Geosci. Model Dev. Discuss., doi:10.5194/gmd-2017-24, 2017
Manuscript under review for journal Geosci. Model Dev.
Discussion started: 28 February 2017

Geoscientific
Model Development
Discussions
Open Access

The Palaeoclimate and Terrestrial Exoplanet Radiative Transfer Model Intercomparison Project (PALAEOTRIP): experimental design and protocols

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Abstract. Accurate radiative transfer calculation is fundamental to all climate modelling. For deep palaeoclimate, and increasingly terrestrial exoplanet climate science, this brings both the joy and the challenge of exotic atmospheric compositions. The challenge here is that most standard radiation codes for climate modelling have been developed for modern atmospheric conditions, and may perform poorly away from these. The palaeoclimate or exoclimate modeller must either rely on these or use bespoke radiation codes, and in both cases rely on either blind faith or *ad hoc* testing of the code. In this paper, we describe the protocols for the Palaeoclimate and Terrestrial Exoplanet Radiative Transfer Model Intercomparison Project (PALAEOTRIP) to systematically address this. This will compare as many radiation codes used for palaeoclimate or exoplanets as possible, with the aim to constrain the ranges of far-from-modern atmospheric compositions in which the codes perform well. This paper describes the experimental protocol and invites community participation in the project through 2017.

1 Introduction

Earth's atmospheric composition has varied dramatically through time, and yet-to-be-discovered terrestrial exoplanets will add untold diversity. A typical model of late Archean atmospheric composition, for example, would be of 30,000 ppm CO_2, 1000 ppm CH_4, no oxygen or ozone and an unknown nitrogen inventory, whereas escape from 'snowball Earth' glaciation may take 0.1 bar CO_2. A fundamental part of the palaeoclimate problem, and equivalently the exo-climate problem, may be stated as: given some atmospheric composition, what was the energy balance of the planet? Or equivalently: for given atmospheric composition and incident solar flux, what was the surface temperature?

This is a conceptually simple physics problem. An atmospheric composition and structure needs to be given, then the radiation field must be simulated, the equations for which are well known (e.g. Goody and Yung, 1989). Regrettably, implementation is far from simple. Millions of gas absorption lines from numerous gases are relevant to the climate problem. Herculean work has assembled most of these into large and oft-revised databases (e.g. Rothman et al., 2013). From these databases, absorption cross sections may be calculated as a function of temperature and pressure. Even these cross sections, calculated with standard assumptions regarding the shape of absorption lines, have some notable disagreement with observations and smoothly varying "continuum" absorption must be added to produce realistic cross sections. Armed with cross sections, the radiative transfer equations may then be solved at the natural resolution of the lines—a so-called line-by-line calculation. Alas, these can take time on the order of the order one to ten hours for a single column, hence are too slow by many orders of magnitude to be used in a climate model.

In a general circulation model (GCM), the radiative transfer for a single column must be evaluated in a fraction of a second. Consequently, simplifications must be made in the treatment of the radiative transfer and the spectral dependence must be heavily parameterized. To optimise efficiency, these parameterizations are made for limited ranges of atmospheric composition or, equivalently, for certain column abundances of absorbing molecules. Often, these parameterizations were made a decade or more ago, with poor documentation. Where an older (and likely faster) GCM is used for palaeoclimate research, one is automatically in the situation of using a legacy radiation code.

At the other end of the modelling spectrum, there still exists a cottage industry of bespoke development of fast-enough radiative transfer codes for deep palaeoclimate, planetary atmospheres, or other obscure radiative transfer problems, where all the required steps are made ad hoc. However, this can mean that the resources required to sufficiently test the code are unavailable locally.

Three broad classes of problem arise. First, whilst excellent parametrization is possible within design ranges, some parameterizations do not perform as well as a third-party user may hope. For example, intercomparison of radiation codes used for the IPCC Forth Assessment Report (Collins et al., 2006) showed that many codes simulated the changes due to a doubling of carbon dioxide poorly. Second, performance of codes will decrease outside design ranges, which often includes the regions that we are interested in for palaeoclimate (e.g. Goldblatt et al., 2009b). Third, errors are made in parameterizations (especially in bespoke codes) which can remain undetected through review and for some years afterwards.

