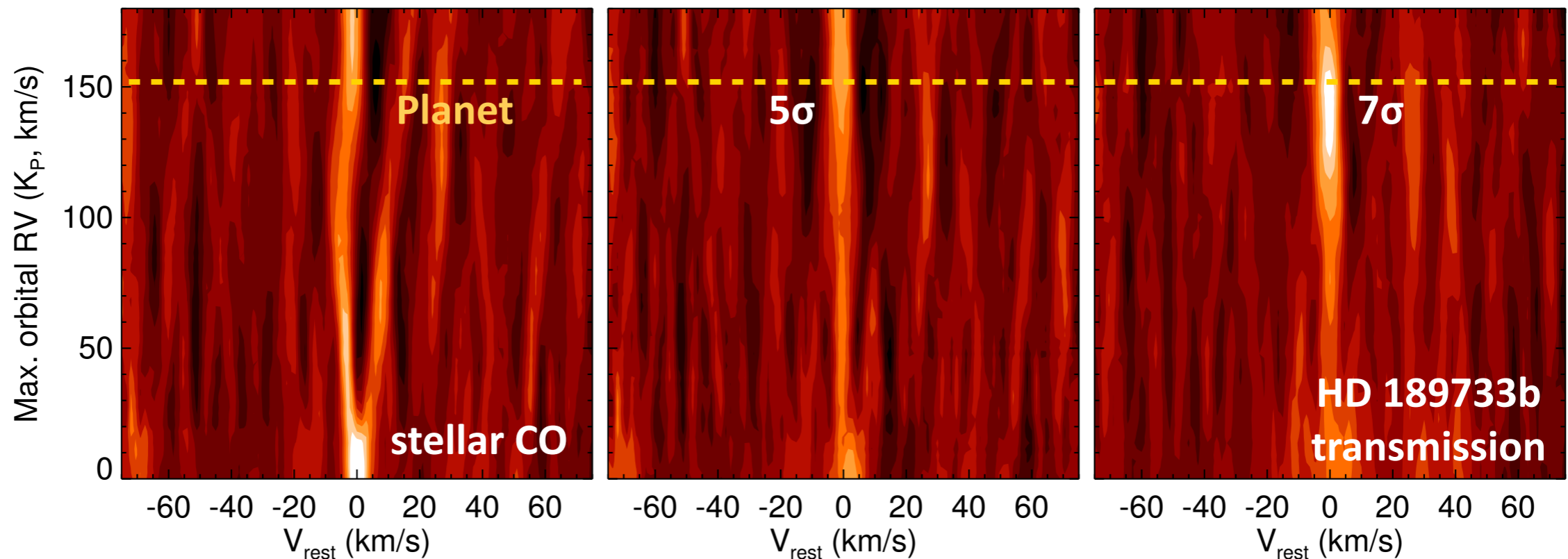


Spectrum as $f(\phi, \mu)$
Planet occupancy (0,1)
Doppler shift (rotation)

Uncorrected

1D line modelling

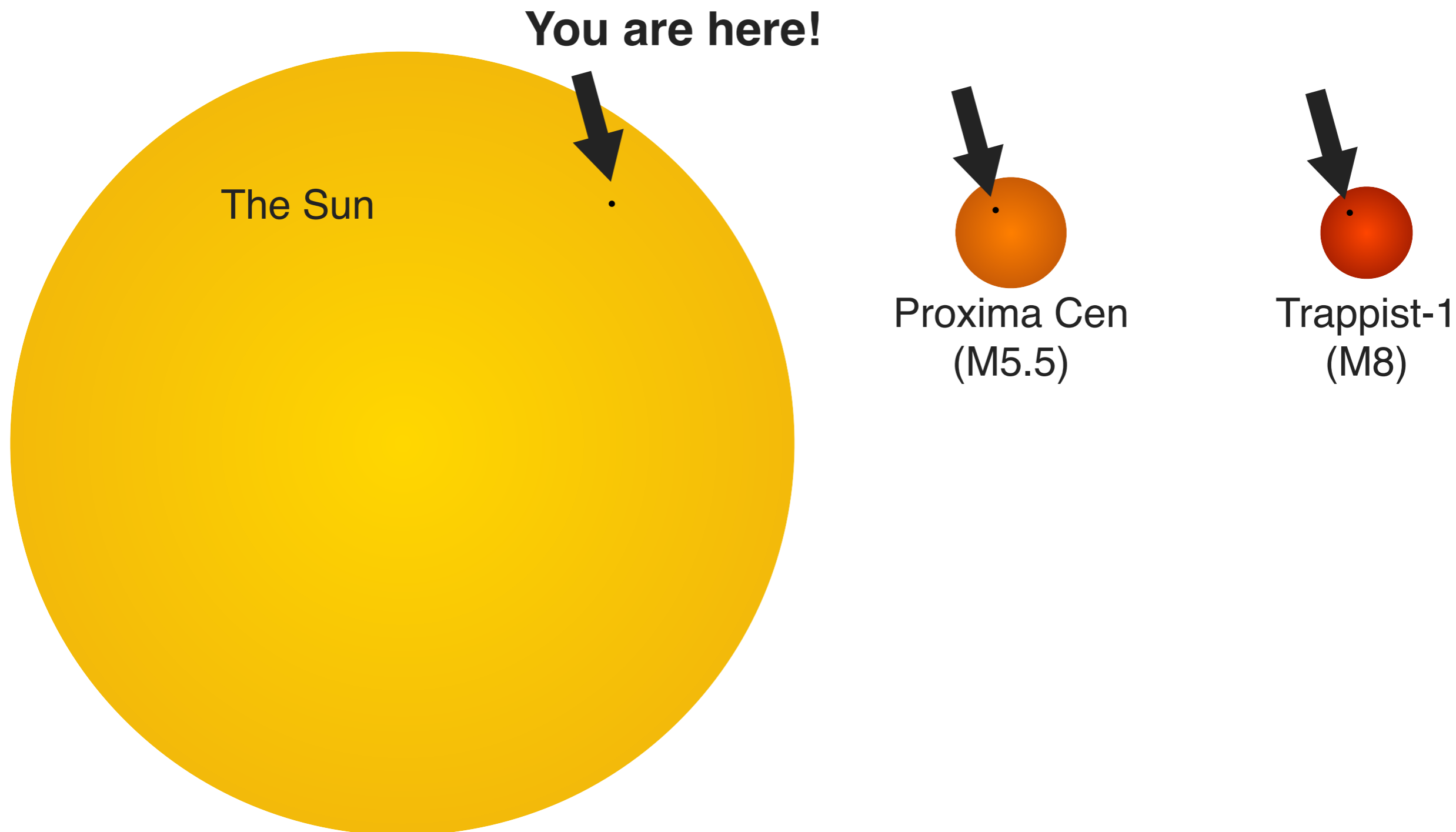
3D stellar modelling



Bridging the gap towards habitable planets

(in the next 10-15 years)

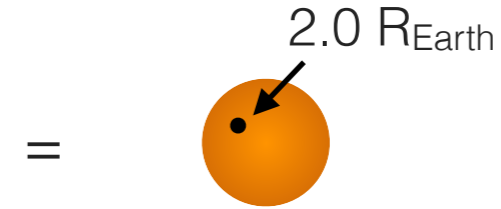
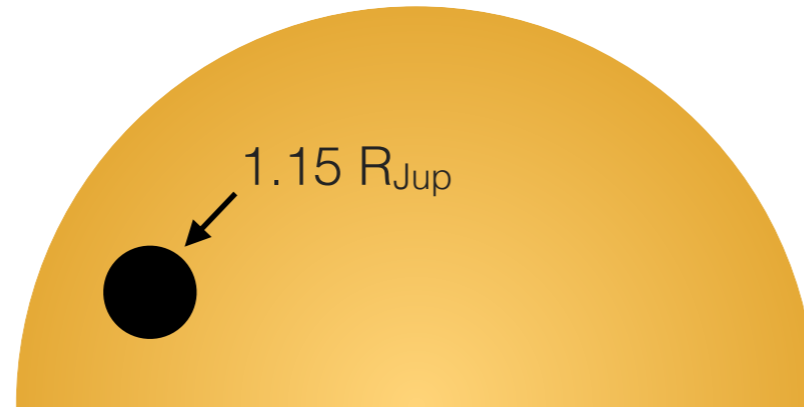
Planets around M-dwarf stars



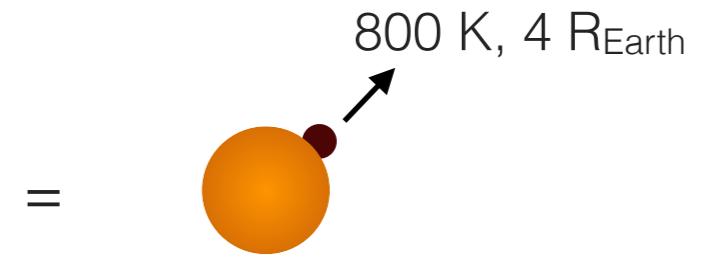
The key sample: M-dwarf planets

M-dwarfs are *smaller* and *cooler* than the Sun, but still bright in the infrared
Warm sub-Neptunes around (nearby) M-dwarfs are within reach of current techniques

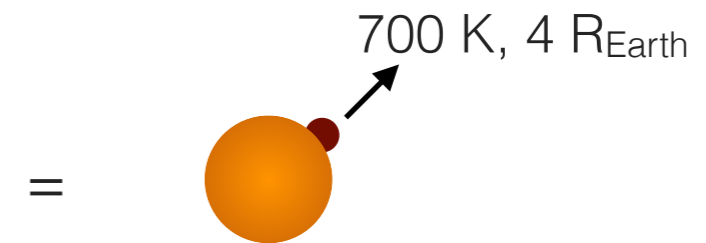
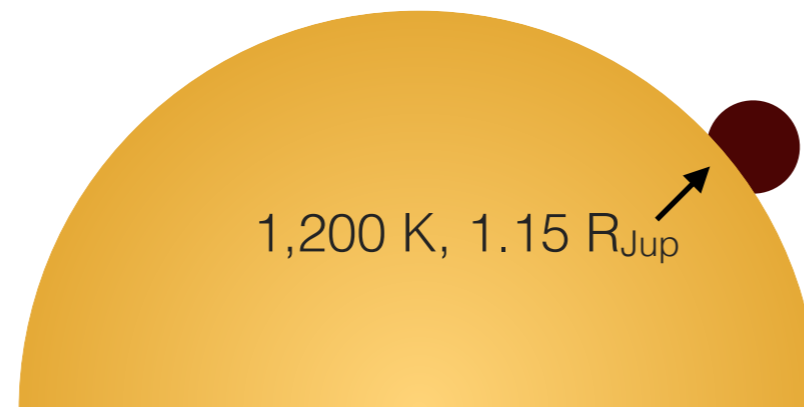
Transit
1.3% depth



