Transmission spectra of multi-dimensional atmospheric simulations: computation and applications

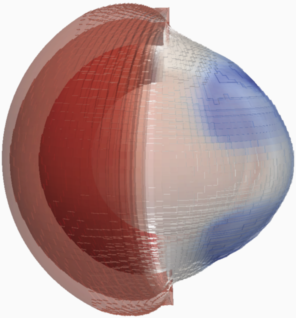
TauREx (1D/2D) & Pytmosph3R 2.0

Aurélien Falco (LAB Bordeaux - ECLIPSE team - Whiplash ERC)

Atmospheric model

Transmission spectrum

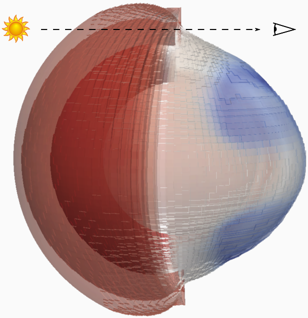
- Atmospheric grid



Atmospheric model

Transmission spectrum

$$\left.\begin{array}{l}\text{- Atmospheric grid}\\ \text{- Rays of light}\end{array}\right\}\text{Optical depth}\xrightarrow[\textit{integral}]{}\text{Transmittance}\rightarrow\text{Spectrum}$$



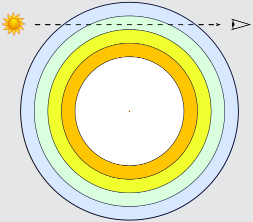
Atmospheric model

Transmission spectrum

$$\left.\begin{array}{l}\text{- Atmospheric grid}\\ \text{- Rays of light}\end{array}\right\}\text{Optical depth}\xrightarrow[\textit{integral}]{}\text{Transmittance}\rightarrow\text{Spectrum}$$

1D

- Very fast
- Retrievals
- Biases (Pluriel et al., 2020)



Atmospheric model

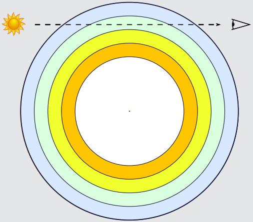
Transmission spectrum

- Atmospheric grid
- Rays of light

} Optical depth $\xrightarrow[\textit{integral}]{}$ Transmittance → Spectrum

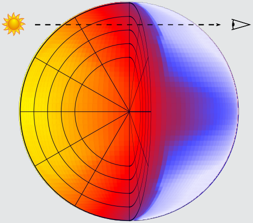
1D

- Very fast
- Retrievals
- Biases (Pluriel et al., 2020)



3D

- Realistic structure
- Too slow for retrievals (?)



Atmospheric model

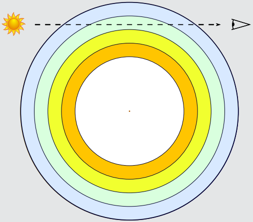
Transmission spectrum

- Atmospheric grid
- Rays of light

$\left.\right\}$ Optical depth $\xrightarrow[\textit{integral}]{}$ Transmittance → Spectrum

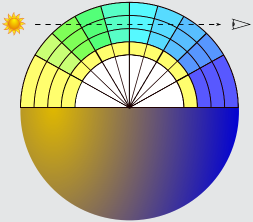
1D

- Very fast
- Retrievals
- Biases (Pluriel et al., 2020)



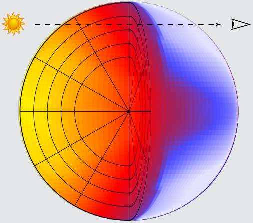
2D

- Fast enough (for retrievals)
- Day-night dichotomy of Ultra Hot Jupiters



3D

- Realistic structure
- Too slow for retrievals (?)



