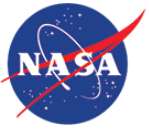

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Cerberus

Overview of the atmospheric retrieval and its application to the Excalibur datasets

Background image credit: Rowan Swain

Parameter retrieval

A step towards data interpretation / A few words of caution

- This excalibur module is not meant to fully automate the atmospheric interpretation
  - Its purpose is to provide guidance towards the latter
- Recovered values will never be: 'Le Truth'
  - If one seeks the absolute 'Truth', Science is not the discipline in the first place. We make assumptions where there is label that says 'unknown', we build on previous work. Similarly to an asymptotic behavior, we are progressing towards it with infinite steps.
  - Acknowledging assumptions or limitations inherent to the mathematical formulation of Nature or the ones pertaining to data quality is a step towards the 'Truth'. Ignoring or denying them is certainly not approaching it.

Cerberus

Overview

- Forward Models:

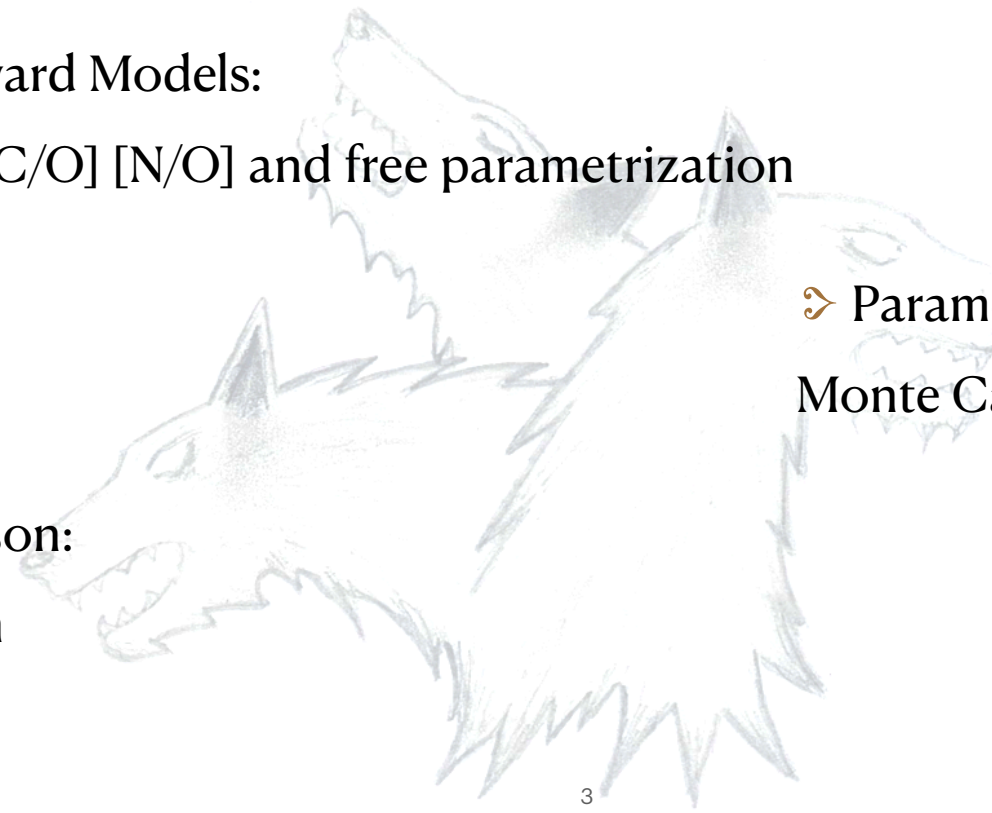
  [X/H] [C/O] [N/O] and free parametrization

- Parameter constraints:

  Monte Carlo Markov Chain sampling

- Model Comparison:

  Bayesian formalism



Cerberus

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(tough to forget assumptions, there s always a term that is a nightmare to evaluate)

Model Comparison

Just apply a formula?

- Whether you are computing a $\chi 2$ or an evidence, the main question is:
  - How do I compare models as fairly as possible?

