Exoplanet Transit Spectroscopy Models for JWST

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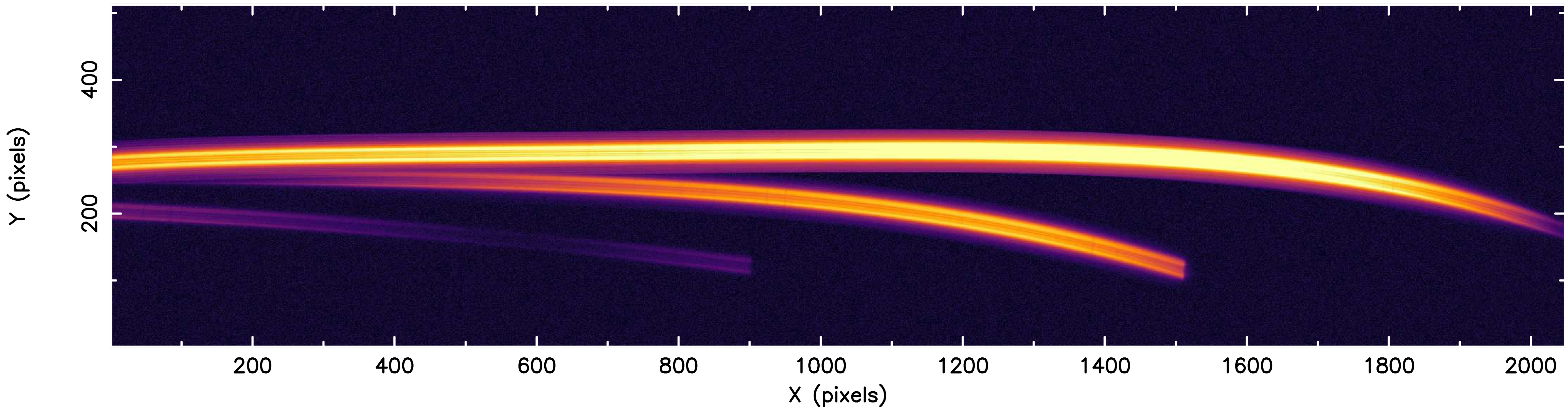

FIGURE 1: A simulation of a high signal-to-noise spectrum of a T=6000K main sequence dwarf with a transiting exoplanet. Three spectral orders have been simulated, including instrument throughput.

Abstract

JWST will deliver unprecedented observations of transiting exoplanets. Canada's instrumentation contribution is NIRISS which has a Single Object Slitless Spectrograph (SOSS) mode developed to optimize observations of transiting exoplanet host stars with R 700 from 0.8 to 2.8 μm. SOSS will deliver spectro-photometric transit lightcurves with 2000 band passes. The observations will be used to probe the thermal structure and chemical composition of the upper atmosphere of distant worlds by measuring the radius of exoplanet (r/R*) vs wavelength. Extracting r/R* is typically done via a transit-model that incorporates the stellar profile via limb-darkening to disentangle r/R* and b. Measurements with thousand bandpasses presents a challenge as each bandpass model has correlated wavelength dependent parameters due to limb-darkening and wavelength independent parameters such as b. We present new software algorithms that fit JWST-like observations and compute r/R* posteriors versus wavelength.

Introduction

The James Webb Space Telescope (JWST) is a large infrared telescope with a 6.5 m primary mirror. The telescope will be launched on an Ariane 5 rocket from French Guiana in October of 2018. One of the main uses of JWST will be to study the atmospheres of exoplanets. The primary method will be via transit spectroscopy. When an exoplanet passes in front of its host star a transit is produced. Some of the starlight will pass through the atmosphere of the planet and imprint absorption and scattering features into the star spectrum. From a careful analysis of the transit shape and depth, a spectrum of a portion of the atmosphere can be recovered.

The Canadian Space Agency (CSA) is providing the Fine Guidance Sensor (FGS) and one of the telescopes four instruments: the Near Infrared Imager and Slitless Spectrograph (NIRISS). The Single Object Slitless Spectroscopy (SOSS) mode of NIRISS provides high-throughput with the ability to observe bright (J~7) stars and will have the capability of detecting a thin atmosphere around a potentially habitable, earth-sized exoplanet under favourable conditions.

