

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

Andrea Bocchieri  ¹, **Quentin Changeat**  ², **Lorenzo V. Mugnai**  ^{3,4,5}, and **Enzo Pascale**  ¹

1 Department of Physics, La Sapienza Università di Roma, Piazzale Aldo Moro 2, Roma, 00185, Italy **2** European Space Agency (ESA), ESA Office, Space Telescope Science Institute (STScI), Baltimore, MD, 21218, USA **3** School of Physics and Astronomy, Cardiff University, Queens Buildings, The Parade, Cardiff, CF24 3AA, UK **4** Department of Physics and Astronomy, University College London, Gower Street, London, WC1E 6BT, UK **5** INAF, Osservatorio Astronomico di Palermo, Piazza del Parlamento 1, Palermo, I-90134, Italy

DOI: N/A

Software

- [Review](#) 
- [Repository](#) 
- [Archive](#) 

Editor: [Open Journals](#) 

Reviewers:

- [@openjournals](#)

Submitted: 01 January 1970

Published: 01 January 1970

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

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 $\text{H}_2\text{-H}_2$ and $\text{H}_2\text{-He}$ 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)
$\text{H}_2\text{-H}_2$	Abel et al. (2011), Fletcher et al. (2018)
$\text{H}_2\text{-He}$	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 [exoddb.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. With MultiNest, we set the evidence tolerance to 0.5 and sample the parameter space through 1500 live points. With emcee, we utilize 100 walkers and run two independent chains, each to convergence, where we adopt the default convergence criteria of the [autoemcee](#) package, i.e. the Geweke convergence diagnostic ([Geweke, 1991](#)) is $z\text{-score} < 2.0$ and the Gelman-Rubin rank diagnostic ([Gelman & Rubin, 1992](#)) is $\hat{r} < 1.01$. When iterating the chains, we increase the number of steps by multiplying the number of steps of the previous iteration by a growth factor of 2, a parameter that we have added to the taurex-emcee plugin as the default value of 10 was too conservative for our tests. 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
$\text{H}_2\text{O}, \text{CH}_4$	6,550	7,505
$\text{H}_2\text{O}, \text{CH}_4, \text{CO}$	15,247	10,093
$\text{H}_2\text{O}, \text{CH}_4, \text{CO}, \text{CO}_2$	14,930	12,847
$\text{H}_2\text{O}, \text{CH}_4, \text{CO}, \text{CO}_2, \text{NH}_3$	30,151	17,097

MultiNest is faster than emcee for all the retrievals bar the one with H_2O and CH_4 , where the computational time is around 15 minutes longer. Additionally, runtimes with MultiNest scale slower with the increase in dimensionality of the parameter space. Finally, the first retrieval

with emcee is slower than the second as the chains may require more iterations to converge based on the realization of the random walkers.

Figures can be included like this:

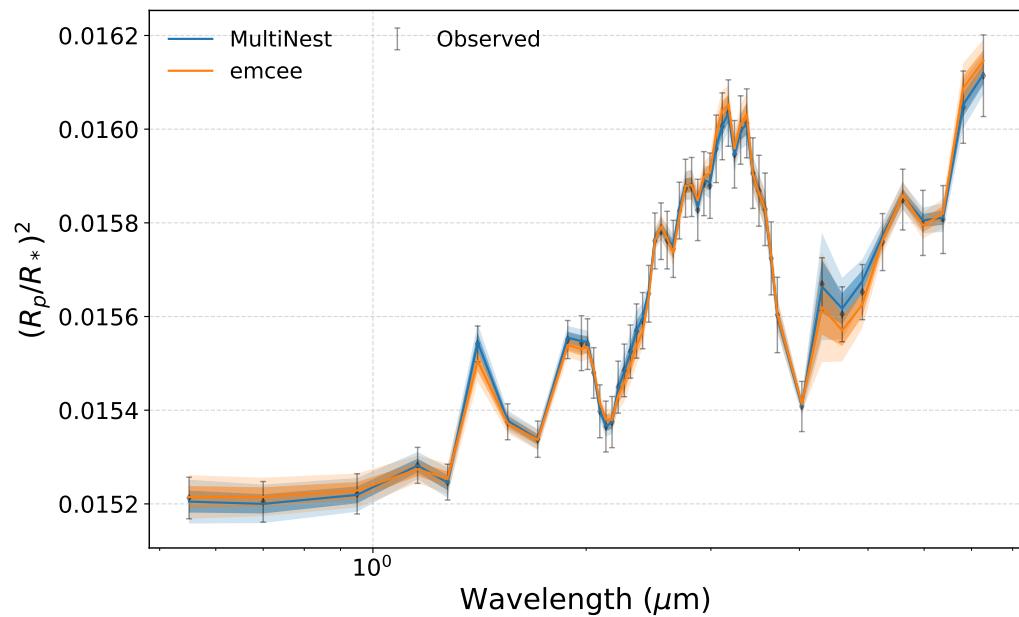


Figure 1: Caption for spectrum figure.

and referenced from text using [Figure 1](#).

