Modeling atmospheres

CEA/MDLS: P. Tremblin

European Research Council
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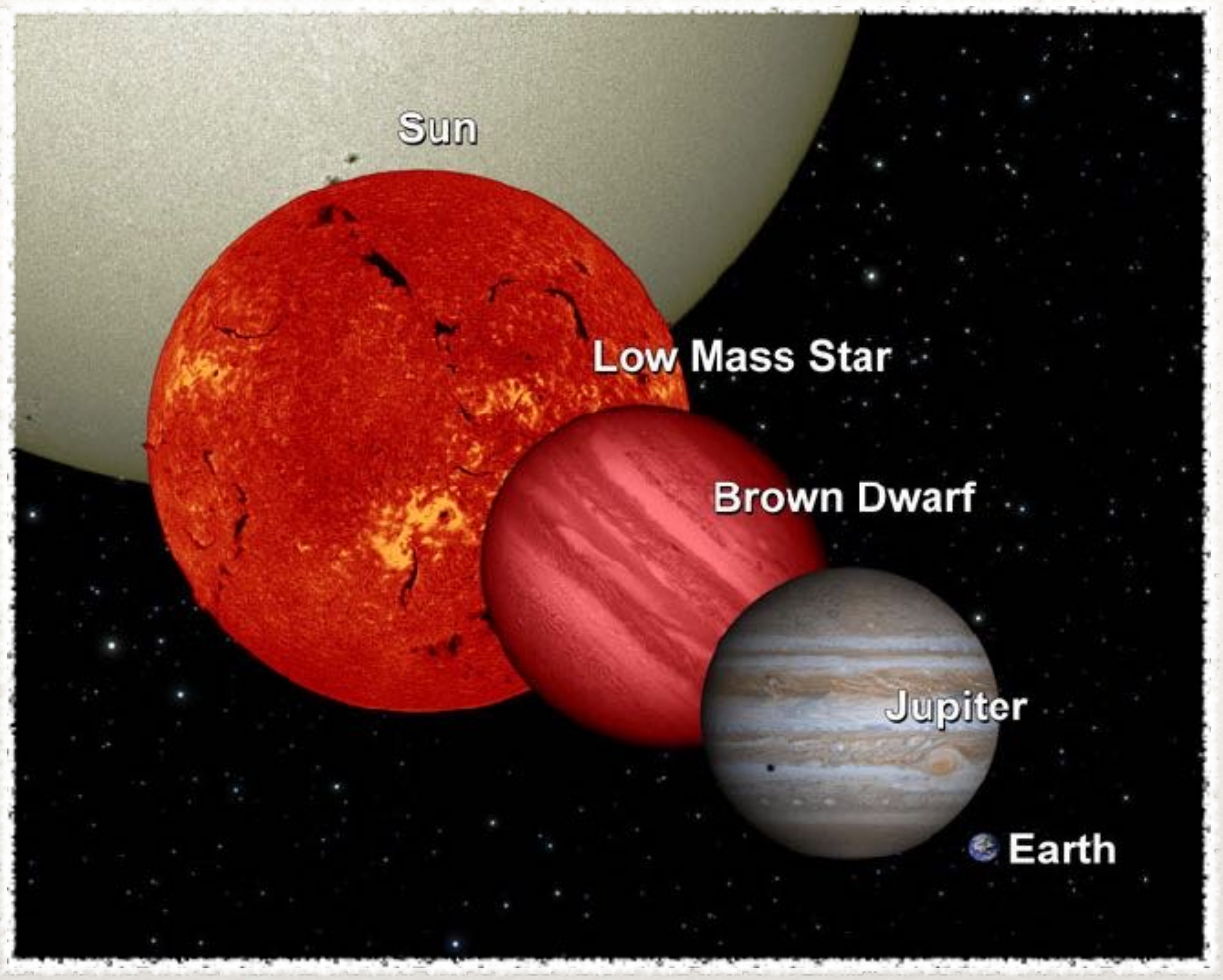
MAISON DE LA SIMULATION

What is an exoplanet?

- Brown dwarfs

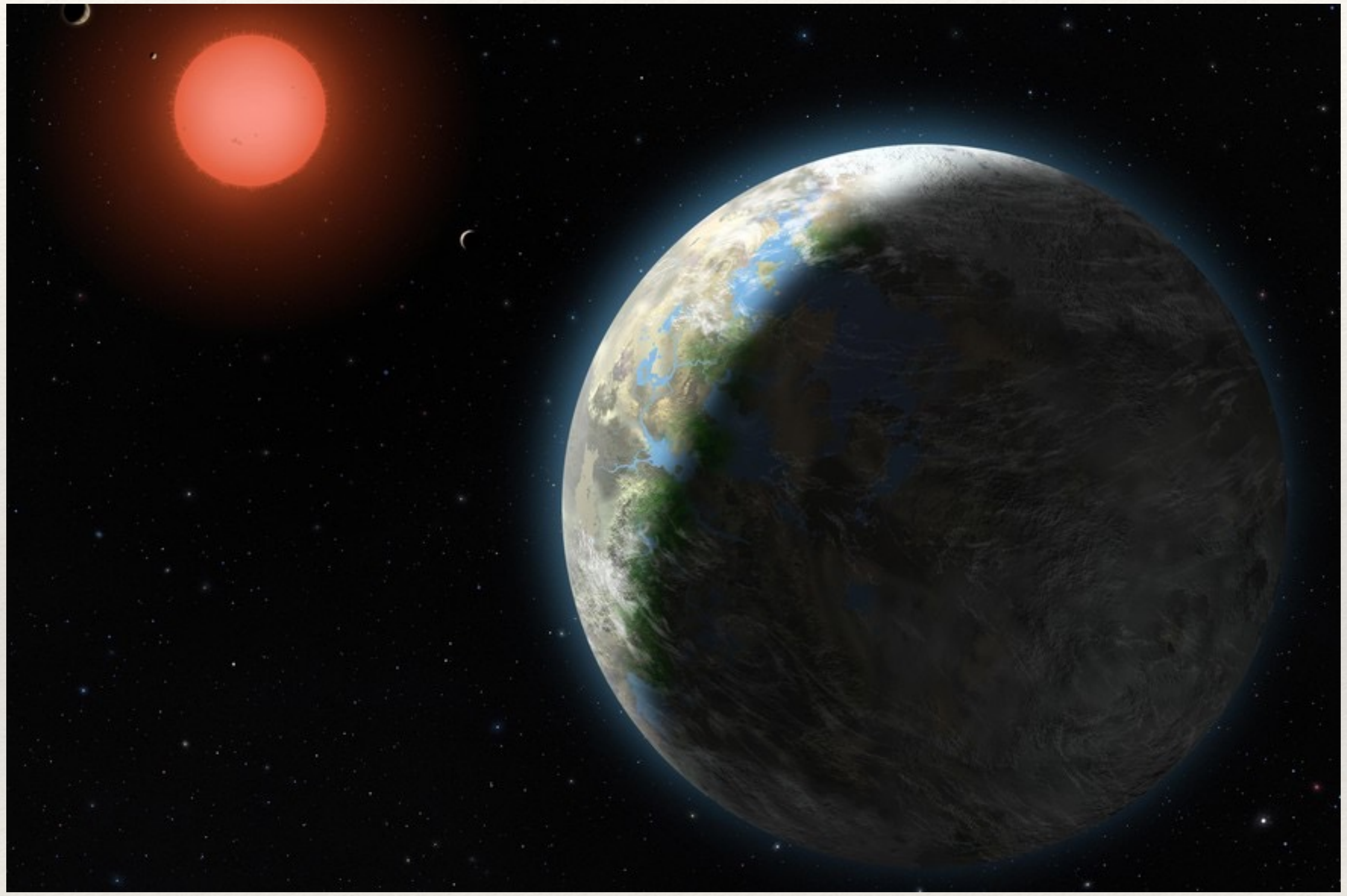


- Theoretically proposed by Kumar and Hayashi & Nakano in the 1960s
- Discovered in 1995 Rebolo et al./Nakajima et al.

- Form like star: grav. Collapse in a molecular cloud
- No H burning
- Cooling sequence between Teff~2500K Teff~250K
- Fuzzy difference with giant planets (good proxy for atmospheres!)

➢ Definition

- An exoplanet is a planet that does not orbit around the Sun but around another star (well sort of…, modulo brown dwarfs)



➢ Definition

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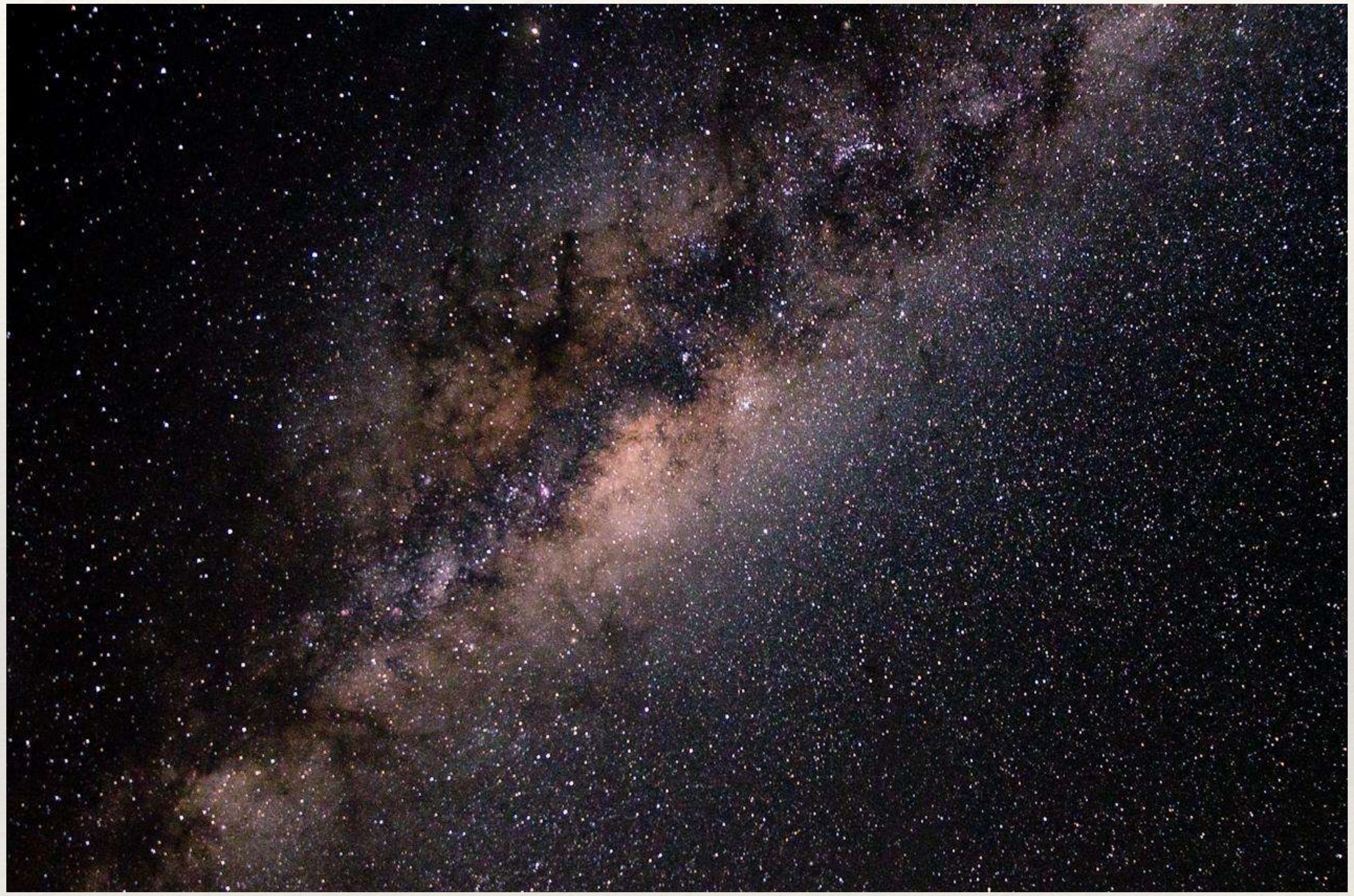
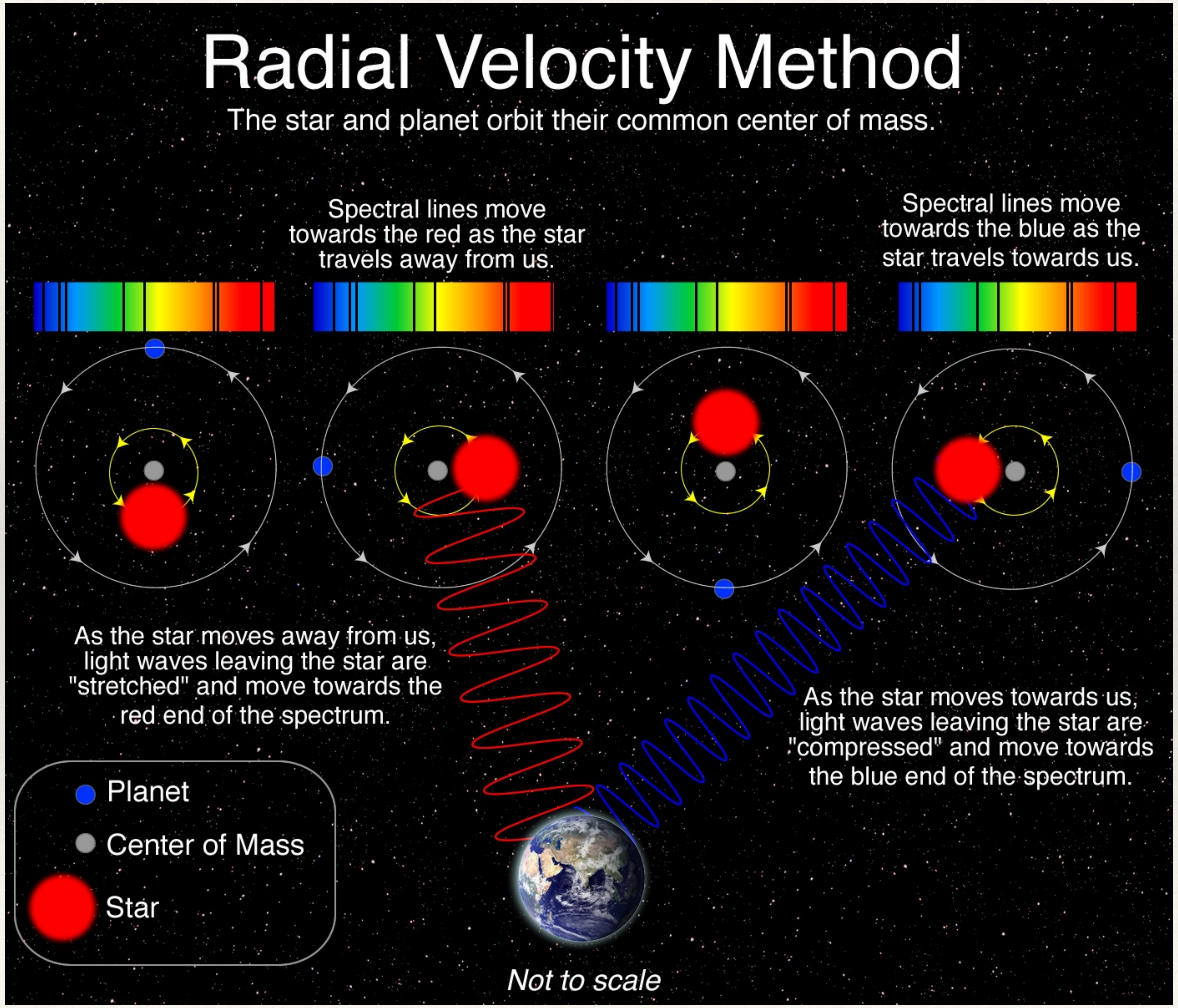


–Quite hard to find in the sky…

➢ A bit of history…

- Once upon a time, there were astronomers who have imagined an undirect detection method: the radial-velocity method

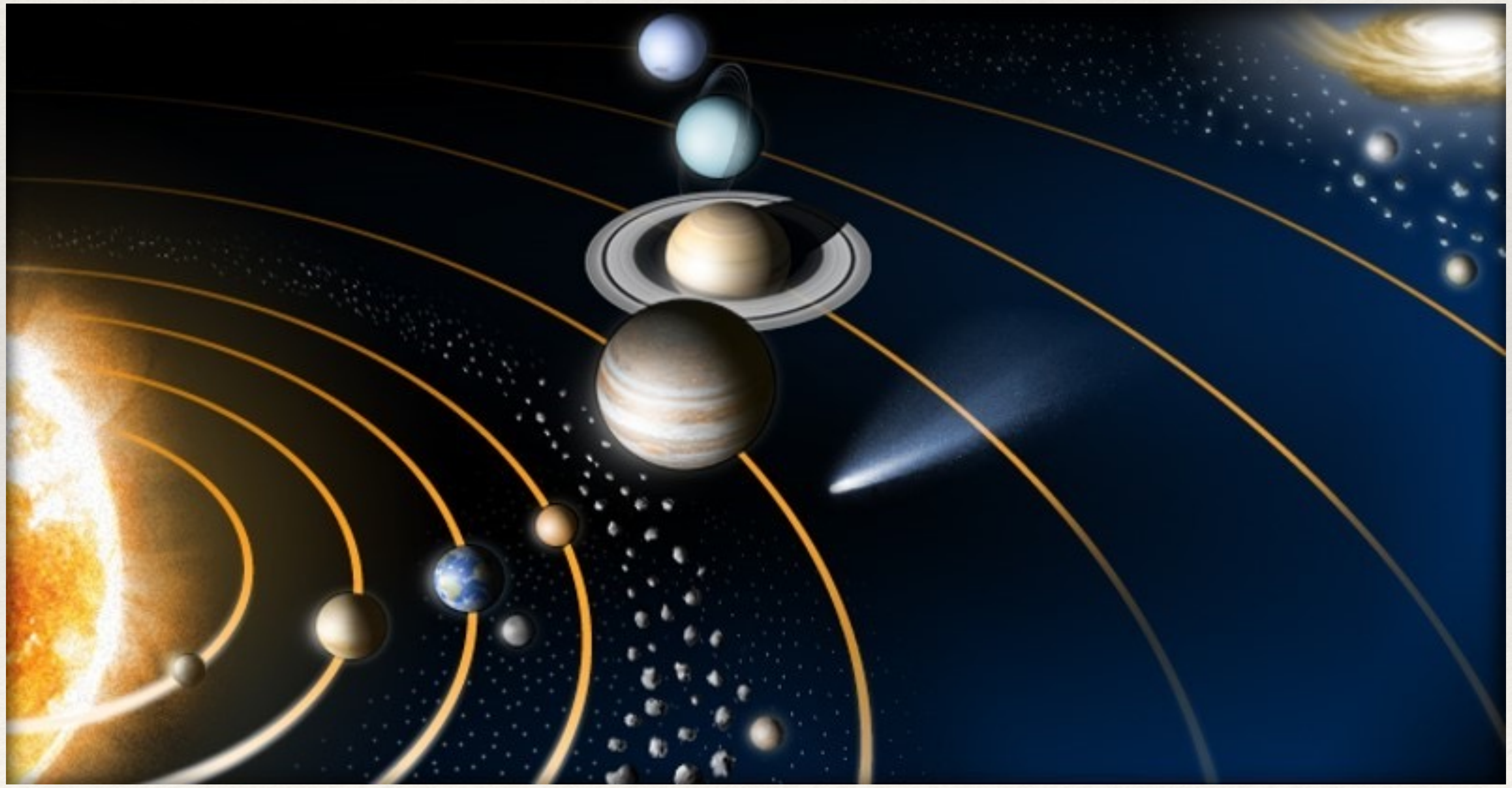


A bit of history…

- In the end of 80's early 90's, astronomers knew that their detectors were sensitive enough to detect this kind of signal.
- Many teams around the world started to collect data and look for planets. But no robust detection has been made in the beginning…
- Why ?

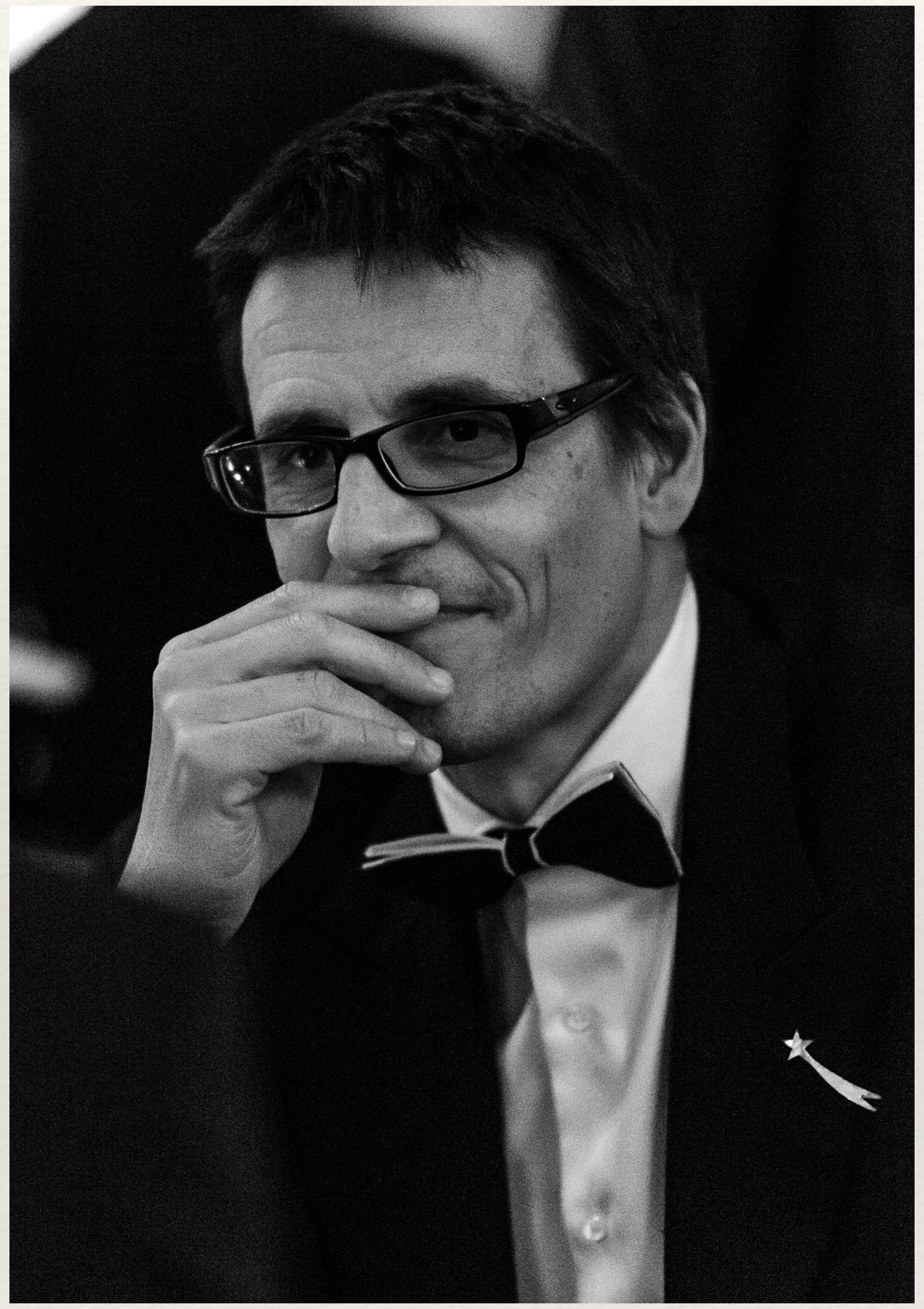
➢ A bit of history…

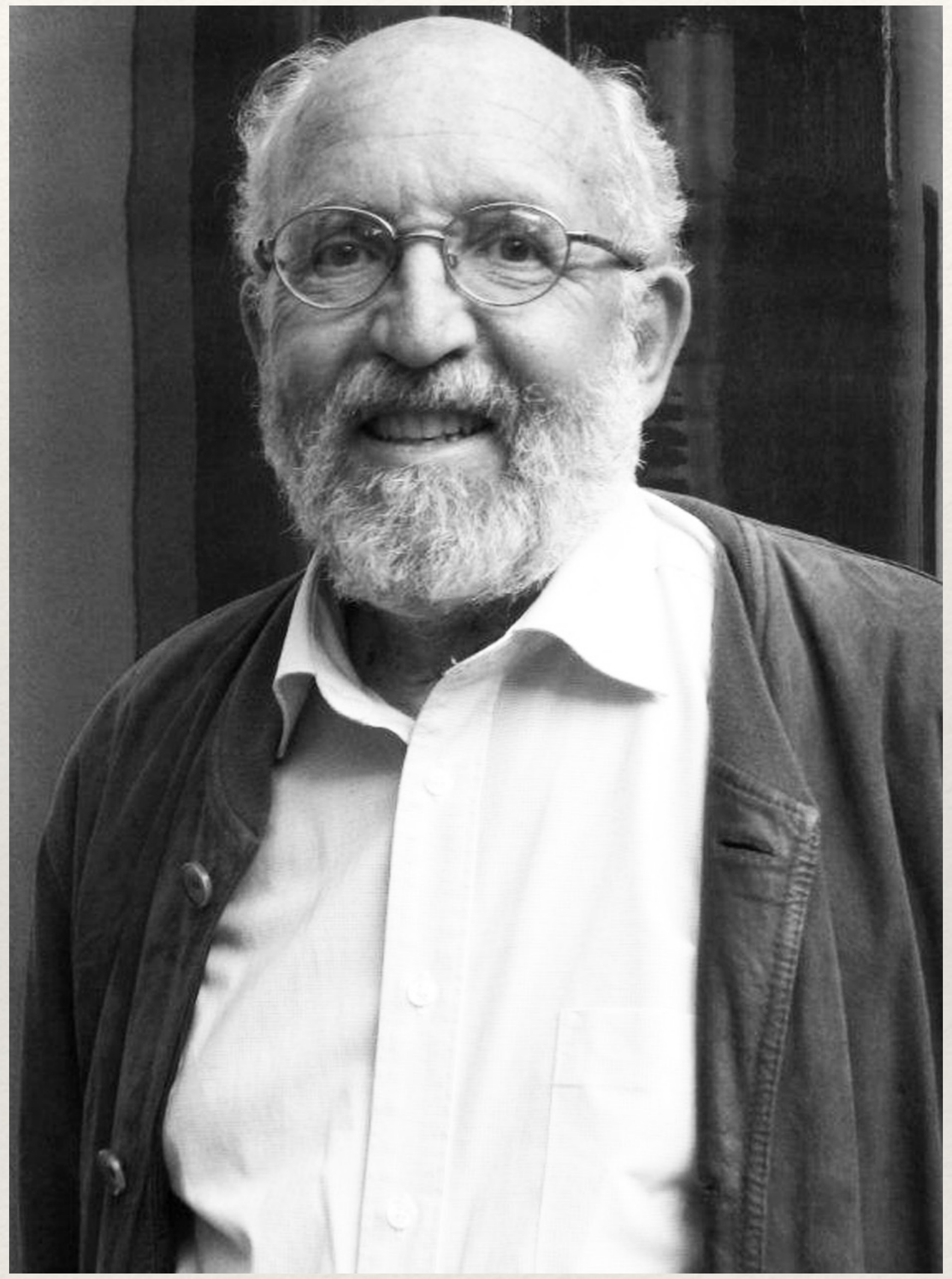
- In the end of 80's early 90's, astronomers knew that their detectors were sensitive enough to detect this kind of signal.
- Many teams around the world started to collect data and look for planets. But no robust detection has been in the beginning…
- Why ? You need the big guy, like Jupiter for the star to move



➢ A bit of history…

- In 94/95, Didier Queloz and Michel Mayor were actually analysing their data on the fly with the Elodie spectrograph at Observatoire de Haute Provence.