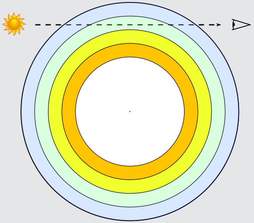
Atmospheric model

Transmission spectrum

$$\left.\begin{array}{l}\text{- Atmospheric grid}\\ \text{- Rays of light}\end{array}\right\}\text{Optical depth}\xrightarrow[\textit{integral}]{}\text{Transmittance}\rightarrow\text{Spectrum}$$

1D (TauREx)

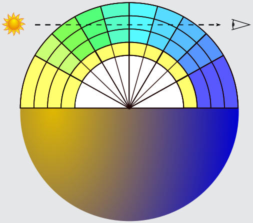
- $N_{z,\mathrm{lay}}$ layers (ℓ)



(Al-Refaie et al., 2019)

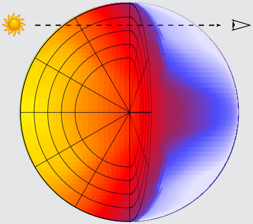
2D (TauREx)

- $N_{z,\mathrm{lay}}$ layers (ℓ)
- N_α slices (solar zenith angle)



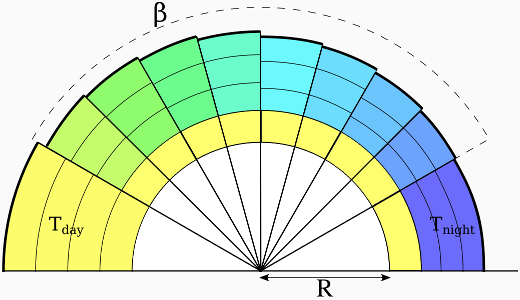
3D (Pytmosph3R)

- $N_{z,\mathrm{lay}}$ layers (ℓ)
- N_{lat} latitudes (ϕ)
- N_{lon} longitudes (λ)



(Caldas et al., 2019)

Coordinate system: from levels to altitude coordinates



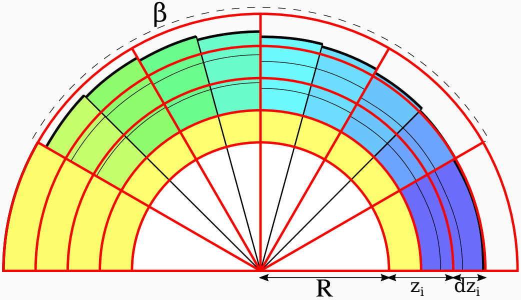
Coordinate system

- Radial coordinate: layers & levels (l)
- Horizontal grid: (α^*) in 2D or (ϕ, λ) in 3D

Input data for each cell (l) or (l, α^*) or (l, ϕ, λ)

- Pressure
- Temperature
- Gas Volume Mixing Ratios
- Aerosols Mass Mixing Ratios

Coordinate system: from levels to altitude coordinates



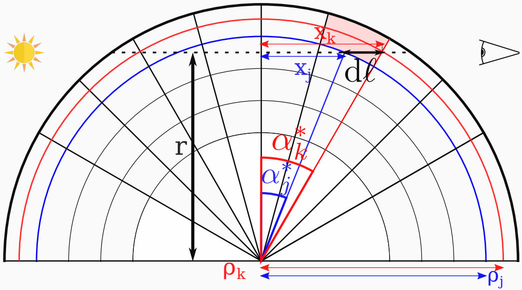
Coordinate system

- Radial coordinate: altitude (z)
- Horizontal grid: $\left(\alpha^*\right)$ in 2D or (ϕ, λ) in 3D

Interpolation of (z, ϕ, λ) using altitude

- Pressure
- Temperature
- Gas Volume Mixing Ratios
- Aerosols Mass Mixing Ratios

Rays subdivision through the altitude-based grid



Compute intersection points coordinates

1D

- Circles at each altitude (point j in blue)

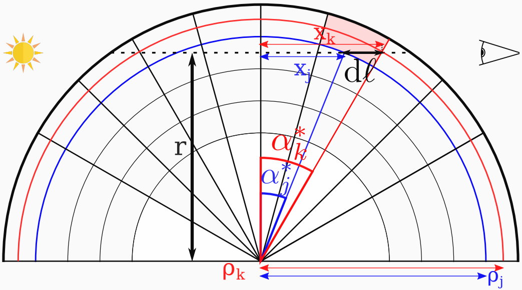
2D

- Circles at each altitude (point j in blue)
- Solar zenith angle lines (point k in red)

3D

- Spheres at each altitude (point j in blue)
- Latitudinal cones (point k in red)
- Longitudinal planes (point k in red)

