The Journal of Open Source Software

POSEIDON: A Multidimensional Atmospheric Retrieval Code for Exoplanet Spectra

Ryan J. MacDonald [1,2,3]

1 Department of Astronomy, University of Michigan, 1085 S. University Ave., Ann Arbor, MI 48109, USA **2** NHFP Sagan Fellow **3** Department of Astronomy and Carl Sagan Institute, Cornell University, 122 Sciences Drive, Ithaca, NY 14853, USA

DOI: 10.21105/joss.04873

Software

- Review
- Repository
- Archive

Editor: Dan Foreman-Mackey

Reviewers:

- @ideasrule
- @LorenzoMugnai

Submitted: 24 August 2022
Published: 13 January 2023

In partnership with

AMERICAN ASTRONOMICAL SOCIETY

This article and software are linked with research article DOI 10.3847/1538-4357/ac47fe, published in the Astrophysical Journal.

Summary

Exoplanet atmospheres are a dynamic and fast-changing field at the frontier of modern astronomy. Telescope observations can reveal the chemical composition, temperature, cloud properties, and (potentially) the habitability of these remote worlds. Astronomers can measure these atmospheric properties by observing how the fraction of starlight blocked by a planet passing in front of its host star changes with wavelength — a technique called transmission spectroscopy. Since the wavelengths where different atoms and molecules absorb are already known (from laboratory measurements or quantum mechanics), astronomers can compare models of exoplanet spectra to observations to infer the chemical composition of exoplanets.

POSEIDON is a Python package for the modelling and analysis of exoplanet spectra. POSEIDON has two main functions: (i) computation of model spectra for 1D, 2D, or 3D exoplanet atmospheres; and (ii) a Bayesian fitting routine ('atmospheric retrieval') that can infer the range of atmospheric properties consistent with an observed exoplanet spectrum.

Exoplanet Modelling and Atmospheric Retrieval with POSEIDON

The first major use case for POSEIDON is 'forward modelling' — illustrated on the left of Figure 1. A user can generate a model planet spectrum, for a given star-planet system, by providing a specific set of atmospheric properties (e.g. the chemical composition and temperature). The forward model mode allows users to explore how atmospheric properties alter an exoplanet spectrum and to produce predicted model spectra for observing proposals. The required input files (pre-computed stellar grids and an opacity database) are available to download from an online repository (linked in the documentation).

The second major use case for POSEIDON is atmospheric retrieval — illustrated on the right of Figure 1. To initialise a retrieval, a user provides an observed exoplanet spectrum and the range of atmospheric properties to be explored (i.e. the prior ranges for a set of free parameters defining a model). A Bayesian statistical sampling algorithm — nominally `PyMultiNest` (Buchner et al., 2014) — then repeatedly calls the forward model, comparing the generated spectrum to the observations, until the parameter space is fully explored and a convergence criteria reached. The main outputs of an atmospheric retrieval are the posterior probability distributions of the model parameters and the model's Bayesian evidence. The Bayesian evidences from multiple retrievals, in turn, can be subsequently compared to compute a detection significance for each model component (e.g. the statistical confidence for a molecule being present in the planetary atmosphere).