- Usual ingredients:
  - Residuals between data and model ✓
  - Noise (data uncertainty) normalization ✓
  - Penalty taking into account the model's degree of freedom ✗

Example of the problematic

Fiction, any resemblance with reality is unfortunate.

A ~~friend~~ acquaintance, ~~theorist~~ scientist who thinks that calling himself a theorist (without any knowledge of what theory is) sounds cool:

J

Or alternatively, picture someone you know that matches the description:

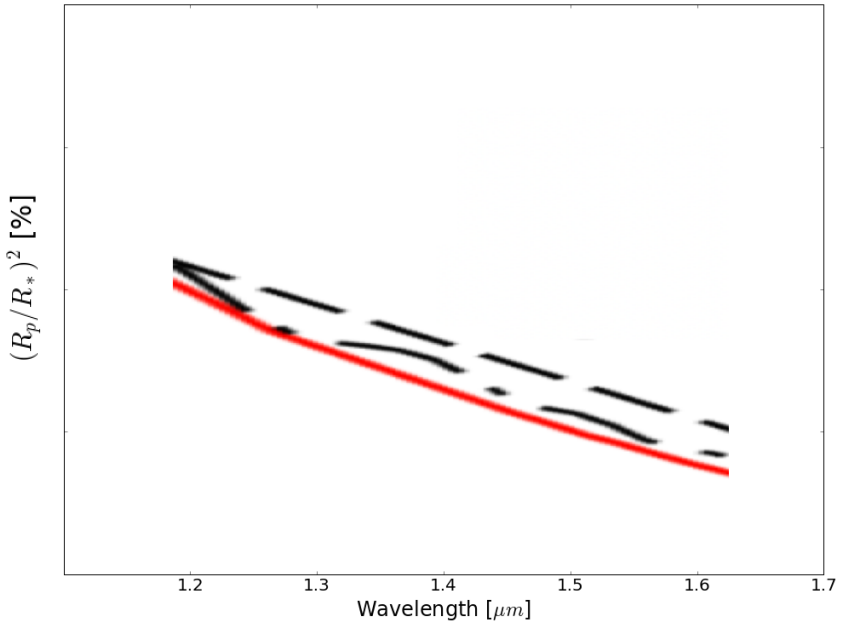
Example of the problematic

J's favorite sample model (wiggling dash dotted line)

- Haze particle size distribution
  - > 2
- T-matrix code
  - > 2
- Haze particle density profile
  - ~ 100

