ROCKE-3D tutorial

michael.way@nasa.gov kostas.tsigaridis@columbia.edu

igor.aleinov@columbia.edu tom.clune@nasa.gov c.m.colose@nasa.gov

vincent.kofman@nasa.gov anthony.leboissetier@nasa.gov

Link to May 2024 tutorial:

https://www.youtube.com/playlist?list=PLpMmnV3HS7r3ryMbNOPynfSrZY4w7mHoB

Link to May 2023 tutorial:

https://www.youtube.com/playlist?list=PLpMmnV3HS7r2XdvFwfQzbM344x6wcD41K

Link to May 2021 tutorial:

https://www.youtube.com/playlist?list=PLpMmnV3HS7r3KGXX8hmIBR3grXNu5hfW-

Link to May 2020 tutorial:

https://www.youtube.com/playlist?list=PLpMmnV3HS7r2djsCJ2OHAVbBA52zp4EHB

Link to May 2019 tutorial:

https://www.youtube.com/playlist?list=PLpMmnV3HS7r3jlWHp2j-M1MtMIk1CB25B

Link to May 2018 tutorial:

https://www.youtube.com/playlist?list=PLpMmnV3HS7r36l1qX_3cNV7CinX2qaS7W

How to join the tutorial

The Zoom link is TBD

Please **mute** your microphone at all times unless you need to speak.

E-mail one of us if your problems persist:

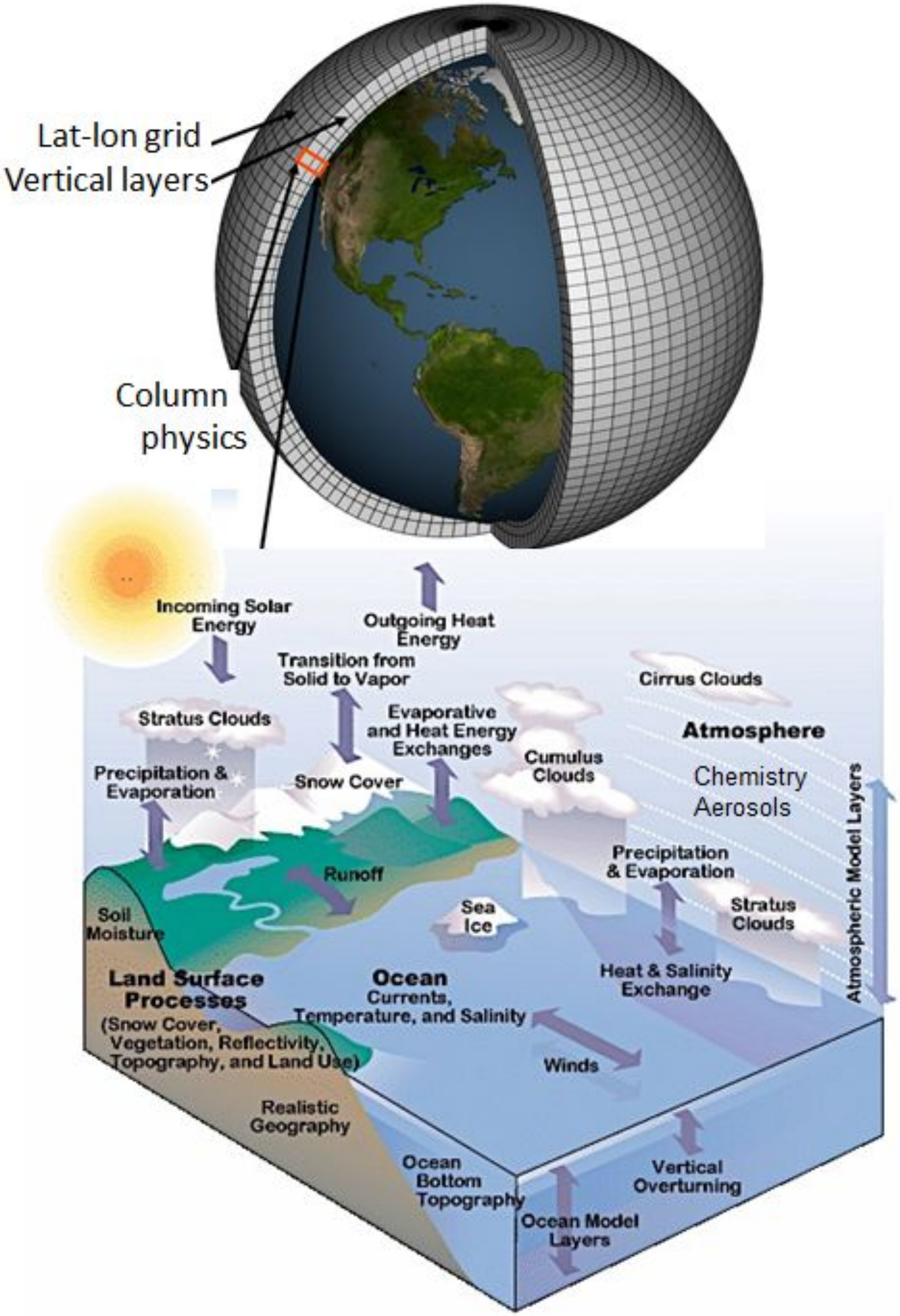
michael.way@nasa.gov, kostas.tsigaridis@columbia.edu, igor.aleinov@columbia.edu

Tuesday Schedule (US Eastern Time Zone)

- 10:00-10:45: Intro & tutorial (Mike & Kostas)
- 10:45-11:00: Break
- 11:00-11:45: Tutorial (Kostas)
- 11:45-13:00: Lunch break
- 13:00-13:45: Tutorial (Tony & Mike), Q&A
- 13:45-14:00: Break
- 14:00-15:00: Q&A

Wednesday Schedule (US Eastern Time Zone)

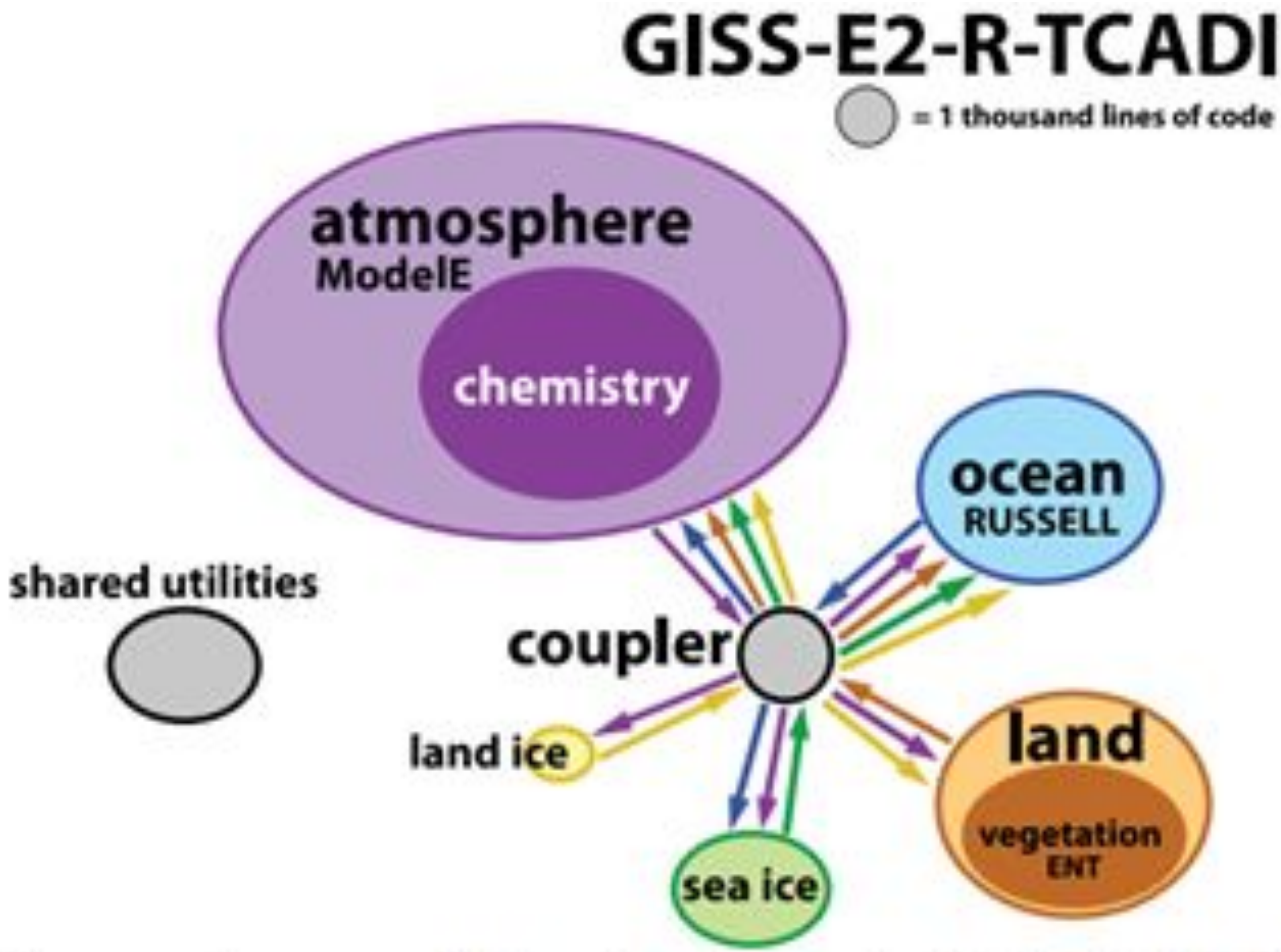
- 10:00-10:05: Good Morning
- 10:05-10:25: Tom Clune (Mike) on Calendar
- 10:25-10:45: Aleinov on ground hydrology
- 10:45-11:00: Break
- 11:00-11:20: Eric Wolf on Radiation
- 11:20-12:00: Vincent Kofman: Planetary Spectrum Generator & ROCKE3D
- 12:00-13:00: Lunch
- 13:00-13:45: Chris Colose: How to create a new planet
- 13:45-14:00: Break
- 14:00-15:00: Q&A



Limitations of 3D global climate models (GCMs):

- Time scales simulated (max ~10^4 yr so far)
- Vertical range (~65 km for ours) – can't simulate escape, only mixing ratios in stratosphere
- Limited to shallow atmospheres (our GCM, anyway) – no mini-Neptunes or larger

GISS ModelE (Schmidt et al., 2014)



Alexander and Easterbrook, GMD, 2015

What is ROCKE-3D good for?

ROCKE-3D (Way et al., 2017)

The Astrophysical Journal Supplement Series, 231:12 (22pp), 2017 July https://doi.org/10.3847/1538-4365/aa7a06

CrossMark

Resolving Orbital and Climate Keys of Earth and Extraterrestrial Environments with Dynamics (ROCKE-3D) 1.0: A General Circulation Model for Simulating the Climates of Rocky Planets

M. J. Way[1,2], I. Aleinov[1,3], David S. Amundsen[1,4], M. A. Chandler[1,3], T. L. Clune[5], A. D. Del Genio[1], Y. Fujii[1], M. Kelley[1], N. Y. Kiang[1], L. Sohl[1,3], and K. Tsigaridis[1,3]
[1] NASA Goddard Institute for Space Studies, New York, NY 10025, USA
[2] Department of Physics and Astronomy, Uppsala University, Uppsala, SE-75120, Sweden
[3] Center for Climate Systems Research, Columbia University, New York, NY 10025, USA
[4] Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10025, USA
[5] Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, USA
Received 2017 February 24; revised 2017 May 31; accepted 2017 June 14; published 2017 July 20

has modeled the atmospheres of:

What is ROCKE-3D good for?

- Earth: 2.9Ga to the present (Del Genio et al. 2018):

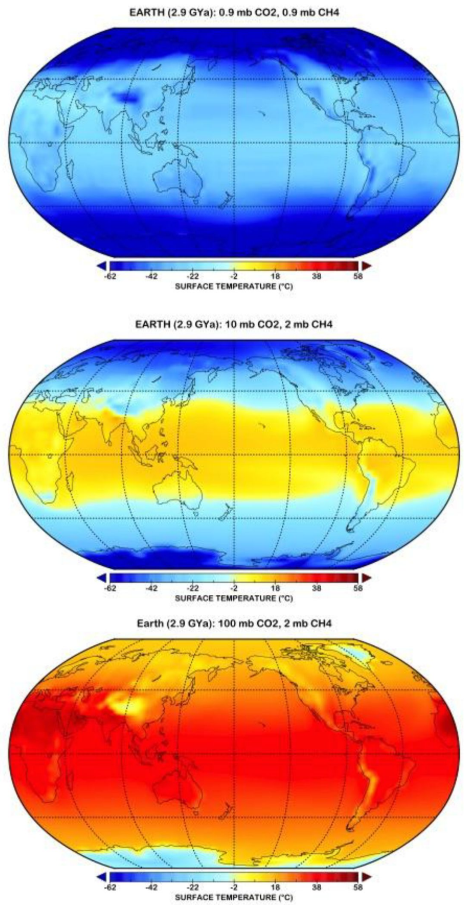


Figure 5. 2.9 Gya Archean Earth surface temperature simulated by the ROCKE-3D GCM (*Way et al.*, 2017) assuming atmospheric compositions for Cases (upper) A, (middle) B, and (lower) C of *Charnay et al.* (2013) and the solar spectrum from *Claire et al.* (2012). Uncertainties due to the unknown land-ocean distribution are a few degrees. Simulations courtesy of Michael Way.

What is ROCKE-3D good for?

- Ancient Venus (Way et al. 2016)

AGU PUBLICATIONS

Geophysical Research Letters

RESEARCH LETTER

10.1002/2016GL069790

Key Points:

- Venus may have had a climate with liquid water on its surface for approximately two billion years
- The rotation rate and topography of Venus play crucial roles in its surface temperature and moisture
- Young Venus-like exoplanets may be considered candidates for the search for life beyond Earth

Was Venus the first habitable world of our solar system?

M. J. Way[1,2], Anthony D. Del Genio[1], Nancy Y. Kiang[1], Linda E. Sohl[1,3], David H. Grinspoon[4], Igor Aleinov[1,3], Maxwell Kelley[1], and Thomas Clune[5]

[1]NASA Goddard Institute for Space Studies, New York, New York, USA, [2]Department of Astronomy and Space Physics, Uppsala University, Uppsala, Sweden, [3]Center for Climate Systems Research, Columbia University, New York, New York, USA, [4]Planetary Science Institute, Tucson, Arizona, USA, [5]Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, Maryland, USA

Table 1. Paleo-Venus Experimental Setups and Results[a]

Simulation	Topography	Spectrum/Flux/S0X	Rotation Period	*T* (min)	*T* (max)	*T* (avg)	Time (avg)
A	Venus	2.900 Gya/2001/1.46	Modern Venus	−22°C	36°C	11°C	1/6 day
B	Venus	0.715 Gya/2357/1.70	Modern Venus	−17°C	35°C	15°C	1/6 day
C	Earth	2.900 Gya/2001/1.46	Modern Venus	−13°C	46°C	23°C	1/6 day
D	Venus	2.900 Gya/2001/1.46	16 × Earth	27°C	84°C	56°C	1/8 day

Mars pressure seasonal cycle

- Modern/Ancient Mars w/o CO2 clouds
  (I. Aleinov -> Tomorrow)

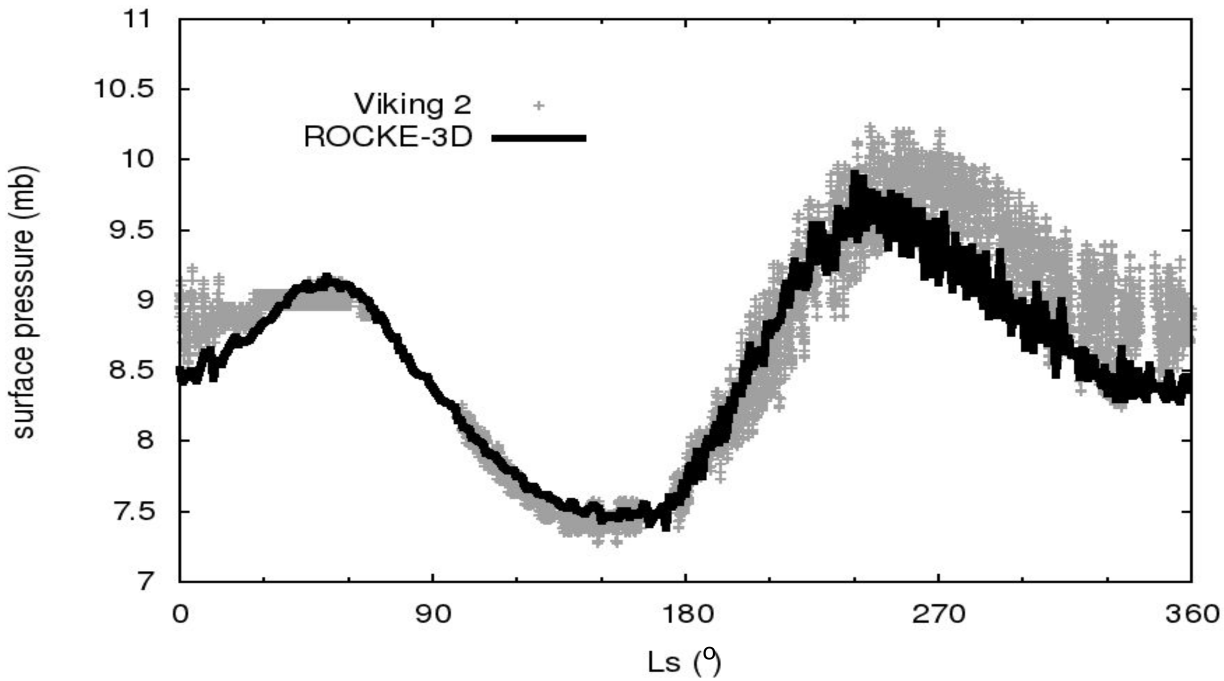


Figure 6. Annual cycle of Mars surface pressure, as measured by the Viking 2 lander (gray crosses) (Hess et al. 1977; Tillman 1989), and surface pressure simulated by ROCKE-3D (black solid line).

What is ROCKE-3D good for?

- Hypothetical Venus-like worlds (near M-dwarfs)
  - Kepler 1649b (Kane et al. 2018):

The Astrophysical Journal, 869:46 (9pp), 2018 December 10 https://doi.org/10.3847/1538-4357/aaec68

CrossMark

Climate Modeling of a Potential ExoVenus

Stephen R. Kane[1], Alma Y. Ceja[1], Michael J. Way[2,3], and Elisa V. Quintana[4]
[1] Department of Earth Sciences, University of California, Riverside, CA 92521, USA; skane@ucr.edu
[2] NASA Goddard Institute for Space Studies, New York, NY 10025, USA
[3] Department of Physics and Astronomy, Uppsala University, Uppsala, SE-75120, Sweden
[4] NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA
Received 2018 September 20; revised 2018 October 24; accepted 2018 October 25; published 2018 December 11

Table 1
Parameters of ROCKE-3D Simulations

ID	P (days)	F_p ($F_\oplus$)	Topo[a]	CO_2 (ppmv)	CH_4 (ppmv)	Orbits[b]	T_{mean}[c] (°C)	T_{min} (°C)	T_{max} (°C)	Bal[d] ($W\ m^{-2}$)	H_2O_{strat}[e] ($kg\ kg^{-1}$)	H_2O_{surf}[f] ($kg\ kg^{-1}$)
1	8.6	2.3	1	400	1	300	90.2	81.2	112.5	103	0.379	0.4845
2	8.6	2.3	3	400	1	66	84.3	42.4	212.4	214	0.099	0.1168
3	8.6	2.3	3	100	0	116	128.9	67.3	285.4	137	0.271	0.3456
4	8.6	2.0	1	400	1	486	91.8	83.5	111.8	77	0.423	0.5214
5	8.6	1.8	1	400	1	634	90.8	83.1	110.2	63	0.434	0.5061
6	8.6	1.6	1	400	1	752	88.0	81.3	102.7	59	0.411	0.4562
7	8.6	1.4	1	400	1	2031	64.1	57.7	72.0	35	0.026	0.1623
8	8.6	1.0	2	400	1	2345	4.3	−54.1	46.9	−3	0.000078	0.0064
9	16.0	1.47	2	400	1	2055	58.3	33.5	91.7	9	0.038	0.1052
10	50.0	1.4	1	376	0	6354	59.0	56.3	61.9	0.3	0.027	0.1226

What is ROCKE-3D good for?

