1. ABOUT THE DATASET

Title: 3D simulations of the exoplanet TRAPPIST-1e using WACCM6

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2. TERMS OF USE

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3. PROJECT AND FUNDING INFORMATION

Title: 3D simulations of oxygenated rocky planetary climates and observational predictions

Dates: 10/2019 – 05/2023

Funding organisation: STFC

Grant no.: ST/T506230/1

4. CONTENTS

Simulation File description

See the data file table on the next page for a list of files associated with each simulation scenario. The prefix (b.e21.BWma1850.f19_g17) for the filenames describes a B case from CESM2.1.3 using the BWma1850 compset (see the CESM2 compsets here https://docs.cesm.ucar.edu/models/cesm2/config/compsets.html). The grid is f19_g17, which has 144 longitude grid points and 96 latitude grid points.

Each case has three files. This includes a 10-year time-average of 'h0' files, a 10-year time-average of 'h1' files, and a single h1 file. h0 files are monthly mean files. h1 files are snapshot files providing instantaneous output required for simulating transmission spectra and emission spectra. Each simulation was run for a minimum of 250 years. Each h0 file has 269 or more variables, whilst each h1 file has 62 variables.

To read in and analyse data, the Python programming code can be used with the xarray package. Example scripts can be found at https://zenodo.org/doi/10.5281/zenodo.5809268 and https://github.com/exo-cesm/CESM2.1.3/tree/main/Tidally_locked_exoplanets. An example script to take snapshot (h1) files and convert them to .gcm binary files, which can then be uploaded to PSG, can be found at https://zenodo.org/records/7066518.

Data file table

Simulation name	Files
P19 PI	b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.cam.h0.0320-0329.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.cam.h1.0320-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.cam.h1.0320-0329.nc
P19 10% PAL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.10pc_o2.cam.h0.0350-0359.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.10pc_o2.cam.h1.0350-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.10pc_o2.cam.h1.0350-0359.nc
P19 1% PAL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.1pc_o2.cam.h0.0310-0319.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.1pc_o2.cam.h1.0310-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.1pc_o2.cam.h1.0310-0319.nc
P19 0.1% PAL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.0.1pc_o2.cam.h0.0300-0309.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.0.1pc_o2.cam.h1.0300-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.0.1pc_o2.cam.h1.0300-0309.nc
P19 no TL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.no_T_lock.cam.h0.0280-0289.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.no_T_lock.cam.h1.0280-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.P19.no_T_lock.cam.h1.0280-0289.nc
W21 PI	b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.cam.h0.0293-0302.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.cam.h1.0293-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.cam.h1.0293-0302.nc
W21 10% PAL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.10pc_o2.cam.h0.0300-0309.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.10pc_o2.cam.h1.0300-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.10pc_o2.cam.h1.0300-0309.nc
W21 1% PAL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.1pc_o2.cam.h0.0271-0280.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.1pc_o2.cam.h1.0271-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.1pc_o2.cam.h1.0271-0280.nc
W21 0.1% PAL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.0.1pc_o2.cam.h0.0250-0259.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.0.1pc_o2.cam.h1.0250-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.0.1pc_o2.cam.h1.0250-0259.nc
W21 no TL	b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.no_T_lock.cam.h0.0310-0319.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.no_T_lock.cam.h1.0310-01-01-00000.nc b.e21.BWma1850.f19_g17.TRAPPIST1_e.W21.no_T_lock.cam.h1.0310-0319.nc

Solar file description

Two files are used as the stellar spectrum input into the WACCM6 model to represent the star TRAPPIST-1. These are: TRAPPIST1_flux_at_e_P19.nc, and TRAPPIST1_flux_at_e_W21.nc. TRAPPIST1_flux_at_e_P19.nc is rescaled and rebinned model 1A from Peacock *et al*. (2019), whilst TRAPPIST1_flux_at_e_W21.nc is rescaled and rebinned from Wilson *et al*. (2021a).

References are below, including Peacock *et al*. (2020) and Wilson *et al*. (2021b) which are the data references for the TRAPPIST-1 spectra:

- Peacock, S., Barman, T., Shkolnik, E.L., Hauschildt, P.H. and Baron, E., 2019. Predicting the extreme ultraviolet radiation environment of exoplanets around low-mass stars: the TRAPPIST-1 system. The Astrophysical Journal, 871(2), p.235.
- Peacock, S. 2020, Habitable Zones and M dwarf Activity across Time ("HAZMAT"), STScI/MAST, doi: 10.17909/T9-J6BZ-5G89.

- Wilson, D.J., Froning, C.S., Duvvuri, G.M., France, K., Youngblood, A., Schneider, P.C., Berta-Thompson, Z., Brown, A., Buccino, A.P., Hawley, S. and Irwin, J., 2021a. The mega-muscles spectral energy distribution of trappist-1. The Astrophysical Journal, 911(1), p.18.
- Wilson, D. J., Froning, C., Duvvuri, G., et al. 2021b, Mega-MUSCLES Semi-empirical SED of TRAPPIST-1, Version 1, Zenodo, doi: 10.5281/zenodo.4556130.

5. METHODS

The data was generated using the CESM2.1.3 code (https://escomp.github.io/CESM/versions/cesm2.1/html/downloading_cesm.html) on computing nodes at the University of Leeds ARC4 supercomputer (https://arcdocs.leeds.ac.uk/systems/arc4.html). Each simulation used a BWma1850 compset, which is a WACCM6 configuration that approximates the climate of Earth in the year 1850, with cyclic conditions each simulation year. This compset was then altered to simulate possible climate scenarios of the exoplanet TRAPPIST-1e. The exact source code and file changes required for each case can be found on GitHub at https://github.com/exo-cesm/CESM2.1.3/tree/main/Tidally_locked_exoplanets. When crashes occurred in the model due to instabilities, the timestep was decreased until stability was reached, and then the model was returned to its default timestep. This was done by setting the following variables in the 'user_nl_cam' file:

&dyn_fv_inparm
fv_nspltvrm = 64
fv_nsplit = 64
fv_nspltrac = 64
/

before removing these variables from user_nl_cam in a branch simulation.

netCDF Operators (NCOs) were used to condense the data through a time average. E.g., the command:

ncra file1.nc file2.nc file3.nc file4.nc file1-4.nc

produces *file1-4.nc* which is a time-average of file1.nc, file2.nc file3.nc, and file4.nc.

Dan Marsh, Catherine Walsh, and Allison Youngblood, all consulted on the production of the data and its analysis.

More detailed information on methods and setup can be found on GitHub https://github.com/exo-cesm/CESM2.1.3/tree/main/Tidally_locked_exoplanets and in the associated article: Cooke GJ et al. 2023, Degenerate interpretations of O_3 spectral features in exoplanet atmosphere observations due to stellar UV uncertainties: a 3D case study with TRAPPIST-1e, *The Astrophysical Journal*, 2023 (Accepted).