Thermal emission
relative to star
(2.3 μm)
140 ppm



Thermal emission
relative to star
(3.5 μm)
470 ppm

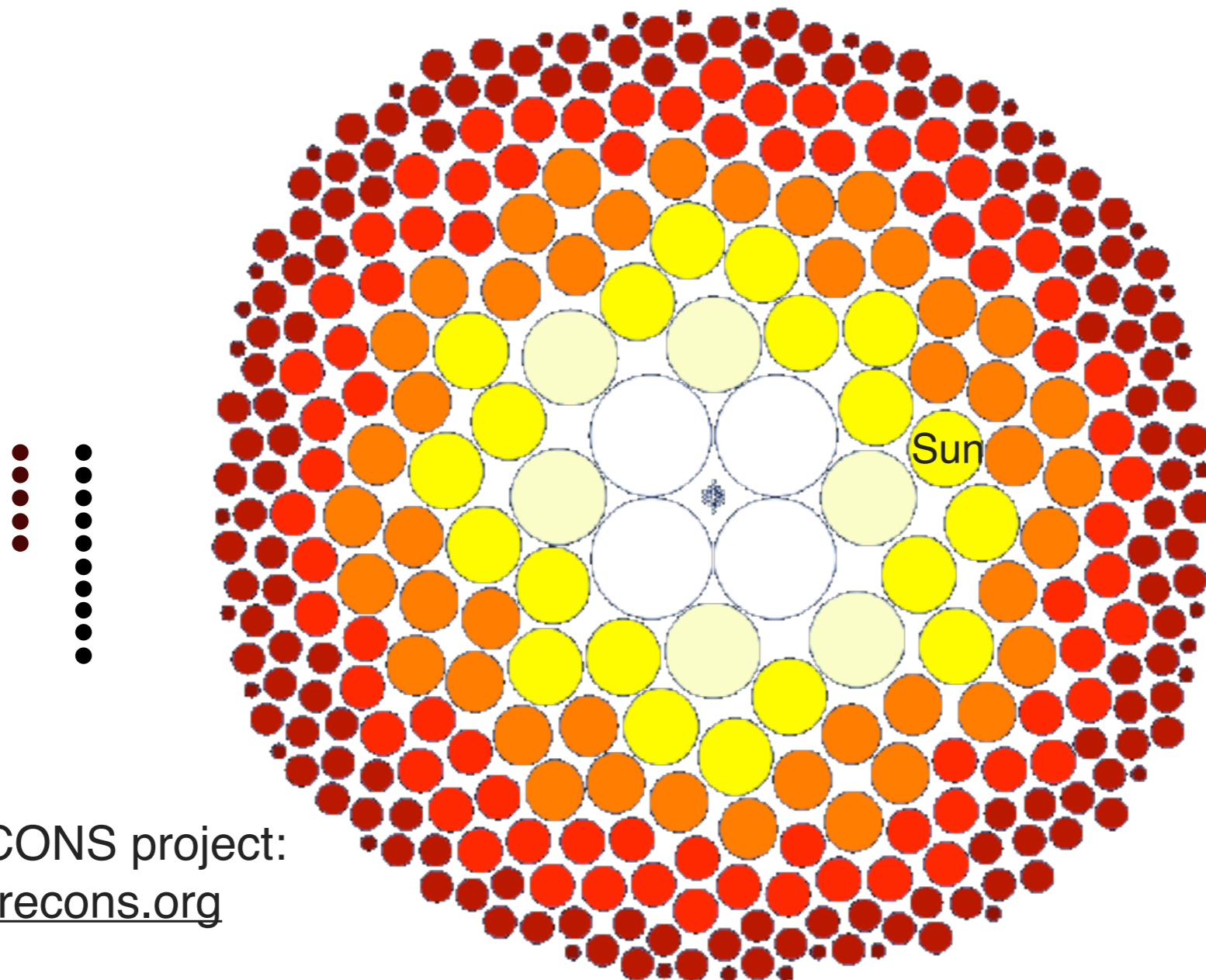


Solar-type star

M5.5 star

Planets around M-dwarf stars are abundant

Dressing & Charbonneau (2015): 2.5 planets / star, 30% in the classic habitable zone
M-dwarf stars are abundant \Rightarrow Temperate M-dwarf planets are nearby



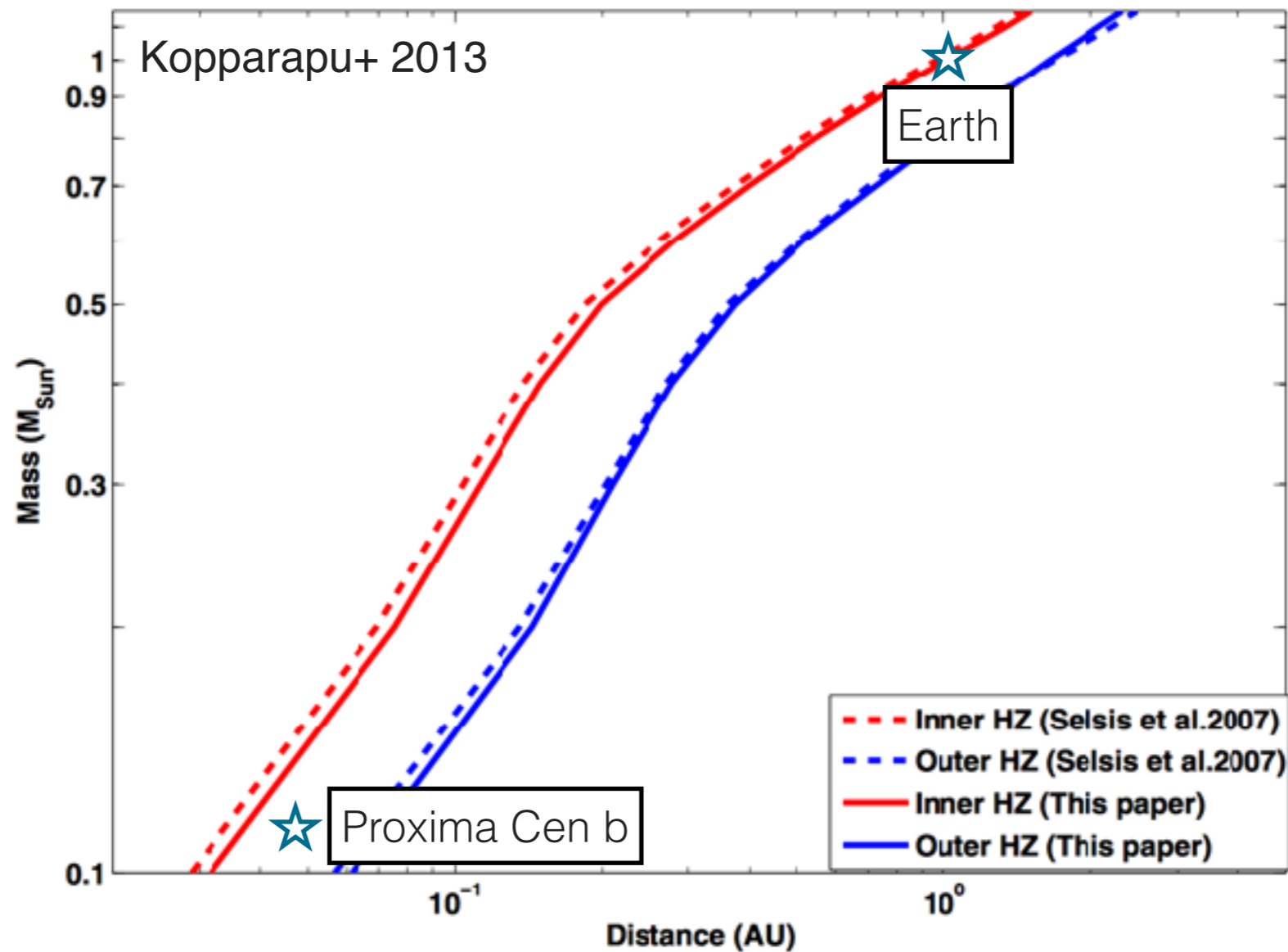
The RECONS project:
www.recons.org

WD:20
O:0
B:0
A:4
F:6
G:20
K:44
M:248
L:5
T:10
Planets:70+8

Current (incomplete) census: 70 planets within 10 pc, 35 within 5 pc
Notable examples: Proxima Cen b,c (1.3 pc) & Trappist-1 a-g (12 pc)

Habitable zones around M-dwarfs

Habitable zone (Earth-based) moves inward with decreasing stellar mass
Potentially habitable planets orbit very close to M-dwarfs