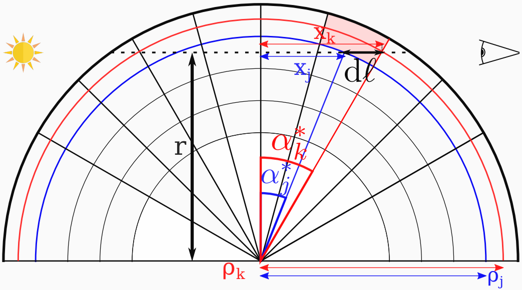
Rays subdivision through the altitude-based grid



Distance between points ($\Delta\ell$)

- Sort points according to their distance x to the terminator
- Cartesian distance $d\ell$ between two successive points
- Coordinates of each cell (2D/3D)
  - List for each ray (to get P, T, x)
  - Global dictionary for computing opacities (to avoid computing twice a cell)

Optical depth



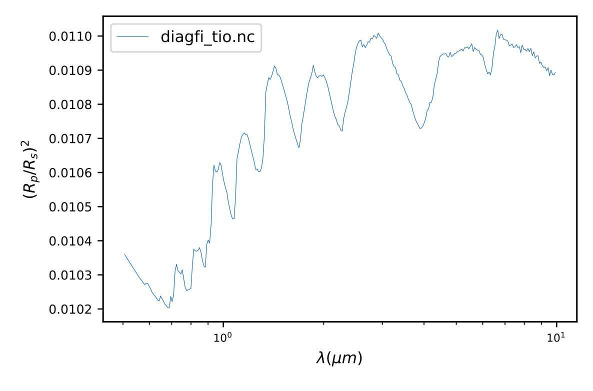
$$\tau_\lambda(\rho,\theta) = \sum_{c \in Cells[\rho,\theta],\, d\ell \in \Delta\ell[\rho,\theta]} \frac{P[c]}{k_B T[c]} \left(\sum_m \chi_m[c]\sigma_{m,\lambda} + \sum_{j<N_{con}} k_{mie,j} \right) d\ell \tag{1}$$

- $d\ell$ is the length of the segment of the ray at coordinates c
- `Exo_k` (Leconte, 2020) handles the opacities:
    - Correlated-k and cross-sections tables from multiple sources
    - Molecular, continuum absorptions, Rayleigh and Mie scatterings...

Integral → transmission spectrum

$$\Delta_\lambda = \frac{{R_p}^2 + \sum_{\rho,\theta} \left(1 - e^{-\tau_\lambda(\rho,\theta)}\right) S_\rho}{{R_s}^2}, \tag{2}$$

with $S_\rho = 2\frac{(\rho + \mathrm{d}\rho/2)\,\mathrm{d}\rho}{N_\theta}$, where N_θ is the number of angular points in the grid of rays



