CINECA INA17_C3B15a: report and preliminary results

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1 Scientific Rationale

The search for exoplanets is a new-born field of astrophysics, whose importance can be hardly overstated. Currently, more than 5000 planets (or candidates) have been discovered and even more are expected in the near future with the launch of new generation space facilities. In this framework, where new data are about to come and need to be analyzed, a theoretical approach via numerical computation becomes mandatory, in order to plan and develop observational protocols, identify peculiar cases, and have hints about some of the phenomena only partly understood.

The project focuses on Super Earths (rocky planets whose mass is in the 1-10 Earth masses range, and whose radius is in the 0.8-2 Earth radii range), a class of planets that is absent in our Solar System. This is particularly interesting from the perspective of planet formation theory, as more and more Super Earths are being observed to orbit stars in the Milky Way. Their characterization could thus place constraints on the formation of the Solar System itself, and could question the robustness of currently accepted formation theories. Super Earths are predicted to have large surface gravities and are likely to exist in a wide range of atmospheres: some of them could retain a thick H-rich atmosphere, others could have a stronger resemblance to Earth, or show a large abundance of complex molecules in their atmospheres. Many Super Earths are also predicted to be potentially habitable planets, as they were found to float in the habitable zone of their host star.

M stars (T_{eff}=3900/2400 K) could be possible hosts for such habitable planets. Despite the fact that a habitable planet orbiting an M star is likely to be tidally locked with the star itself (i.e. it shows always the same hemisphere to the star during its orbit), advection winds could allow a redistribution of heat throughout the surface and could, by principle, allow the presence of life. M stars, however, are very active and that could also potentially threaten life on such planets. This is a highly debated topic of current exoplanetary science.

2 Current Project Status

Researchers and PhD students belonging to an Italian collaboration among the Observatories of Padua, Palermo, and Cagliari built from scratch a 1D structure code which accounts for both radiative transfer and convective adjustment. We chose to call it `MAGRATHEA` to quote Douglas Adams's *Hitchhikers Guide to the Galaxy*, in which the ancient planet Magrathea is considered the home of the industry of "custom-made planet building". This is, in a sense, what our code is supposed to do when it will be fully developed.

The radiative subroutine `ExART` can calculate up and down fluxes at each atmospheric layer using absorption spectra previously adapted via k distribution method. The only input it requires is a set of 14 values, each one representing the radiation of the host star integrated in the 14 bands where the k distributions are calculated. The k distribution approach is fast, flexible, and generally accurate. It reduces by orders of magnitude the computational time and the volume of data that it is usually occupied by a whole set of absorption spectra, necessary in order to retrieve the fluxes at each layer of the atmosphere. This technique also allows the radiative code to equally consider input absorption spectra at various pressures.

The thermo-convective subroutine `THERMOCON` was written to manage convective adjustment, following the approach proposed originally by Manabe and Strickler [1964], and it is coupled to the radiative counterpart. At present time, this code allows to model cloud-free atmospheres spanning a wide range of parameters, such as pressure, temperature, and stellar irradiation.

The code is written in Fortran 90 and is now parallelized through the MPI paradigm so that different models could be run at the same time, one model for each CPU involved.

The final goal of the project is to study the role of the chemical composition, pressure, and planetary/stellar parameters on the atmospheric thermal profiles. The results of the broad model grid allowed us to study the structure of Super Earths atmospheres and the potential habitability on the surface of such planets. The adopted compositions are selected within a database of CO_2, N_2, and H_2O molecules, typical of Mars-like and Early Earth atmospheres. A thermo-convective code coupled with a radiative routine will be used to retrieve such temperatures profiles, running about 17000 models of primordial Earth-like planets and Super Earths, while spanning a wide range of parameters.

3 CINECA Runs

A grid of 17280 models was run at CINECA Galileo cluster, within the *Accordo Quadro INAF-CINECA (2017)* agreement. The grid was formed by all combinations of the input parameters reported in Table 1. The chemical database available at the time of computing was composed by CO_2, H_2O, and N_2 as filling gas. A Python routine was built to create the input files that `MAGRATHEA` would then assume for each model.

The planetary radius is retrieved from the planetary mass using the input density, following the approach presented in Seager et al. [2007].

In order to consider plausible ground pressures when modeling theoretical exoplanets, we chose to determine the ground pressure of the atmosphere on an exoplanet basing our calculations on the ratio of the Earth's atmospheric mass to the planetary mass. Considering $M_{atm,\oplus} \approx 5.15 \cdot 10^{18}\ kg$ and $M_\oplus \approx 5.97 \cdot 10^{24}\ kg$, this ratio r is:

$$r = M_{atm,\oplus}/M_\oplus = 8.6 \cdot 10^{-7} \tag{1}$$

When changing the planetary mass, we imposed that the mass of the planetary atmosphere should change accordingly to keep the ratio r constant. Thus:

Table 1: Input parameters of the dry grid of models. See the text for the meaning of S_{maxg}, S_{rg}, and α.

