The Open-source Bayesian Atmospheric Radiative Transfer (BART) Code to Model Exoplanet Atmospheres

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Exoplanetary Atmospheres and Habitability

Nice, France - 16/10/2015

Atmospheric Modeling:

- Radiative transfer. H*ere!*
- Cloud formation. *D. Homeier*
- Magnetic fields. *R. Estrela*
- Circulation dynamics.
- Scattering.
- Thermal equilibrium.
- Photo-chemistry.
- Vertical mixing.

} *Grassi, Tsai, Blecic, Blumenthal, Hébrard, Venot, Hu*

The Problem of Exoplanet Atmospheric Modeling:

- Low S/N observations.
- Photometry: few, broadband points. (e.g., Spitzer)
- Spectra: low resolution, span. (e.g., Hubble's WFC3)

Two approaches:

Forward Modeling:

- Physically-motivated (+)
- Self-consistent (+)
- Non-exhaustive (–)
- Not necessarily unique solution (–)

Retrieval (e.g., Bayesian):

- Statistically robust (+)
- Data driven (+)
- Computationally intensive (–)
- Not necessarily self-consistent (–)

Either way, **we need to know the physics well.**

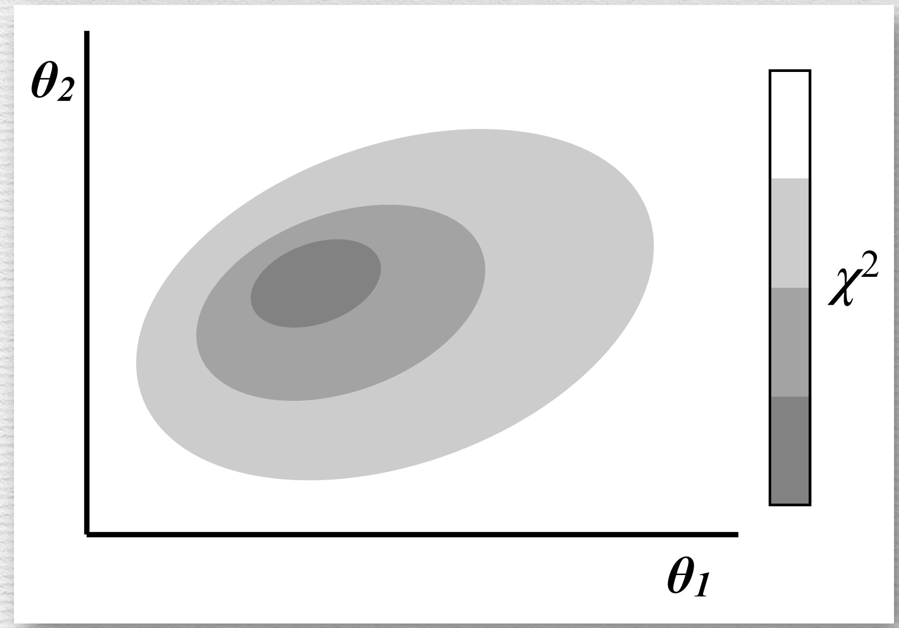
Bayesian Statistics: Uncertainties estimation:

Markov-chain Monte Carlo algorithm:

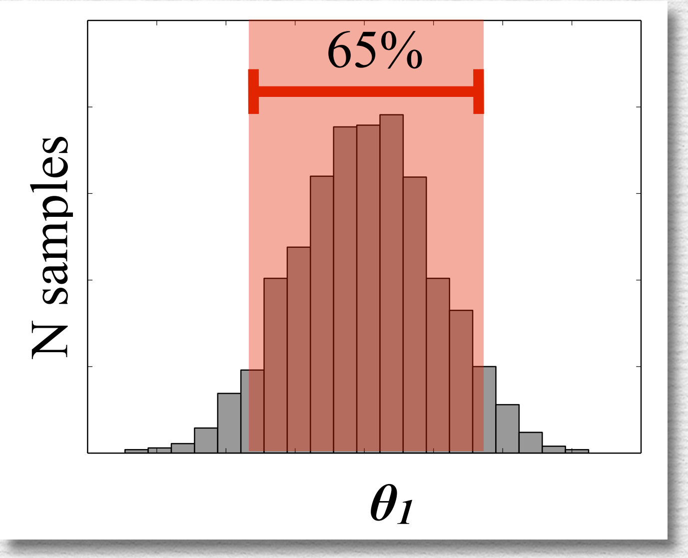
- Random sampling: Markov chain (10^5–10^6 samples).
- Accept/reject ∝ goodness of fit (χ^2).
- Posterior distribution ∝ parameter uncertainties.

$$\chi^2(\theta_1, \theta_2|\mathbf{d}) = \sum_i \frac{(m_i - d_i)^2}{\sigma_i^2}$$

Posterior:

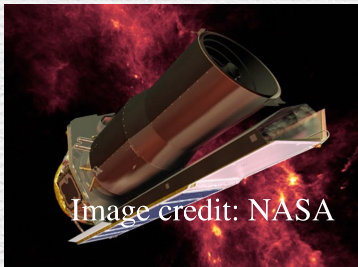


Marginal posterior:

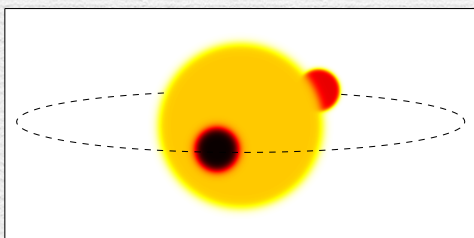


Exoplanet Characterization:

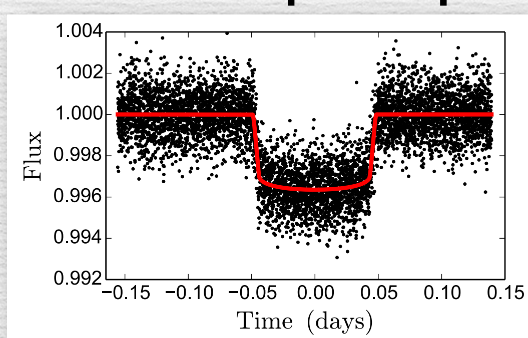
Observations:



Transiting systems:

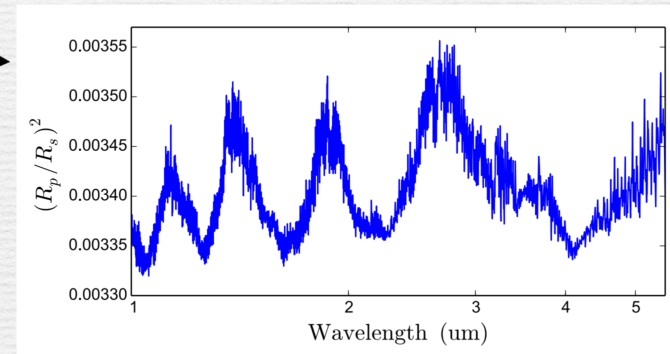


Transit/eclipse depths:

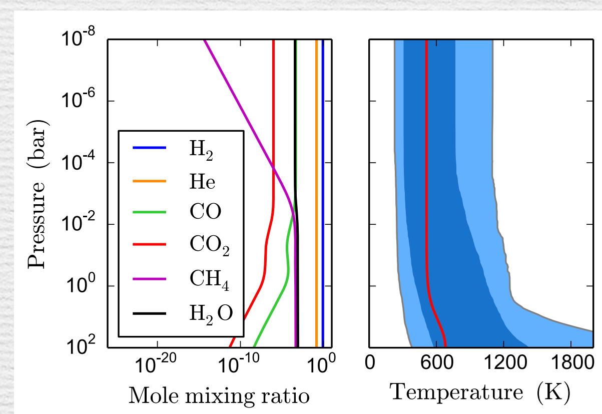


Modeling:

Transmission/emission spectra:

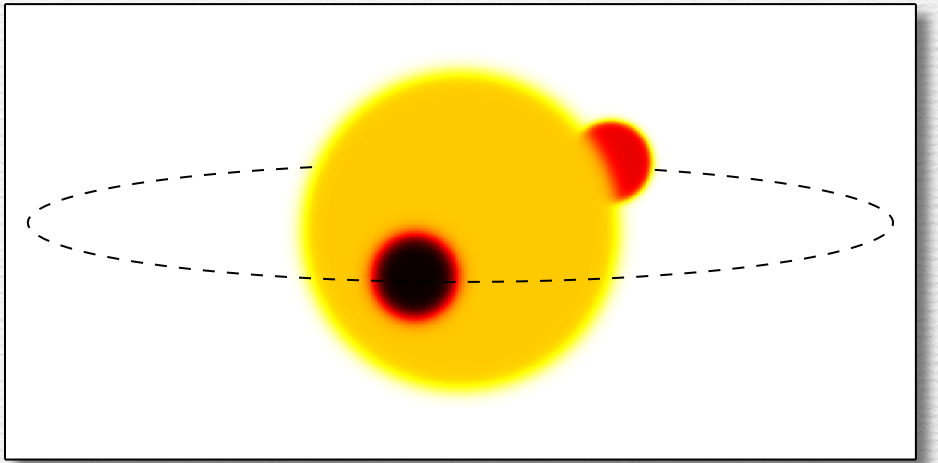


Atmospheric characterization:

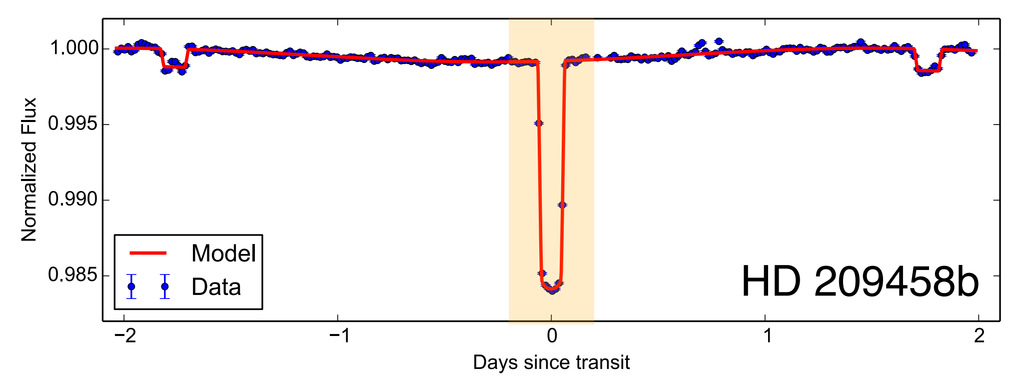


Transiting Exoplanets:

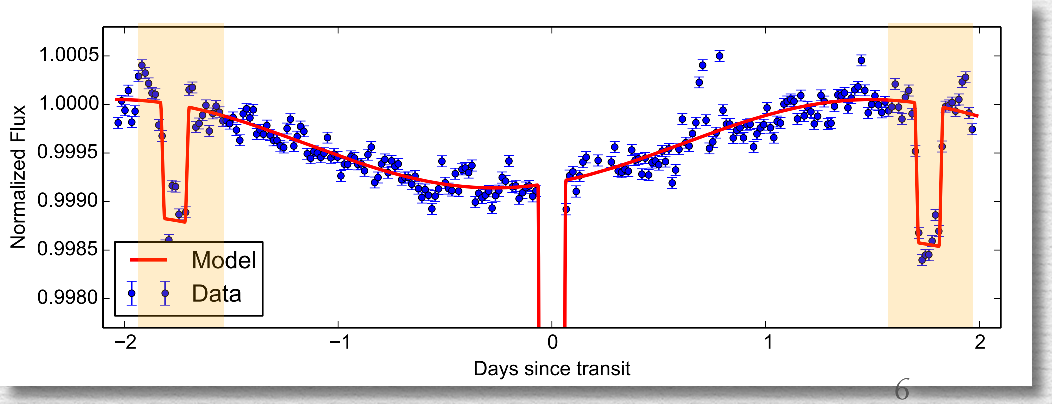
Planets that pass in front and behind their host star.



IR Photometric time-series:



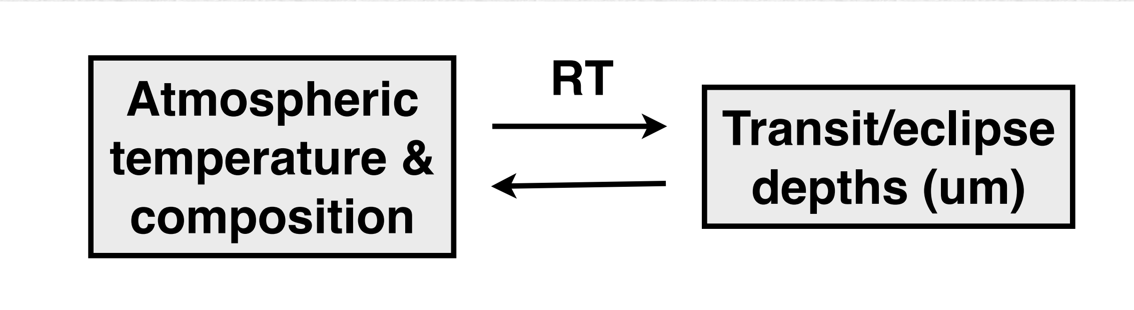
$$\text{Transit depth} = \frac{\Delta F}{F} \approx \left(\frac{R_p}{R_s}\right)^2$$



$$\text{Eclipse depth} = \frac{\Delta F}{F} \approx \frac{F_p}{F_s}$$

Atmospheric Modeling:

The problem:



Our solution:
- Radiative Transfer
- Thermo-chemical equilibrium
- (Bayesian) Statistics

Radiative Transfer:
- Atmospheric model
- Species databases
- Observing geometry

Atmospheric model:
- Temperature
- Species abundances

Bayesian Atmospheric Radiative Transfer (BART) project.
Harrington, Cubillos, Blecic et al.

Precursors:
Madhusudhan & Seager (2009),
Line et al. (2013),
Benneke & Seager (2012),
Waldmann et al. (2015).

Atmospheric Modeling:

Bayesian Atmospheric Radiative Transfer (BART):

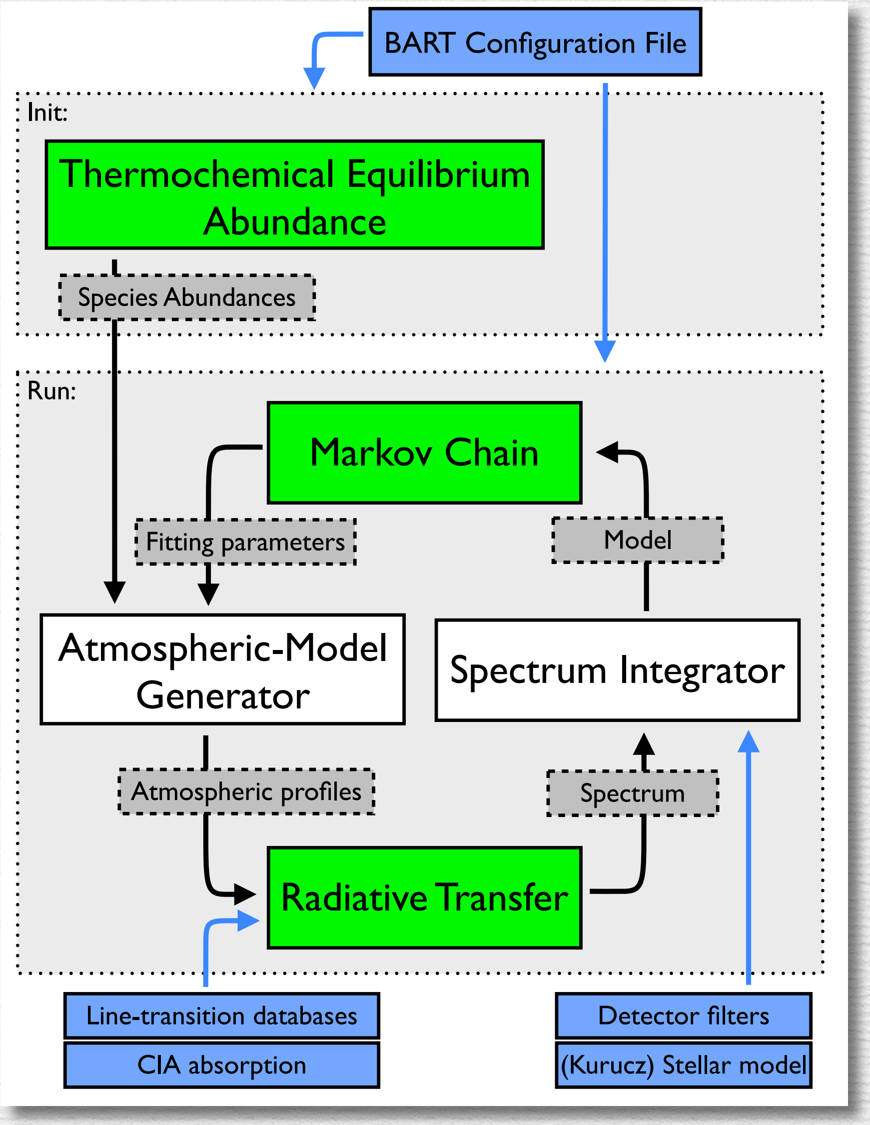
github.com/exosports/BART

GitHub

- Open-source Open-development.
- Documented.
- User interaction at the ‘Python’ level.

python™

- Modular, independent, sub-modules:
  - Thermochemical-equilibrium chemistry.
  - Radiative-transfer.
  - Bayesian statistics.