Models accuracy

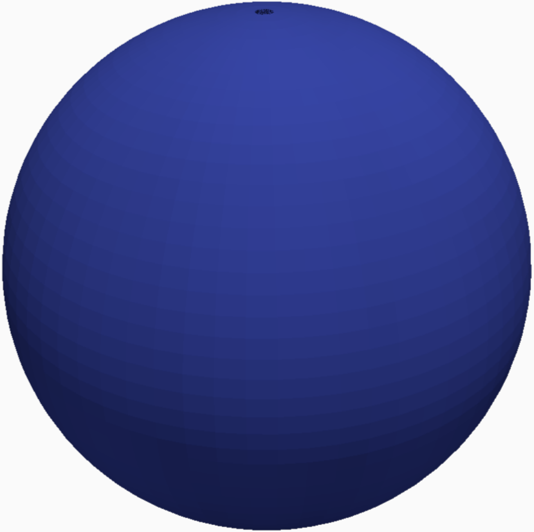
Three models

- 1D
- 2D
- 3D

Test cases

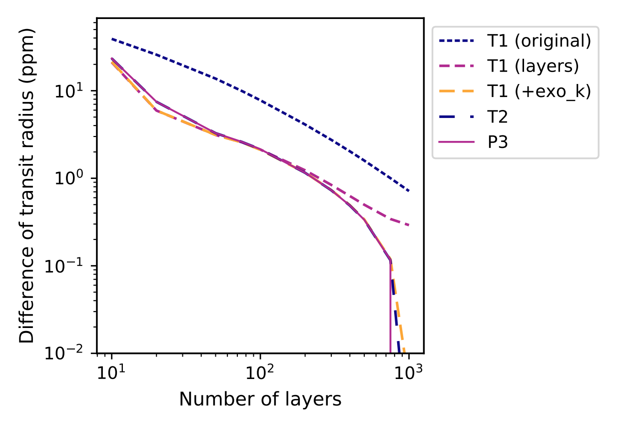
- Isothermal atmosphere
- 2D temperature map (day → night)
- 3D GCM (WASP-121b)

Isothermal atmosphere

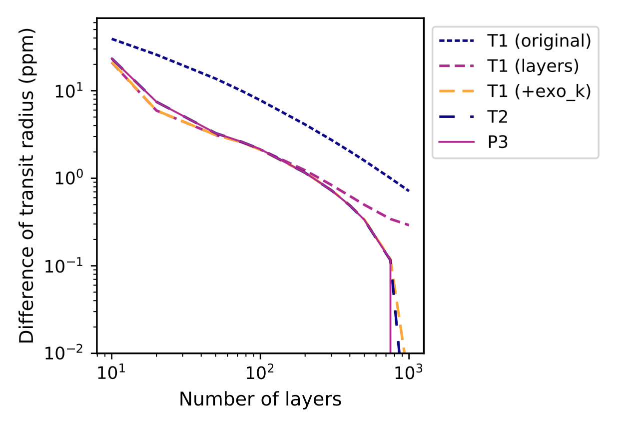


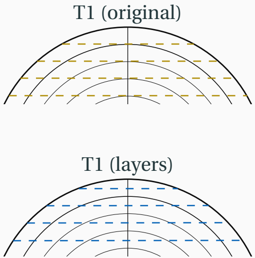
T = 2500K

Isothermal (T = 2500K)

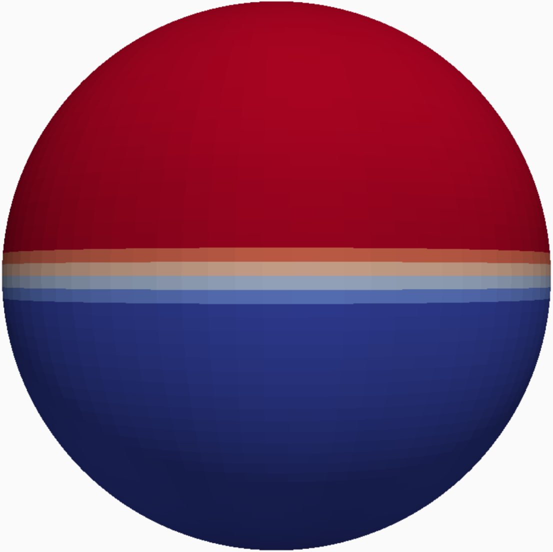


Isothermal (T = 2500K)