- Proxima Centauri b type systems (Del Genio et al. 2019) up to 10bar N_2/CO_2

ASTROBIOLOGY
Volume 19, Number 2, 2019

DOI: 10.1089/ast.2017.1760

Research Article

Habitable Climate Scenarios for Proxima Centauri b with a Dynamic Ocean

Anthony D. Del Genio,[1] Michael J. Way,[1] David S. Amundsen,[1,2] Igor Aleinov,[1,3] Maxwell Kelley,[1,4] Nancy Y. Kiang,[1] and Thomas L. Clune[5]

TABLE 4. DESCRIPTION OF GENERAL CIRCULATION MODEL SIMULATIONS

No.	*Name*	*Description*
1	Control	0.984 bar, N_2 + 376 ppmv CO_2 atmosphere, dynamic ocean, aquaplanet, synchronous rotation, S_o = 881.7 W/m^2, S = 35.4 psu
2	Thermo	Like Control but with a thermodynamic ocean
3	Control-High	Like Control but with S_o = 956 W/m^2
4	Control-Thin@	Like Control but with 0.1 bar N_2 + 376 ppmv CO_2
5	Control-Thick#@	Like Control but with 10 bar N_2 + 376 ppmv CO_2
6	Archean Low*	Like Control but 638 ppmv CO_2, 450 ppmv CH_4
7	Archean Med*	Like Control but 900 ppmv CO_2, 900 ppmv CH_4
8	Archean Med NoCH$_4$*@	Like Archean Med but 0 ppmv CH_4
9	Archean High*	Like Control but 10,000 ppmv CO_2, 2000 ppmv CH_4
10	Pure CO_2+@	Like Control but 0.984 bar pure CO_2 atmosphere
11	Control-Shallow@	Like Control but with a 158 m depth ocean
12	Control-Deep@	Like Control but with a 2052 m depth ocean
13	Zero Salinity	Like Control but S = 0 psu
14	High Salinity	Like Control but S = 230 psu
15	3:2e0	Like Control but in 3:2 resonance with e = 0
16	3:2e30	Like Control but in 3:2 resonance with e = 0.30
17	Day-Ocean	Like Control but with Earth land–ocean distribution and substellar point over Pacific
18	Day-Land	Like Day-Ocean but substellar point over Africa

What is ROCKE-3D good for?

- Ancient Lunar Atmosphere (Aleinov et al. 2019)

Geophysical Research Letters

Research Letter | Full Access

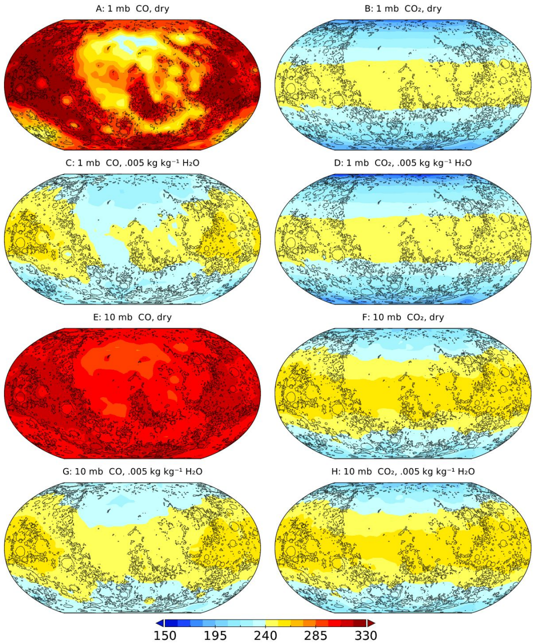
Modeling a Transient Secondary Paleo-Lunar Atmosphere: 3-D Simulations and Analysis

I. Aleinov, M.J. Way, C. Harman, K. Tsigaridis, E.T. Wolf, G. Gronoff

First published: 01 May 2019 | https://doi.org/10.1029/2019GL082494

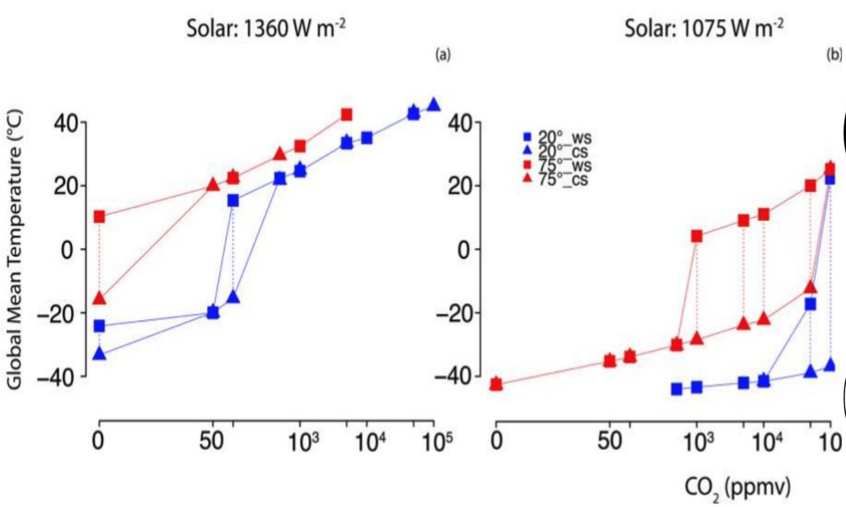
Go here for SFX Go here for SFX

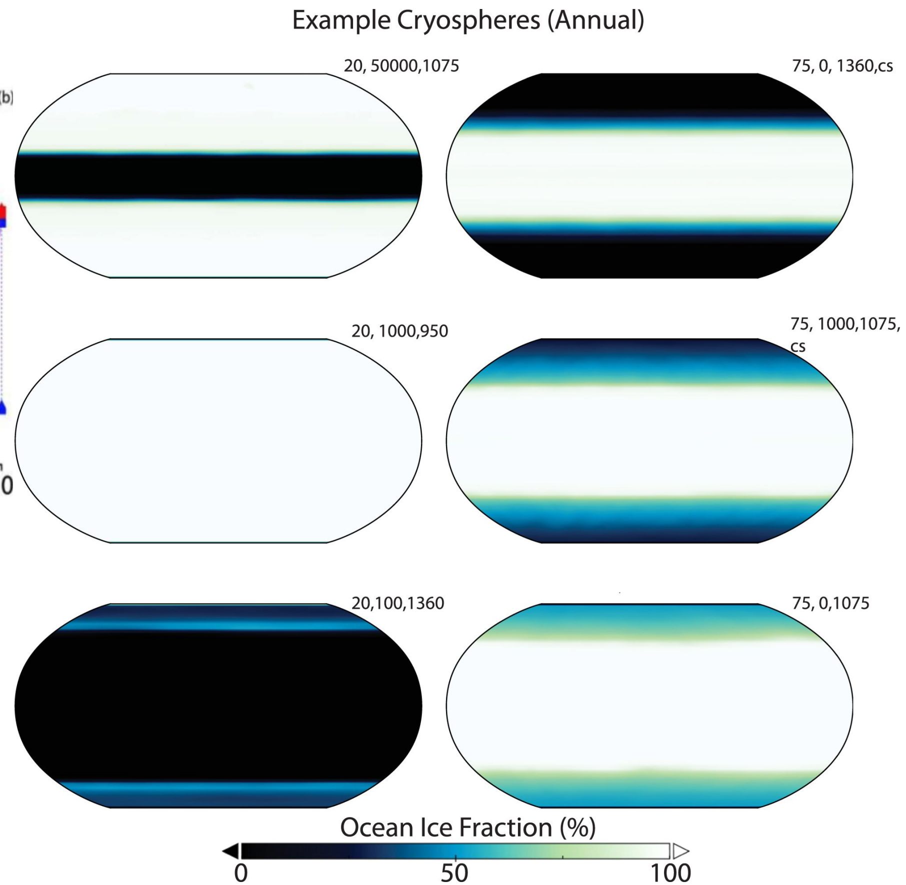
This article has been accepted for publication and undergone full peer review but has not been through the copyediting, typesetting, pagination and proofreading process, which may lead to differences between this version and the Version of Record. Please cite this article as doi: 10.1029/2019GL082494



What is ROCKE-3D good for?

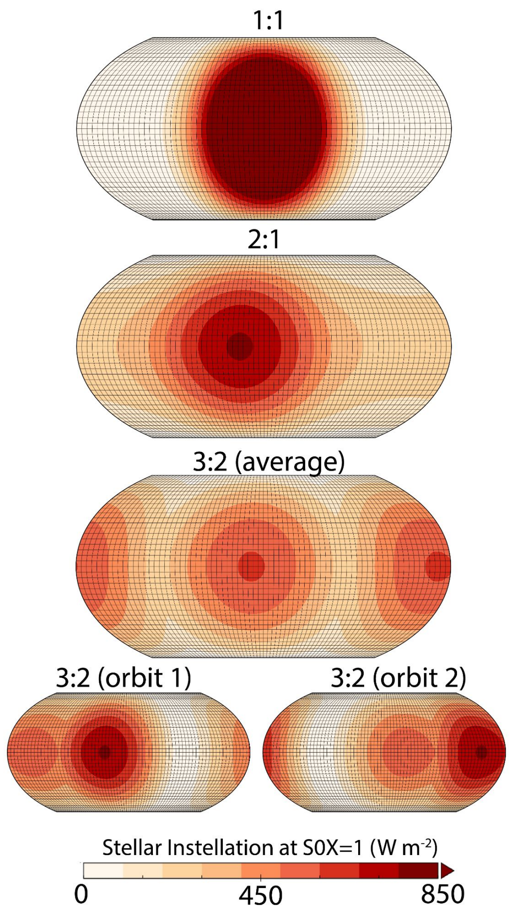
- Obliquity Studies (Colose et al. 2019 ApJ)
- ROCKE-3D has hysteresis

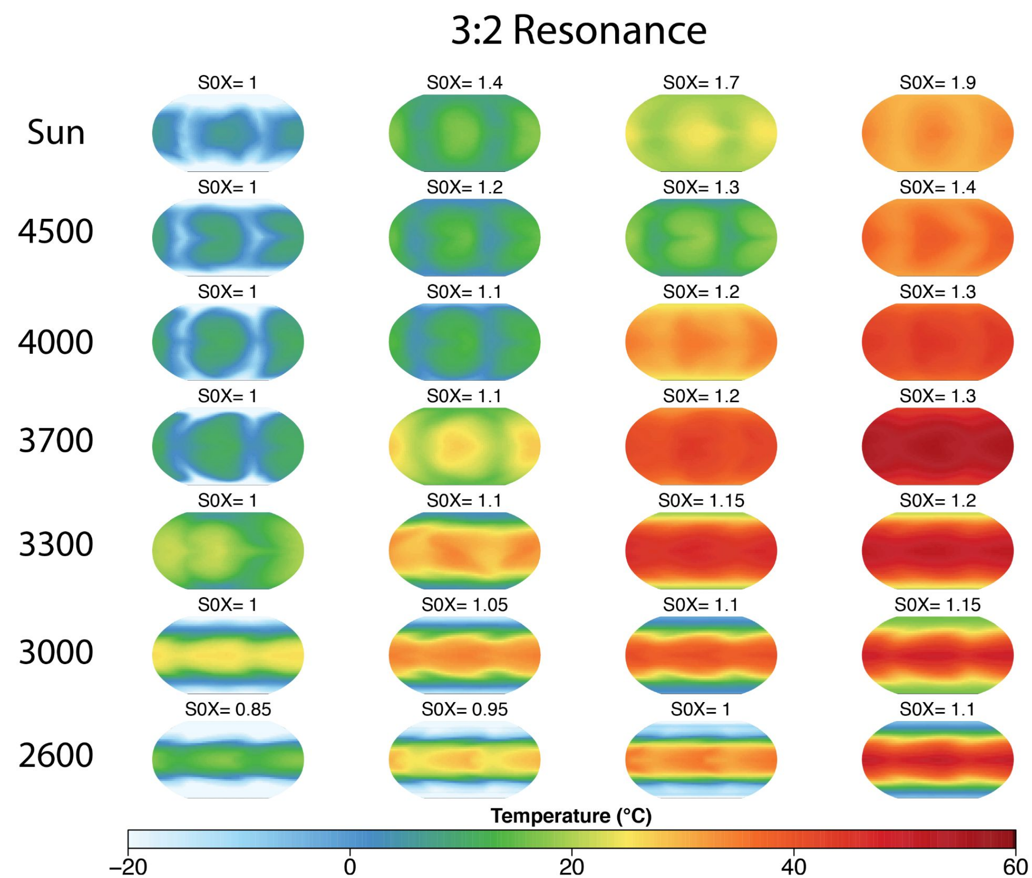




What is ROCKE-3D good for?

- Spin-orbit resonances (Colose et al. 2021 ApJ)
- Geothermal heating can be applied





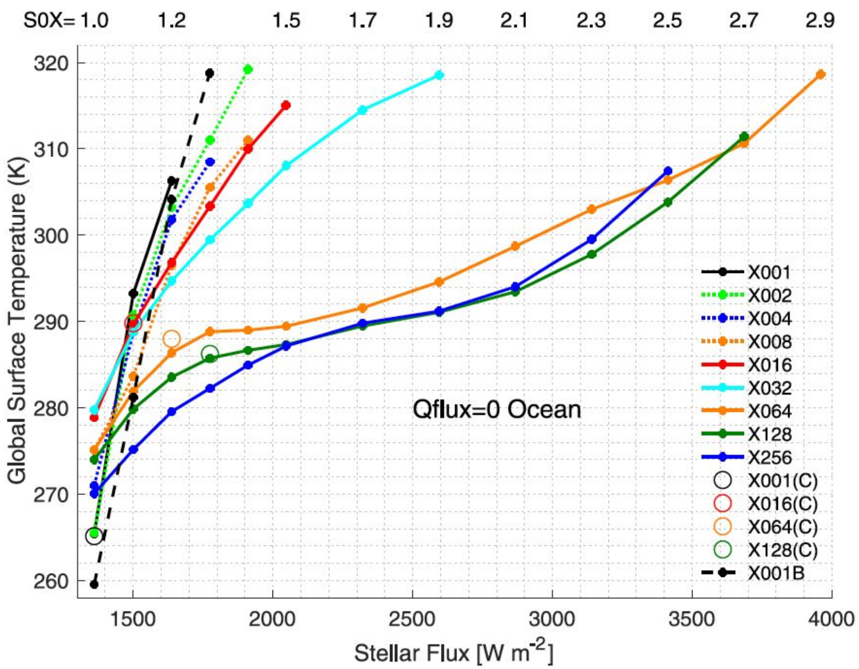
What is ROCKE-3D good for?

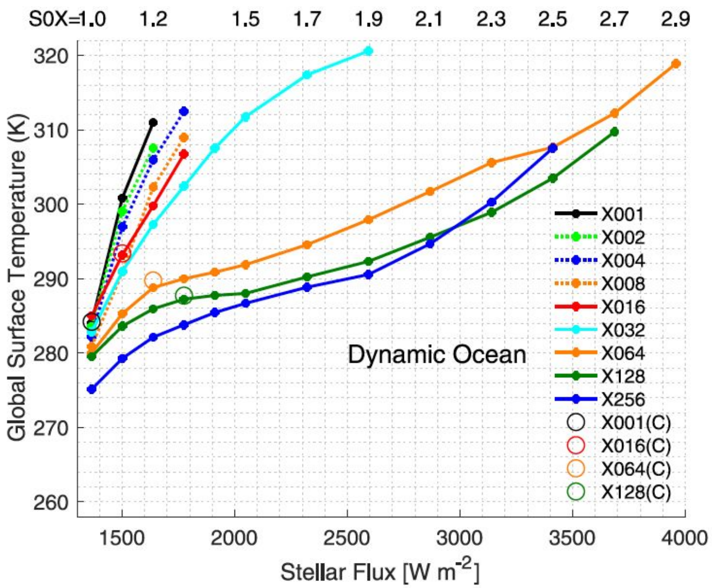
- Parameter Ensembles (Way et al. 2018 ApJS)

Climates of Warm Earth-like Planets I: 3-D Model Simulations

M.J. Way,[1,2] Anthony D. Del Genio,[1] Igor Aleinov,[1,3] Thomas L. Clune,[4] Maxwell Kelley,[1] and Nancy Y. Kiang[1]

[1] NASA Goddard Institute for Space Studies, 2880 Broadway, New York, NY, 10025, USA
[2] Department of Physics and Astronomy, Uppsala University, Uppsala, 75120, Sweden
[3] Center for Climate Systems Research, Columbia University, New York, NY 10025, USA
[4] Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, USA





Why Tell You About These Papers?!

- The fastest and most reliable means to get a new planet running after this tutorial is to find a similar one from our previous papers

- You can find the rundecks, boundary condition files, and model output for most of our papers on-line:

- https://portal.nccs.nasa.gov/GISS_modelE/ROCKE-3D/publication-supplements/

What is ROCKE-3D good for?

Caveats?

There are a limited number of types of atmospheres and stellar spectra available. We will discuss them later, time permitting.

What it should NOT be used for

Variable atmospheric mass for mix of constituents

- mean atmospheric molecular weight changing, etc.

Super Earths

Where thin atmospheric approximation **invalid**

Super thick oceans? (See Tony Leboissetier's slides)

Not above temps of 400K & not below 100K (except Titan)

Really cold planets (ocean freezing to bottom = model crash)

Fast spinning planets (Grid resolution)

Mini-Neptunes and above (gas giants, etc.)

- remember the ROCKE-3D acronym: **R**esolving **O**rbital & **C**limate **K**eys of **E**arth & **E**xtraterrestrial **E**nvironments

south pole anomaly

limitations in atmospheric constituents (radiation & chem)

Where to?

- GISS contacts
  - Clouds: Andy Ackerman
  - Chemistry: Kostas & Sonny
  - Aerosols: Kostas Tsigaridis
  - Various planets, orbits, etc.: Mike Way
  - Radiation: Eric Wolf (Andy Lacis for GISS Radiation)
  - Atmospheric composition: Kostas Tsigaridis
  - Debugging: Igor Aleinov, Kostas, Mike (use sparingly!)
  - Calendar/Rotation issues: Tom Clune
  - Biology: Nancy Kiang
  - Land: Igor Aleinov
  - Ocean/Sea Ice: Tony Leboissetier
  - Panoply: Robert Schmunk

Code Repository Server at GISS

- https://simplex.giss.nasa.gov
- https://simplex.giss.nasa.gov/gcm/ROCKE-3D/

Model Documentation (what little there is):

Planet_1.0 dynamic ocean rundeck:
https://simplex.giss.nasa.gov/gcm/decks/P1SoM40_html/index.html

Model_E2 Earth rundeck:
https://simplex.giss.nasa.gov/gcm/decks/E6F40_html/index.html

Latest snapshots: what does this really mean?
https://simplex.giss.nasa.gov/snapshots/

ROCKE-3D snapshots: https://simplex.giss.nasa.gov/snapshots/

Released versions of ROCKE-3D code

- modelE2_planet_1.1.tgz - version 1.1 of ROCKE-3D model
- modelE2_planet_2.0.tgz - version 2.0 of ROCKE-3D model

Updated versions of the code

- modelE2_planet_1.0_patches_2024.05.26_07.50.01.tgz - patched version 1.0 of ROCKE-3D model as it is currently used in our planetary simulations.

Frozen versions:

modelE2_planet_1.1 is similar with planet_1.0, with backported fixes from modelE2_planet_2.0. No change in answers, unless opted in. This is the workhorse moving forward.

Under development version:

modelE2_planet_1.0_patches is planet_1.1 as it further evolves. This will mainly include bug fixes and compatibility updates for the latest compilers. The date will change, so don't bookmark the file, rather the snapshots page.

Model Versions/Names

GISS ModelE

- GISS ModelE2
- GISS-E2-[RH] (CMIP5)
- GISS-E2.1 (CMIP6)
- ROCKE-3D
  - planet_1.0 (GISS ModelE2)
  - planet_2.0 (GISS ModelE2.1 + tracersE3)
  - planet_3.0 (GISS ModelE3)
  - planet (development)
- NINT, OMA, MATRIX

Terminology and file system structure

- .modelErc
  - $HOME/.modelErc
- ROCKE-3D
  - $HOME/modelE2_planet_1.0
- Template rundecks
  - $HOME/modelE2_planet_1.0/templates
- Rundecks
  - $HOME/modelE2_planet_1.0/decks
- Source code
  - $HOME/modelE2_planet_1.0/model (and sub-dirs)

Input and output locations

- Shared input files
  - Location defined by $GCMSEARCHPATH in .modelErc
  - Relative path in rundecks (do not start with /).
- User-defined input files
  - Anywhere accessible to the model while running.
  - Absolute path in rundecks (start with /).

- Output files
  - In subdirs, as defined by $SAVEDISK in .modelErc
  - Also soft-linked in the decks directory, under runid.

Overview of the rundeck: runid.R

- Documentation
- Preprocessor Options
- Object modules
  - Files to be compiled
- Components
- Component Options
- Data input files
  - Emissions
  - Boundary conditions
  - …
- Label and Namelist
  - run name (runid)
- PARAMETERS … END_PARAMETERS
  - Runtime parameters (variables in FORTRAN)
- INPUTZ
  - Start/end times

Key planet_1.0 template rundecks

- Planet_1.0
  - P4SM40 (prescribed sea surface temperatures)
  - P4SqM40 (Earth Q-flux heat surface fluxes)
  - P1SoM40 (Fully coupled/dynamic ocean)
  - PS_Mars (Dune/Desert Planet no ocean)

If you want to use ANYTHING else in the templates directory PLEASE ask us about it first!