Radiative Transfer:

The radiative-transfer equation describes how light propagates, as it travels through a medium:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -\kappa_\nu (I_\nu - B_\nu(T))$$

path — T, p, composition

Not really new science,

... but **must be efficient** (if MCMC)**.**

- Each species has an specific absorption pattern in the spectrum.

The Transit code:

- Solves 1D, line-by-line radiative-transfer equation.
- Produces transmission (transit) or emission (eclipse) spectra.
- Open-source, documented.

github.com/exosports/transit

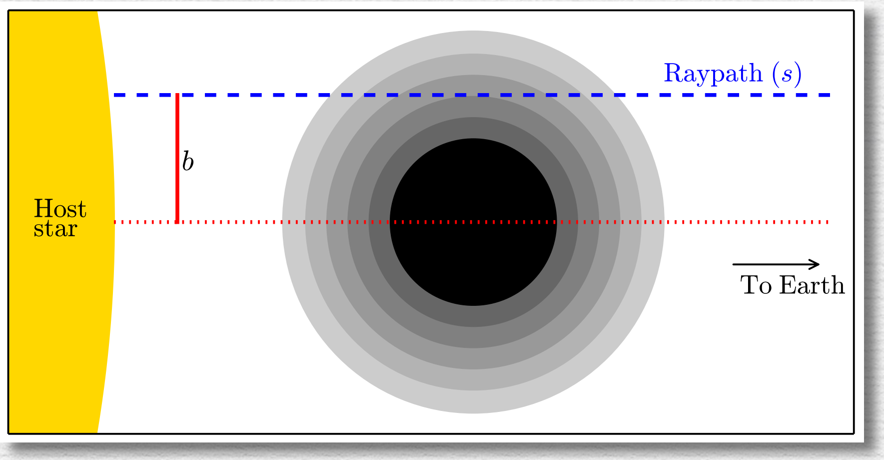
GitHub

Inputs:

- One-dimensional atmospheric model (T, p, abundances).
- Species opacity databases.

Radiative Transfer:

Transit Observing Geometry:



- 1D spherical-shells model
- Parallel rays

Transmission spectrum:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -\kappa_\nu (I_\nu - B_\nu(T))$$

Transit depth

$$M_\nu = \frac{\Delta F}{F_s} = \frac{1}{R_s^2}\left[R_{\rm top}^2 - 2\int_0^{R_{\rm top}} \exp(-\tau_\nu) b \mathrm{d}b\right]$$

$$\mathrm{d}\tau_\nu = \kappa_\nu \mathrm{d}s$$

Atmospheric Model:

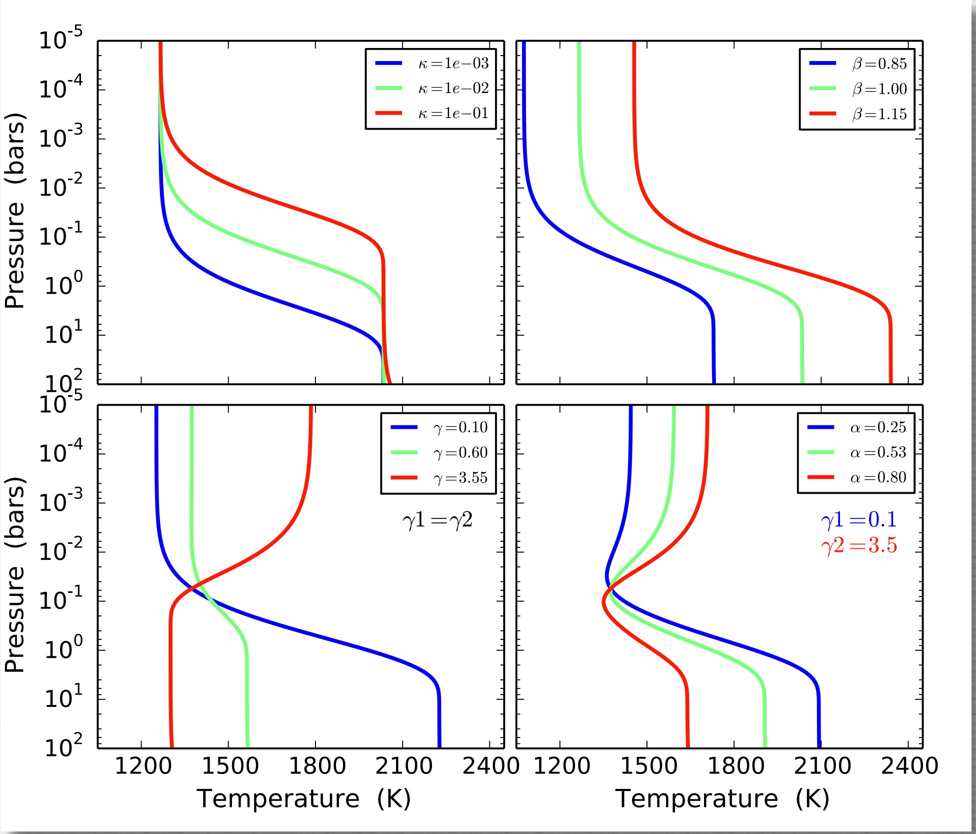
Temperature-profile model:

Three-stream Eddington approximation (Parmentier & Guillot 2014, Line et al. 2013):

$$T^4(p) = \frac{3T_{\rm int}^4}{4}\left(\frac{2}{3}+\tau\right) + \frac{3T_{\rm irr}^4}{4}(1-\alpha)\xi_{\gamma 1}(\tau) + \frac{3T_{\rm irr}^4}{4}\alpha\xi_{\gamma 2}(\tau)$$

- Stellar ($T_{\rm irr}$) and internal ($T_{\rm int}$) heating sources.

- IR (κ_{IR}) and optical mean opacities (κ_v)



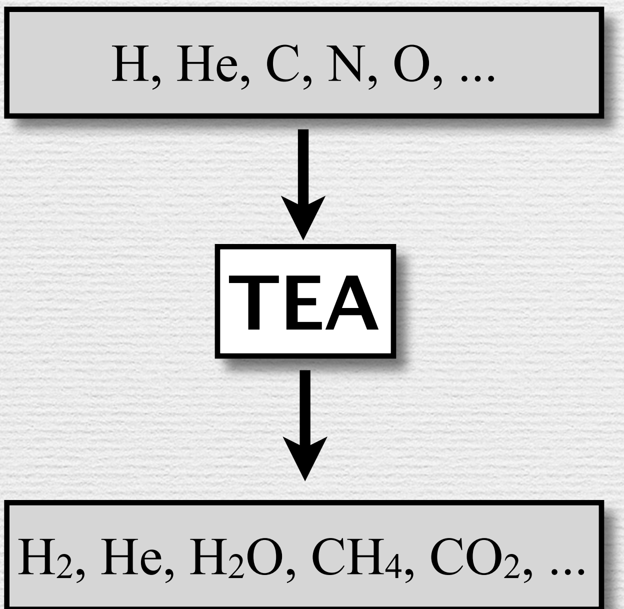
Atmospheric Model:

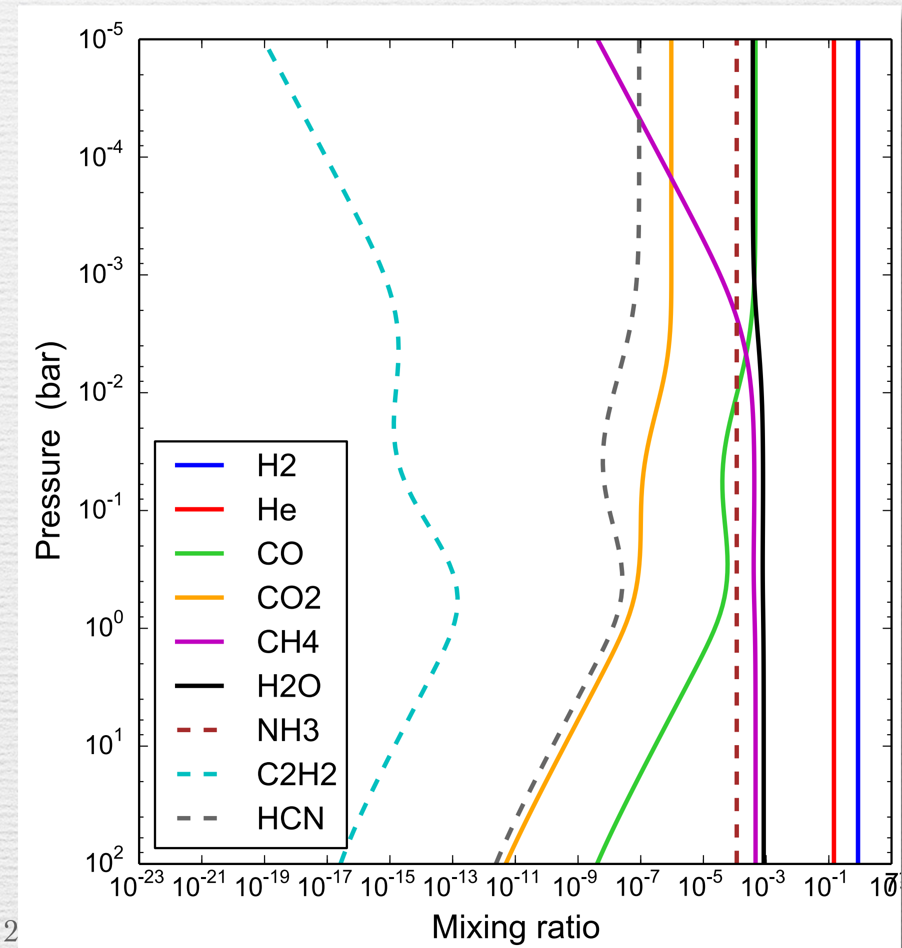
Thermochemical-Equilibrium Abundance (TEA) code: (Blecic et al. 2015a)

- Calculate species abundances (for given *T*, *p*).
- Python open-source code:

github.com/dzesmin/TEA

- Gibbs free energy minimization:





Radiative Transfer:

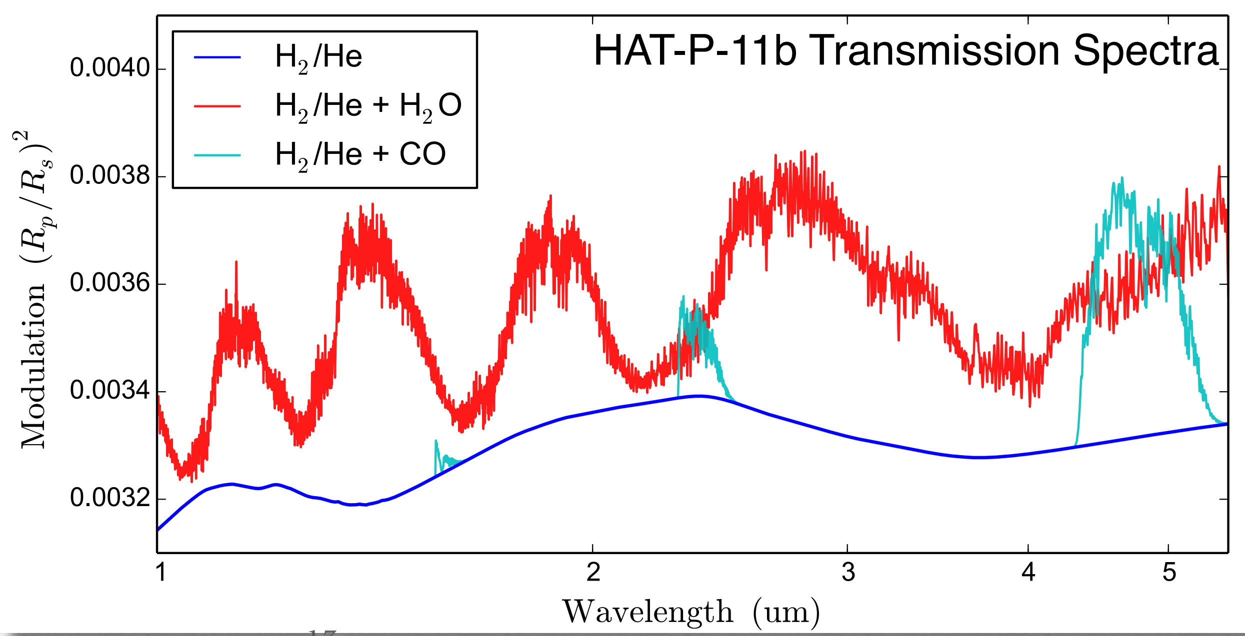
Opacity databases:

- Collision-induced absorption (CIA, Borysow et al., Richard et al. 2012):
  - Smooth variation.
  - Main species: H_2, He.

- Quantum electronic, rotational, vibrational transitions (Rothman et al. 2010, 2013):
  - Discrete lines/bands.
  - Main species:

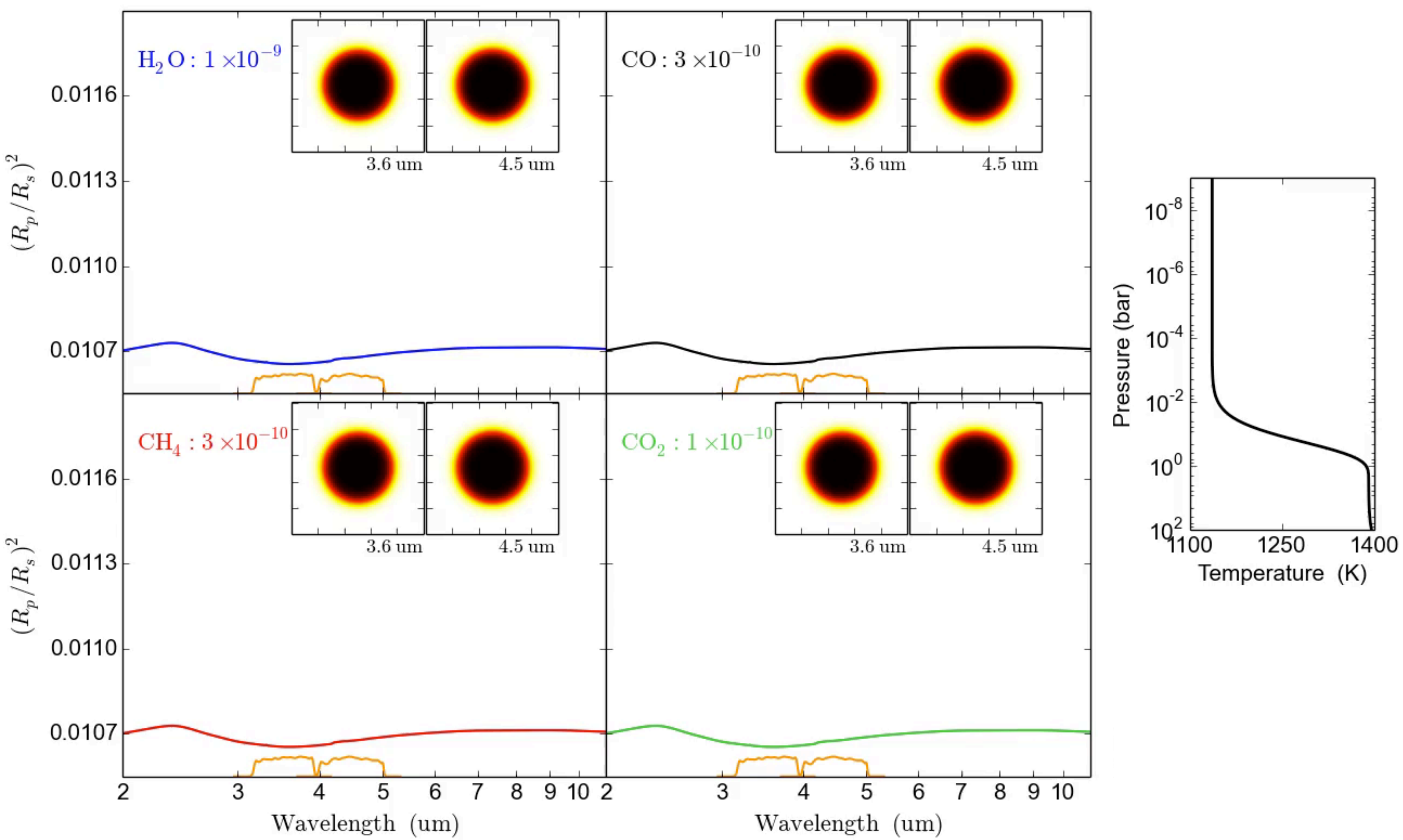
    H_2O, CH_4, CO, CO_2,

    NH_3, C_2H_2, C_2H_4, ...