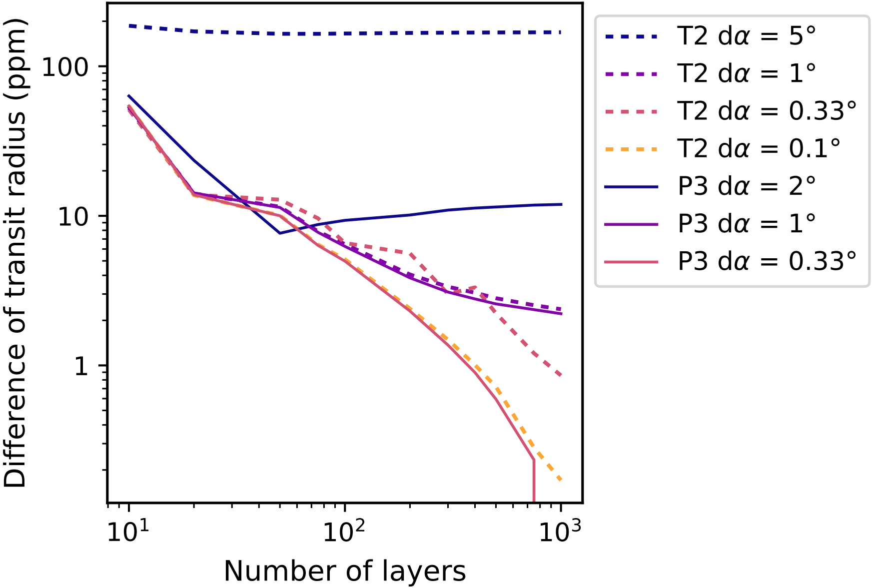




2D



T_{day}	T_{night}	T_{deep}
3300	500	2500


Difference of transit radius (ppm)
100
10
1
10^1
10^2
10^3
Number of layers
T2 dα = 5°
T2 dα = 1°
T2 dα = 0.33°
T2 dα = 0.1°
P3 dα = 2°
P3 dα = 1°
P3 dα = 0.33°

2D retrievals: performance of TauREx models

Retrievals → run many times one model

Optical depth

$$\mathcal{O}\left(\left(\frac{N_{z,\mathrm{lay}}^2}{2}+N_{z,\mathrm{lay}}\cdot N_\alpha\right)\cdot N_\lambda\right)$$

Interpolation of the opacities

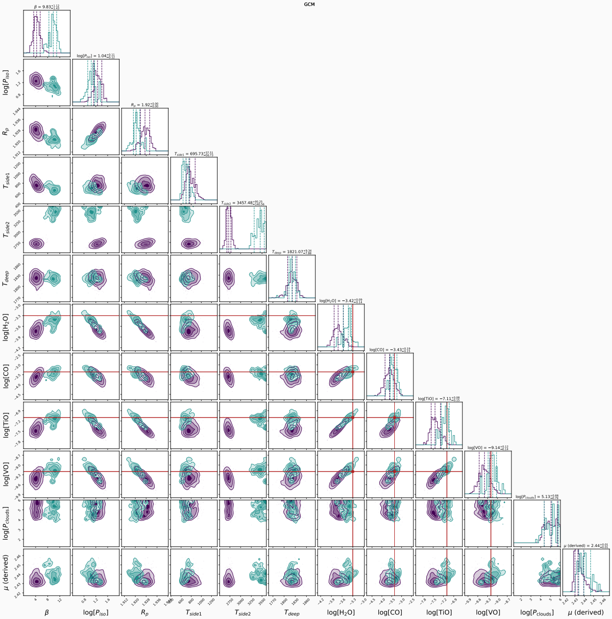
$$\mathcal{O}\left(C\cdot N_{z,\mathrm{lay}}\cdot N_\alpha\cdot N_\lambda\cdot N_{\mathrm{mol}}\right)$$

$N_{z,\mathrm{lay}}$: number of layers ; N_α: number of angles ; N_λ: number of wavelengths ; N_{mol}: number of molecules

		N_α (2D)			
$N_{z,\mathrm{lay}}$	1D	2	10	20	30
100	**0.26**	0.52	1.20	1.99	**2.80**
200	0.78	1.73	3.05	4.72	6.32

Table 1: Average time (s) to run one TauREx model. Molecular absorption only (no Rayleigh scattering nor CIA), with four molecules on 39124 wavelengths from 0.3 to 15 μm.

2D retrieval of WASP-121b



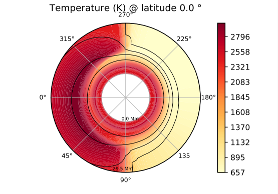
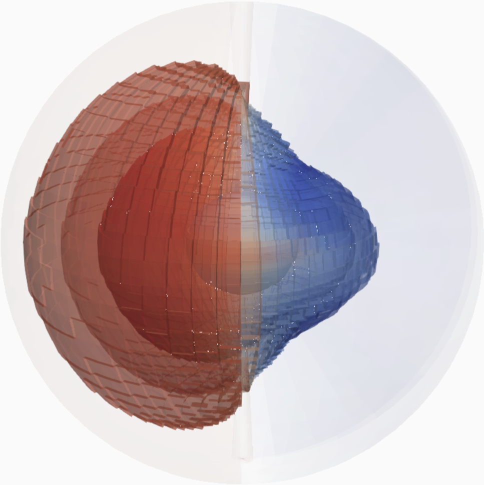