- Planet_2.0 will have many more rundeck options.
- Never confuse a template with a working rundeck!

Key planet_2.0 template rundecks

P2{G,S}{A,x,N}{p,q,o}{F,M}40

Component	Explanation
Model version	P1: Template configuration of ROCKE-3D version 1.0 (planet_1.0; Way et al., 2017)
	P2: Template configuration of ROCKE-3D version 2.0 (planet_2.0; this work)
Radiation	G: GISS radiation
	S: SOCRATES radiation
Atmosphere[a]	A: Atmosphere of preindustrial Earth (year 1850), as described by GISS ModelE CMIP6 simulations
	x: Same as A, without a) aerosols; b) O_3; c) stratospheric H_2O formation from CH_4 oxidation
	N: Same as x, with O_2 and Ar replaced by N_2
Ocean	p: prescribed sea surface temperature and sea ice extent and thickness
	q: Q-flux ocean, 100m mixed layer depth
	o: dynamic ocean; see next line for resolution
Resolution	M40: atmosphere: 4°x5° with 40 layers to 0.1 hPa; ocean, if o configuration: 4°x5° with 13 layers
	F40: atmosphere: 2°x2.5° with 40 layers to 0.1 hPa; ocean, if o configuration: 1°x1.25° with 40 layers

[a]: In the text these configurations are frequently named Earth's (A), planet_1.0 (x), and anoxic (N) atmospheres.

Rundeck details

- Go into detail of P1SoM40 rundeck
- Then compare P4SqM40 rundeck with P1SoM40
- Then compare P1SoM40 with PS_Mars
- Complete list of variables:

https://simplex.giss.nasa.gov/gcm/decks/P1SoM40_html/index.html

Rundeck start/stop times

```
&INPUTZ

YEARI=1897,MONTHI=1,DATEI=1,HOURI=0, ! pick IYEAR1=YEARI (default) or < YEARI

YEARE=1910,MONTHE=1,DATEE=1,HOURE=0,KDIAG=12*0,9,

ISTART=2,IRANDI=0,YEARE=1897,MONTHE=1,DATEE=1,HOURE=1,

/
```

- `master_yr=1850`

Let’s now run the first hour of 2 rundecks.

Running new rundecks

- P4SM40 (prescribed sea surface temperatures)
- P4SqM40 (Earth Q-flux heat surface fluxes)
- P1SoM40 (Fully coupled/dynamic ocean)
- PS_Mars (Dune/Desert Planet no ocean)

Remember how you did it before:

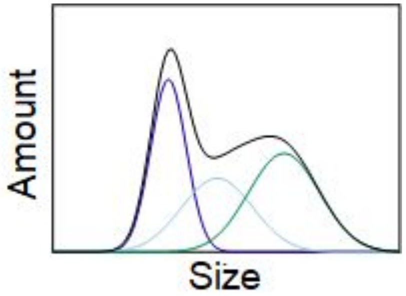
https://docs.google.com/document/d/1yyI0CDx1wEYbwqRsbvczXpdW2teePZ_NgIePTLFHtNA/view

```
cd /home/username/modelE2_planet_1.0/decks
make rundeck RUNSRC=P1SoM40 RUN=P1SoM40_Test
../exec/get_input_data -w P1SoM40_Test /home/username/ModelE_Support/prod_input_files
make clean; make -j setup RUN=P1SoM40_Test
../exec/runE P1SoM40_Test -cold-restart -np 2
```

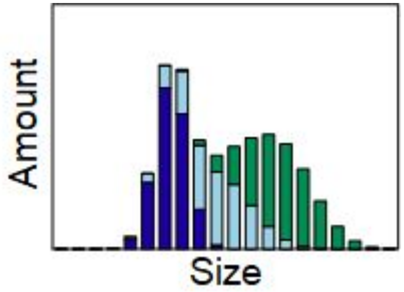
Running with tracers

- Chemistry: CBM4, KPP under development
- Aerosols
  - OMA: One-moment aerosols

  - MATRIX: Modal, resolves mixing state



  - TOMAS: Sectional
    (abandoned following E2.1/planet_2.0)



Atmospheric composition of new planets

Not everything that matters for climate is uniformly distributed in a planetary atmosphere.

CH_4?

O_3

Dust

Sea salt

Other aerosols

} **Clouds!**

Random thoughts

- The I file
- The lock file
- COMPILE_WITH_TRAPS=YES EXTRA_FFLAGS=”-O0 -g” (make clean before AND after!!!)
- ../exec/sswE RUNID (to stop a job gracefully)

ROCKE-3D Ocean types

- **Prescribed Sea Surface Temperatures**
  - modern Earth
  - Computationally cheap
- **Q-flux/mixed layer/slab ocean**
  - In the exoplanet realm normally means NO horizontal heat transport between grid cells
  - For Earth-like simulations the heat transport is prescribed.
  - Computationally cheap
- **Fully-Coupled dynamic ocean**
  - NOT computationally cheap, but most realistic
- **Standalone ocean**
  - prescribed atmosphere
  - computationally cheapest

Fully-coupled ocean runs

- Start from P1SoM40.R *(dynamic ocean run)*
- Key differences from P4SqM40.R *(Q-flux run)*:

1) model source files

```
OCN_DRV                              ! driver for ocean-grid components
OLAYERS                              ! ocean layering options
OCEAN_COM  OGEOM                     ! dynamic ocean modules
OCNDYN OCNDYN2  OTIDELL              ! dynamic ocean routines
OCN_Interp                           ! dynamic ocean routines
OSTRAITS_COM  OSTRAITS               ! straits parameterization
OCNKPP                               ! ocean vertical mixing
OCNMESO OCNTDMIX OCNGM               ! ocean mesoscale mixing
```

2) parameters

- KOCEAN=1

Fully-coupled ocean runs

3) input files

- *OIC* (temperature and salinity in very strange units, initial conditions only)
- *TOPO_OC* (ocean topography)
- *OSTRAITS* (ocean cells connected through land)
- No partial land/ocean cells

Ocean model: future updates

Coming next in Planet2.0:

- **Quasi-hydrostatic ocean model**
  - useful for planets/icy moons with deep ocean (~10-100km)
  - full treatment of the Coriolis force
  - relaxation of the shallow water approximation
- **Geothermal Heating**
- **More options for mesoscale diffusivity**
- **Ocean bottom/coastal drag**
- **Improved sea ice thermodynamics/dynamics**
- **Variable gravity**

Change of topography

- TOPO
- TOPO_OC
- RVR (River directions).
- NAMERVR (River names; there has to be at least one).
- variable_lk=1; set to zero for non-variable lakes (expanding/contracting).
- If generate new or remove ocean grid cells, OIC also needs to be changed.
- GLMELT needs to change if land/sea mask changes drastically. Points where glacier calving might be problematic
- wsn_max (max snow depth) set to 2m by default.
  - ONLY use if you have an ocean, otherwise set to 0.
- nrad=5 (default) use 1 in cases where model is unstable

Change of orbital parameters & other

- planetName
- eccentricity
- obliquity
- Calendar fun:
  - siderialorbitalPeriod
  - siderialrotationPeriod
  - quantizeYearLength (for tidally-locked planets)

- GHG file versus the X variables below
- CH4X, CO2X, N2OX, etc. as seen by the radiation.
- Physical properties of the atmospheric mixture (such as molecular mass and heat capacity) should be set explicitly in model/shared/PlanetParams_mod.F90
- For our solar system in the present epoch, the only thing other than orbital parameters is to change planet_s0. Nothing else is needed, if the solar spectrum is the same.

Single-column model (SCM)

- Essentially converts the 3D model to 1D, using the same model code.
- Exists for Planet_1.0 in Beta, but not currently being used by the ROCKE-3D Team.
- Runs on your laptop!

In the event of a crash?

ROCKE-3D document on known crash solutions.

Very useful when you push the model outside of its comfort zone:

https://docs.google.com/document/d/1Hvy9vW9m8YiN8_wf7SnulWIEcoXjgHT88C_o73-sbqw/view

Output and post-processing

- <runid>.PRT file
- MONYYYY.zzzRUNID.nc
- rsf files (KRSF: save rsf every KRSF months)
- fort.[12].nc files (alternate save every NDISK timesteps)
- acc files (KCOPY=0 no acc, =1 acc)
  - scaleacc: generate aij (and the like) files
  - sumfiles: generate temporally averaged acc files
- diffreport
- Panoply (http://www.giss.nasa.gov/tools/panoply)
- ncview

Post-Processing: NetCDF Diagnostics

The ROCKE-3D GCM contains the following diagnostics files from **scaleacc**:

Remember we have this:

https://simplex.giss.nasa.gov/gcm/decks/P1SoM40_html/index.html

Most commonly used diagnostics:

- aij: atmospheric model, 2D longitude vs. latitude variables
    - https://docs.google.com/spreadsheets/d/1Sp01pwCv8Vr4kLnR7fTz0IPHzdU6FjoD4OFlc4YICCo/view#gid=0
- aj: atmospheric model, 1D longitudinally averaged variables vs. latitude
- ajl: atmospheric model, 2D longitudinally averaged latitude vs. pressure variables
    - https://docs.google.com/spreadsheets/d/1HZ0oQRQre_v1e4fH0Pwf2y2-uMBluvujin97ogdYlf4/view#gid=0
- agc: atmospheric model, 2D longitudinally averaged latitude vs. pressure general circulation variables
- aijk: atmospheric model, 3D longitude-latitude-pressure variables
- aijl: atmospheric model, 3D longitude-latitude-model level variables
    - https://docs.google.com/spreadsheets/d/1R3bCQ1BA3ukS-aPPomORvLeSr0_QqGM6azFvkuI3DQY/view#gid=0
- ojl: dynamic ocean, 2D longitudinally averaged latitude vs. depth variables
- oijl: dynamic ocean, 3D longitude-latitude-depth variables

Post-Processing: NetCDF Diagnostics

diagnostics available in some simulations:

- adiurn: atmospheric model, diurnal cycles at selected gridpoints
- hdiurn: atmospheric model, hourly timeseries at selected gridpoints
- otj: Ocean R, northward transports
- oij: Ocean R, longitude-latitude
- olnst: Ocean R, straits
- toijl: Ocean R, longitude-latitude-depth tracer fields
- icij: Viscous-plastic ice dynamics, longitude-latitude fields
- areg: atmospheric model, aj diagnostics for predefined regions
- consrv: atmospheric model, conservation quantities on the budget grid
- tconsrv: atmospheric model, tracer conservation quantities on the budget grid
- tajl: atmospheric model, latitude-height tracer fields (budget latitude bands)
- taij: atmospheric model, longitude-latitude tracer fields (or on the cubed-sphere grid if applicable)
- taijl: atmospheric model, longitude-latitude-height tracer fields (or on the cubed-sphere grid if applicable)
- **all: output ALL available diagnostics above.**

Source Code Structure

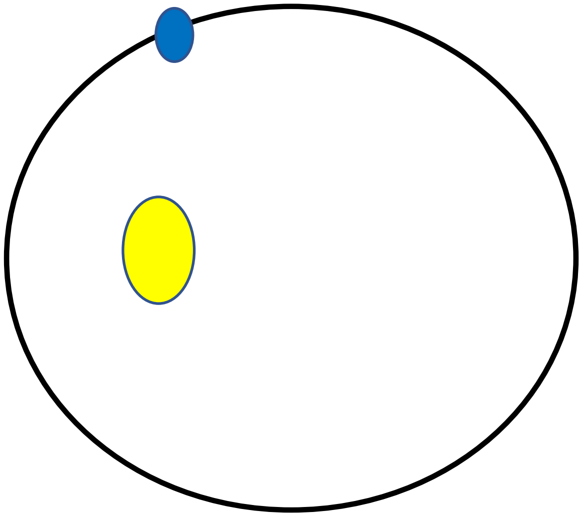
- `#include "rundeck_opts.h“`
- The XXX_COM and XXX_DRV files
- Constants_mod.F90 and PlanetParams_mod.F90,
- Adding diagnostics (DEFACC.f)

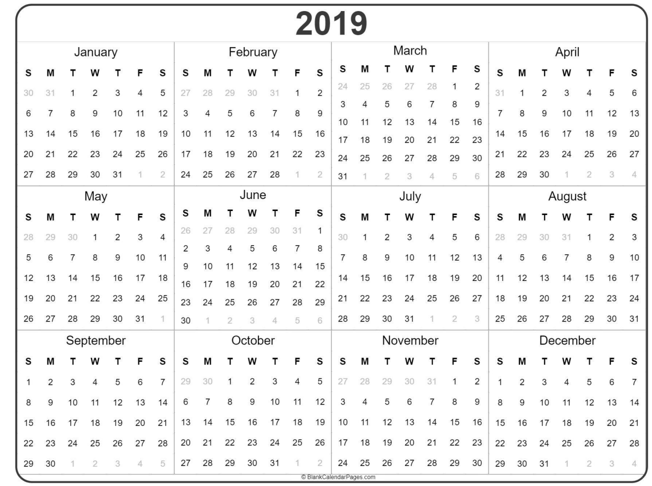
Day 2

- 10:00-10:05: Good Morning
- 10:05-10:25: Tom Clune (Mike) on Calendar
- 10:25-10:45: Aleinov on ground hydrology
- 10:45-11:00: Break
- 11:00-11:20: Eric Wolf (Radiation)
- 11:20-12:00: Vincent Kofman: Planetary Spectrum Generator & ROCKE-3D
- 12:00-13:00: Lunch
- 13:00-13:45: Colose: How to create a new planet
- 13:45-14:00: Break
- 14:00-15:00: Q&A

ModelE
Orbits & Calendars

Tom Clune (GMAO) <Mike Way filling in>





Absolute
Model
Time

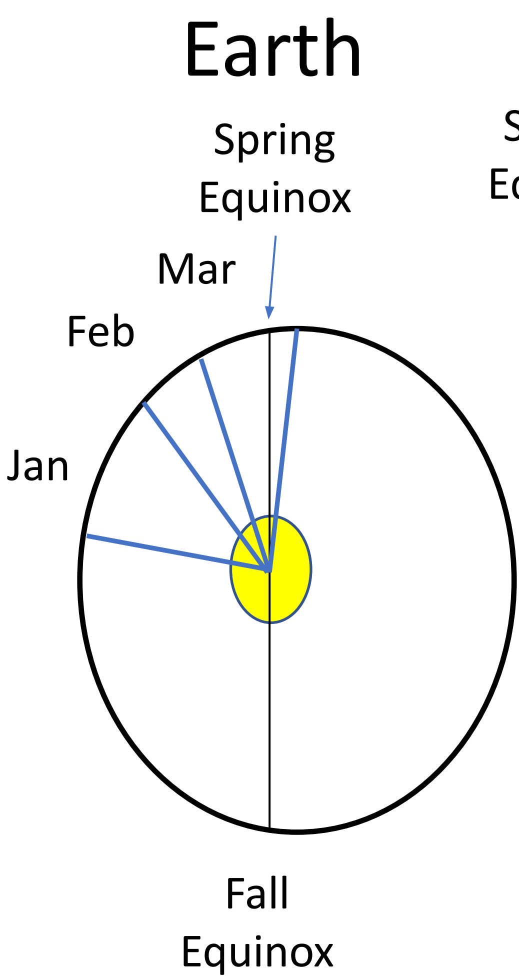
ORBIT

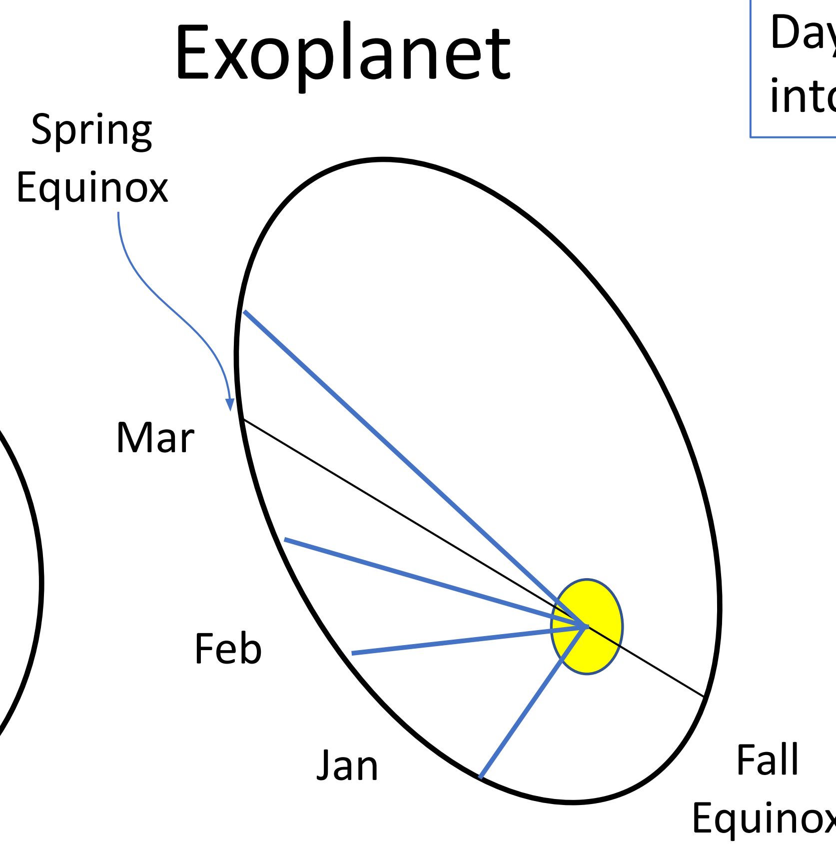
Calendar

Distance
Hour Angle
Declination Angle

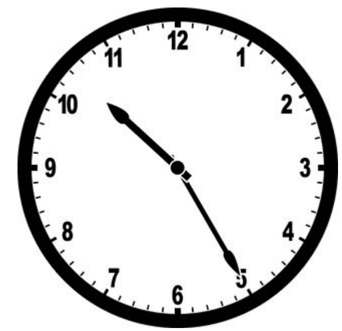
Year
Month
Date
Day Of Year
Hour
Seconds

Exoplanet years are divided into 12 months. The angle (solar longitude) subtended by each month is (approximately) the same as the corresponding month for the Earth.





Days are subdivided into 24 equal "hours".



Hour angle is 180° for prime meridian at 0h Jan 01.

Note: orbital period is "adjusted" to be an integral multiple of rotation period.

Problems …

The conventional Earth-like calendars work well when:

$$|\omega_{\mathbf{orbit}}| \ll |\omega_{\mathbf{planet}}|$$

This allows:

1. Integral number of solar days per year (with minor adjustment)
2. Division of year into 12 roughly equal months that have *many* days each.

This assumption fails badly for slow rotators including tidally locked planets.