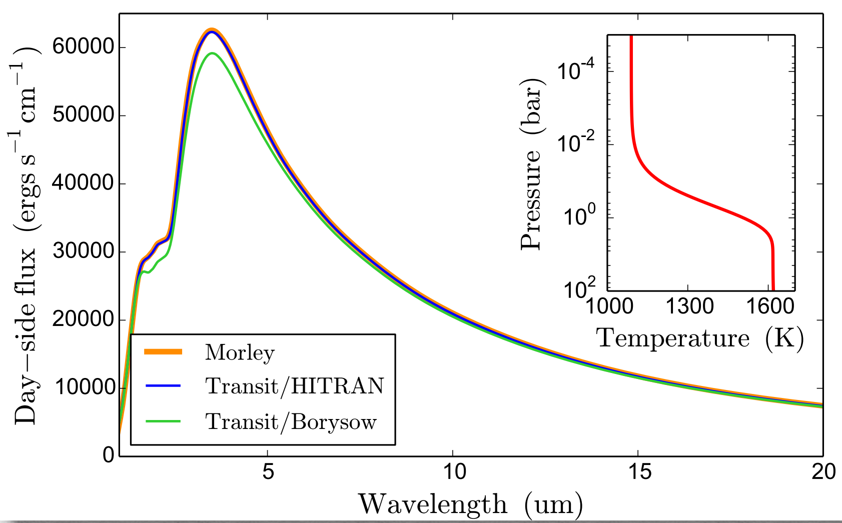
Radiative Transfer:

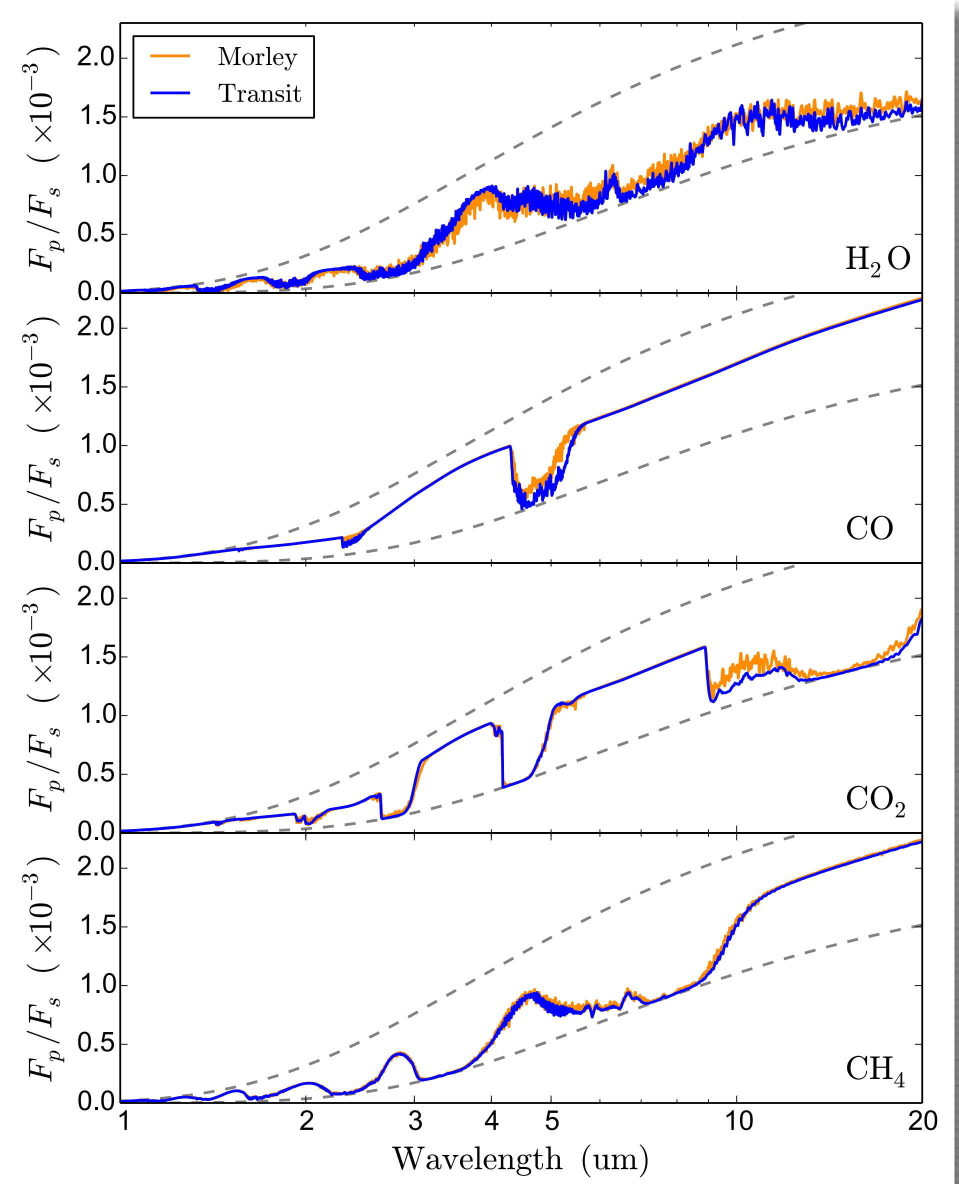
Transmission spectra:



Radiative Transfer: Validation

Our models agree to a few percent with those of C. Morley (in prep.).





Statistical Package:

Multi-Core Markov-chain Monte Carlo (MC³): (Cubillos et al. 2015a, in prep.)

- **General** package for model-parameter estimation**.**
- Single/Parallel processor (MPI).
- Python/C open-source project:

  github.com/pcubillos/mccubed

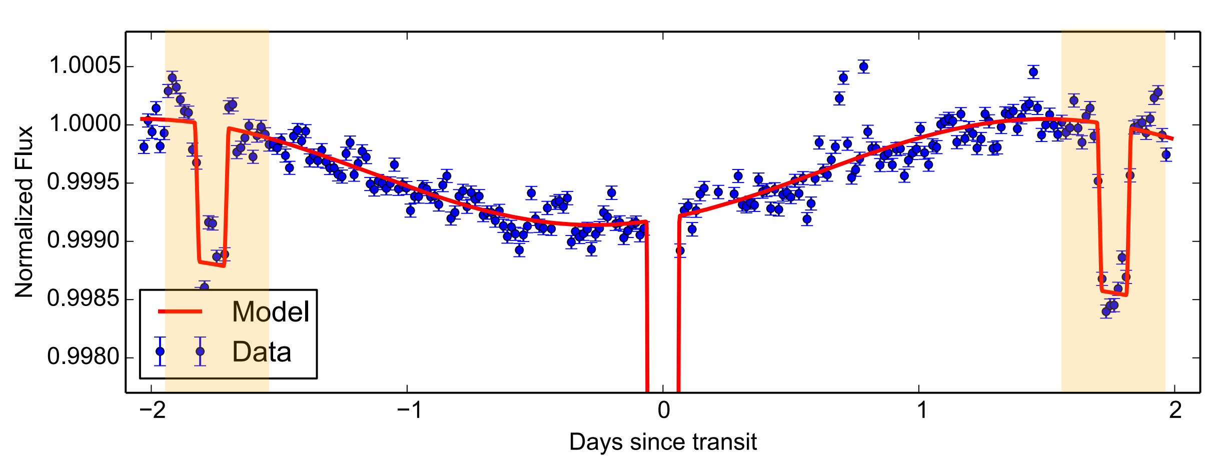
- Differential-Evolution MCMC (Braak 2006)**.**
- Gelman-Rubin MCMC convergence (Gelman & Rubin 1992)**.**