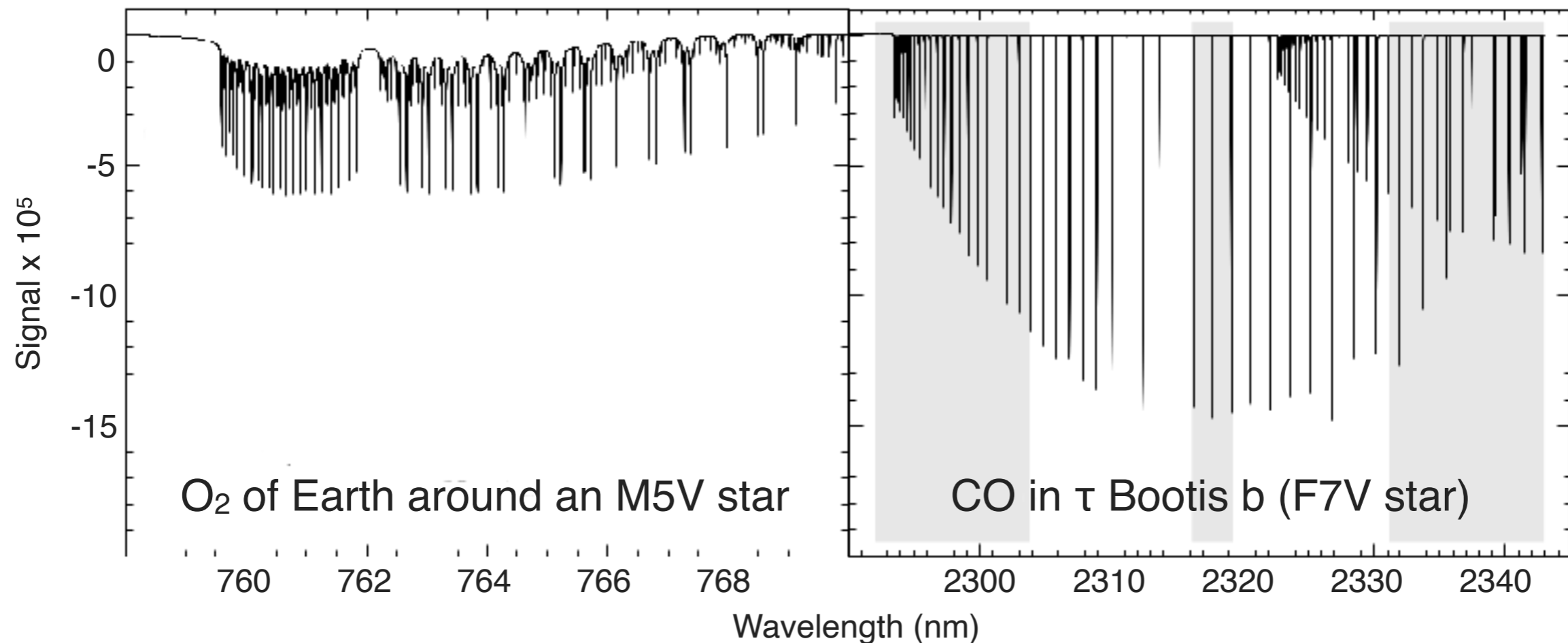
Key observational consequences

Temperate planets have an increased probability to transit M-dwarfs
Transits repeat every few days only and can be stacked quickly to increase S/N

Transiting terrestrial planets around M dwarfs

Oxygen in high-resolution transmission spectra

Average line depth is 1/3 of the CO dayside signal from τ Boo b



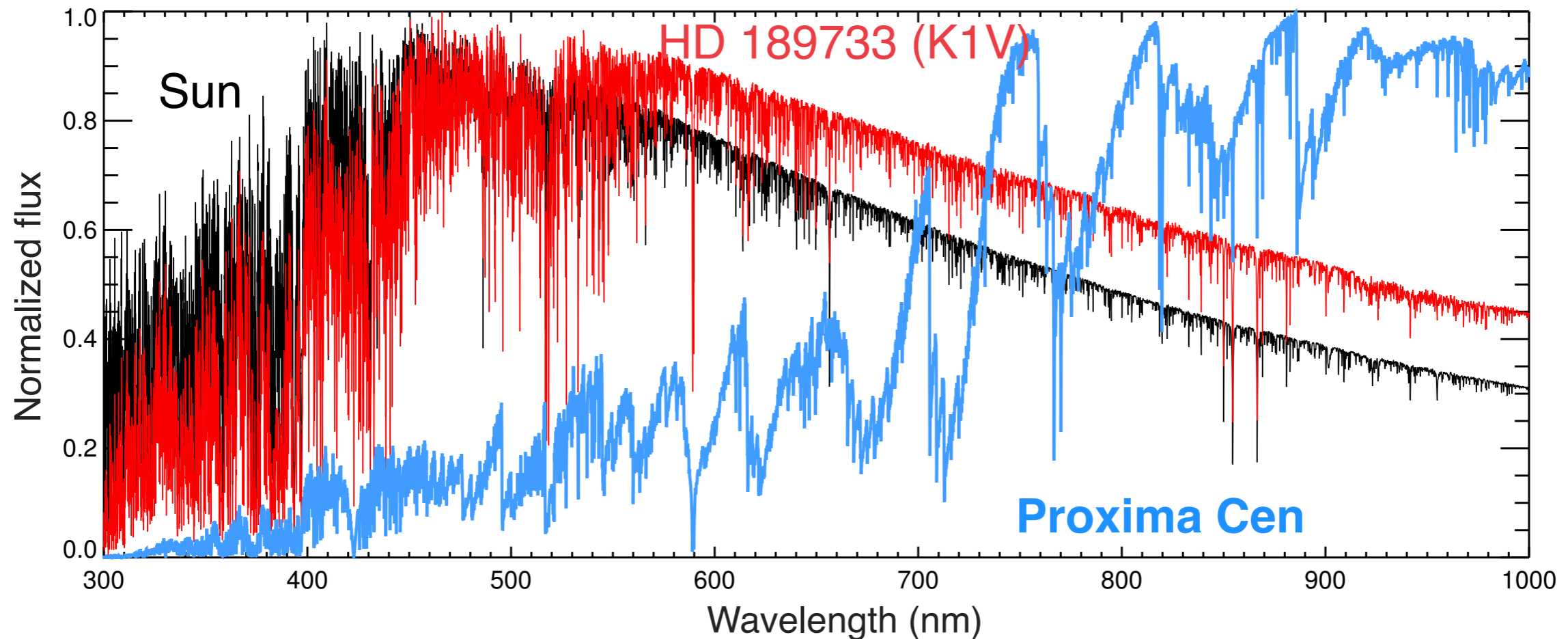
Challenge: even the closest M-dwarf is much fainter than τ Boo (at least 6 magnitudes)
Extremely Large Telescopes + Hi-res spectroscopy are needed to reach the S/N

39m E-ELT, 30 transits (3 years) \Rightarrow 3σ detection

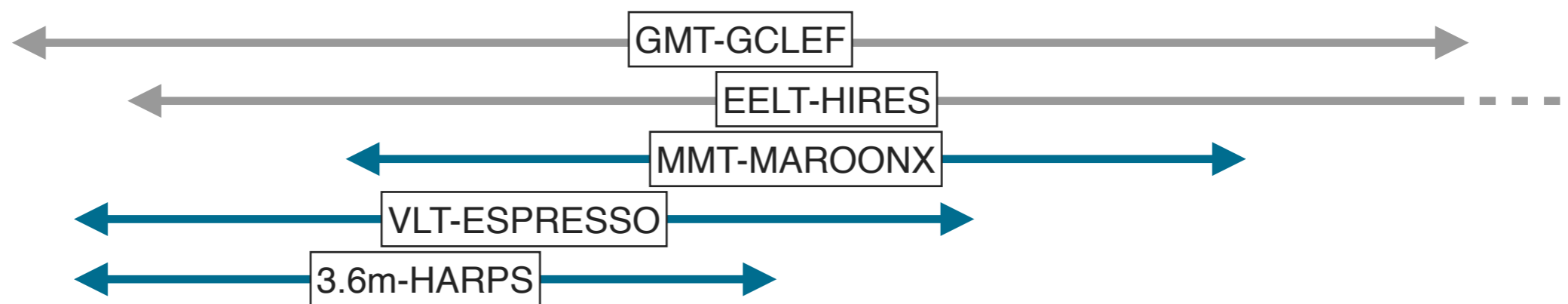
High instrumental efficiency and RV separation from telluric oxygen is key
(Snellen+13, Rodler & Lopez-Morales14; Serindag & Snellen 19; Lopez-Morales+19)

Reflected light from Proxima Centauri b

The star is faint in the optical (B=12.95, V=11.13, R=9.45) \Rightarrow low S/N



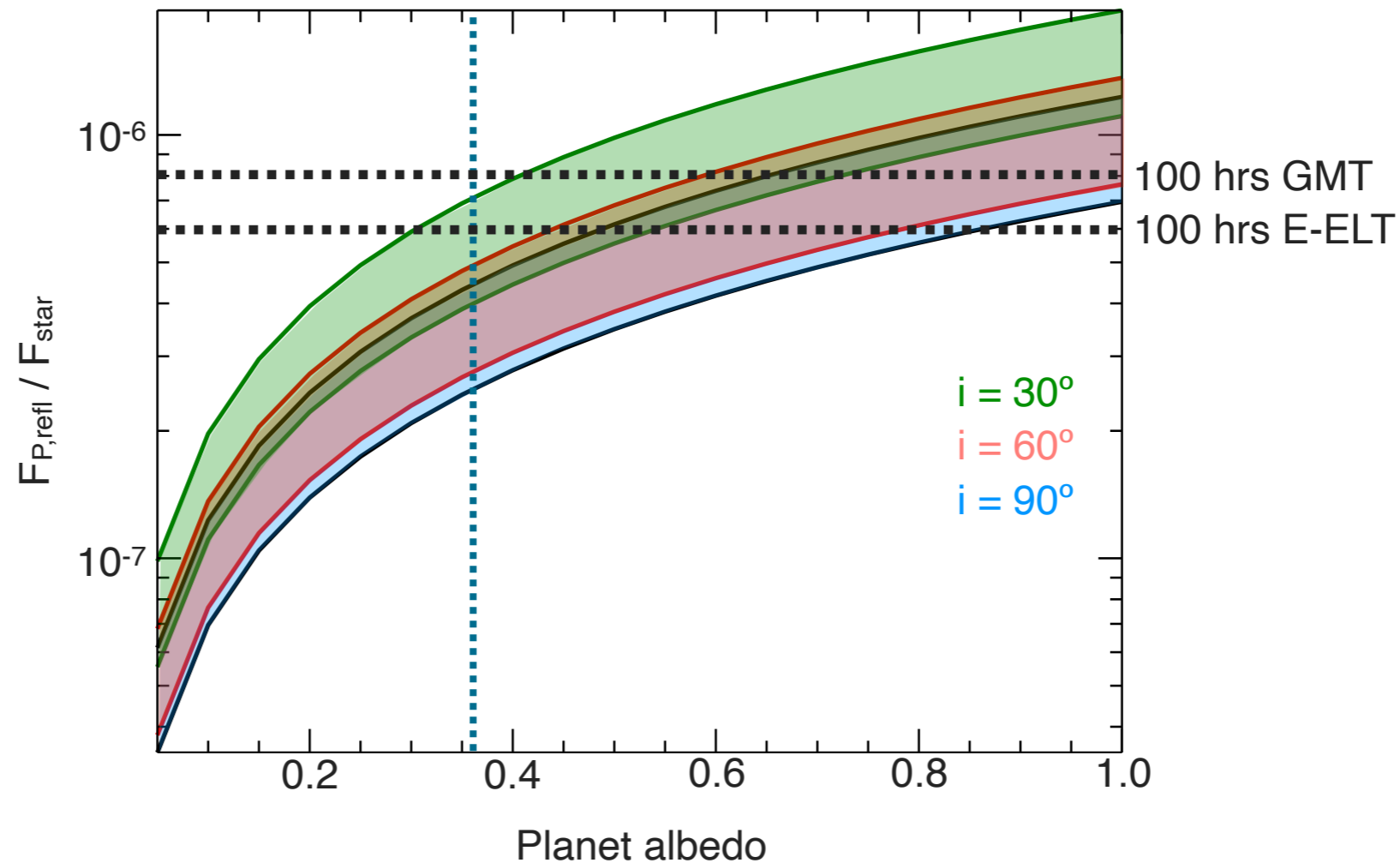
Current spectrographs are starting to be optimised to observe M dwarfs