Treatment of slow rotators

- Calendar years always* have at least 120 *calendar* days.
  - *Calendar* days and *solar* days are distinct
    - ***Be wary of "diurnal" diagnostics***
  - Monthly averages mays also be misleading – a given longitude may experience daylight for an entire "month" even at the equator!
- For very slow rotators (e.g., Venus)
  - Must deactivate orbit "quantization"
  - Seasons "float" from (calendar) year to (calendar) year
  - *Entire (calendar) years may have a day/night bias*
    - Must run large number of cal. years to get valid "annual" averages
    - Ideally the least-common-multiple of orbit year and physical day
      - For Venus we typical use 50 orbits to get reasonable statistics

*override option exists

Basic orbit rundeck parameters

- planetName=… (something other than ‘Earth’)
- obliquity=… degrees - default is modern Earth
- eccentricity=… default is modern Earth
- longitudeAtPeriapsis=… in degrees – default is modern Earth
- siderealOrbitalPeriod=…in seconds – default is model Earth year 365*24*3600)
  - <u>Automatically adjusted to quantize year</u>
- siderealRotationPeriod= in seconds – default is model Earth day ~86163.934
- quantizeYearLength= ‘true’ or ‘false’ (default is ‘true’)
- EOT (‘off’ / ‘naive’ / ‘on’) equation-of-time
  - important for high-eccentricity slow rotators)
  - Default is ‘on’ for non-Earth on Planet_2.0 branch (“naive” on Planet_1.0)
- Rarely used:
  - meanDistance=…(AU): S0X or planet_s0 equivalent.
  - hourAngleOffset=… (move prime-meridian, e.g., for topography)

Boundary Conditions Files

- Compare P1SoM40 with:
  - https://portal.nccs.nasa.gov/GISS_modelE/ROCKE-3D/publication-supplements/ /Way2020JGRP-Venus_Habitable_Climate_Scenarios/RUNDECKS/
  - Aquaplanet (24_V4101eoDOFP3Od_X001M2.R)
    - AIC: set winds (u,v) to zero
    - TOPO_OC and OIC depth
  - Venus 310m ocean (23_V4101eoDOFP3Od_X001J.R)
    - River directions file (in Planet_2.0 this is optional)
  - Venus Land planet (21_V4101eoDOFP3Od_X001LAR.R)

Boundary Conditions Files

- Compare P1SoM40 with:
    - https://portal.nccs.nasa.gov/GISS_modelE/ROCKE-3D/publication-supplements/Habitable_Climate_Scenarios_for_Proxima_Centauri_B/RUNDECKS/
    - Tidally Locked Proxima Centauri (with CO_2 atm)
        - aquaplanet (01_Control_ProxCenb04bHR_TL.R)
        - earth topography (longitude) (17_Day_Ocean_ProxCenb06b2HR_TL.R)
        - spectral files documentation
            - https://docs.google.com/document/d/15AYsvIrmOBQ4b5yIw3yJJV4cvkjcdJ0Z2gREKmIVVHs/edit
        - model/shared/PlanetParams_mod.F90

rsf files: bootstrapping from previous run

- rsf files (KRSF: See Slide 40)
- useful for small changes between configurations
- Can save time to reach equilibrium
- Must have same B.C. files, but can change:
  - orbital parameters
  - insolation
- Must use rsf file in place of AIC input file
- ISTART=9 (continue previous run)
- ISTART=8 (new run, ground hydrology reset)

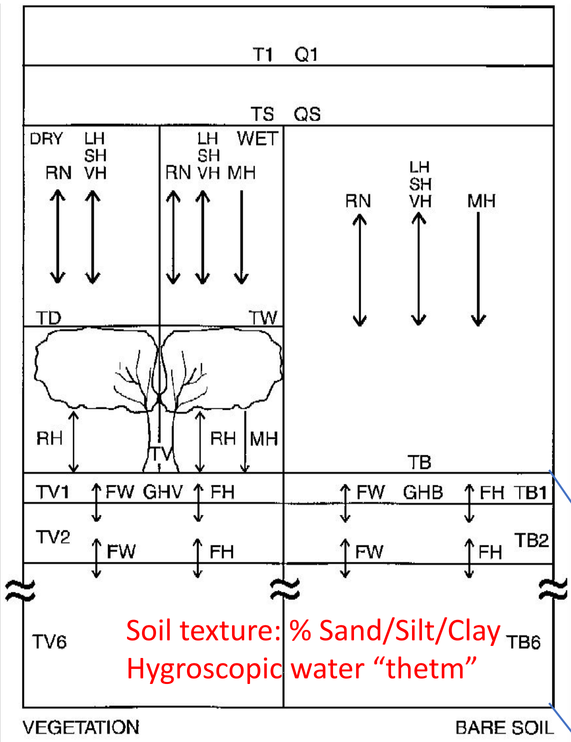
ROCKE-3D

GISS ModelE

Land Hydrology

(Rosenzweig & Abramopoulos 1997; Schmidt et al. 2006)

- 6 soil layers to 3.5 m depth
- 3 snow layers
- Vegetation canopy layer
- Aerodynamic evaporation from soil, snow and wet canopy
- Transpiration from dry canopy
- Infiltration / capillary rise / runoff



RN – net radiation
LH – latent heat flux
SH -- sensible heat flux
VH – heat of water vapor (planet 3.0)
MH – heat of precipitation
TD – temperature of dry canopy
TB – temperature of bare soil
TV1-6 – temperatures of soil layer under vegetation
FW – water flux between soil layers
GHV – heat flux into vegetated land
FH – heat flux between soil layers
TB1-6 – temperatures of bare soil layers
TS, QS – temperature and water vapor mixing ratio of surface
T1, Q1 – temperature and water vapor mixing ratio of first atmosphere layer

	soil depth (m)
	0.0
1	-0.09999996
2	-0.27254396
3	-0.57025843
4	-1.08394717
5	-1.97028677
6	-3.49961317

Lake water balance = soil run-off – evaporation + precipitation +/- transport
Maximum 95% of grid cell area

- Circular surface with conical bottom above soil, default slope R/H = 2000.
- Becomes cylinder when lake becomes small
- Can evaporate completely.
- **NEW: Automatic river directions from topography (#define RVR_ELEV)**

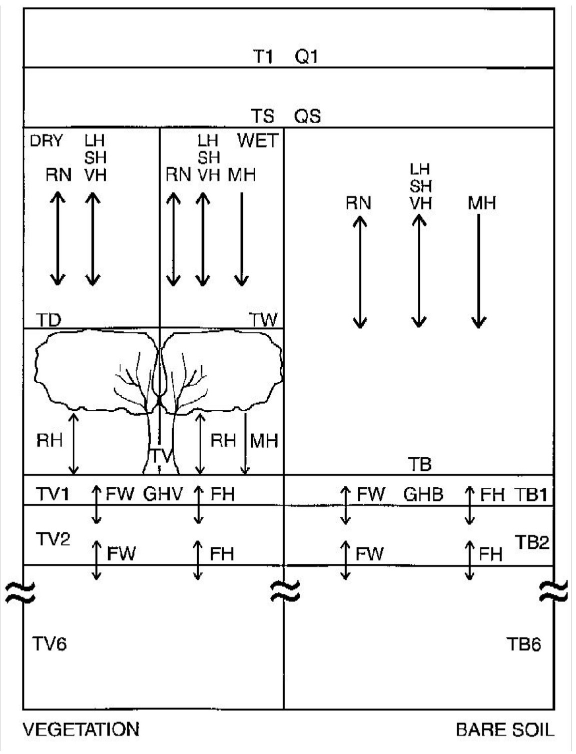
ROCKE-3D

GISS ModelE

Land Hydrology

(Rosenzweig & Abramopoulos 1997; Schmidt et al. 2006)

- 6 soil layers to 3.5 m depth
- 3 snow layers
- Vegetation canopy layer
- Aerodynamic evaporation from soil, snow and wet canopy
- Transpiration from dry canopy
- Infiltration / capillary rise / runoff



Total water balance =

qatm (atmosphere vapor)
+ cldw (clouds)
+ snowdp (snow)
+ gwtr (water in soil)
+ mwl (lakes+rivers, units different)

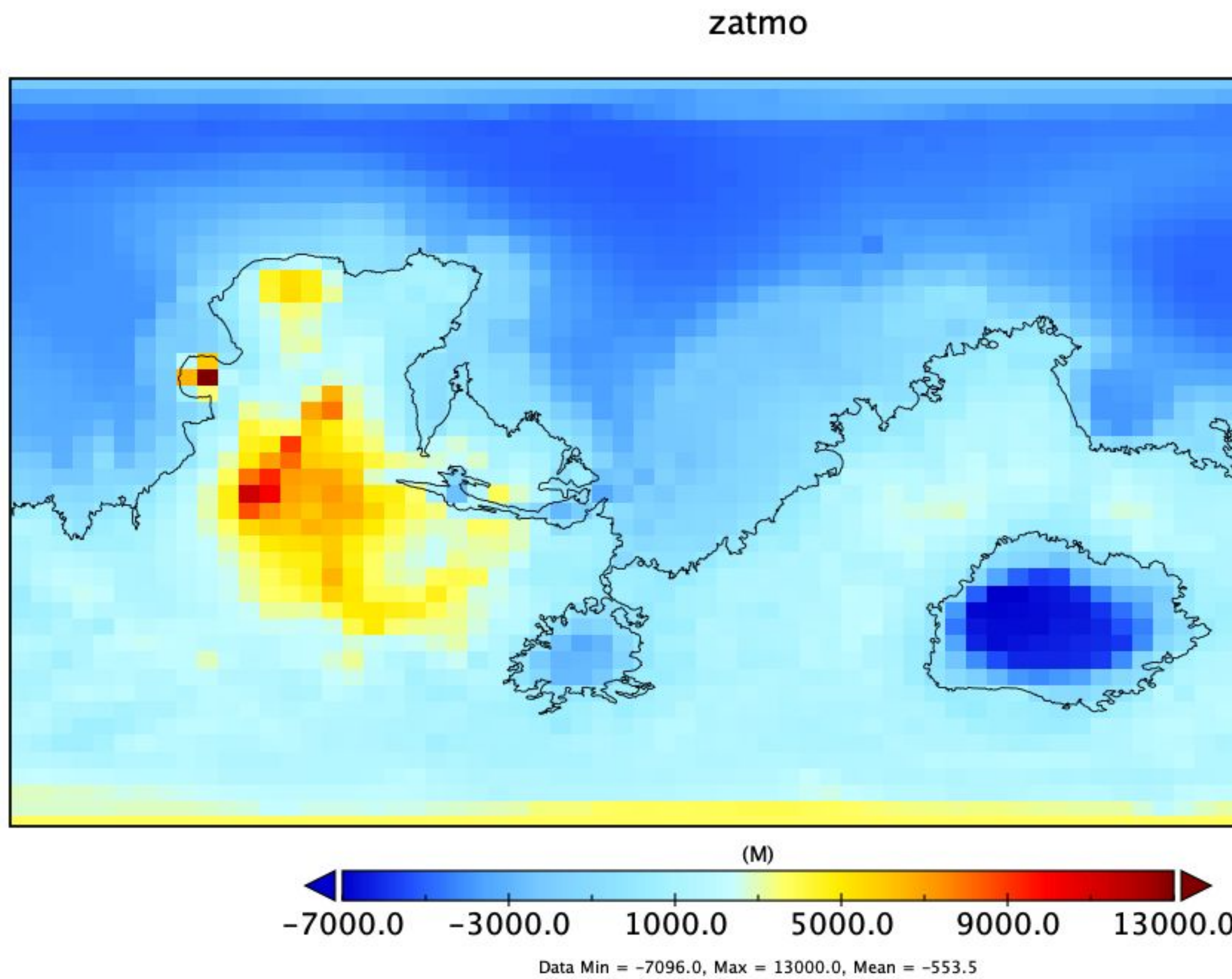
Soil "available water" (liquid) =

gwtr (water in soil)
– gice (frozen water in soil)
– thetm (hygroscopic water)

Input files

VEG = vegetation +albedo
TOP_INDEX = standard deviation of topography
SOIL = soil textures + slope
ROUGH = roughness length (can be generated from topography)
SOILIC = initial conditions for ground hydrology

PS_Mars topography



PS_Mars ground hydrology (SOIL)

SOIL=planet/desert_world/soil_allsand.nc

$ ncdump -h soil_allsand.nc

```
netcdf soil_allsand {
dimensions:
   lon = 72 ; West-East resolution
   lat = 46 ; South-North resolution
   ngm = 6 ; number of layers
   imt = 5 ; number of textures: sand, silt, clay, peat, rock
variables:
   float lon(lon) ;
       lon:units = "degrees_east" ;
   float lat(lat) ;
       lat:units = "degrees_north" ;
   float dz(ngm, lat, lon) ; thickness of layers (m)
   float q(ngm, imt, lat, lon) ; soil textures (centers) (fractions)
   float qk(ngm, imt, lat, lon) ; soil textures (edges) (fractions)
   float sl(lat, lon) ; typical slope
}
```

PS_Mars ground hydrology (SOILIC)

SOILIC=planet/desert_world/soilic_drysoil.nc

$ ncdump -h soilic_drysoil.nc

```
netcdf soilic_drysoil {
dimensions:
	jm = 46 ; West-East resolution
	im = 72 ; South-North resolution
	ngm = 6 ; number of layers
variables:
	double wetness(jm, im, ngm) ; wetness (0-1)
	double snow(jm, im) ; snow water equivalent (m)
	double temp(jm, im, ngm) ; soil temperature (o C)
// global attributes:
		:NCO = "3.9.9" ;
}
```

PS_Mars ground hydrology (VEG)

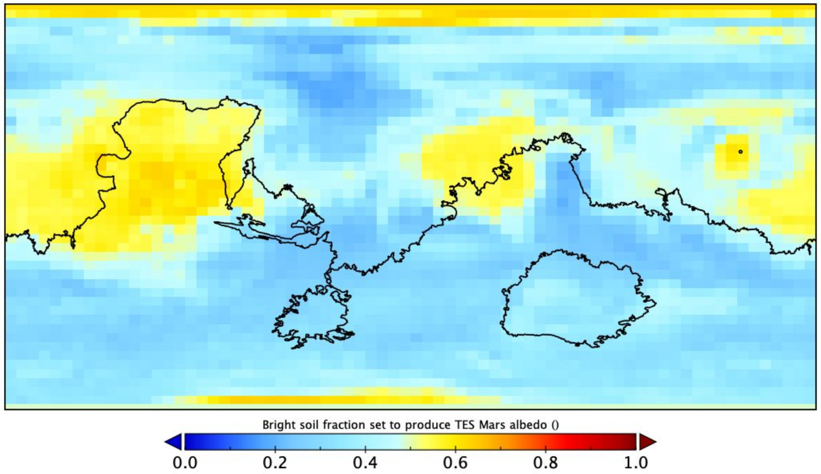
VEG=planet/Mars/veg_Mars_TES_albedo_EntPFT_72x46.nc

```
$ ncdump -h veg_Mars_TES_albedo_EntPFT_72x46.nc
netcdf veg_Mars_TES_albedo_EntPFT_72x46 {
dimensions:
        lon = 72 ;
        lat = 46 ;
variables:
        float lon(lon) ;
        float lat(lat) ;
        float bare_bright(lat, lon) ;
                bare_bright:long_name = "Bright soil fraction set to produce TES Mars albedo" ;
                bare_bright:units = "1" ;
        float bare_dark(lat, lon) ;
                bare_dark:long_name = "Dark soil fraction set to produce TES Mars albedo" ;
                bare_dark:units = "1" ;
// global attributes:
}
```

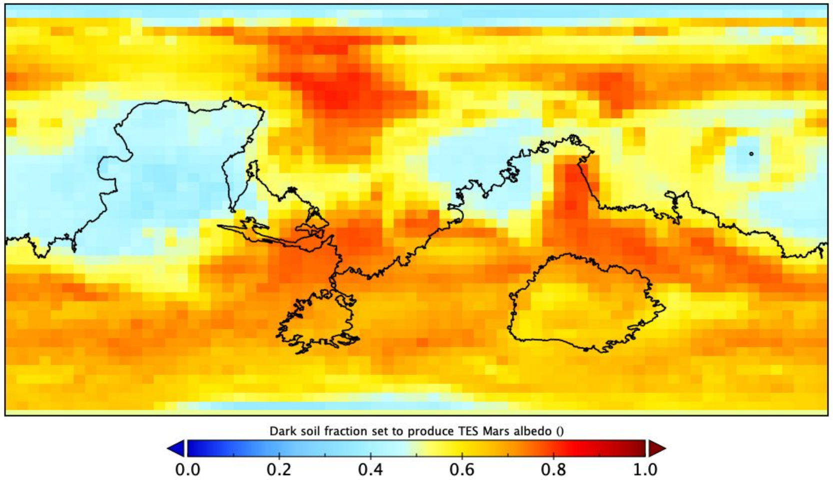
PS_Mars albedo

VEG=planet/Mars/veg_Mars_TES_albedo_72x46.nc

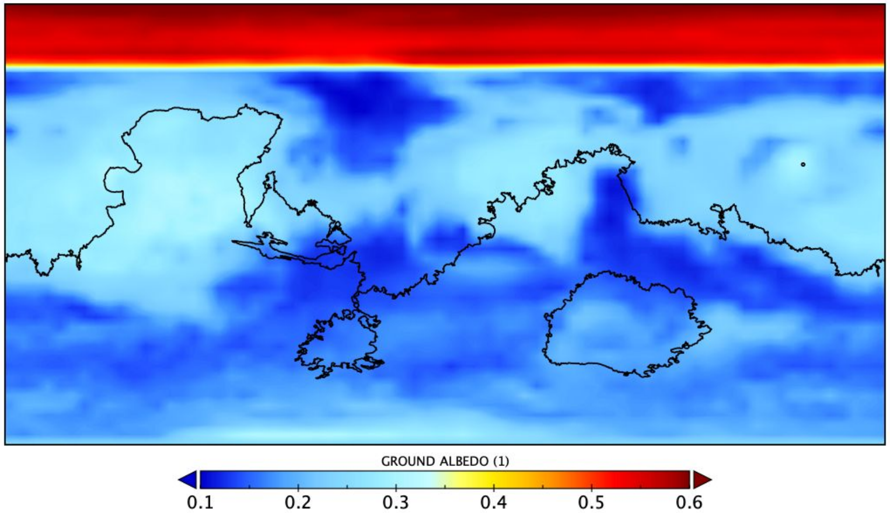
bright soil fraction (albedo = 0.5)



dark soil fraction (albedo = 0)



ROCKE-3D ground albedo (March)



Computed ground albedo is a combination of dark and bright soil
+ snow/CO2 ice effect

PS_Mars params …

```
#define PLANET_PARAMS likeMars
…………………………………………..
!------------------
planetName = 'Mars' ! Construct a calendar …
! The following sets the various orbital parameters
! source: http://en.wikipedia.org/wiki/Mars
eccentricity = 0.093
obliquity = 25.19d0 ! degrees
longitudeAtPeriapsis = 251.0 ! degrees
siderealOrbitalPeriod  = 59354294.4 ! seconds
siderealRotationPeriod = 88642.6848 ! seconds
quantizeYearLength='true' ! Or false
meanDistance = 1.52366231 ! AU (can use planet_s0 = ...  instead)
!------------------
```

PS_Mars diagnostics

```
Planet :: Mars
   Mean solar day:
          88775.1850588159       (sec)
          1.02749056781037       (Earth days)
   SiderealRotationPeriod:
          88642.6847826087       (sec)
          1.02595699979871       (Earth days)
   SiderealOrbitalPeriod:
          59390598.8043478       (sec)
          687.391189865137       (Earth days)
   meanDistance (AU)          :   1.52366231000000
   Precession (degs from VE)  :   251.000000000000
    Solar Days per year:          669
  Eccentricity:  9.300000000000000E-002
  Obliquity (degs):   25.1900000000000
Fixed orbital parameters for planet.
  Eccentricity:  9.300000000000000E-002
  Obliquity (degs):   25.1900000000000
  Longitude at periapsis (degs from ve):   251.000000000000
```

PRT diagnostics for Mars

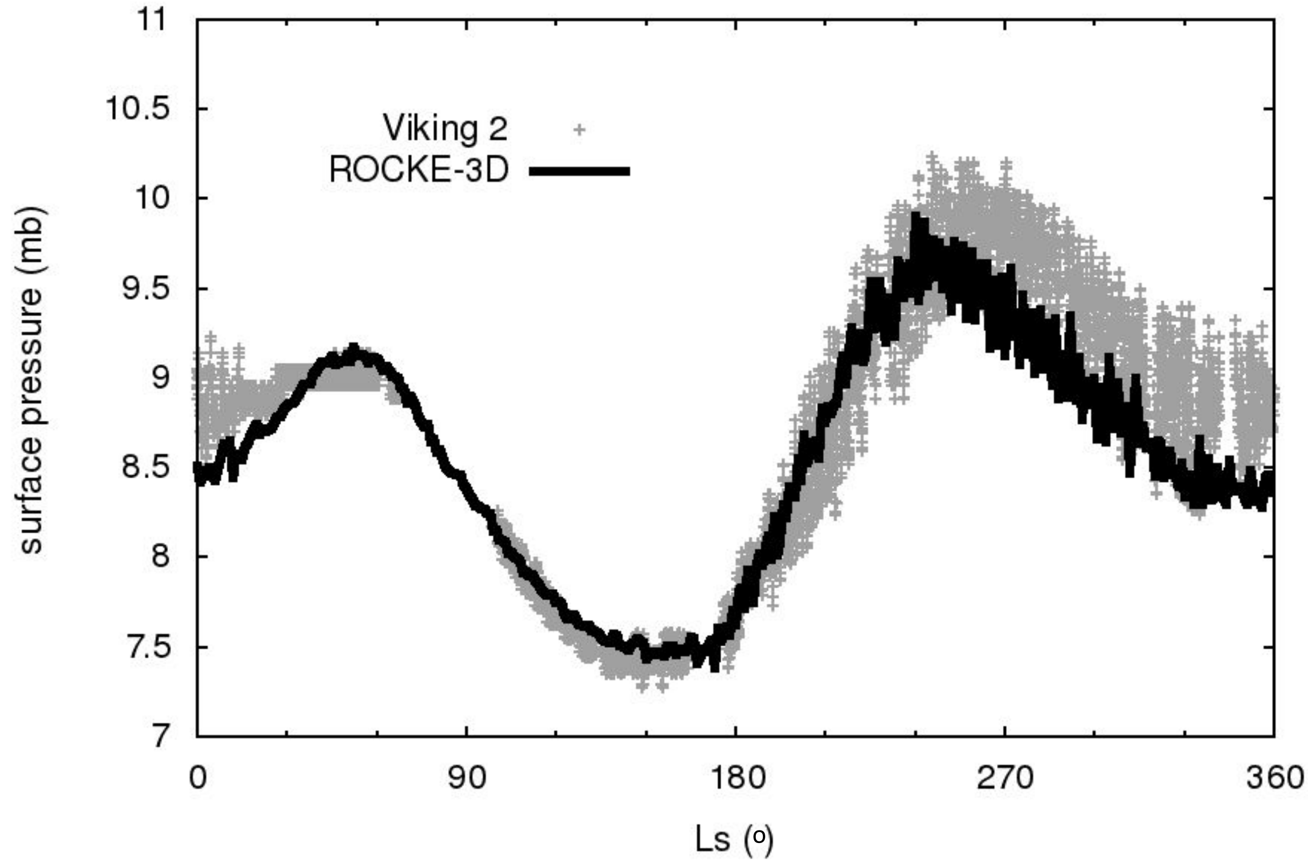
Calendar for Year: 2000

Calendar year length (sec): 59390598.8043

Full Name	Abbr	# days	1st day	mid day	lst day
January	JAN	49	1	25	49
February	FEB	45	50	72	94
March	MAR	54	95	121	148
April	APR	56	149	176	204
May	MAY	62	205	235	266
June	JUN	64	267	298	330
July	JUL	65	331	363	395
August	AUG	63	396	427	458
September	SEP	58	459	487	516
October	OCT	55	517	544	571
November	NOV	49	572	596	620
December	DEC	49	621	645	669

apsis........................06-31
periapsis.....................12-12
vernal equinox................03-52
summer solstice...............07-09
winter solstice...............12-41
autumnal equinox..............10-02

