Data detrending techniques for high-precision exoplanet spectroscopy

Giuseppe Morello
Bât 703 – Pe 37D

Scientific career

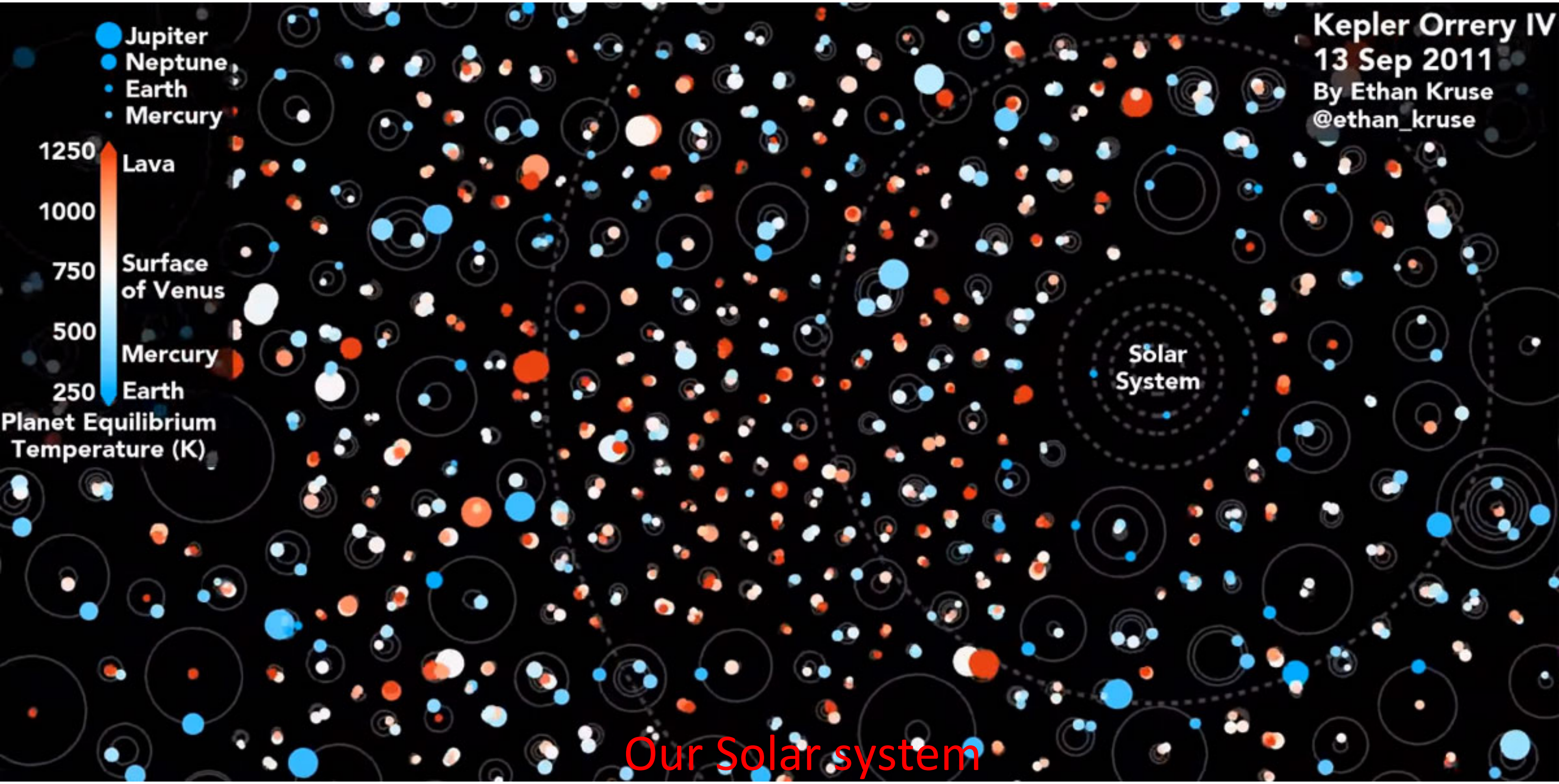
- PhD, UCL , Oct. 2013 – Oct. 2016
  I. D. Howarth & G. Tinetti

- IPAC Fellowship, Caltech, Jan.-Jul. 2016
  P. W. Morris & S. D. Van Dyk
  (automated classification and clustering: kNN, SVM, SOM, …)

- Post-doc, UCL, Nov. 2016 – Oct. 2017
  G. Tinetti

- Post-doc, CEA Saclay, Nov. 2017 – ongoing
  Pierre-Olivier Lagage

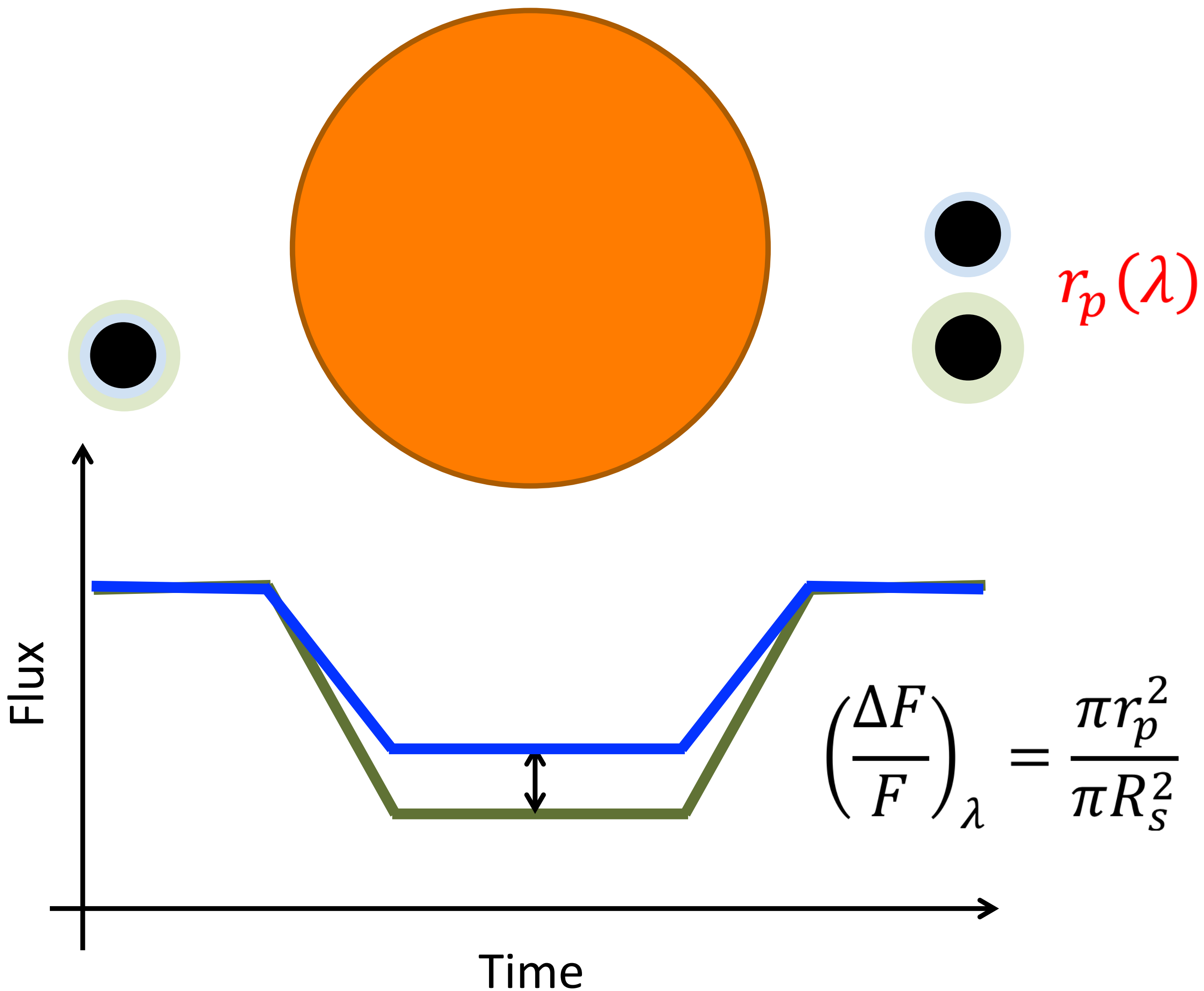
Exoplanets variety

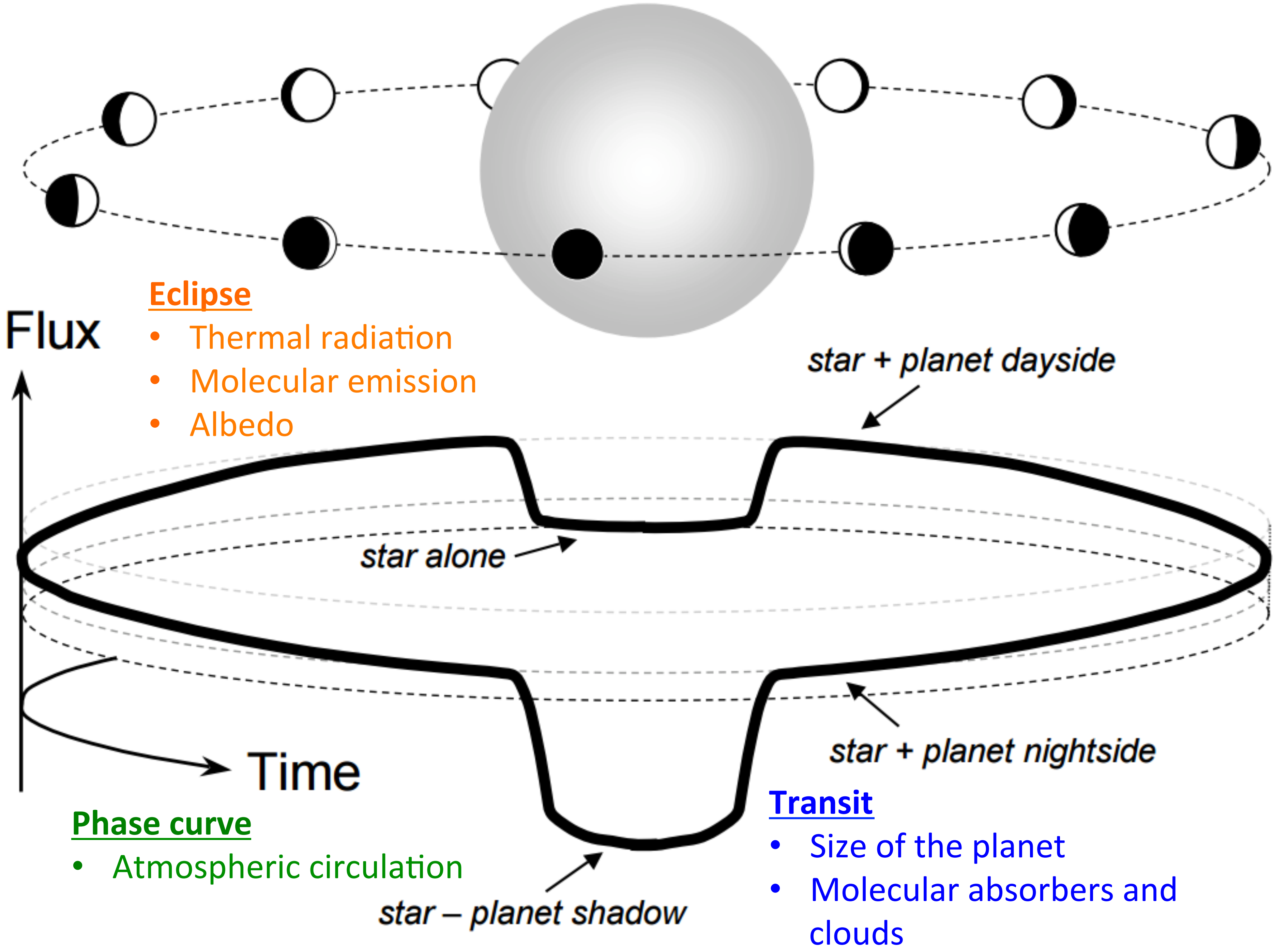


Our Solar system

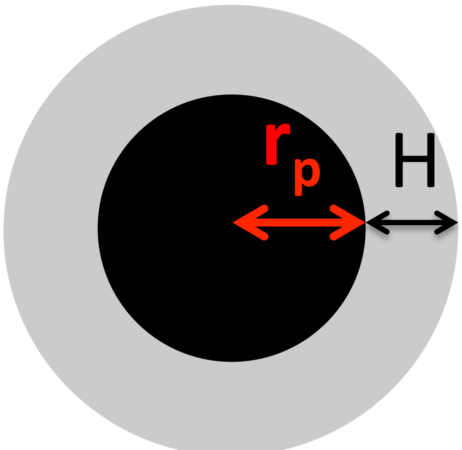
Distances not to scale

Transit of an exoplanet with atmosphere




Eclipse
Thermal radiation
Molecular emission
Albedo
Flux
star + planet dayside
star alone
Time
star + planet nightside
Transit
Size of the planet
Molecular absorbers and clouds
Phase curve
Atmospheric circulation
star – planet shadow

Atmospheric absorption



$$\left(\frac{\Delta F}{F}\right)_{atm} \approx \frac{2\pi r_p H}{\pi R_s^2}\kappa(\lambda)$$

$$H = \frac{KT}{\mu g}$$

Required precision of 10 – 100 parts per million (ppm)!

planet	$r_p\ (km)$	$g\ (m/s^2)$	$T(K)$	μ	$h\ (km)$	$\frac{\Delta F_{atm}}{F}\ (10^{-4},\ \mathfrak{K}=1)$
Earth	6400	9,8	300	28 u	9	0,0024
Jupiter	71500	25	140	2 u	23	0,069
HD189733b	90000	18	570	2 u	131	0,84

Brown et al. 2001

Technical and astrophysical challenges

1 Removing the instrument systematics
(Spitzer, Hubble ~ 100 – 1000 ppm)

2 Accurate modeling the astrophysical scenario:
stellar limb-darkening, activity, etc. (~ 100 – 1000 ppm)

3 Interpreting the atmospheric spectrum:
many chemical species, parameter degeneracies, low signal-to-noise data, sparse wavelength coverage, etc.