The palaeoclimate or exoplanet modeller is thus in a bind. The science interest is in novel atmospheric compositions, whose radiation properties are outside the intuition of most non-specialists. It would be prudent to test *any* fast radiation code that one planned to use against a well-trusted line-by-line code across the parameter space of interest; however, doing this requires both the specialist knowledge in radiative transfer, the local availability of such a mode and a lot of time and energy. All of these can be hard to come by.

With the Palaeoclimate and Terrestrial Exoplanet Radiative Transfer Model Intercomparison Project (PALAEOTRIP), we hope to alleviate this problem. Our aim is to test a large number of fast radiation codes, both GCM and bespoke, against line-by-line models for a wide range of conditions applicable to palaeoclimate and terrestrial exoplanet research. Such intercomparison studies have a long history in application to modern conditions and anthropogenic global change (e.g. Ellingson et al., 1991; Fouquart et al., 1991; Collins et al., 2006; Pincus et al., 2016) and have contributed markedly to improvements in the fidelity of radiation codes and thus the robustness of climate models. Our hope is that exporting such systematic intercomparison to deep palaeoclimate and exoplanets will yield similar improvements. In this paper, we describe the experimental design and protocol[1]. Up-to-date project information will be available at www.palaeotrip.org throughout the project.

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[1] Community input on the experimental design and protocols can, at this stage, be provided via the open peer review process "discussion" phase of *Geoscientific Model Development*. These will be considered final in post review manuscript.

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2 Experimental Design

2.1 Philosophy

The standard method of radiative transfer intercomparison is to compare model output—especially changes in fluxes in response to changes atmospheric composition—calculated on *fixed* atmospheric profiles. The use of fixed profiles is essential to isolate the fidelity of the radiative transfer codes (to be evaluated) from the myriad of other processes that determine the atmospheric profile. This methodology has a long history (e.g. Ellingson et al., 1991; Fouquart et al., 1991); see Collins et al. (2006) for an in-depth discussion of this methodology. We use instantaneous (unadjusted) radiative forcings; the most modern radiative transfer intercomparison project for IPCC class models (Pincus et al., 2016) additionally use *effective radiative forcings* that account for a variety of rapid adjustments in GCMs. Our method here corresponds to the (Pincus et al., 2016) assessment of "parametrization error".

Twelve sets of experiments, each of which varies a parameter of key importance for palaeoclimate and Earth-like exoplanets, should be performed. The choice of parameter space represents a range of mainstream assumptions about atmospheric composition through Earth history. We have explored all of this parameter space previously: see Goldblatt et al. (2009b) and Byrne and Goldblatt (2014a, b) for well mixed greenhouse gases, Goldblatt and Zahnle (2011b, a) for clouds and Goldblatt et al. (2009a) for varying atmospheric pressure. One class of model atmospheres that we exclude is H_2 dominated atmospheres (Wordsworth and Pierrehumbert, 2013), because variation in mean molecular weight will mean that air-broadened line shapes may not be appropriate and thus a majority of codes may not perform well (that is, these atmospheres require rather specialist treatment, beyond the scope of this intercomparison). Our hope it that by assembling and analyzing results from many radiative transfer codes outside of modern conditions, we will both help future investigators to make an educated choice of which radiative transfer code is applicable for a particular experiment, and inform model developers of opportunities for improvement of models.

All of the required input files for the project are available at www.palaeotrip.org, and as an online supplement to this paper.

2.2 Model atmosphere

2.2.1 Atmospheric profile

All experiments use a Global Annual Mean (GAM) profile. This based on a profile derived from averaging of reanalysis data by Byrne and Goldblatt (2014a). This specific profile should be used, and none substituted for it. Experiments 1–4, 6–8 and 10 use the GAM profile unmodified, whereas experiments 5 and 9 modify it as described for experiment 5.