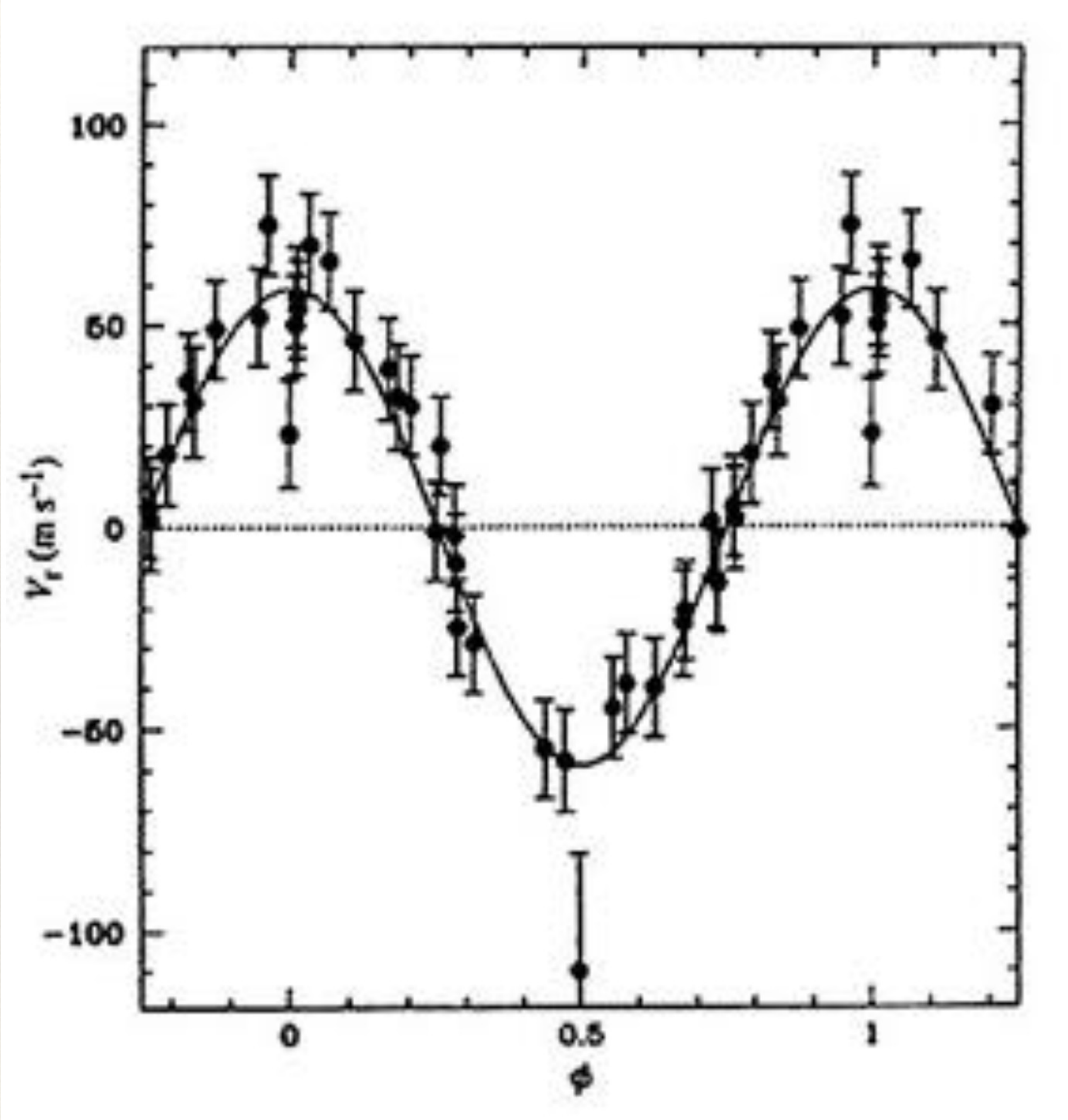




–… and found a tiny signal in their data…

➤ A bit of history…

- After almost one year checking their data, they extract this signal from the star 51 Pegasus



–… and found that an object (51 peg b) is orbiting with a period of only **4.2 days**

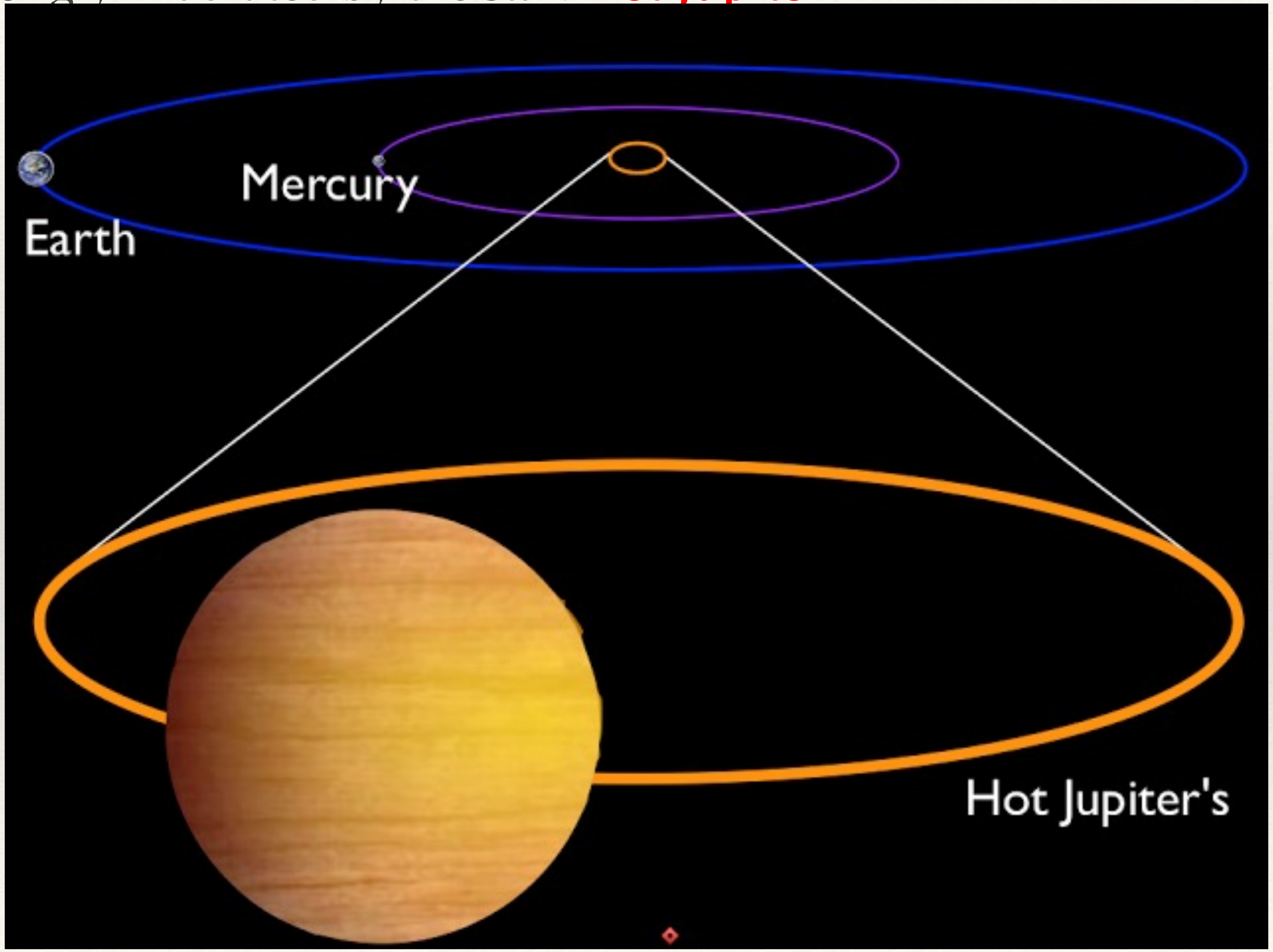
A bit of history…

–How do we get the orbit of the object?

- How do we get the mass of the object?

➢ A bit of history…

- Minimum mass of 0.5 mass of Jupiter orbiting at 0.05 au of the star…
- Strongly irradiated by the star: **Hot Jupiter**



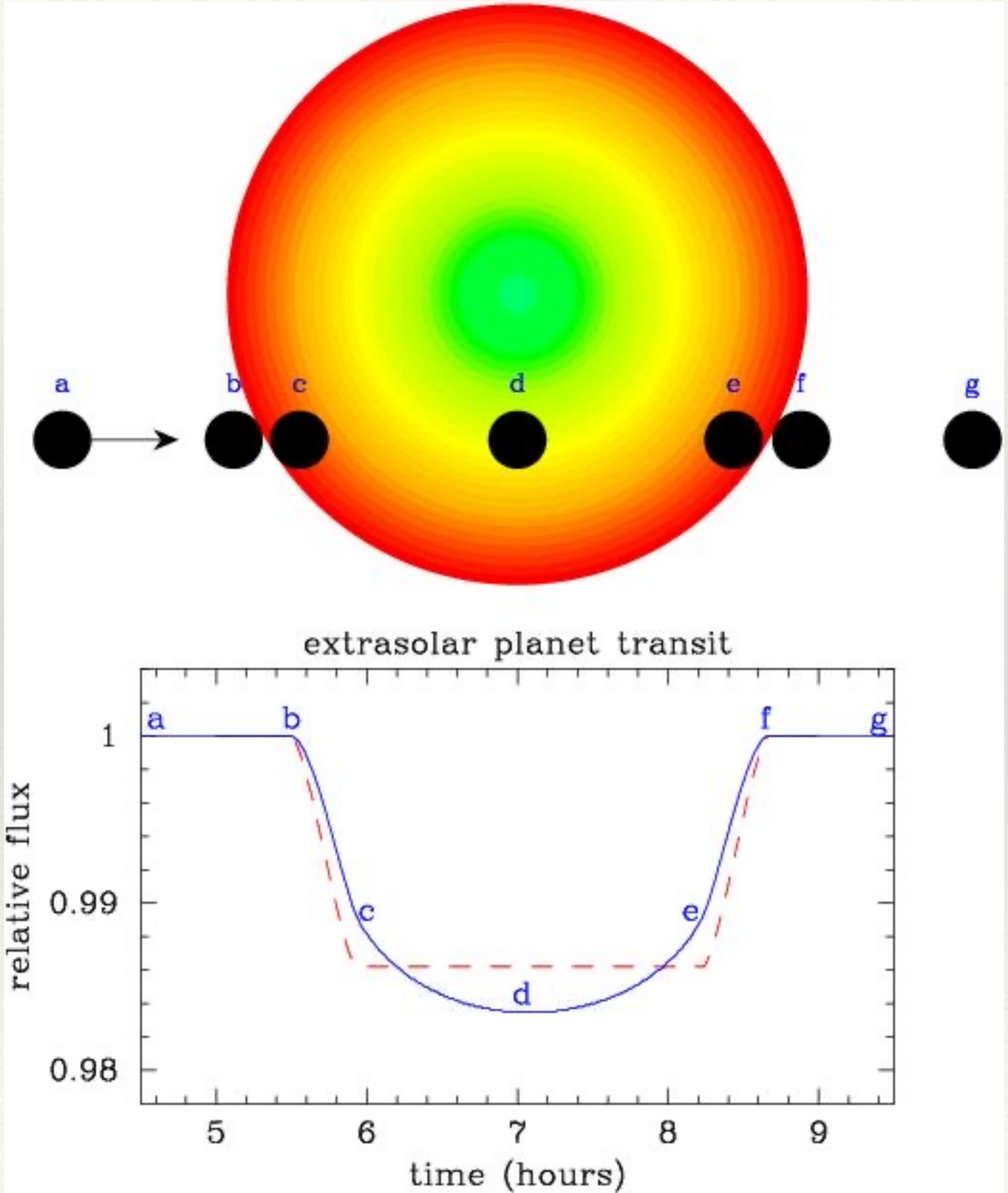
➢ A bit of history…

- Nobody has ever predicted this kind of planets to exist: a huge part of the astrophysics community (and the press) was not ready to accept this detection:

  - Instrumental error? (the signal around 51 peg was immediatly confirmed by competitors, Marcy's group)
  - Astrophysical artifact? E.g. from the atmosphere of the star? star spots ?
  - A binary star?

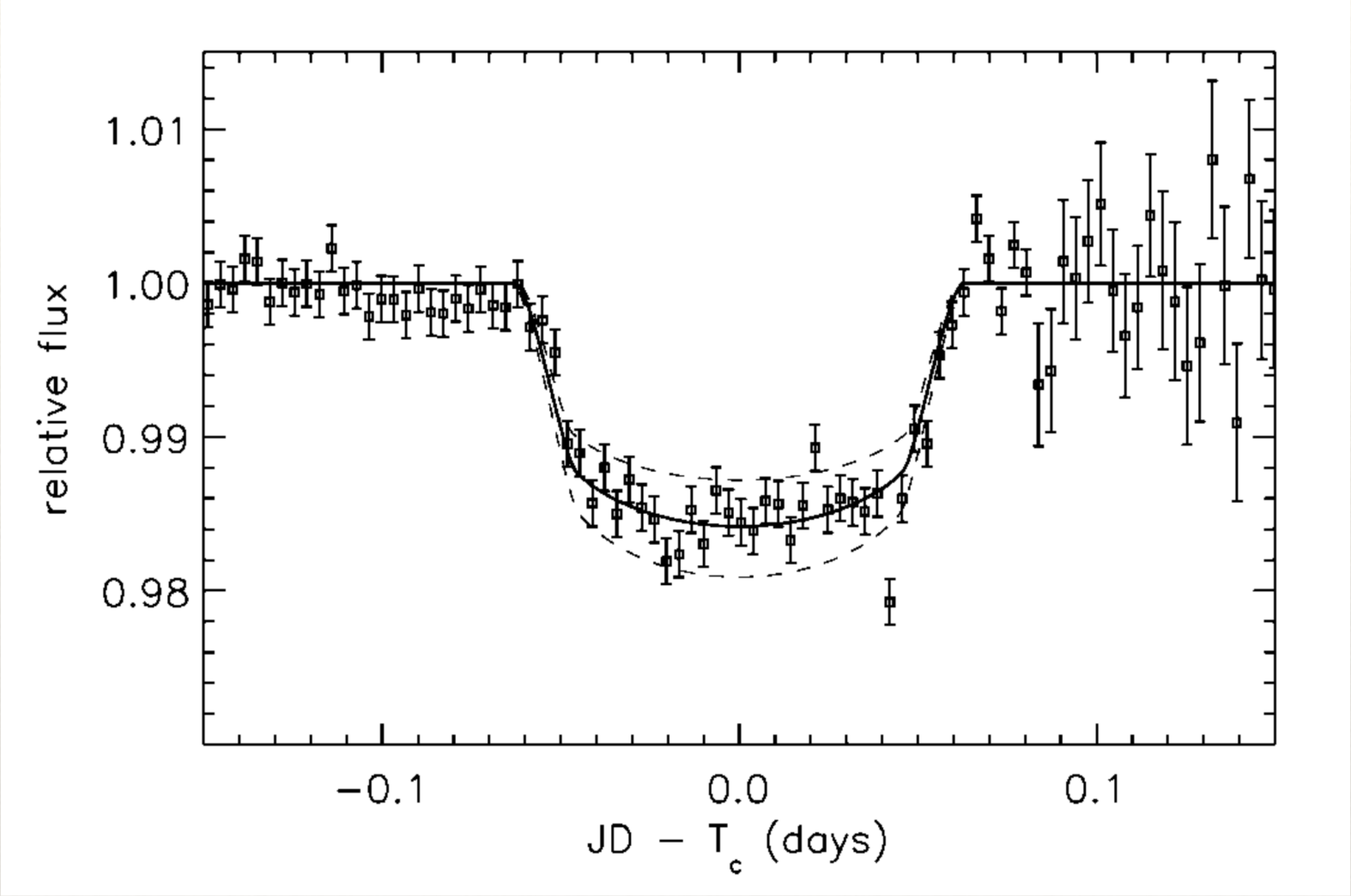
➢ A bit of history… part 2

- Once upon a time, there were astronmers who imagined a second undirect detection technique: the transit method



➢ A bit of history… part 2

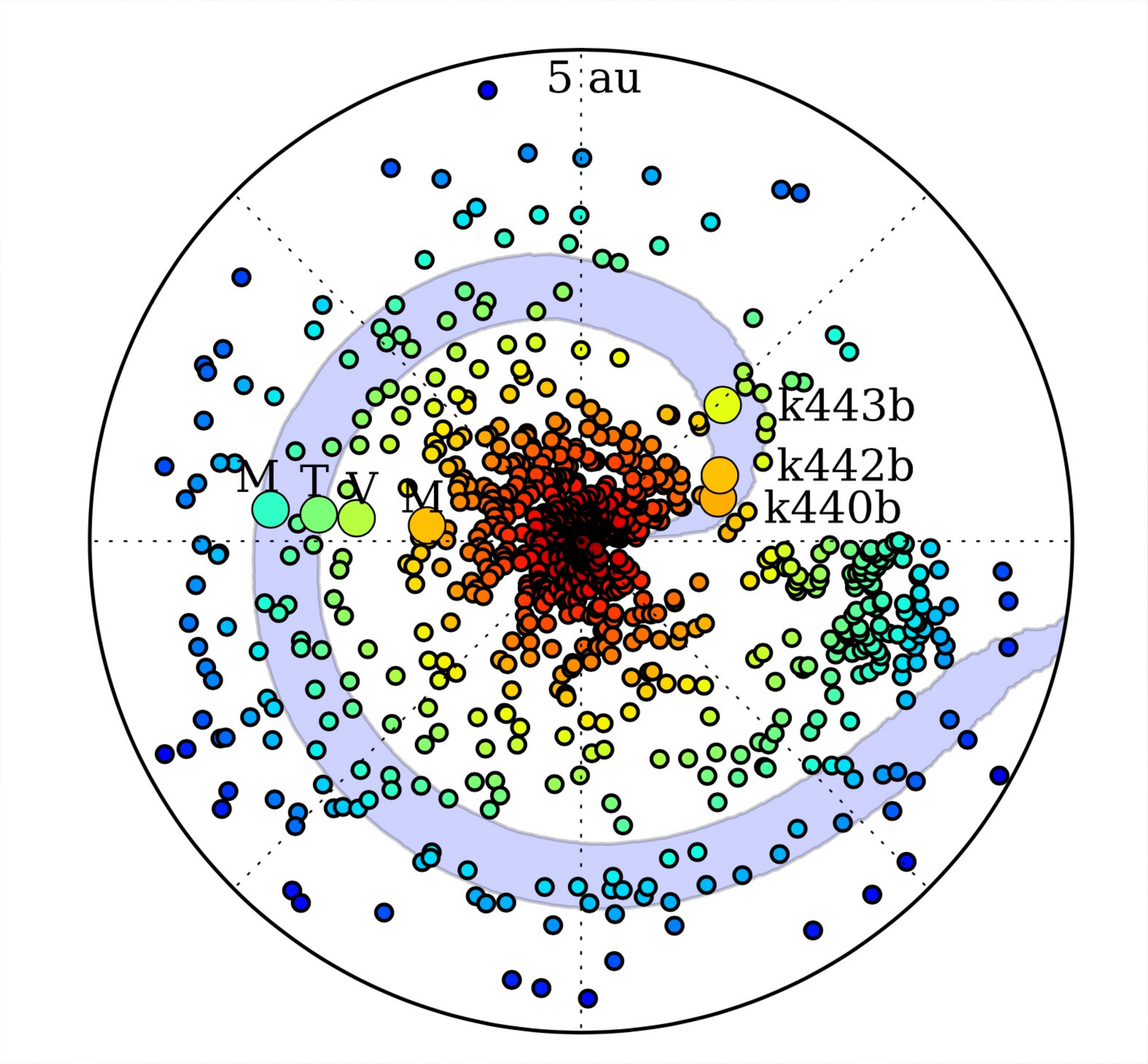
- Astronomers had to wait until 1999 for the first detection by this method, a 0.7 Jupiter-mass hot jupiter called HD209458b



–Finally confirming the existence of exoplanets!

➢ A bit of history… part 2

- Since then astronomers have observed up to **5600 exoplanets** with an important diversity in terms of mass, radius, orbits, etc… with a few rocky planets in the habitable zone of their parent stars:



➢ But a big challenge: the inflated radius of hot jupiter

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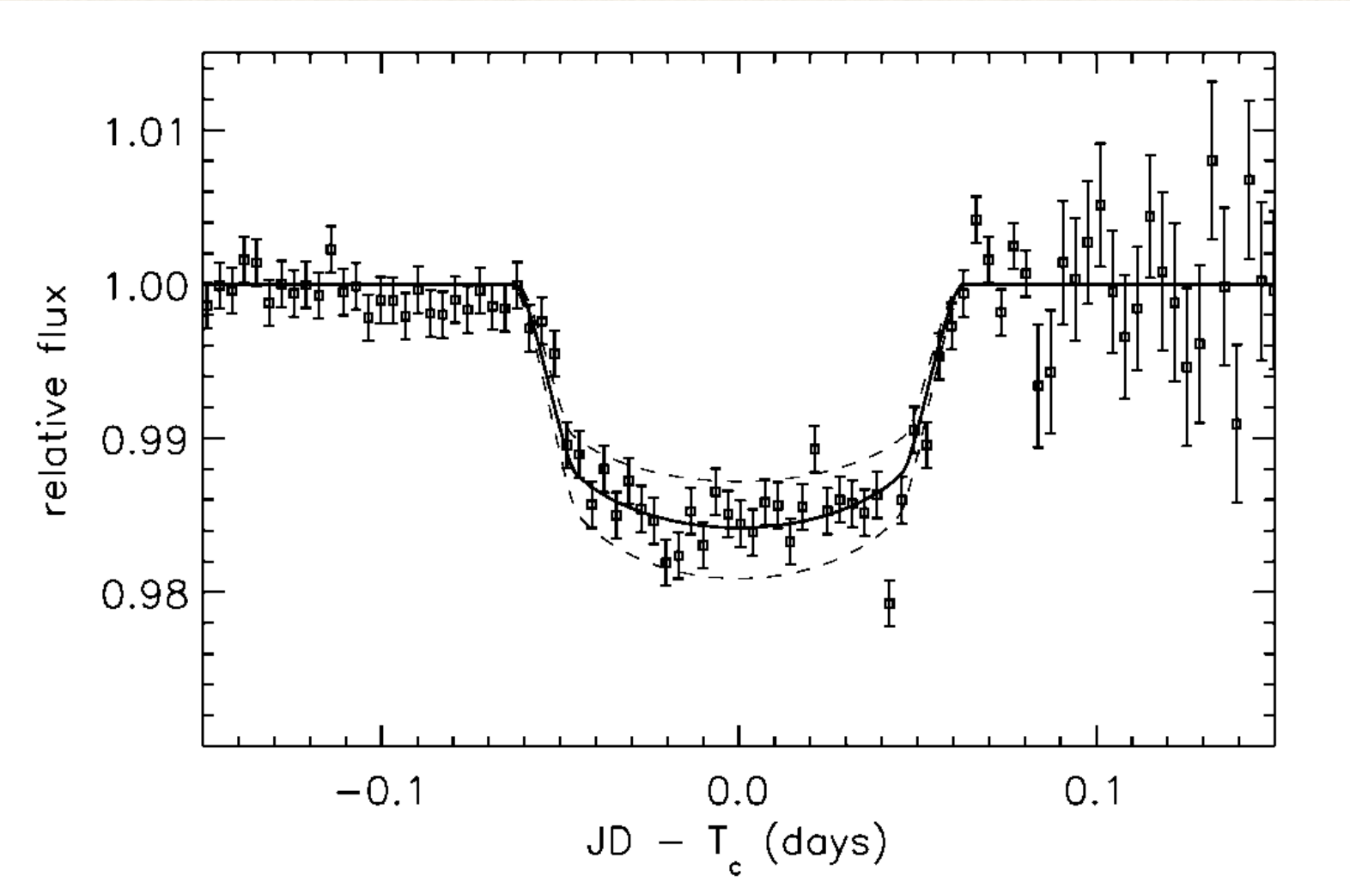