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

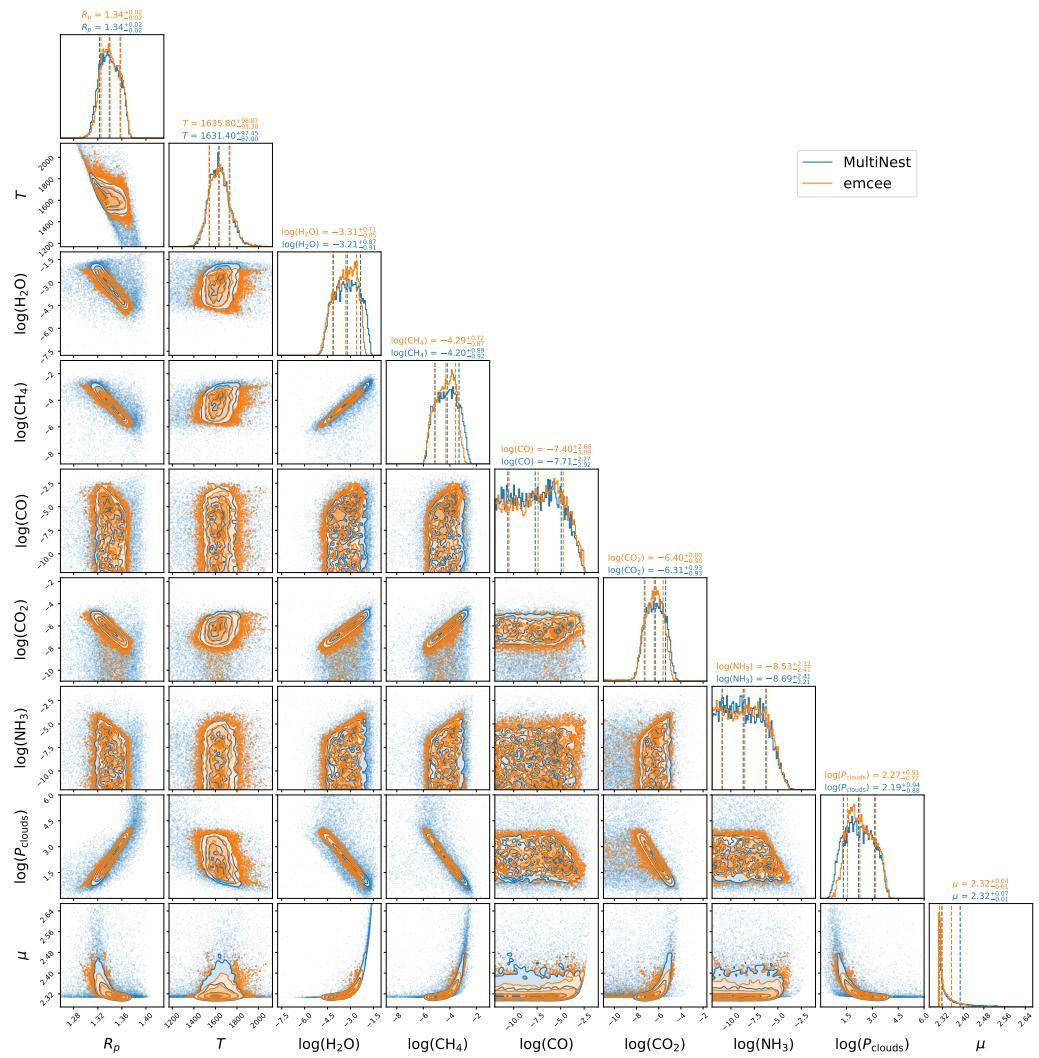


Figure 2: Caption for posteriors figure.

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).

Acknowledgements

This work was supported by the Italian Space Agency (ASI) with Ariel grant n. 2021.5.HH.0.