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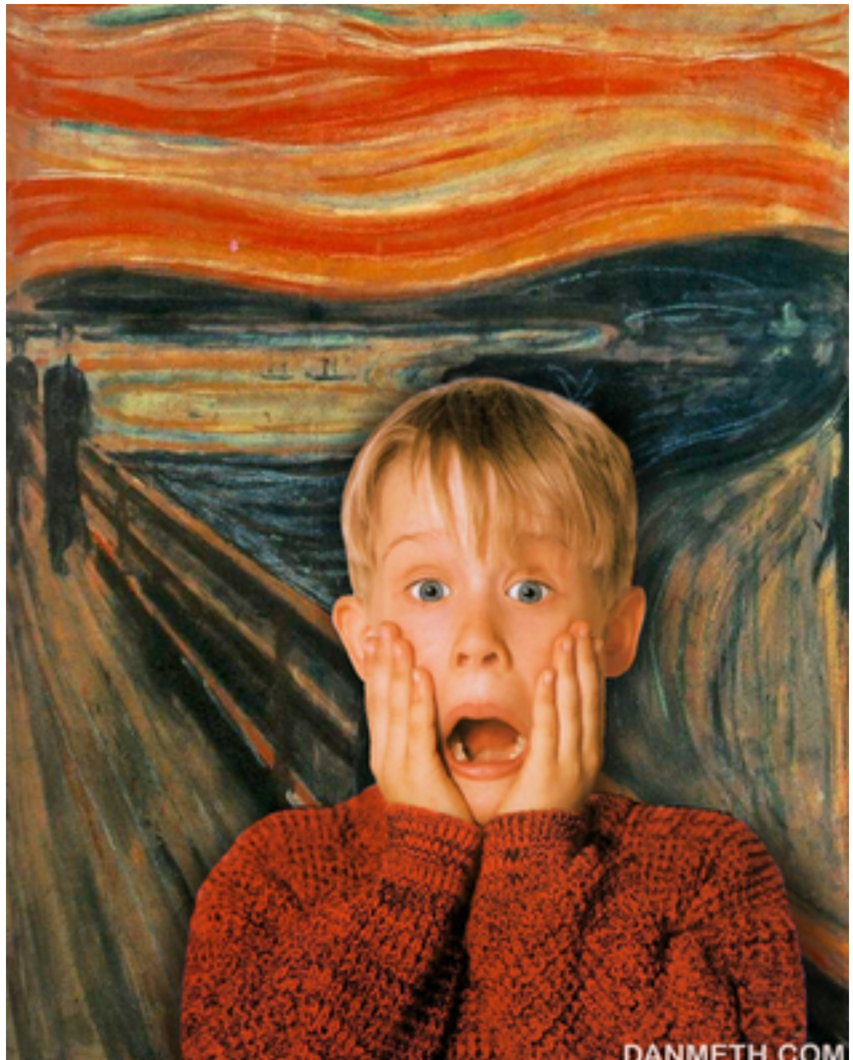
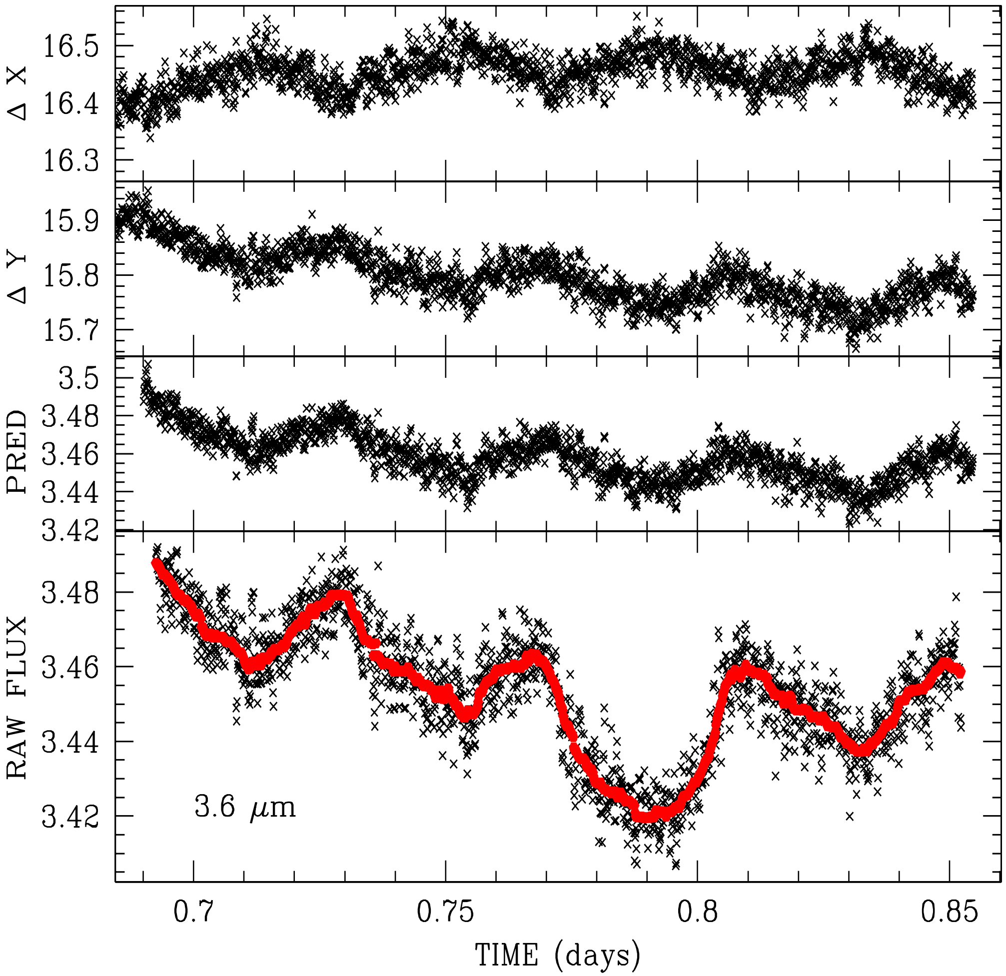
Removing the instrument systematics

(Spitzer, Hubble ~ 100 – 1000 ppm)



Data detrending: parametric



Example: Spitzer/IRAC -> division by a polynomial function of centroid coordinates.

1. Optical State Vector (OSV): detector temperature, inclination, point spread function, etc.
2. Measured flux is correlated with OSV parameters
3. Parametric correction based on those parameters.

Some controversial results in the literature (corrections beyond the well-known instrument response)

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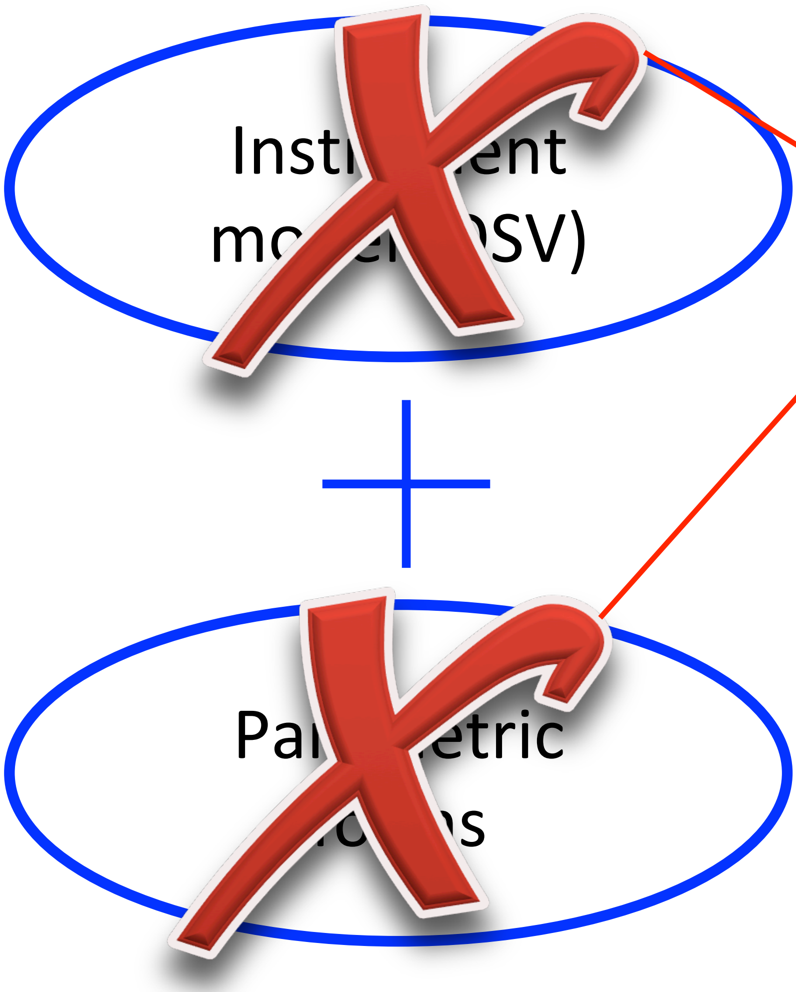
Data detrending: blind



Blind

e.g., Fourier, Wavelet Filters,
Principal Component Analysis (PCA),
Independent Component Analysis (ICA)

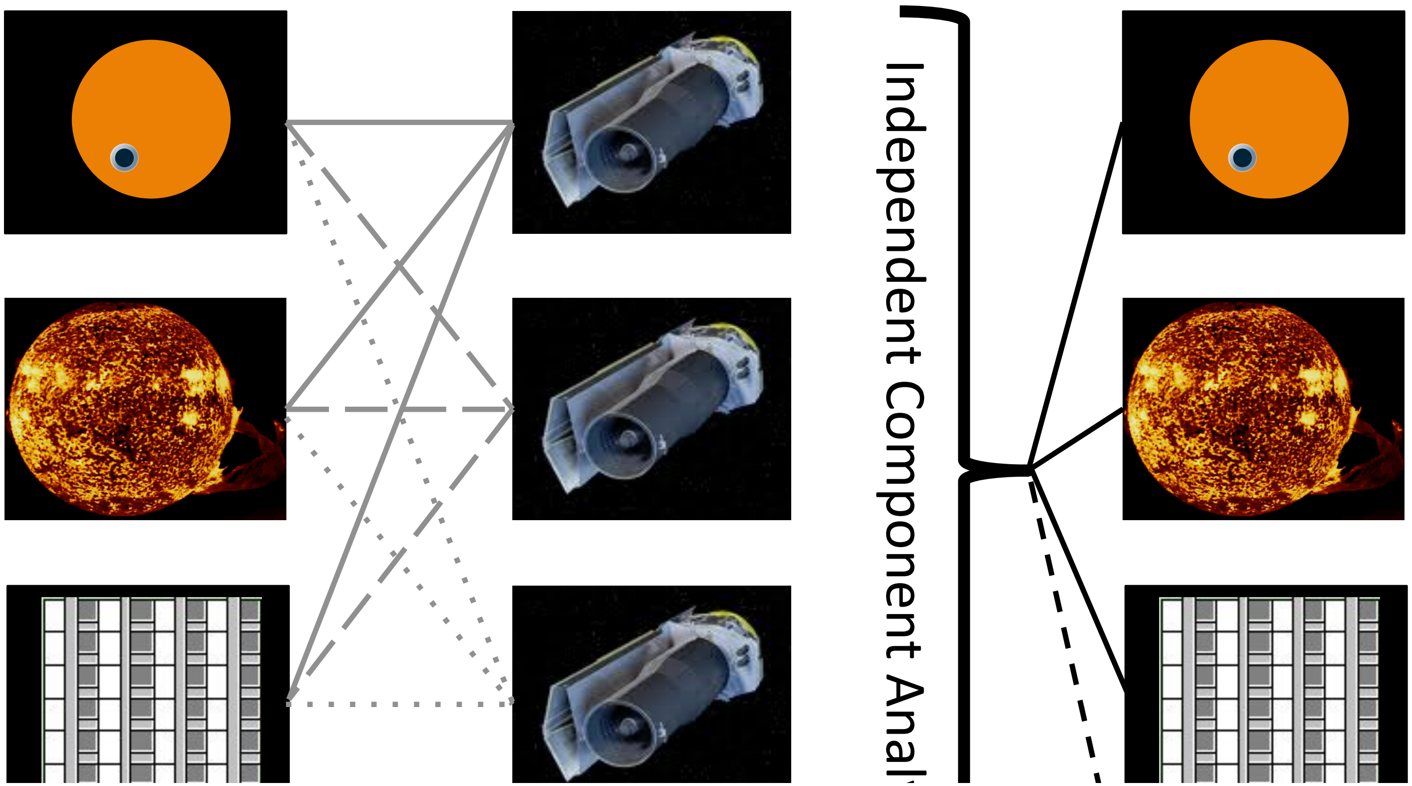
Highest degree of objectivity

Consistent results

Non-parametric

e.g., Spatial Weighting Functions (Ballard et al. 2010), BLISS mapping (Stevenson et al. 2012), Gaussian Processes (GPs, Gibson et al. 2012, Evans et al. 2015)

1 Independent Component Analysis



observations

signals

$$X = AS$$

mixing matrix

Minimize mutual information

$$S = A^{-1}X$$

UNKNOWN

1

ICA: statistics (1)

$$H(\mathbf{y}) = -\sum_k p(\mathbf{y}_k)\log p(\mathbf{y}_k)$$ Shannon entropy

It is the statistical measure of uncertainty associated with a random variable.

$$I(y_1, y_2, ..., y_n) = \sum_{i=1}^{n} H(y_i) - H(\mathbf{y})$$ mutual information

