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Atmospheric Retrievals with petitRADTRANS

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Summary

`petitRADTRANS` (pRT) is a fast radiative transfer code used for computing emission and transmission spectra of exoplanet atmospheres (Mollière et al., 2019), combining a FORTRAN back end with a Python based user interface. These spectra can be used as a forward model for fitting spectroscopic data using Monte Carlo techniques, commonly referred to as an atmospheric retrieval (Madhusudhan & Seager, 2009). The retrieval module of pRT combines fast pRT with the `MultiNest` (J. Buchner et al., 2014; F. Feroz et al., 2009; Farhan Feroz et al., 2019; F. Feroz & Hobson, 2008) and `Ultranest` (J. Buchner et al., 2014; Johannes Buchner, 2019) nested sampling codes, allowing for fast atmospheric retrievals on a large range of different types of exoplanet data. Both samplers also offer MPI implementations, allowing for easy parallelisation across a large cluster.

Statement of need

Atmospheric retrievals are a cornerstone of exoplanet atmospheric characterisation. pRT is a powerful and user-friendly tool, and is unique in its abilities to characterise exoplanets in both emission and transmission. Various thermal structures, chemistry and cloud parameterisations and opacity calculation methods can be combined and used to statistically identify the most favoured model for a given atmosphere. With increasing volumes of both ground- and space-based spectra available, it is necessary for exoplanet researchers to have access to a range of characterisation tools.

petitRADTANS Retrieval Module

The `Retrieval` module combines the `RadTrans` forward modelling class with a nested sampler via a likelihood function to perform an atmospheric retrieval. Datasets, priors and other retrieval hyper parameters are set through the `RetrievalConfig` class, while the `models` module includes a range of complete atmospheric models that can be fit to the data. Users can also define their own model function, making use of temperature profiles from the `physics` module and chemistry parameterisations from the `chemistry` module.

Multiple datasets can be included into a single retrieval, with each dataset receiving its own `RadTrans` object used for the radiative transfer calculation, allowing for highly flexible retrievals where multiple spectral resolutions, wavelength ranges and even atmospheric models can be combined in a single retrieval. Each dataset can also receive scaling factors (for the flux, uncertainties or both), error inflation factors and offsets. The model functions are used to compute a spectrum $\vec{S}$, which is convolved to the instrumental resolution and binned to the wavelength bins of the data using a custom binning function to account for non-uniform bin

sizes. The resulting spectrum compared to the data with flux $\vec{F}$ and covariance $\mathbf{C}$ in the likelihood function:

$$-2\log\mathcal{L} = \left(\vec{S}-\vec{F}\right)^T \mathbf{C}^{-1}\left(\vec{S}-\vec{F}\right) + \log\left(2\pi\det\left(\mathbf{C}\right)\right). \quad (1)$$

The second term is included in the likelihood to allow for uncertainties to vary as a free parameter during the retrieval, and penalizes overly large uncertainties.

pRT can compute spectra either using line-by-line calculations, or using correlated-k (c-k) tables for defining the opacities of molecular species. We include up-to-date correlated-k line lists from Exomol (Chubb et al., 2020; McKemmish et al., 2016; Polyansky et al., 2018; Tennyson & Yurchenko, 2012) and HITEMP (Rothman et al., 2010), with the full set of available opacities listed in the online documentation. The exo-k package is used to resample the the correlated-k opacity tables to a lower spectral resolution in order to reduce the computation time (Leconte, 2021). Combining the c-k opacities of multiple species requires mixing the distributions in g space. Previously, this was accomplished by taking 1000 samples of each distribution. This sampling process resulted in non-deterministic spectral calculations, resulting in unexpected behaviour from the nested sampling process, as the same set of parameters could result in varying log-likelihood. This has been updated to fully mix the c-k distributions. Considering the first species, the second species is added in, and the resulting grid is sorted. The cumulative opacity grid is then mixed with the next species, a process which iterates until every species with significant opacity contributions ($>0.1\%$ of the current opacity in any bin) is mixed in to the opacity grid. Once complete, the resulting grid is linearly interpolated back to the 16 g points at each pressure and frequency bin as required by pRT. This fully deterministic process stabilized the log-likelihood calculations in the retrievals, and resulted in a 5$\times$ improvement in the speed of the c-k mixing function.

Various thermal, chemical and cloud parameterisations are available in pRT. Built in temperature profiles range from interpolated splines to physically motivated profiles as in Guillot (2010) and Mollière et al. (2020). Equilibrium and disequilibrium chemistry can be interpolated from a pre-computed grid on-the-fly. Chemical abundances can also be freely retrieved, with the additional possibility of using a combination of free and chemically consistent abundances. Cloud parametersiations range from a 'grey' continuum opacity applied at all wavelengths, to clouds parameterised as in (**ackermann2001?**), using log-normal or Hansen (1971) particle size distributions with real optical opacities for different compositions and particle shapes, and including self-scattering. Included in pRT is an option to use an adaptive pressure grid with a higher resolution around the location of the cloud base, and a lower resolution elsewhere. The higher resolution grid is 10 times as fine as the remaining grid, and replaces one grid cell above and below the cloud base layer, as well as the cloud base layer cell itself. This allows for more precise positioning of the cloud layers within the atmosphere.