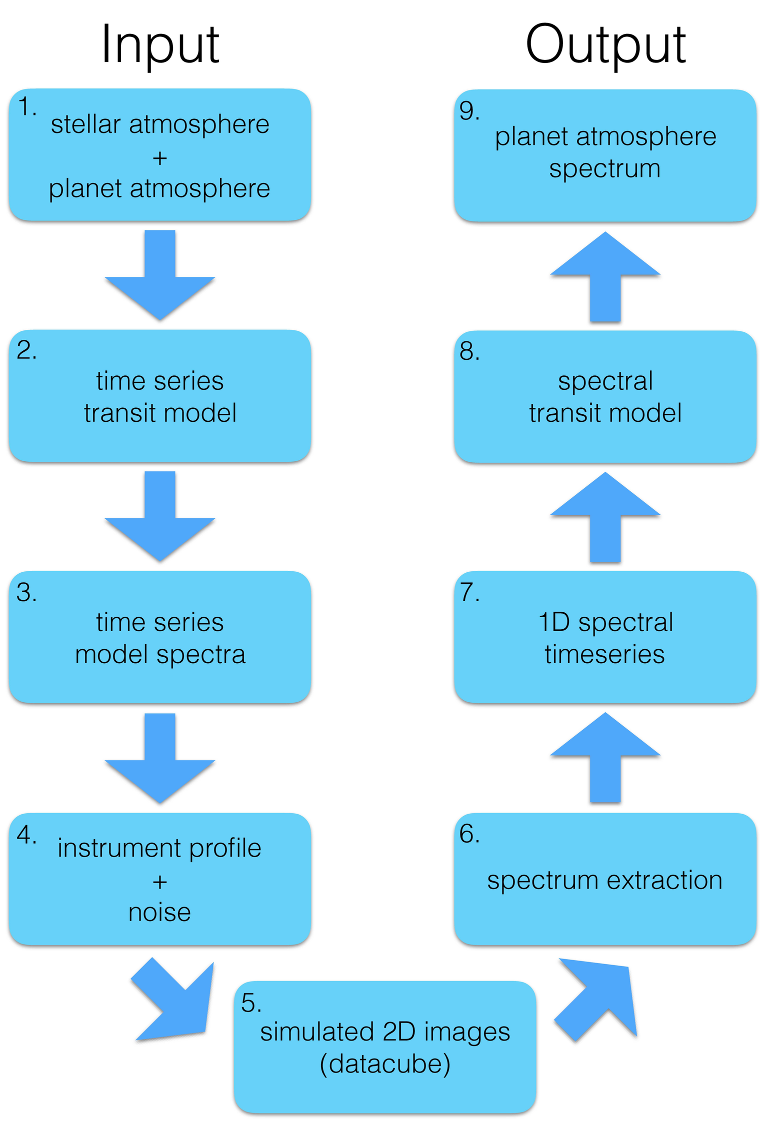

FIGURE 2: Workflow. The diagram gives an overview of our end-to-end simulations and extraction tools. Each step has a seperate modular tool developed for spectral transit observations.

In preparation for science operations and observations of transiting exoplanets we have developed a suite of software tools to generate 2D spectrum images and to extract and analyze observations from the SOSS mode. All source code has been made open source and is available to the community via github: **https://github.com/jasonfrowe/jwst** Comments and contributions are welcome.