Figure 1: Input simulation

T_{day}	T_{night}	T_{deep}
3453	695	1821
2721	769	1821

Table 2: Retrieved temperatures

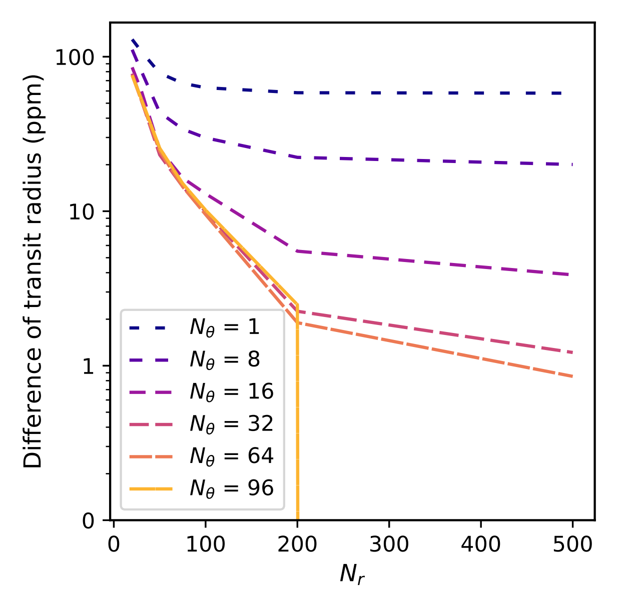
3D (T_{eq} = 2100 K)

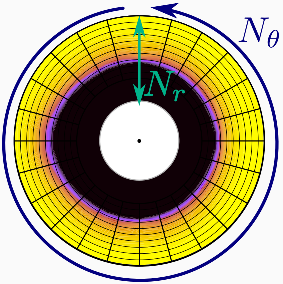


Pytmosph3R 2.0 - Pytmosph3R 1.3

~10-50 ppm

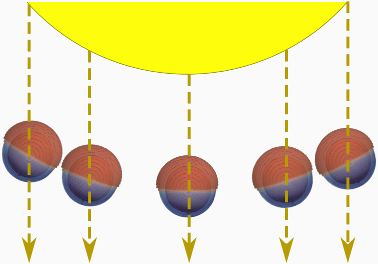
3D (T_{eq} = 2100 K)





