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SpectralModel: a high-resolution framework for petitRADTRANS 3

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Summary

Atmospheric characterisation from spectroscopic data is a key to understand planetary formation. Two types of observations can be performed for this kind of analysis. Space-based observations (e.g., using the James Webb Space Telescope, JWST), are not impeded by the Earth's atmosphere, but are currently limited to low resolving powers (< 3000), which can lead to ambiguities in some species detections. Ground-based observations (e.g., using the Very Large Telescope, VLT), on the other hand, can benefit from large resolving powers ($\approx 10^5$), allowing for unambiguous species detection, but are impacted by telluric spectral lines. `petitRADTRANS` (pRT) is a radiative transfer package used for computing emission or transmission spectra of planetary atmospheres (Mollière et al., 2019). The package has a non-negligible user base, the original article being cited in 264 refereed works at the time of writing. pRT is already relatively easy to use on space-based, low-resolution observations. However, while the package technically has the capacity to analyse high-resolution spectra, thanks to its ability to incorporate high-resolution ($\mathcal{R} = 10^6$) line lists, ground-based observations analysis is a complex and challenging task. The new `SpectralModel` object provides a powerful and flexible framework that streamlines the setup necessary to model and retrieve high-resolution spectra.

Statement of need

Calculating a spectrum using pRT's core object `Radtrans` is a two-step process in which the user first instantiates the object, giving parameters that control the loading of opacities. The second step is for the user to call one of the `Radtrans` function, giving "spectral" parameters such as the temperatures or the mass fractions of the atmosphere, that will be used in combination with the loaded opacities to generate the spectrum.

However, these two steps are by themselves often insufficient to build a spectrum in a real-life scenario. The spectral parameters may individually rely on arbitrarily complex models requiring their own parameters, and may depend on each other. For example, getting mass fractions from equilibrium chemistry requires knowing the temperature profile, and the mean molar mass requires knowing the mass fractions (see e.g. the built-in pRT functions). Common operations such as convolving the spectrum, scaling it to stellar flux, or more specifically for high-resolution spectra, Doppler-shifting the spectrum and including the transit effect, must be done by post-processing the `Radtrans`-generated spectrum. Finally, using a retrieval requires to code a "retrieval model" including all the steps described above. This induces, especially for first-time users, a significant setup cost. The alternative is to use one of pRT's built-in models, but this lacks flexibility.

The `SpectralModel` object extends the base capabilities of the petitRADTRANS package by providing a standardized but flexible framework for spectral calculations. It has been especially designed to effectively erase the setup cost of modelling the spectral Doppler-shift,

the transit effect, and of implementing the preparation step necessary for ground-based high-resolution observations analysis. `SpectralModel` is also interfaced with pRT's `retrieval` module (Nasedkin et al., 2024), and as such is an easy-to-use tool to perform both high- and low-resolution atmospheric retrievals. Compared to other commonly used spectral modelling packages, for example ATMOSPHERIX (Klein et al., 2023), Brewster (Burningham et al., 2021), CHIMERA (Line et al., 2013), PSG (Villanueva et al., 2018), NEMESIS (Irwin et al., 2008), PICASO (Batalha et al., 2019), PLATON (Zhang et al., 2020), POSEIDON (MacDonald, 2023), TauREx (Al-Refaie et al., 2021), petitRADTRANS is currently, to our knowledge, the only one able to both generate time-varying high-resolution spectra and retrieve the corresponding data out-of-the-box[1].

The combination of ease-of-use and flexibility offered by `SpectralModel` makes it a powerful tool for high-resolution (but also low-resolution) atmospheric characterisation. With the upcoming first light of a new generation of ground based telescopes, such as the Extremely Large Telescope, `SpectralModel` makes petitRADTRANS ready for the new scientific discoveries that will be unveiled in the next era of high-resolution observations.

The `SpectralModel` object

Spectral parameter calculation framework

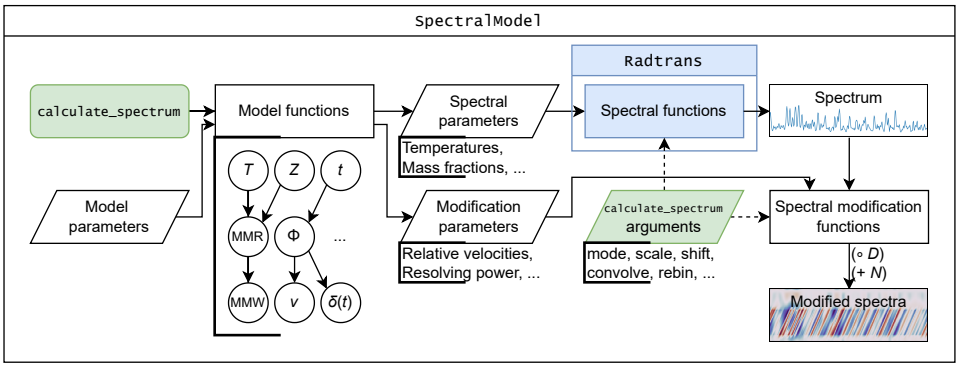

Figure 1: Flowchart of `SpectralModel.calculate_spectrum` function. The annotation below the model functions represents an example of execution order of these function after topological sorting, involving the temperature (T), the metallicity (Z), the time (t), the mass fractions (MMR), the mean molar masses (MMW), the orbital phases (ϕ), the relative velocities (v), and the transit effect (δ). Additional deformations (D) and noise (N) can also be included.