Parameters	**#**	**Notes/Values**
Planetary Mass ($M_\oplus$)	3	1, 5, 10
$T_\star$ (K)	9	$\Delta T = 500\ K$ from 3000 to 7000 K
Distances (AU)	4	From 0.8 S_{maxg} to 1.2 S_{rg}
X_{CO_2}	5	0.0001, 0.01, 0.1, 0.5, 0.9
Pressure Factors α	4	0.3,1,3,10
Albedo	2	0.1, 0.3
Emissivity	2	0, 2/3
Water vapor	2	dry, wet (RH 60%)

$$M_{atm,pl} = r \cdot M_{pl} \tag{2}$$

This leads to $M_{atm,5\ M_\oplus} \approx 2.57 \cdot 10^{19}\ kg$ and $M_{atm,10\ M_\oplus} \approx 5.15 \cdot 10^{19}\ kg$.

The four atmospheric mass factors (hereafter α_i) can be now considered to retrieve the desired ground pressures for each planetary mass, following this equation:

$$P_{gr,i}\ [Pa] = \alpha_i \cdot \frac{M_{atm,pl}\ [kg]\ g_{pl}\ [m\ s^{-2}]}{4\pi(R_{pl}\ [m])^2} \tag{3}$$

As for the distance from the star, the code bases its calculations on the boundaries for the habitable zone provided by Kopparapu et al. [2013] for irradiance S at the runaway greenhouse limit (S_{rg}, inner boundary), and for S at the maximum greenhouse limit (S_{maxg}, outer boundary). Those depend on the temperature of the star and need to be calculated for each stellar temperature in the grid.

We defined two two points at $S_{eff} = 1.2\ S_{rg}$ (shortest distance - highest irradiation) and $S_{eff} = 0.8\ S_{maxg}$ (higher distance - lowest irradiation) for each stellar temperature, and then select other 2 points equally spaced between the two limits.

The distances at each effective stellar flux are then retrieved by solving the formula (where $T_\star$ is in K, and $R_\star$ is in $R_\oplus$ units):

$$d\ [AU] = \sqrt{\frac{L_\star}{S_{eff}}} = \sqrt{\frac{(T_\star/5778)^4 \cdot R_\star^2}{S_{eff}}} \tag{4}$$

If water vapor was present in the atmosphere, its distribution was not uniform. The humidity value $h(i)$ at every boundary layer $i = 1...nz$ is defined as (following the approach proposed by Manabe and Wetherald [1967]):

$$h(i) = RH \frac{Q(i) - 0.02}{1.00 - 0.02} \tag{5}$$

Where the factor RH is the user-provided relative humidity at the surface. For the wet models in the grid, we used a standard value of the relative humidity $RH = 60\%$.

The array $Q(i) = \frac{P_0(i)}{P_0(nz)}$ for $i = 1...nz$ is the ratio between the input (dry) global pressure of the layer and the input (dry) ground pressure, fixed for the entire run. Any value of $Q(i)$ lower than 0.02 (higher altitudes) is forced to be equal to 0.02 itself, thus resulting in dry layers at low pressures.

4 Analysis

The analysis of such a large number of models was executed in two ways: first, a qualitative study of visual comparison of the various features of the output profiles (an example is shown in Figure 1), then a more thorough principal component analysis to detect the parameters that most play a role in changing a pressure-temperature profile.

In general, the largest impact on the atmospheric profile is caused by the irradiance: the more photons an atmosphere receives from the star, the hotter it will be. Secondary changes in the shape of the profile are caused by the chemical composition of the atmosphere and are further enhanced by the stellar temperature (which changes the wavelength peak of the blackbody radiation). CO_2 is effective in shielding the surface from the radiation, absorbing or scattering the majority of the flux in the upper layers, allowing the tropospheres to be more temperate. This may lead to ground temperatures well below the range of habitability, experiencing a scenario similar to the maximum greenhouse, even without including the formation of clouds in the atmosphere.

Water vapor is set to be more abundant, by construction, in the lower layers of the atmosphere: here, it can produce extreme variations in the shape of the profile compared to the modeled dry analog, and in particular, it increases the temperature at the ground boundary layer. This contributes to an increase of the frequency of unstable models (which would require more water vapor than it is physically possible) or surface temperatures hotter than 500 K, threshold over which `MAGRATHEA` loses its reliability because of the lack of precalculated opacity tables in those regions. For habitability purposes, the positive feedback between water vapor and the temperature is a demonstration of the runaway greenhouse process.