The Journal of Open Source Software

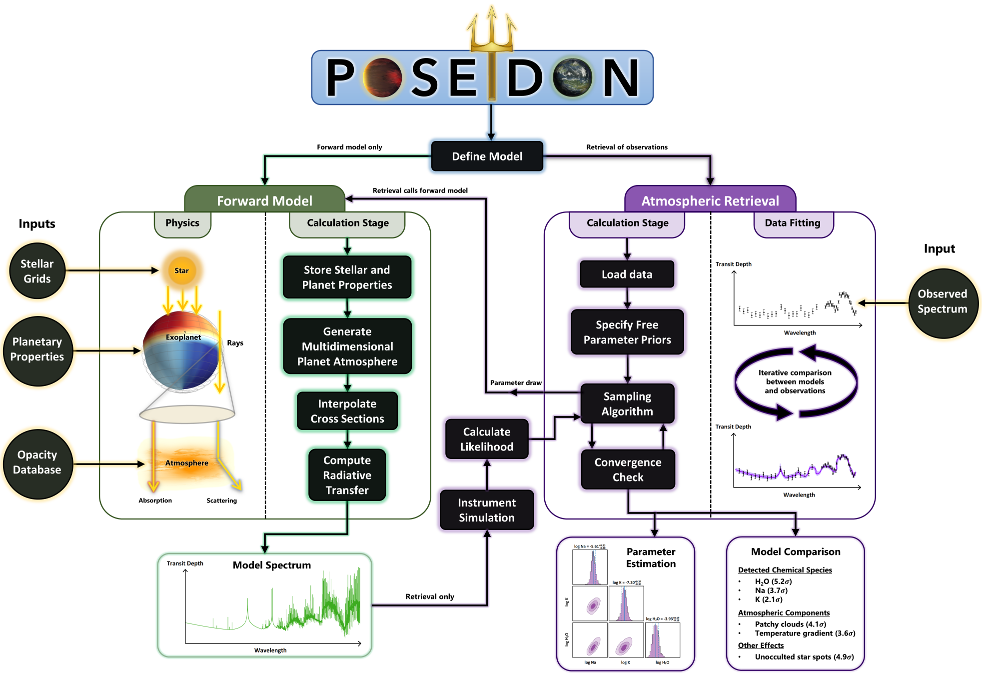

Figure 1: Schematic architecture of the POSEIDON atmospheric retrieval code. Users can call POSEIDON in two main ways: (i) to generate a model exoplanet spectrum for a specified planet atmosphere (green arrows); or (ii) to fit an observed exoplanet spectrum by statistical sampling of a model's atmospheric properties (purple arrows). The diagram highlights code inputs (circles), algorithm steps (rectangles), and code outputs (bottom green or purple boxes).

POSEIDON was first described in the exoplanet literature by (MacDonald & Madhusudhan, 2017). Since then, the code has been used in 17 peer-reviewed publications (e.g., Alam et al., 2021; Kaltenegger et al., 2020; Sedaghati et al., 2017). Most recently, a detailed description of POSEIDON's new multidimensional forward model, TRIDENT, was provided by (MacDonald & Lewis, 2022).

Statement of Need

Recent years have seen a substantial improvement in the number of high-quality exoplanet spectra. In particular, the newly operational JWST and a profusion of high-resolution ground-based spectrographs offer an abundance of exoplanet data. The accurate interpretation of such data requires a retrieval code that can rapidly explore complex parameter spaces describing a rich variety of atmospheric phenomena.

POSEIDON provides the capability to model and retrieve transmission spectra of planets with inhomogeneous temperatures, compositions, and cloud properties (i.e. 2D or 3D models). Several studies have highlighted that not including these multidimensional effects can bias retrieval inferences (e.g., Caldas et al., 2019; Line & Parmentier, 2016; MacDonald et al., 2020; Pluriel et al., 2022). However, existing open-source exoplanet retrieval codes assume 1D atmospheres for computational efficiency. POSEIDON, therefore, offers an open-source implementation of state-of-the-art multidimensional retrieval methods (see MacDonald & Lewis, 2022 and MacDonald & Lewis, in prep.) to aid the interpretation of high-quality exoplanet spectra.

In a 1D configuration, POSEIDON compares well with other retrieval codes. When applied to Hubble Space Telescope observations, POSEIDON produces consistent retrieval results with the ATMO and NEMESIS retrieval codes (Lewis et al., 2020; Rathcke et al., 2021). Recently, (Barstow et al., 2022) presented a comparison of five exoplanet retrieval codes, including POSEIDON, which demonstrated good agreement on simulated Ariel (Tinetti et al., 2020) transmission spectra. POSEIDON also offers exceptional computational performance: a single 1D forward model over a wavelength range sufficient for JWST analyses takes 70 ms (see MacDonald & Lewis, 2022, Appendix D), while publication-quality 1D retrievals typically take an hour or less. POSEIDON also supports multi-core retrievals via PyMultiNest's MPI implementation, which achieves a roughly linear speed-up in the number of cores. Therefore, POSEIDON allows users to readily explore 1D retrievals on personal laptops while scaling up to multidimensional retrievals on modest clusters.