- Number of parameters: ~500

A single set of parameters, 4 nodes of 128 CPU cores and 12 hours later



Example of the problematic

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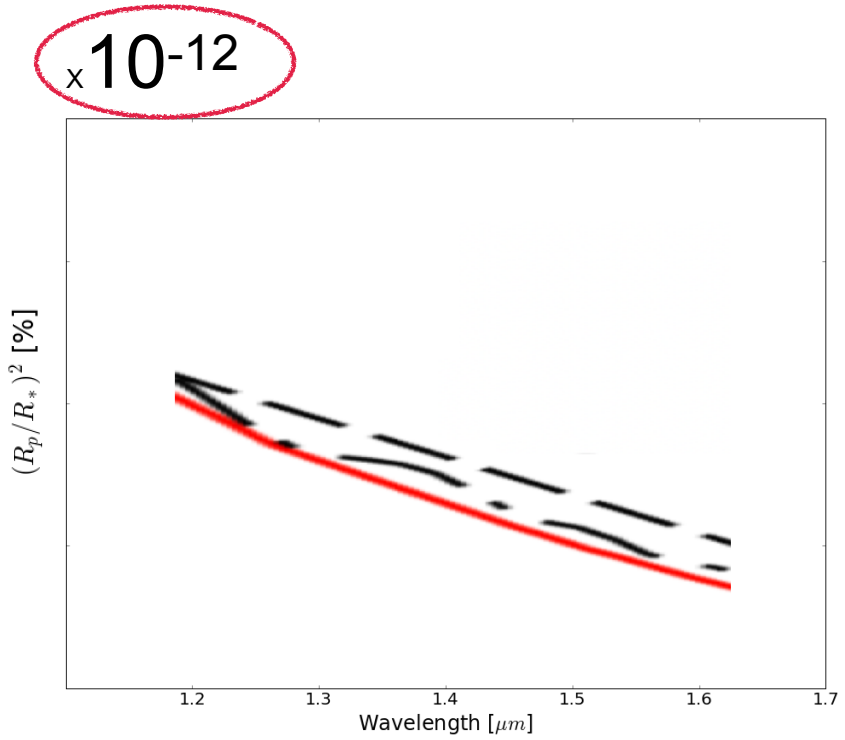
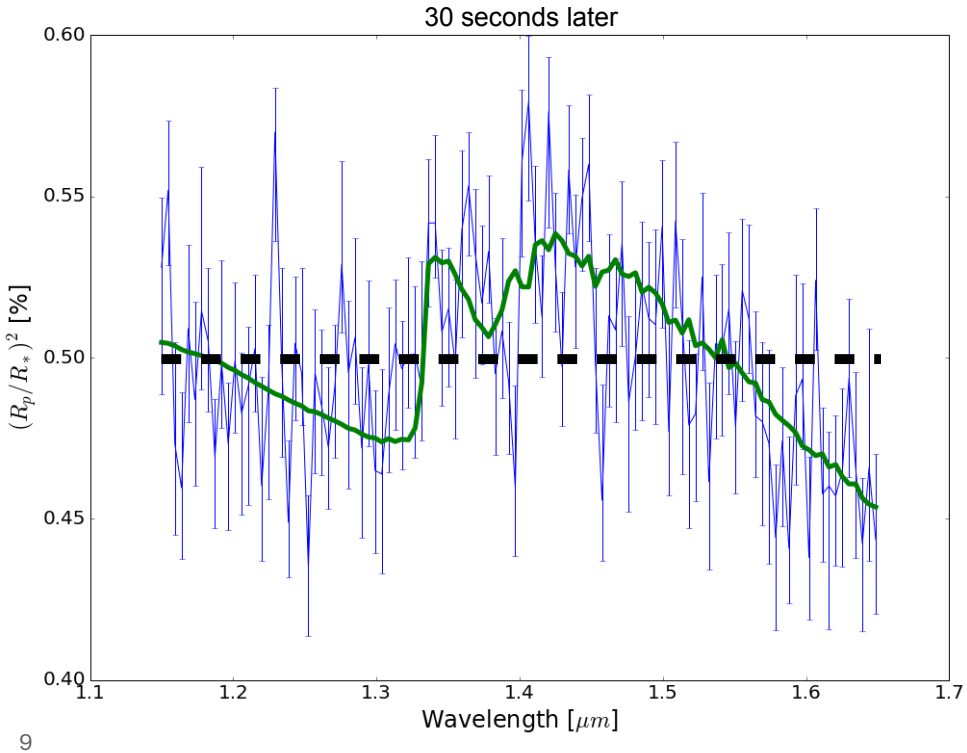


Example of the problematic

J's favorite effective model (another formulation)

- d/dλ (J's model) = 0
- Number of parameters: 1



Model Comparison

DoF of J's model?

- Haze particle size distribution
  - > 2
- T-matrix code
  - > 2
- Haze particle density profile
  - ~ 100

- Number of parameters: ~500

$d/d\lambda$ (J's model) = 0

Number of parameters: 1

Model Comparison

A few concluding points

- Exoplanet models we use against data have complexity (number of effective degrees of freedom) changing as we sample the parameter space
- One can use an equivalent of the local Fisher matrix to proper balance model comparison

- For J or anyone tempted to go that way: number of parameters > number data points is not very serious
- Data quality should guide setting appropriate priors, but also building **reasonable parametrized forward models**