Gain in S/N from cross-correlating with thousands of lines: 65-80x

Reflected light from Proxima Centauri b

The planet/star contrast is between 7×10^{-7} and 2×10^{-6} times the albedo



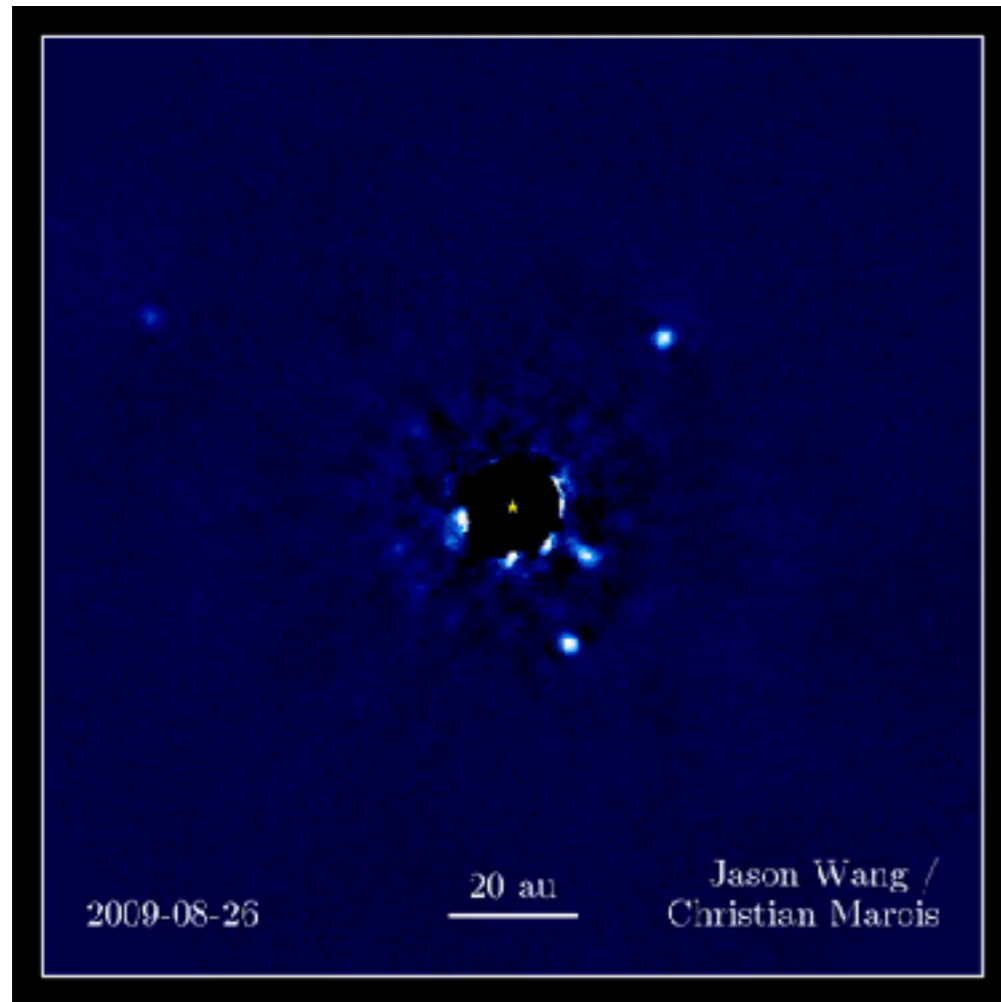
High-resolution spectroscopy (350-1000nm, 10% throughput):
challenging even with 100 hours of Extremely Giant Telescopes

Combining spectral and spatial resolution

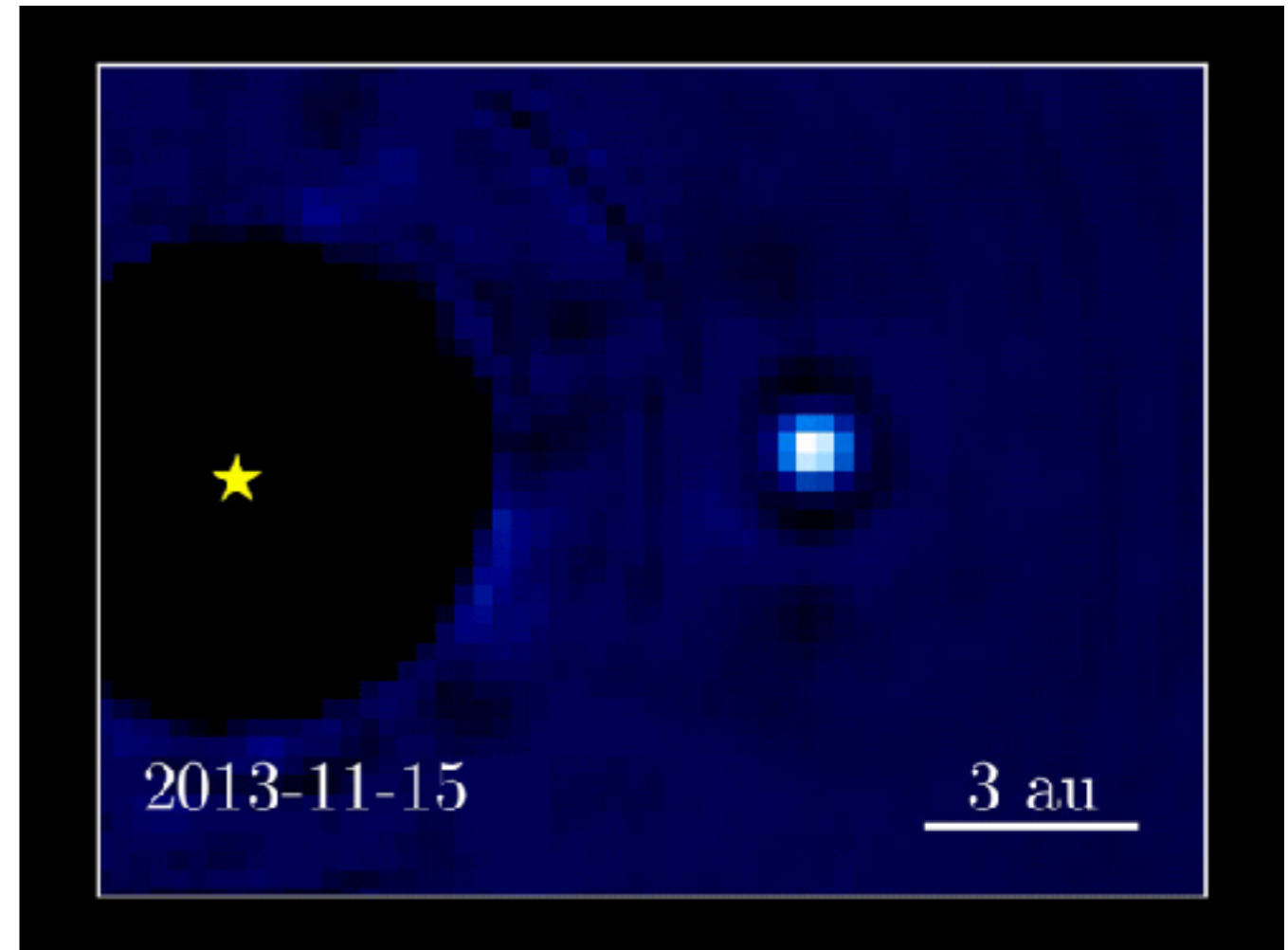
Direct imaging state-of-the-art
Playing with the S/N formula
Simulations and future prospects

Direct imaging of exoplanets

Technology can detect planets 1 million times fainter than the star
Some of these planets can be seen orbiting their star!



HR 8799 b-c-d-e
Seen “face on”