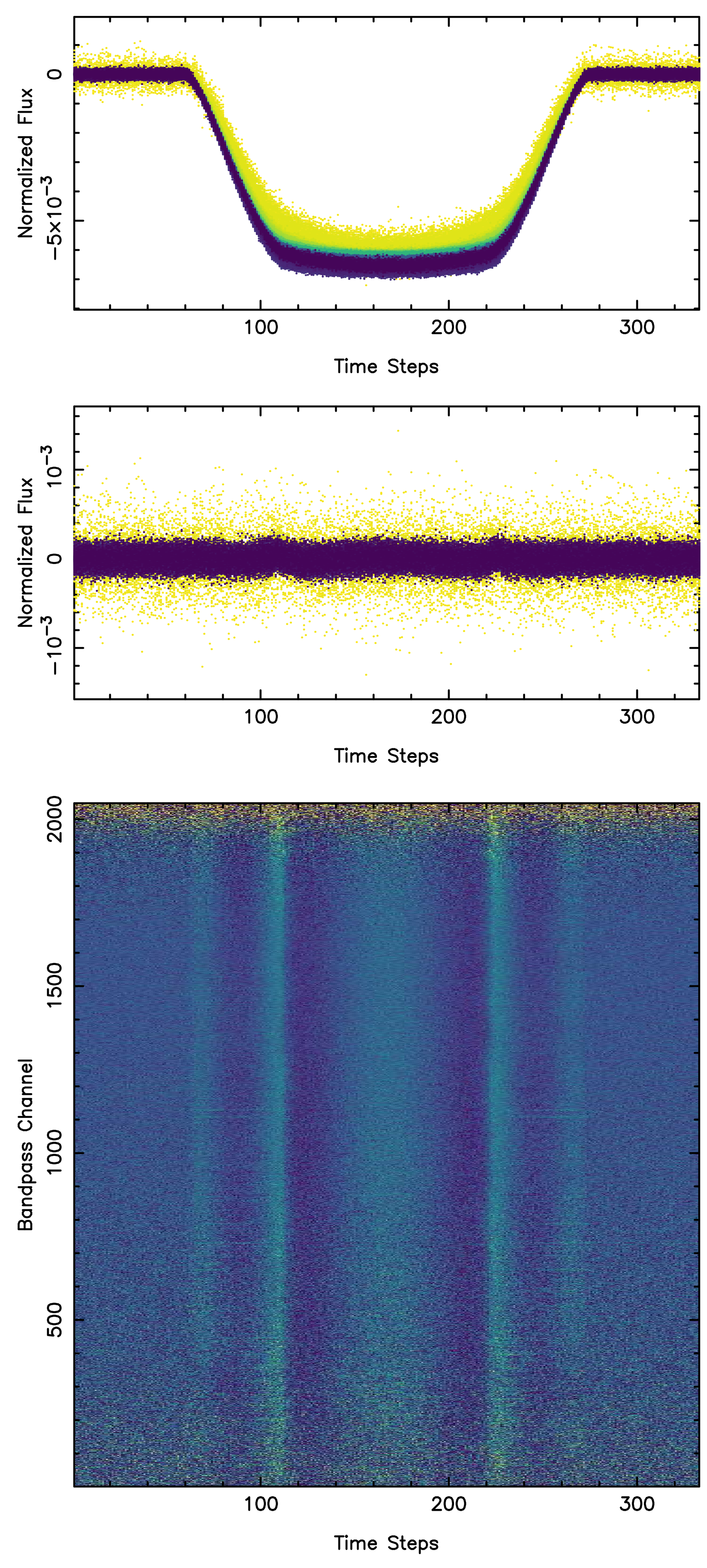

FIGURE 3: The top panel shows the extracted simulated transit lightcurves ranging from 0.8 μm (yellow) to 2.8 μm (dark purple). Each time step corresponds to 15 seconds with a total duration of 1.2 hours. The middle panel shows the residuals after subtraction of the best fit spectral transit model. The kinks seen at the location of the ingress and egress are due to a mismatch to the adopted limb-darkening model. The bottom panel shows the residuals as a function of bandpass with channel 1 corresponding of 0.8 μm and channel 2048 corresponding to 2.8 μm. Data are simulated with a non-linear model and extracted using a quadratic model. A quadratic model is typically adopted when modeling transit lightcurves.

End-to-End Simulation Workflow

Simulated observations use high resolution (R $\sim$ 500 000) ATLAS-9 models for the host star calculated at 18 surface angles to allow for the calculation of wavelength dependent limb-darkening coefficients. Transit models use a quadratic limb-darkening law with high-resolution (R $\sim$ 100 000) exoplanet atmosphere models (B. Benneke) to produce time series spectroscopic models that are: drizzled across multiple orders to match the NIRISS-SOSS pixel resolution; convolved with the instrument PSF; multiplied by the instrument response function with noise sources added. The resultant datacube is a realistic representation of JWST NIRISS observations. A single slice is shown in Figure 1. An overview of our end-to-end model is shown in Figure 2.

The datacube is analyzed to extract time-series 1D spectra. This is equivalent to having a transit model for each observed resolution element. For SOSS this means more than 2000 simultaneous transit light-curves, each observed with a different bandpass. The top panel of Figure 3 shows the extracted transit lightcurve for each bandpass for simulations of GJ 436b.