Cerberus

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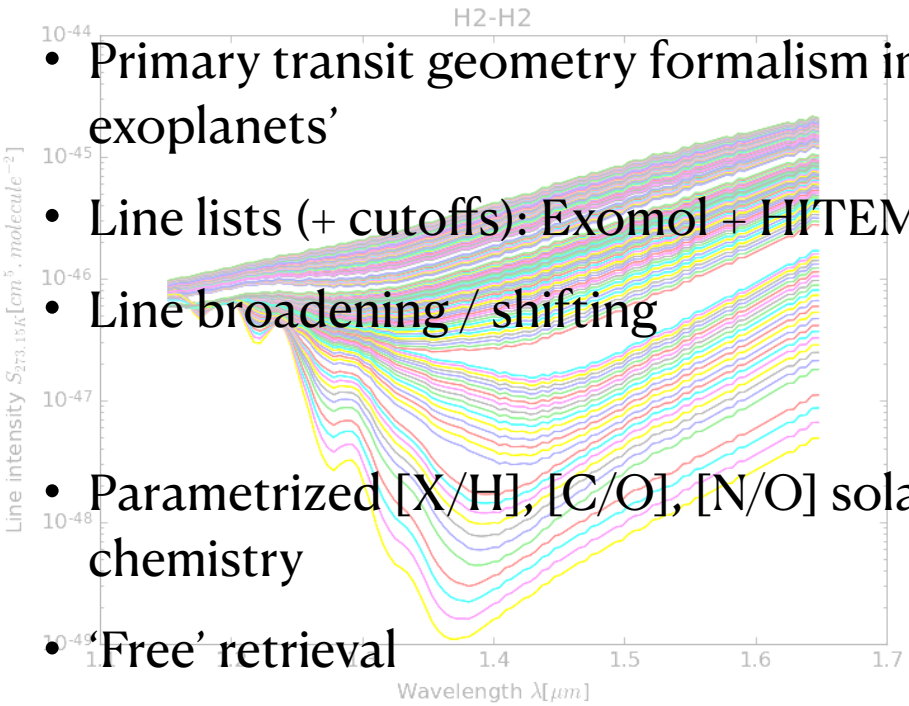
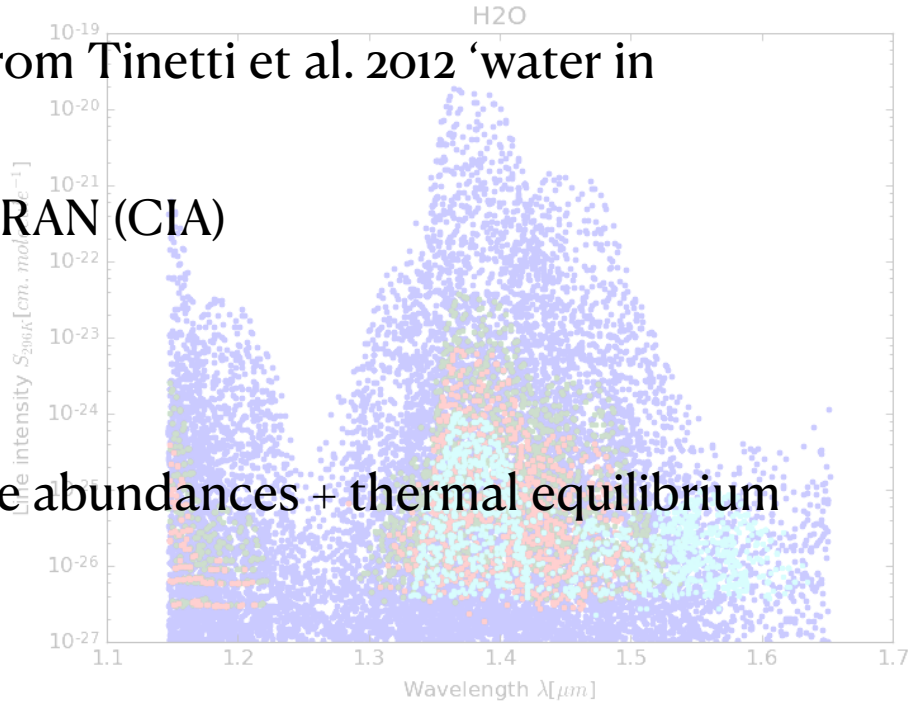
Forward models

HST/G141





- Primary transit geometry formalism inherits from Tinetti et al. 2012 ‘water in exoplanets’
- Line lists (+ cutoffs): Exomol + HITEMP + HITRAN (CIA)
- Line broadening / shifting
- Parametrized [X/H], [C/O], [N/O] solar relative abundances + thermal equilibrium chemistry
- ‘Free’ retrieval

Initial study questions

HST/G141

- How does the atmospheric interpretation react to uniformly reduced datasets?
- If we stray away from the usual super hot Jupiter assumptions on chemistry, which should break for a large fraction of the targets already observed by HST, where do we end?
- Is there any hint of departures from the typical water or nothing spectrum in those data?