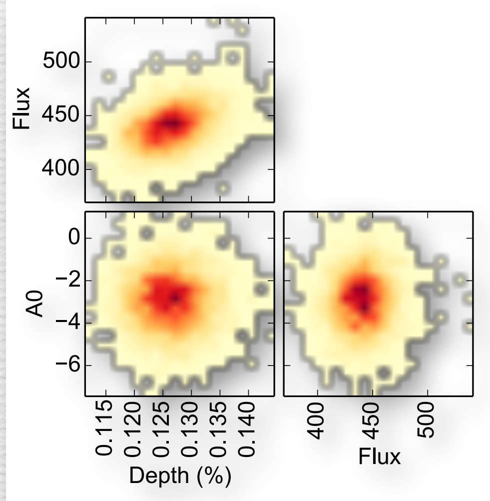
Statistical Package:

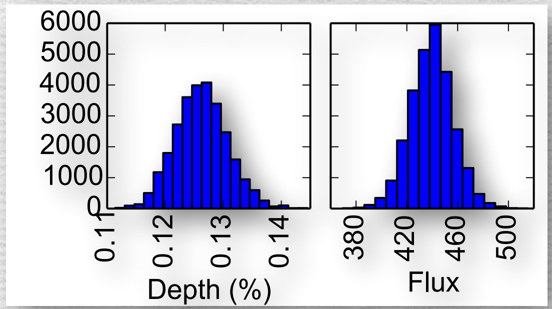
Multi-Core Markov-chain Monte Carlo (MC³): (Cubillos et al. 2015a, in prep.)

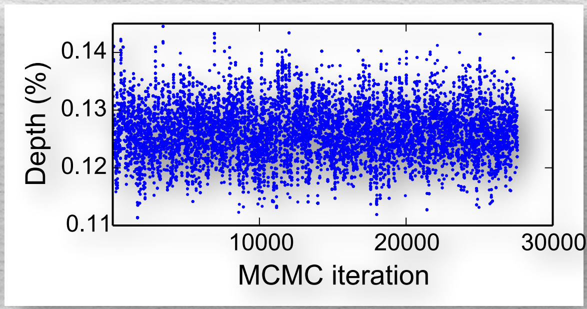
github.com/pcubillos/mccubed

HD 209458b Spitzer 4.5 um phase curve:









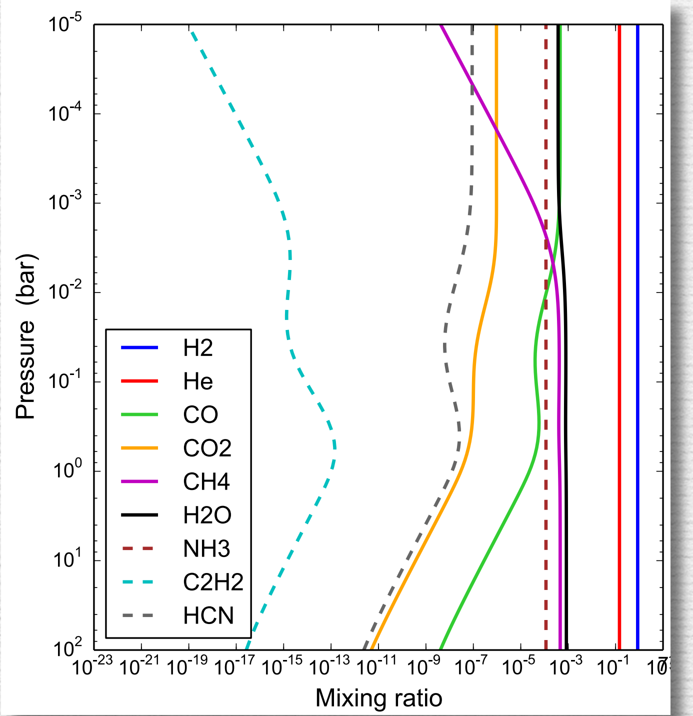
Bayesian Atmospheric Radiative Transfer (BART):

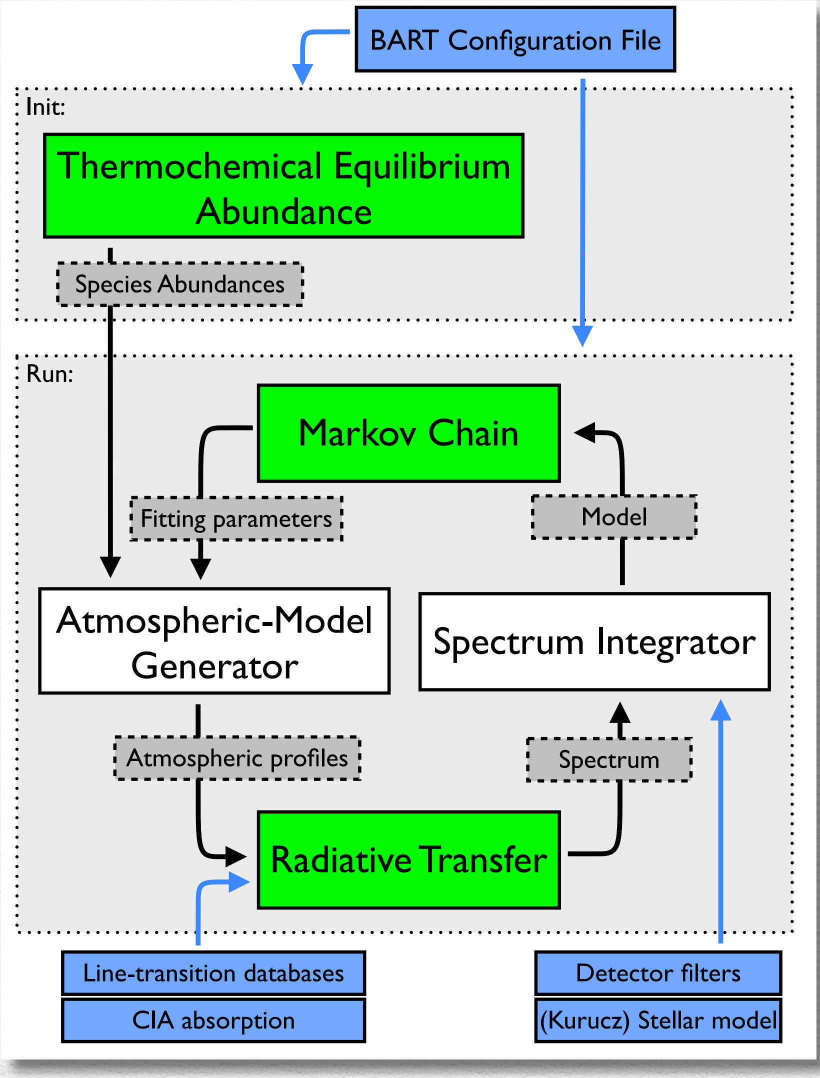
Free parameters:

- $T(p)$ parameters (3–5 parameters).
- Abundance parameters for each species:

  $\log(f_{H2O})$, $\log(f_{CH4})$, ...
- Radius-pressure reference point:

  $\mathrm{rad}_0 = \mathrm{rad}(p_0)$





HAT-P-11b: Transit Observations

Neptune-like planet:

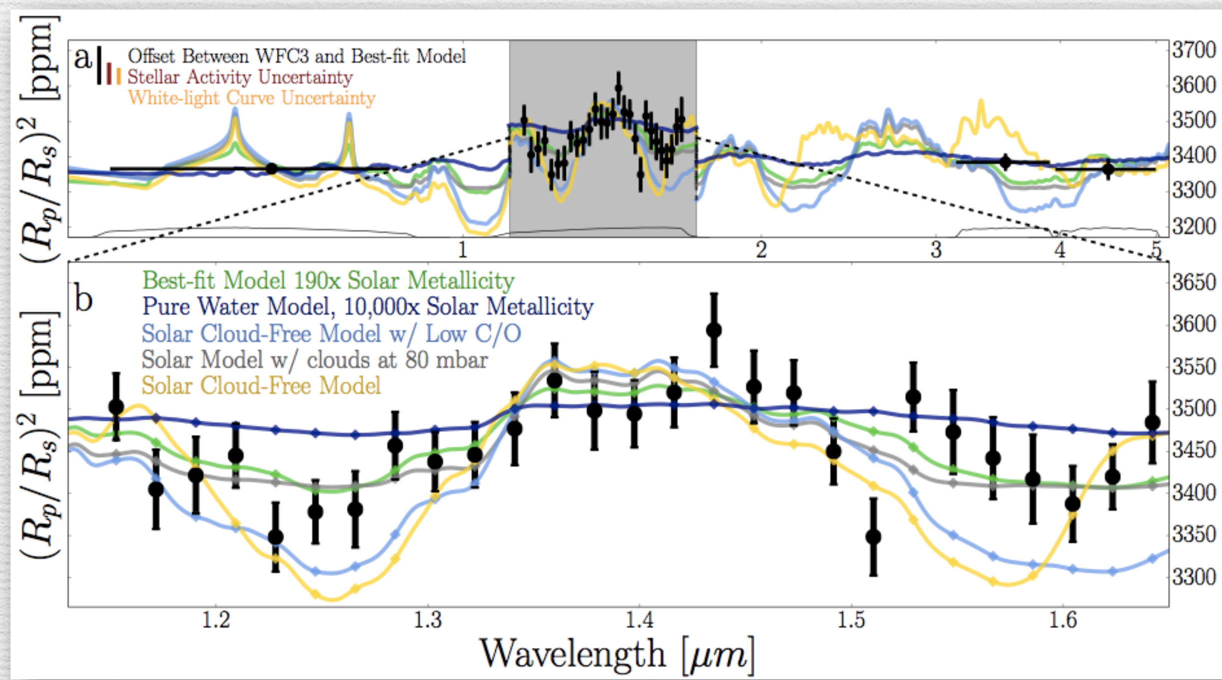
- 26 M_{Earth}, 4.7 R_{Earth}.
- 900 K equilibrium temperature.
- 5-day orbit period.

(Bakos et al. 2010)

Transit observations:

- Kepler 0.64 um.
- Hubble's WCF3 1.1–1.7 um.
- Spitzer 3.6 & 4.5 um.

(Fraine et al. 2014)



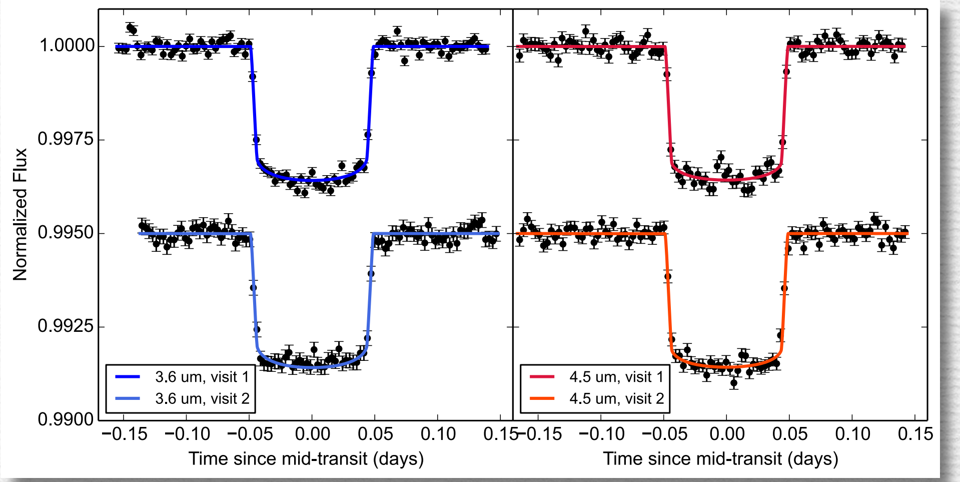
Atmospheric characterization with the SCARLET code:

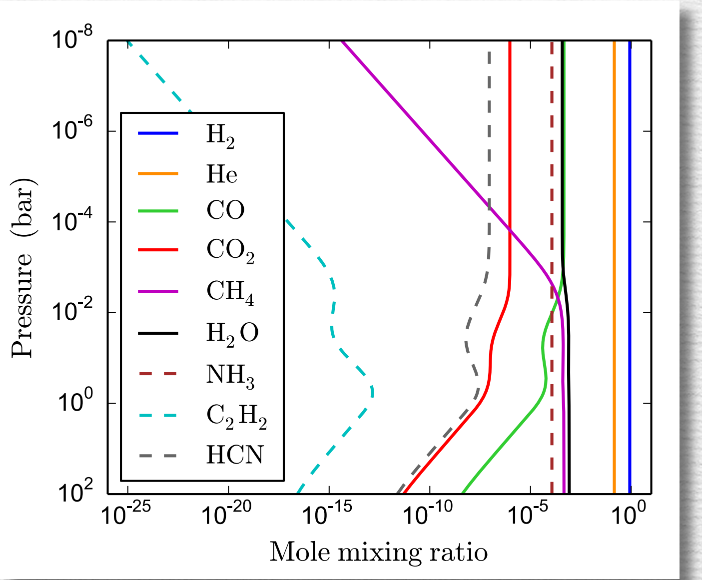
Benneke et al.

HAT-P-11b: Transit Observations

Re-analyze Spitzer 3.6 and 4.5 um data:

Wavelength (um)	Transit depth	R_p/R_s
3.6	0.00335 ± 0.00002	0.05791 ± 0.00022
4.5	0.00338 ± 0.00003	0.05816 ± 0.00025





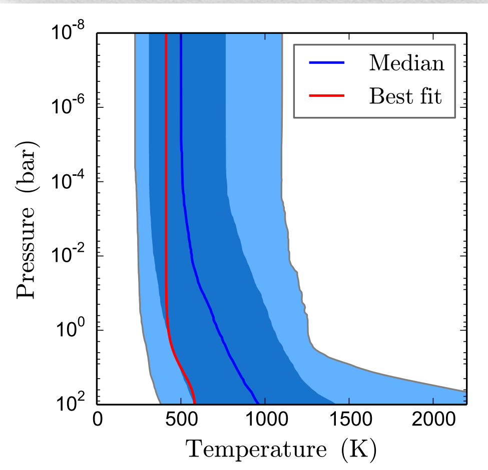
BART fitting parameters:

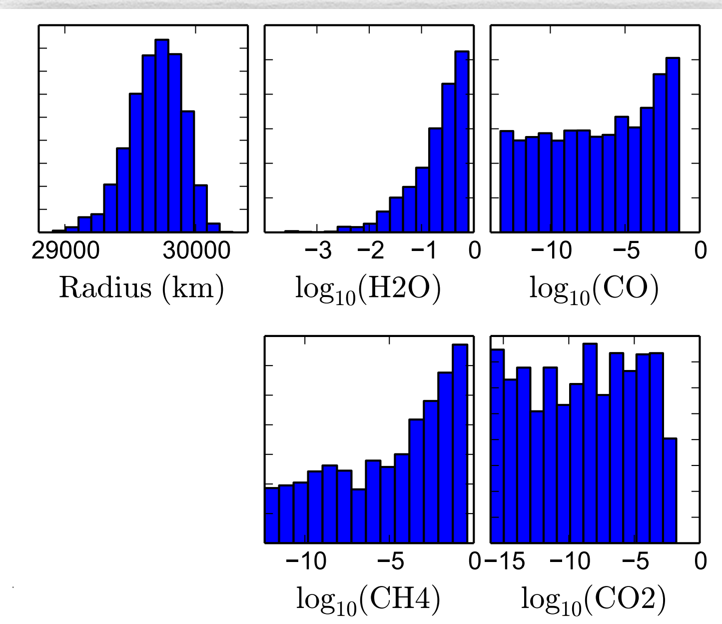
- H_2O, CH_4, CO, and CO_2 abundances **(4)**.
- Temperature-profile params **(3)**.
- Altitude at 0.1 bar **(1)**.