References

- Abel, M., Frommhold, L., Li, X., & Hunt, K. L. C. (2011). Collision-induced absorption by H₂ pairs: From hundreds to thousands of kelvin. *The Journal of Physical Chemistry A*, 115(25), 6805–6812. <https://doi.org/10.1021/jp109441f>
- Abel, M., Frommhold, L., Li, X., & Hunt, K. L. C. (2012). Infrared absorption by collisional H₂-He complexes at temperatures up to 9000 k and frequencies from 0 to 20,000 cm⁻¹. *The Journal of Chemical Physics*, 136(4), 044319. <https://doi.org/10.1063/1.3676405>
- Al-Refaie, A. F., Changeat, Q., Waldmann, I. P., & al., et. (2021). TauREx 3: A Fast, Dynamic, and Extendable Framework for Retrievals. 917(1), 37. <https://doi.org/10.3847/1538-4357/ac0252>
- Al-Refaie, A., Changeat, Q., Venot, O., & al., et. (2020). TauREx 3.1 - Extending atmospheric retrieval with plugins. *European Planetary Science Congress*, EPSC2020–669. <https://doi.org/10.5194/epsc2020-669>
- Barstow, J. K., Changeat, Q., Garland, R., & al., et. (2020). A comparison of exoplanet spectroscopic retrieval tools. 493(4), 4884–4909. <https://doi.org/10.1093/mnras/staa548>
- Bocchieri, A., Mugnai, L. V., Pascale, E., & al., et. (2023). Detecting molecules in Ariel low resolution transmission spectra. *Experimental Astronomy*, 56(2–3), 605–644. <https://doi.org/10.1007/s10686-023-09911-x>
- Changeat, Q., Al-Refaie, A., Mugnai, L. V., & al., et. (2020). Alfnoor: A Retrieval Simulation of the Ariel Target List. 160(2), 80. <https://doi.org/10.3847/1538-3881/ab9a53>
- Coles, P. A., Yurchenko, S. N., & Tennyson, J. (2019). ExoMol molecular line lists - XXXV. A rotation-vibration line list for hot ammonia. 490(4), 4638–4647. <https://doi.org/10.1093/mnras/stz2778>
- Edwards, B., Mugnai, L., Tinetti, G., & al., et. (2019). An Updated Study of Potential Targets for Ariel. 157(6), 242. <https://doi.org/10.3847/1538-3881/ab1cb9>
- Feroz, F., Hobson, M. P., & Bridges, M. (2009). MULTINEST: an efficient and robust Bayesian inference tool for cosmology and particle physics. 398(4), 1601–1614. <https://doi.org/10.1111/j.1365-2966.2009.14548.x>
- Feroz, Farhan, Hobson, M. P., Cameron, E., & al., et. (2019). Importance Nested Sampling and the MultiNest Algorithm. *The Open Journal of Astrophysics*, 2(1), 10. <https://doi.org/10.4236/oja.20190201002>

[//doi.org/10.21105/astro.1306.2144](https://doi.org/10.21105/astro.1306.2144)

- Fletcher, L. N., Gustafsson, M., & Orton, G. S. (2018). Hydrogen Dimers in Giant-planet Infrared Spectra. *235*(1), 24. <https://doi.org/10.3847/1538-4365/aaa07a>
- Foreman-Mackey, D., Hogg, D. W., Lang, D., & al., et. (2013). emcee: The MCMC Hammer. *125*(925), 306. <https://doi.org/10.1086/670067>
- Gelman, A., & Rubin, D. B. (1992). Inference from Iterative Simulation Using Multiple Sequences. *Statistical Science*, *7*, 457–472. <https://doi.org/10.1214/ss/1177011136>
- Geweke, J. (1991). *Evaluating the accuracy of sampling-based approaches to the calculation of posterior moments* (Staff Report No. 148). Federal Reserve Bank of Minneapolis. <https://ideas.repec.org/p/fip/fedmsr/148.html>
- Goodman, J., & Weare, J. (2010). Ensemble samplers with affine invariance. *Communications in Applied Mathematics and Computational Science*, *5*(1), 65–80. <https://doi.org/10.2140/camcos.2010.5.65>
- Li, G., Gordon, I. E., Rothman, L. S., & al., et. (2015). Rovibrational Line Lists for Nine Isotopologues of the CO Molecule in the X $^1\Sigma^+$ Ground Electronic State. *216*(1), 15. <https://doi.org/10.1088/0067-0049/216/1/15>
- Mugnai, L. V., Bocchieri, A., & Pascale, E. (2023). ExoRad 2.0: The generic point source radiometric model. *The Journal of Open Source Software*, *8*(89), 5348. <https://doi.org/10.21105/joss.05348>
- Mugnai, L. V., Pascale, E., Edwards, B., & al., et. (2020). ArielRad: the Ariel radio-metric model. *Experimental Astronomy*, *50*(2-3), 303–328. <https://doi.org/10.1007/s10686-020-09676-7>
- Polyansky, O. L., Kyuberis, A. A., Zobov, N. F., & al., et. (2018). ExoMol molecular line lists XXX: a complete high-accuracy line list for water. *480*(2), 2597–2608. <https://doi.org/10.1093/mnras/sty1877>
- Rothman, L. S., Gordon, I. E., Barber, R. J., Dothe, H., Gamache, R. R., Goldman, A., Perevalov, V. I., Tashkun, S. A., & Tennyson, J. (2010). HITEMP, the high-temperature molecular spectroscopic database. *111*, 2139–2150. <https://doi.org/10.1016/j.jqsrt.2010.05.001>
- Tinetti, G., Drossart, P., Eccleston, P., & al., et. (2018). A chemical survey of exoplanets with ARIEL. *Experimental Astronomy*, *46*(1), 135–209. <https://doi.org/10.1007/s10686-018-9598-x>
- Tinetti, G., Eccleston, P., Haswell, C., & al., et. (2021). Ariel: Enabling planetary science across light-years. *arXiv e-Prints*, arXiv:2104.04824. <https://doi.org/10.48550/arXiv.2104.04824>
- Yurchenko, S. N., Amundsen, D. S., Tennyson, J., & al., et. (2017). A hybrid line list for CH₄ and hot methane continuum. *605*, A95. <https://doi.org/10.1051/0004-6361/201731026>