Spectral Transit Model

The developed spectro-photometric transit model is parameterized by the orbital period (P), center of transit time ($T0$), impact parameter (b), scaled planetary radius, $R_{\mathrm{P}}/R_{\star}$, eccentricity, normalization factor based on out-of-transit flux, limb-darkening co-efficients, radial velocity, planet albedo, ellipsoidal variations, secondary eclipse depth and dilution from photometric crowding. The model can handle multiple planets with non-interacting Keplerian orbits with implicit input of transit timing variations. Each parameter can be fitted bolometrically or per bandpass. Our model also includes a Gaussian Process correlated noise model via two hyperparameters to describe a squared exponential kernel. Correlated noise is expected due to astrophysical phenomena such as star spots. Gaussian priors for any and all model parameters can be specified.

With 2048 bandpasses, a minimum model to properly model a transiting exoplanet requires P, $T0$, b, 2048 parameters for $R_{\mathrm{P}}/R_{\star}$, $2{\times}2048$ limb-darkening parameters and 2048 normalization parameters. As the impact parameter is independent of wavelength, most model parameters are correlated, thus 8195 parameters need be simultaneously fitted.

To solve the computational problem of finding a best fit solution we:

- Find a best fit transit model for a white-light integrated transit curve
- Fit each bandpass independently with the impact parameter fixed to the white-light solution
- Refine all parameters simultaneously with a limited memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm.

The choice of L-BFGS requires the calculation of numerical gradients, which have been internally optimized though parallelization with OPEN-MP directives and cached calculations to minimize duplication. With 20 CPUs, a bestfit solution for a JWST SOSS observation of a single transit with the assumption of independent Gaussian uncertainties can be completed in 2 to 4 hours. When a full GP co-variance is invoked, computational run times are approximately 10 times slower. Our programs also include the ability to bin data to enable *quick-look* computations.

Posteriors for model parameters are computed from Markov-Chain-Monte-Carlo. A deMCMC approach has been adopted to handled correlated parameters. To obtain convergence with 8195 free parameters, chain with lengths of $\sim$ 10M are required. The computational overhead for a full calculation is on the timescale of two weeks.

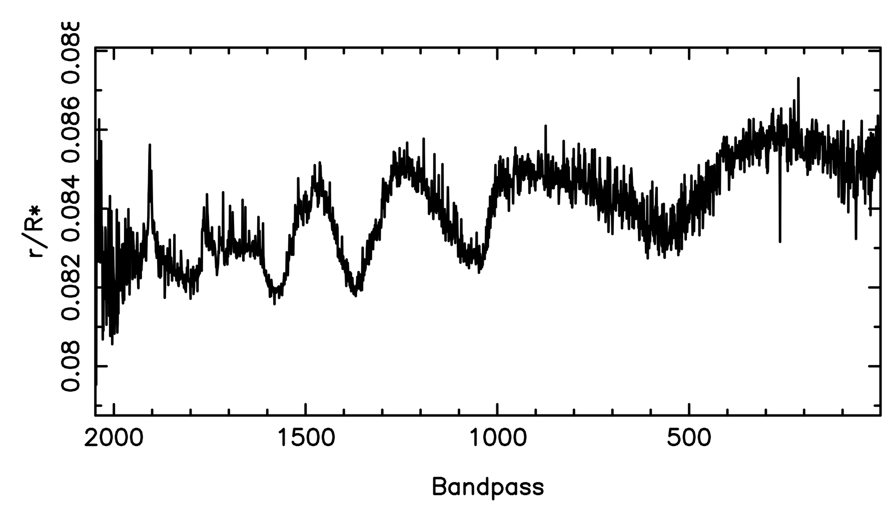

FIGURE 4: Recovered $R_{\mathrm{P}}/R_{\star}$for high signal to noise simulations of GJ 436. Bandpass 1 through 2048 corresponds covers 2.8 μm to 0.8 μm.

Figure 4 shows the recovered spectrum for our simulated dataset of GJ-436b as parameterized by $R_{\mathrm{P}}/R_{\star}$, which agrees well with our input spectra. We are still in the process of investigating systematic errors due to the choice of a quadratic limb-darkening model. We are also investigating the use of GPU computing for matrix inversion to improve GP run times. Questions? Just ask!