

NEMESISPY: A Python package for simulating and retrieving exoplanetary spectra

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DOI: [10.21105/joss.06874](https://doi.org/10.21105/joss.06874)

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Submitted: 10 March 2024

Published: 08 September 2024

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Summary

Spectra of exoplanets allow us to probe their atmospheres' composition and thermal structure and, when applicable, their surface conditions (Burrows, 2014). Spectroscopic characterisation of a large population of exoplanets may help us understand the origin and evolution of planetary systems (Chachan et al., 2023; Madhusudhan et al., 2017; Mordasini et al., 2016). The extraction of information from spectral data is known as atmospheric retrievals (e.g., Irwin et al., 2008; Line et al., 2013; Madhusudhan & Seager, 2009), which can be divided into two steps: forward modelling and model fitting. At a minimum, the forward modelling step requires an atmospheric model for the observed planet and a radiative transfer pipeline that can calculate model spectra given some input atmospheric model. The model fitting step typically requires a Bayesian parameter inference algorithm that can constrain the free parameters of the forward model by fitting the observed spectra. Atmospheric retrieval pipelines have long been applied to the spectral analysis of the Earth and other solar system planets, and the discovery of exoplanets further ignited the development of new retrieval pipelines with varying focus and functionalities (MacDonald & Batalha, 2023).

NEMESISPY is a Python package developed to perform parametric atmospheric modelling and radiative transfer calculation for the retrievals of exoplanetary spectra. It is a recent development of the well-established Fortran NEMESIS library (Irwin et al., 2008), which has been applied to the atmospheric retrievals of both solar system planets and exoplanets employing numerous different observing geometries (Barstow et al., 2014, 2016; Barstow, 2020; Irwin et al., 2020; James et al., 2023; Krissansen-Totton et al., 2018; Lee et al., 2012; Teanby et al., 2012). NEMESISPY can be easily interfaced with Bayesian inference algorithms to retrieve atmospheric properties from spectroscopic observations. Recently, NEMESISPY has been applied to the retrievals of Hubble and Spitzer data of a hot Jupiter (Yang et al., 2023), as well as to JWST/Mid-Infrared Instrument (JWST/MIRI) data of a hot Jupiter (Yang et al., 2024).

Statement of need

NEMESISPY has three distinguishing features as an exoplanetary retrieval pipeline. Firstly, NEMESISPY inherits the fast correlated-k (Lacis & Oinas, 1991) radiative transfer routine from the Fortran NEMESIS library (Irwin et al., 2008), which has been extensively validated against other radiative transfer codes (Barstow et al., 2020). Secondly, NEMESISPY employs a just-in-time compiler (Lam et al., 2015), which compiles the most computationally expensive routines to machine code at run time. Combined with extensive code refactoring, NEMESISPY is significantly faster than the Fortran NEMESIS library. Such speed improvement is crucial for analysing exoplanetary spectra using sampling-based Bayesian parameter estimation (e.g., Feroz & Hobson, 2008), which typically involves the computation of millions of model spectra.

Thirdly, NEMESISPY implements several parametric atmospheric temperature models from Yang et al. (2023). These routines are particularly useful for retrieving spectroscopic phase curves of hot Jupiters, which are emission spectra observed at multiple orbital phases and can enable detailed atmospheric characterisation.

NEMESISPY contains several general-purpose routines for atmospheric modelling and spectral simulations. The modular nature of the package means that subroutines can be easily called on their own. Currently, NEMESISPY has an easy-to-use API for simulating emission spectra and phase curves of hot Jupiters from arbitrary input atmospheric models, and new features are being actively developed, such as multiple scattering in radiative transfer calculation, an API for transmission spectra, and the line-by-line radiative transfer method. NEMESISPY has already enabled two scientific publications (Yang et al., 2023; Yang et al., 2024) and is used in numerous ongoing exoplanetary data analysis projects. The combination of well-tested core radiative transfer routines, accelerated computational speed, and packaged modular design is ideal for tackling the influx of JWST data of exoplanets.

State of the field

For a review of exoplanet atmospheric retrieval codes with comparable functionalities to NEMESISPY, we refer the reader to the comprehensive catalogue in MacDonald & Batalha (2023).

Acknowledgements

The authors express gratitude to the developers of many open-source Python packages used by NEMESISPY, in particular, numpy (Harris et al., 2020), SciPy (Virtanen et al., 2020), Numba (Lam et al., 2015) and Matplotlib (Hunter, 2007). The authors also express gratitude to the many developers of the open-source Fortran NEMESIS library (Irwin et al., 2008).