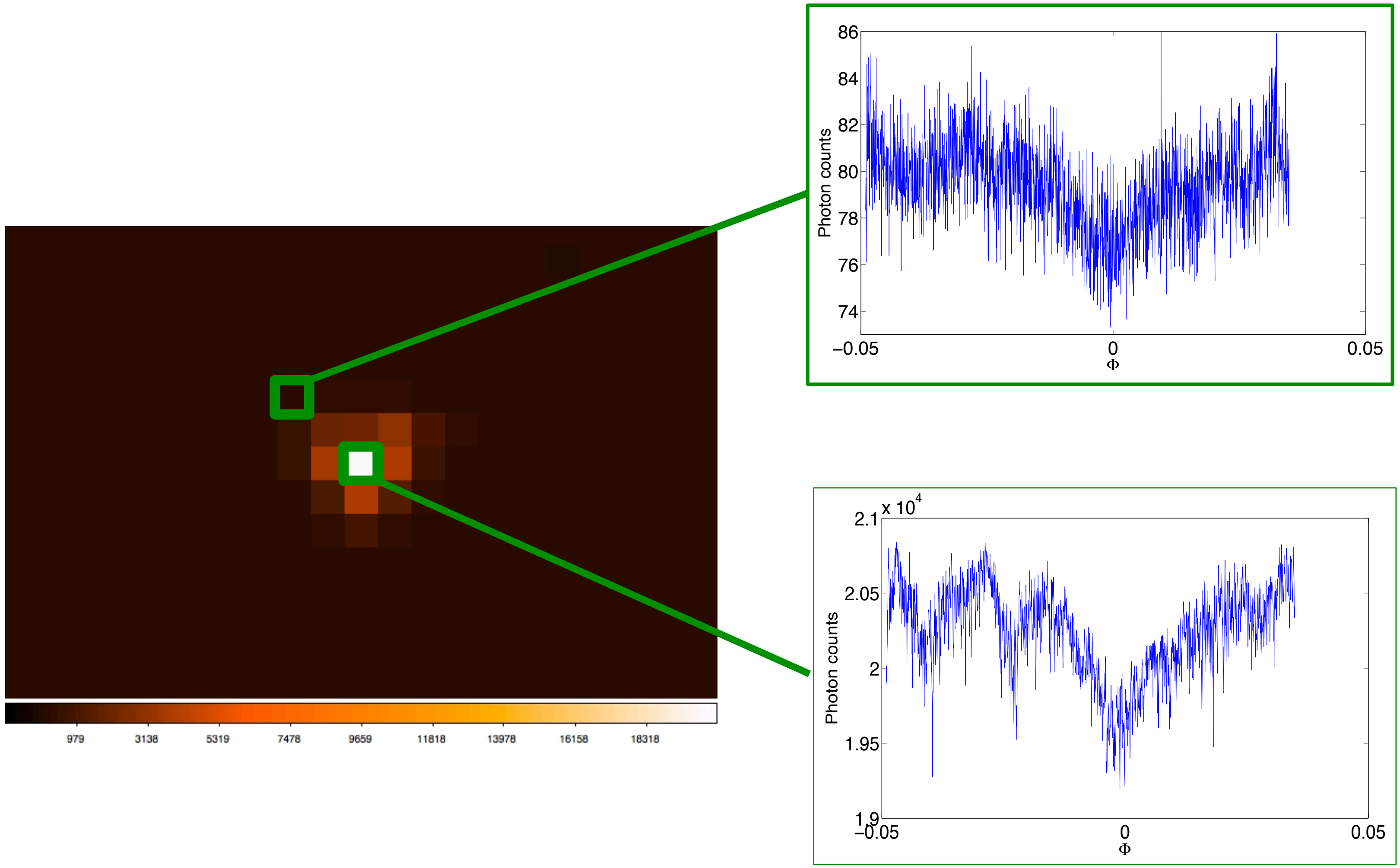
maximum independence = minimum mutual information

$$I(s_1, s_2, ..., s_n) = \sum_i H(s_i) - H(\mathbf{x}) - log|det(\mathbf{W})|$$

1

Pixel-ICA

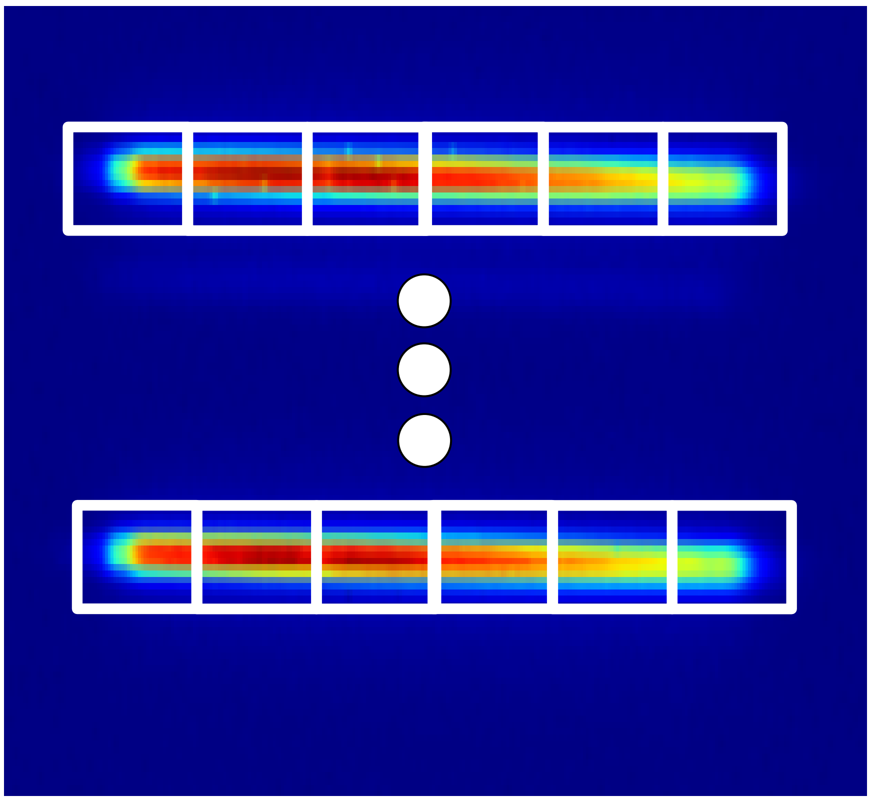
Application to Spitzer/IRAC observations

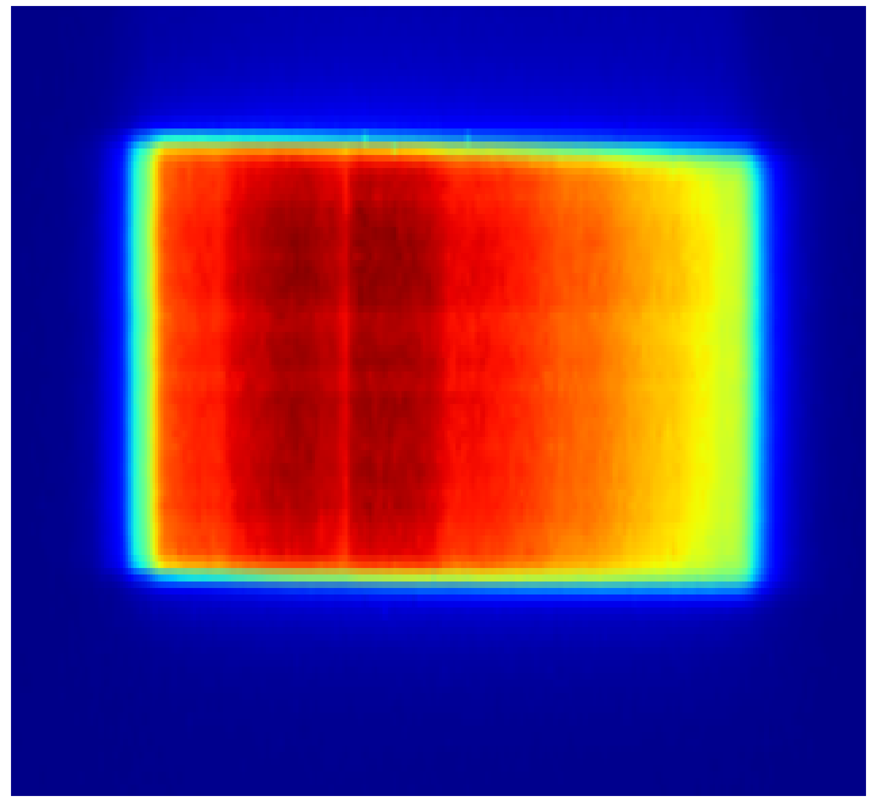


Morello et al. 2014, 2015, 2016; Morello 2015

Stripe-ICA

Application to HST/WFC3 observations

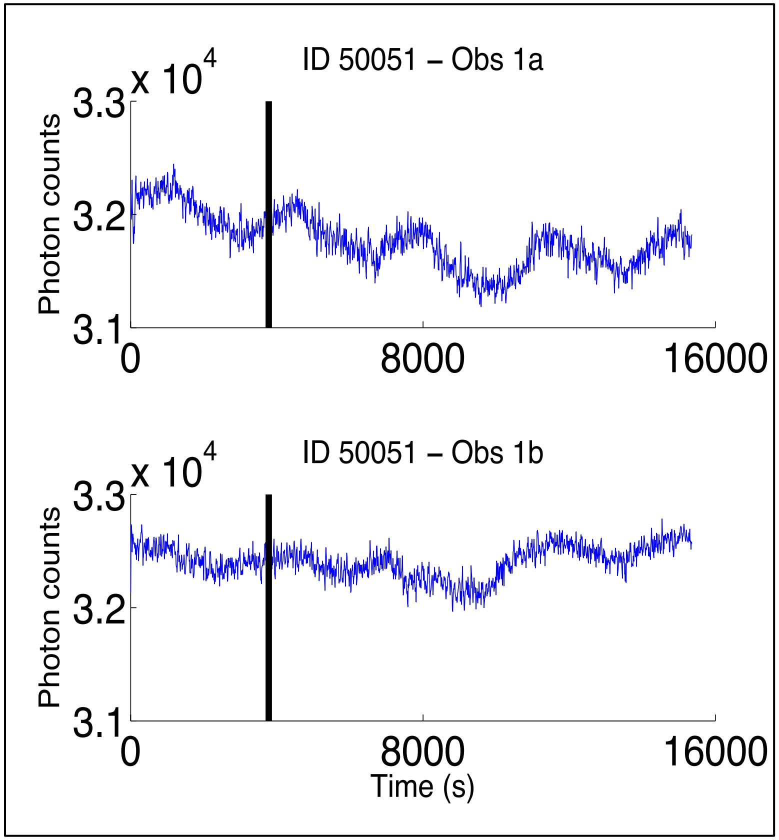




Damiano, Morello et al. 2017

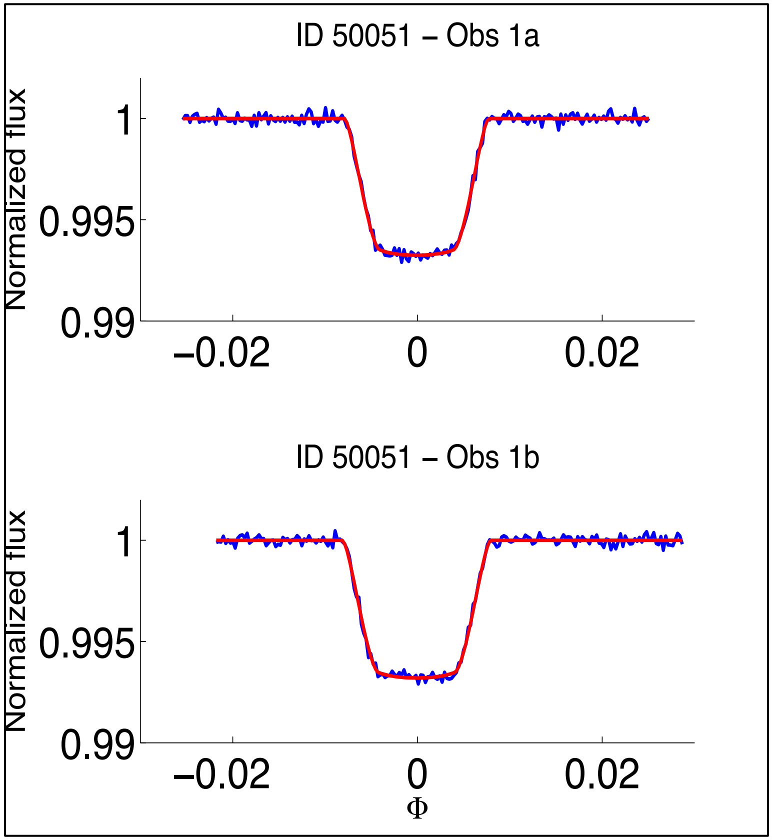
1 Spitzer/IRAC observations at 3.6 μm of GJ436b