Mars pressure seasonal cycle

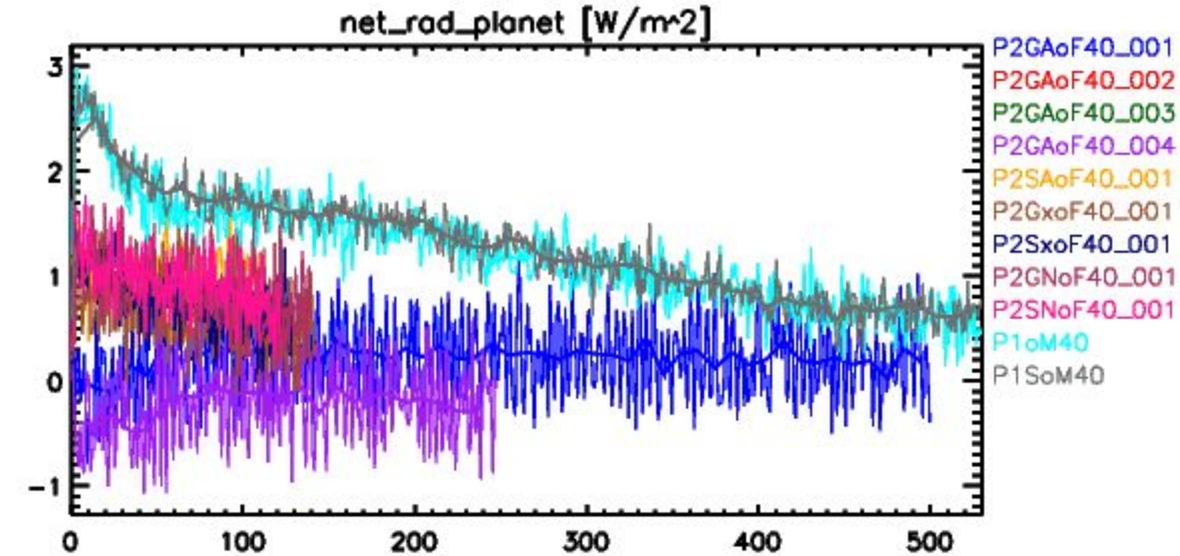


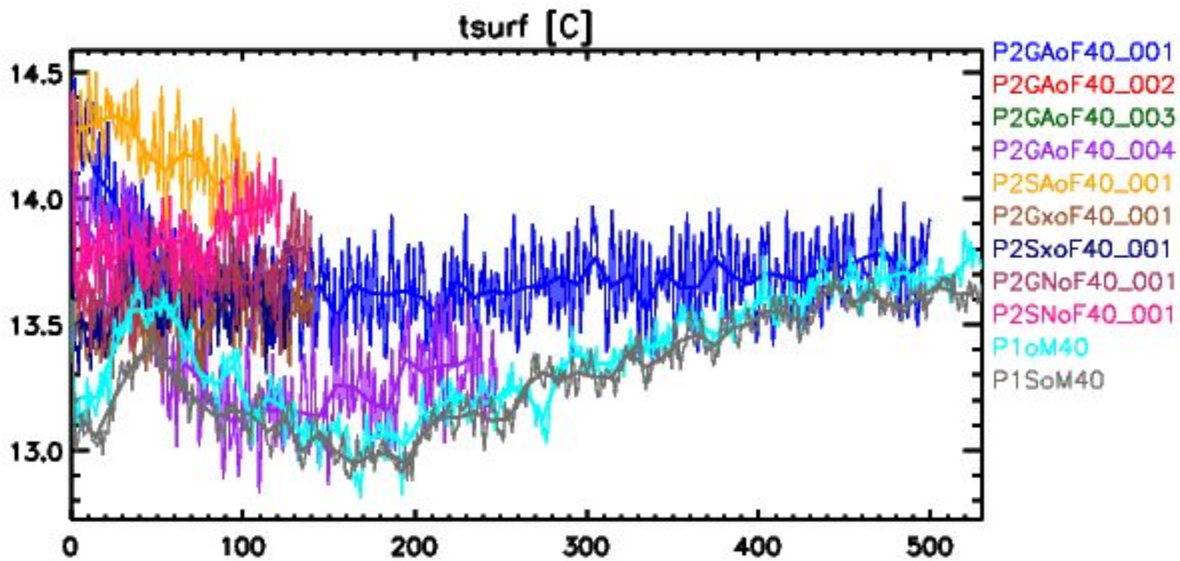
Annual cycle of Mars surface pressure, as measured by the Viking 2 lander (gray crosses) (Hess et al. 1977; Tillman 1989), and surface pressure simulated by ROCKE-3D (black solid line).

Post Processing Analysis

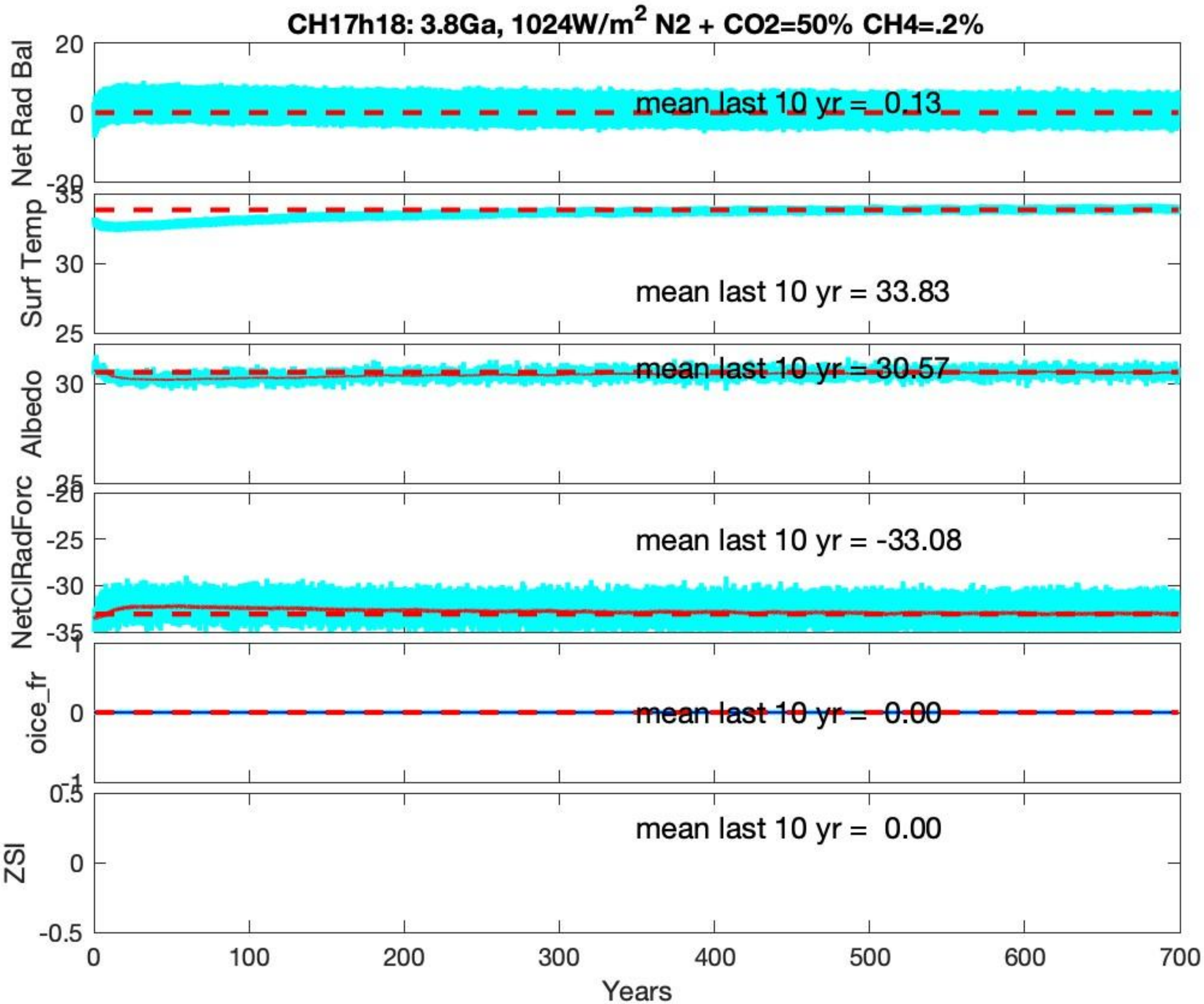
- How do we decide something is in equilibrium?
  - Radiative equilibrium (atm + ocean)
  - Hydrological equilibrium

    (could be 1000s of yrs)

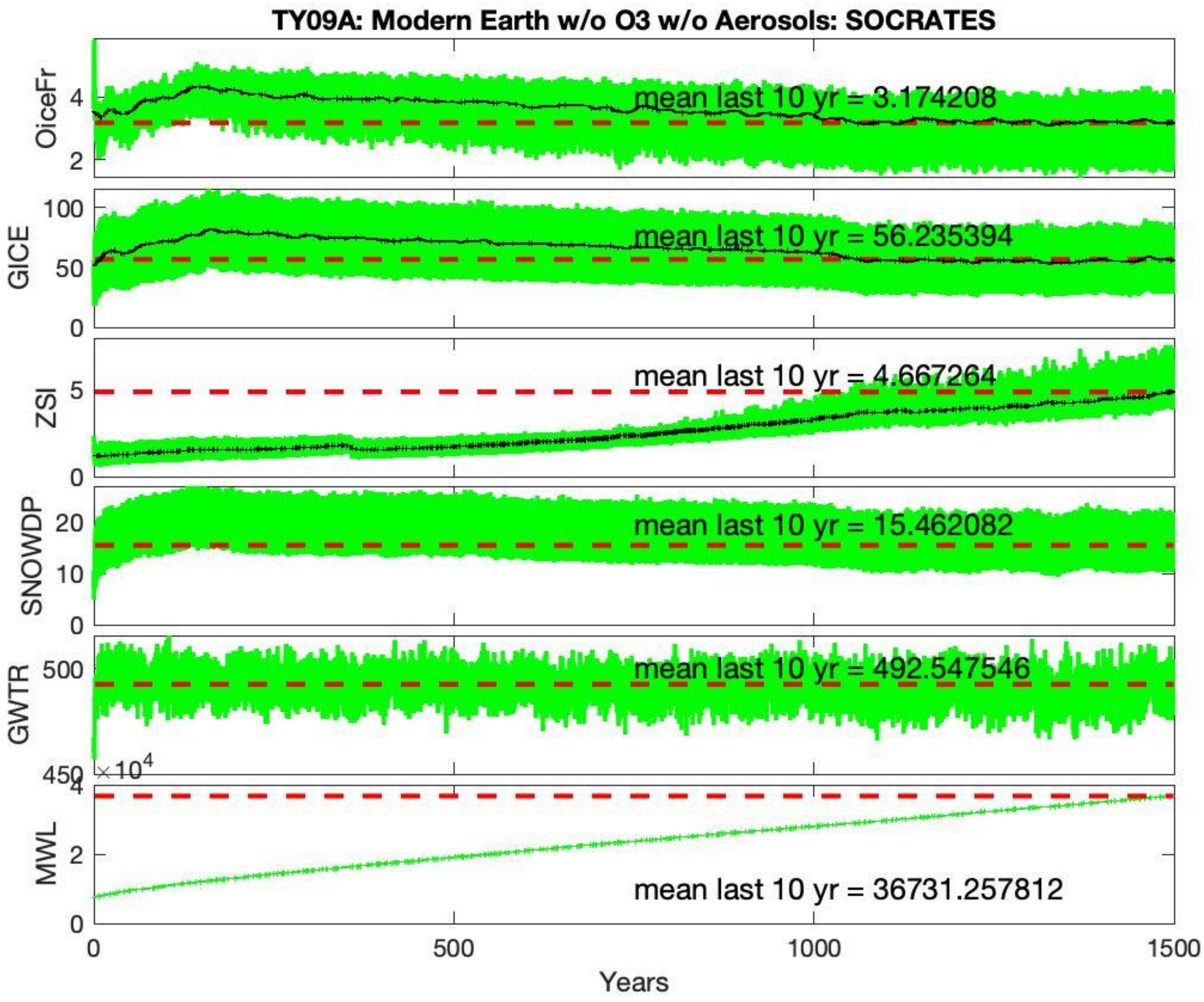




Hydrological Equilibrium Example



Hydrological Equilibrium Example

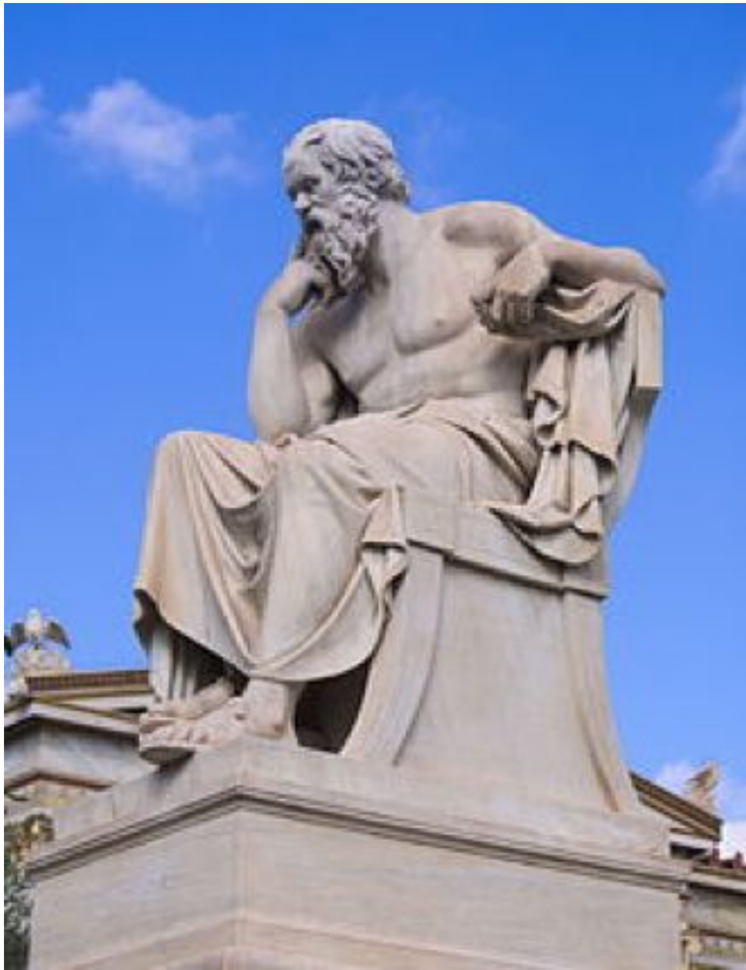


Radiative Transfer: SOCRATES

Suite **O**f **C**ommunity **RA**diative **T**ransfer codes based on **E**dwards and **S**lingo

SOCRATES

The radiative transfer component of ROCKE-3D

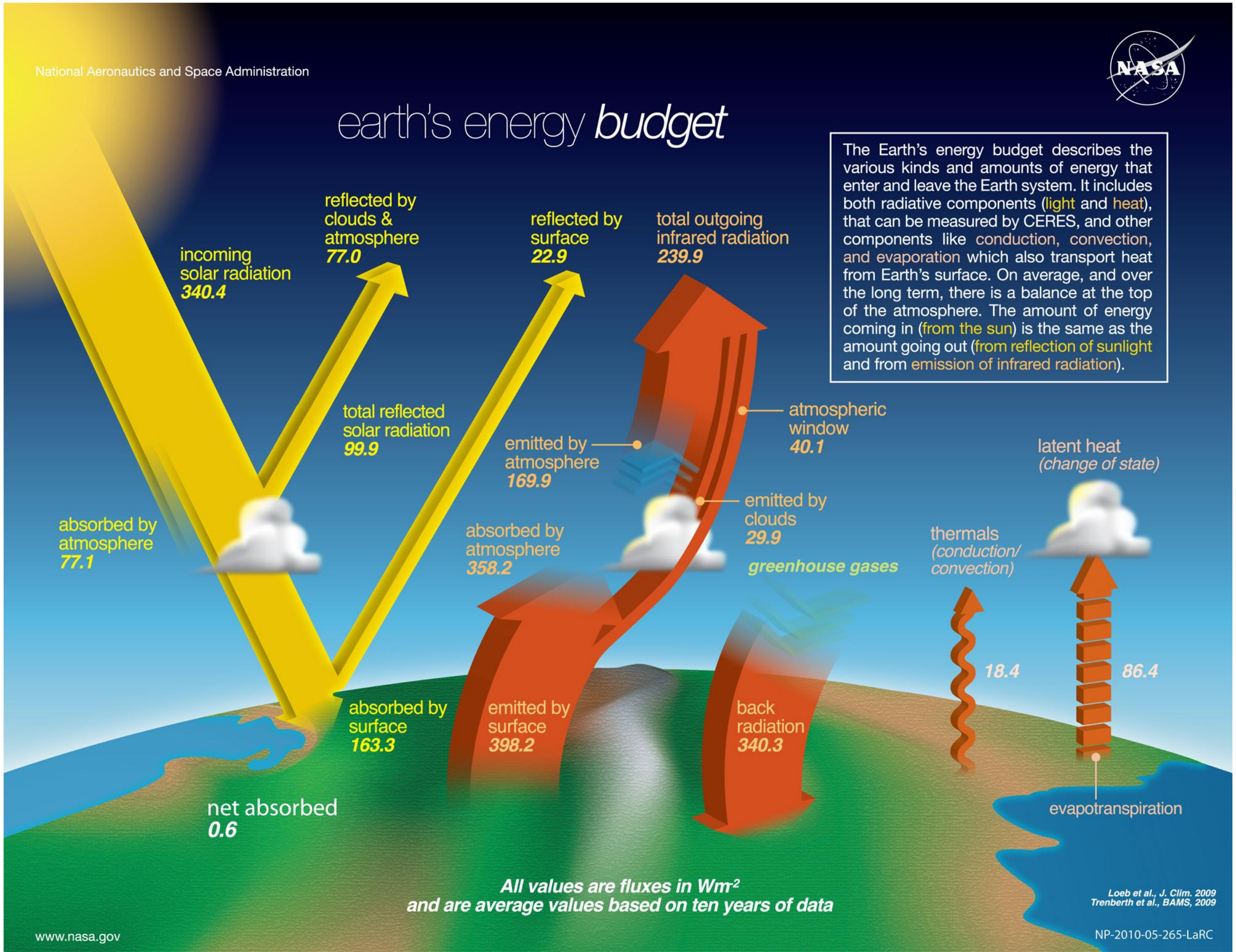


What is Radiative Transfer?

The transfer of electromagnetic energy through a medium.

Radiative transfer in large part determines the energy balance of planets.

This balance can be very different for other planets compared to Earth!



What is Radiative Transfer?