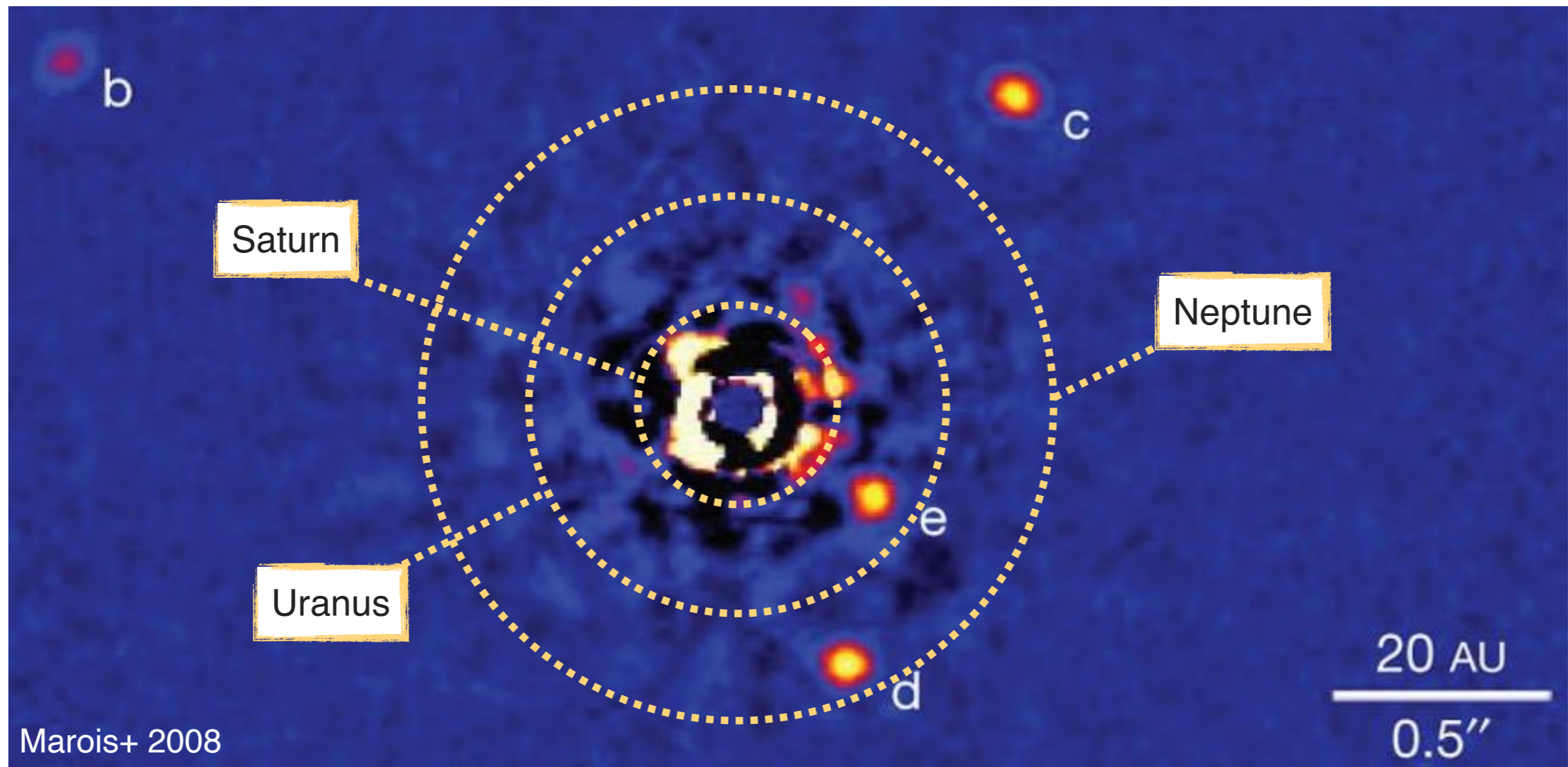


β Pictoris b
Seen “edge on”

Direct spectroscopy of young giant exoplanets

Possible with state-of-the-art instrumentation (SPHERE, GPI) at low spectral resolution

Direct imaging of HR 8799 system: 4 planets

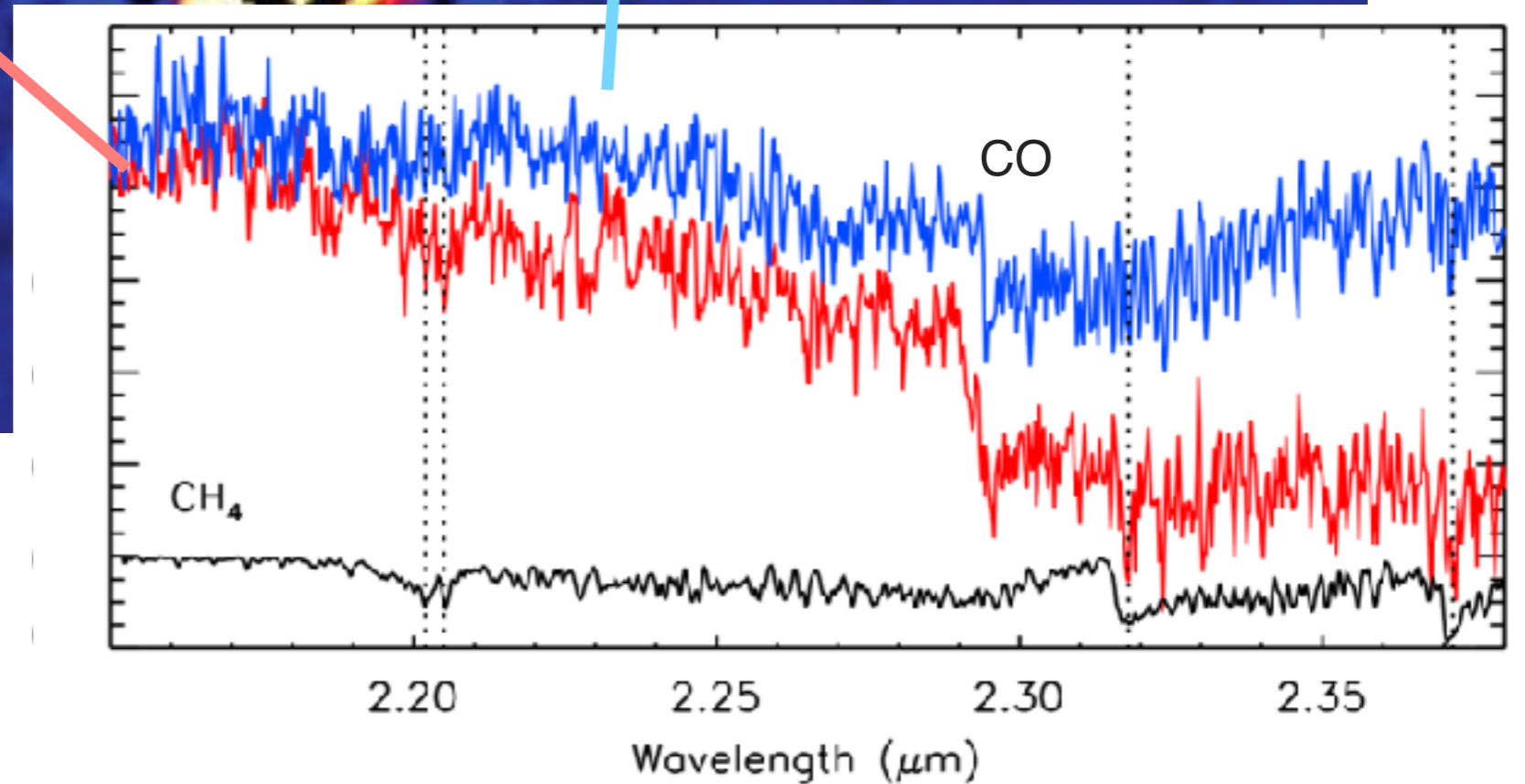
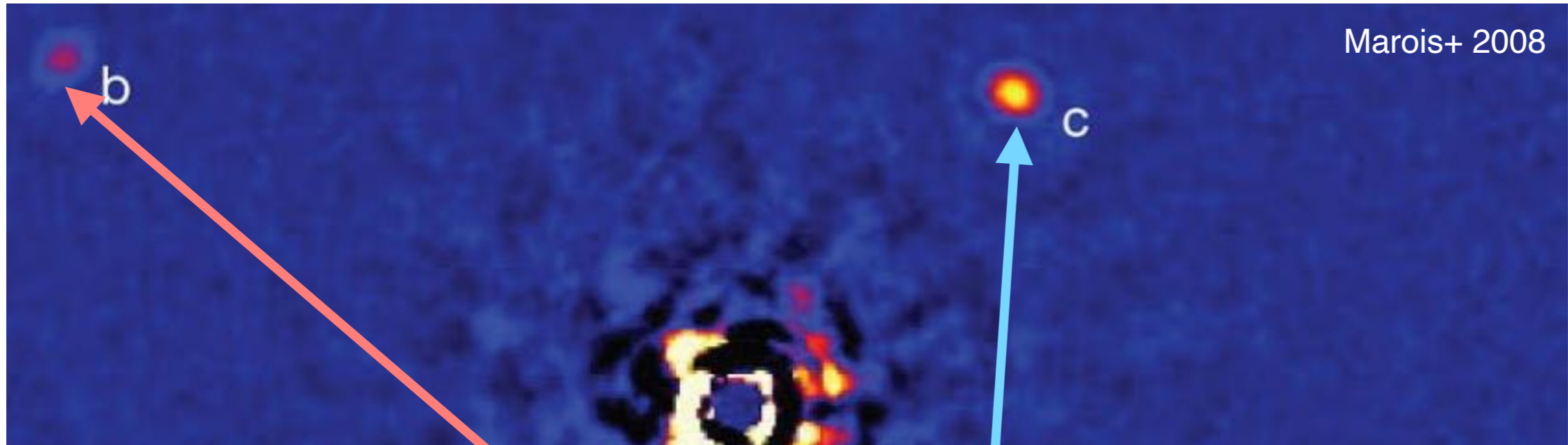


Only possible for **young planets** (still contracting) on **wide orbits** (far from the star)
Observations possible down to planet / star contrasts of 10^{-6} (1 ppm)

Our Solar System would be well below our sensitivity

Direct spectroscopy of young giant exoplanets

Keck-OSIRIS K-band spectrum of HR 8799 b,c at medium resolution (R=4,000)
(Konopacky+ 2015)