Future Developments

POSEIDON v1.0 officially supports the modelling and retrieval of exoplanet transmission spectra in 1D, 2D, and 3D. The initial release also includes a beta version of thermal emission spectra modelling and retrieval (for cloud-free, 1D atmospheres, with no scattering), which will be developed further in future releases. Suggestions for additional features are more than welcome.

Documentation

Documentation for POSEIDON, with step-by-step tutorials illustrating research applications, is available at https://poseidon-retrievals.readthedocs.io/en/latest/.

Similar Tools

The following exoplanet retrieval codes are open source: PLATON (Zhang et al., 2019, 2020), petitRADTRANS (Mollière et al., 2019), CHIMERA (Line et al., 2013), TauRex (Al-Refaie et al., 2021; Waldmann et al., 2015), NEMESIS (Irwin et al., 2008) Pyrat Bay (Cubillos & Blecic, 2021), and BART (Harrington et al., 2022)

Acknowledgements

RJM expresses gratitude to the developers of many open source Python packages used by POSEIDON, in particular Numba (Lam et al., 2015), numpy (Harris et al., 2020), Matplotlib (Hunter, 2007), SciPy (Virtanen et al., 2020), and Spectres (Carnall, 2017).

RJM acknowledges financial support from the UK's Science and Technology Facilities Council (STFC) during the early development of POSEIDON and support from NASA Grant 80NSSC20K0586 issued through the James Webb Space Telescope Guaranteed Time Observer Program. Most recently, RJM acknowledges support from NASA through the NASA Hubble Fellowship grant HST-HF2-51513.001 awarded by the Space Telescope Science Institute, which is operated by the Association of Universities for Research in Astronomy, Inc., for NASA, under contract NAS5-26555. RJM is especially grateful to Lorenzo Mugnai and Michael Zhang for excellent and helpful referee reports, and to the editor, Dan Foreman-Mackey, for his tireless efforts to encourage new people to join the open source community in astronomy. RJM thanks Nikole Lewis, Ishan Mishra, Jonathan Gomez Barrientos, John Kappelmeier, Antonia Peters, Kath Landgren, and Ruizhe Wang for helpful discussions.

References

Alam, M. K., López-Morales, M., MacDonald, R. J., Nikolov, N., Kirk, J., Goyal, J. M., Sing, D. K., Wakeford, H. R., Rathcke, A. D., Deming, D. L., Sanz-Forcada, J., Lewis, N. K., Barstow, J. K., Mikal-Evans, T., & Buchhave, L. A. (2021). Evidence of a Clear Atmosphere for

WASP-62b: The Only Known Transiting Gas Giant in the JWST Continuous Viewing Zone. *Astrophysical Journal Letters*, *906*(2), L10. https://doi.org/10.3847/2041-8213/abd18e

Al-Refaie, A. F., Changeat, Q., Waldmann, I. P., & Tinetti, G. (2021). TauREx 3: A Fast, Dynamic, and Extendable Framework for Retrievals. *Astrophysical Journal*, *917*(1), 37. https://doi.org/10.3847/1538-4357/ac0252

Barstow, J. K., Changeat, Q., Chubb, K. L., Cubillos, P. E., Edwards, B., MacDonald, R. J., Min, M., & Waldmann, I. P. (2022). A retrieval challenge exercise for the Ariel mission. *Experimental Astronomy*, *53*(2), 447–471. https://doi.org/10.1007/s10686-021-09821-w