2.2.2 Line data

Line-by-line codes should use line data from HITRAN2012 (e.g. Rothman et al., 2013).

Bespoke, GCM and legacy radiation codes will use a variety of line data. It is acceptable to submit either the most current/standard version, or a variety of versions corresponding to different applications. The model version number/name, a a brief description and/or link to the full description should be included as metadata with the model output, especially the version number/name of the code.

2.2.3 Stellar fluxes

Stellar fluxes are supplied for both the Sun and and example M-star (ADLeo). Where a solar flux is specified ad-hoc, these should be used. As with line data, these may be pre-set in some bespoke, legacy and GCM codes: use the standard configuration and include whatever description possible. Where it is impractical to modify the stellar flux, perform experiments 1–5 and 9–12 only.

2.2.4 Clouds

Experiments with both low and high clouds are included. Calculations should be done with a single profile, with a cloud fraction of unity. Clouds may be specified in different ways in different radiation codes; the nominal descriptions here should be matched as well as possible given how clouds are specified in the particular radiation code, and appropriate description provided as metadata.

Vertical position: if clouds are specified in a layer, low clouds should be in the 800–825 hPa layer, high clouds in the 250–300 hPa layer. If they are specified on levels, they should be at 812.5 hPa and 275 hPa, and can be specified with minimal vertical extent (or extent not exceeding the boundaries of the layer).

Low clouds are taken to be made of liquid water droplets. Thus cloud particles are well described as Mie spheres, so consistent specification across models should be straightforward. A standard low cloud should have a water path of $40\,\mathrm{g\,m^{-2}}$ and effective radius of $10\,\mu$m (Goldblatt and Zahnle, 2011b). Single scattering properties from a Mie code can be provided by the PALAEOTRIP team if requested.

High clouds are taken to be made of ice crystals, and are thus more complicated to describe, as there are a variety of ice habits which are all non-spherical. The normal parameter to describe the size of particles is the effective diameter, D_{eff}. A standard high cloud should have a water path of $20\,\mathrm{g\,m^{-2}}$ and effective diameter of $70\,\mu$m (Goldblatt and Zahnle, 2011b). Where single scattering properties need to be specified, these should use the “general habit mixture” from Baum et al. (2014) which are available for all sizes required from http://www.ssec.wisc.edu/ice_models/polarization.html.

2.2.5 Miscellaneous details

A solar zenith angle of 60° should be used for all experiments. The surface should be black for thermal calculations and have a grey albedo of 0.12 in solar calculations. If a combined solar-thermal calculation is performed, the separation between solar and thermal albedos should be at $3\,\mu$m.

2.3 Experiments

In addition to standard conditions, four sets of clear-sky experiments applicable to palaeoclimate should be performed:

1. Standard conditions
2. Varying the concentrations of well-mixed greenhouse gases (WMGHG).
3. Varying the amount of water vapour.
4. Switching atmospheric ozone and oxygen on/off.
5. Varying the surface pressure.

A further three clear-sky experiments applicable to exoplanets should be performed, with the solar spectrum is replaced with an M-star spectrum. This is relevant because it will be relatively easy to find and observe planets receiving the same insolation as Earth around M-stars, but this stellar spectrum is significantly to the red of the solar spectrum (so less Rayleigh scattering but more water absorption are expected):

6. Standard conditions, with M-star spectrum.
7. Varying the amount of water vapour, with M-star spectrum.
8. Varying the surface pressure, with M-star spectrum.

Four experiments with clouds should be performed, to test the representation of cloud radiative properties. All should use standard conditions with a solar spectrum:

9. Inclusion of a low level (e.g. stratus) cloud, with fixed droplet size distribution and varying cloud water path.
10. Inclusion of a low level (e.g. stratus) cloud, with fixed cloud water path and varying droplet size distribution.
11. Inclusion of a high level (e.g. cirrus) cloud, with fixed droplet size distribution and varying cloud water path.
12. Inclusion of a high level (e.g. cirrus) cloud, with fixed cloud water path and varying droplet size distribution.