`SpectralModel` provides a framework to automatise the calculation of the spectral parameters. Each spectral parameter is linked to a function, called here "model function", which calculates its value. This feature can be extended to the parameters required for these functions, and so on. Before calculating spectra, the function's execution order is automatically determined through a topological sorting algorithm[2] (Kahn, 1962). `SpectralModel` comes with built-in functions (Blain et al., 2024) for all the spectral parameters, so that the object can be used "out-of-the-box". Parameters that ultimately do not depend on any function are called "model parameters", and must be given during instantiation.

[1] ATMOSPHERIX is able to make cross-correlation analysis of high-resolution spectra, but relies on petitRADTRANS to generate its templates. HYDRA-H (Gandhi et al., 2019) is a code able to perform high-resolution data retrievals, but is not publicly available. The other cited packages may have out-of-the-box single-time high-resolution spectral generation capabilities, but no time-varying high-resolution data retrieval framework, similarly to petitRADTRANS before the implementation of `SpectralModel`.

[2] Cyclic dependencies are not supported.

In addition, `SpectralModel` provides built-in functions (Blain et al., 2024) to scale, convolve, Doppler-shift, rebin, include planet transit effect, and prepare a spectrum after it has been calculated. Similarly to model functions, these "spectral modification functions" must be given, if used, their own model parameters during instantiation.

The spectral calculation is done within the `calculate_spectrum` function (see Figure 1). The spectral mode (emission or transmission), as well as which of the spectral modification to activate (i.e. only scaling, or both convolving and rebinning, etc.), are controlled through the function's arguments ("spectral modification parameters").

Interface with pRT's `retrieval` module

In order to be able to perform high-resolution data retrievals, the `Retrieval` object has been extended to support spectra with up to 3 dimensions, intended to be spectral order, exposure (time), and spectral pixel (wavelength). Several improvements to the module have been implemented as well:

- The retrieved data can now be provided as arrays instead of requiring a file.
- Custom `Radtrans` (or by extension `SpectralModel`) objects can now be used for retrievals.

In addition, `SpectralModel`'s model parameters and spectral modification functions can be advantageously used to simplify the retrieval setup compared to `Radtrans`'. This removes the need for several steps:

- building the `RetrievalConfig` object, as this has been automated,
- declaring the fixed parameters, as all model parameters that are not retrieved parameters are *de facto* fixed parameters,
- writing the retrieval model function, as it is given by the `SpectralModel` itself.

Ground-based high-resolution spectra contain telluric and stellar lines that must be removed. This is usually done with a "preparing" pipeline (also called "detrending" or "pre-processing" pipeline). To this end, a new `retrieval.preparing` sub-module has been implemented, containing the "Polyfit" pipeline (Blain et al., 2024) and the "SysRem" pipeline (Tamuz et al., 2005). To perform a retrieval when the data are prepared with "Polyfit", the forward model must be prepared in the same way (Blain et al., 2024). This forward model preparation step can be activated when calculating a spectrum with `SpectralModel`.

Other features

Telluric lines, noise, and other deformations can be included in a `SpectralModel` object. A time-varying airmass can be added as model parameter to better model the telluric lines.

A command-line interface (CLI) with ESO's SKYCALC sky model calculator has been implemented, adapting the CLI provided on the ESO's website.

SpectralModel comes with a class method which takes into account the (uniform) prior range of the radial velocity semi-amplitude (K_p), the rest frame velocity shift ($V_{\rm rest}$), and the mid transit time offset (T_0) to automatically calculate the optimal wavelength range to load, reducing memory usage.

The petitRADTRANS 3 update

Fully and seamlessly implementing `SpectralModel` into pRT required major changes and refactors to pRT's code. The changes focus on optimisations (both for speed and RAM usage) for high-resolution spectra computing, but this also impacts the correlated-k (low-resolution) part of the code. Overall, computation times for a typical spectral calculation between version 2 and version 3 have been divided by two, and RAM usage reduced by 30%. To speed-up "input data" (opacities, pre-calculated equilibrium chemistry table, star spectra table) loading

times, pRT's loading system has been overhauled and the loaded files have been converted from a mix of ASCII, Fortran unformatted and HDF5 files to HDF5-only. Opacities now also follow an extended ExoMol database naming and structure convention. The package's installation process has been made compatible with Python ≥ 3.12[3]. Finally, several quality-of-life features (e.g., missing requested opacities can be automatically downloaded from the project's Keeper library, or the `Planet` object) have been implemented.

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[3] pRT 2 used the `numpy.distutils` module to compile its Fortran extensions. This module is deprecated and is removed for Python 3.12. pRT 3 uses the Meson build system instead, with almost unnoticeable changes for users.

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