Photometric data are fully incorporated into the retrieval process. The spectral model is multiplied by a filter transmission profile from the SVO database using the `species` package (Stolker et al., 2020). This results in accurate synthetic photometry, which can be compared to the values specied by the user with the `add_photometry` function.

Publication ready summary plots of best fits, temperature and abundance profiles and corner plots can be automatically generated. Multiple retrieval results can be combined in the plots for model intercomparisons. Such results have been benchmarked against other widely used retrieval codes, in particular as part of the JWST Early Release Science program (Wellbanks et al, in prep).

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References

Buchner, Johannes. (2019). Collaborative Nested Sampling: Big Data versus Complex Physical Models. *131*(1004), 108005. https://doi.org/10.1088/1538-3873/aae7fc

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. *564*, A125. https://doi.org/10.1051/0004-6361/201322971

Chubb, K. L., Rocchetto, M., Al-Refaie, A. F., Waldmann, I., Min, M., Barstow, J., Molliére, P., Phillips, M. W., Tennyson, J., & Yurchenko, S. N. (2020). The ExoMolOP Database: Cross-sections and k-tables for Molecules of Interest in High-Temperature Exoplanet Atmospheres. *A&A*.

Feroz, F., & Hobson, M. P. (2008). Multimodal nested sampling: An efficient and robust alternative to Markov Chain Monte Carlo methods for astronomical data analyses. *384*(2), 449–463. https://doi.org/10.1111/j.1365-2966.2007.12353.x

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., & Pettitt, A. N. (2019). Importance Nested Sampling and the MultiNest Algorithm. *The Open Journal of Astrophysics*, *2*(1), 10. https://doi.org/10.21105/astro.1306.2144

Guillot, T. (2010). On the radiative equilibrium of irradiated planetary atmospheres. *520*, A27. https://doi.org/10.1051/0004-6361/200913396

Hansen, J. E. (1971). Multiple Scattering of Polarized Light in Planetary Atmospheres Part II. Sunlight Reflected by Terrestrial Water Clouds. *Journal of Atmospheric Sciences*, *28*(8), 1400–1426. https://doi.org/10.1175/1520-0469(1971)028%3C1400:MSOPLI%3E2.0.CO;2

Leconte, J. (2021). Spectral binning of precomputed correlated-k coefficients. *645*, A20. https://doi.org/10.1051/0004-6361/202039040

Madhusudhan, N., & Seager, S. (2009). A Temperature and Abundance Retrieval Method for Exoplanet Atmospheres. *707*(1), 24–39. https://doi.org/10.1088/0004-637X/707/1/24

McKemmish, L. K., Yurchenko, S. N., & Tennyson, J. (2016). ExoMol Molecular linelists – XVIII. The spectrum of Vanadium Oxide. *Mon. Not. R. Astron. Soc.*, *463*, 771–793. https://doi.org/10.1093/mnras/stw1969

Mollière, P., Stolker, T., Lacour, S., Otten, G. P. P. L., Shangguan, J., Charnay, B., Molyarova, T., Nowak, M., Henning, Th., Marleau, G.-D., Semenov, D. A., van Dishoeck, E., Eisenhauer, F., Garcia, P., Garcia Lopez, R., Girard, J. H., Greenbaum, A. Z., Hinkley, S., Kervella, P., … Zurlo, A. (2020). Retrieving scattering clouds and disequilibrium chemistry in the atmosphere of HR 8799e. *640*, A131. https://doi.org/10.1051/0004-6361/202038325

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

Polyansky, O. L., Kyuberis, A. A., Zobov, N. F., Tennyson, J., Yurchenko, S. N., & Lodi, L. (2018). ExoMol molecular line lists XXX: A complete high-accuracy line list for water. *Mon. Not. R. Astron. Soc.*, *480*, 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

Stolker, T., Quanz, S. P., Todorov, K. O., Kühn, J., Mollière, P., Meyer, M. R., Currie, T., Daemgen, S., & Lavie, B. (2020). MIRACLES: atmospheric characterization of directly imaged planets and substellar companions at 4-5 μm. I. Photometric analysis of β Pic b, HIP 65426 b, PZ Tel B, and HD 206893 B. *635*, A182. https://doi.org/10.1051/0004-6361/201937159

Tennyson, J., & Yurchenko, S. N. (2012). ExoMol: Molecular line lists for exoplanet and other atmospheres. *425*(1), 21–33. https://doi.org/10.1111/j.1365-2966.2012.21440.x