References

- Barstow, J. K. (2020). Unveiling cloudy exoplanets: The influence of cloud model choices on retrieval solutions. *Monthly Notices of the Royal Astronomical Society*, 497(4), 4183–4195. <https://doi.org/10.1093/mnras/staa2219>
- Barstow, J. K., Aigrain, S., Irwin, P. G. J., Hackler, T., Fletcher, L. N., Lee, J. M., & Gibson, N. P. (2014). CLOUDS ON THE HOT JUPITER HD189733b: CONSTRAINTS FROM THE REFLECTION SPECTRUM. *The Astrophysical Journal*, 786(2), 154. <https://doi.org/10.1088/0004-637X/786/2/154>
- Barstow, J. K., Aigrain, S., Irwin, P. G. J., & Sing, D. K. (2016). A CONSISTENT RETRIEVAL ANALYSIS OF 10 HOT JUPITERS OBSERVED IN TRANSMISSION. *The Astrophysical Journal*, 834(1), 50. <https://doi.org/10.3847/1538-4357/834/1/50>
- Barstow, J. K., Changeat, Q., Garland, R., Line, M. R., Rocchetto, M., & Waldmann, I. P. (2020). A comparison of exoplanet spectroscopic retrieval tools. *Monthly Notices of the Royal Astronomical Society*, 493(4), 4884–4909. <https://doi.org/10.1093/mnras/staa548>
- Burrows, A. S. (2014). Spectra as windows into exoplanet atmospheres. *Proceedings of the National Academy of Sciences*, 111(35), 12601–12609. <https://doi.org/10.1073/pnas.1304208111>
- Chachan, Y., Knutson, H. A., Lothringer, J., & Blake, G. A. (2023). Breaking Degeneracies in Formation Histories by Measuring Refractory Content in Gas Giants. *The Astrophysical Journal*, 943(2), 112. <https://doi.org/10.3847/1538-4357/aca614>

- Feroz, F., & Hobson, M. P. (2008). Multimodal nested sampling: An efficient and robust alternative to Markov Chain Monte Carlo methods for astronomical data analyses. *Monthly Notices of the Royal Astronomical Society*, 384(2), 449–463. <https://doi.org/10.1111/j.1365-2966.2007.12353.x>
- Harris, C. R., Millman, K. J., van der Walt, S. J., Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., van Kerkwijk, M. H., Brett, M., Haldane, A., del Río, J. F., Wiebe, M., Peterson, P., ... Oliphant, T. E. (2020). Array programming with NumPy. *Nature*, 585(7825), 357–362. <https://doi.org/10.1038/s41586-020-2649-2>
- Hunter, J. D. (2007). Matplotlib: A 2D Graphics Environment. *Computing in Science & Engineering*, 9(3), 90–95. <https://doi.org/10.1109/MCSE.2007.55>
- Irwin, P. G. J., Parmentier, V., Taylor, J., Barstow, J., Aigrain, S., Lee, E., & Garland, R. (2020). 2.5D retrieval of atmospheric properties from exoplanet phase curves: Application to WASP-43b observations. *Monthly Notices of the Royal Astronomical Society*, 493(1), 106–125. <https://doi.org/10.1093/mnras/staa238>
- Irwin, P. G. J., Teanby, N. A., de Kok, R., Fletcher, L. N., Howett, C. J. A., Tsang, C. C. C., Wilson, C. F., Calcutt, S. B., Nixon, C. A., & Parrish, P. D. (2008). The NEMESIS planetary atmosphere radiative transfer and retrieval tool. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 109(6), 1136–1150. <https://doi.org/10.1016/j.jqsrt.2007.11.006>
- James, A., Irwin, P. G. J., Dobinson, J., Wong, M. H., Tsubota, T. K., Simon, A. A., Fletcher, L. N., Roman, M. T., Teanby, N. A., Toledo, D., & Orton, G. S. (2023). The Temporal Brightening of Uranus' Northern Polar Hood From HST/WFC3 and HST/STIS Observations. *Journal of Geophysical Research: Planets*, 128(10), e2023JE007904. <https://doi.org/10.1029/2023JE007904>
- Krissansen-Totton, J., Garland, R., Irwin, P., & Catling, D. C. (2018). Detectability of Biosignatures in Anoxic Atmospheres with the James Webb Space Telescope: A TRAPPIST-1e Case Study. *The Astronomical Journal*, 156(3), 114. <https://doi.org/10.3847/1538-3881/aad564>
- Lacis, A. A., & Oinas, V. (1991). A description of the correlated k distribution method for modeling nongray gaseous absorption, thermal emission, and multiple scattering in vertically inhomogeneous atmospheres. *Journal of Geophysical Research*, 96(D5), 9027. <https://doi.org/10.1029/90JD01945>
- Lam, S. K., Pitrou, A., & Seibert, S. (2015). Numba: A LLVM-based Python JIT compiler. *Proceedings of the Second Workshop on the LLVM Compiler Infrastructure in HPC*, 1–6. <https://doi.org/10.1145/2833157.2833162>
- Lee, J.-M., Fletcher, L. N., & Irwin, P. G. J. (2012). Optimal estimation retrievals of the atmospheric structure and composition of HD 189733b from secondary eclipse spectroscopy: Exoplanet retrieval from transit spectroscopy. *Monthly Notices of the Royal Astronomical Society*, 420(1), 170–182. <https://doi.org/10.1111/j.1365-2966.2011.20013.x>
- Line, M. R., Wolf, A. S., Zhang, X., Knutson, H., Kammer, J. A., Ellison, E., Deroo, P., Crisp, D., & Yung, Y. L. (2013). A SYSTEMATIC RETRIEVAL ANALYSIS OF SECONDARY ECLIPSE SPECTRA. I. A COMPARISON OF ATMOSPHERIC RETRIEVAL TECHNIQUES. *The Astrophysical Journal*, 775(2), 137. <https://doi.org/10.1088/0004-637X/775/2/137>
- MacDonald, R. J., & Batalha, N. E. (2023). A Catalog of Exoplanet Atmospheric Retrieval Codes. *Research Notes of the AAS*, 7(3), 54. <https://doi.org/10.3847/2515-5172/acc46a>
- Madhusudhan, N., Bitsch, B., Johansen, A., & Eriksson, L. (2017). Atmospheric signatures of giant exoplanet formation by pebble accretion. *Monthly Notices of the Royal Astronomical Society*, 469(4), 4102–4115. <https://doi.org/10.1093/mnras/stx1139>