Raw lightcurves



ICA

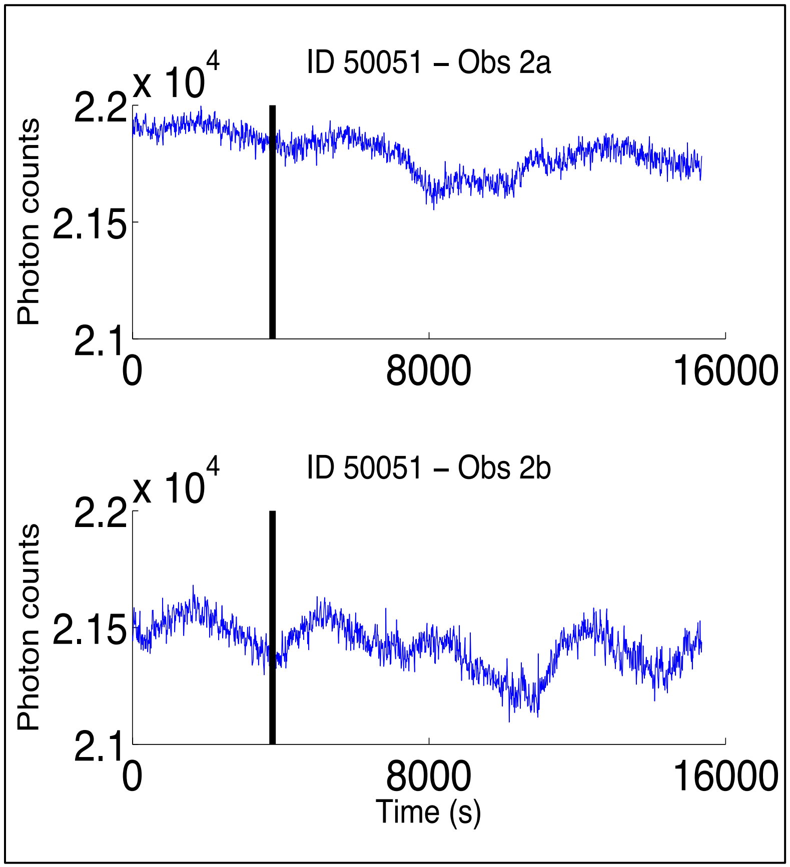
Detrended lightcurves + models



Morello et al. 2015

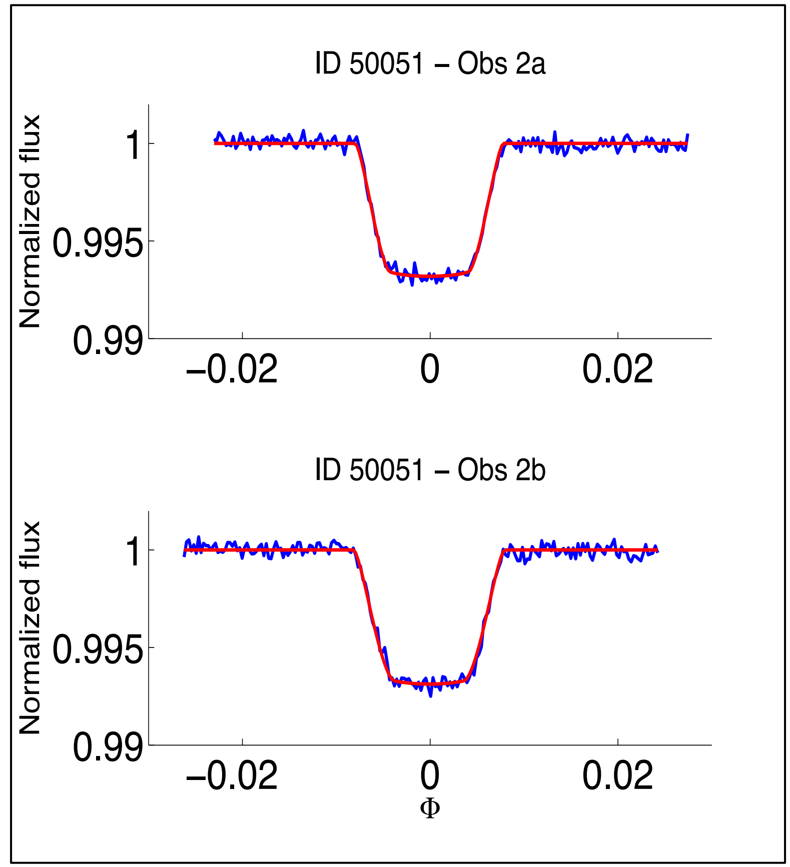
Spitzer/IRAC observations at 4.5 μm of GJ436b

Raw lightcurves



ICA

Detrended lightcurves + models



Morello et al. 2015

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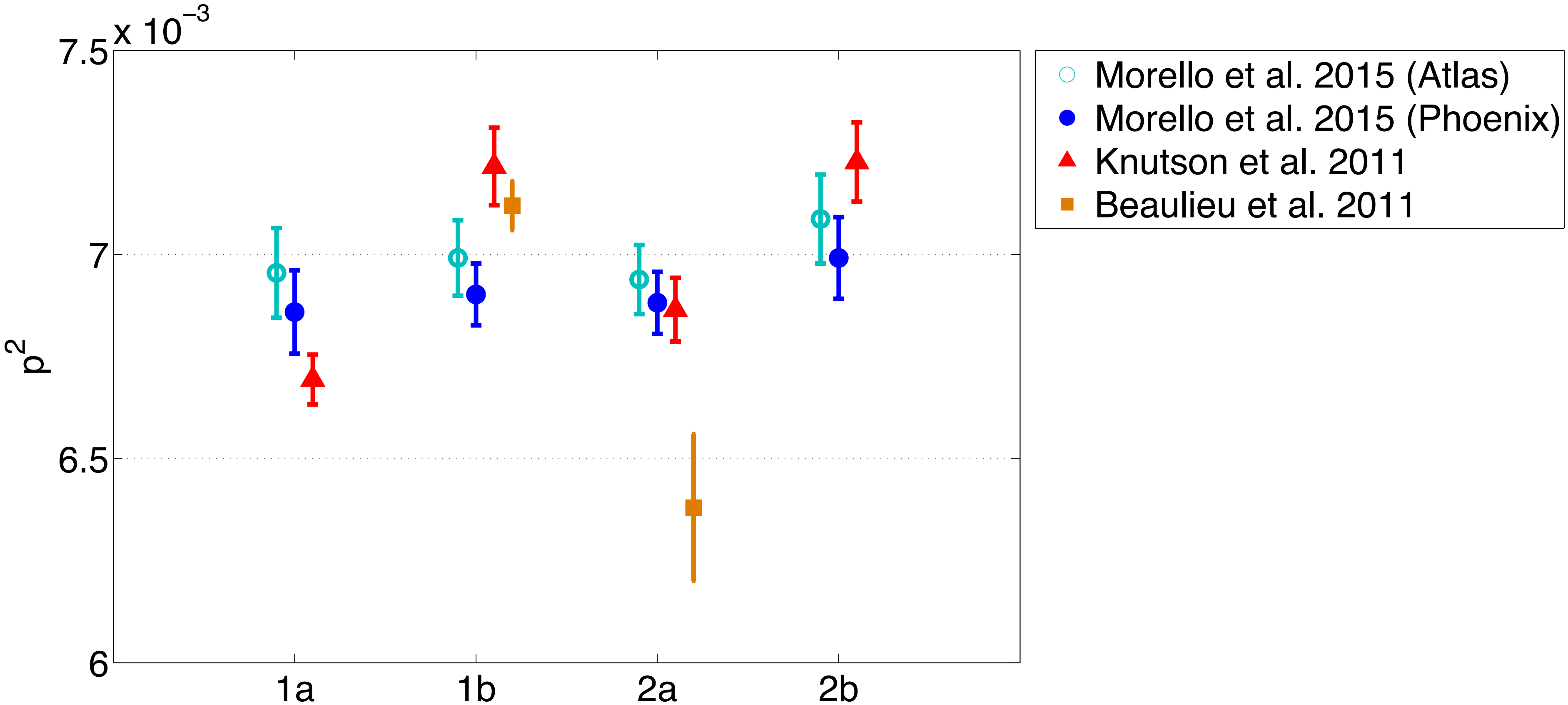
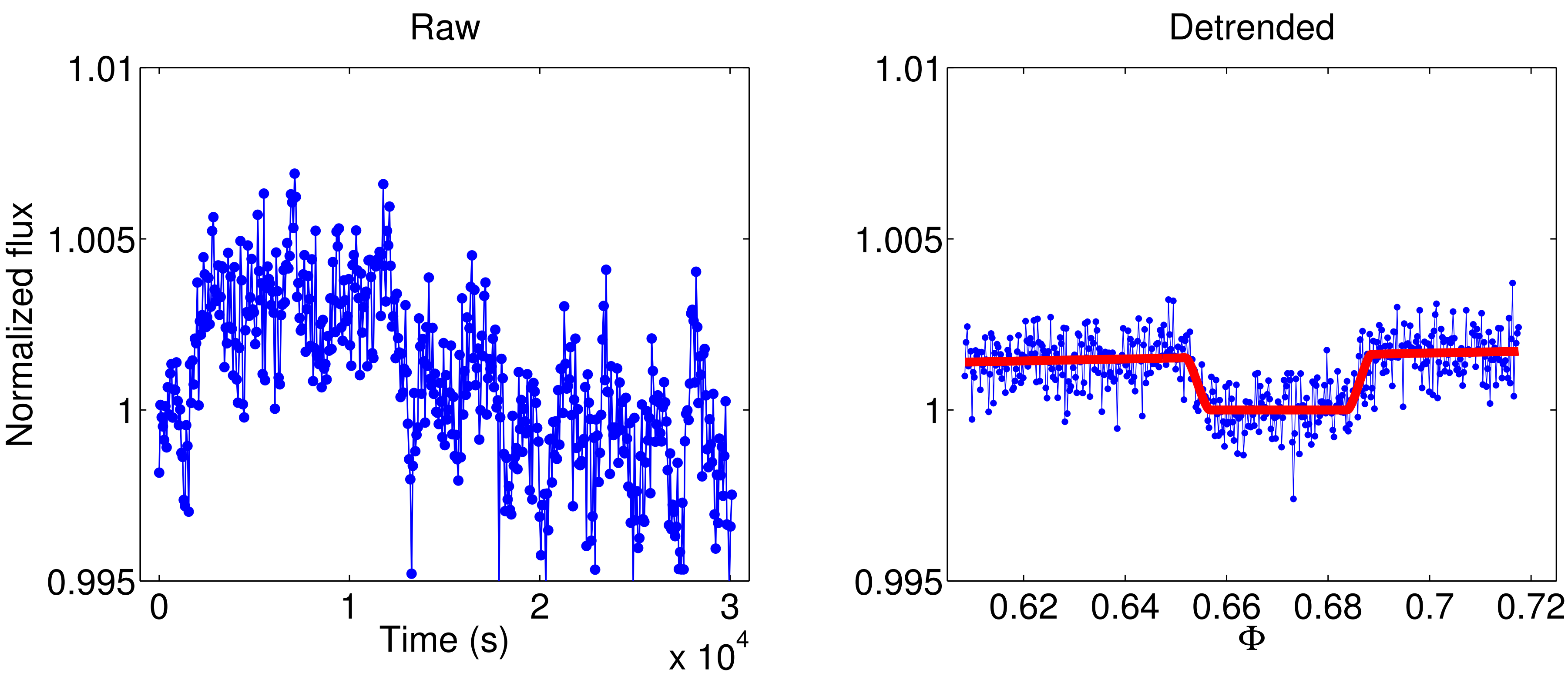
Spitzer/IRAC observations of GJ436b - Results