Forward models

From HST to ARIEL/CASE

- While HST has set up extraordinary and unexpected grounds for exoplanet atmosphere characterization
  - Basic modeling has to grow (wider range of wavelength, probability of more than one or two absorbing species showing up —> tie everything up with appropriated chemistry)
  - More detailed modeling (T-P profile interaction with gas chemistry and condensate formation)
  - Keep an open but cautious mind, there is a balance to find between what the data are telling you and what you would like them to tell you
- Retrieval speed...

Cerberus

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Monte Carlo Markov Chains

About Metropolis Hasting (MH) sampling

- MH is slow but safe
- MH will not hide multimodal marginalized posteriors

- Nested sampling is way less time consuming than MH because it was successfully built for this very purpose, it comes at a price
- Nested sampling is a very efficient and reliable tool, **as long as their user know what they re doing:**

Monte Carlo Markov Chains

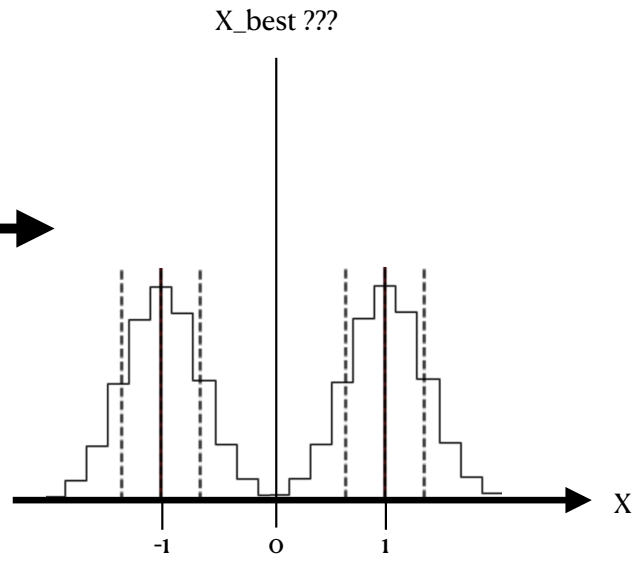
Nested sampling

- Nested sampling is a very efficient and reliable tool, **as long as their user know what they re doing:**
  - Do you know the behavior of your model and did you pass it to your nested sampler so that he can build a proper hierarchy of nests?
  - If you find out that a nested sampler and a MH sampler don't give you the same answer, there is a problem, and the problem is not the type of sampler, it is your understanding of the tool you used
  - Nested sampler do not give better posteriors / correlation plots because they look like wikipedia 2D Gaussian distribution. They give what you voluntarily or not assume when pressing the button. Not knowing what the blackbox does if a crucial info is missing, (like the covariance matrix of your model for nested samplers) might give you nice looking plots, but that s the full extent of your result

Monte Carlo Markov Chains

Multimodal marginalized PDF

- Underlying physics: x^2
- Data = 1 +/- some gaussian random noise
- J is applying what he learned about MCMC:
  - x_best = median(sample values)



Monte Carlo Markov Chains

Multimodal marginalized PDF

- More than often, if your sampler hasn't completely distorted your solution space without you knowing it, you ll end up with multiple solutions competing one with another
- In Cerberus the parameter recovery is subdivided into multiple steps, one is dedicated to separate modes and compare their evidence

- It is not wise to quote the median value of your samples as the most likely estimate without understanding your marginalized PDF

Concluding remarks

Preparing for ARIEL/CASE

- HST/G141 sample of ~60 targets was a start but we will ingest thousands of targets for CASE
- Challenges for Cerberus are
  - CPU time
  - Forward modeling: TP profile, gas + condensate chemistry as a full package
  - Exploring solutions for planetary systems that have widely different physical properties