Scattering/Absorption

by gases (N_2, CO_2, H_2O, etc)

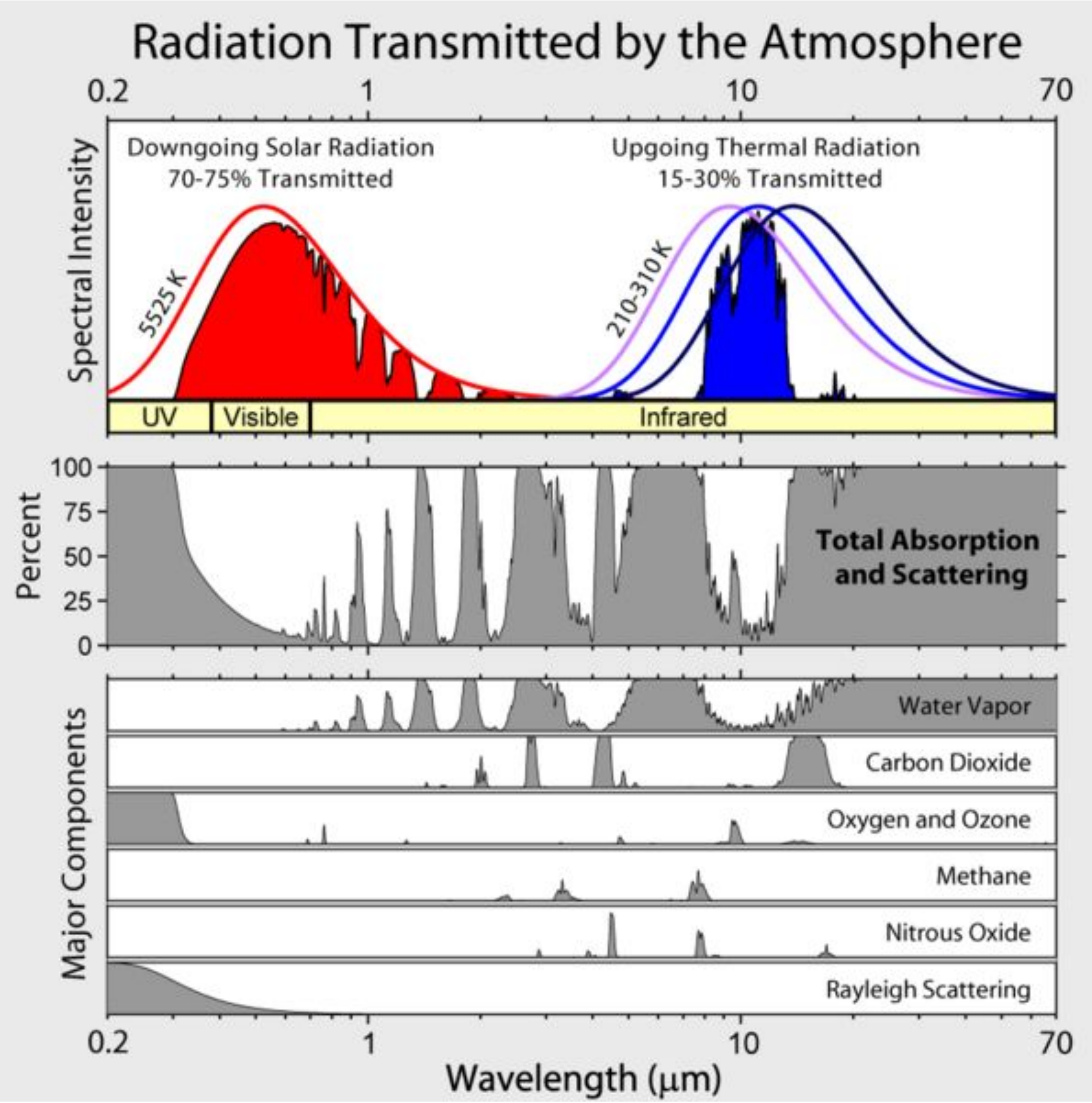
by aerosols (clouds, hazes, etc)

Emission/Reflection

by surfaces (ice, land, ocean)

by the atmosphere itself

Other planets may have very different incident stellar flux, gases, aerosols, and surface properties!



Radiative Transfer: SOCRATES

SOCRATES: a radiative transfer model designed for use in 3-D climate models

requirements: *flexible, fast, accurate*

key terms

spectral files: tailored sets of gas and aerosol absorption coefficients used in SOCRATES (must be set in rundeck, *spectral_file_lw*, *spectral_file_sw*)

stellar spectra: incident stellar energy spectra, convolved with shortwave spectral files (*solar_spec*)

incident stellar flux: the total amount of stellar energy reaching a planet (*planet_s0*)

Important SOCRATES Resources

ROCKE-3D/SOCRATES User guide

(how to setup SOCRATES within ROCKE-3D)

https://docs.google.com/document/d/1B80VTwyxwnozNt5rNry0ICWvz-UWO-bAWZjMTyfhVfA/edit

ROCKE-3D/SOCRATES List Of Spectral Files

(a list and description of gas absorption files and stellar spectra available)

https://docs.google.com/document/d/15AYsvIrmOBQ4b5yIw3yJJV4cvkjcdJ0Z2gREKmIVVHs/edit#heading=h.dpunmplojmki

SOCRATES technical manual guide

(the gory technical description of the inner workings of SOCRATES, provided by the UK Met Office)

http://homepages.see.leeds.ac.uk/~lecsjed/winscpuse/socrates_techguide.pdf

SOCRATES user guide

(users guide for advanced applications of SOCRATES, provided by the UK Met Office)

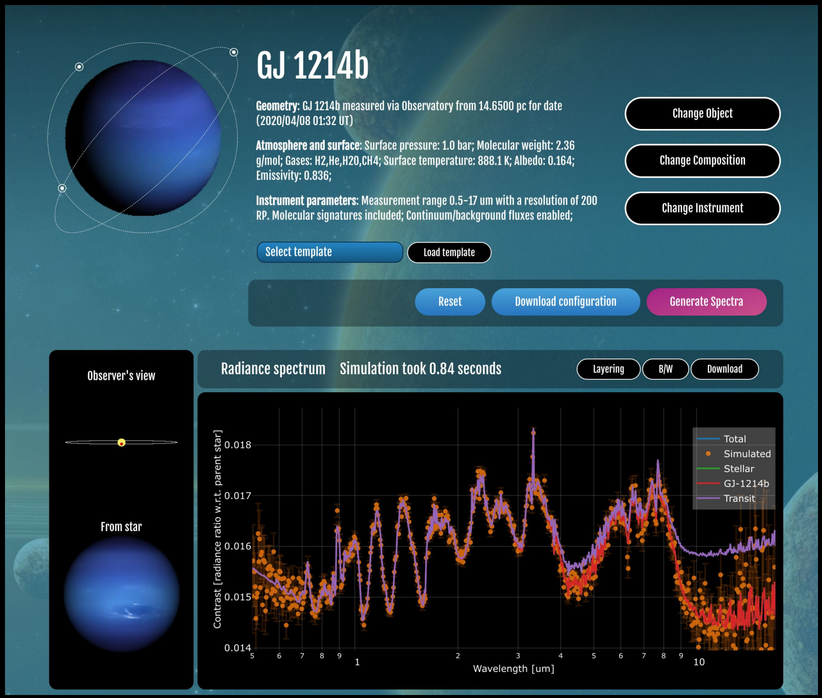
http://homepages.see.leeds.ac.uk/~lecsjed/winscpuse/socrates_userguide.pdf

Using the Planetary Spectrum Generator to study 3D inputs of Exoplanets

Vincent Kofman
Villanueva, Fauchez, & the PSG team

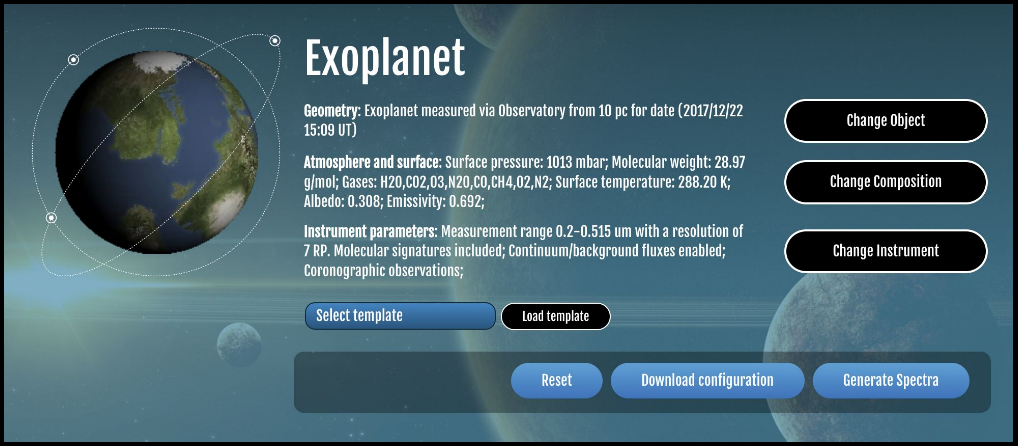
the Planetary Spectrum Generator

- PSG is a free radiative transfer tool (UV-radio, ground/space telescopes & orbiters).
- Contains most Solar system object and all confirmed exoplanets
- Noise simulator for different instrument types and background noise sources
- Capable of grid-based retrievals & bulk analysis (~millions of spectra) through cluster-hosted API calls
- GlobES module for ingesting results from Global Circulation Models

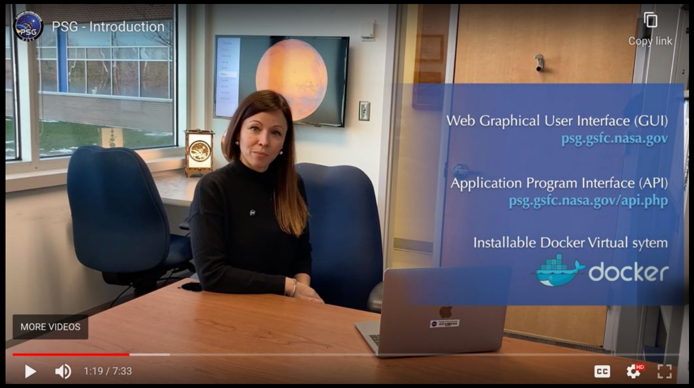


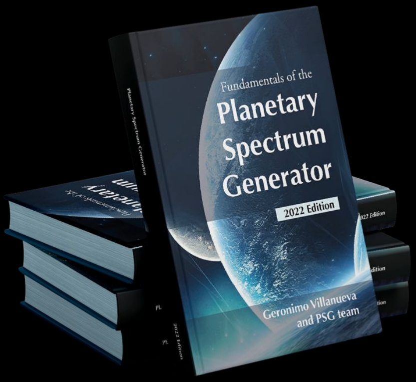
https://psg.gsfc.nasa.gov/

the Planetary Spectrum Generator



- Fully free and online simulations accessible with a user-friendly web interface (also from mobile devices)
- Extensive documentation – Handbook, many tutorial videos and online documentation freely available





https://psg.gsfc.nasa.gov/

the Planetary Spectrum Generator

Code repository

https://github.com/nasapsg/globes

Main site

https://psg.gsfc.nasa.gov/

PSG tutorial, handbook, parameter list

https://youtu.be/cojqtJjBxQg?feature=shared

https://psg.gsfc.nasa.gov/images/help/handbook.pdf

https://psg.gsfc.nasa.gov/helpapi.php#parameters

the Planetary Spectrum Generator

Code repository

https://github.com/nasapsg/globes

Main site

https://psg.gsfc.nasa.gov/

PSG tutorial, handbook, parameter list

https://youtu.be/cojqtJjBxQg?feature=shared

https://psg.gsfc.nasa.gov/images/help/handbook.pdf

https://psg

The pale blue dot: using the Planetary Spectrum Generator to simulate signals from hyper realistic exo-Earths

Kofman[1,2], Villanueva[1], Fauchez[1,2], Mandell[1], Johnson[3], Payne[1], Latouf[1,4], Kelkar[1,5]
1: NASA Goddard Space Flight Center, 8800 Greenbelt Rd, Greenbelt, MD, 20771, USA
2: Physics Department, College of Arts and Science, American University, 4400 Massachusetts Ave NW, Washington, DC 20016
3: Dept. Physics and Astronomy, University of Las Vegas, 4505 S. Maryland Pkwy. Las Vegas, NV 89154, USA
4: George Mason University, 4400 University Drive, Fairfax, VA, 22030, USA
5: IISER, Indian Institute of Science Education and Research, Dr. Homi Bhabha Road, Pune, 411008, India

Draft version May 29, 2024
Typeset using LaTeX **twocolumn** style in AASTeX631

From General Circulation Models (GCMs) to Exoplanet Spectra with the Global Emission Spectra (GlobES)

Thomas J. Fauchez,[1,2,3] Geronimo L. Villanueva,[4,3] Vincent Kofman,[4,2,3] Ravi K. Kopparapu,[4] and Gabrielle Suissa

[1] *NASA Goddard Space Flight Center 8800 Greenbelt Road Greenbelt, MD 20771, USA*
[2] *Integrated Space Science and Technology Institute, Department of Physics, American University, Washington DC*
[3] *NASA GSFC Sellers Exoplanet Environments Collaboration*
[4] *NASA Goddard Space Flight Center, Greenbelt, MD, USA.*

Outline

- General principles of PSG and GlobES

- Use cases
  1. Transiting Trappist 1e
  2. Observations of direct imaging
  3. Phase curve of Trappist 1b

- Demonstration

Modeling Atmospheric Absorption

- Ephemeris and flux calculation
  - Planet and stellar size, distance and location in the sky
  - Photon budget as function of wavelength
- Radiative transfer code
  - Atmospheric structure and abundances
  - Molecular databases & physical processes
  - Retrieval of atmospheric chemical and physical conditions
- Instrument, detector, and noise model
  - Wavelength range, throughput, sensitivity
  - Detector type, quantum efficiency, telescope temperature
  - Noise sources, signal strengths

PSG: Operation principles

- Configuration file contains all input for the simulation
- Use the interface to modify and run the config or edit using text editor -> upload or send API command
- Reproducible, shareable, easy to modify and test importance different molecules/physical phenomena

1. Load template config
2. Translate netCDF to PSG binary
3. Test in GlobES interface

Configuration file - example

- ATMOSPHERE
- GENERATOR
- GEOMETRY
- SURFACE
- OBJECT
- RETRIEVAL

```
<OBJECT-OBS-LONGITUDE>-38.583984
<OBJECT-OBS-LATITUDE>7.44873
<OBJECT-SOLAR-LONGITUDE>-46.21
<OBJECT-SOLAR-LATITUDE>0.4
<GENERATOR-GAS-MODEL>Y
<ATMOSPHERE-NAERO>1
<SURFACE-MODEL>Cox-Munk,8.0
<ATMOSPHERE-NMAX>4
<ATMOSPHERE-LMAX>60
<OBJECT-DATE>2008/03/19 15:00:00
<OBJECT>Planet
<OBJECT>Planet
<OBJECT-NAME>Earth
<OBJECT-DIAMETER>12742
<OBJECT-GRAVITY>9.8
<OBJECT-GRAVITY-UNIT>g
<OBJECT-STAR-DISTANCE>1.0
<OBJECT-STAR-VELOCITY>0.0
<OBJECT-STAR-TYPE>G
<OBJECT-STAR-TEMPERATURE>5777
<OBJECT-STAR-RADIUS>1.0
<OBJECT-OBS-VELOCITY>0.0
<OBJECT-PERIOD>58.646
<OBJECT-STAR-METALLICITY>0.0
<OBJECT-INCLINATION>90.00
<OBJECT-ECCENTRICITY>0.00000
<OBJECT-PERIAPSIS>0.00
<GEOMETRY>Observatory
<GEOMETRY-OFFSET-NS>0.0
<GEOMETRY-OFFSET-EW>0.0
```

```
<ATMOSPHERE-STRUCTURE>Equilibrium
<ATMOSPHERE-DESCRIPTION>NASA/MERRA2 / GFS / NCEP / US Weather
Service
<ATMOSPHERE-PRESSURE>1.00
<ATMOSPHERE-PUNIT>bar
<ATMOSPHERE-TEMPERATURE>300
<ATMOSPHERE-WEIGHT>28.97
<ATMOSPHERE-NGAS>6
<ATMOSPHERE-AEROS>SeaSalt
<ATMOSPHERE-ATYPE>AFCRL_Seasalt_HRI
<ATMOSPHERE-AABUN>5
<ATMOSPHERE-AUNIT>ppb
<ATMOSPHERE-ASIZE>0.078
<ATMOSPHERE-ASUNI>um
<ATMOSPHERE-CONTINUUM>Rayleigh,Refraction,CIA_all,UV_all
<ATMOSPHERE-LAYERS>72
<ATMOSPHERE-GAS>CO2,N2O,N2,O2,H2O,O3
<ATMOSPHERE-TYPE>HIT[2],HIT[4],HIT[22],HIT[7],HIT[1],HIT[3]
<ATMOSPHERE-ABUN>400,.3,78.1,20.9,1,1,1.5
<ATMOSPHERE-UNIT>ppm,ppm,pct,pct,scl,scl
<ATMOSPHERE-GCM-
PARAMETERS>144,91,72,-180,-90,2.5,2.0,Surf_Ocean,Surf_Snow,Sur
f_Soil,Surf_Forest,Surf_Grass,Temperature,Pressure,Water,Water
Ice,H2O,O3
<SURFACE-TEMPERATURE>300
<SURFACE-ALBEDO>0.3928
<SURFACE-EMISSIVITY>0.000
<SURFACE-PHASEMODEL>ISO
<SURFACE-GAS-RATIO>1.0
<SURFACE-GAS-UNIT>ratio
```

```
<SURFACE-NSURF>5
<SURFACE-SURF>Ocean,Snow,Grass,Soil,Forest
<SURFACE-
TYPE>Albedo_GSFC,Albedo_GSFC,Albedo_GSFC,Albedo_GSFC,Albedo_GSFC
<SURFACE-
ABUN>1.02991e-01,8.97009e-01,0.00000e+00,0.00000e+00,0.00000e+00
<SURFACE-UNIT>scl,scl,scl,scl,scl
<GENERATOR-BEAM>1
<GENERATOR-BEAM-UNIT>diameter
<GENERATOR-CONT-MODEL>Y
<GENERATOR-RANGE1>450
<GENERATOR-RANGE2>650
<GENERATOR-RANGEUNIT>nm
<GENERATOR-RESOLUTION>100
<GENERATOR-RESOLUTIONUNIT>nm
<GENERATOR-RADUNITS>Wsrm2um
<GENERATOR-DIAMTELE>6.5
<GENERATOR-LOGRAD>N
<GENERATOR-CONT-STELLAR>N
<GENERATOR-TRANS-APPLY>N
<GENERATOR-TRANS-SHOW>N
<GENERATOR-TRANS>02-01
<GENERATOR-NOISE>NO
<GENERATOR-NOISE2>1
<GENERATOR-NOISETIME>0.4
<GENERATOR-NOISEOTEMP>300
<GENERATOR-NOISEOEFF>1
```

Translating netCDF into the PSG binary format

<ATMOSPHERE-GCM-PARAMETERS>144,91,72,-180,-90,2.5,2.0,Surf_Ocean,Surf_Snow,Surf_Soil,Surf_Forest,Surf_Grass,Temperature,Pressure,Water,WaterIce,H2O,O3

```python
    infile  = 'Fig_2/data/ground_03.dat'
    data_s = np.fromfile(infile, dtype=np.float32)

    with open(outfile, 'xb') as fo:
        fo.write(bytes('<BINARY>',encoding = 'utf-8'))
        fo.write(np.array(data_s[2:-2],order='C'))
        fo.write(np.array(t_map,order='C'))
        fo.write(np.array(p_map,order='C'))
        fo.write(np.array(lq_map,order='C'))
        fo.write(np.array(ic_map,order='C'))
        fo.write(np.array(h2o_map,order='C'))
        fo.write(np.array(o3_map,order='C'))
        fo.write(bytes('</BINARY>',encoding = 'utf-8'))
```

```
      0  3C42 494E 4152 593E 0000  <BINARY>
     10  0000 0000 0000 0000 0000
8787570  F0C1 0000 F0C1 89A9 72C1  ..  ....r.
8787580  633F DDC0 9F23 C7C1 0000  c?...#..
8787590  F0C1 5596 9AC1 5D81 1EC1  ..U...]. .
8787600  7393 97C1 DB58 C6C1 B6F4  s....X....
8787610  DAC0 42F9 0BC1 04E1 48C1  ..B. . .H.
8787620  498D 68C0 9418 85C1 4128  I.h.. ..A(
8787630  DDC1 66E0 E4C1 FCC1 EDC1  ..f.......
8787640  3E22 6AC1 E094 86C0 AE32  >"j......2
8787650  45C0 6A2E 61C0 86C8 0EC1  E.j.a... .
8787660  E394 D1C1 5AF3 2CC1 82ED  ....Z.,...
```

https://github.com/nasapsg/globes/blob/main/gcm_rocke3d

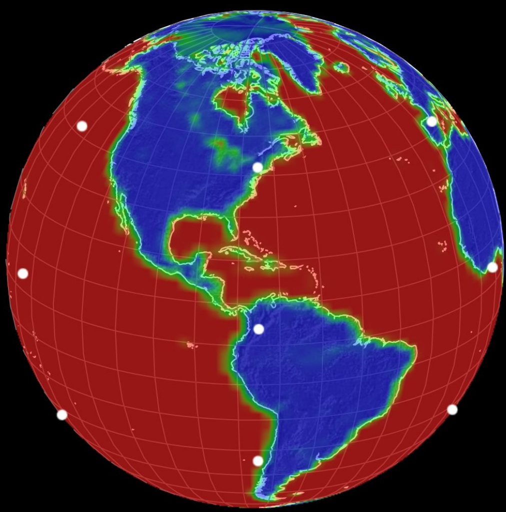
GlobES interface and GCM files

2. Check if inputs read correctly

Variable
Surf_Ocean
Altitude
Surface
Topography
Earth's topography
Show winds
2D Interpolation
Show data-points

GCM data
Select a source

1. Upload binary file and configuration



East longitude / Latitude: -30.9 30.9 surf_ocean [part]: 1
Atmospheric data: NASA/MERRA2 / GFS / NCEP / US Weather Service
surf_ocean (0 to 1 part)

3. Verify calculation parameters

Parameters of the spectroscopic 3D synthesis

The parameters of the (exo)planet and its host star are as defined in the Target and Geometry section of PSG. This also includes the observational conditions (e.g., distance to the object, inclination, phase), while in this section, the user can also quickly define observational mode (i.e., transit, direct imaging and phase). However, it is important that the user verifies the parameters in the Target and Geometry section. The atmosphere and surface information will be as defined in the Atmosphere and Surface section, while the algorithm will use the 3D atmospheric data defined in this section to establish the vertical profiles at each location.

