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taurex-emcee: a TauREx 3.1 plugin for the emcee sampler

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Summary

taurex-emcee is a plugin for the TauREx 3.1 atmospheric retrieval framework (A. F. Al-Refaie et al., 2021) that extends the choice of sampling methods available to the user. The plugin provides an interface to the emcee sampler (Foreman-Mackey et al., 2013), a popular affine-invariant ensemble sampler widely used in the astronomy community. Running the sampler to convergence is automated through the autoemcee package, which also supports parallelization with MPI. Thus, the taurex-emcee plugin allows users to easily launch parallelized retrievals of atmospheric spectra with emcee. This enables reliable, efficient, and fast retrievals, especially when coupled with TauREx's GPU-accelerated forward models (A. Al-Refaie et al., 2020).

taurex-emcee is released under the BSD 3-Clause license and is available on GitHub. The plugin can be installed from the source code or from PyPI, so it can be installed as `pip install taurex-emcee`. The documentation is available on readthedocs, including a quick-start guide, a tutorial, a description of the software functionalities, and guidelines for developers. The documentation is continuously updated and is versioned to match the software releases.

Benchmark

We benchmarked the taurex-emcee plugin against the MultiNest sampler (F. Feroz et al., 2009; Farhan Feroz et al., 2019), natively implemented in TauREx 3, on a synthetic transmission spectrum of the hot Jupiter HD 209458b. The aim being first to assess the computational time of the two samplers on a controlled case, second to assess the consistency of the results from the retrievals. The synthetic spectrum and the retrievals were performed on a single node of the Sapienza University of Rome Melodie server, equipped with one NVIDIA A40 GPU. The high-resolution forward spectrum was generated assuming stellar and planetary parameters of HD 209458b from Edwards et al. (2019), reported in Table 1, and a gaseous atmosphere with hydrogen and helium at a ratio $H_2/He = 0.172$ and an isothermal temperature profile.

Table 1: Summary of the selected target's properties

R_p [R_J]	M_p [M_J]	T_p [K]	P [d]	R_s [$R_\odot$]	Mag K	T_s [K]	M_s [$M_\odot$]
1.35	0.71	1613	3.52	1.18	6.31	6,086	1.18

The atmosphere is simulated with five molecular species as trace gases: H_2O (100 ppm),

CH_4 (10 ppm), CO (1 ppm), CO_2 (0.1 ppm), and NH_3 (0.01 ppm). Molecular abundances are assumed constant with altitude. Cross sections at a resolution of 15,000 are used for all species, as given in Table 2. Collision-induced absorption (CIA) with H_2–H_2 and H_2–He and Rayleigh scattering are included in the calculation. We also include grey opaque clouds with a cloud-top pressure of 1000 Pa. Finally, 100 pressure layers are used to sample the atmosphere, from 1 Pa to 10^6 Pa, uniformly in log-space.

Table 2: Cross sections and CIA used in the simulations

Opacity	Reference(s)
H_2-H_2	Abel et al. (2011), Fletcher et al. (2018)
H_2-He	Abel et al. (2012)
H_2O	Polyansky et al. (2018)
NH_3	Coles et al. (2019)
CO	Li et al. (2015)
CO_2	Rothman et al. (2010)
CH_4	Yurchenko et al. (2017)

To simulate the observation of the transmission spectrum, we assume an observation by the `Ariel` space mission (Tinetti et al., 2021, 2018) in Tier 2 mode (Edwards et al., 2019). We utilize radiometric estimates of the total noise on one observation of HD 209458b obtained with `ArielRad` (Mugnai et al., 2020), the `Ariel` radiometric simulator now available at the online exodb.space website. `ArielRad` is based on the generic point source radiometric model `ExoRad2` (Mugnai et al., 2023), adapted with the `Ariel` payload configuration. The software versions used are: `ExoRad2` v2.1.113, `ArielRad-payloads` v0.0.17, and `ArielRad` v2.4.26.

In our retrieval benchmarks, we attempt to constrain the abundances of the trace gases, alongside the temperature profile, the planetary radius, and the cloud-top pressure. We perform five retrievals each with `MultiNest` and `emcee`, with increasing number of molecules included in the free parameters (the other molecules being fixed to their true values), from only H_2O to all five trace gases.