General Notes:

- Experiments 1–4, 6–8 and 10–12 all use the Global Annual Mean temperature-pressure (T-p) profile. Climatological profiles of water vapour and ozone are supplied. Experiments 5 and 9 use modifications of the GAM profile.
- Experiments 6–8 use the M-star spectrum, all others use the solar spectrum.
- The runcode is a unique identifier for each run, which should be used as the name of the output file for each run (e.g. `runcode.dat`). These all begin `PT` (for palaeotrip, and to avoid starting a filename with a number), followed by the number of the experiment and the run number (x) within each experiment, counting from the lowest value of any quantity varied.

Experiment 1 (Standard Conditions): GAM profile with climatological water and ozone abundances. Volume mixing ratios of WMGHGs: 400×10^{-6} CO_2, 1×10^{-6} CH_4, and 1×10^{-6} N_2O. Oxygen mixing ratio is 0.21, and the remainder of the atmosphere is nitrogen. Runcode: `PT1`.

Experiment 2: The concentration of each WMGHG should be varied in series (with the other two held at standard conditions). The ranges used should be: CO_2 from 10^{-9} to 10^{-1}, CH_4 from 10^{-9} to 10^{-2} and N_2O from 10^{-9} to 10^{-2}. The lower end of each range is selected for minimal radiative significance of that gas (see Byrne and Goldblatt, 2014b). The upper limit is an arbitrary guess at an upper bound for an Earth-like planet. Models should be run with concentrations evenly spaced in log units, with five runs per one log unit (e.g. $\{1 \times 10^{-9.0}, 1 \times 10^{-8.8}, 1 \times 10^{-8.6}, 1 \times 10^{-8.4}, 1 \times 10^{-8.2}, 1 \times 10^{-8.0}, \dots\}$). Runcodes: `PT2a`_*x*, `PT2b`_*x*, `PT2c`_*x* for CO_2, CH_4 and N_2O respectively.

Experiment 3 The water vapour mixing ratio should be changed by a constant factor, with all other gases as standard conditions. The factors to use should be 0.1 to 10, which correspond to the differences between saturation vapour pressures from 255 K to 330 K. Models should be run with concentrations evenly spaced in log units, with five runs per one log unit. Runcodes: `PT3`_*x*

Experiment 4 Absorption by atmospheric oxygen and ozone should be turned off, with all other conditions as standard. Note there is no change to the T-p profile. Runcodes: `PT4`

Experiment 5 The surface pressure is varied between 0.1 and 10 bars. This is done by multiplying the pressure vector in the GAM profile by a factor $0.1 \leq y \leq 10$, and dividing mixing ratio vectors of minor absorbing species (CO_2, CH_4, N_2O and O_3) by y so that the mass of each absorber is conserved. Absorption by atmospheric oxygen should be turned off. Models should be run with y evenly spaced in log units, with five runs per one log unit. Runcodes: `PT5`_*x*

Experiments 6 As experiment 1, with Mstar spectrum. Runcode: `PT6`

Experiments 7 As experiment 3, with Mstar spectrum. Runcodes: `PT7`_*x*.

Experiments 8 As experiment 5, with Mstar spectrum. Runcodes: `PT7`_*x*.

Experiments 9 A low altitude cloud is added to the standard profile (experiment 1). Water path should vary between 10 and 100 $g\,m^{-2}$, with 11 values evenly spaced in log space ([10.00, 12.59, 15.85, 19.95, 25.12, 31.62, 39.81, 50.12, 63.10, 79.43, 100.00]). Standard effective radius of 10 μm. Runcodes: `PT9`_*x*.

Experiments 10 A low altitude cloud is added to the standard profile (experiment 1). Fixed water path of 40 $g\,m^{-2}$. Effective radius should vary between 5 and 25 μm in 1 μm steps. Runcodes: `PT10`_*x*.