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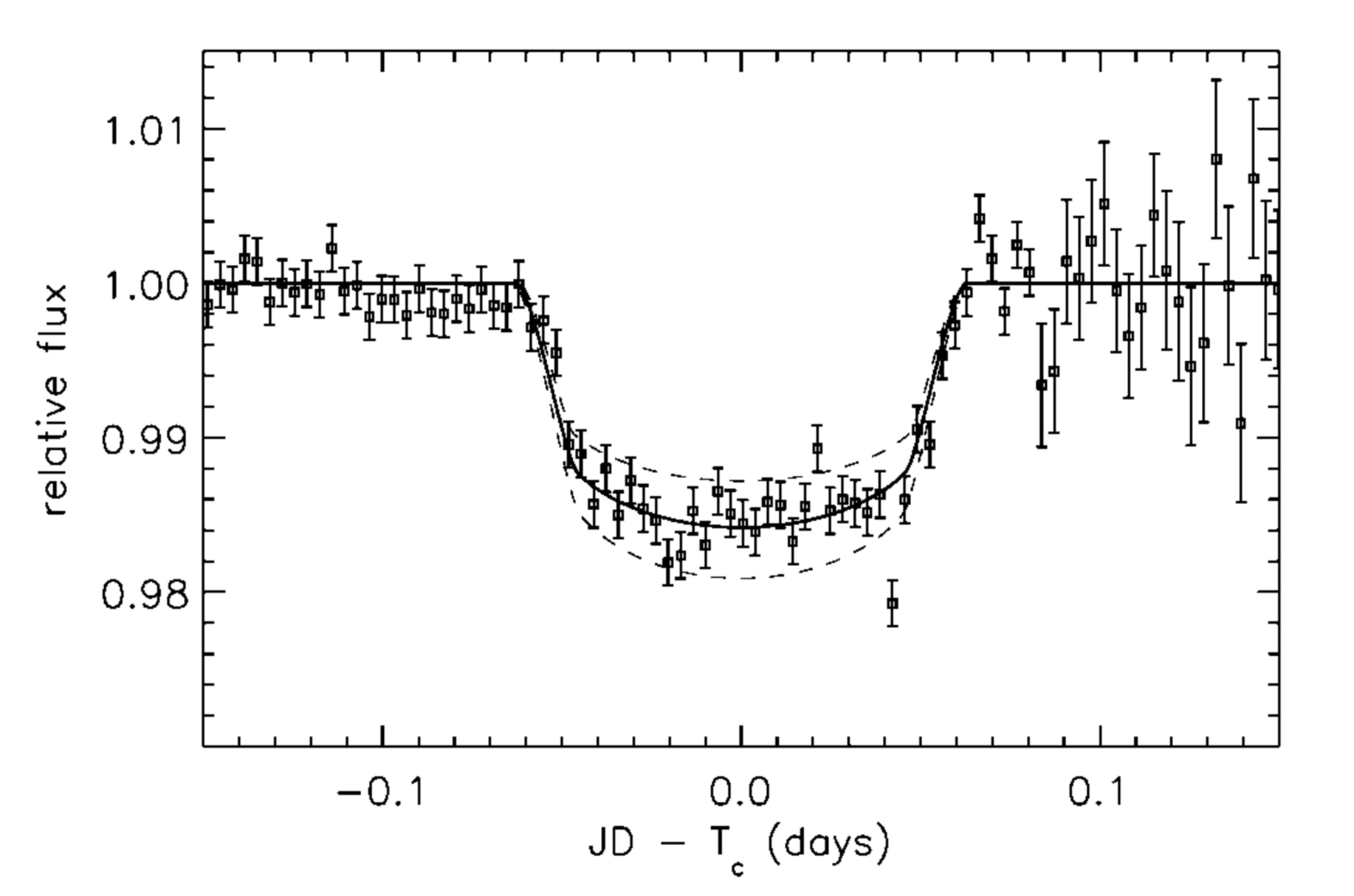
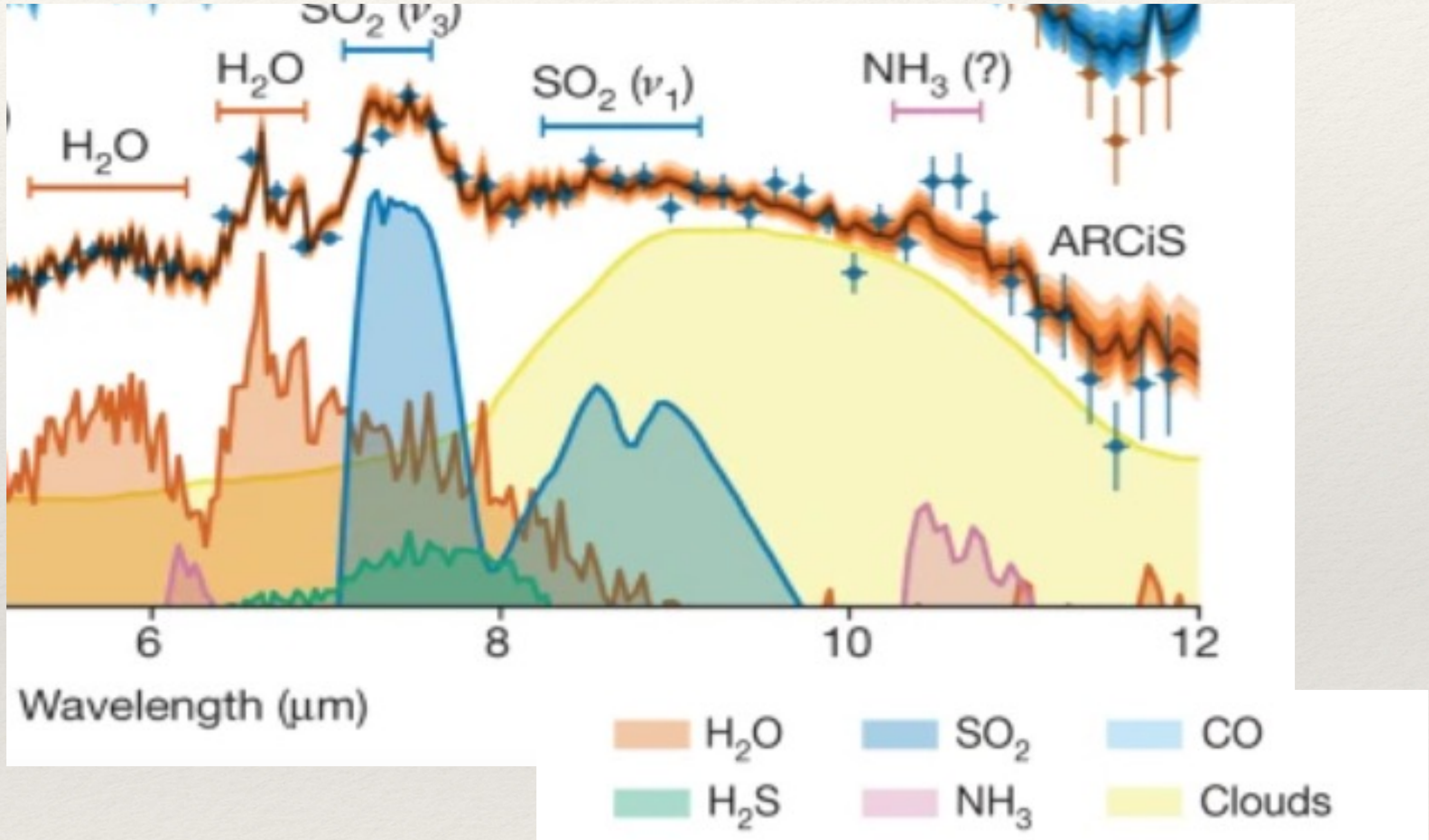


- R = 1.4 Rjup



SO_2, silicate clouds, but no CH_4 detected in a warm Neptune

A. Dyrek et al. 2023 , Nature

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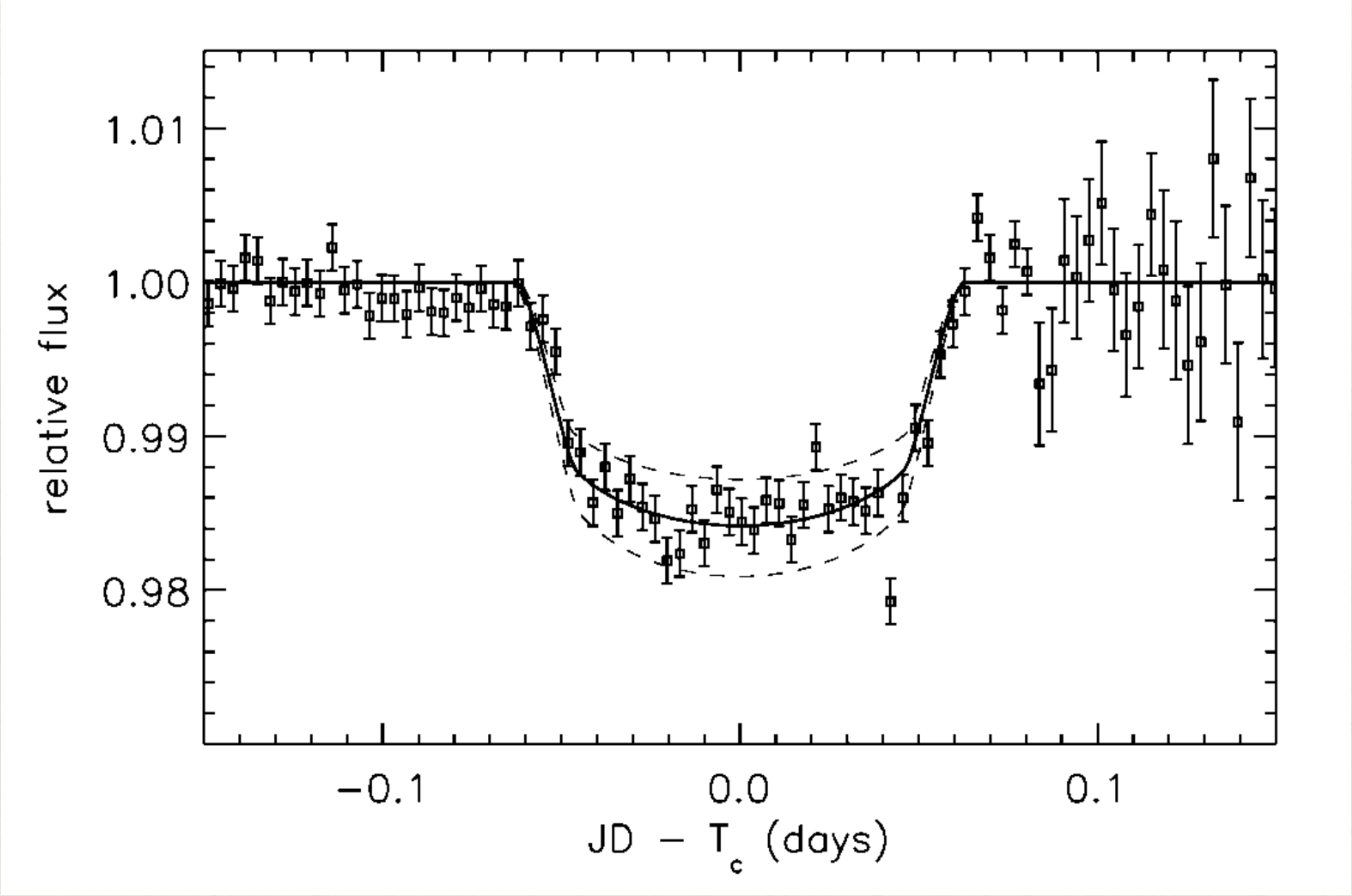

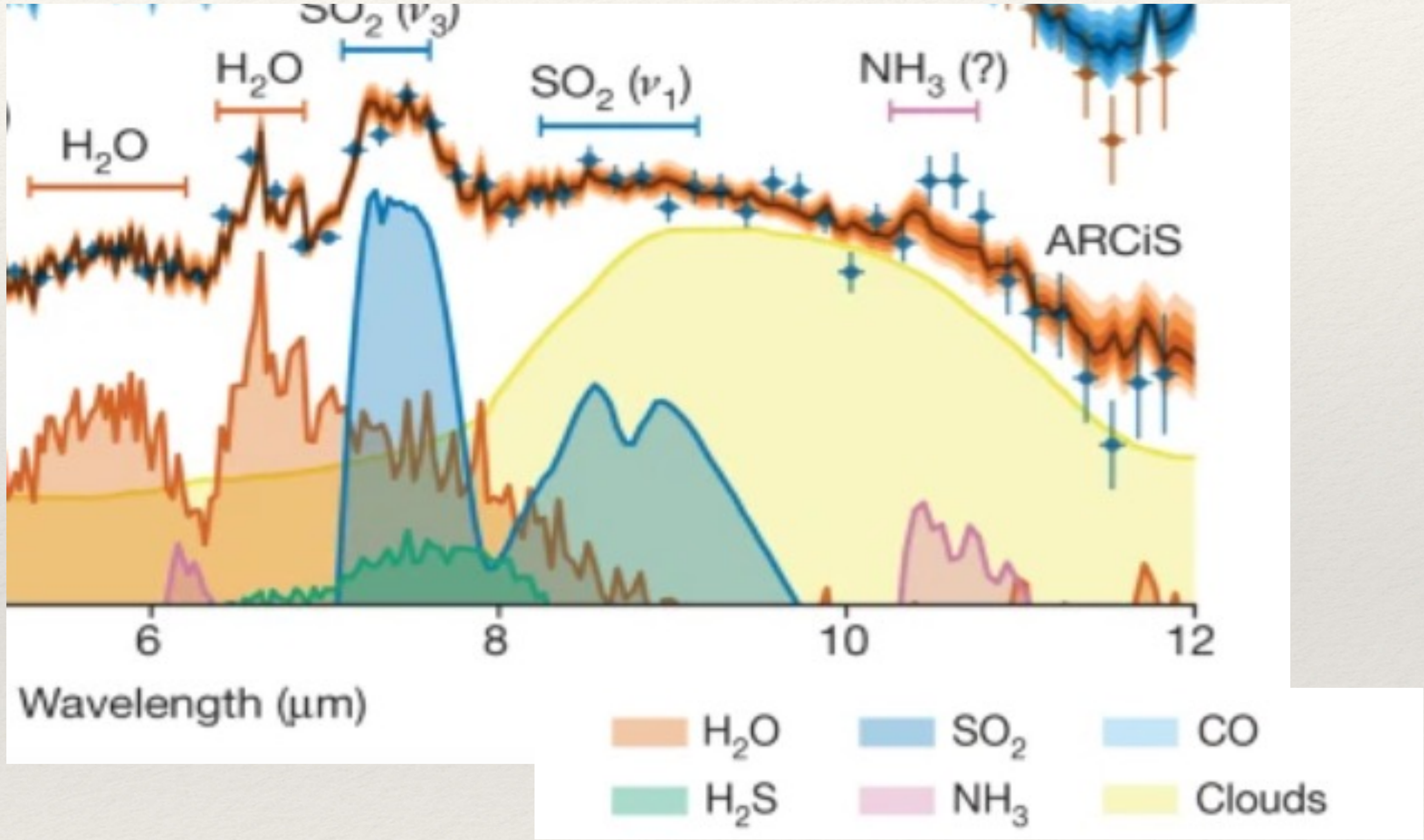

SO_2, silicate clouds, but no CH_4 detected in a warm Neptune

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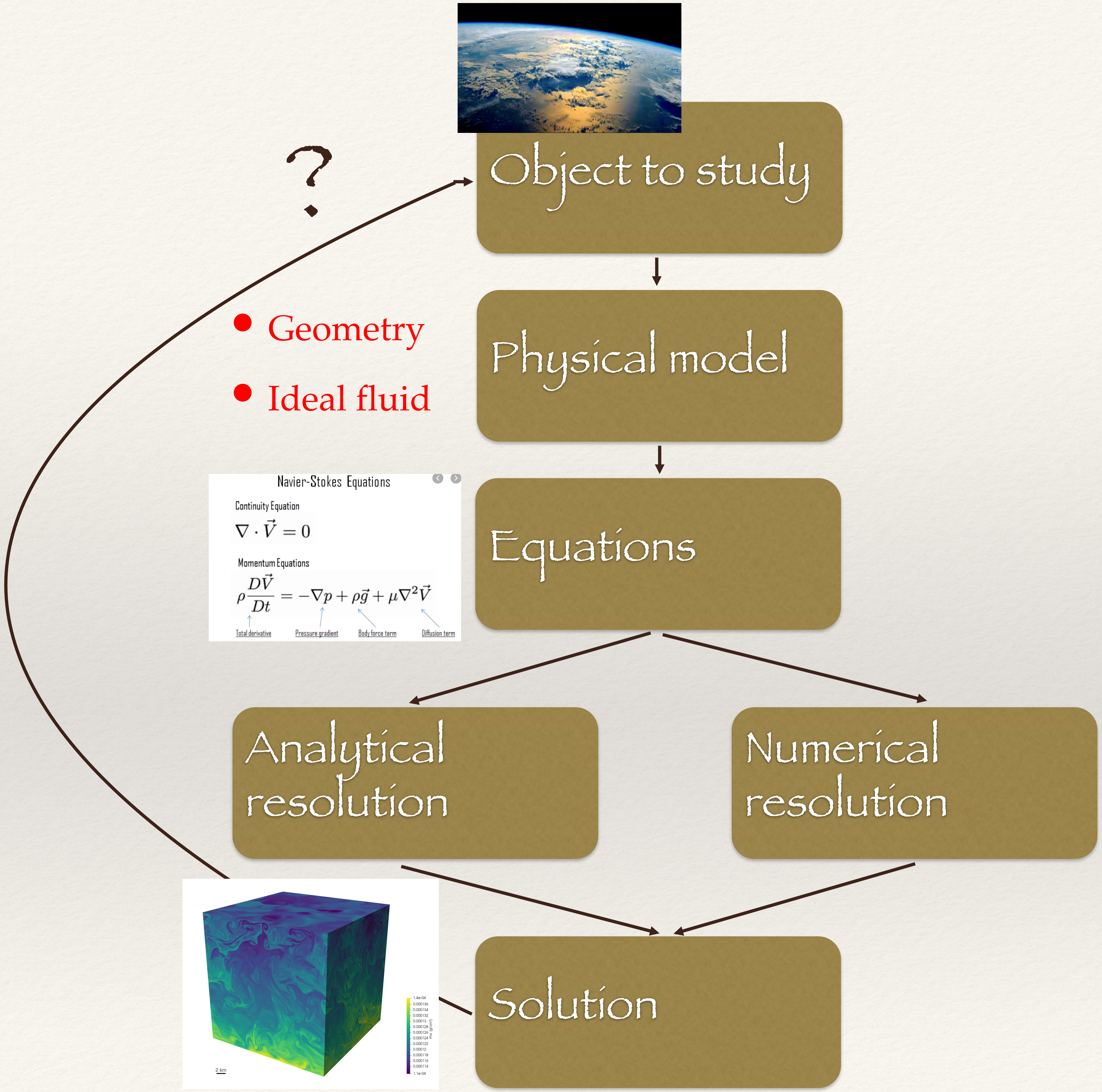
- R = 1.4 Rjup

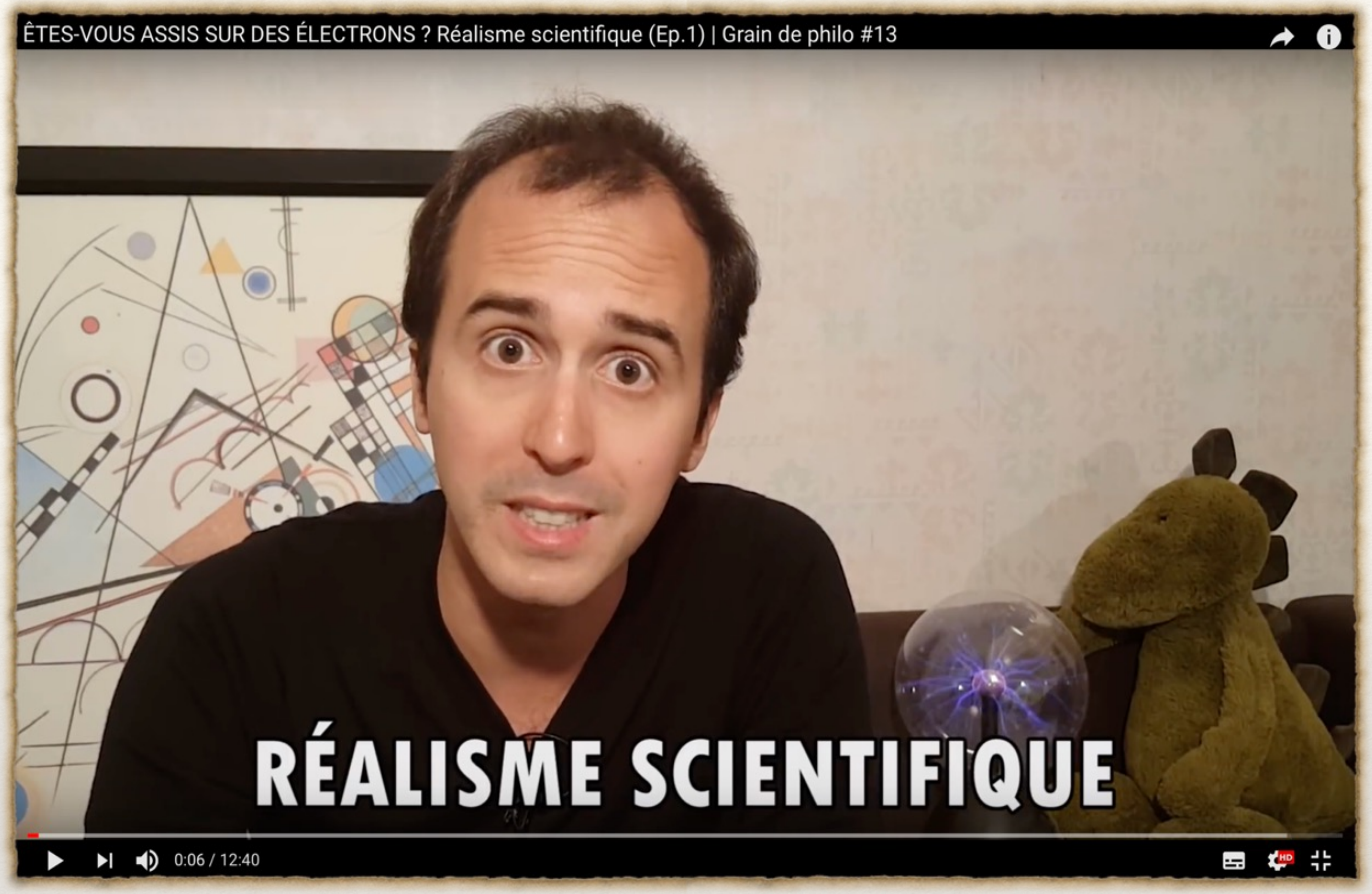
- Need a hot deep atmosphere for the exoplanet!

Modeling atmospheres

What is happening in an atmosphere?



Object to study
Physical model
Equations
Analytical resolution
Numerical resolution
Solution
?
Geometry
Ideal fluid
Navier-Stokes Equations
Continuity Equation
$\nabla \cdot \vec{V} = 0$
Momentum Equations
$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \rho \vec{g} + \mu \nabla^2 \vec{V}$
Total derivative
Pressure gradient
Body force term
Diffusion term



Réaliste ou anti-réaliste ?

Monsieur Phi

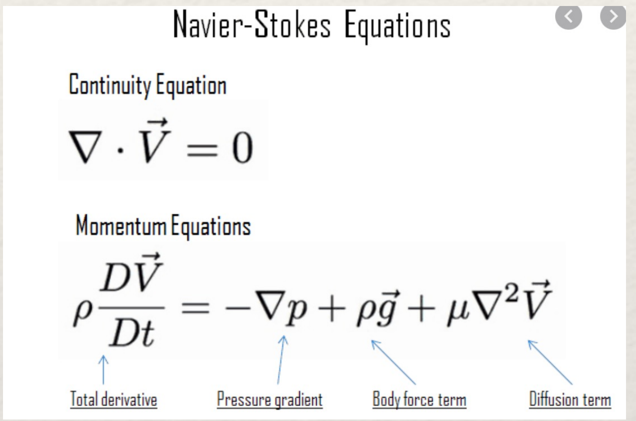
https://youtu.be/9-ILAnAW8us

Object to study

Physical model

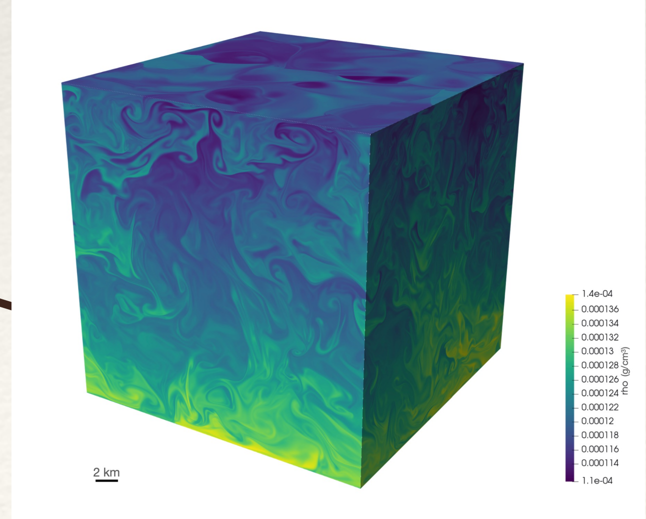
- Geometry
- Ideal fluid

Equations



Analytical resolution

Numerical resolution



Solution

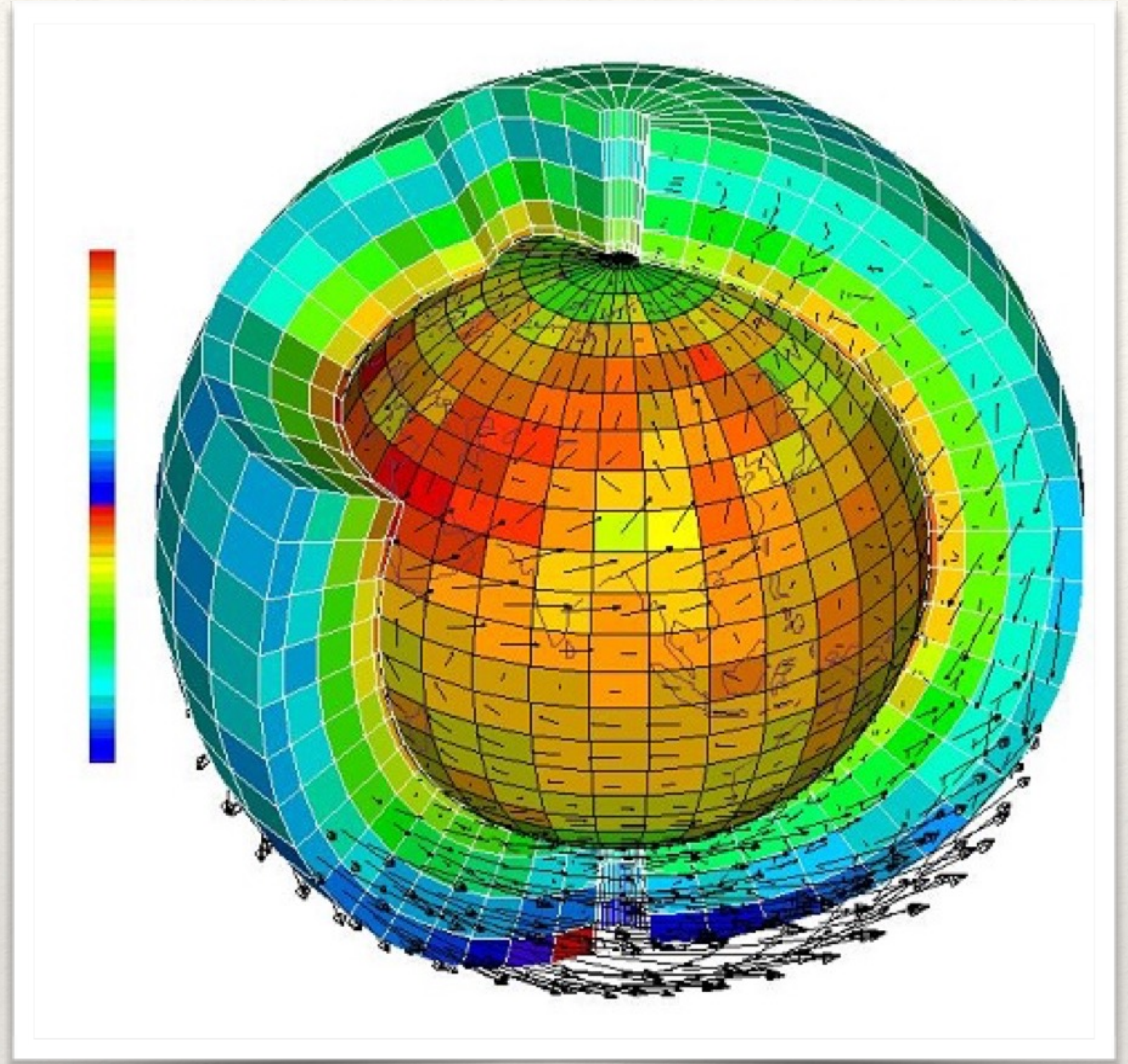
?

?