MultiNest config, emcee config…

As a first comparison, we report in Table 3 the computational time of the retrievals with the two samplers.

Table 3: Runtime of the retrievals with `emcee` and `MultiNest` samplers.

Fitted molecules	Emcee [s]	MultiNest [s]
H_2O	16,465	5,423
H_2O, CH_4	6,550	7,505
H_2O, CH_4, CO	15,247	10,093
H_2O, CH_4, CO, CO_2	14,930	12,847
H_2O, CH_4, CO, CO_2, NH_3	30,151	17,097

Figures can be included like this:

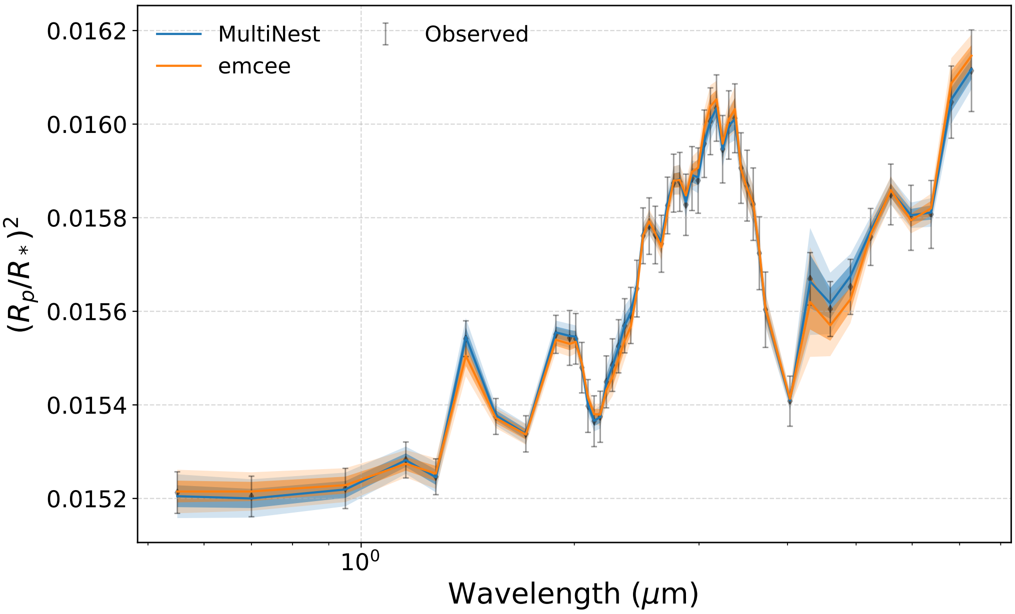

Figure 1: Caption for spectrum figure.

and referenced from text using Figure 1.

Figure sizes can be customized by adding an optional second parameter:

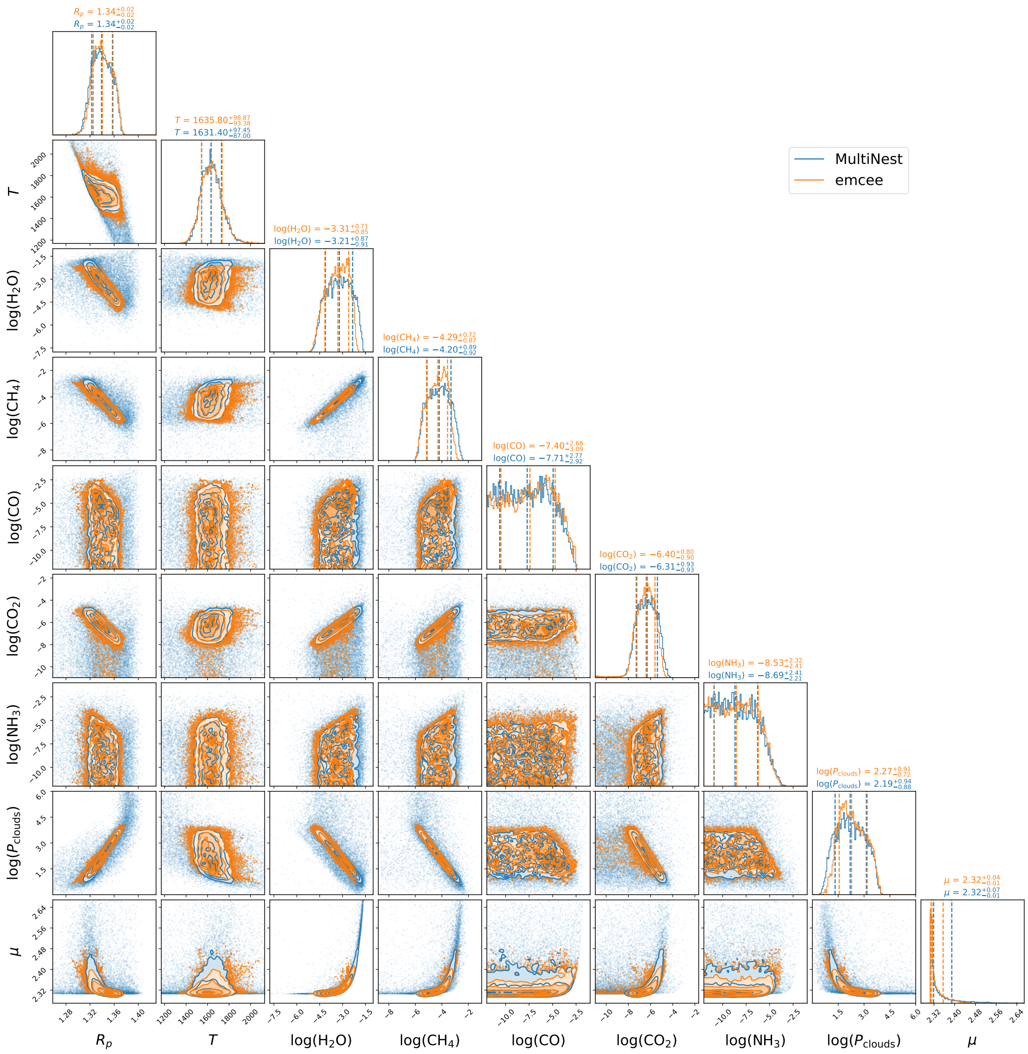

Figure 2: Caption for posteriors figure.

and referenced from text using Figure 2.

Statement of need

Optimized sampling methods are a key component of any retrieval code. Nested samplers (F. Feroz et al., 2009; Farhan Feroz et al., 2019) are a powerful and robust sampling method, successfully applied to the retrieval of exoplanet atmospheric spectra (Barstow et al., 2020; Bocchieri et al., 2023; Changeat et al., 2020). TauREx 3.1 natively implements a suite of nested samplers, including the MultiNest sampler, or makes them available as plugins, such as the UltraNest sampler. The primary target of nested samplers is the efficient calculation of the Bayesian `evidence`, whilst the inference of the `posterior` is a by-product. This is regarded as a key advantage of nested samplers, as the `evidence` can be readily used for model selection. However, the `evidence` is not always required, and the interpretation of the `posterior` from nested samplers necessitates some care. Additionally, algorithmic assumptions of nested samplers may require to tailor the priors to explore the parameter space thoroughly.

Where the inference of the Bayesian `posterior` is the primary target, a well-established alternative to nested samplers are a family of Markov chain Monte Carlo methods known as affine-invariant ensemble samplers (Goodman & Weare, 2010). The implementation in emcee (Foreman-Mackey et al., 2013) is a popular choice in the astronomy community, as it takes care of the heavy lifting of the sampling process, is well documented, and is straightforward to utilize. To date, the `emcee` sampler is not natively implemented in the TauREx 3.1 retrieval framework, nor elsewhere in other retrieval codes, to the knowledge of the authors. To fill this gap, we developed the `taurex-emcee` plugin, which interfaces the `emcee` sampler to TauREx. Key advantages of `taurex-emcee` are that it affords a more straightforward interpretation of the `posterior` and is more robust to the choice of priors. However, the current implementation is not intended to explore multimodal `posteriors`, for which nested samplers will inevitably be more efficient. Moreover, we caveat that it may require substantial computational time to sample high-dimensional parameter spaces with `emcee`, which can be mitigated by coupling `taurex-emcee` with TauREx's GPU-accelerated forward models (A. Al-Refaie et al., 2020).

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