If the emissivity of the atmosphere is non-null, the greenhouse effect of carbon dioxide and water vapor is even more effective in heating the whole atmosphere.

Any variation in pressure does not change dramatically the shape of the profile, nor its ground temperature. This value, on the other hand, plays a role in defining the habitability range of each modeled atmosphere. For lower pressures, it is more likely to have unstable atmospheres, since less water is required to effectively reach the maximum volume mixing ratio allowed by the other species.

A more detailed view of the atmospheric composition affects the ground temperature at the end of a `MAGRATHEA` run can be seen in Figure 2.

To be able to compare the results of these radiative-convective models with observed spectra of even warmer Super Earths, an extension towards hotter temperatures is required and, in fact, already scheduled for the next future.

It may also be necessary to loosen the requirement that imposes N_2 as a filling gas, adding the partial pressure of water vapor to the ones of the other dry components. This would, of course, increase the mass of the atmosphere in time, and its pressure subsequently: in

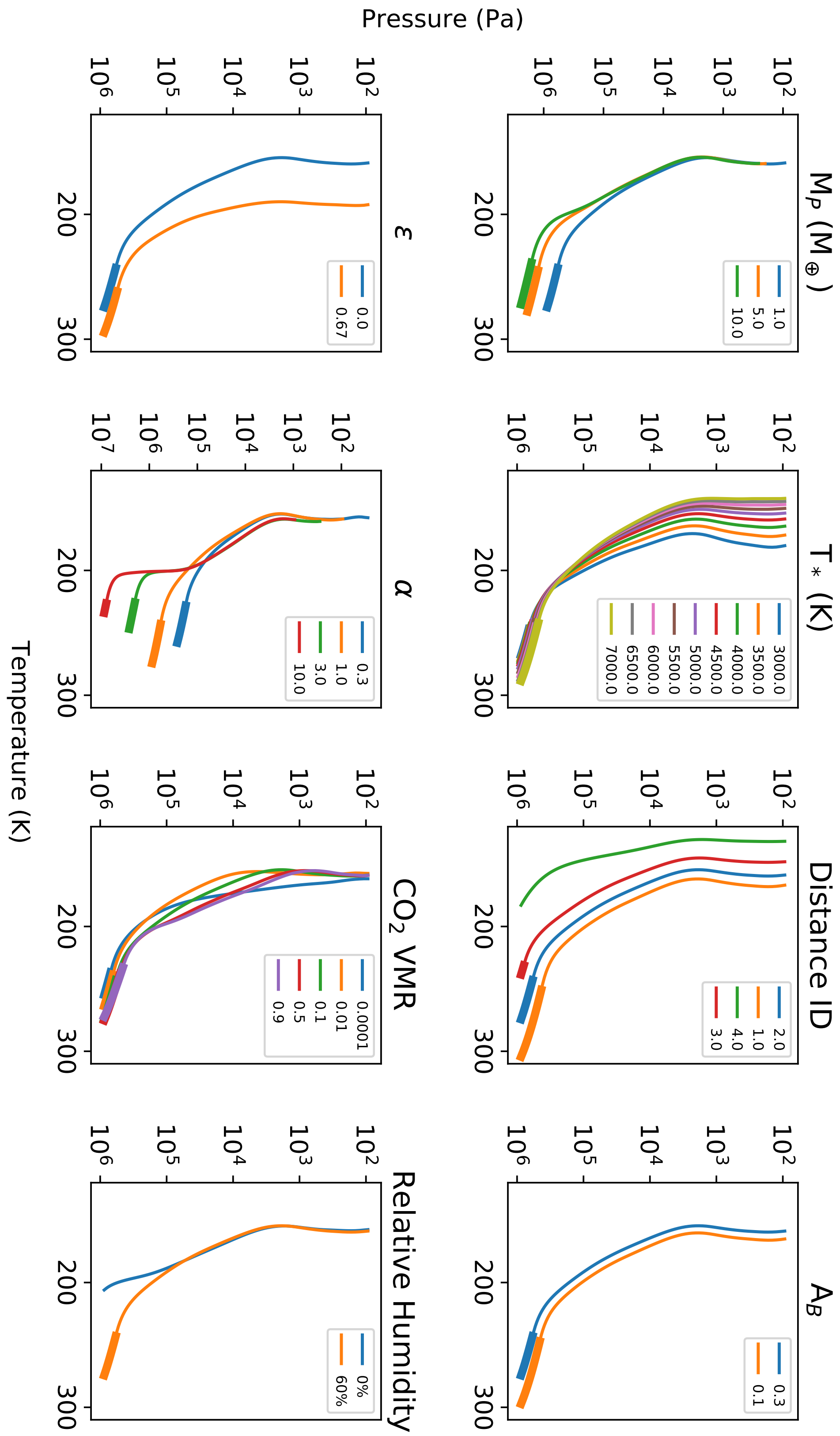

Figure 1: A handful of pressure-temperature profiles retrieved in the runs. In the various subplots, everything is held fixed but the parameter whose impact must be studied. This is shown as a title of the subplot.