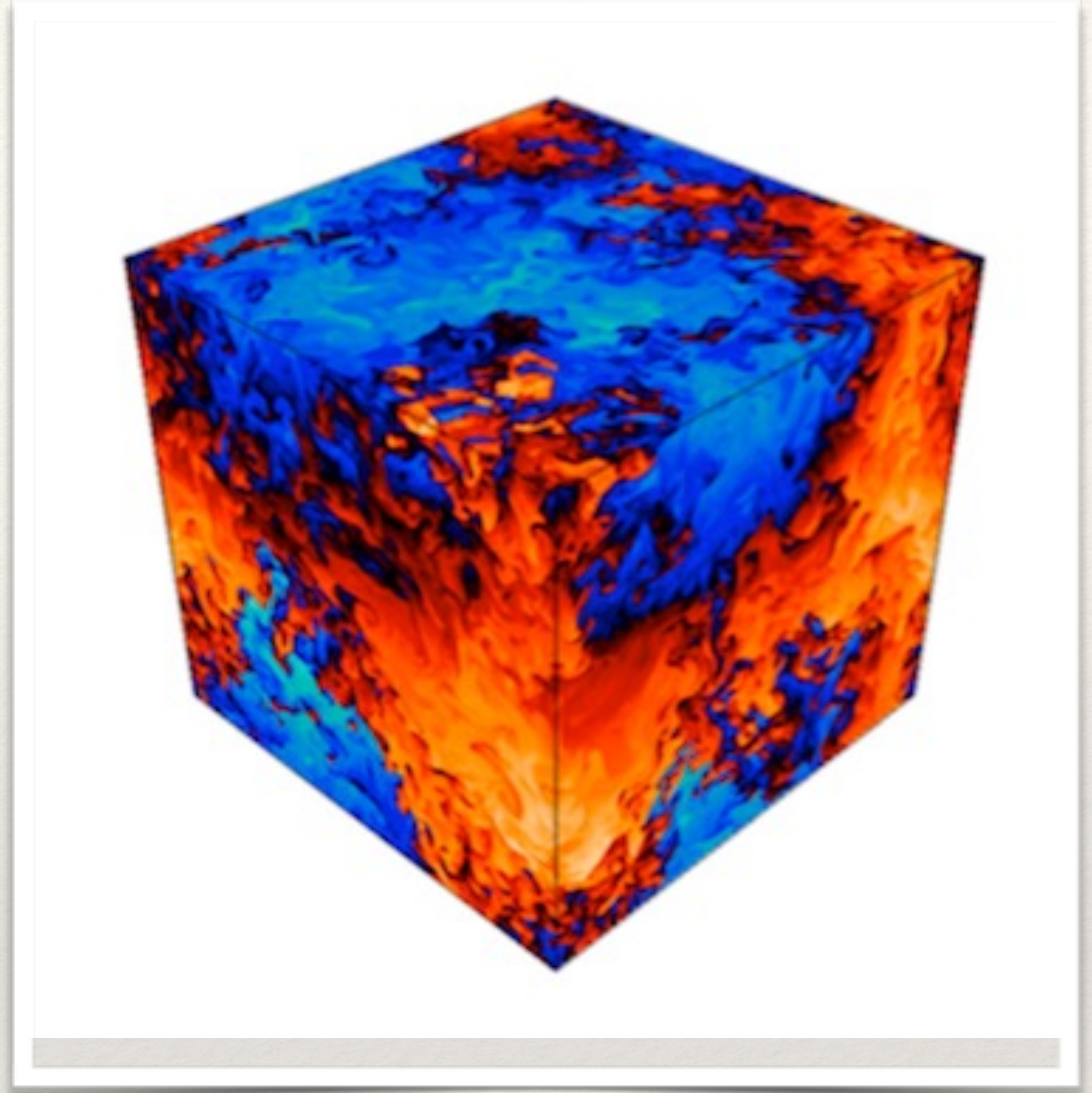
?

?

➢ 3D global and local models



Large scale circulation (climate)



Small scale convection (weather)

No! (not yet)

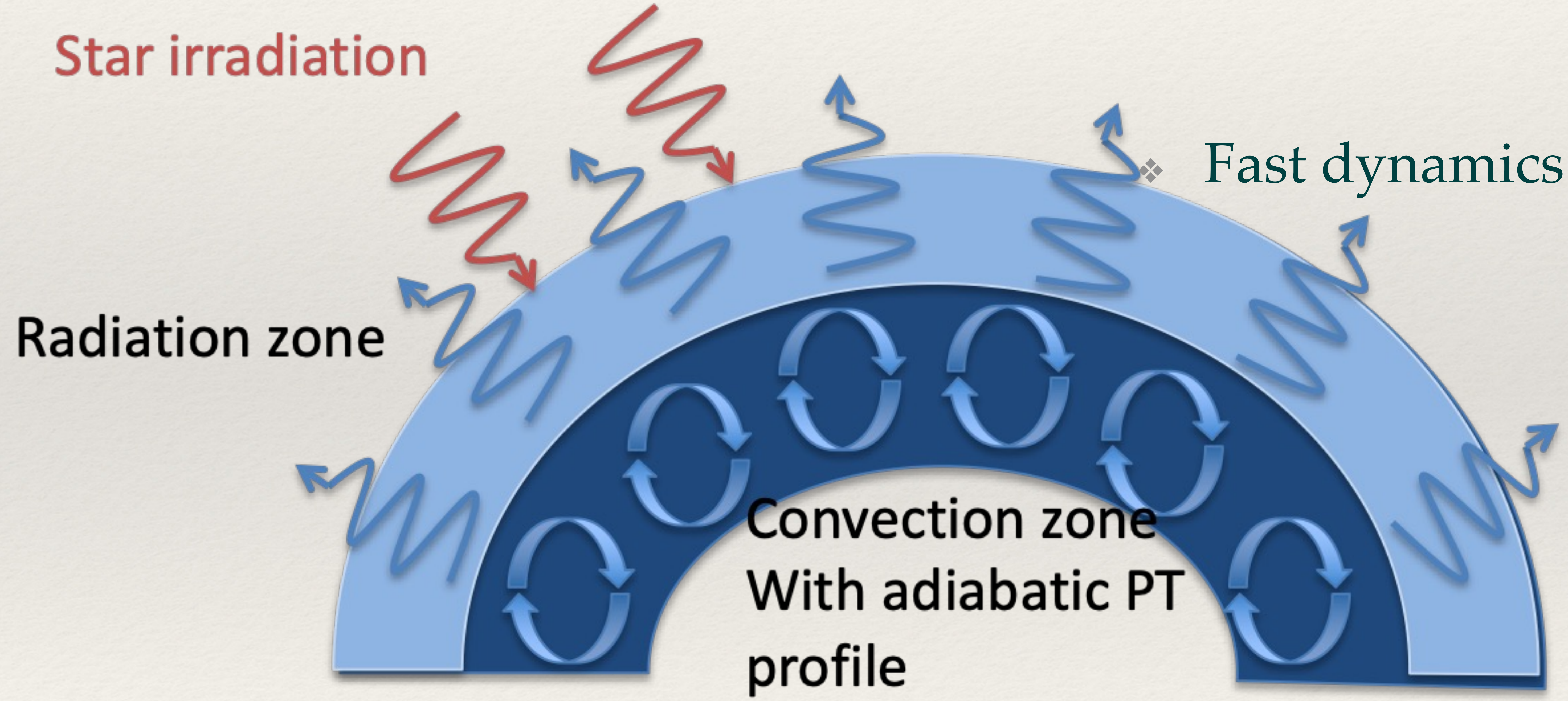
Astérix Theorem

« Le truc le plus fondamental pour un/une chercheur/euse »

➢ 1D radiative-convective equilibrium

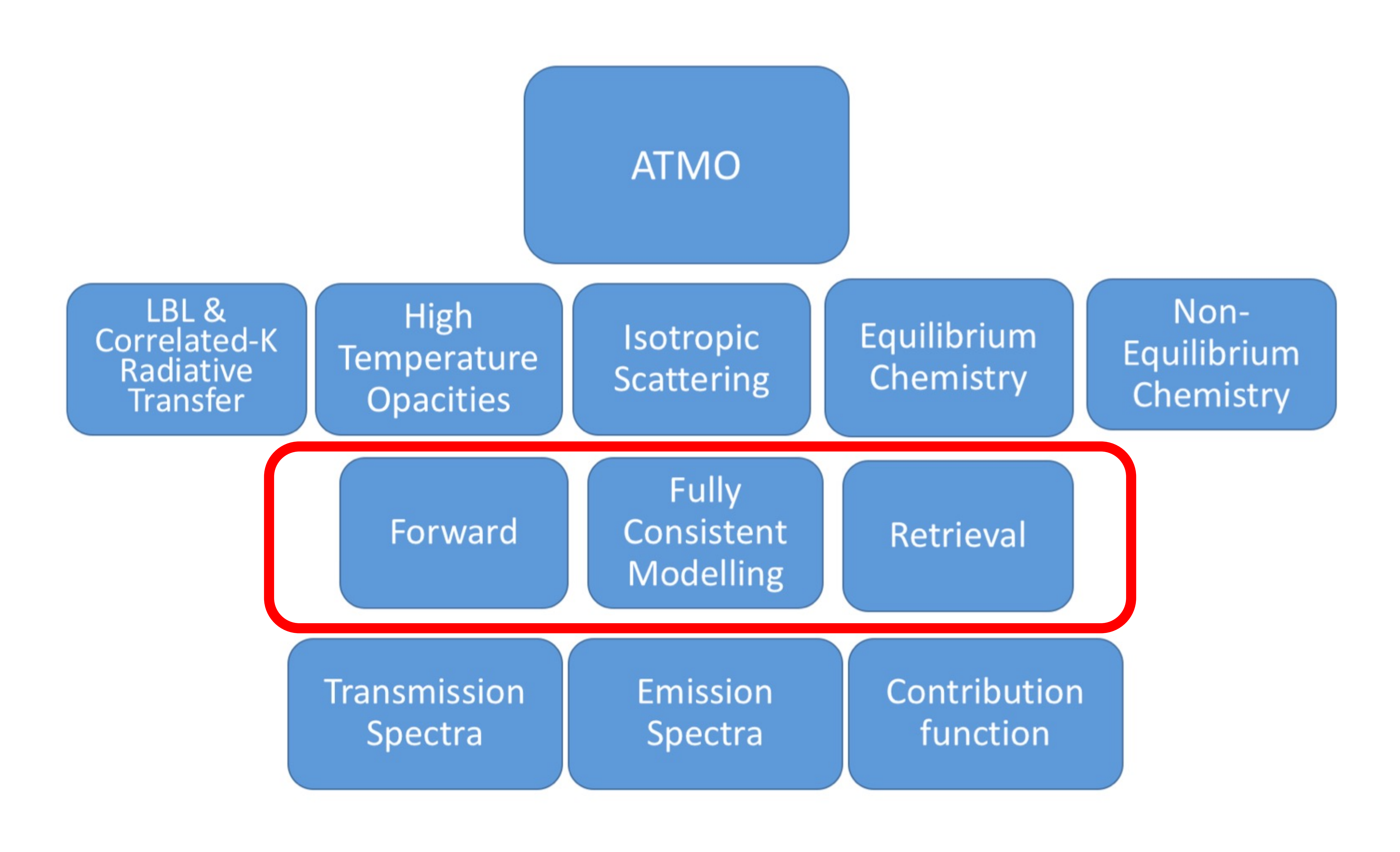
What you want to get:
- Pressure P
- Temperature T

What you need to solve (steady state):
- Hydrostatic balance
- Energy conservation



- Fast dynamics in the upper atmosphere
- Slow dynamics in the deep atmosphere
- But need radiative transfer, chemistry, convective parametrization!

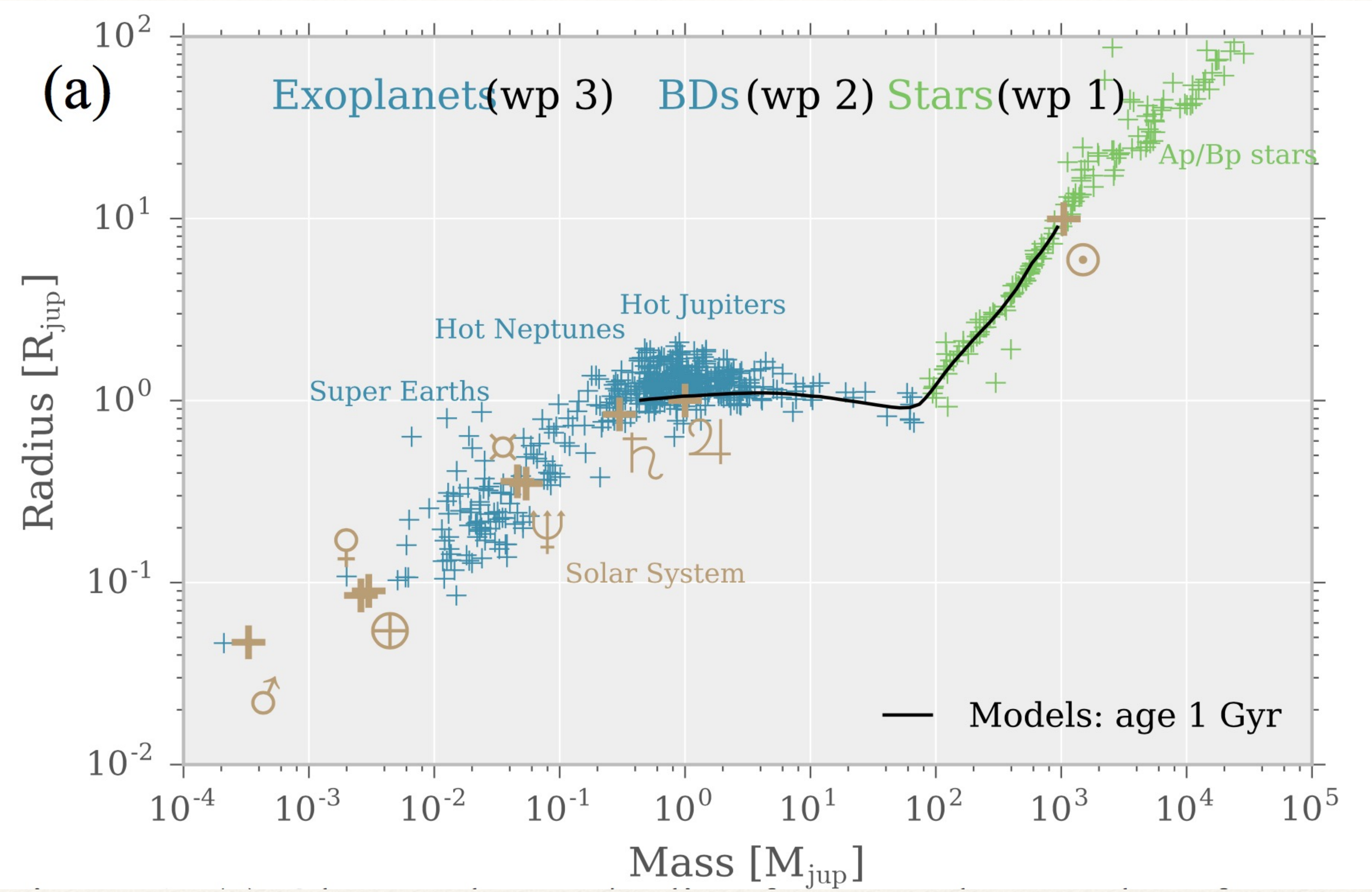
➢ 1D radiative-convective equilibrium, the ATMO code



Pressure/temperature and dynamics

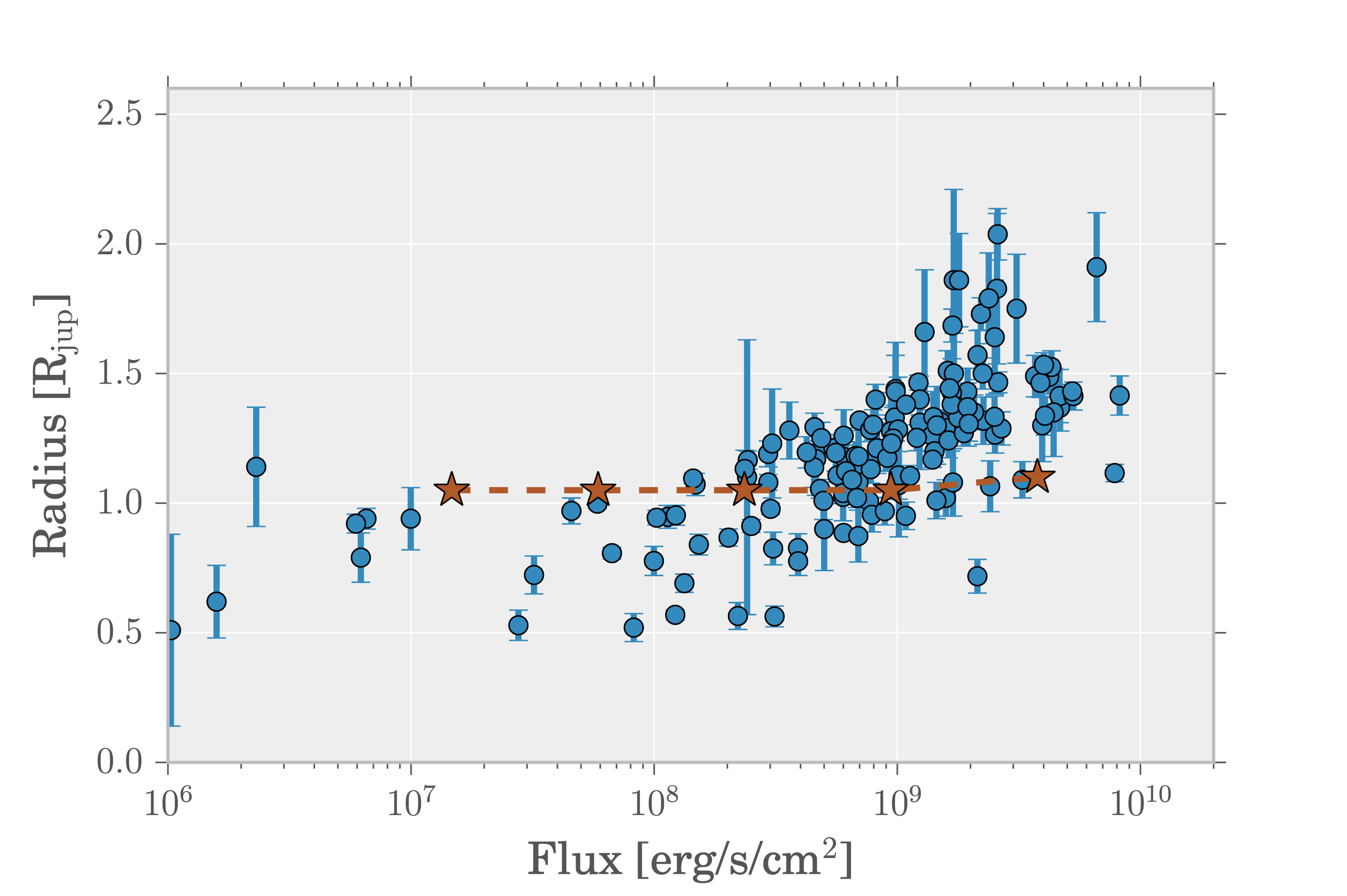
➢ Radius inflation, why is it a challenge?

- We know very well what the radius of ball of gas should be:



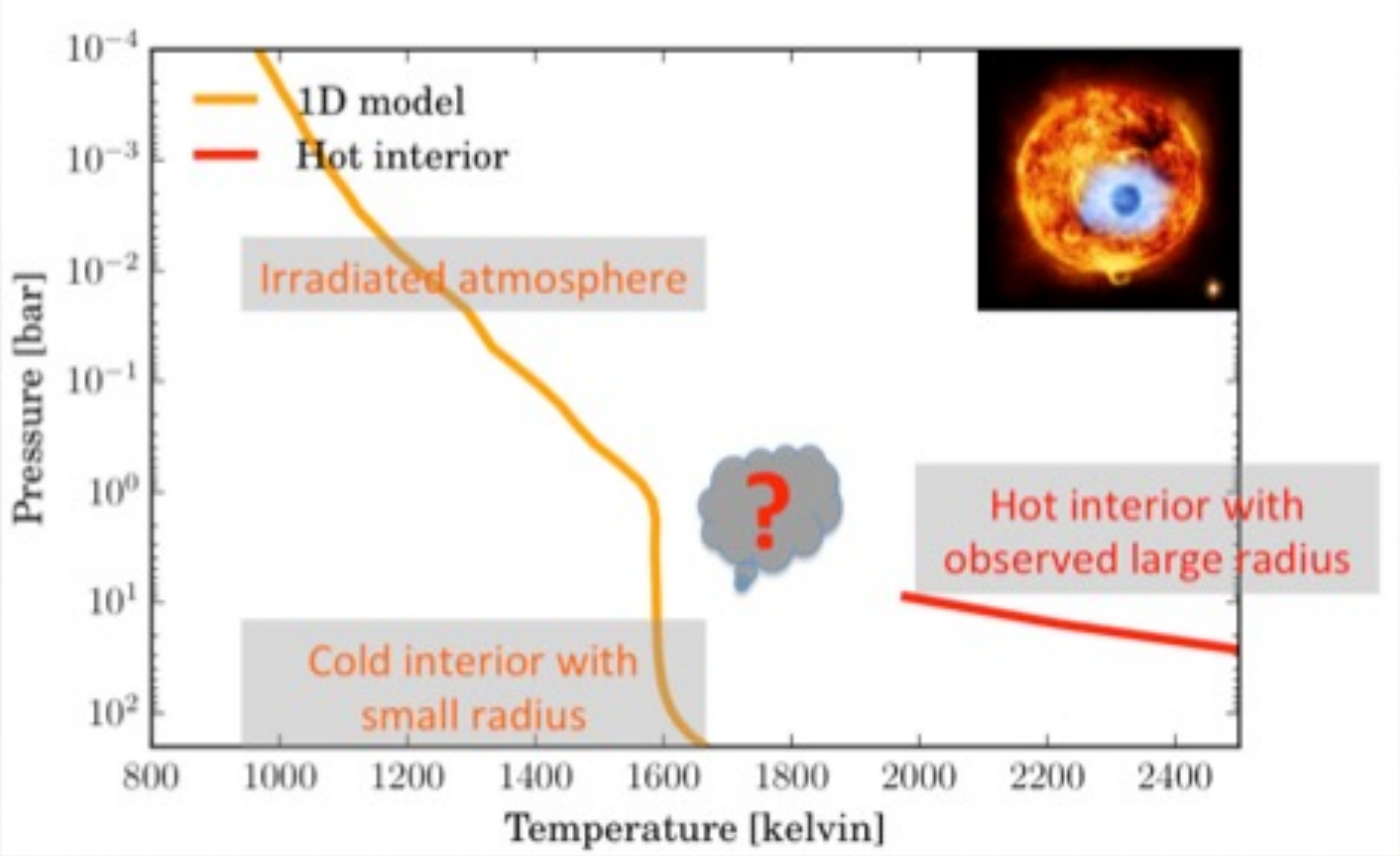
➢ Radius inflation, why is it a challenge?

- We know very well what the radius of ball of gas should be
- And we do not know why irradiated hot jupiters are bigger with increasing irradiation



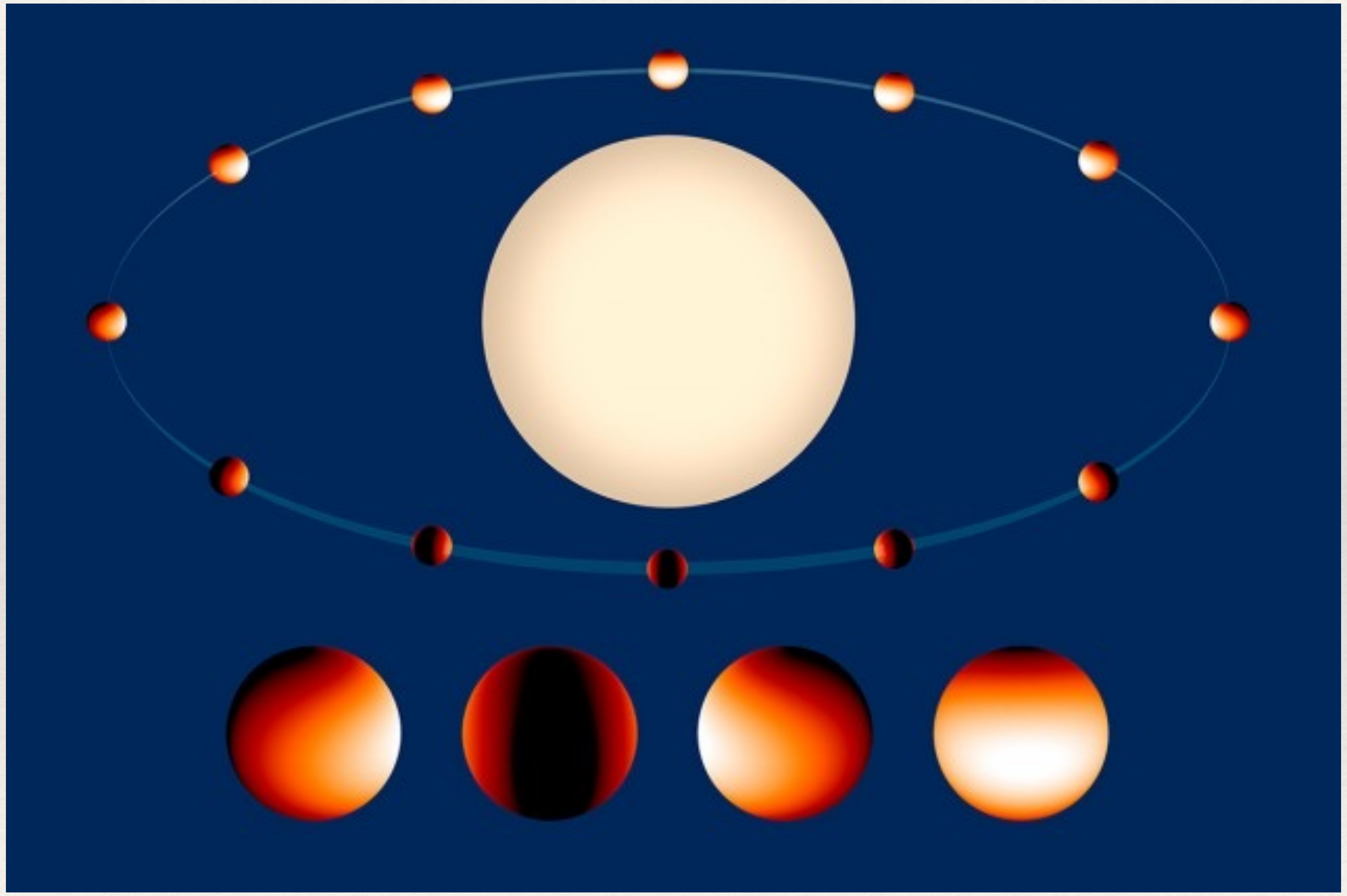
➢ Radius inflation, why is it a challenge?