Morello et al. 2015

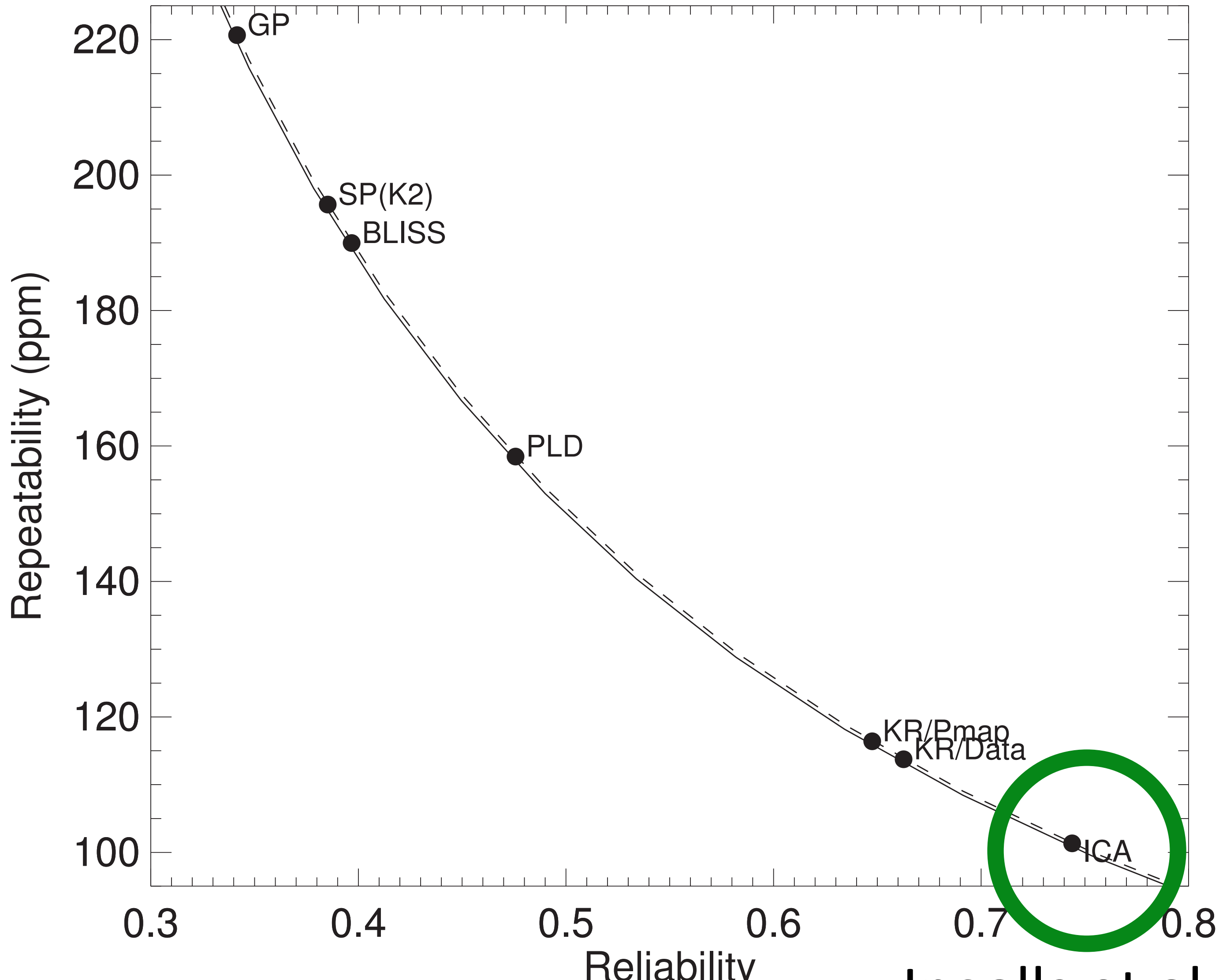
Secondary eclipse of XO3b



Morello et al. 2016

1 IRAC data challenge: eclipses of XO3b

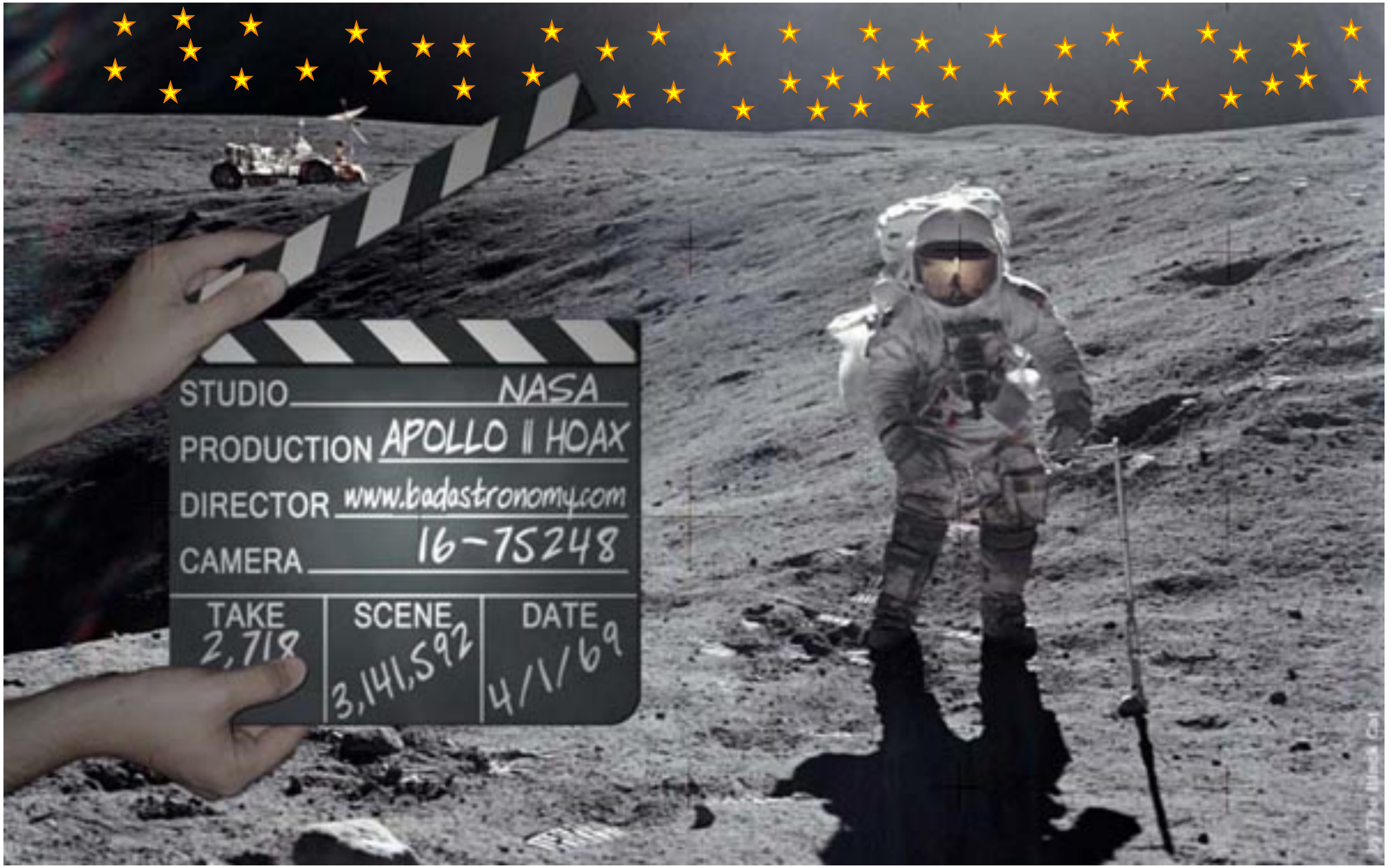
The Astronomical Journal, 152:44 (27pp), 2016 August



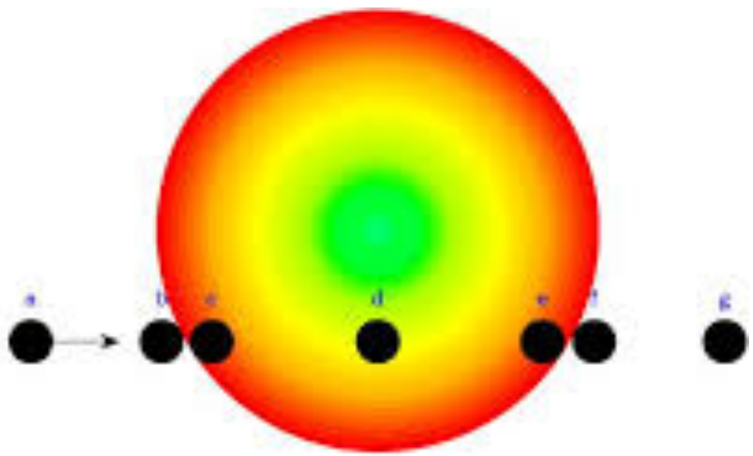
Ingalls et al. 2016

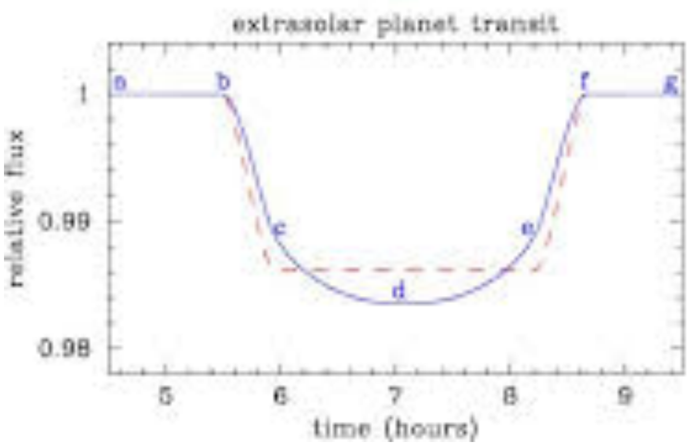
2 Accurate modeling the astrophysical scenario:

stellar limb-darkening, activity, etc. (~ 100 – 1000 ppm)



Stellar limb darkening (1)





$$F\left(p^2, z(t), I_\lambda^*(\mu)\right)$$

$$\left(\frac{R_p}{R_*}\right)^2, \frac{a}{R_*}, i, P, t_0, e, \omega, c_1, c_2, c_3, c_4$$

Four-coefficient law (Claret 2000)

$$\frac{I_\lambda(\mu)}{I_\lambda(1)} = 1 - \sum_{n=1}^{4} c_n\left(1 - \mu^{n/2}\right)$$

$$\mu = \sqrt{1 - r^2}$$

Stellar limb darkening (2)

PROBLEM:
parameter degeneracies!

$$F\left(p^2, z(t), I_\lambda^*(\mu)\right)$$

$$\left(\frac{R_p}{R_*}\right)^2, \frac{a}{R_*}, i, P, t_0, e, \omega, c_1, c_2, c_3, c_4$$

SOLUTIONS (to date):