Buchner, J., Georgakakis, A., Nandra, K., Hsu, L., Rangel, C., Brightman, M., Merloni, A., Salvato, M., Donley, J., & Kocevski, D. (2014). X-ray spectral modelling of the AGN obscuring region in the CDFS: Bayesian model selection and catalogue. *Astronomy & Astrophysics*, *564*, A125. https://doi.org/10.1051/0004-6361/201322971

Caldas, A., Leconte, J., Selsis, F., Waldmann, I. P., Bordé, P., Rocchetto, M., & Charnay, B. (2019). Effects of a fully 3D atmospheric structure on exoplanet transmission spectra: retrieval biases due to day-night temperature gradients. *Astronomy & Astrophysics*, *623*, A161. https://doi.org/10.1051/0004-6361/201834384

Carnall, A. C. (2017). SpectRes: A Fast Spectral Resampling Tool in Python. *arXiv e-Prints*, arXiv:1705.05165. https://arxiv.org/abs/1705.05165

Cubillos, P. E., & Blecic, J. (2021). The PYRAT BAY framework for exoplanet atmospheric modelling: a population study of Hubble/WFC3 transmission spectra. *Monthly Notices of the Royal Astronomical Society*, *505*(2), 2675–2702. https://doi.org/10.1093/mnras/stab1405

Harrington, J., Himes, M. D., Cubillos, P. E., Blecic, J., Rojo, P. M., Challener, R. C., Lust, N. B., Bowman, M. O., Blumenthal, S. D., Dobbs-Dixon, I., Foster, A. S. D., Foster, A. J., Green, M. R., Loredo, T. J., McIntyre, K. J., Stemm, M. M., & Wright, D. C. (2022). An Open-source Bayesian Atmospheric Radiative Transfer (BART) Code. I. Design, Tests, and Application to Exoplanet HD 189733b. *Planetary Science Journal*, *3*(4), 80. https://doi.org/10.3847/PSJ/ac3513

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 and Engineering*, *9*(3), 90–95. https://doi.org/10.1109/MCSE.2007.55

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*, 1136–1150. https://doi.org/10.1016/j.jqsrt.2007.11.006

Kaltenegger, L., MacDonald, R. J., Kozakis, T., Lewis, N. K., Mamajek, E. E., McDowell, J. C., & Vanderburg, A. (2020). The White Dwarf Opportunity: Robust Detections of Molecules in Earth-like Exoplanet Atmospheres with the James Webb Space Telescope. *Astrophysical Journal Letters*, *901*(1), L1. https://doi.org/10.3847/2041-8213/aba9d3

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.

Lewis, N. K., Wakeford, H. R., MacDonald, R. J., Goyal, J. M., Sing, D. K., Barstow, J., Powell, D., Kataria, T., Mishra, I., Marley, M. S., Batalha, N. E., Moses, J. I., Gao, P., Wilson, T. J., Chubb, K. L., Mikal-Evans, T., Nikolov, N., Pirzkal, N., Spake, J. J., …

Zhang, X. (2020). Into the UV: The Atmosphere of the Hot Jupiter HAT-P-41b Revealed. *Astrophysical Journal Letters*, *902*(1), L19. https://doi.org/10.3847/2041-8213/abb77f

Line, M. R., & Parmentier, V. (2016). The Influence of Nonuniform Cloud Cover on Transit Transmission Spectra. *Astrophysical Journal*, *820*(1), 78. https://doi.org/10.3847/0004-637X/820/1/78

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. *Astrophysical Journal*, *775*(2), 137. https://doi.org/10.1088/0004-637X/775/2/137

MacDonald, R. J., Goyal, J. M., & Lewis, N. K. (2020). Why Is it So Cold in Here? Explaining the Cold Temperatures Retrieved from Transmission Spectra of Exoplanet Atmospheres. *Astrophysical Journal Letters*, *893*(2), L43. https://doi.org/10.3847/2041-8213/ab8238