- We do not know why irradiated hot jupiters are bigger with increasing irradiation
- 1D (forward) atmospheric models do not work, too cold in the deep atmosphere



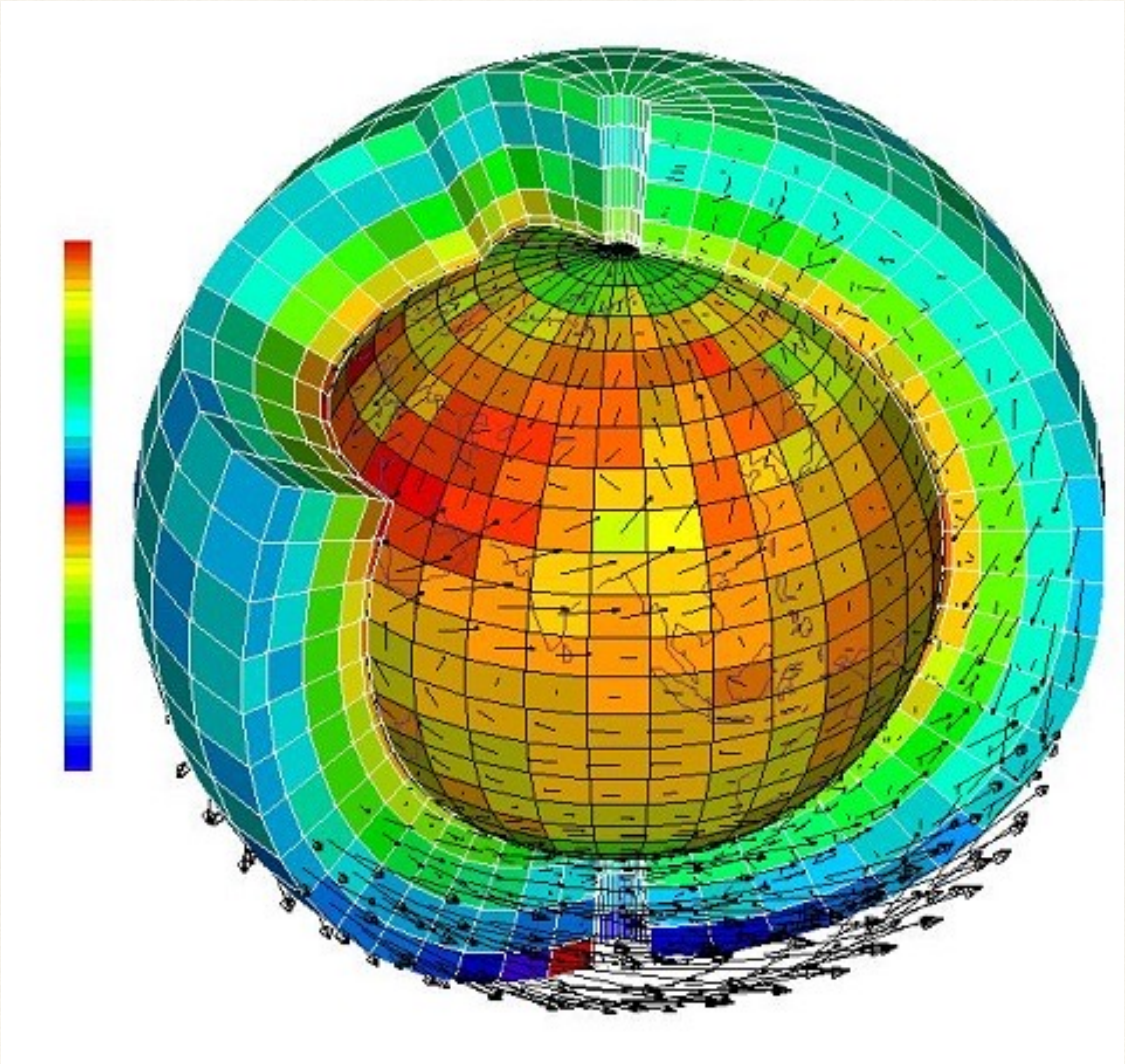
➢ Asymetric irradiation of tidally locked hot jupiter

- A hot dayside and a cold nightside implies pressure gradients and winds
- 3D atmospheric models to study the circulation



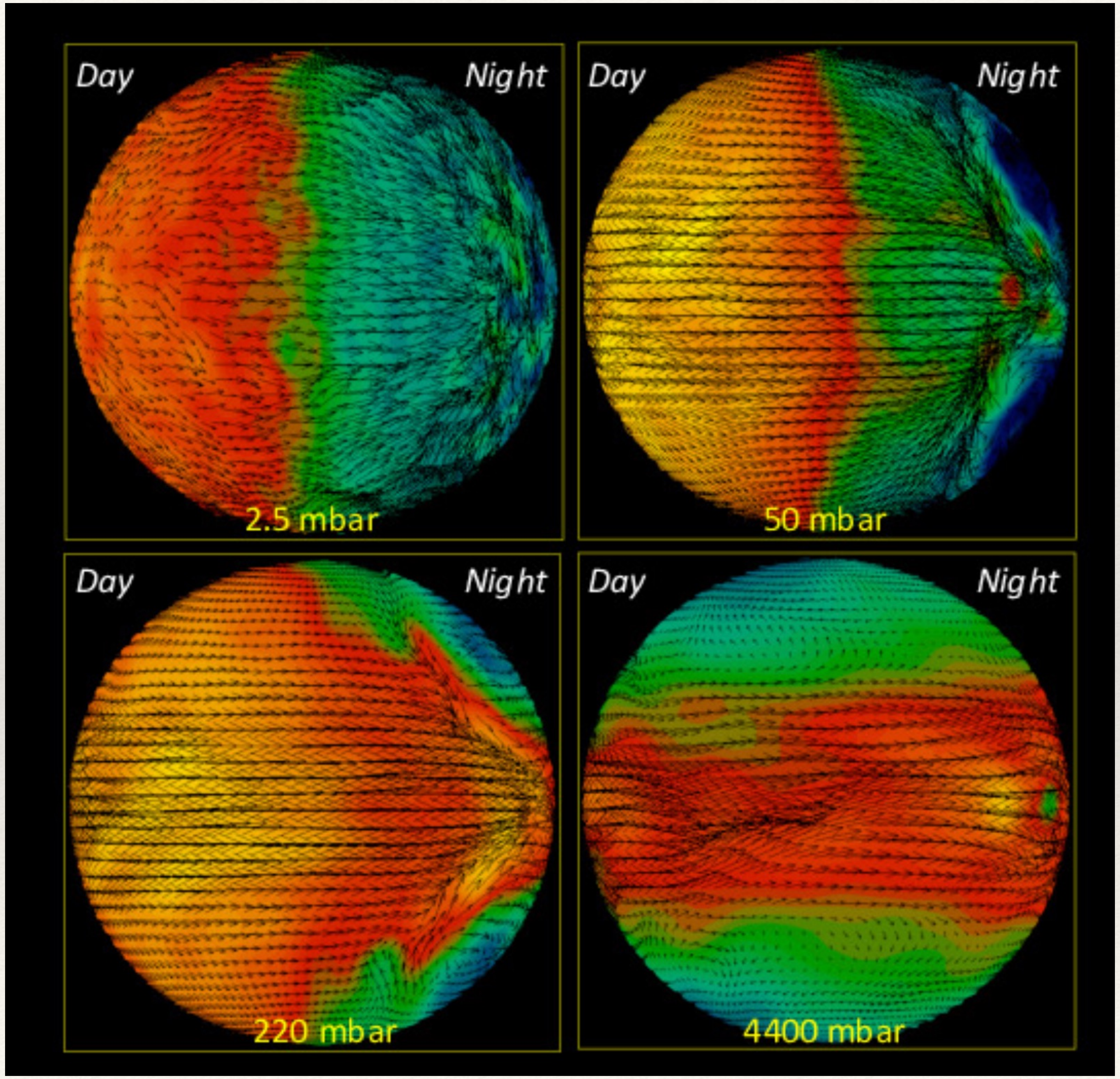
➢ Asymetric irradiation of tidally locked hot jupiter

- A hot dayside and a cold nightside implies pressure gradients and winds
- 3D atmospheric models to study the circulation: time-dependent Euler equations in spherical coordinates)



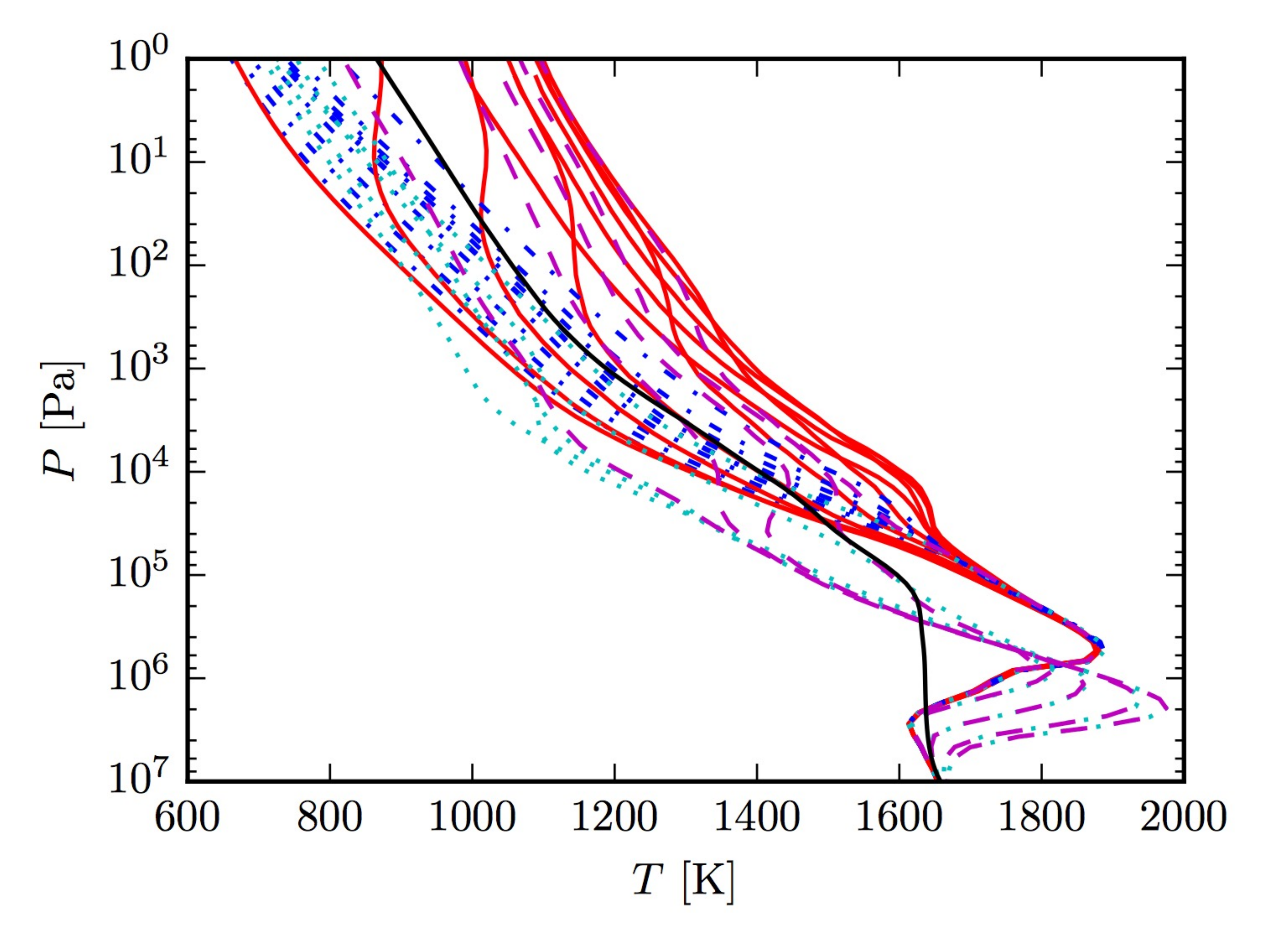
➢ Asymetric irradiation of tidally locked hot jupiter

- 3D atmospheric models to study the circulation, evolution in time to get the steady state



➢ Asymetric irradiation of tidally locked hot jupiter

- Does it work ? No…



- Parmentier et al. 2016: cold deep atmosphere (cannot explain inflation) but provide cloud trap

–Can you guess why ?

➢ 1D radiative-convective equilibrium

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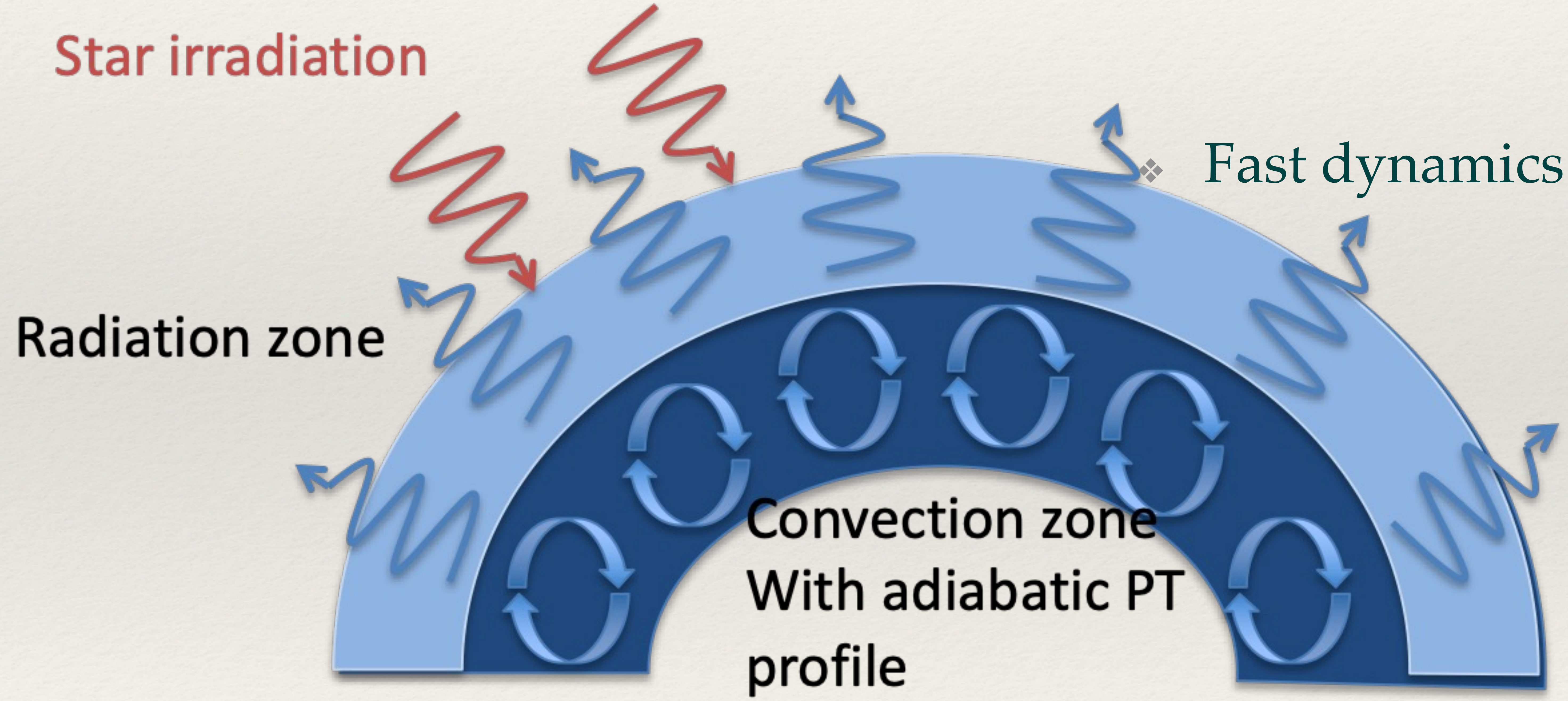
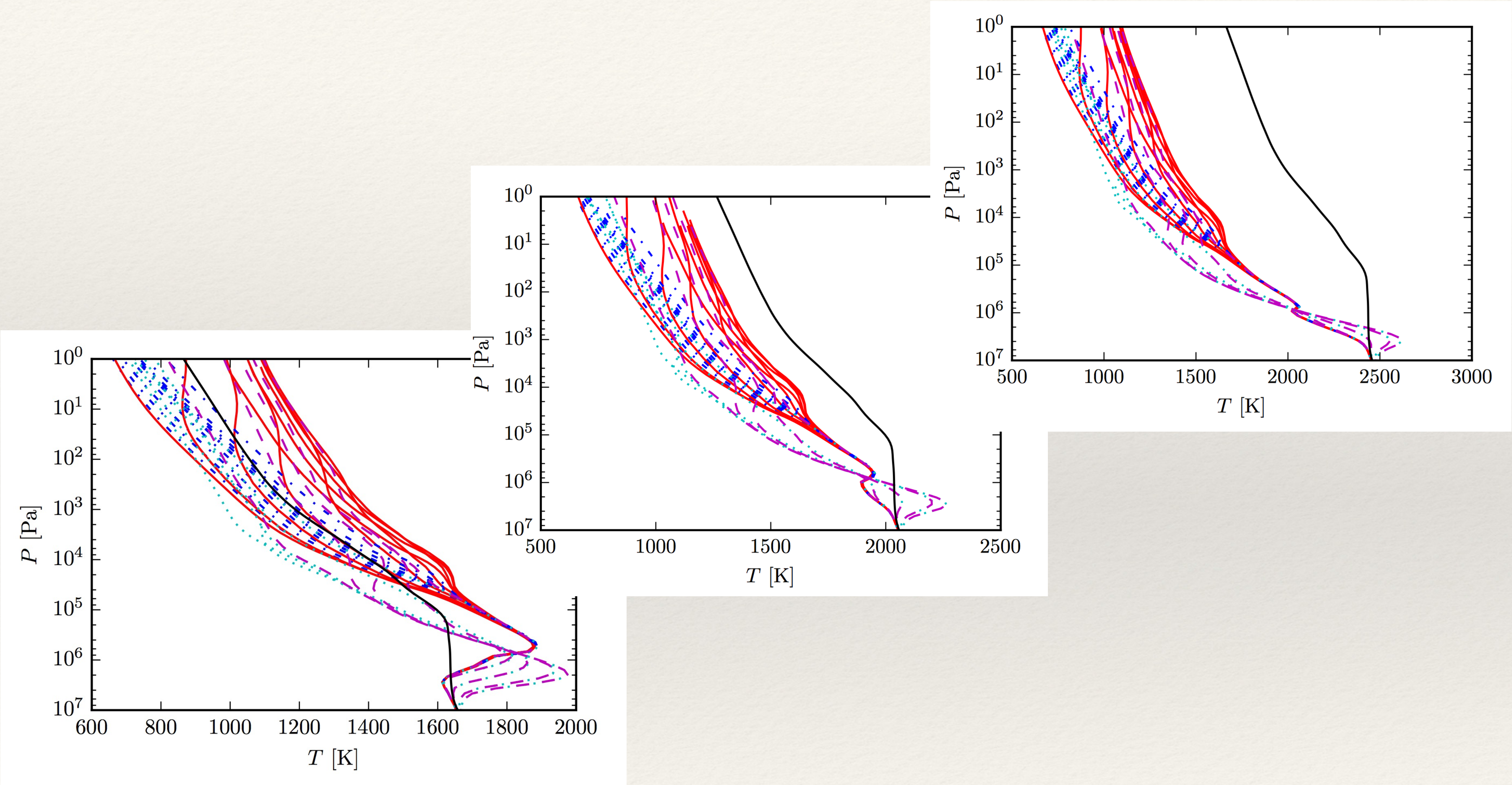


- Fast dynamics in the upper atmosphere
- Slow dynamics in the deep atmosphere

➢ Asymetric irradiation of tidally locked hot jupiter

- The deep atmosphere is not converged in time because of computation limitation

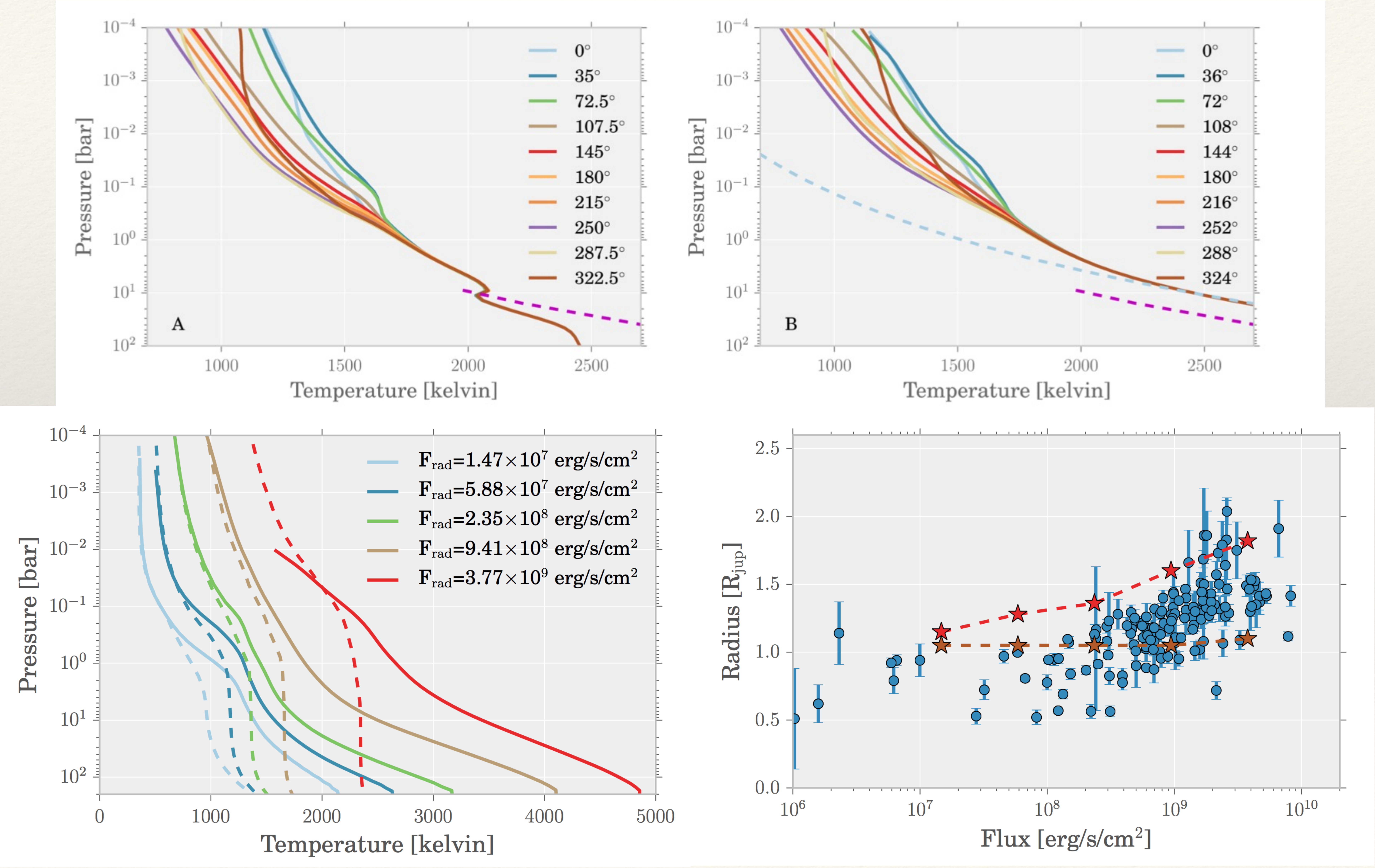


➢ Asymetric irradiation of tidally locked hot jupiter

- Need to construct a 2D steady state circulation model at the equator
  - Keep the steady state nature of the 1D model
  - Can take into account the asymetric irradiation as a 3D model
  - (Tremblin et al. 2017)

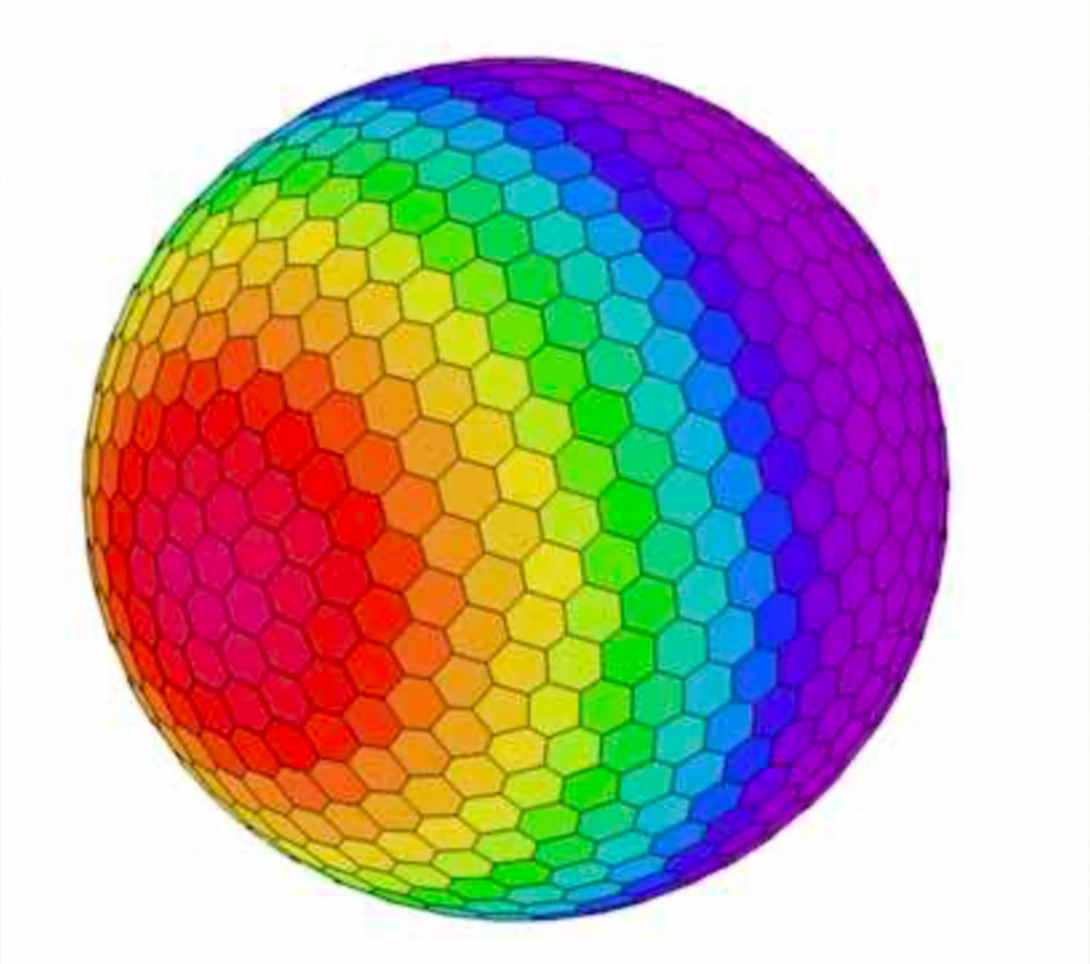
➢ Asymetric irradiation of tidally locked hot jupiter

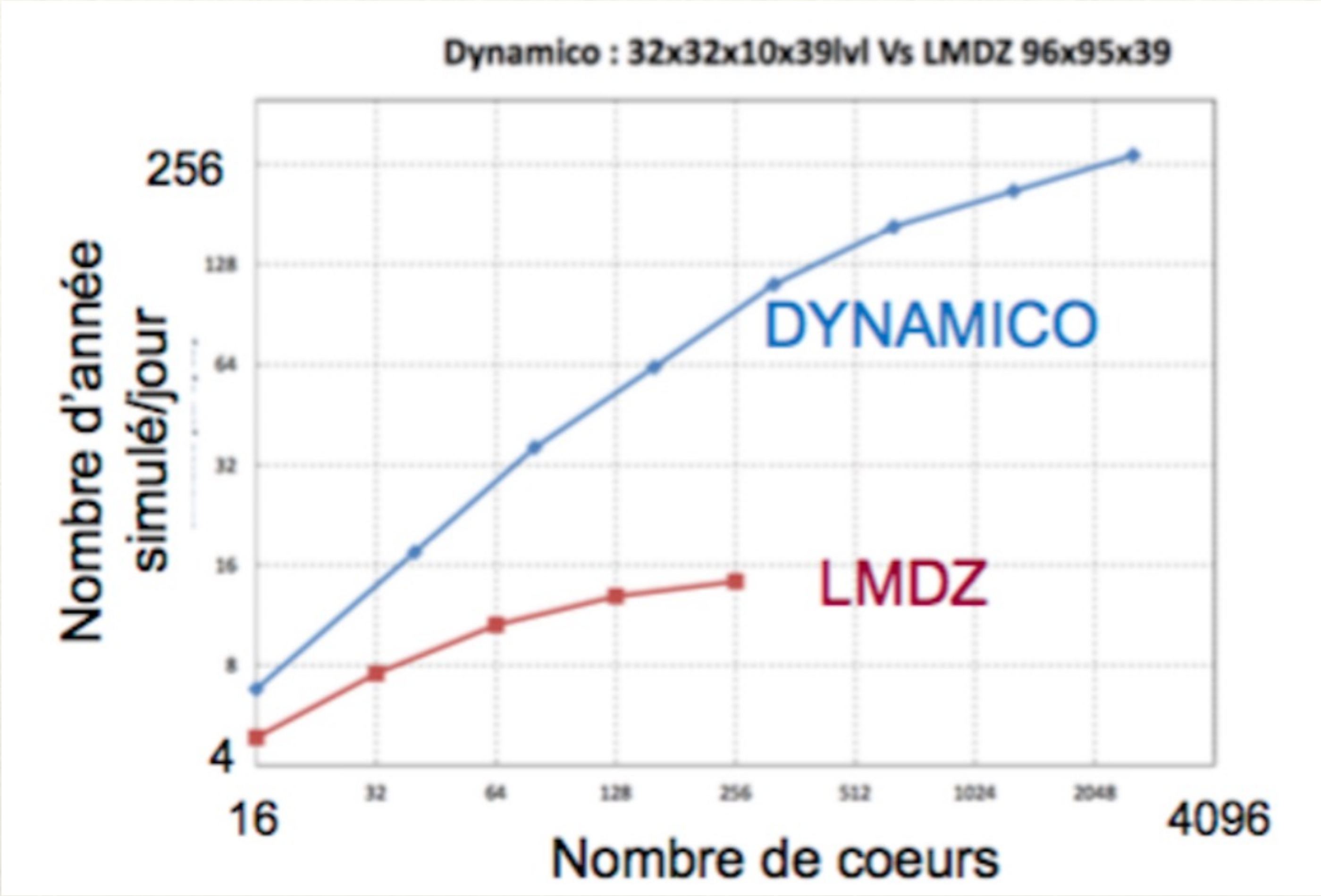
- Get a hot deep interior because of vertical mass flows !



