NEMESISPY: A Python package for simulating and retrieving exoplanetary spectra

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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).

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