Limb-darkening coefficients

1. from stellar-atmosphere models

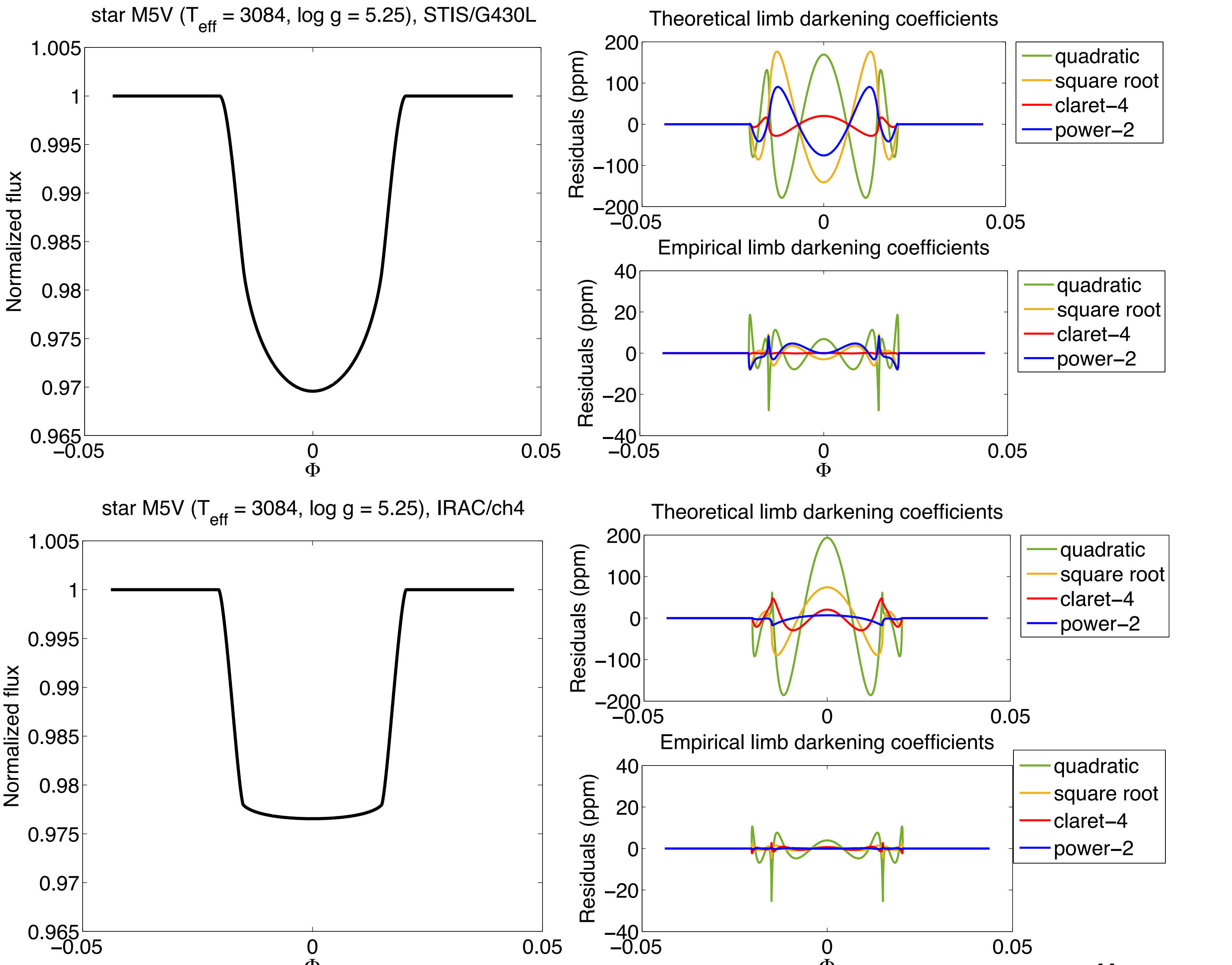
No empirical verification

2. free parameters in light-curve fits, but linear or two-coefficient laws

Inadequate for certain passbands

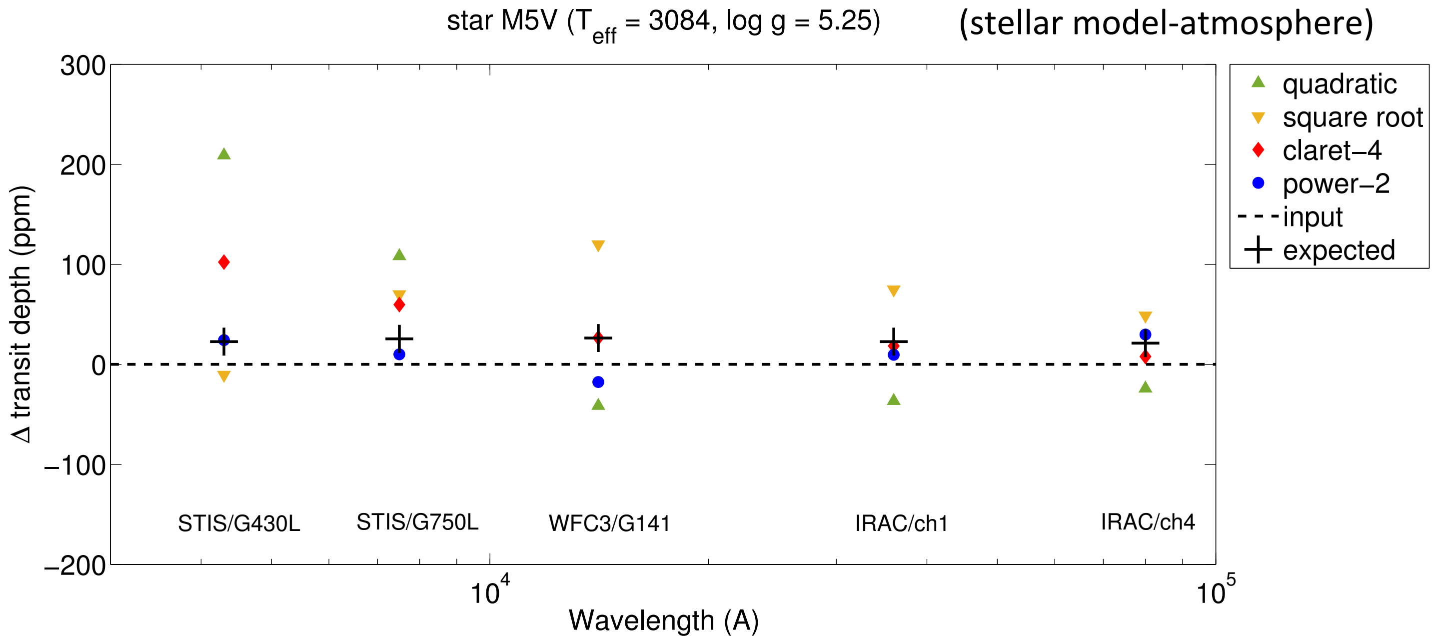
Potential biases in transit depth

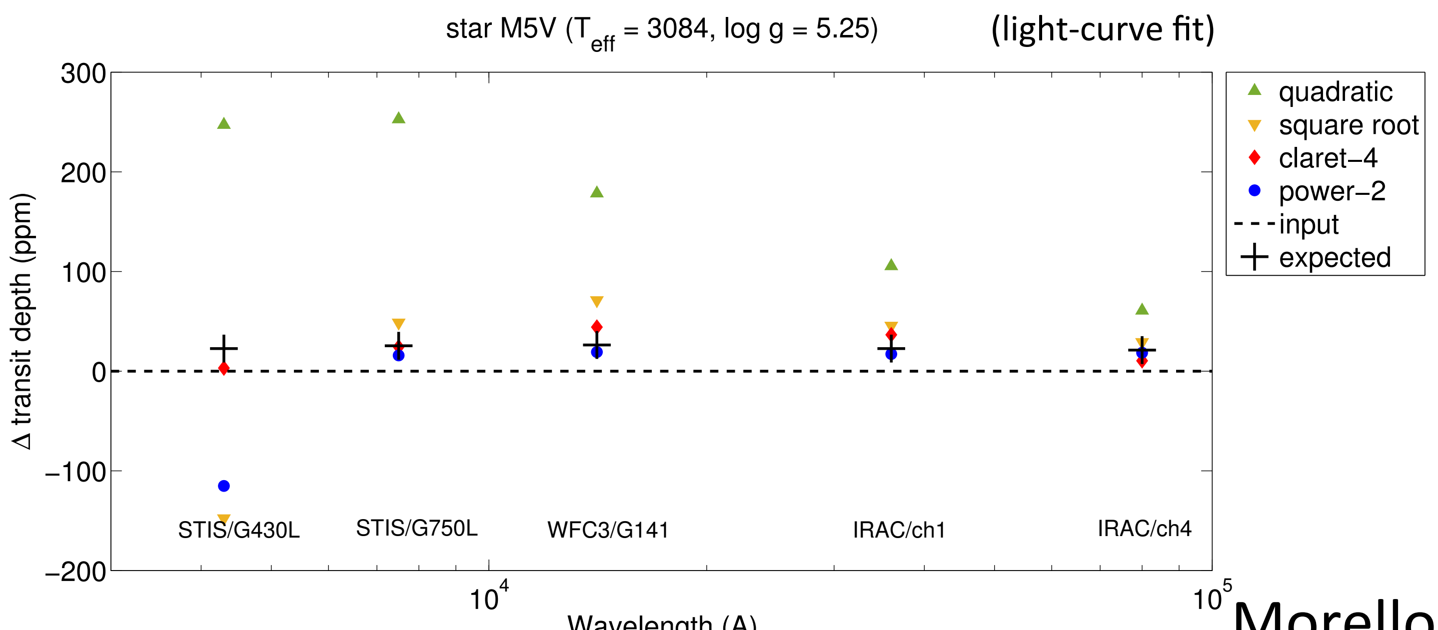
2 Stellar limb-darkening (3)



Morello et al. 2017

2 Stellar limb-darkening (4)





Morello et al. 2017

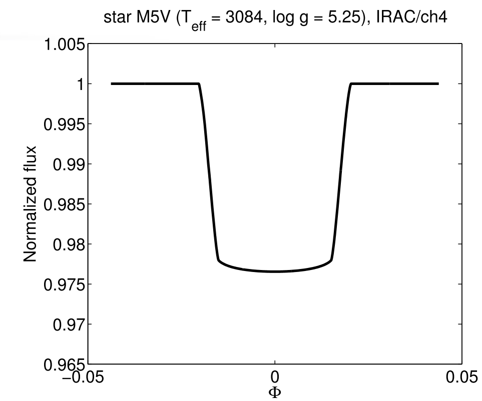
SEA BASS

2

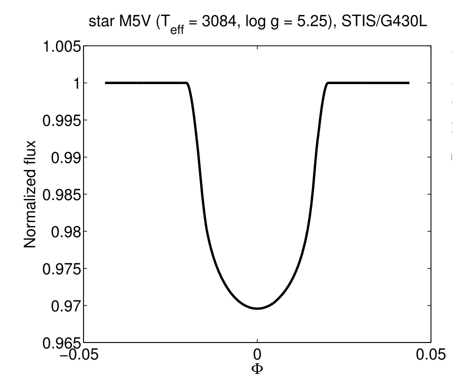
Stellar and **E**xoplanetary **A**tmospheres
Bayesian **A**nalysis **S**imultaneous **S**pectroscopy

INFRARED TRANSITS
- ✓ Two-coefficient limb-darkening laws,
  or
- ✓ Fixed limb-darkening coefficients

=> geometric parameters (orbital, transit duration)



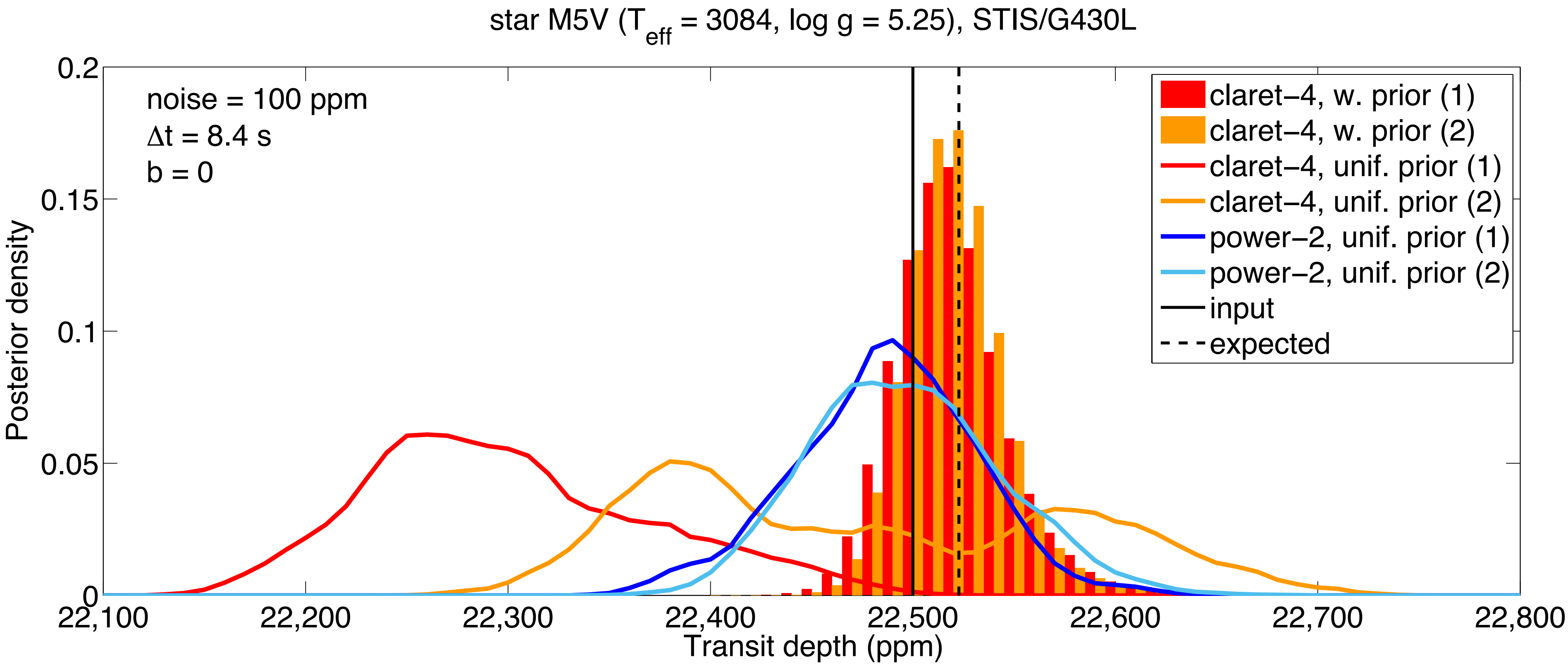
VISIBLE TRANSITS
- ✓ Informative Bayesian priors on the geometric parameters
- ✓ Fully empirical four-coefficient limb-darkening



Morello et al. 2017; Morello, arXiv:1712.09393

2

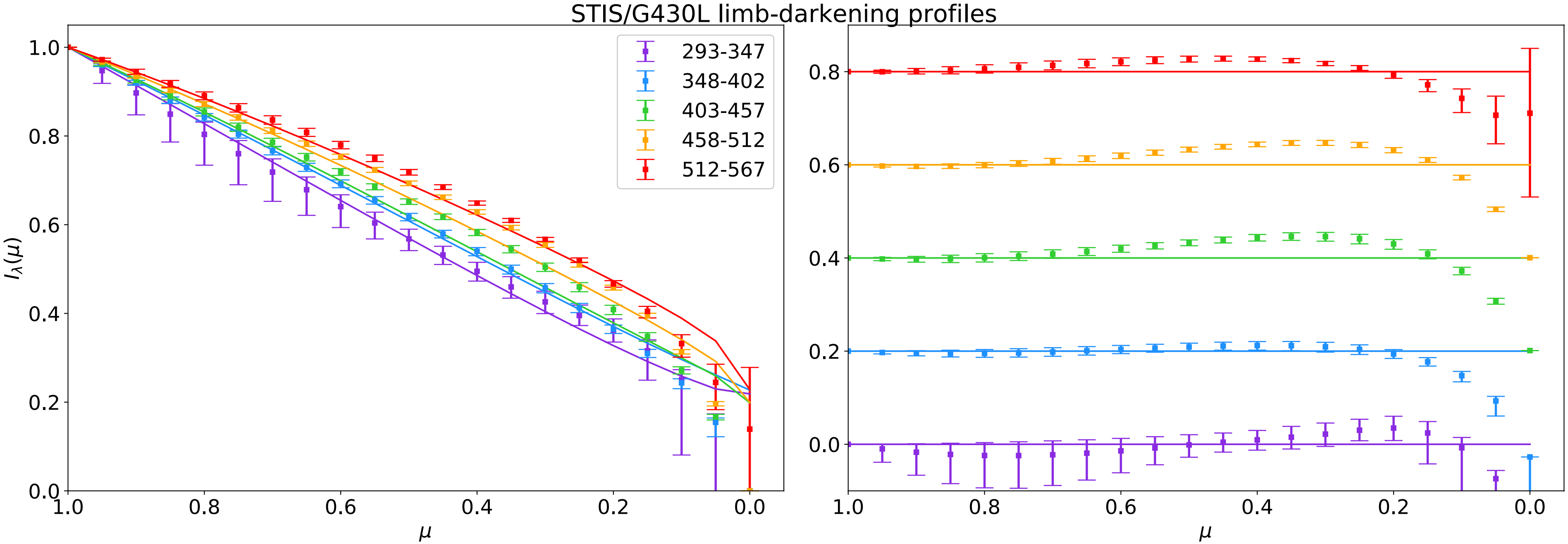
SEA BASS: simulations



Morello et al. 2017

2

SEA BASS: HD20458 l-d profile



Morello, arXiv:1712.09393

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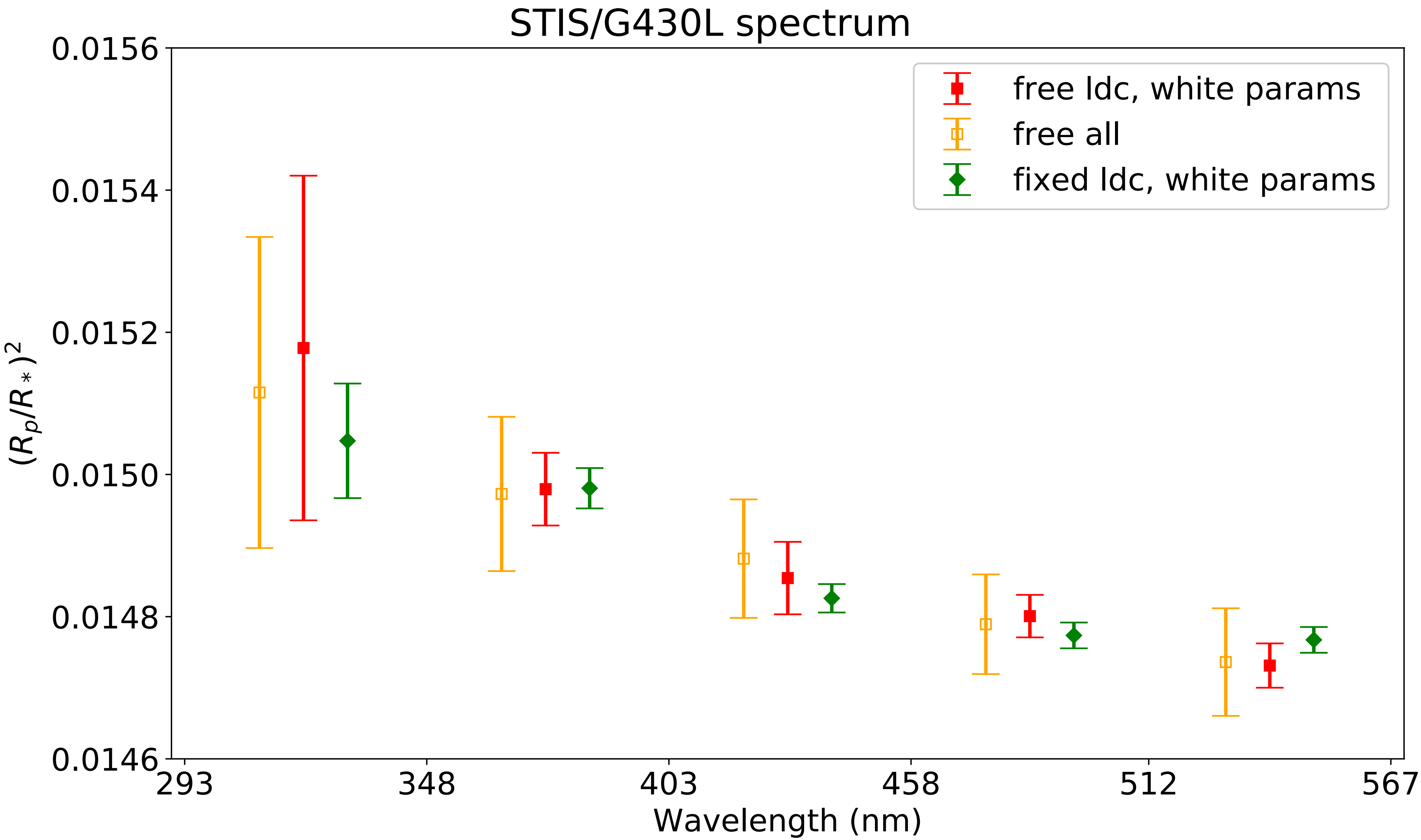
SEA BASS: HD20458b spectrum