Geometry Current: Disk emission | Primary transit | Disk emission | Phase: 0.0

Atmosphere Molecules: CO2,N2O,N2,O2,H2O,O3 | Aerosols: SeaSalt,Water,WaterIce | Change

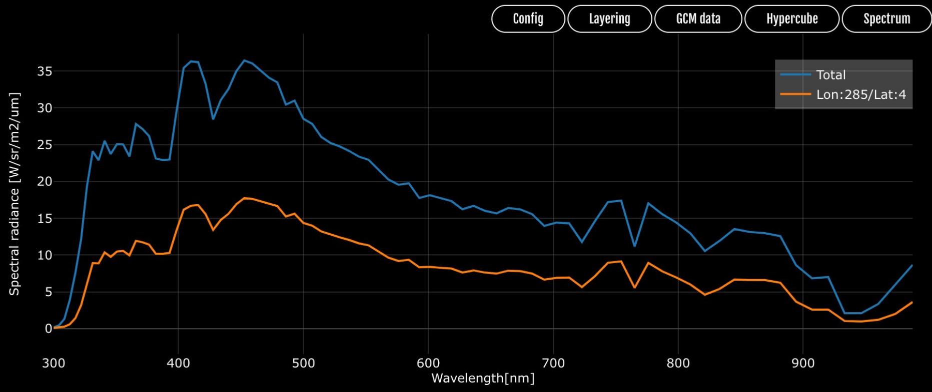
Instrument Wavelength: 300-1000 nm, resolution 70 RP | Change

Spatial binning 20 Higher binning leads to faster calculations, yet degraded regional details

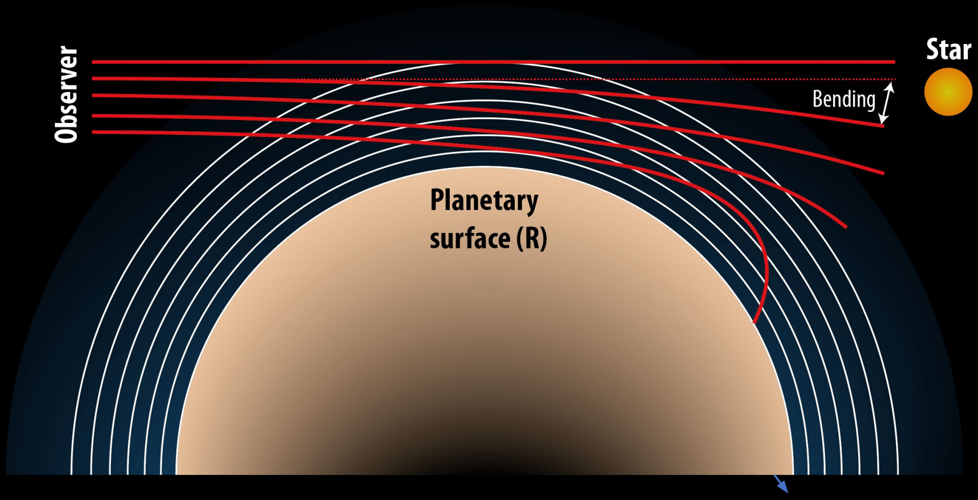
4. Run!!

Generate 3D Spectra

5. Save results



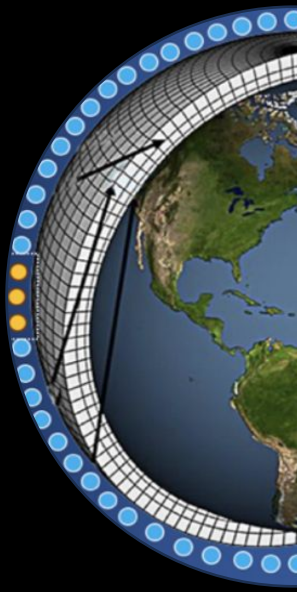
1. Synthesizing transit spectra

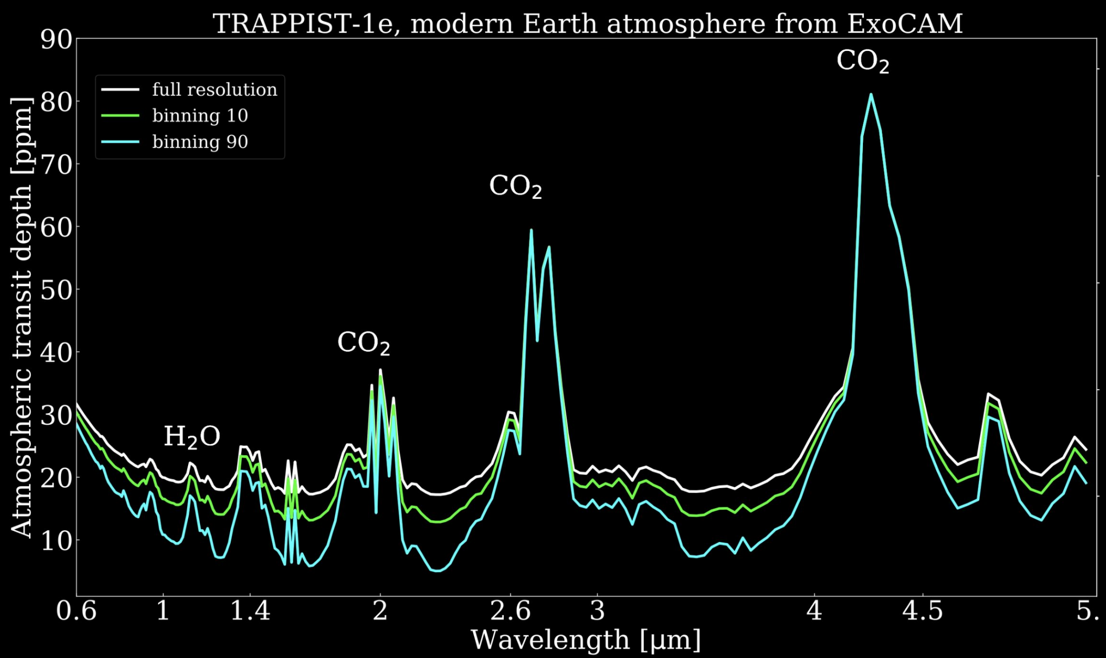


- Transit modeling follows extinction of light across an atmosphere
- Important to consider layering, spherical effects, and refraction of light
- Opacity sources: molecules, clouds, hazes

1. Synthesizing transit spectra

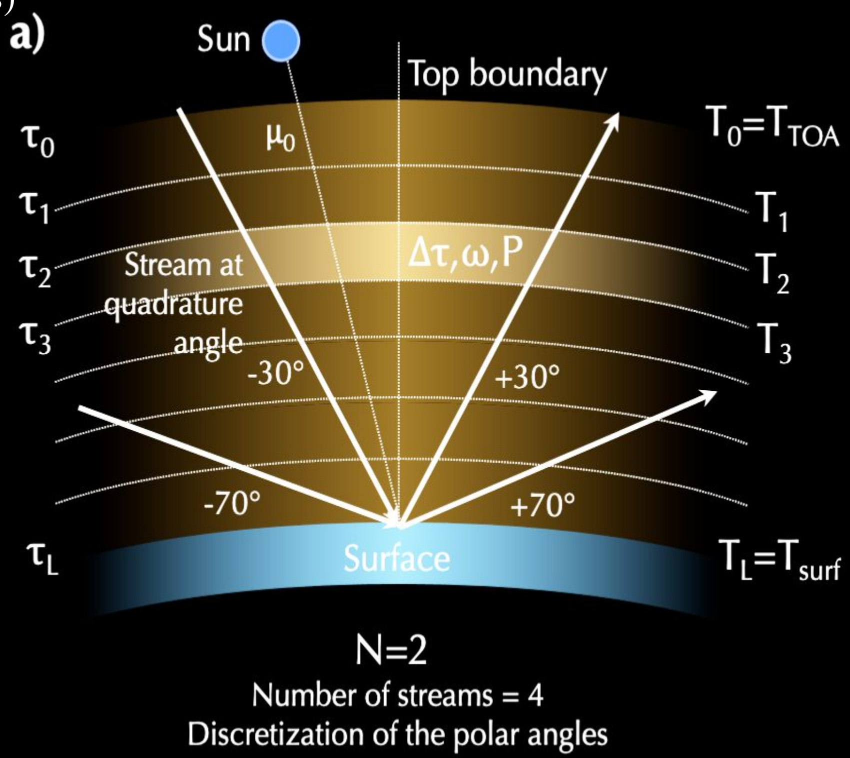
- Clouds across the terminator
- The average of the planet may result in underestimation of cloud opacity

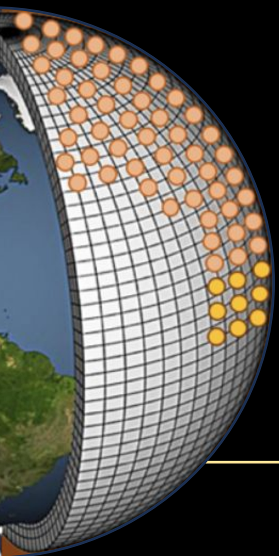




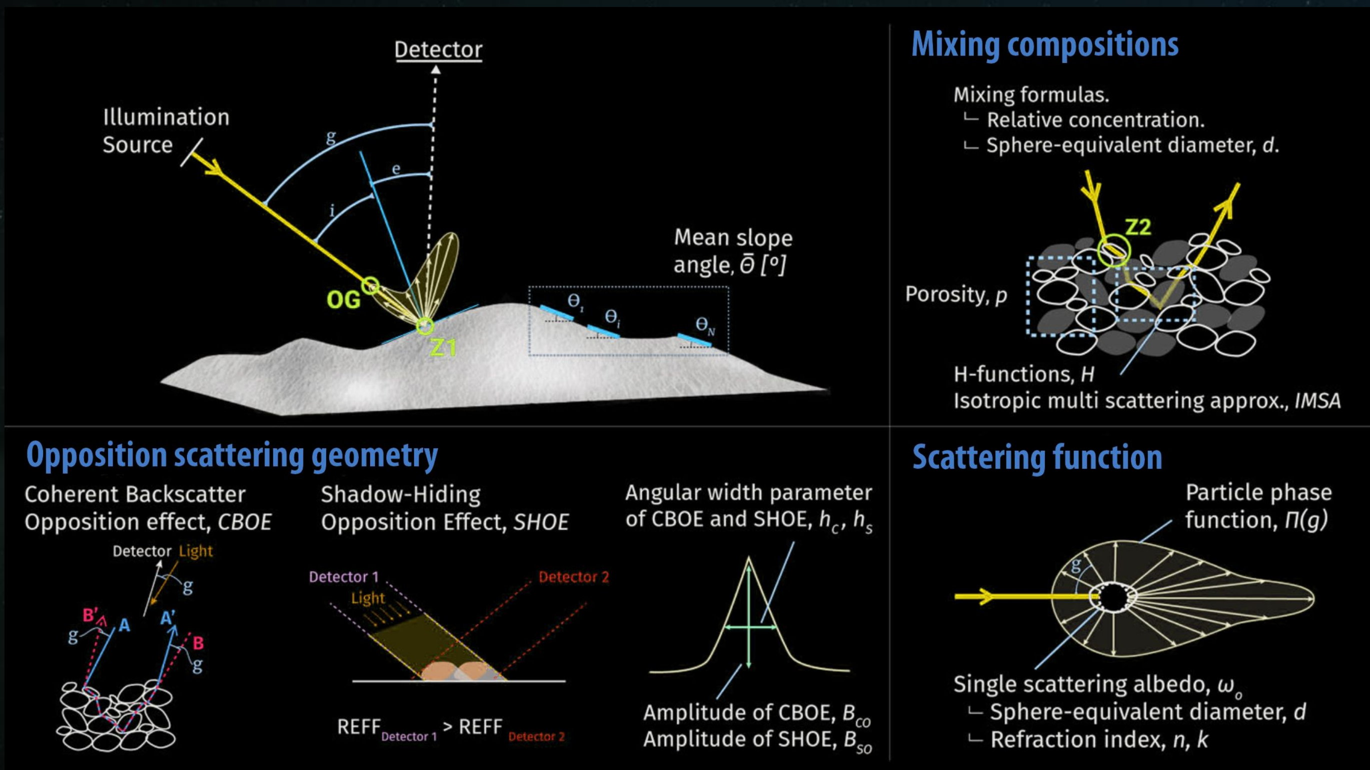
2. Direct imaging simulations

- Requires balancing of light streams in the atmosphere considering multiple scattering to obtain intensity
- Surface modeling (e.g., glint, Fresnel effects) and scattering models have notable effects.
- Earth: Strong local variations dominate the spectra -> 1D approximation insufficient





Advanced scattering models



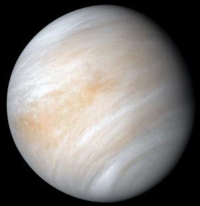
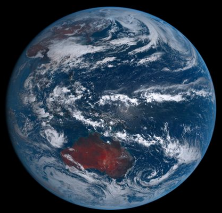
Adapted from Pommerol et al. 2019

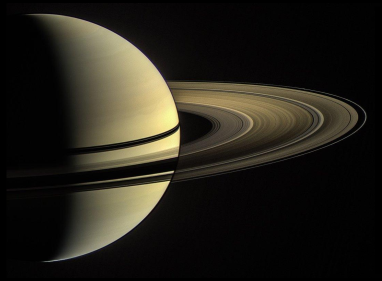
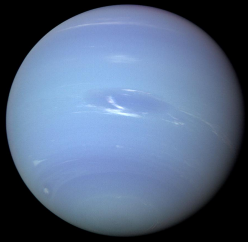
3D and integrated surface modeling with many available phase functions, mixing and component properties.

PSG permits Lambert, Hapke, Lommel-Seeliger, ocean glint, Fresnel, surface scattering modelling.

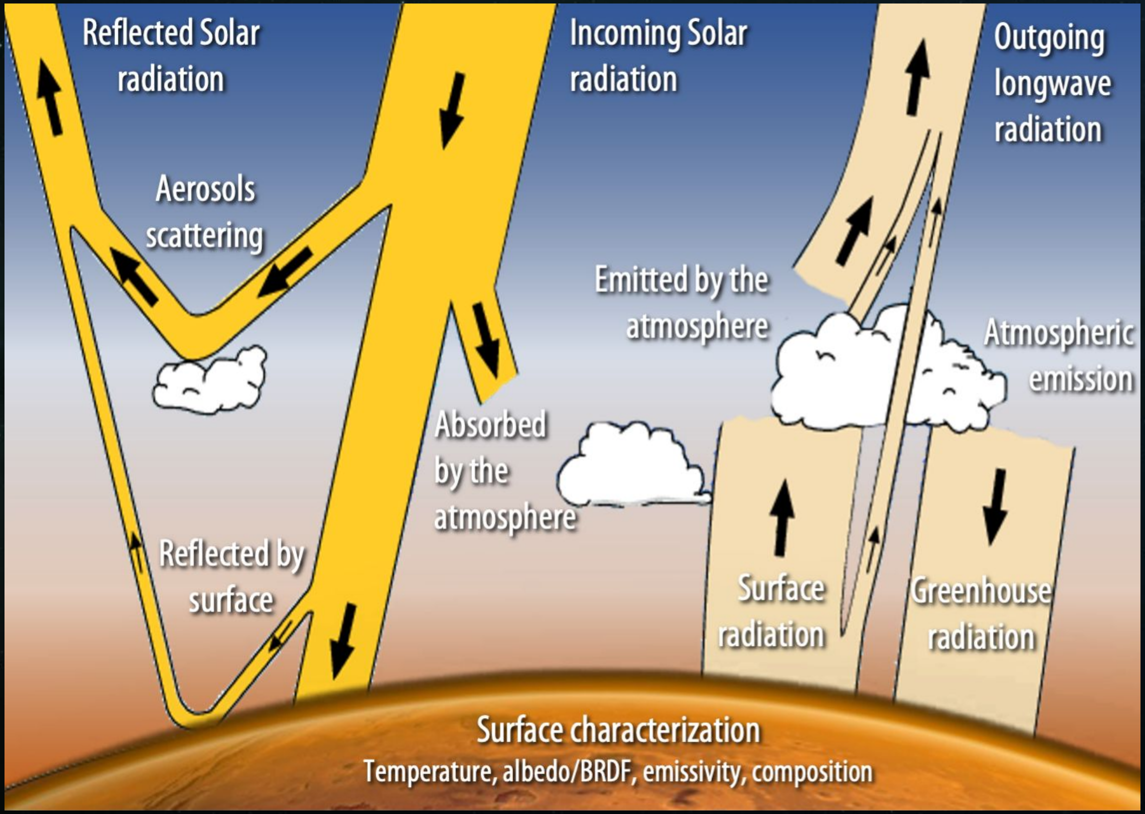
2. Direct imaging simulations
why 3D and clouds?