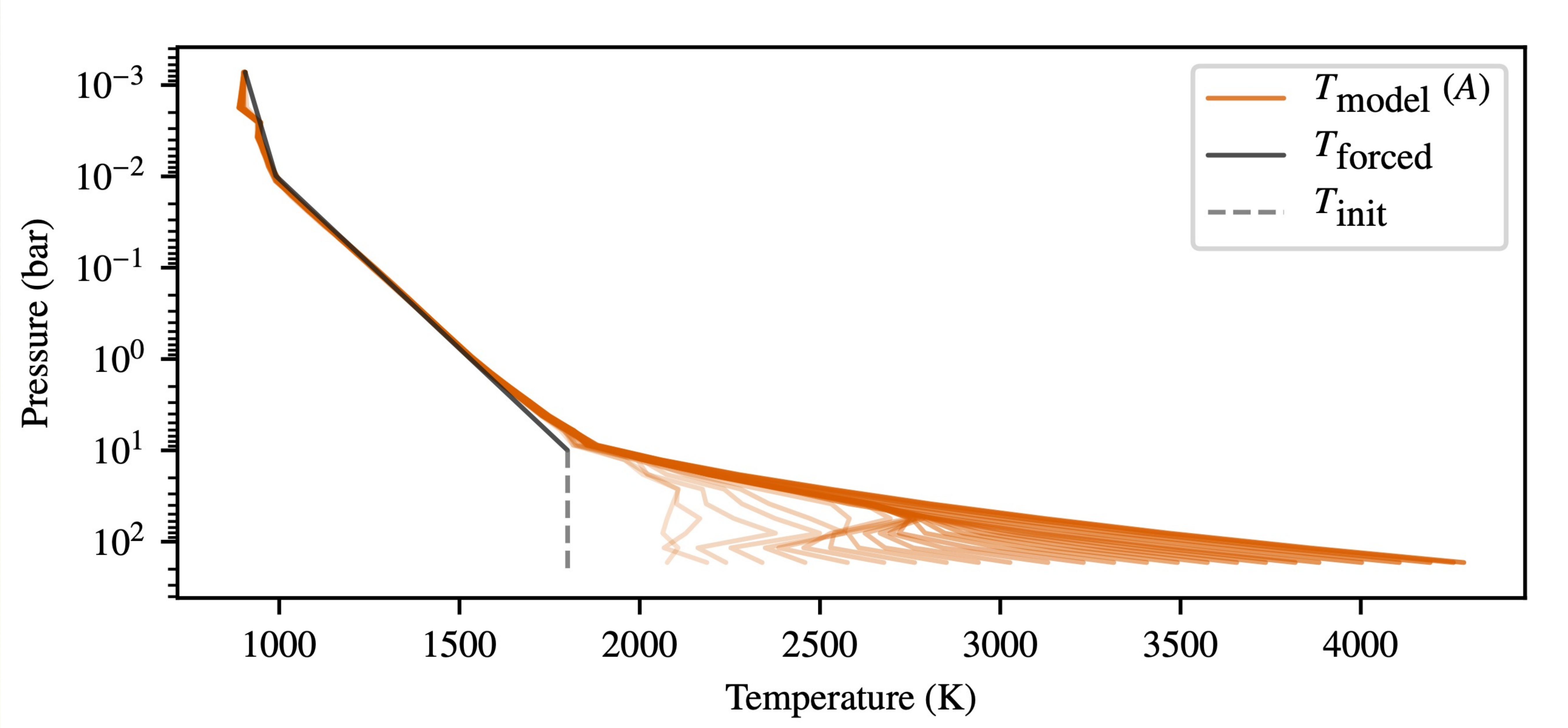
➢ With 3D models: « paleoclimate » simulation of hot jupiters

- Sainsbury-Martinez et al. 2019 (Dynamico code, Earth climate)





- High Performance Computing
- 3000 years instead of 300 days



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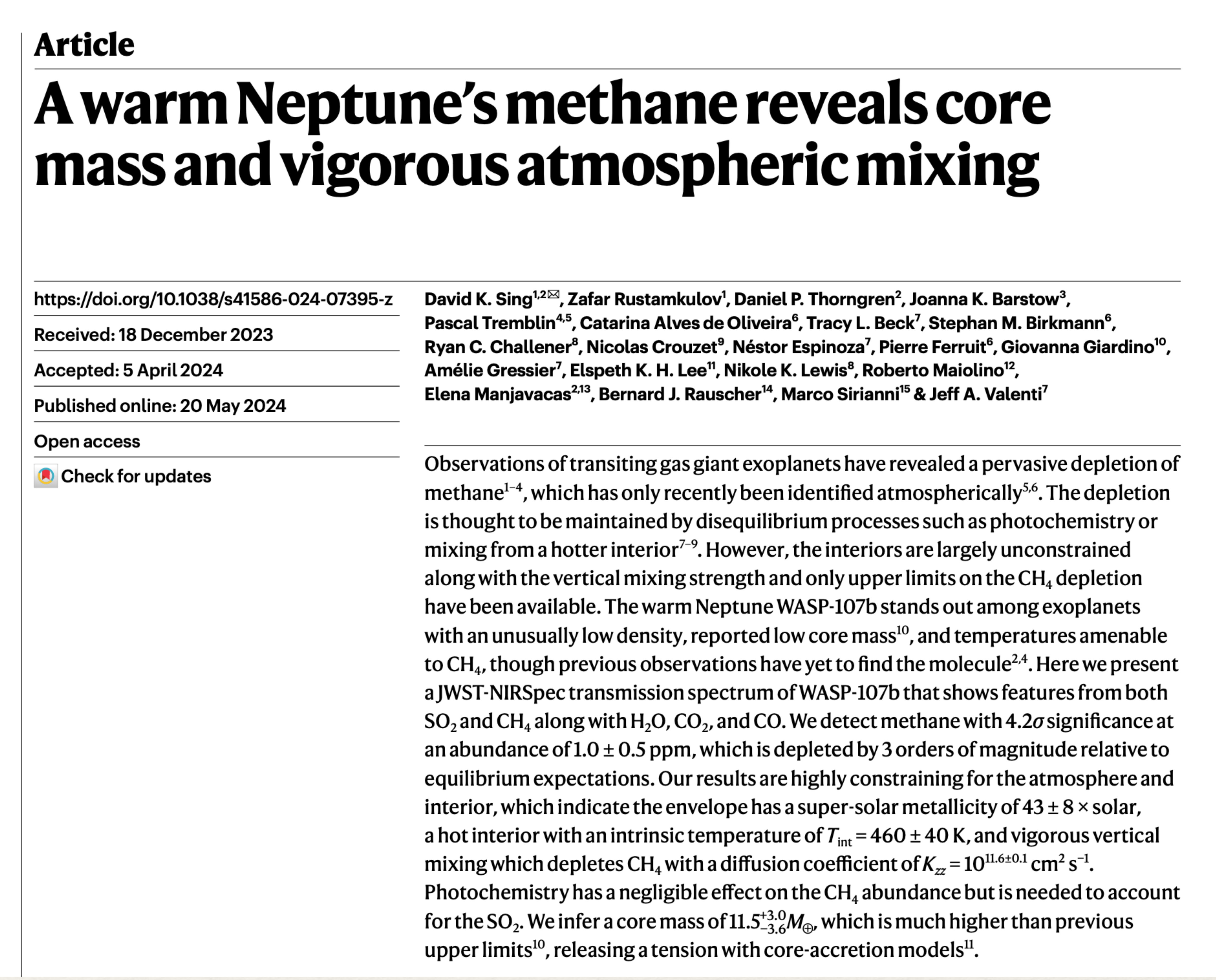
Article

A warm Neptune's methane reveals core mass and vigorous atmospheric mixing

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Check for updates

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Observations of transiting gas giant exoplanets have revealed a pervasive depletion of methane[1–4], which has only recently been identified atmospherically[5,6]. The depletion is thought to be maintained by disequilibrium processes such as photochemistry or mixing from a hotter interior[7–9]. However, the interiors are largely unconstrained along with the vertical mixing strength and only upper limits on the CH_4 depletion have been available. The warm Neptune WASP-107b stands out among exoplanets with an unusually low density, reported low core mass[10], and temperatures amenable to CH_4, though previous observations have yet to find the molecule[2,4]. Here we present a JWST-NIRSpec transmission spectrum of WASP-107b that shows features from both SO_2 and CH_4 along with H_2O, CO_2, and CO. We detect methane with 4.2σ significance at an abundance of 1.0 ± 0.5 ppm, which is depleted by 3 orders of magnitude relative to equilibrium expectations. Our results are highly constraining for the atmosphere and interior, which indicate the envelope has a super-solar metallicity of 43 ± 8 × solar, a hot interior with an intrinsic temperature of T_{int} = 460 ± 40 K, and vigorous vertical mixing which depletes CH_4 with a diffusion coefficient of $K_{zz} = 10^{11.6\pm0.1}$ cm^2 s^{-1}. Photochemistry has a negligible effect on the CH_4 abundance but is needed to account for the SO_2. We infer a core mass of $11.5^{+3.0}_{-3.6} M_\oplus$, which is much higher than previous upper limits[10], releasing a tension with core-accretion models[11].

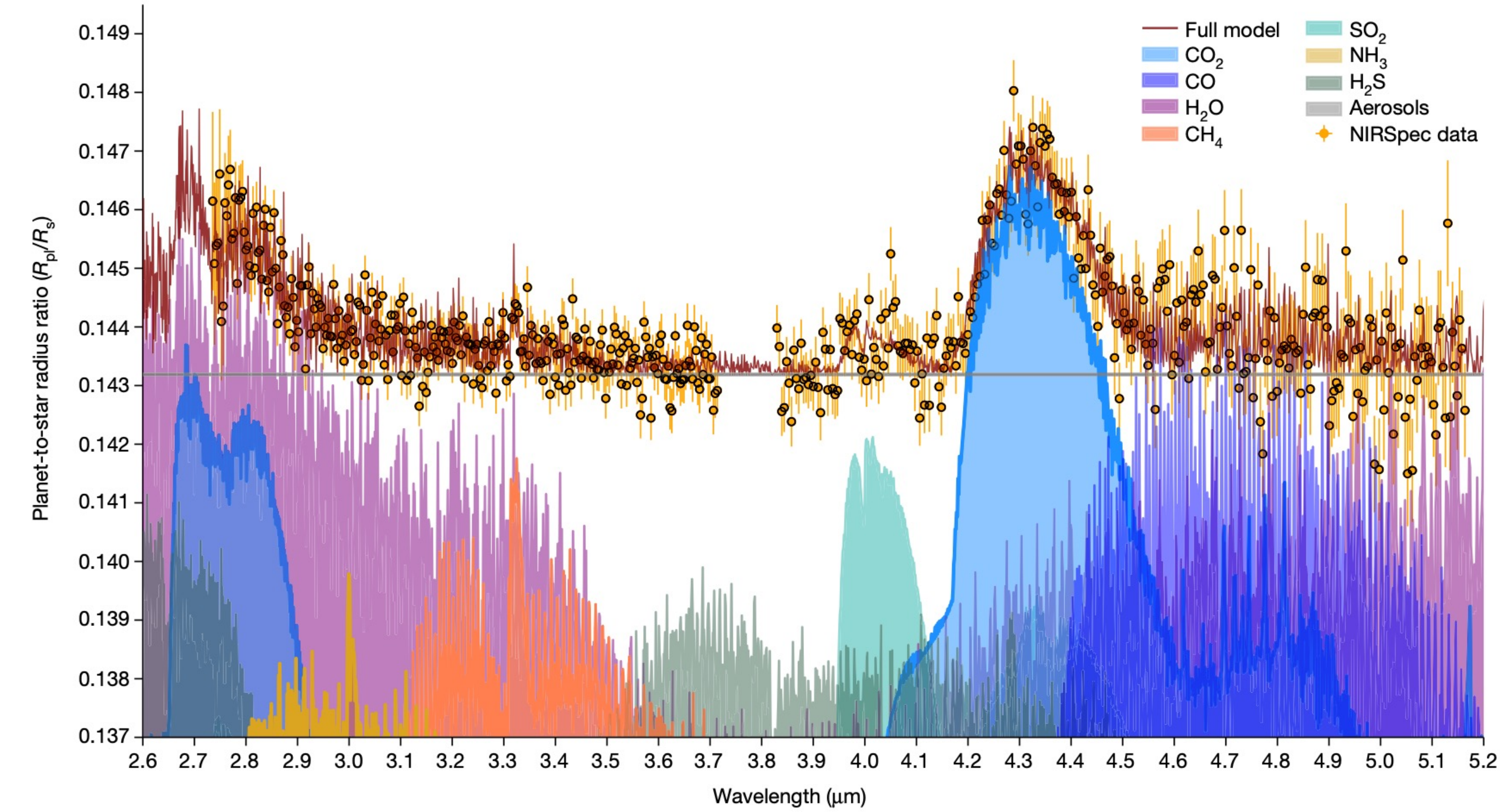
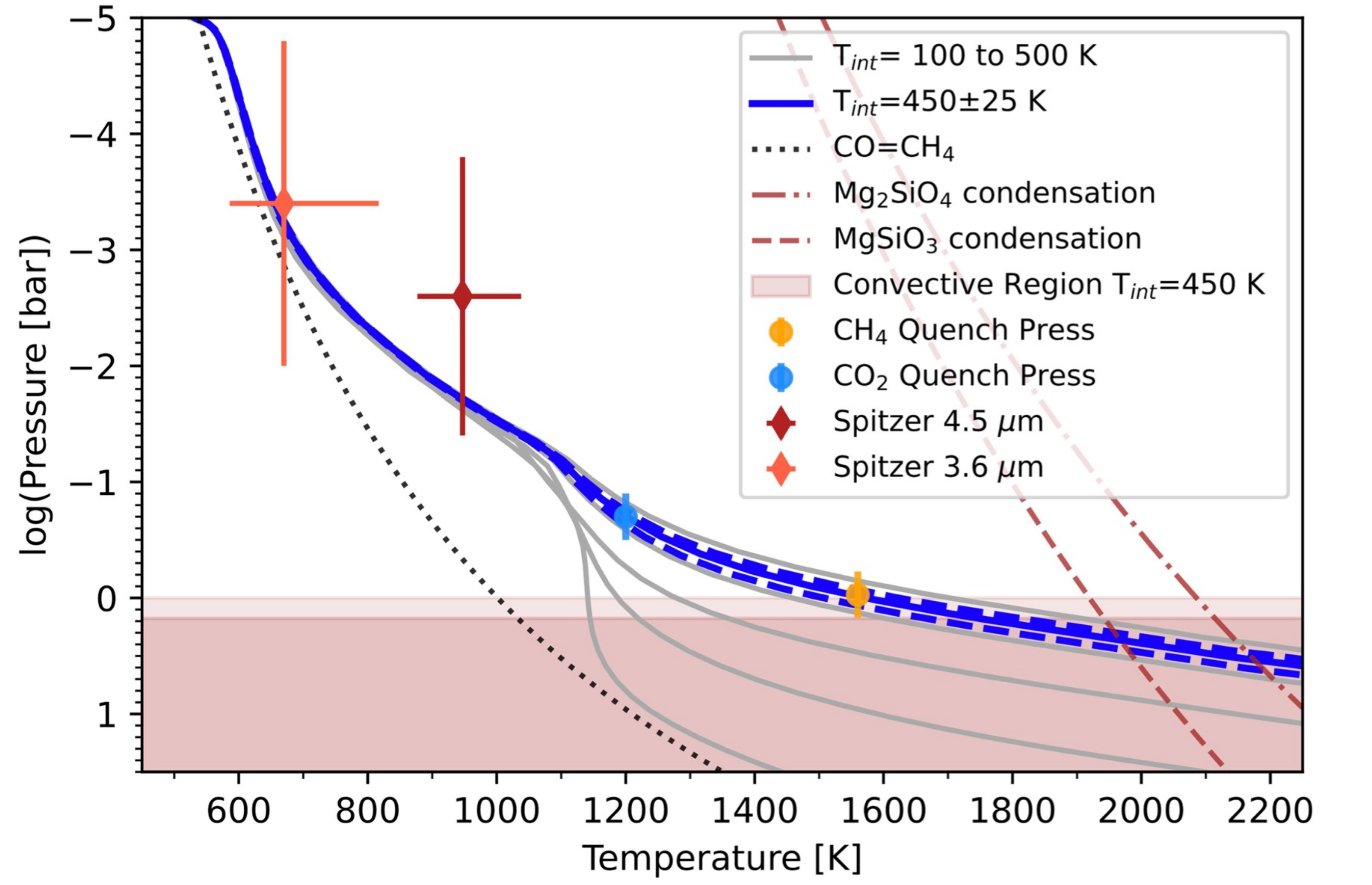


Fig. 2 | WASP-107b transmission spectral measurements. JWST-NIRSpec transmission spectrum and the 1σ uncertainties. The best-fit ATMO[32] model is also plotted, and the individual contributions for each molecular species are shown.

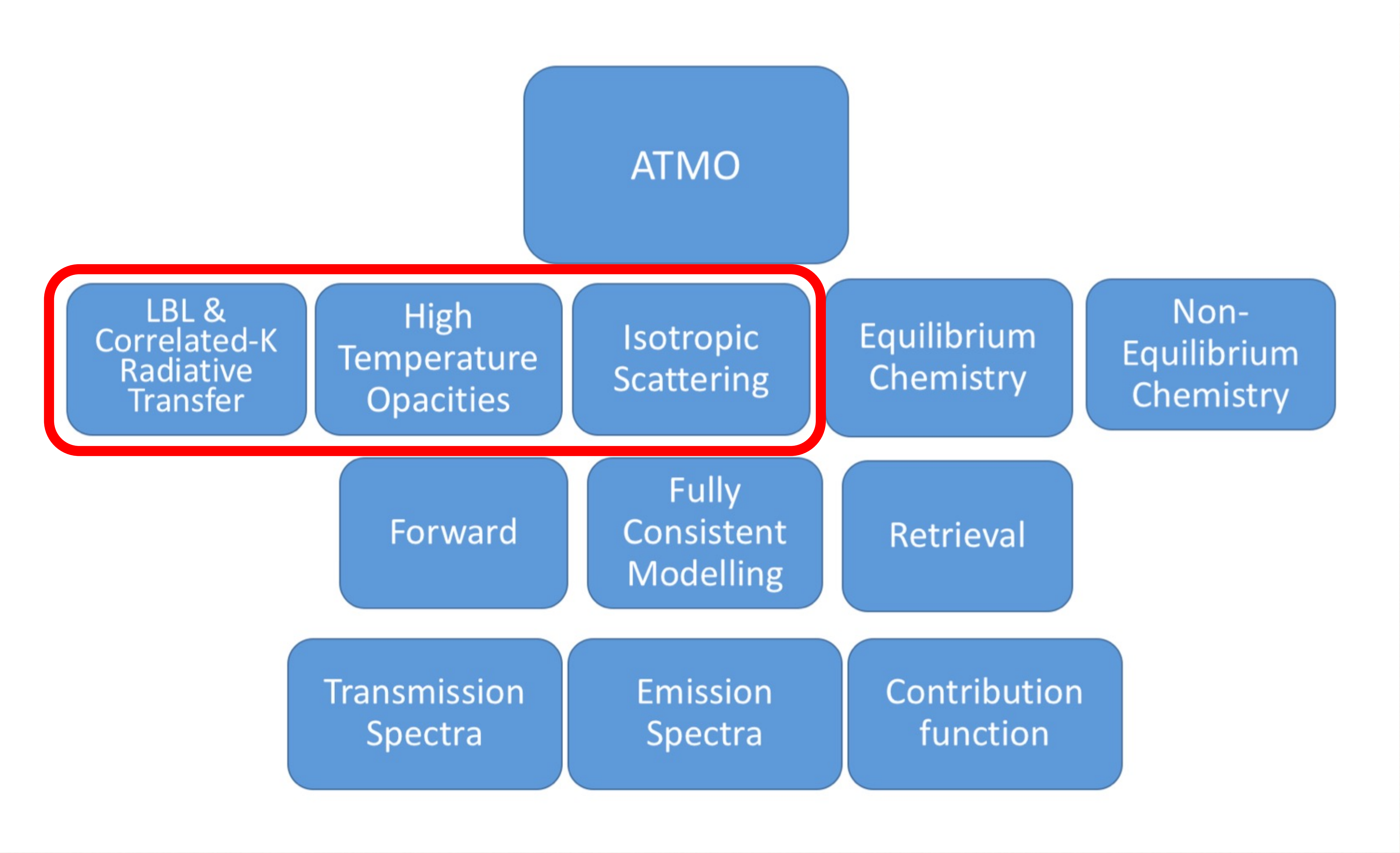


Extended Data Fig. 6 | Pressure-Temperature Profiles. Shown are P-T profiles in radiative-convective equilibrium with T_{int} values ranging from 100 to 500 K (grey). The T-P with the best-fit T_{int} is shown (blue), with a shaded region showing where the model is dominated by convection. The quench pressures for CO_2 and CH_4 are also depicted along with Mg-Si condensation curves (dashed, dot dashed lines). The equilibrium CH_4=CO equal-abundance curve is also shown (dotted line), with the CH_4 abundance dropping at increased temperatures. The brightness temperatures measured from Spitzer secondary eclipse observations are shown from ref. 123. The corresponding pressures and ranges are derived from the best-fit model contribution function, with the y-axis range encapsulating 80% of the total emitted flux. The Spitzer brightness temperatures are consistent with the best-fitting T_{int} = 460K T-P profile.

- Sing et al. 2023 Nature (JWST / NIRSPEC + ATMO retrieval)

Radiative transfer

➢ 1D radiative-convective equilibrium, the ATMO code



➢ Radiative transfer

give me the 3D time dependent radiative transfer equation, with showing all the variables on which depends the specific intensity

A common 3D, time-dependent radiative transfer equation (RTE) written for the **specific intensity** is:

$$\frac{1}{c}\frac{\partial I_\nu(\mathbf{x},\mathbf{n},t)}{\partial t} + \mathbf{n}\cdot\nabla_{\mathbf{x}} I_\nu(\mathbf{x},\mathbf{n},t) = -\chi_\nu(\mathbf{x},\mathbf{n},t)\, I_\nu(\mathbf{x},\mathbf{n},t) + \eta_\nu(\mathbf{x},\mathbf{n},t),$$

where the **specific intensity** depends on all of

$$I_\nu \equiv I_\nu(\mathbf{x},\mathbf{n},t) \quad \text{with} \quad \mathbf{x}=(x,y,z)\in\mathbb{R}^3, \quad \mathbf{n}\in S^2, \quad t\in\mathbb{R}, \quad \nu\in\mathbb{R}^+.$$

More explicitly (showing frequency as well):

$$\frac{1}{c}\frac{\partial I(\mathbf{x},\mathbf{n},\nu,t)}{\partial t} + \mathbf{n}\cdot\nabla_{\mathbf{x}} I(\mathbf{x},\mathbf{n},\nu,t) = -\chi(\mathbf{x},\mathbf{n},\nu,t)\, I(\mathbf{x},\mathbf{n},\nu,t) + \eta(\mathbf{x},\mathbf{n},\nu,t).$$

Meaning of symbols

- $I(\mathbf{x},\mathbf{n},\nu,t)$: specific intensity at position $\mathbf{x}$, propagation direction $\mathbf{n}$ (unit vector), frequency ν, time t.
- c: speed of light.
- $\nabla_{\mathbf{x}}$: spatial gradient (3D).
- $\chi(\mathbf{x},\mathbf{n},\nu,t)$: extinction coefficient (absorption + out-scattering) $[\text{length}^{-1}]$.
- $\eta(\mathbf{x},\mathbf{n},\nu,t)$: emissivity (includes true emission + in-scattering source term if you fold it in).

If you want the version where scattering is written explicitly (rather than hidden inside η), tell me whether you want **elastic scattering** and whether you prefer the equation in **wavelength** λ or **frequency** ν.

❖ Why is it complicated ?

➢ Radiative transfer

give a simplified version with the following assumption:
* stationary
* 1D plane-parallel
* local thermodynamical equilibrium
* 2-stream approximation

Under those assumptions you typically write a **grey, stationary, 1D plane–parallel** transfer equation for two discrete directions $\mu = \pm 1/\sqrt{3}$ (Eddington 2-stream). Let z be the vertical coordinate and τ the (grey) optical depth defined by

$$d\tau = \chi(z)\, dz,$$

with χ the extinction coefficient.

Two-stream RTE (LTE source)

LTE $\Rightarrow$ source function $S = B(T)$ (Planck function; in grey form you can think of B integrated over frequency).

For the two intensities $I_+(\tau) \equiv I(\tau, \mu)$ with $\mu = +1/\sqrt{3}$ (upward) and $I_-(\tau) \equiv I(\tau, -\mu)$ with $\mu = +1/\sqrt{3}$ (downward), the stationary 1D RTE becomes:

$$\mu \frac{dI_+}{d\tau} = I_+ - B(T(\tau)),$$

$$-\mu \frac{dI_-}{d\tau} = I_- - B(T(\tau)),$$

❖ (Careful with LLM: I did not ask for a grey model, neither to neglect scattering!)

➢ Radiative transfer

Pa

give a simplified version with the following assumption:
* stationary
* 1D plane-parallel
* local thermodynamical equilibrium
* 2-stream approximation

Under those assumptions you typically write a **grey, stationary, 1D plane–parallel** transfer equation for two discrete directions $\mu = \pm 1/\sqrt{3}$ (Eddington 2-stream). Let z be the vertical coordinate and τ the (grey) optical depth defined by

$$d\tau = \chi(z)\, dz,$$

with χ the extinction coefficient.

Two-stream RTE (LTE source)

LTE $\Rightarrow$ source function $S = B(T)$ (Planck function; in grey form you can think of B integrated over frequency).