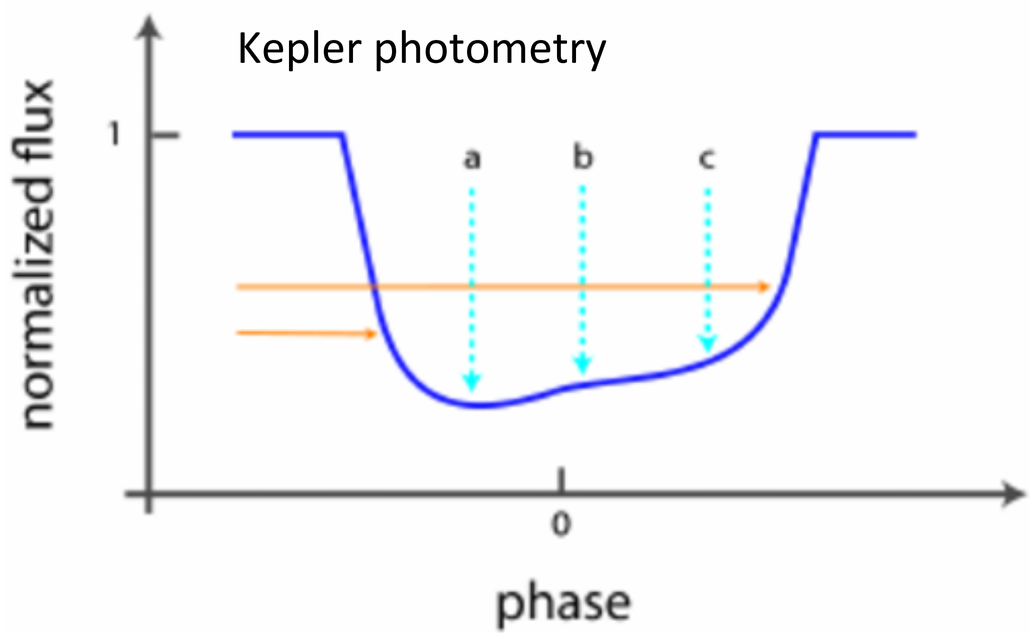


Morello, arXiv:1712.09393

State-of-the-art scientific results

Rapid rotators: KOI13

- Stellar oblateness
- Gravity darkening
- Rossiter–McLaughlin effect



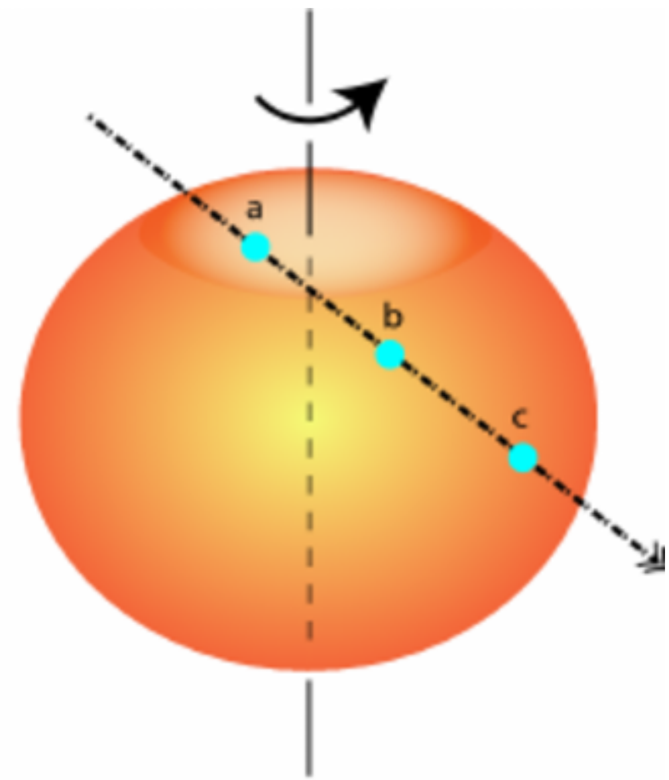


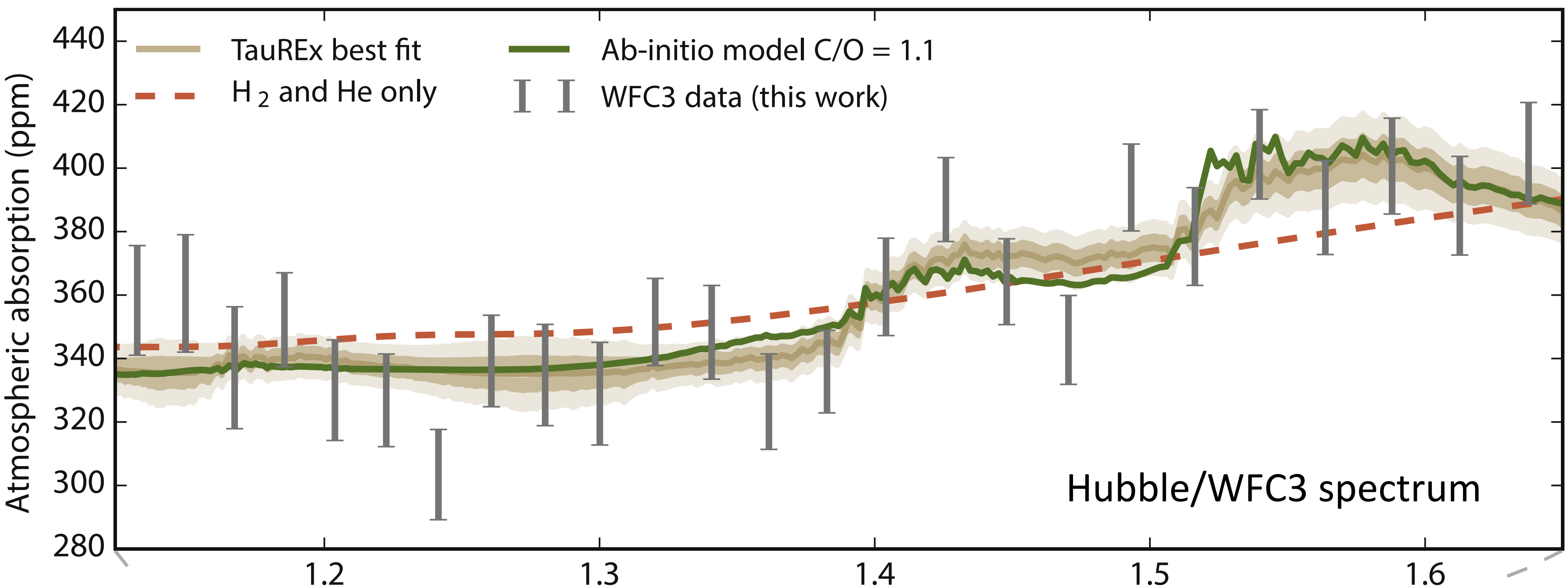
Image credit: Szabo et al. 2013

Absolute system dimensions determined from star's projected equatorial rotational speed

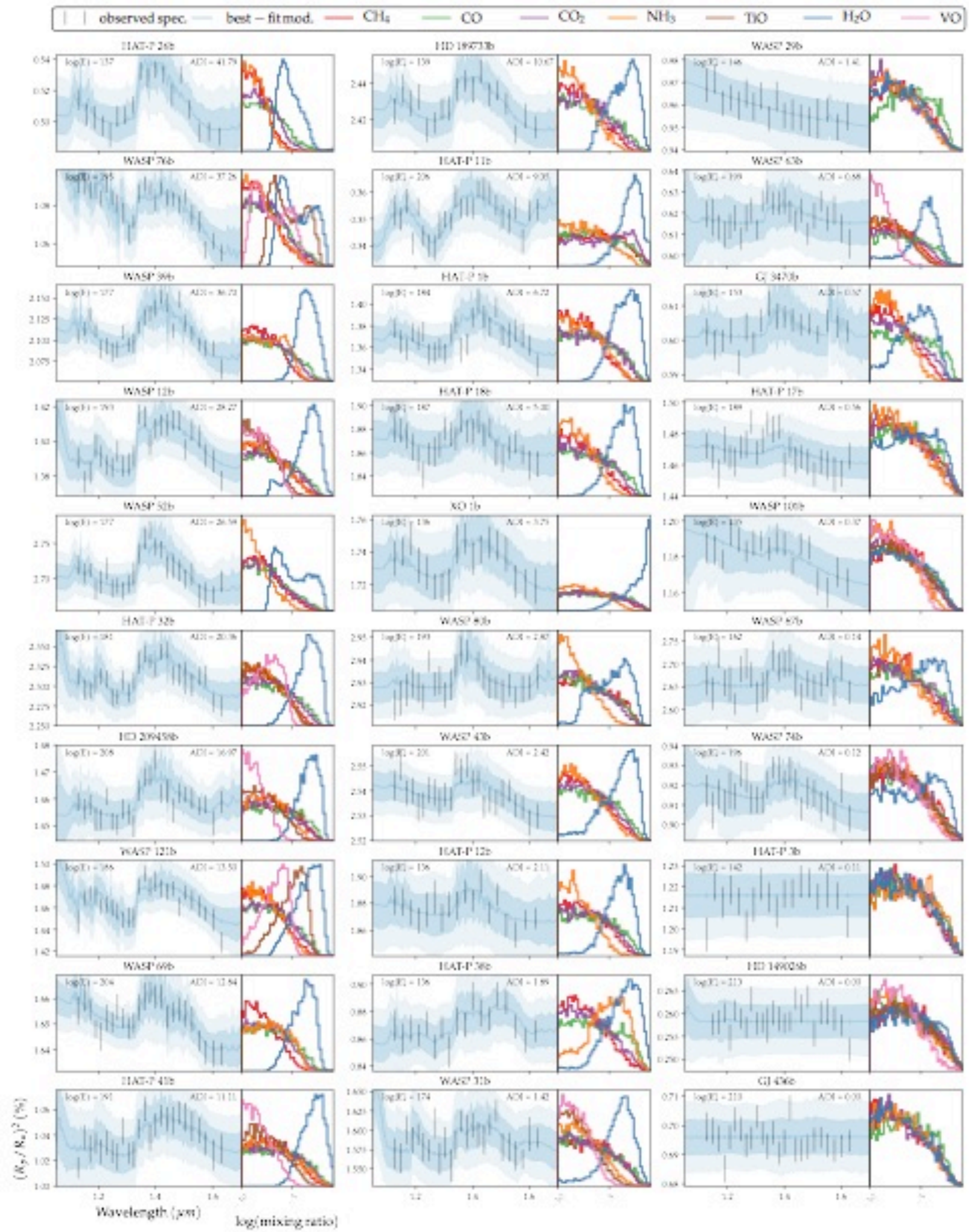
Howarth & Morello 2017

Atmosphere around super-Earth 55 Cnc e

Star: $T_{\rm eff} = 5200\,K,\ M_* = 0.91\,M_\odot,\ R_* = 0.94\,R_\odot$
Planet: $T_{\rm eq} = 1950\,K,\ M_p = 8.1\,M_\oplus,\ R_p = 2.0\,M_\oplus$
Orbital: $a = 0.01545\,AU = 3.523\,R_*,\ P = 0.7365417\,\text{days}$



Tsiaras et al. 2016



A POPULATION STUDY OF HOT JUPITER ATMOSPHERES

- Largest catalogue of exoplanet atmospheres (30 planets);
- Observed with Hubble/WFC3;
- H_2O, TiO, VO detections;
- No clouds in very hot planets;
- Atmospheric Detectability Index (ADI) not correlated with S/N

Tsiaras et al., arXiv:1704.05413

Conclusions

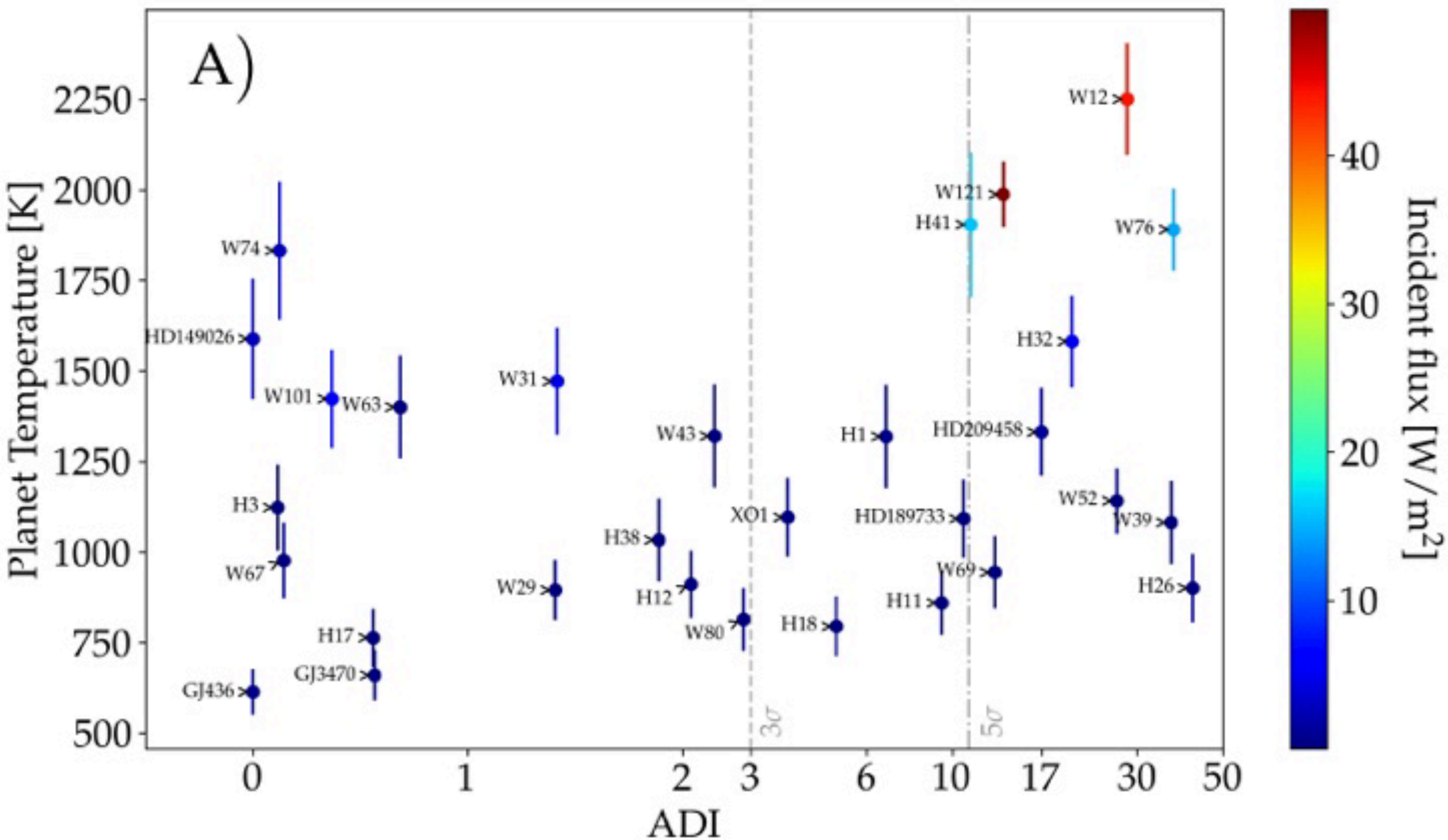
TO DATE

- Transit/eclipse/phase curve spectroscopy for exoplanets atmospheric characterisation;
- High-performance, objective (blind) data detrending methods: pixel-ICA, stripe-ICA;
- High-precision and accuracy empirical star's limb-darkening: SEA BASS;
- Scientific results: individual targets (KOI13, 55 Cnc e), catalog (30 planets)

FUTURE PROJECTS

- JWST data detrending pipelines
- Observational techniques for stellar activity, non-spherical bodies, etc.
- Catalog: higher-quality data, larger wavelength coverage and sample of exoplanets;
- Correlations, link with formation and evolution.