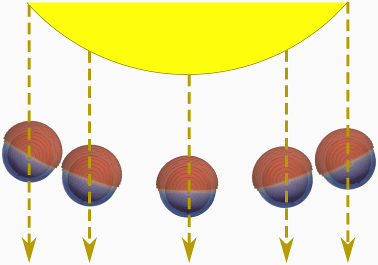
GCM resolution
100x32x64

Rotation of the planet during transit: WASP-121b

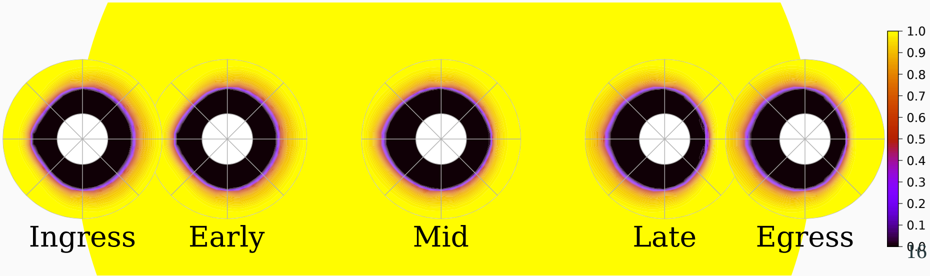


	Ingress	Early	Mid	Late	Egress
Orbital phase ϕ	$-15°$	$-13°$	$0°$	$+13°$	$15°$

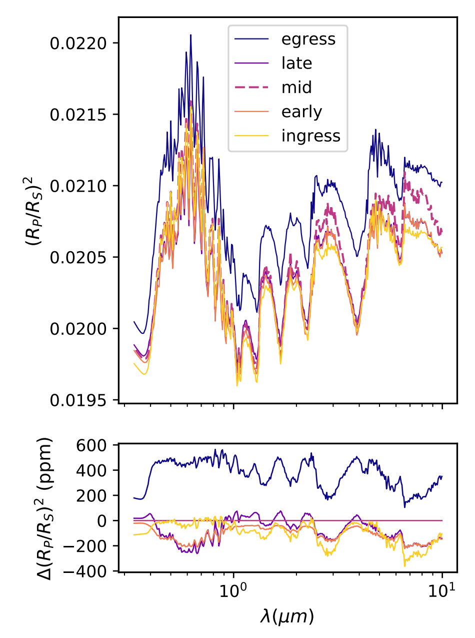
Rotation of the planet during transit: WASP-121b

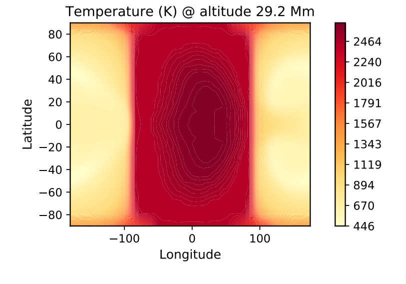


	Ingress	Early	Mid	Late	Egress
Orbital phase ϕ	$-15°$	$-13°$	$0°$	$+13°$	$15°$



Rotation of the planet during transit





Conclusion

Three models

- 1D & 2D with TauREx
- 3D with Pytmosph3R

Conclusion

Three models

- 1D & 2D with TauREx
- 3D with Pytmosph3R

2D (TauREx)

- Validated in isothermal with TauREx (1D), in 2D with Pytmosph3R
- Fast enough for retrievals (Zingales et al. (2021) in prep)

Conclusion

Three models

- 1D & 2D with TauREx
- 3D with Pytmosph3R

2D (TauREx)

- Validated in isothermal with TauREx (1D), in 2D with Pytmosph3R
- Fast enough for retrievals (Zingales et al. (2021) in prep)

3D (Pytmosph3R)

- Rotation: infer asymmetric east-west characteristics of the atmosphere

Conclusion

Three models

- 1D & 2D with TauREx
- 3D with Pytmosph3R

2D (TauREx)

- Validated in isothermal with TauREx (1D), in 2D with Pytmosph3R
- Fast enough for retrievals (Zingales et al. (2021) in prep)

3D (Pytmosph3R)

- Rotation: infer asymmetric east-west characteristics of the atmosphere

http://perso.astrophy.u-bordeaux.fr/~jleconte/pytmosph3r-doc/index.html

New release very soon!

- Papers under reviews (Falco et al., 2021; Pluriel et al., 2021)
- Parallel
- Emission
- Lightcurve

Al-Refaie, A. F., Changeat, Q., Waldmann, I. P., and Tinetti, G. (2019). TauREx III: A fast, dynamic and extendable framework for retrievals.

Caldas, A., Leconte, J., Selsis, F., Waldmann, I., Bordé, P., Rocchetto, M., and Charnay, B. (2019). Effects of a fully 3D atmospheric structure on exoplanet transmission spectra: retrieval biases due to day–night temperature gradients. *Astronomy & Astrophysics*, 623:A161.

Falco, A., Zingales, T., Pluriel, W., and Leconte, J. (2021). Computation of transmission spectra using a 1D, 2D or 3D atmospheric structure. *Unpublished manuscript*.

Leconte, J. (2020). Spectral binning of precomputed correlated-k coefficients. *arXiv preprint arXiv:2012.01428*.

Pluriel, W., Leconte, J., Parmentier, V., Zingales, T., and Falco, A. (2021). Evolution of the biases in retrieved atmospheric composition of hot Jupiters. *Unpublished manuscript*.

Pluriel, W., Zingales, T., Leconte, J., and Parmentier, V. (2020). Strong biases in retrieved atmospheric composition caused by day-night chemical heterogeneities. *A&A*, 636:A66.

Zingales, T., Falco, A., Pluriel, W., and Leconte, J. (2021). TauREx 2D: Modelling 2D effects in retrieval. *Unpublished manuscript*.