Experiments 11 A high altitude cloud is added to the standard profile (experiment 1). Water path should vary between 10 and 100 $g\,m^{-2}$, with 11 values evenly spaced in log space. Standard effective diameter of 70 μm. Runcodes: `PT11`_*x*.

Experiments 12 A high altitude cloud is added to the standard profile (experiment 1). Fixed water path of 20 $g\,m^{-2}$. Effective diameter should vary between 20 and 120 μm in 10 μm steps. Runcodes: `PT12`_*x*.

Note that, for most experiments, a literal interpretation of the changes to atmospheric conditions will imply some physical inconsistencies: there is no change in atmospheric pressure when CO_2 mixing ratio increases to 10^{-1}, water vapour may become super-saturated, there is no change to the T-p profile when gas concentrations change. These inconsistencies are tolerated, with the philosophy of designing simple and easy to compare experiments which test the fidelities of the radiation codes, with is best done on fixed profiles.

2.4 Submission of results

To facilitate comparison of many codes, each of which undoubtedly has its own output format, we ask that contributing scientists reformat output into the standard plain text format described below. Not only are these formats simple, but we have provided MATLAB and Python codes which will write them automatically from your output. These scripts, and sample output files, are available at www.palaeotrip.org and included in the supplementary information for this paper.

For spectrally integrated output (dimensions $\mathrm{W\,m^{-2}}$) the PALAEOTRIP data format consists of a plain text file with an ten line header that includes the metadata in Table 2 followed by the data header describing each column, consisting the the variables in Table 1. Each data column is twelve characters long and therefore all quantities will be rounded to twelve figures. The formatting codes accept model output that corresponds to either pressure levels or layers and will automatically distinguish between these (levels are the boundary between model layers). Quantities on layers and levels will be exported to separate data files but in both cases the first column will correspond to the pressure at the level or centre of the layer in pascals. The filename convention is `runcode_levels.txt` and `runcode_layers.txt` (e.g. `PT2a_1_layers.txt`, `PT2a_1_layers.txt`).

For spectrally resolved output (dimensions $\mathrm{W\,m^{-2}\,\mu m^{-1}}$) other than from line-by-line models, where available, a separate file should be provided for each flux, with pressure levels as rows and each spectral bin as a column. Two rows of column headers should give the minimum and maximum wavelength of the spectral bin. Other aspects of the output files should be as the spectrally integrated fluxes. The filename convention is `runcode_variable.txt` (e.g. `PT2a_1_layers.txt`, `PT2a_1_Fswdn.txt`).

All model output should be put into a single `.zip` file called `yourname.zip` and can be uploaded via the palaeotrip website. Include a `readme.txt` file as necessary.

For line-by-line models, spectrally resolved output should be subsampled to $1\,\mathrm{cm^{-1}}$ resolution. Contact the PALAEOTRIP project team directly to discus how to submit this (info@palaeotrip.org).

3 Protocol and information for contributors

The experimental design and protocols for the PALAEOTRIP are described in this paper[2]. If you intend to submit model output to the PALAEOTRIP project, we ask that you register your intention at www.palaeotrip.org. This will ensure that models are not run in duplicate by different groups, and that your model output is expected.

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[2] Community input on the experimental design and protocols can, at this stage, be provided via the open peer review process "discussion" phase of *Geoscientific Model Development*. These will be considered final as described in the post review manuscript.

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Table 1. Model output that will be accepted by PALAEOTRIP.