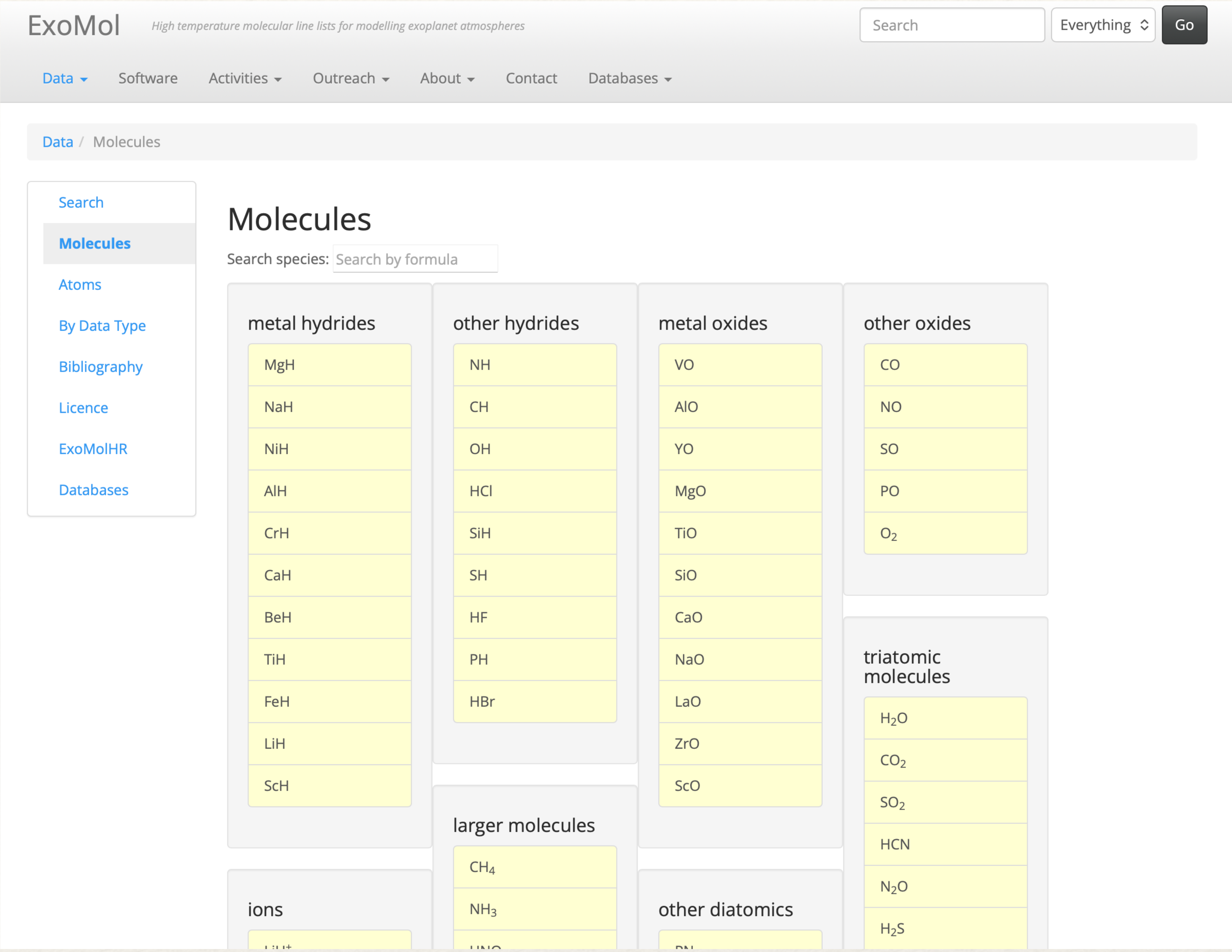
For the two intensities $I_+(\tau) \equiv I(\tau, \mu)$ with $\mu = +1/\sqrt{3}$ (upward) and $I_-(\tau) \equiv I(\tau, -\mu)$ with $\mu = +1/\sqrt{3}$ (downward), the stationary 1D RTE becomes:

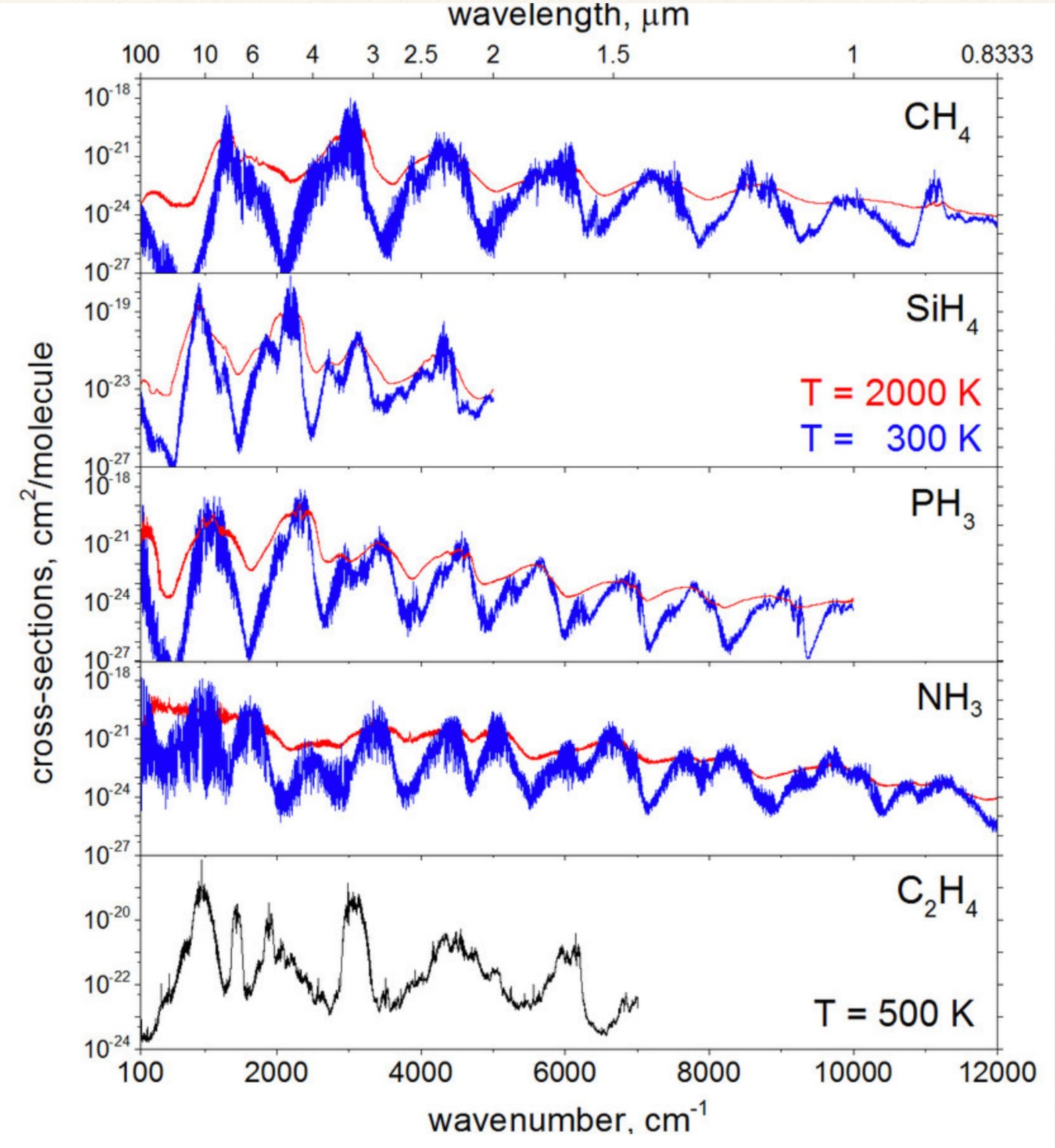
$$\mu \frac{dI_+}{d\tau} = I_+ - B(T(\tau)),$$

$$-\mu \frac{dI_-}{d\tau} = I_- - B(T(\tau)),$$

❖ (Careful with LLM: I did not ask for a grey model, neither to neglect scattering!)

➢ Radiative transfer





Cross sections generated using ExoMol line lists for methane, 10to10 line list [53], silane [72], phosphine [56], ammonia [79] and ethylene [75].

❖ Linelist of molecular absorption are huge!

➢ Radiative transfer

3. Radiative transfer in g-space

Within the band, the spectrally integrated intensity (or flux) is approximated by

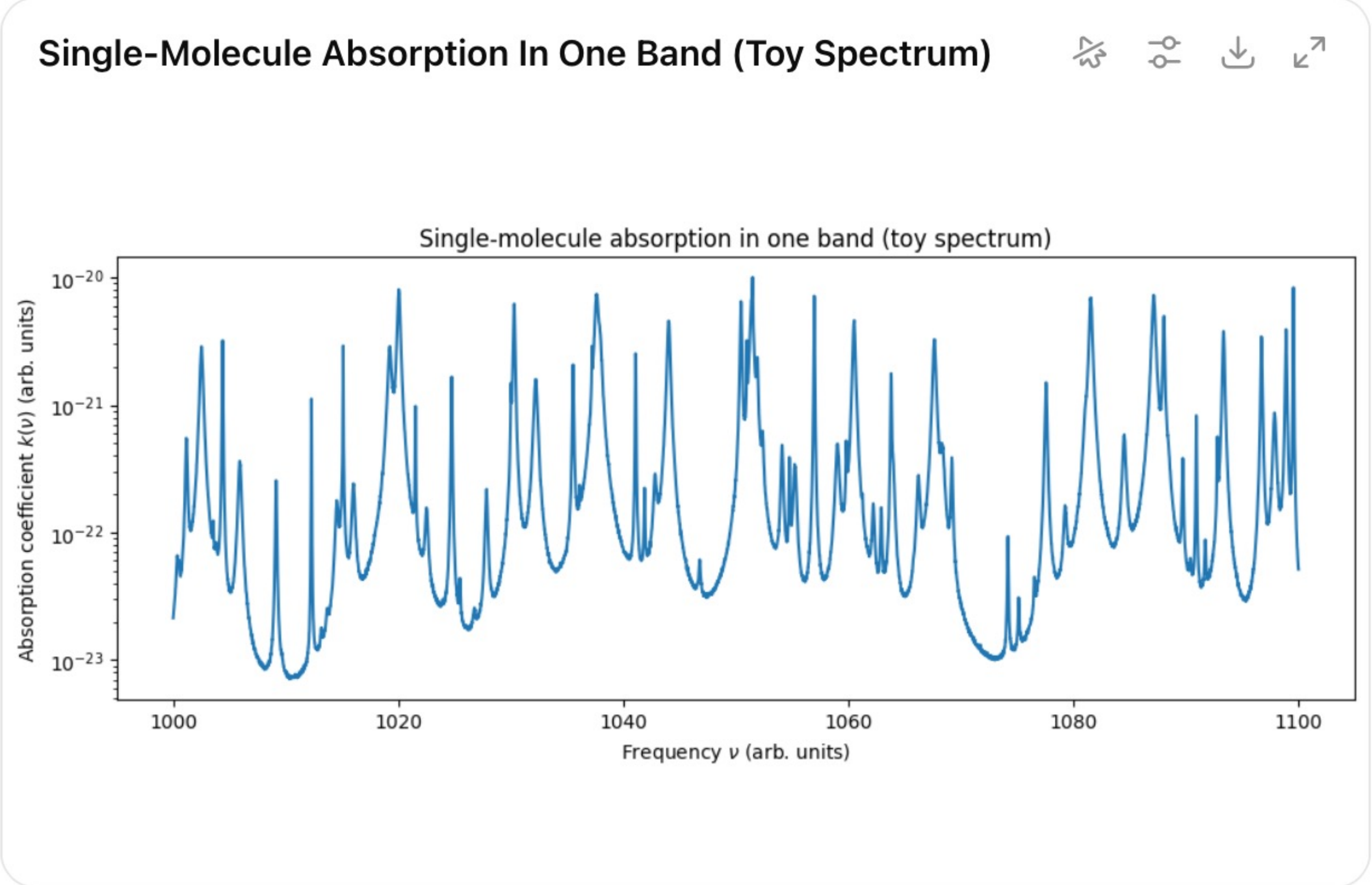
$$\int_{\nu_1}^{\nu_2} I_\nu \, d\nu \;\approx\; \Delta\nu \int_0^1 I(k(g))\; dg.$$

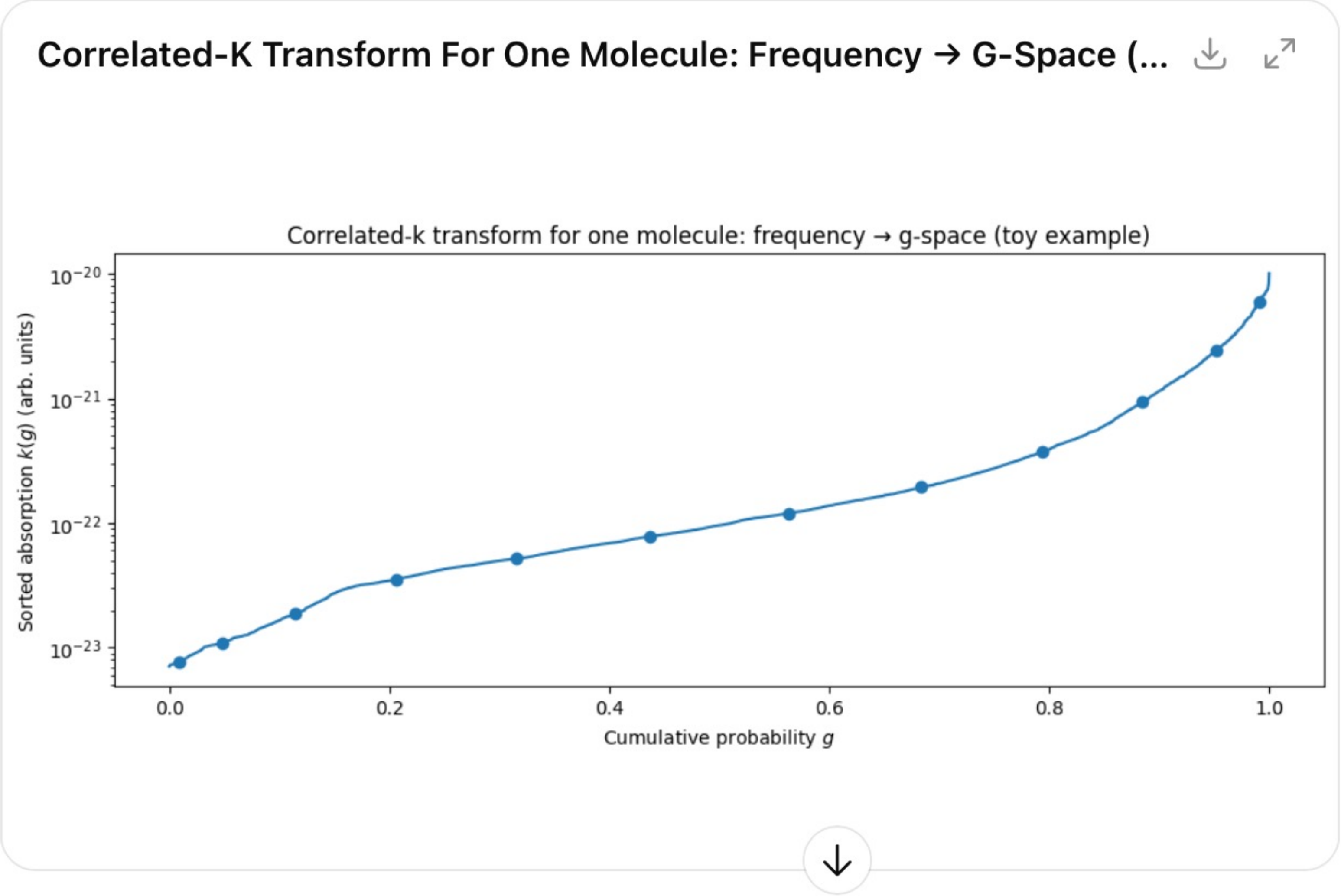
In practice, this integral is evaluated with a small quadrature:

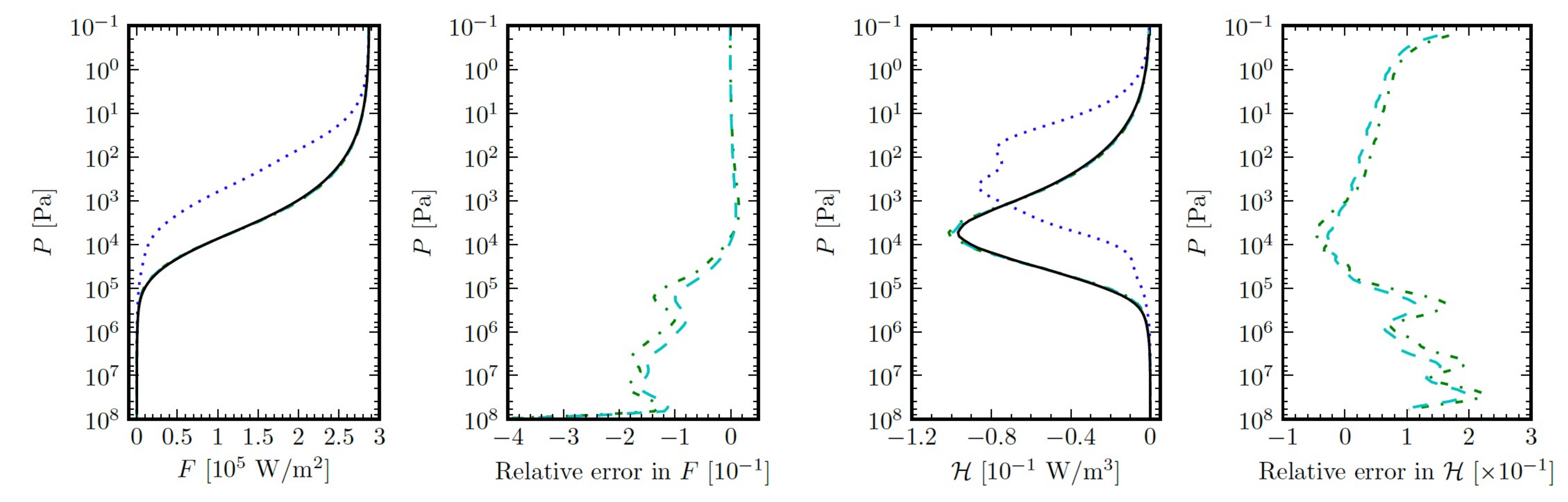
$$\int_0^1 I(k(g))\; dg \;\approx\; \sum_{i=1}^{N_g} w_i \, I(k_i)\,,$$

with typically $N_g \sim 8$–32 points instead of millions of frequency points.

Each quadrature point solves a **standard RTE** with a constant absorption coefficient k_i.







- Binning is bad : need a special treatment (correlated K see e.g. Amundsen et al. 2014)

➢ Radiative transfer

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Article | Published: 06 November 2023

$^{15}NH_3$ in the atmosphere of a cool brown dwarf

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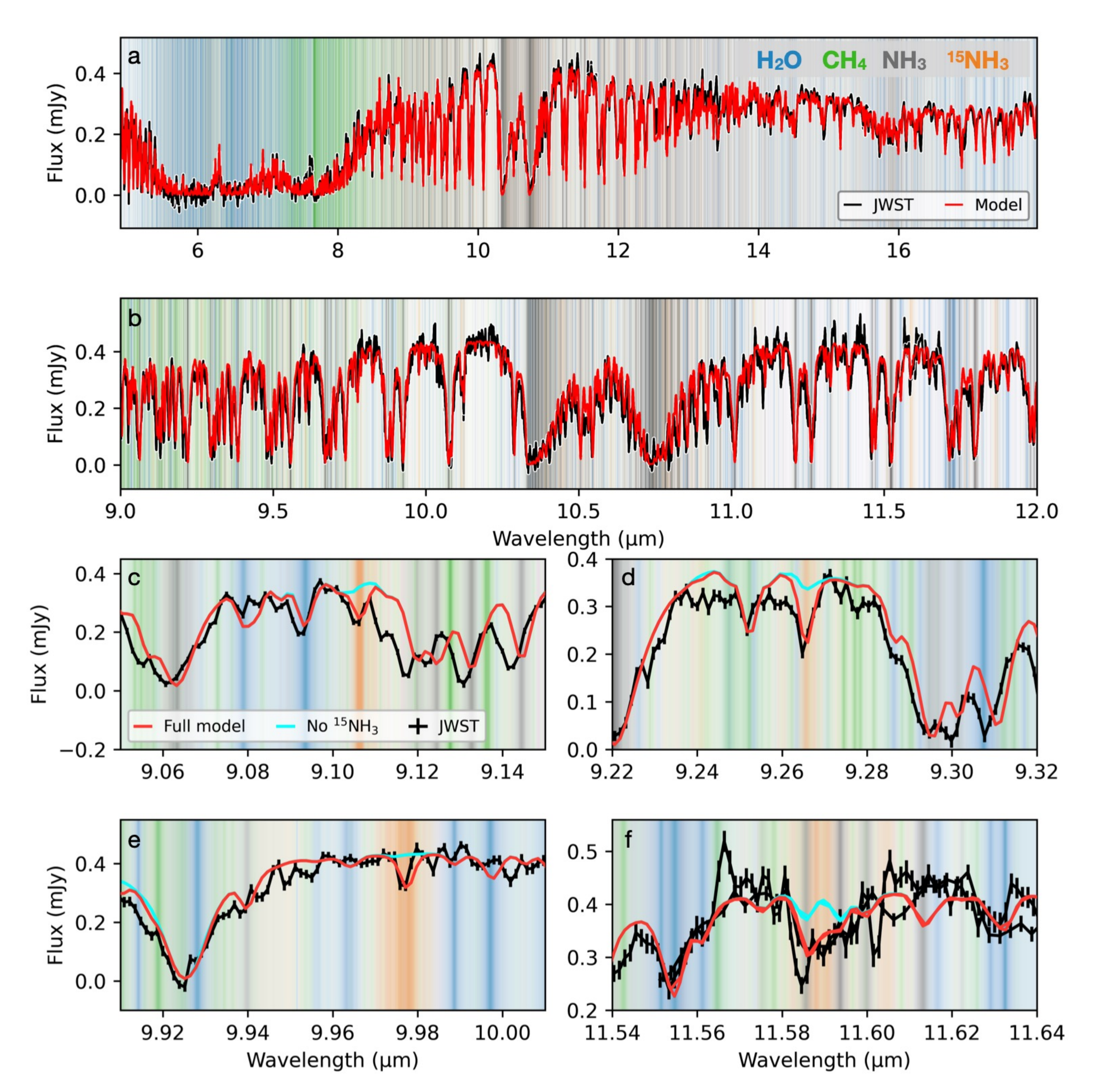
Nature **624**, 263–266 (2023) | Cite this article

Abstract

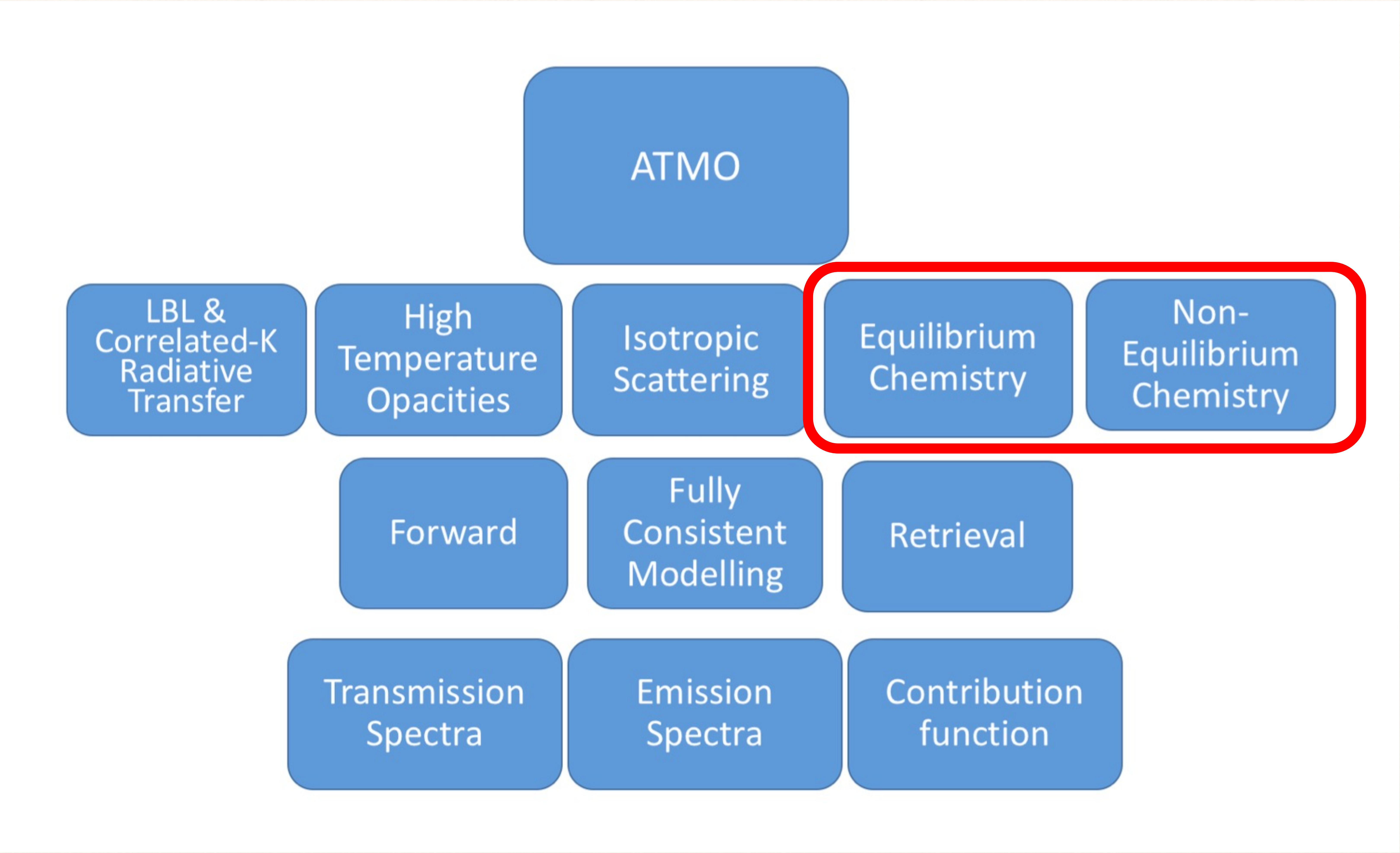
Brown dwarfs serve as ideal laboratories for studying the atmospheres of giant exoplanets on wide orbits, as the governing physical and chemical processes within them are nearly identical[1,2]. Understanding the formation of gas-giant planets is challenging, often involving the endeavour to link atmospheric abundance ratios, such as the carbon-to-oxygen (C/O) ratio, to formation scenarios[3]. However, the complexity of planet formation requires further tracers, as the unambiguous interpretation of the measured C/O ratio is fraught with complexity[4]. Isotope ratios, such as deuterium to hydrogen and $^{14}N/^{15}N$, offer a promising avenue to gain further insight into this formation process, mirroring their use within the Solar System[5,6,7]. For exoplanets, only a handful of constraints on $^{12}C/^{13}C$ exist, pointing to the accretion of ^{13}C-rich ice from beyond the CO iceline of the disks[8,9]. Here we report on the mid-infrared detection of the $^{14}NH_3$ and $^{15}NH_3$ isotopologues in the atmosphere of a cool brown dwarf with an effective temperature of 380 K in a spectrum taken with the Mid-Infrared



❖ High resolution example : detecting isotopes in brown dwarf atmospheres

Chemistry

➢ 1D radiative-convective equilibrium, the ATMO code

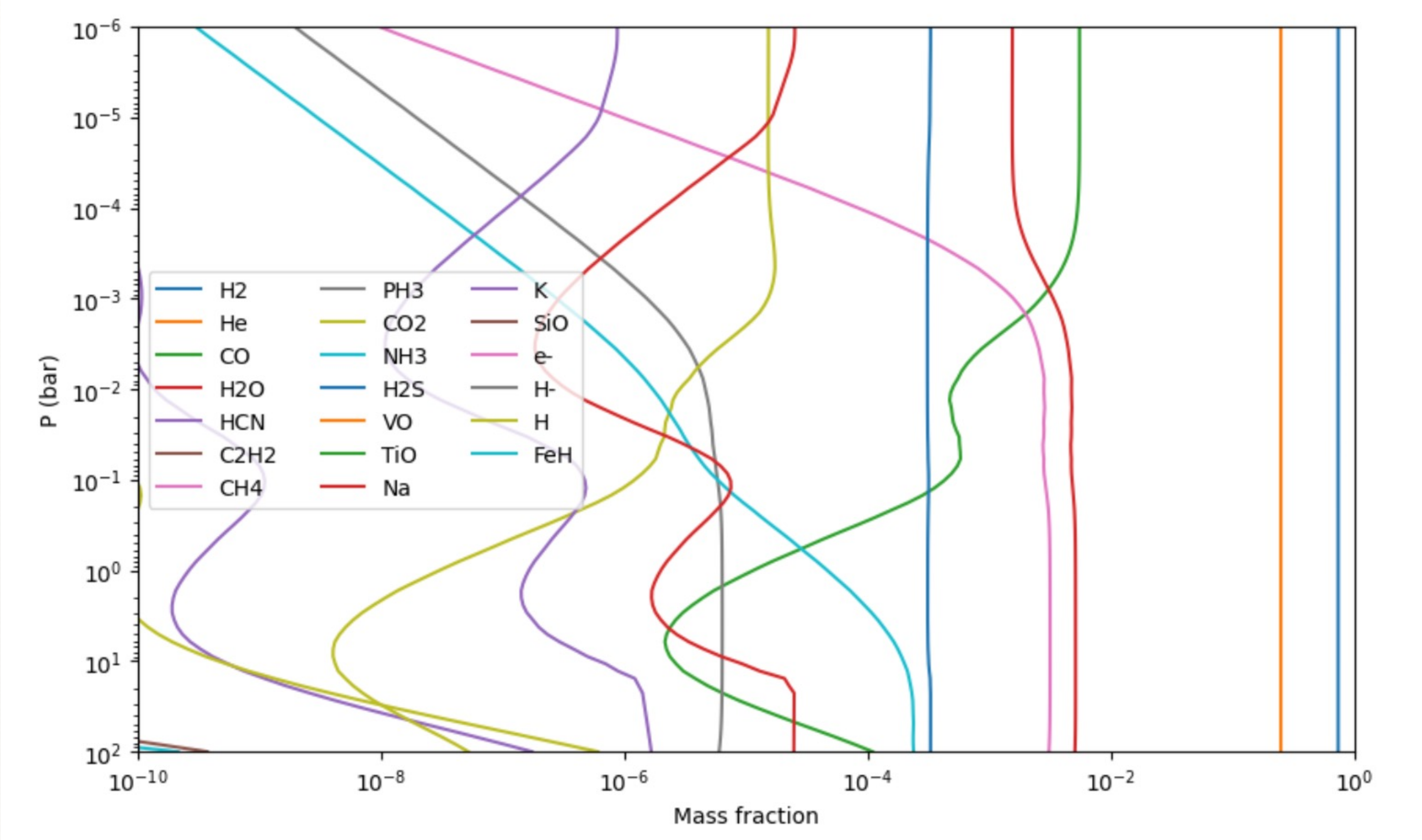


➢ Chemistry

Equilibrium chemistry (including condensation)

Chemical abundances are assumed to be in **thermodynamic equilibrium** at given temperature and pressure, with compositions determined by **minimization of the total Gibbs free energy**.