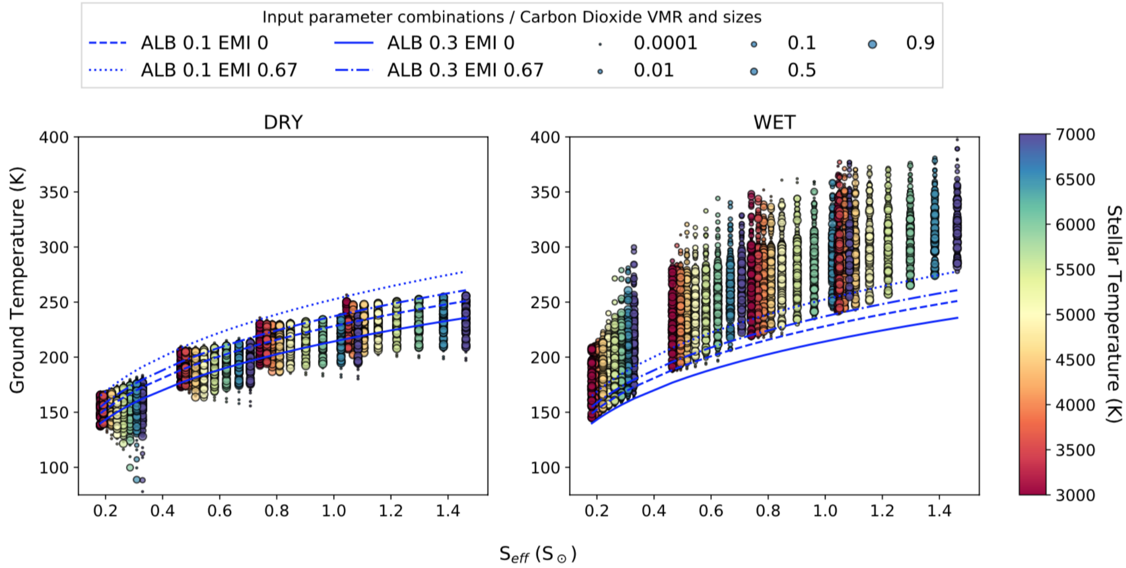

Figure 2: Ground temperature of all models vs stellar irradiation. *Left:* The subset of all the dry models on the theoretical grid. *Right:* The subset of all the wet models of the theoretical grid. Solid, dashed, dash-dotted, and dotted lines represent the trends of the initial temperatures determined by different combinations of the albedo and emissivity values. The size of the dots represents carbon dioxide abundance. The dots are color-coded depending on the stellar temperature.

this case, to avoid abrupt changes in pressure from one boundary layer to the subsequent caused by the increasing water vapor, a dynamic sampling of the boundary layers (at which the temperature must be evaluated) from one iteration to the following must be adopted.

For some cooler profiles, the condensation of both water vapor and carbon dioxide can no longer be neglected, so more accurate modeling of the outer boundary of the habitable zone should require the treatment of cloudy atmospheres. This feature is currently being implemented and validated, so the team will soon be able to repeat some interesting models.

As a consequence, an update of the albedo and the emissivity of cloudy layers may lead to more accurate results when calculating the incoming flux. The treatment of such parameters as wavelength-dependent would lead to much more reliable results.

`MAGRATHEA` should be also coupled with a routine that allows to vary the chemical composition both via equilibrium and non-equilibrium processes. This could allow a more consistent variation of the composition, as well as the production of more species that could be tracers for life. To do this, it is also necessary to include more species in the k-correlated table.

At this point, the pressure-temperature profiles could be fed to a retrieval software to generate theoretical emission spectra for many combinations of input parameters: this would allow to finally couple theory and data.

5 Papers in preparation

This run allowed to complete a Ph.D. project thesis:

1. Alei, E., *Habitability Studies of Super Earths Atmospheres*, Ph.D. Thesis, Università degli Studi di Padova, 2019

Our group should publish one paper:

1. Paper I: *A systematic study of CO2 planetary atmospheres and their link to the stellar environment* - Antonino Petralia, Eleonora Alei, Giambattista Aresu, Cesare Cecchi-Pestellini, Giuseppina Micela, Riccardo Claudi, Angela Ciaravella - under revision by *Monthly Notices of the Royal Astronomical Society*.

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