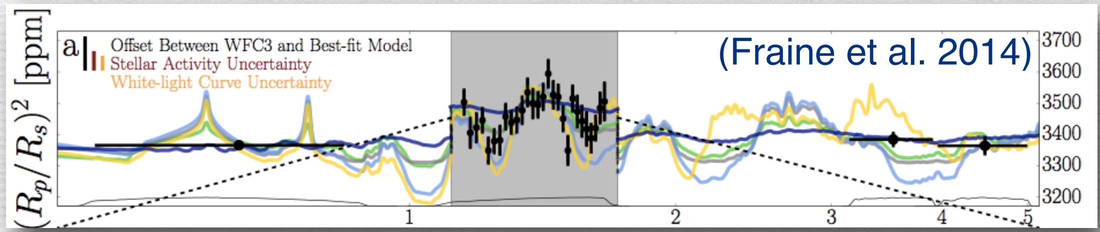
Started from equilibrium abundances.

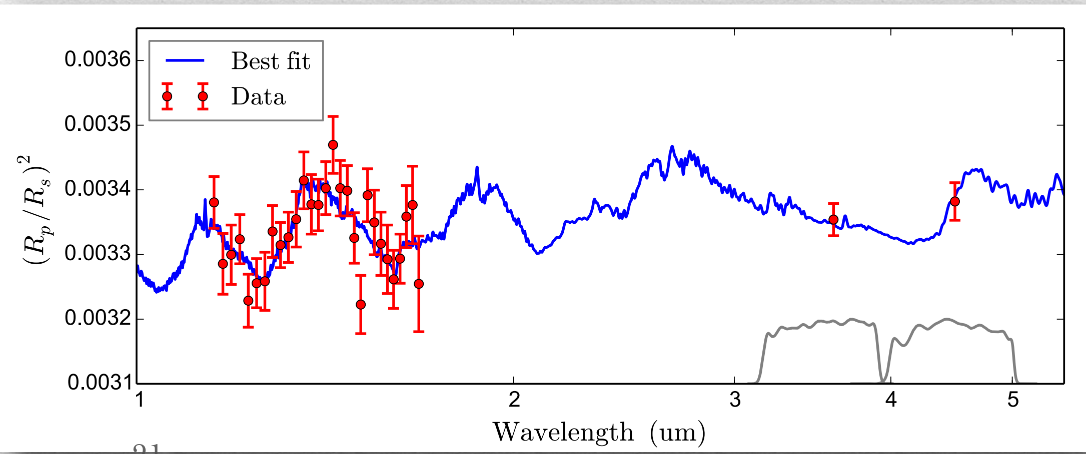
HAT-P-11b: Results

- Constrained the 0.1-bar radius to: 29,750 ± 200 km.
- Determined ~100 x super-solar abundance of H_2O.
- CH_4, CO, CO_2 remained unconstrained.









Replicate the work of Fraine et al. (2014).

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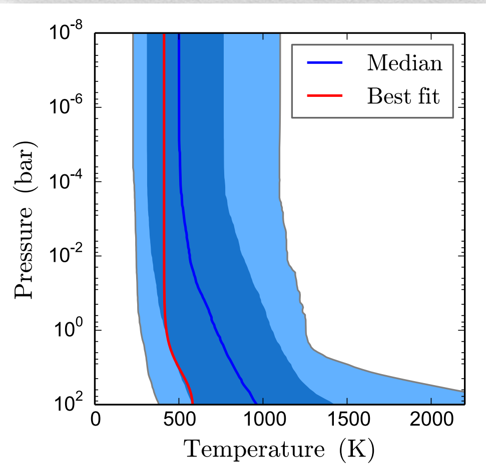

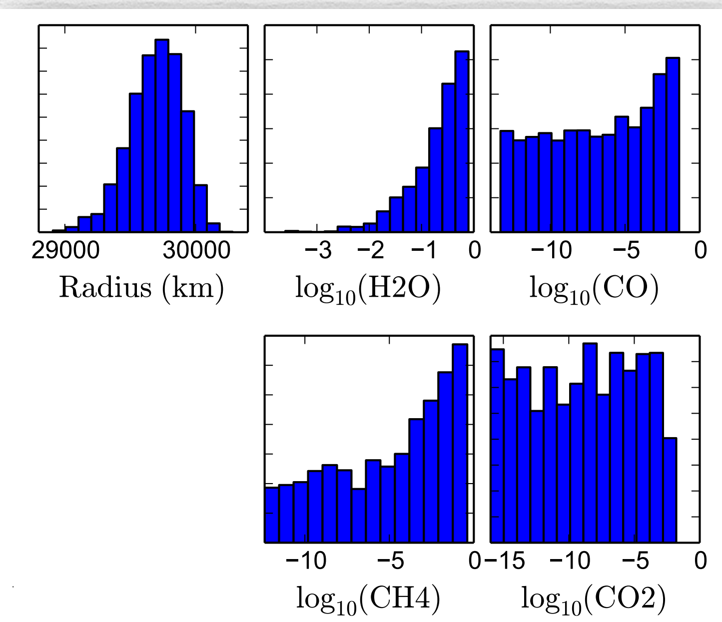

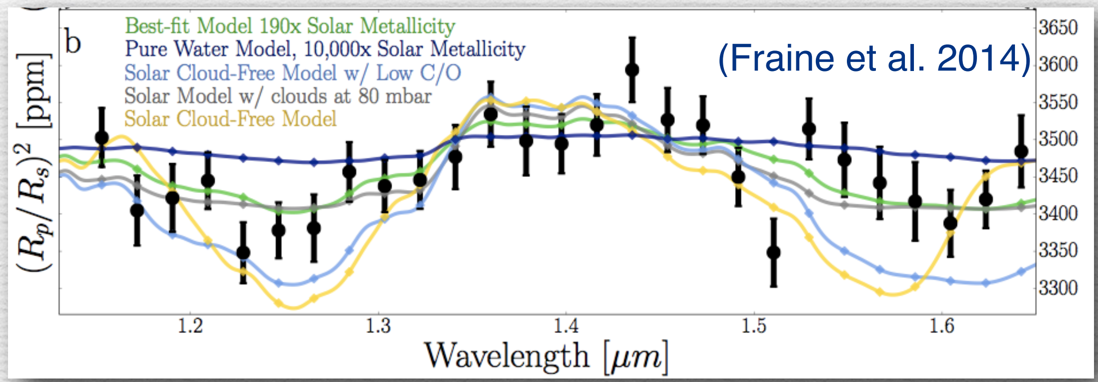

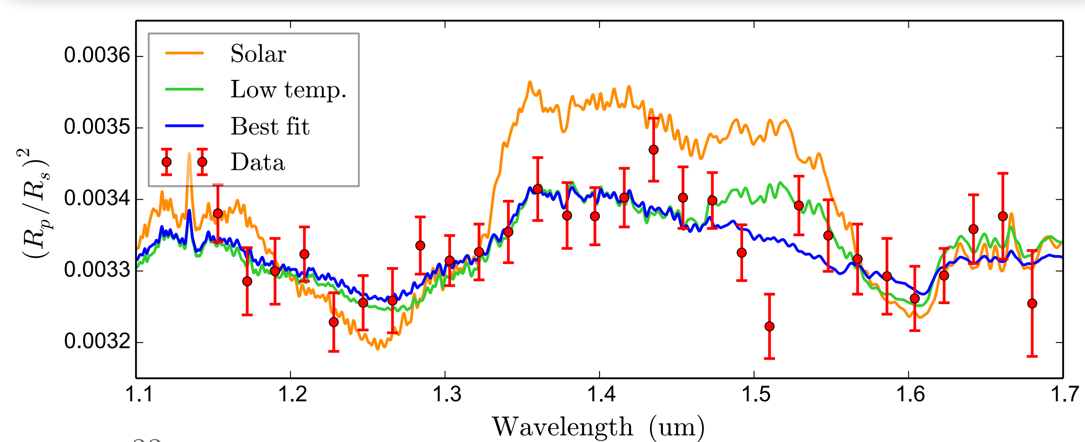

Replicate the work of Fraine et al. (2014).

Conclusions:

- Models can be as complex as the data allow.
- Current exoplanet data is limited in wavelength coverage, wavelength resolution.

Tools for exoplanet characterization:

- We developed an open-source, statistically-robust code to model exoplanet spectra and characterize planetary atmospheres.
- The retrieval analysis has been validated and can reproduce previous results on Neptune planet HAT-P-11b.

github.com/exosports/BART

github.com/pcubillos/MCcubed

github.com/exosports/transit

github.com/dzesmin/TEA

Future development:

- Add Haze/Clouds and Rayleigh models.
- Add chemical disequilibrium: photo-chemistry, vertical mixing.
- Future instrument simulations: JWST & ELTs.