MERCI


A)
Planet Temperature [K]
ADI
Incident flux [W/m^2]
3σ
5σ
W12
W121
H41
W76
W74
HD149026
H32
W31
W101
W63
W43
H1
HD209458
H3
XO1
HD189733
W52
W39
H38
W67
W69
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H12
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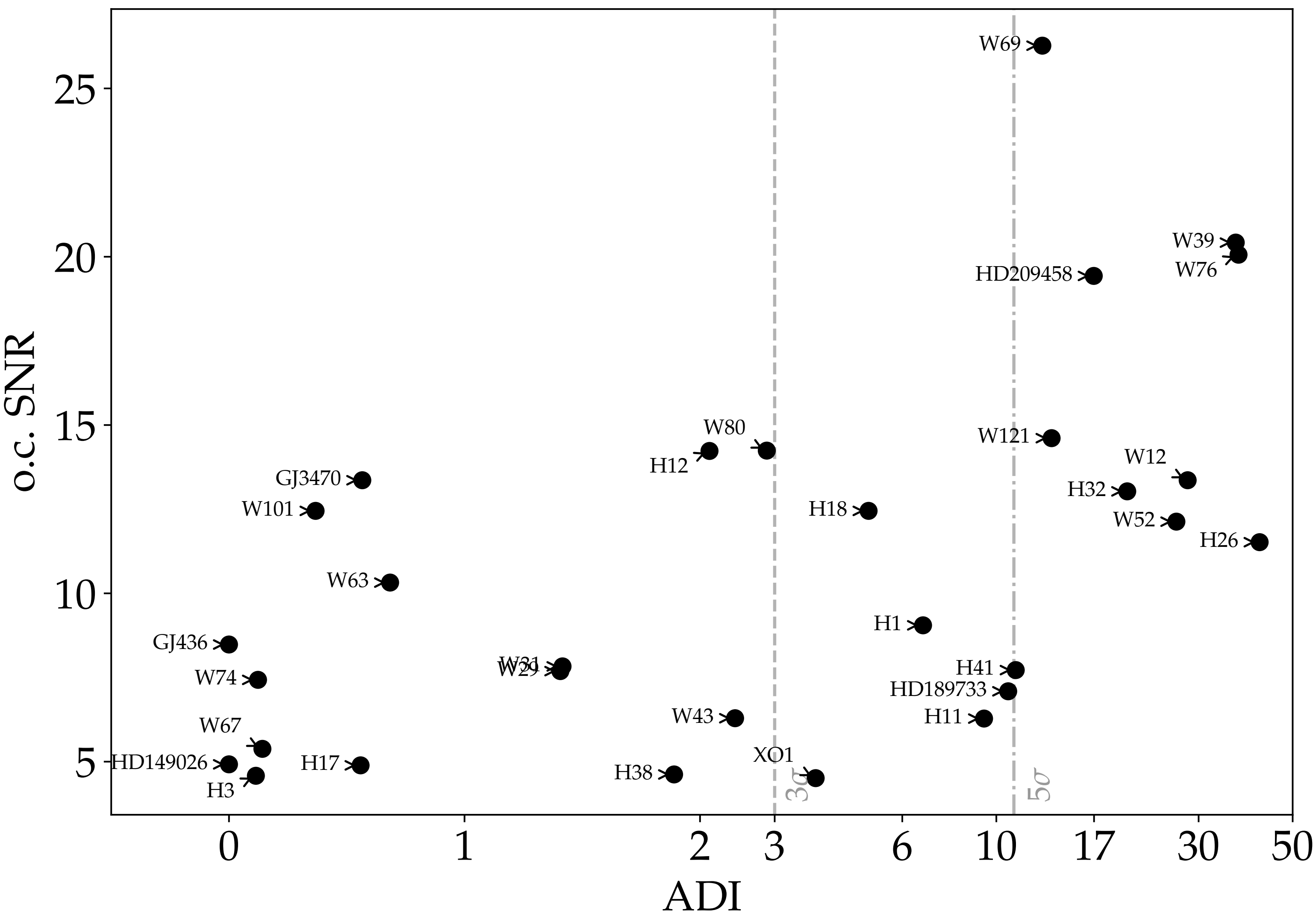
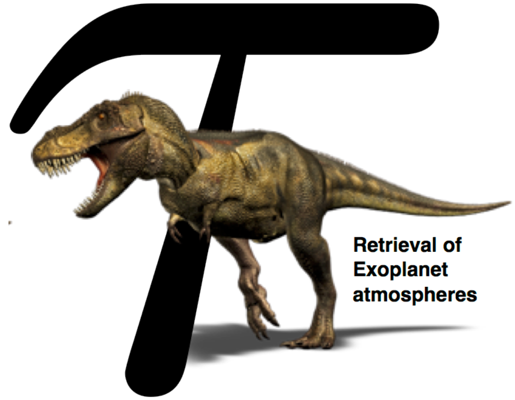
H11
W80
H18
H17
GJ3470
GJ436

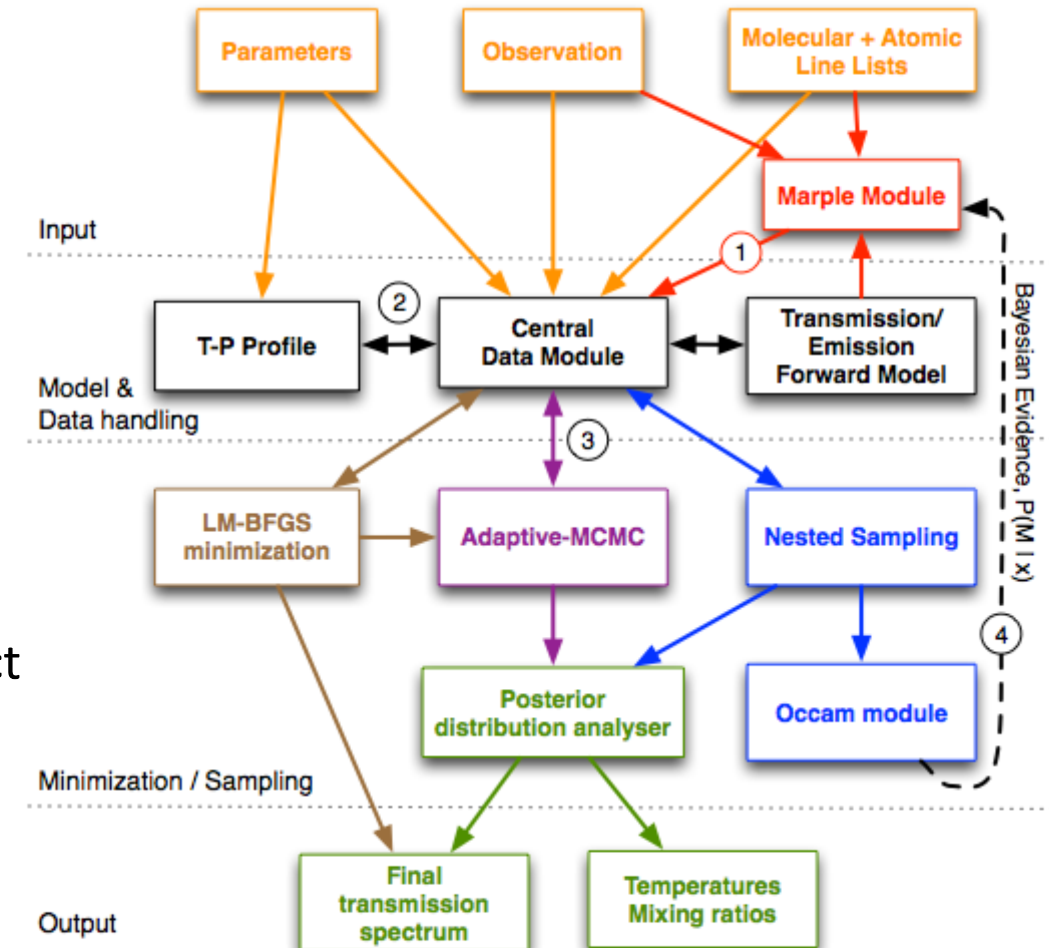


o.c. SNR
ADI
0
1
2
3
6
10
17
30
50
5
10
15
20
25
3σ
5σ
W69
W39
W76
HD209458
W80
H12
W121
W12
H32
W52
H26
GJ3470
W101
H18
W63
H1
GJ436
W31
W29
H41
HD189733
W74
W43
H11
W67
HD149026
H17
H38
XO1
H3

3



- **Fully Bayesian Retrieval**
  - MCMC
  - Nested Sampling
  - Maximum Likelihood
- **Cross-sections** from Hitran/ Hitemp and the ExoMol project
- Prior composition selection through **pattern recognition software**
- **Full parallelisation for cluster computing**



Waldmann et al. 2015a,b; Rocchetto et al. 2016

PCA vs ICA

- Linear transformation of the observations;
- Find a basis of orthogonal components.

PCA

- *Uncorrelatedness*:
  $E\{xy\} = E\{x\} \, E\{y\}$
- Up to 2^{nd}-order statistics
- Pre-processing step for ICA

ICA

- *Independence*:
  $E\{f(x)g(y)\} = E\{f(x)\} \, E\{g(y)\}$
- Higher-order statistics

ICA: statistics (2)

Among all the distributions with fixed mean and covariance, the gaussian distribution has the maximum entropy.

$$J(\mathbf{y}) = H(\mathbf{y}_{gauss}) - H(\mathbf{y})$$ negentropy

- Mutual information and negentropy are hard computing.
- Alternatively, we can maximize non-gaussianity of the source signals, through different estimators.

$$kurt(y) = E(y^4) - 3E(y^2)^2$$ kurtosis

$$J(y) \approx \sum_{i=1}^{p} k_i [E\{G_i(y)\} - E\{G_i(\nu)\}]^2$$ approximated negentropy

Negentropy approximations

$$J(y) \approx \sum_{i=1}^{p} k_i [E\{G_i(y)\} - E\{G_i(\nu)\}]^2$$

contrast functions

random gaussian variable

$$G_i(s) = \log(\cosh s)$$

$$G_i(s) = e^{-\frac{s^2}{2}}$$

$$G_i(s) = s^4$$

Hyvarinen 1999

Time-correlated signals

Joint diagonalization of several time-lagged covariance matrices

$$\mathbf{R}_{\mathbf{x}}(\tau_k) = E(\mathbf{x}(t)\mathbf{x}^T(t+\tau_k)), \quad k = 0, ..., M-1$$

$$\mathbf{R}_{\mathbf{s}}(\tau_k) = \mathbf{A}^T \mathbf{R}_{\mathbf{x}}(\tau_k)\mathbf{A}$$

We adopt MULTICOMBI code (Tichavsky et al. 2006) to perform ICA decomposition.

Interference-to-Signal Ratio

- If the source signals and the true mixing matrix are known, it is possible to test the goodness of the separation:

Normalized gain matrix

$$\tilde{\mathbf{G}} = \hat{\mathbf{W}}\mathbf{A}\mathbf{D}^{\frac{1}{2}}$$

Diagonal matrix of the variances of the estimated source signals

Estimated inverse mixing matrix

True mixing matrix

- In case of perfect demixing, the normalized gain matrix is the identity.

$$\mathbf{ISR}_{ij} = \frac{\tilde{\mathbf{G}}_{ij}^{2}}{\tilde{\mathbf{G}}_{ii}^{2}} \approx \tilde{\mathbf{G}}_{ij}^{2}$$

- For certain algorithms, it is possible to calculate asymptotical expressions for the **ISR** matrix, which are independent on the mixing matrix.

Error bars

$$\sigma_{par} = \sigma_{par,0}\sqrt{\frac{\sigma_0^2 + \sigma_{ICA}^2}{\sigma_0^2}}$$

$$\sigma_{ICA}^2 = f^2\left(\sum_j o_j^2 \mathbf{ISR}_j + \sigma_{ntc-fit}^2\right)$$

MULTICOMBI:

$$\mathbf{ISR} = \frac{\mathbf{ISR}^{EF} + \mathbf{ISR}^{WA}}{2}$$

$$\boxed{\mathbf{ISR}_{i,j} = min\left(\mathbf{ISR}_{i,j}^{EF}, \mathbf{ISR}_{i,j}^{WA}\right)}$$

LILLE
PARIS
STRASBOURG
NANCY
BREST
RENNES
ORLEANS
Seine
Loire
NANTES
DIJON
LYON
BORDEAUX
TOULOUSE
Rhone
NICE
MARSEILLE
AJACCIO