- Molecules vary strongly with position and height on Earth
- For terrestrial planets, ground coverage and clouds dominate the reflectivity
- Inclusion of 3D clouds as they of critical importance in atmospheres:
  - Energy balance
  - Composition (photochemistry, transport of H_2O)
  - Detectability of molecular species

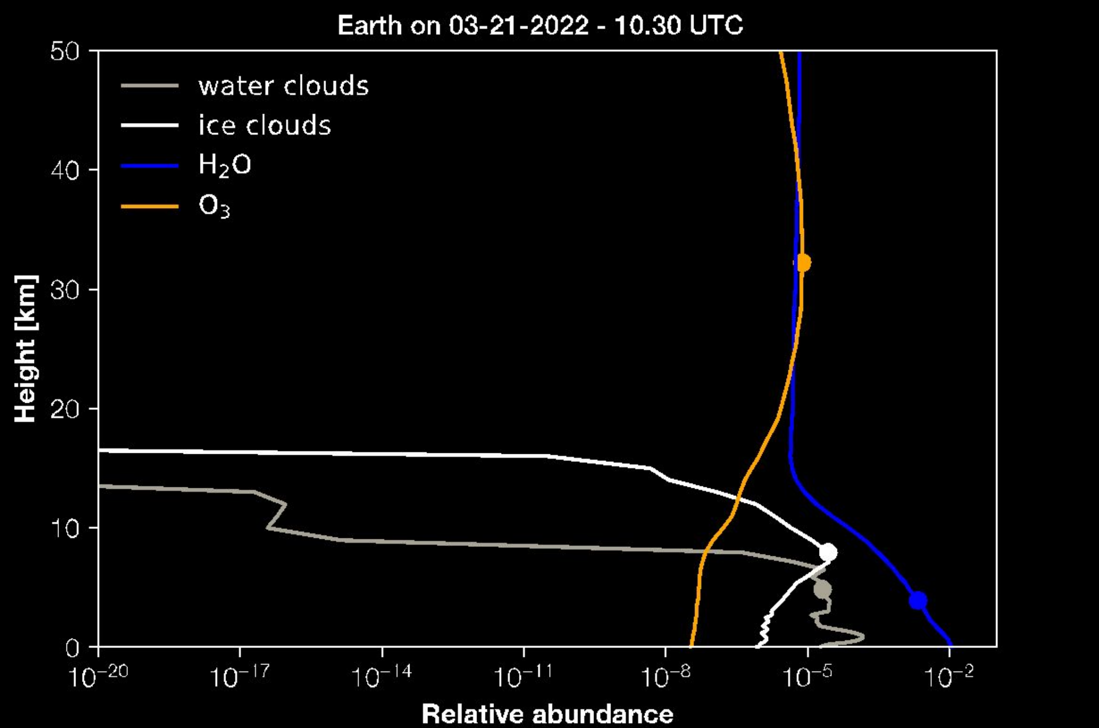
The components in a radiative transfer simulation

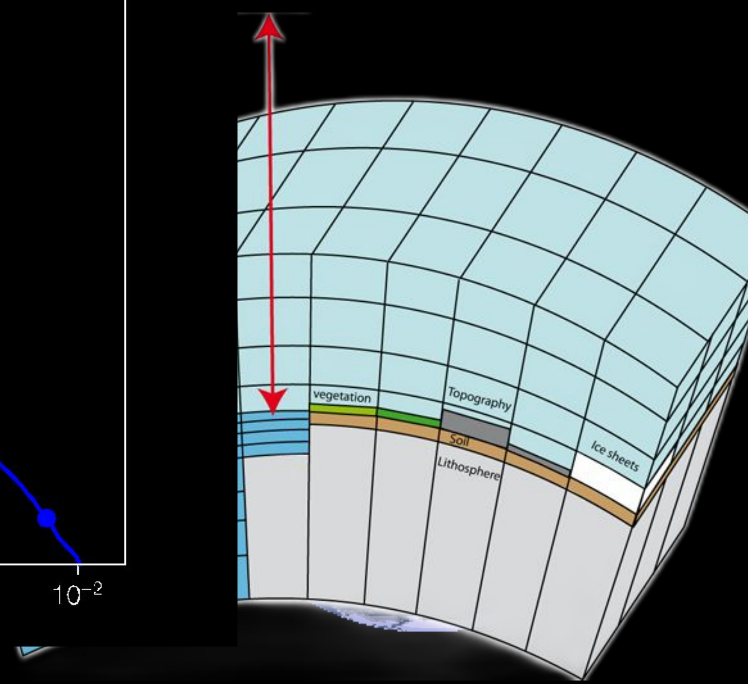


2. Direct Imaging simulations
Earth as a laboratory

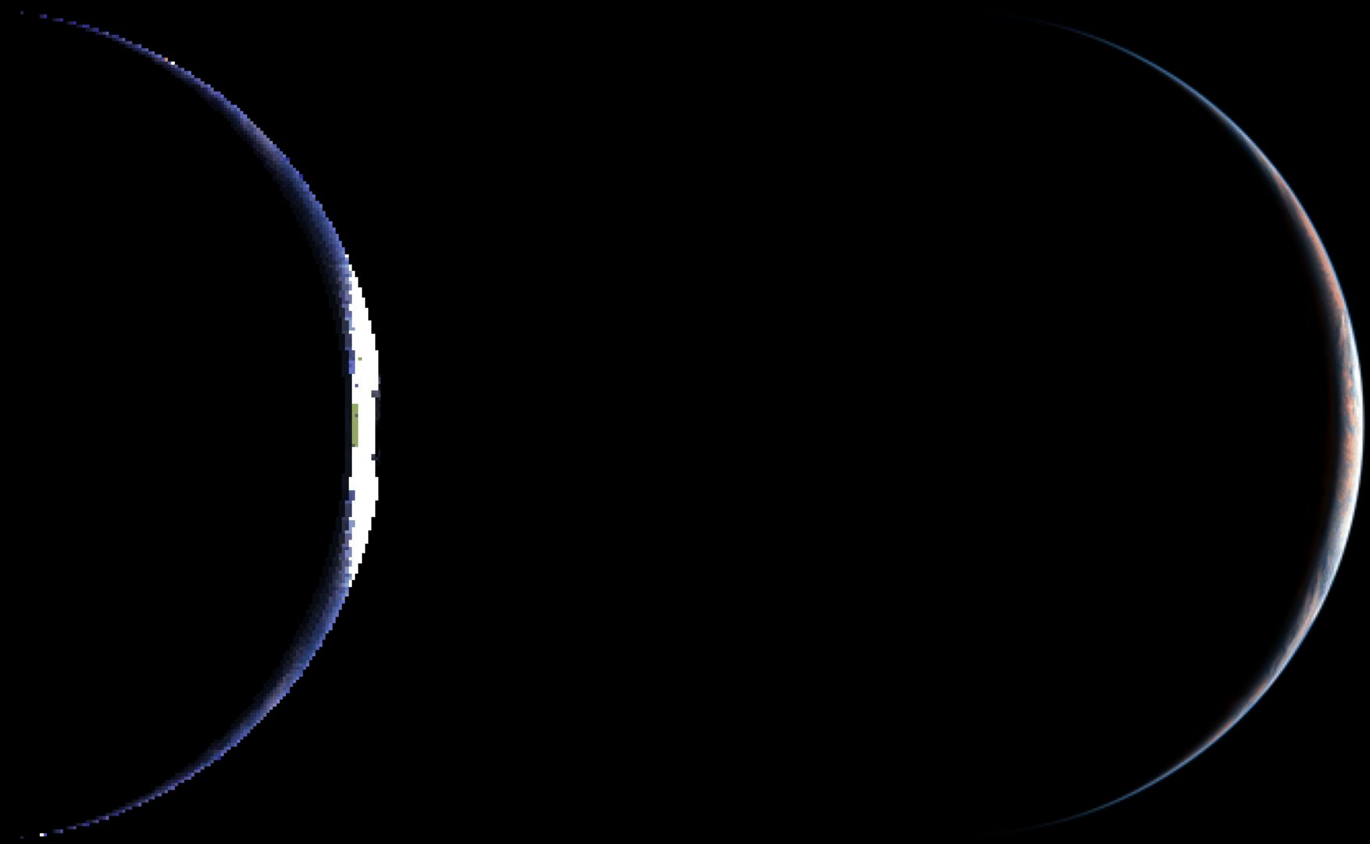
2. Direct Imaging simulations
Earth as a laboratory

- Mc
- H_2(
- Liq



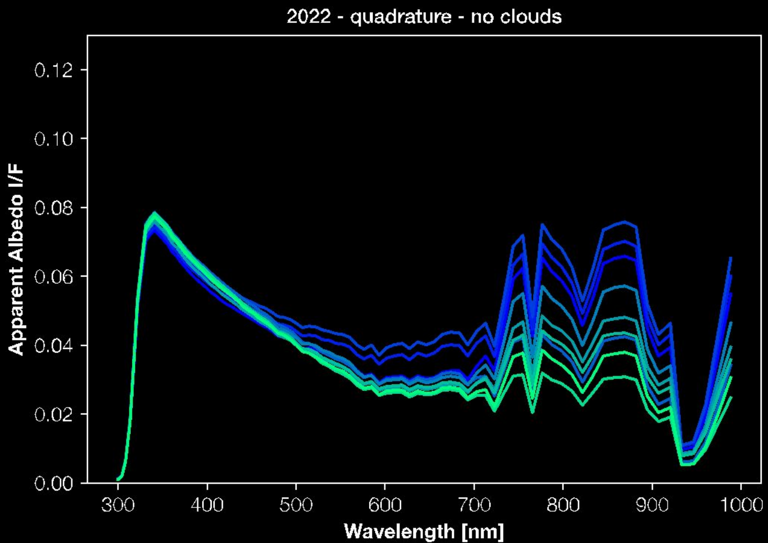


2. Direct imaging simulations

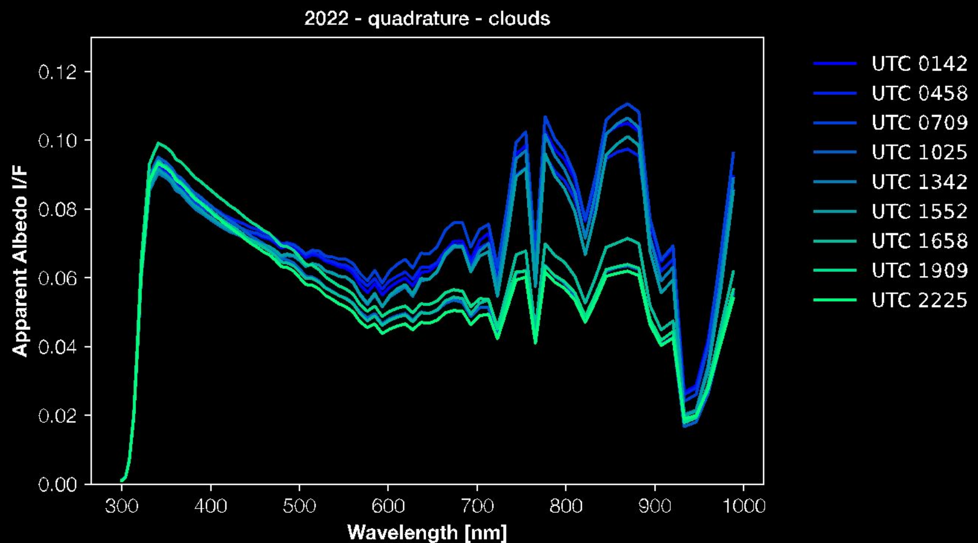


2. Direct Imaging simulations

Ground Variation
variations

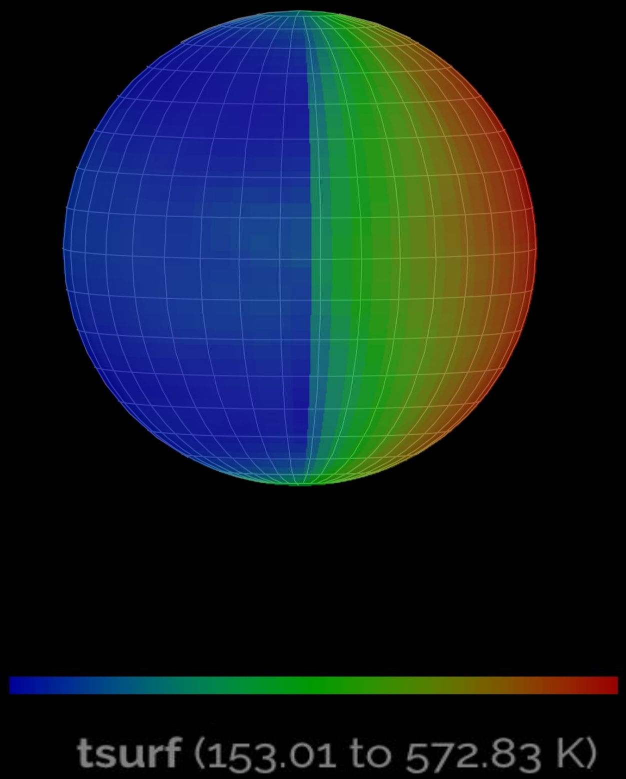


Ground + cloud

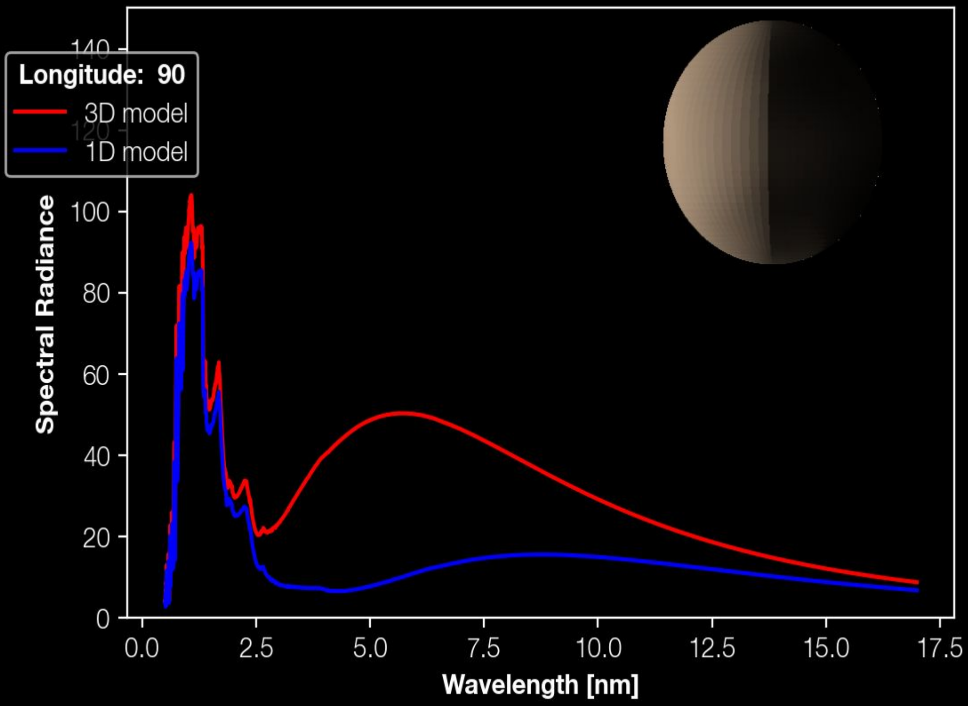


3. Phase curve simulations
Trappist 1b

- Tidally locked rocky planet with a thin CO_2 atmosphere (Turbet+23)
- Phase curve: study the reflected and emitted light from the planet throughout its orbit
- Consider Trappist host star (2566 K) and the planet's black body emission



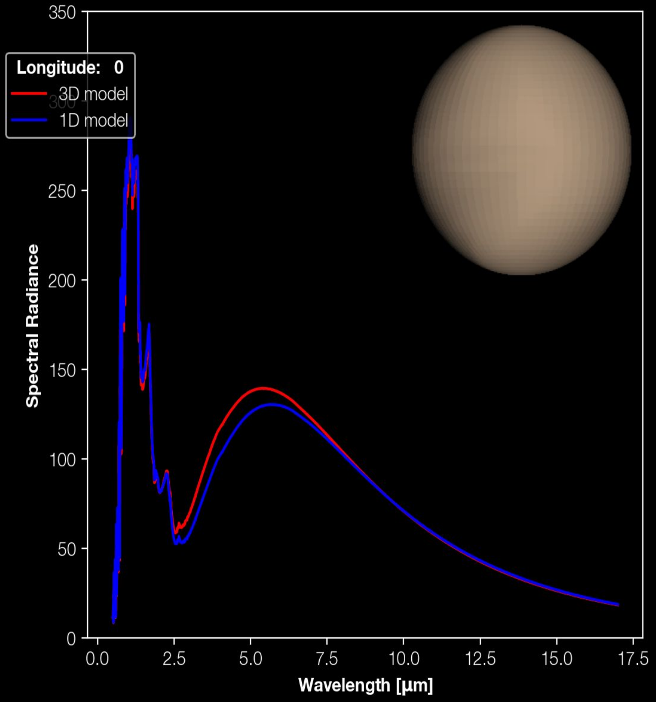
3. Phase curve simulations
Trappist 1b



- Tidally locked rocky planet with a thin CO_2 atmosphere
- 3D model considers ~1700 simulations across the full disk
- 1D model averages the black body temperature

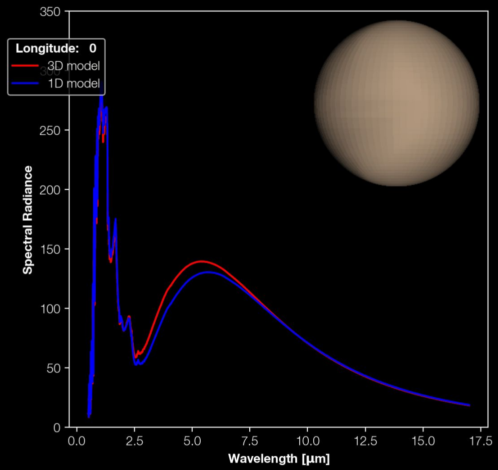
3. Phase curve simulations
Trappist 1b

- Tidally locked rocky planet with a thin CO_2 atmosphere
- Phase curve: study the reflected and emitted light from the planet throughout its orbit
- Consider Trappist host star (2566 K) and the planet's black body emission
- 1D versus 3D show very different spectra and integrated fluxes



Summary

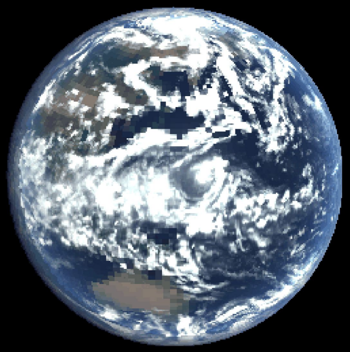
- The Planetary Spectrum Generator enables 3D simulations of (exo)planet atmospheres using different detection methods
- Translate netCDF into binary format
- Load configuration file and check ingestion

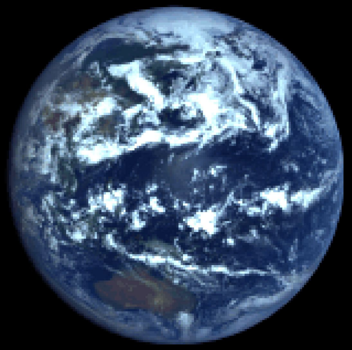


Keep an eye out for our GlobES papers!

Kofman+ *in review*

Fauchez+ *in prep*





```
<ATMOSPHERE-GCM-PARAMETERS>144,91,72,-180,-90,2.5,2.0,Surf_Ocean,Surf_Snow,Surf_Soil,Surf_Forest,Surf_Grass,Temperature,Pressure,Water,WaterIce,H2O,O3
```

ATMOSPHERE-GCM-PARAMETERS		
144, 91, 72, -180, -90, 2.5, 2.0, Surf_Ocean, Surf_Snow, Surf_Soil, Surf_Forest, Surf_Grass, Temperature, Pressure, Water, WaterIce, H2o, O3		
Number of longitudinal points	144	*Required*
Number of latitudinal points	91	*Required*
Number of vertical layers	72	*Required*
Start of longitudinal points	-180	*Required*
Start of latitudinal points	-90	*Required*
Longitudinal resolution	2.5	*Required*
Latitudinal resolution	2.0	*Required*
GCM fields – surface 91*144 4-byte floats	Surf_Ocean Surf_Snow Surf_Soil Surf_Forest Surf_Grass	*Surf_* indicates it describes the surface. Note that the name of these fields are case sensitive. User spectra can be indicated here too.
GCM field – atmosphere 72*91*144 4-byte floats (see text)	Temperature Pressure Water WaterIce H_2O O_3	Temperature, dimensions of 72* 91 *144. For the correct interpretation of temperature and pressure, the keywords should be exactly reproduced. The keyword ‘Wind’, not shown here, is be interpreted as a 2*72*91*144 array (east and south speed in m/s). The names of the aerosols: ‘Water’ and ‘WaterIce’ have to be exactly mentioned here. User spectra can be indicated here too. H_2O and O_3 refer to the molecular species as originally reported in the MERRA-2 data.

It should be noted that the *logarithm* of the abundance and pressure values should be saved in the binary array (*i.e.* this is not the case for the temperature and the wind speeds). The data in the binary should also be saved in 32-bit floating points (4 bytes per number)

Creating a New Planet (step by step)

Creating a New Planet
https://docs.google.com/document/d/1zrXQyEjXLRldWdyiZn2JxxQXz6dU8bayqOltf6eIJgo/edit?usp=sharing

Files for Download for interactive example

https://drive.google.com/open?id=1S2I7FC3m2lbZyFShGQBAvdyiJvMPO2ry

If you want to join along, then beforehand:

1. Download files in link above and put the Proxima rundeck (.R file) in /home/username/modelE2_planet_1.0/decks
2. In your favorite text editor, modify the .R file lines “solar_spec_dir” and “spectral_dir” to the appropriate socrates path, e.g., (‘/home/username/ModelE_support/socrates/stellar_spectra’ or ‘/home/username/ModelE_support/socrates/spectral_files’).
3. Put rest of the files (input files) in /home/username/ModelE_Support/prod_input_files

Creating a New Planet (sanity checks)

Modifying pressure,gravity,radius, and some composition in model/shared/PlanetParams_mod.F90

Key items for consideration in rundeck modification

- Initial condition files (esp. AIC, OIC)
- Planet's topography and ocean state
- Self-consistent input files
- River directions
- Surface conditions (soil, vegetation)

- Total stellar flux
- Greenhouse gas concentrations
- Spectral files/star type
- Orbital parameters
- Thinking ahead about errors/bugs

- ❏ Generating a first acc file → aij (or others) file
- ❏ Getting correct diagnostics
  https://simplex.giss.nasa.gov/gcm/doc/HOWTO/newio.html#scaleacc
- ❏ Checking a few key things from output (e.g., incsw_toa, tsurf, topography, net_rad_planet)
- ❏ Panoply viewer (https://www.giss.nasa.gov/tools/panoply/)

Time Permitting

- Discuss real case scenarios with audience

- Transmission and reflection spectra (Yuka Fujii)
    - https://docs.google.com/document/d/1Kre_HT586XIsodNkeHejTEwYZPQ6cbAs0t9BXU0G054/view
        - PSG supersedes that above (see earlier in the tutorial).

- Using GSFC/NCCS Discover cluster and other tricks of the Planet_1.0 trade:
    - https://docs.google.com/document/d/1iQDq0S5UIqus6dbUUVVQQdP6k8P10vlMCuVqhn2sWpA/view