MacDonald, R. J., & Lewis, N. K. (2022). TRIDENT: A Rapid 3D Radiative-transfer Model for Exoplanet Transmission Spectra. *Astrophysical Journal*, *929*(1), 20. https://doi.org/10.3847/1538-4357/ac47fe

MacDonald, R. J., & Madhusudhan, N. (2017). HD 209458b in new light: evidence of nitrogen chemistry, patchy clouds and sub-solar water. *Monthly Notices of the Royal Astronomical Society*, *469*(2), 1979–1996. https://doi.org/10.1093/mnras/stx804

Mollière, P., Wardenier, J. P., van Boekel, R., Henning, Th., Molaverdikhani, K., & Snellen, I. A. G. (2019). petitRADTRANS. A Python radiative transfer package for exoplanet characterization and retrieval. *Astronomy & Astrophysics*, *627*, A67. https://doi.org/10.1051/0004-6361/201935470

Pluriel, W., Leconte, J., Parmentier, V., Zingales, T., Falco, A., Selsis, F., & Bordé, P. (2022). Toward a multidimensional analysis of transmission spectroscopy. II. Day-night-induced biases in retrievals from hot to ultrahot Jupiters. *Astronomy & Astrophysics*, *658*, A42. https://doi.org/10.1051/0004-6361/202141943

Rathcke, A. D., MacDonald, R. J., Barstow, J. K., Goyal, J. M., Lopez-Morales, M., Mendonça, J. M., Sanz-Forcada, J., Henry, G. W., Sing, D. K., Alam, M. K., Lewis, N. K., Chubb, K. L., Taylor, J., Nikolov, N., & Buchhave, L. A. (2021). HST PanCET Program: A Complete Near-UV to Infrared Transmission Spectrum for the Hot Jupiter WASP-79b. *Astronomical Journal*, *162*(4), 138. https://doi.org/10.3847/1538-3881/ac0e99

Sedaghati, E., Boffin, H. M. J., MacDonald, R. J., Gandhi, S., Madhusudhan, N., Gibson, N. P., Oshagh, M., Claret, A., & Rauer, H. (2017). Detection of titanium oxide in the atmosphere of a hot Jupiter. *Nature*, *549*(7671), 238–241. https://doi.org/10.1038/nature23651

Tinetti, G., Eccleston, P., Haswell, C., Lagage, P.-O., Leconte, J., Lüftinger, T., Micela, G., Min, M., Pilbratt, G., Puig, L., & al., et. (2020). Ariel: Enabling planetary science across light-years. *ESA Ariel Mission Definition Study Report*, arXiv:2104.04824. https://doi.org/10.48550/arXiv.2104.04824

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., … SciPy 1. 0 Contributors. (2020). SciPy 1.0: fundamental algorithms for scientific computing in Python. *Nature Methods*, *17*, 261–272. https://doi.org/10.1038/s41592-019-0686-2

Waldmann, I. P., Tinetti, G., Rocchetto, M., Barton, E. J., Yurchenko, S. N., & Tennyson, J. (2015). Tau-REx I: A Next Generation Retrieval Code for Exoplanetary Atmospheres. *Astrophysical Journal*, *802*(2), 107. https://doi.org/10.1088/0004-637X/802/2/107

Zhang, M., Chachan, Y., Kempton, E. M.-R., & Knutson, H. A. (2019). Forward Modeling and Retrievals with PLATON, a Fast Open-source Tool. *Publications of the Astronomical

Society of the Pacific, *131*(997), 034501. https://doi.org/10.1088/1538-3873/aaf5ad

Zhang, M., Chachan, Y., Kempton, E. M.-R., Knutson, H. A., & Chang, W. (Happy). (2020). PLATON II: New Capabilities and a Comprehensive Retrieval on HD 189733b Transit and Eclipse Data. *Astrophysical Journal*, *899*(1), 27. https://doi.org/10.3847/1538-4357/aba1e6