- Madhusudhan, N., & Seager, S. (2009). A TEMPERATURE AND ABUNDANCE RETRIEVAL METHOD FOR EXOPLANET ATMOSPHERES. *The Astrophysical Journal*, 707(1), 24–39. <https://doi.org/10.1088/0004-637X/707/1/24>
- Mordasini, C., van Boekel, R., Mollière, P., Henning, Th., & Benneke, B. (2016). THE IMPRINT OF EXOPLANET FORMATION HISTORY ON OBSERVABLE PRESENT-DAY SPECTRA OF HOT JUPITERS. *The Astrophysical Journal*, 832(1), 41. <https://doi.org/10.3847/0004-637X/832/1/41>
- Teanby, N. A., Irwin, P. G. J., Nixon, C. A., de Kok, R., Vinatier, S., Coustenis, A., Sefton-Nash, E., Calcutt, S. B., & Flasar, F. M. (2012). Active upper-atmosphere chemistry and dynamics from polar circulation reversal on Titan. *Nature*, 491(7426), 732–735. <https://doi.org/10.1038/nature11611>
- Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., ... van Mulbregt, P. (2020). SciPy 1.0: Fundamental algorithms for scientific computing in Python. *Nature Methods*, 17(3), 261–272. <https://doi.org/10.1038/s41592-019-0686-2>
- Yang, J., Hammond, M., Piette, A. A. A., Blecic, J., Bell, T. J., Irwin, P. G. J., Parmentier, V., Tsai, S.-M., Barstow, J. K., Crouzet, N., Kreidberg, L., Mendonça, J. M., Taylor, J., Baeyens, R., Ohno, K., Teinturier, L., & Nixon, M. C. (2024). Simultaneous retrieval of orbital phase resolved JWST/MIRI emission spectra of the hot Jupiter WASP-43b: Evidence of water, ammonia and carbon monoxide. *Monthly Notices of the Royal Astronomical Society*, stae1427. <https://doi.org/10.1093/mnras/stae1427>
- Yang, J., Irwin, P. G. J., & Barstow, J. K. (2023). Testing 2D temperature models in Bayesian retrievals of atmospheric properties from hot Jupiter phase curves. *Monthly Notices of the Royal Astronomical Society*, 525(4), 5146–5167. <https://doi.org/10.1093/mnras/stad2555>