CO head-band
+
hints of CH₄ in planet b

Combining spectral and spatial resolution

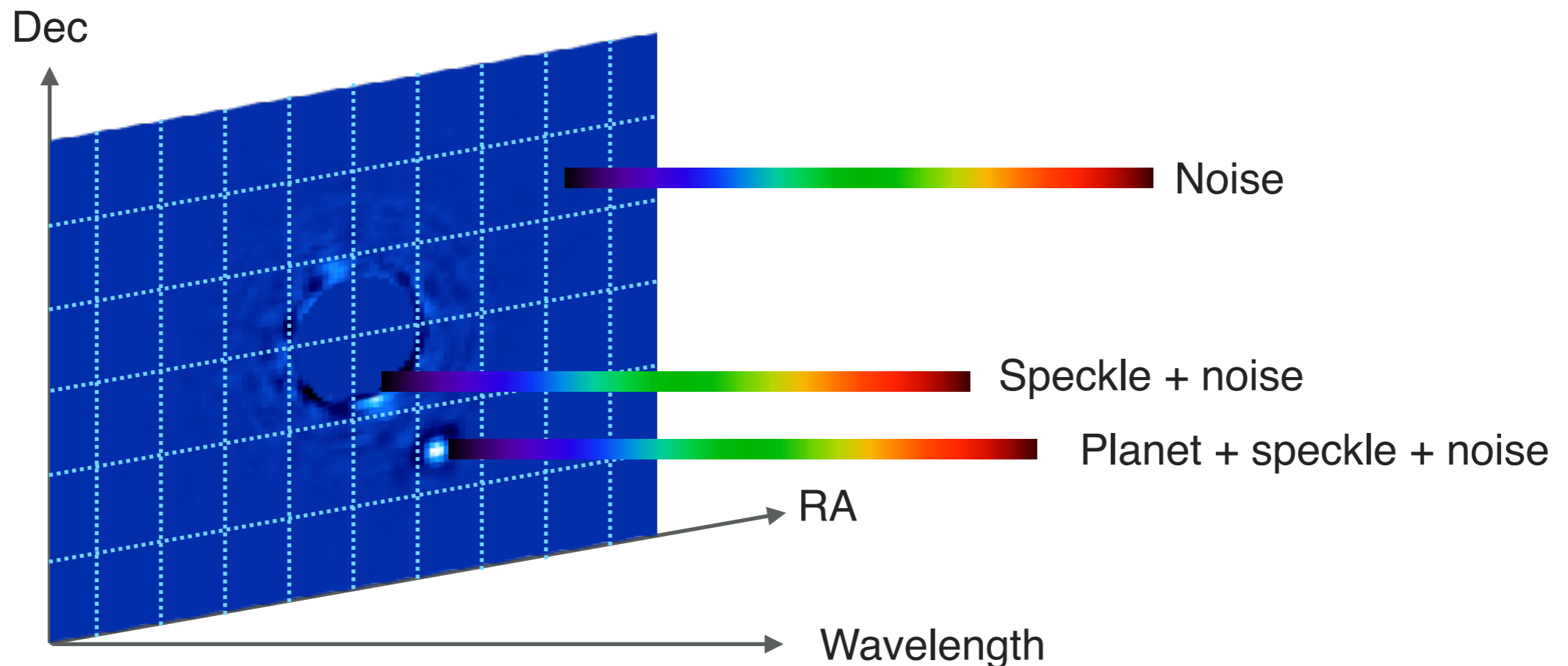
Snellen+ 2014, 2015; Lovis+ 2016; Mawet+ 2017; Wang+ 2017

$$S/N = \frac{S_{\text{planet}}}{\sqrt{S_{\text{star}}/K + \sigma_{\text{bg}}^2 + \sigma_{\text{RN}}^2 + \sigma_{\text{Dark}}}} \sqrt{N_{\text{lines}}}$$

Direct imaging suppression

Cross-correlation gain

Implementation: Integral Field Unit w/ high-res spectroscopic capabilities

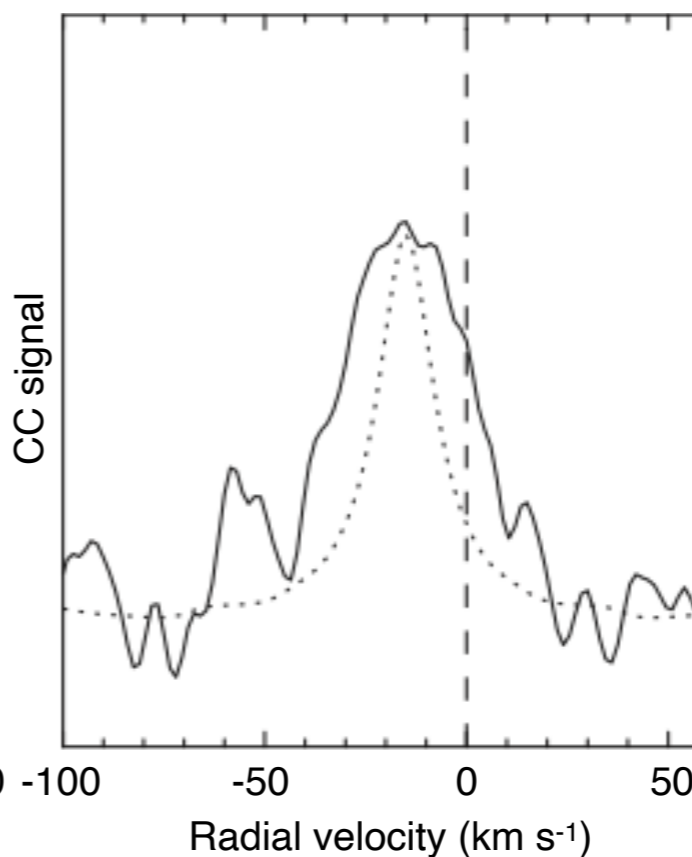
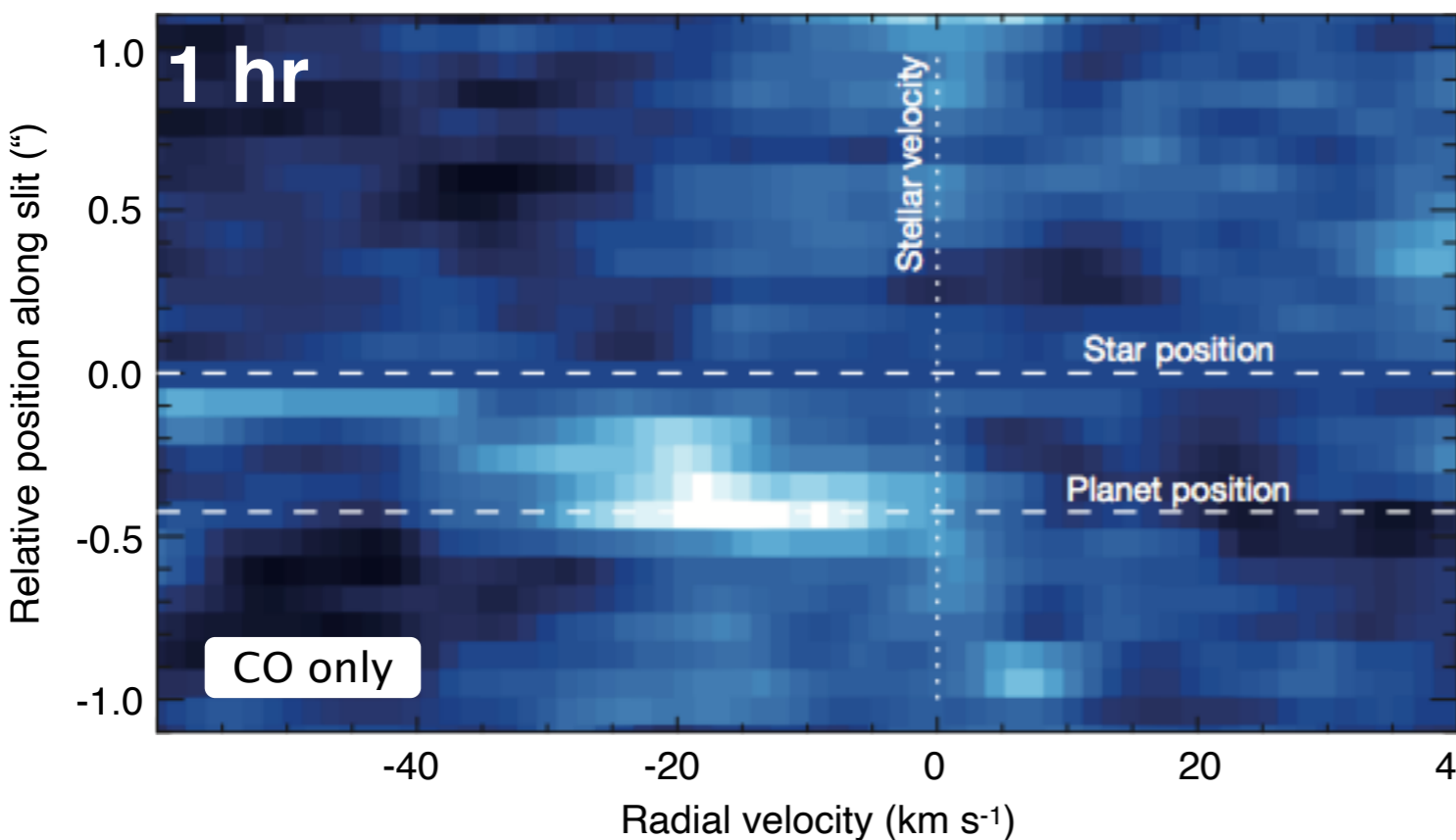
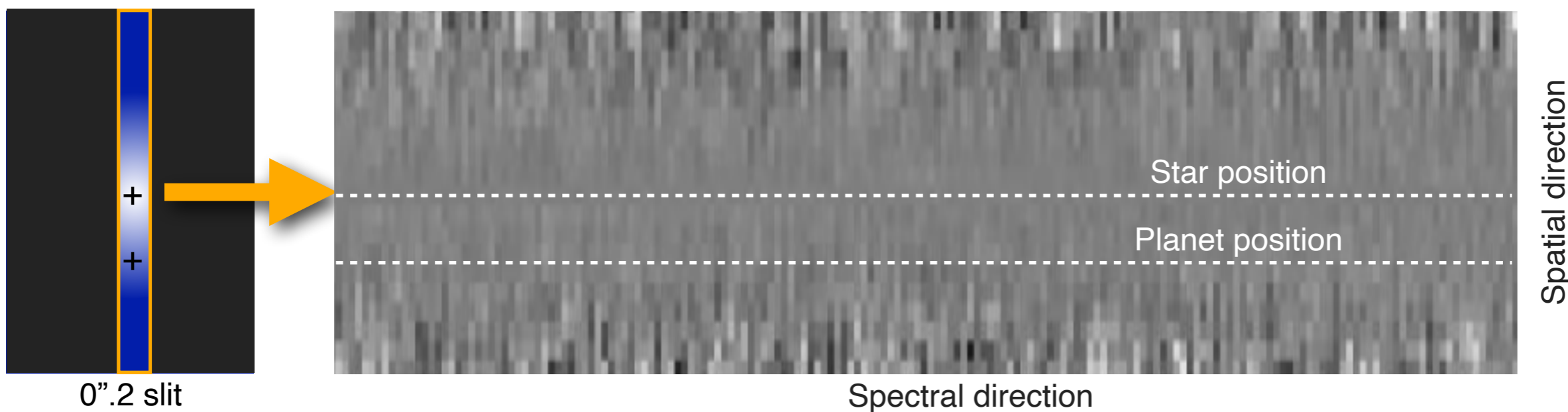


Stage 1: classic AO + DI algorithms to suppress starlight

Stage 2: cross-correlation of residual spectra at each pixel

Testing spectral + spatial resolution: long-slit spectroscopy

CRIRES@VLT, 1hr @ $2.3\mu\text{m}$, seeing 1.0-1.3", 22 spectra (Snellen+ 2014)