Variable	**Description**	**Unit**
Quantities on levels (bold variables are required):		
plevel	pressure on levels (layer bountaries)	Pa
Fswdndir	direct solar flux down	$\mathrm{W\,m^{-2}}$
Fswdndif	difuse solar flux down	$\mathrm{W\,m^{-2}}$
Fswdn	total solar flux down (Fswdndir+Fswdndif)	$\mathrm{W\,m^{-2}}$
Fswup	solar flux up	$\mathrm{W\,m^{-2}}$
Fswnet	net solar flux	$\mathrm{W\,m^{-2}}$
Flwdn	thermal flux down	$\mathrm{W\,m^{-2}}$
Flwup	thermal flux up	$\mathrm{W\,m^{-2}}$
Flwnet	net thermal flux (Flwdn-Flwup)	$\mathrm{W\,m^{-2}}$
Quantities on layers (all should be included if any are)		
player	pressure at layer centre	Pa
Qsolar	solar heating rate	$\mathrm{K\,day^{-1}}$
Qtherm	thermal heating rate	$\mathrm{K\,day^{-1}}$

Table 2. Model metadata to be included with PALAEOTRIP submissions.

Variable	**Metadata Description**
runcode	String with the code of run (see experiment descriptions)
modelname	String with the name (and version number) of model
username	String with your name (e.g. ‘Colin Goldblatt’)
useremail	String with your email (e.g. ‘czg@uvic.ca’)
usernotes	String with any notes about this run

The anticipated timeline of the project is in Table 3. Sadly, few deadlines survive contact with academics, but it is our intention to keep a tight schedule. We will post any updates to www.palaeotrip.org and communicate schedule changes directly to all participating scientists.

We intend that everyone submitting unique model results will be offered authorship on the final paper. Lead authorship will be by one of the project team, who will additionally determine the order of authorship (likely project team followed by contributing scientists, listed alphabetically). This paper will be circulated amongst all co-authors prior to submission.

A motivation of this project is to find out how a variety of radiation codes perform across a range of conditions applicable to palaeoclimate and exoplanets, so that future model users may know the range of conditions across which each model is likely to be accurate. Therefore, it is essential that models are able to be identified in the final paper. The analysis will be restricted to the range of conditions specified here, as an indicator of performance in palaeo- and exoclimate studies. We have no interest

Table 3. Proposed PALAEOTRIP timeline

Timeframe	Activity
January 2017	Submit description/protocol paper
January – March 2017	Review of description/protocol paper. Community feedback on experimental design.
February – March 2017	Respond to review of protocol paper and finalize protocol.
April – July 2017	Contribution of radiative transfer model runs.
May – August 2017	Analysis of model output by PALAEOTRIP team.
August – September 2017	Write results paper, circulate to co-authors.
October 2017	Co-author comments.
November 2017	Revise and submit results paper.

in, or intention of, commenting on the fitness of any model for any other purpose. It is the responsibility of scientist submitting model results to assert that the model can be identified in the final paper.

4 Summary and Discussion

PALAEOTRIP will run twelve controlled experiments addressing the radiative transfer through a subset of conditions expected through Earth's past climate, and applicable to Earth-like exoplanets. We invite community participation in the experiment. Over the course of the next year, the model runs will be performed and compared. The anticipated outcome is that the community will be better informed about the performance of available radiative transfer codes for palaeo- and exoclimate research.

The range of conditions which we have specified experiments for is somewhat "vanilla". It likely does not represent the full range of conditions seen in Earth's past, and will be a tiny fraction of the parameter space for Earth-like exoplanets. This is motivated to get wide participation; that is to specify conditions which most models which derive from Earth atmospheric sciences should be capable of being run for. We anticipate that, if this intercomparison is successful, we may be able to lead a more wide-ranging intercomparison in the future.

5 Code and data availability

A zip file containing the GAM profile and scripts to be used to write model output into the specified format is available in an online supplement to this article. Version 0.9 (i.e. beta version) corresponds to this version, in *Geoscientific Model Development Discussions*. Version 1.0 will accompany the final peer reviewed manuscript in *Geoscientific Model Development*. Updated versions of these will be made available through the project website, www.palaeotrip.org.

Final model output will be available from www.palaeotrip.org and as an online supplement to the paper which will describe the results of the intercomparison.

Author contributions. CG has designed the experiment and is responsible for the scientific content herein. LK has provided technical assistance.

Competing interests. The authors declare that they have no conflict of interest.

Acknowledgements. Financial support has been provided by and NSERC discovery grant and UVic startup funds to CG.

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