When **condensation curves** are crossed, stable condensed phases (liquids/solids) form and **remove elements from the gas phase**, so gas abundances follow both **chemical equilibrium** and **phase equilibrium**.



PetitRadtrans

➢ Chemistry

Out-of-equilibrium (non-equilibrium) chemistry

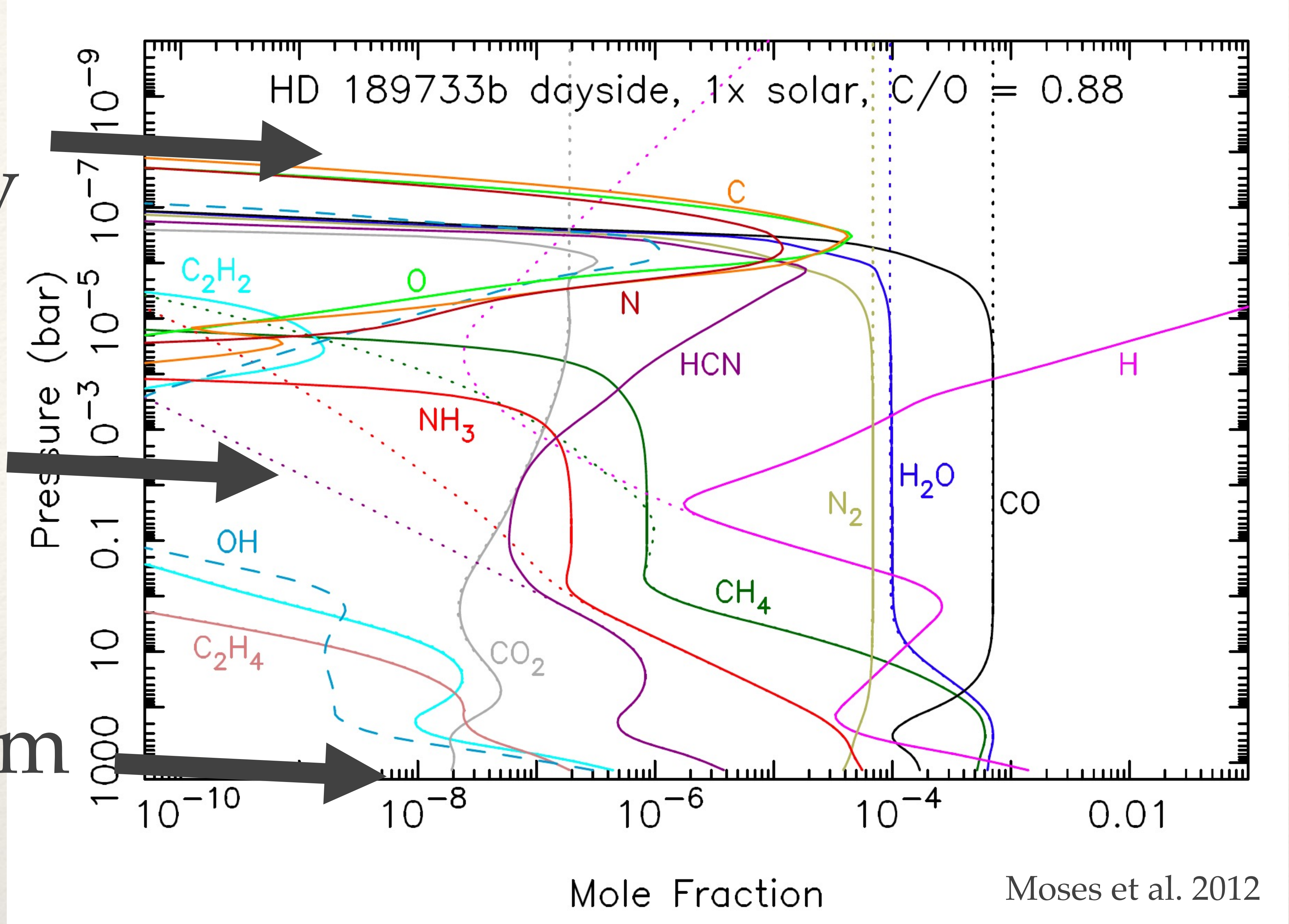
Chemical abundances are **time-dependent** and do **not** relax to thermodynamic equilibrium. They are controlled by **finite reaction rates**, **transport** (mixing, advection), and **external forcing** (e.g. UV radiation), requiring the solution of **kinetic rate equations** rather than Gibbs free-energy minimization.

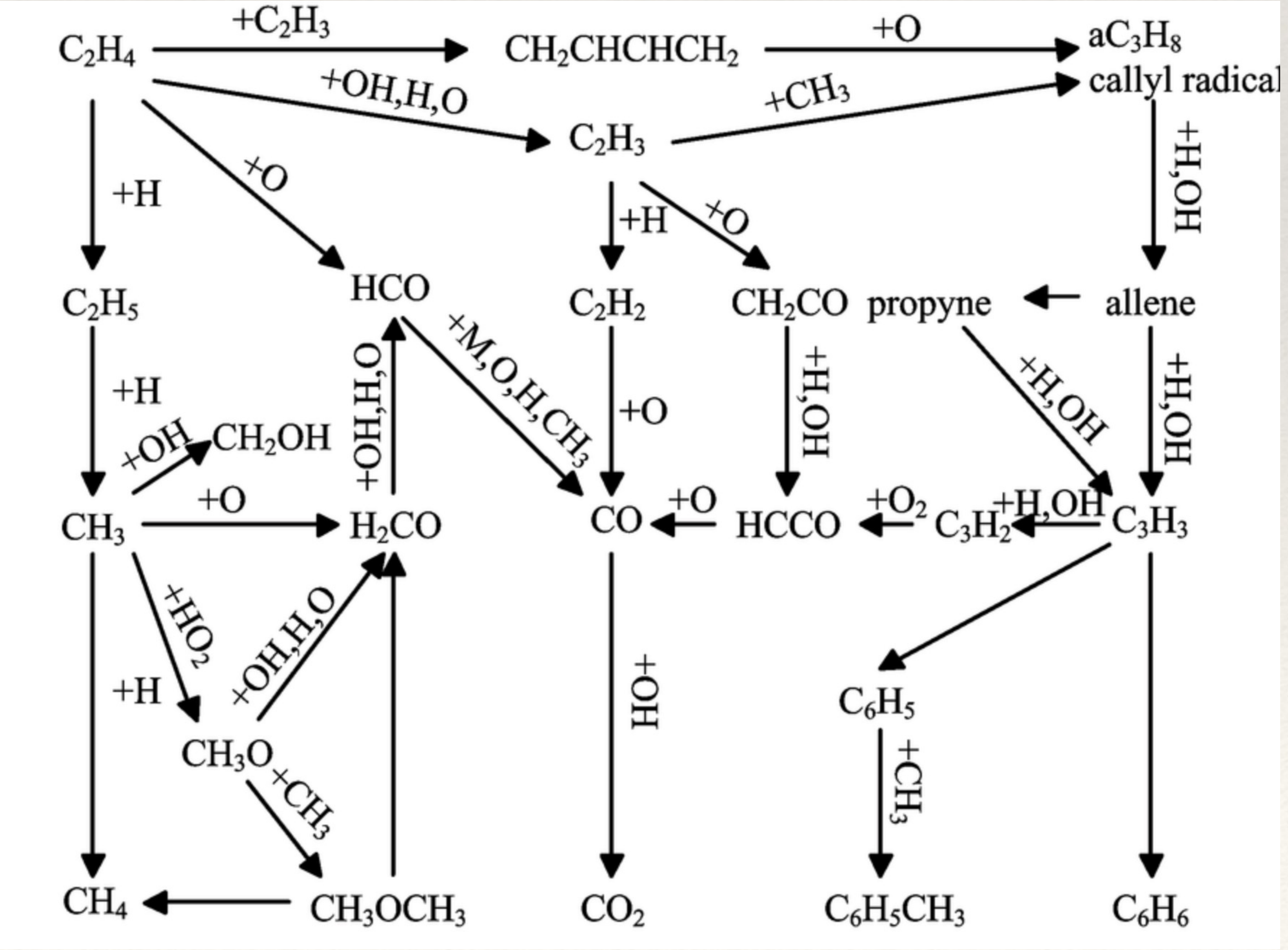
Chemical kinetic networks can include hundred of species and thousands of reactions

Photo-chemistry

mixing

equilibrium





➢ Chemistry

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Article | Open access | Published: 26 April 2023

Photochemically produced SO_2 in the atmosphere of WASP-39b

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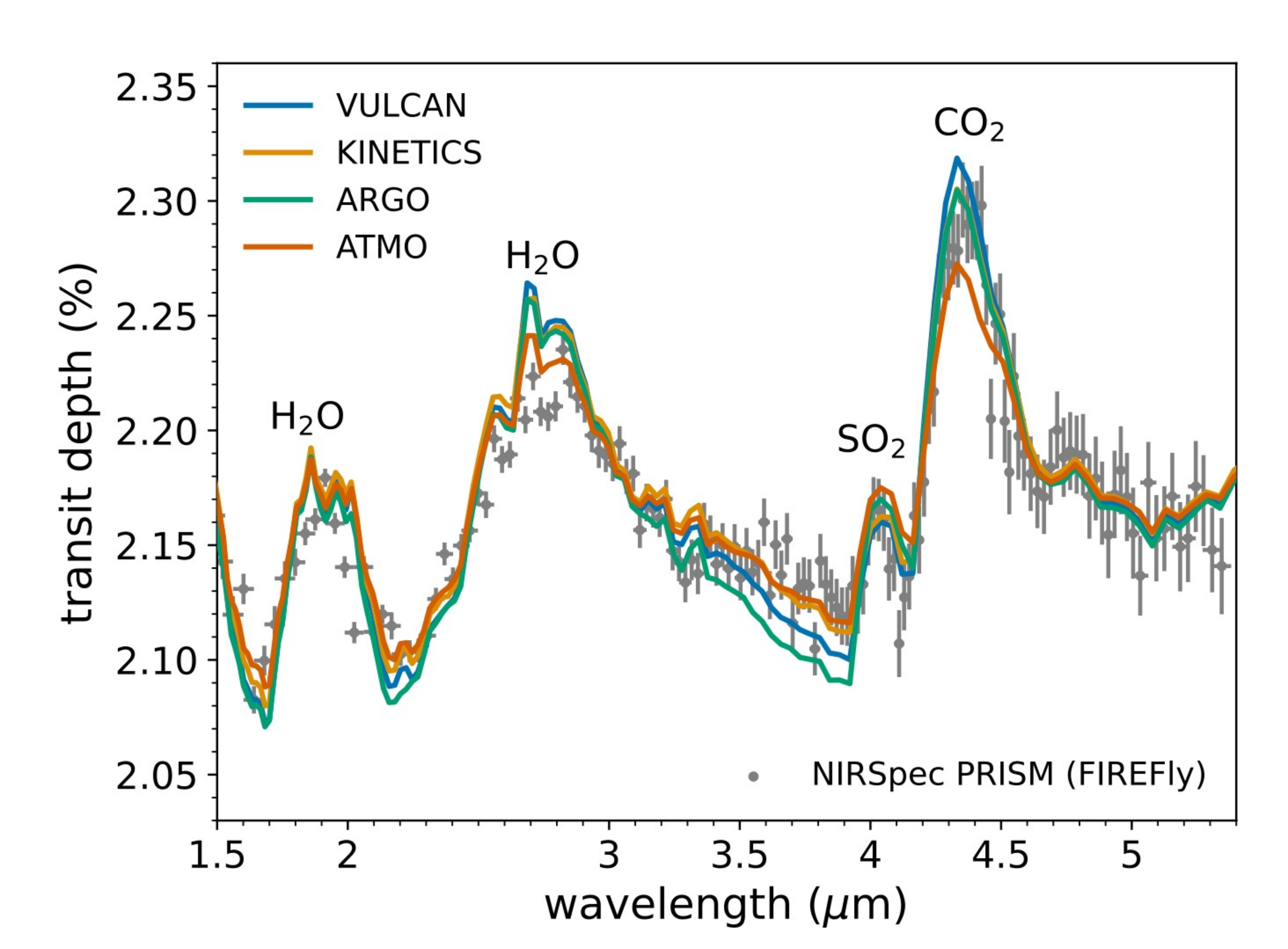
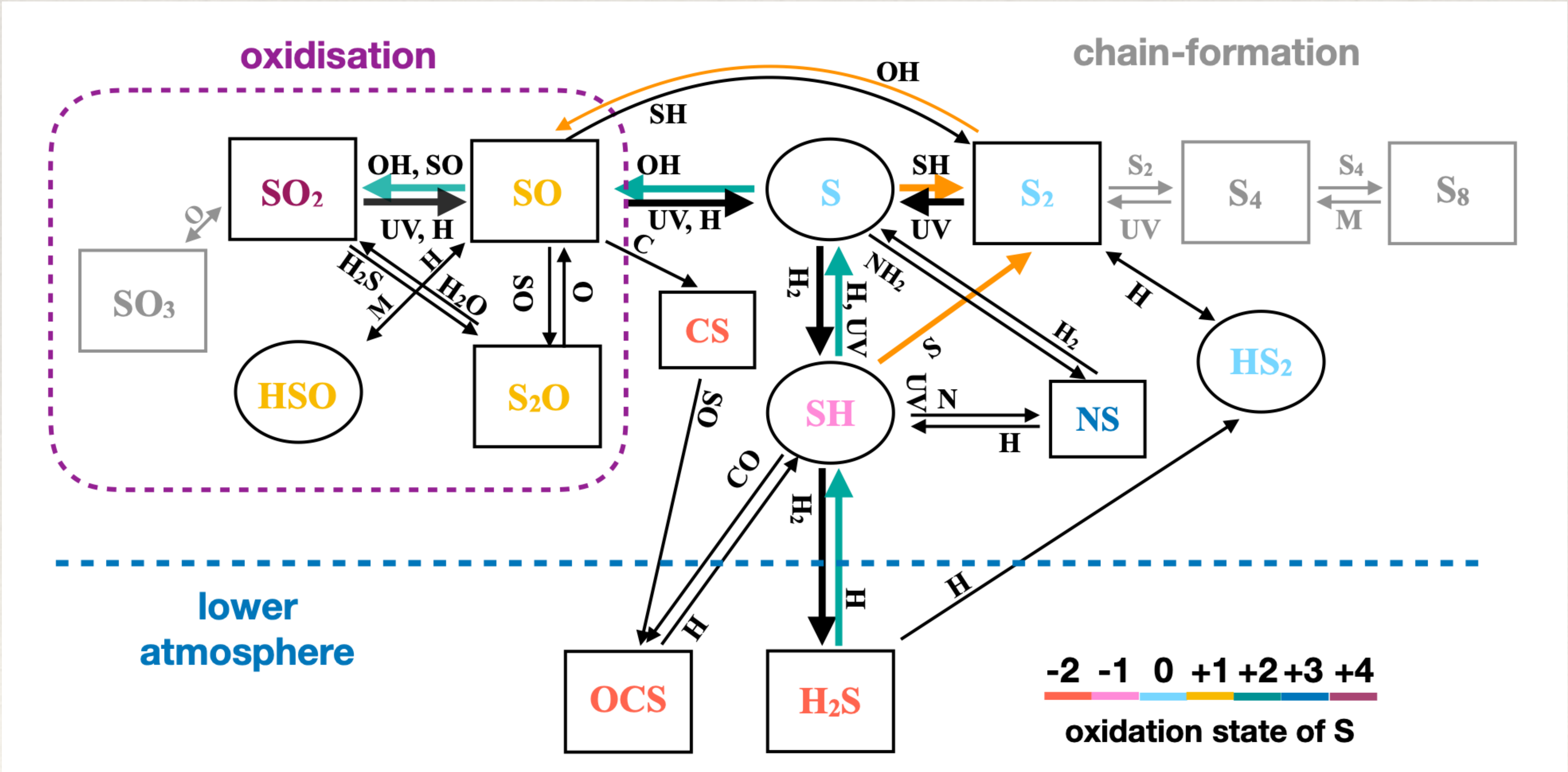
Nature **617**, 483–487 (2023) | Cite this article

Abstract

Photochemistry is a fundamental process of planetary atmospheres that regulates the atmospheric composition and stability[1]. However, no unambiguous photochemical products have been detected in exoplanet atmospheres so far. Recent observations from the JWST Transiting Exoplanet Community Early Release Science Program[2,3] found a spectral absorption feature at 4.05 μm arising from sulfur dioxide (SO_2) in the atmosphere of WASP-39b. WASP-39b is a 1.27-Jupiter-radii, Saturn-mass (0.28 M_J) gas giant exoplanet orbiting a Sun-like star with an equilibrium temperature of around 1,100 K (ref. [4]). The most plausible way of generating SO_2 in such an atmosphere is through photochemical processes[5,6]. Here we show that the SO_2 distribution computed by a suite of photochemical models robustly explains the 4.05-μm spectral feature identified by JWST transmission observations[7] with

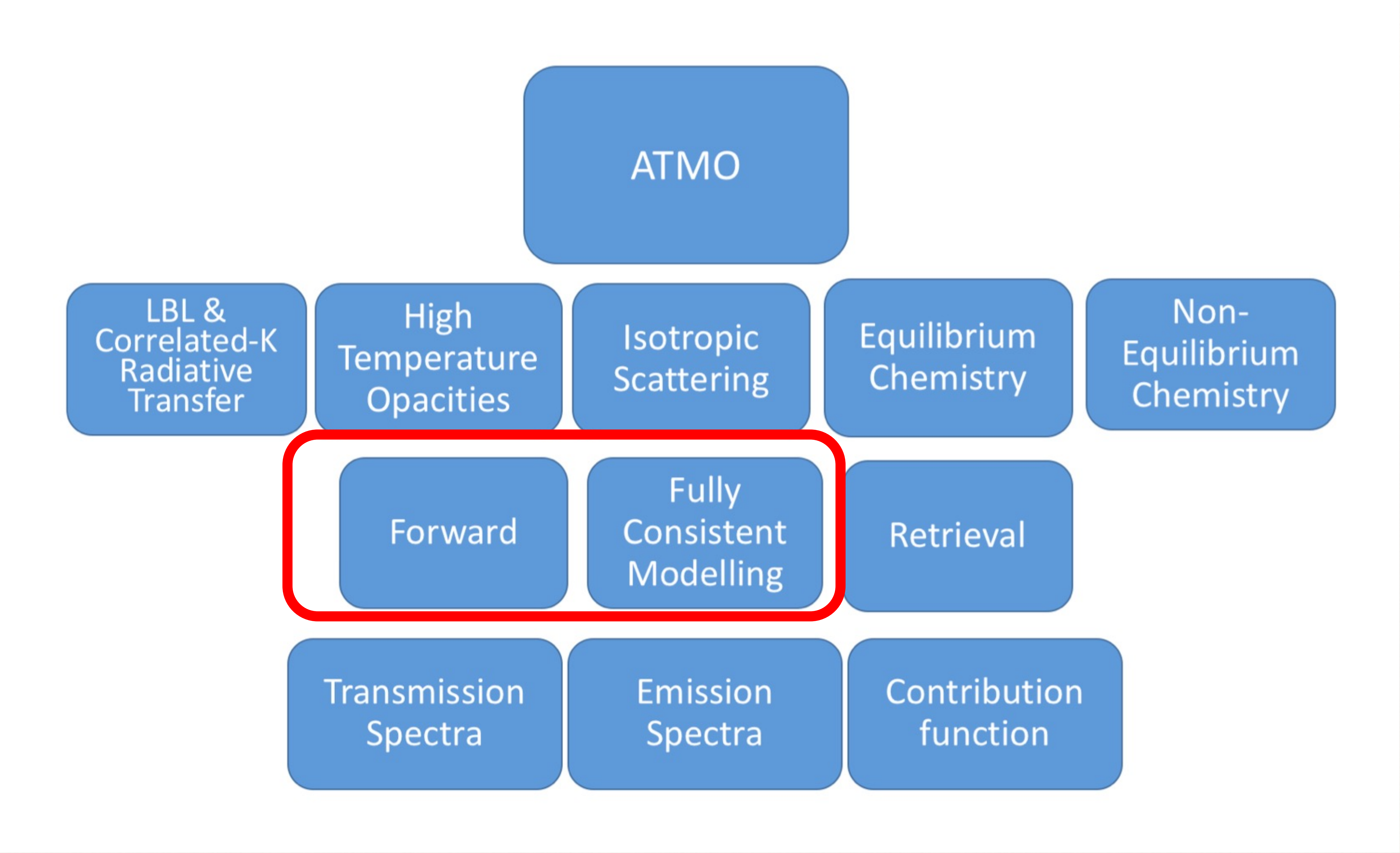




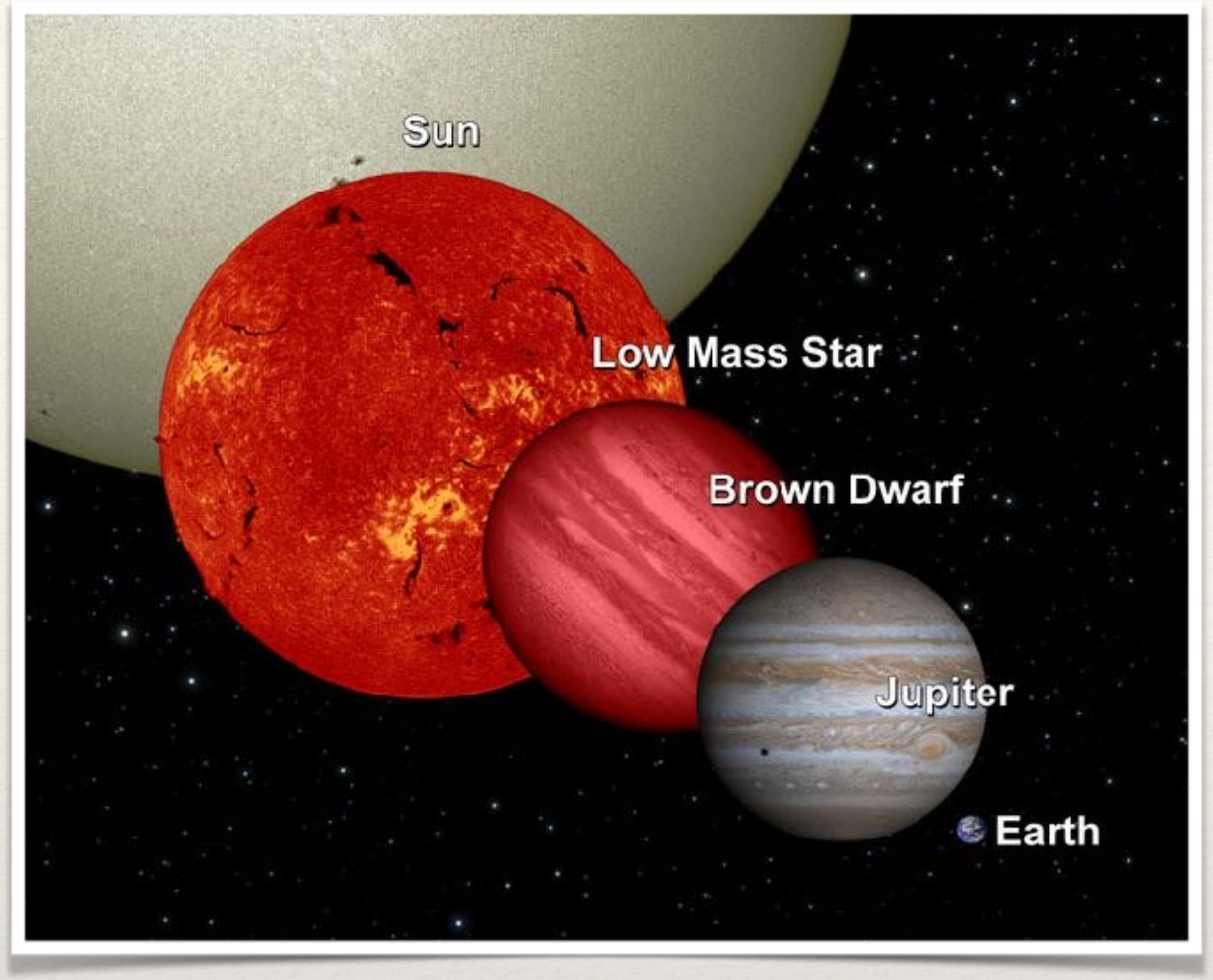
❖ Photo-chemistrty example : detecting SO2 in the atmosphere of wasp39b

Convective parametrization

➢ 1D radiative-convective equilibrium, the ATMO code



- Brown dwarfs



- Theoretically proposed by Kumar and Hayashi & Nakano in the 1960s

- Discovered in 1995 Rebolo et al./Nakajima et al.

- Form like star: grav. Collapse in a molecular cloud
- No H burning
- Cooling sequence between Teff~2500K Teff~250K
- Fuzzy difference with giant planets (good proxy!)

Rocky exoplanets