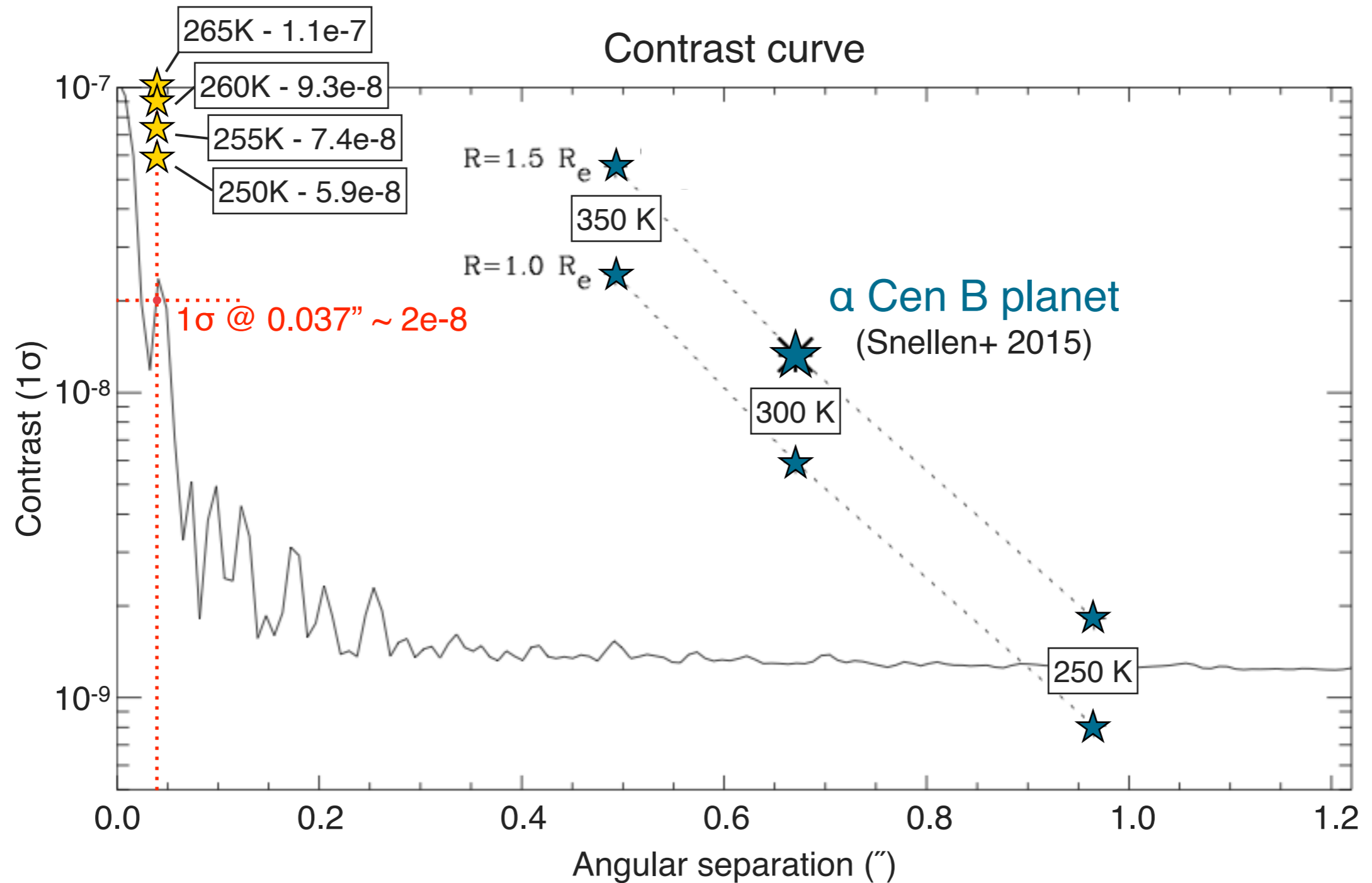
β Pic b

12-21 Myr
 2.6×10^{-4} contrast
S/N = 6.5
FWHM = 27 km/s
 $P_{\text{rot}} \sim 8$ hours

See also Schwarz+ 2015: $\text{H}_2\text{O}+\text{CO}$ in GQ Lupi b, S/N = 12

Thermal emission from Proxima Cen b

$R = 1.1 R_{\oplus}$, $T = 250\text{-}265\text{K}$, $a = 0.0485 \text{ AU} \Rightarrow 0.0373''$ separation (I. Snellen)



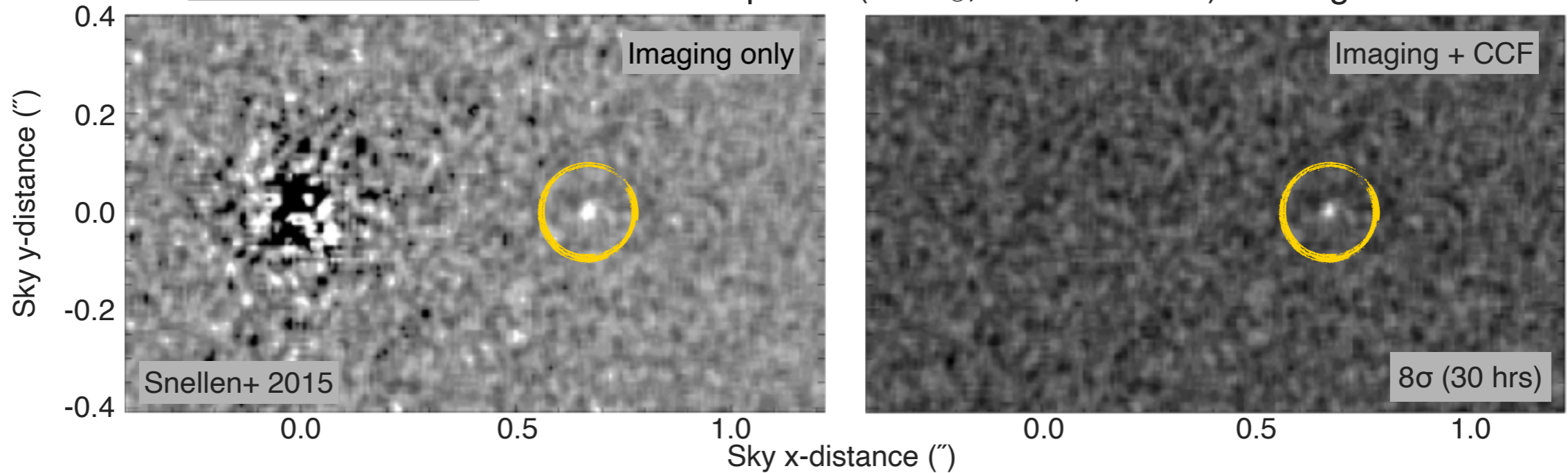
METIS observations centered at $4.85 \mu\text{m}$, 30 hrs

Spectral + spatial resolution with the ELT

Simulating ~30 hours of observations on our nearest neighbours (I. Snellen)

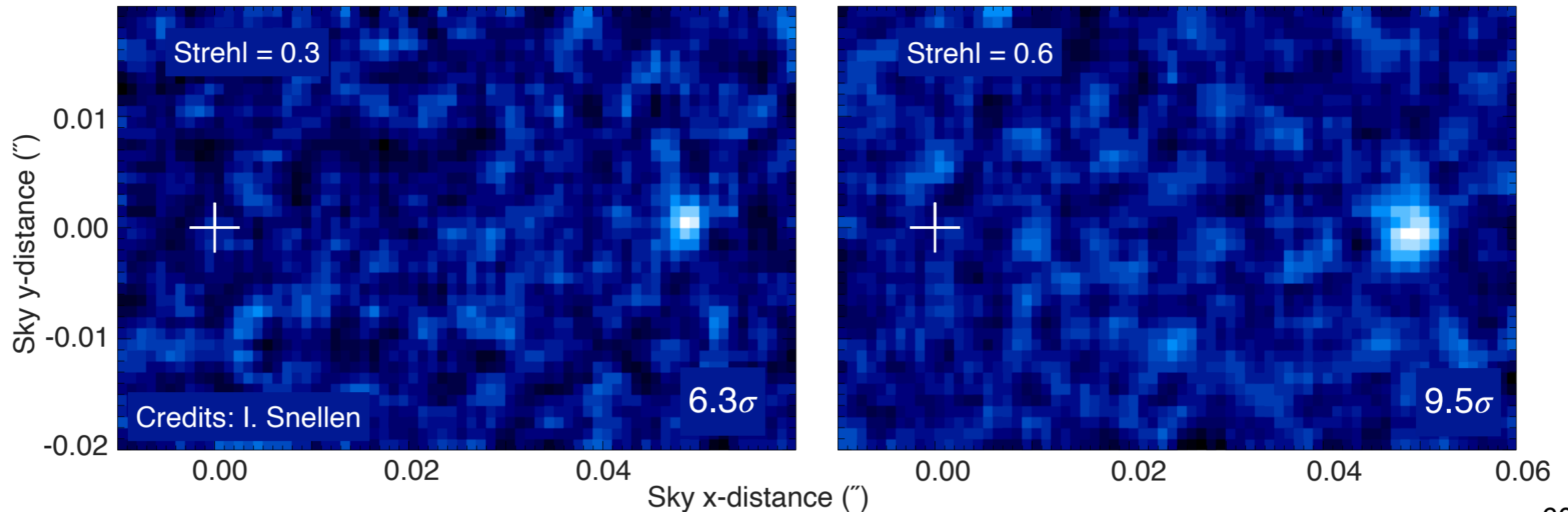
METIS: M band

Thermal emission of “**Earth-like**” planet ($1.5 R_{\oplus}$, 300 K, 30 km/s) orbiting α Cen B



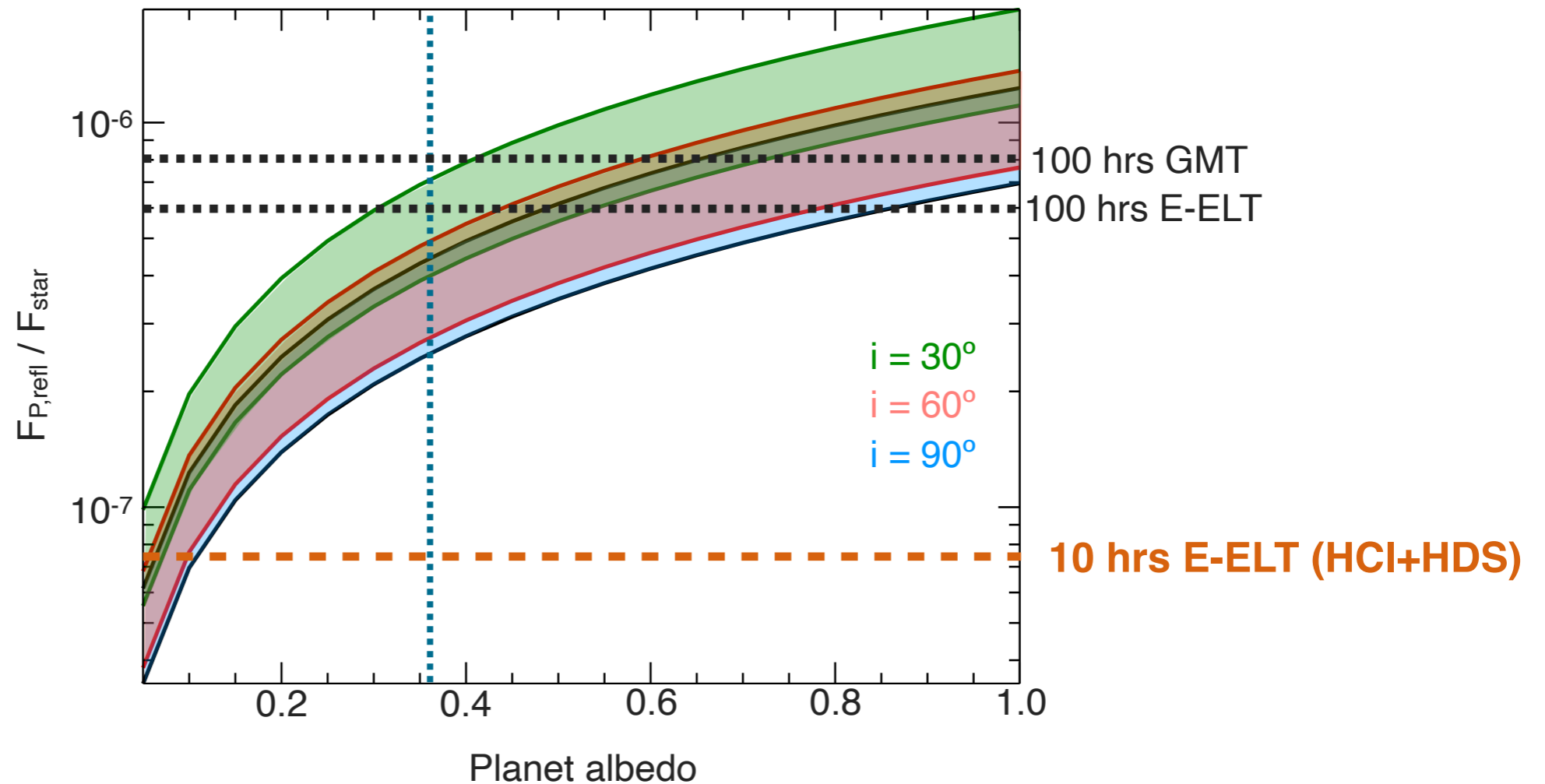
Reflected light from **Proxima Cen b** ($1.1 R_{\oplus}$, 0.048 AU, 40 km/s)

HIRES: 0.5-1.8 μ m



Proxima Centauri b: reflected light

The planet/star contrast is between 7×10^{-7} and 2×10^{-6} times the albedo

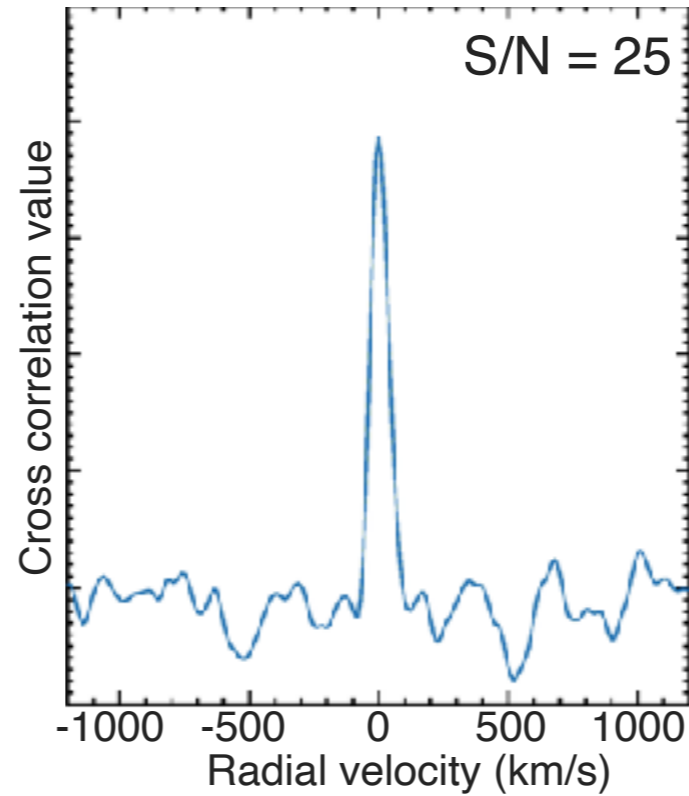
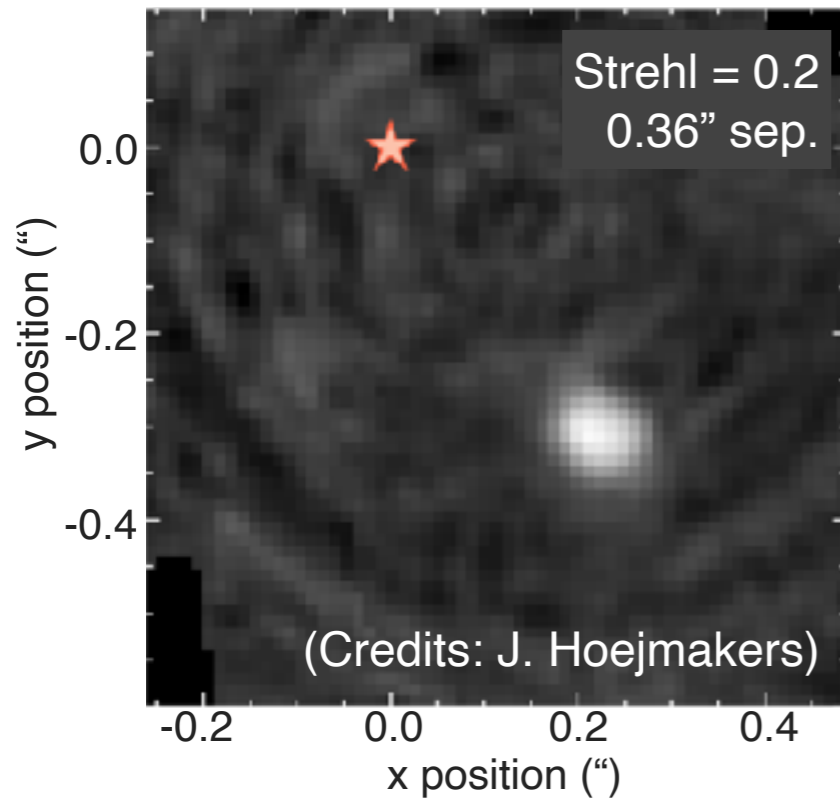


High-resolution spectroscopy only (350-1000nm, 10% throughput):
challenging even with 100 hours of Extremely Giant Telescopes

Spectral and spatial resolution combined would easily succeed!
(Revised Snellen+ 2015 estimates, strehl ratio 0.3, 10% throughput)

Testing spectral + spatial resolution: mid-res IFUs

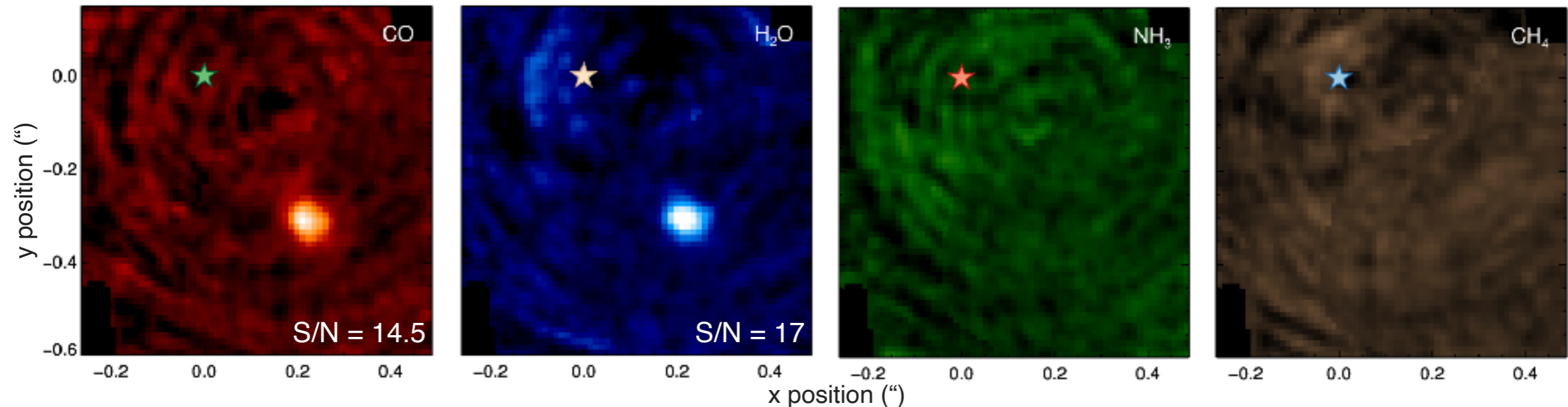
Hoeijmakers+18: Integral Field spectroscopy with VLT/SINFONI



Medium-resolution ($R = 5,000$)
2.5h on β Pic b

1σ limit: <8 ppm!

Molecular "maps" also possible



See also: HR 8799b with Keck/OSIRIS at $R = 5,000$ (Konopacky+ 2013)