Build-a-Planet

ASTRON 5202 Project 4

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1 Introduction and Motivation

This paper presents our investigation into the likely internal structure and composition of the exoplanet TRAPPIST-1b utilizing the academic software ExoPlex. Project 4 tasks us with selecting a likely rocky exoplanet with measured mass and radius from the exoplanet archive to explore its potential structure. We have chosen to focus on TRAPPIST-1b, a planet within the well-studied TRAPPIST-1b system, which has been identified as likely rocky in prior research, as suggested by the project description referencing Fulton et al. (2017), Seager et al. (2007), and Chen and Kipping (2016).

The motivation for this study stems from the fundamental challenge of characterizing exoplanetary interiors based solely on observational data like mass and radius. While these measurements provide crucial information about a planet's average density, they offer limited insight into its internal composition. Specifically, the composition of a dense, iron-rich core and a less dense silicate mantle, which is characteristic of rocky planets. Studying exoplanets like TRAPPIST-1b can provide valuable constraints on planet formation and evolution theories. Understanding the internal structure and composition of these planets helps us assess their potential habitability.

2 Methods

This project employed the `ExoPlex` software to model the internal structure of rocky exoplanets, with a specific focus on TRAPPIST-1b. `ExoPlex` requires inputs such as planet mass and refractory ratios. Specifcally, the iron-to-magnesium molar ratio (Fe/Mg) and silicon-to-magnesium molar ratio (Si/Mg). The software also allows for modifications to the distribution of elements between the core and mantle, such as the molar fraction of iron in the mantle (`mol_frac_Fe_mantle`), and the addition of light elements (silicon, oxygen, sulfur) to the core via weight fractions (`wt_frac_Si_core`, `wt_frac_O_core`, `wt_frac_S_core`). `ExoPlex` computes mineralogical and physical properties such as density, pressure, and gravity as functions of depth and outputs these in .tsv format. Summary outputs include the planet's total radius, core radius fraction, core mass fraction, and central pressure.

All simulations were executed in Python using the command-line format:

```
python Group_4.py --mass=... --FeMg=... --SiMg=...
--mol_frac_Fe_mantle=... --wt_frac_Si_core=...
--wt_frac_O_core=... --wt_frac_S_core=...
```

with appropriate substitutions made based on the simulation goals.

2.1 Warmup Simulations

The initial tasks served as an introduction to `ExoPlex`'s functionality. We first modeled the radii of Earth, Mars, and Mercury using their respective masses: 1.0, 0.107, and 0.055 Earth masses. These simulations employed the default solar refractory ratios (Fe/Mg = 0.9, Si/Mg = 0.9) and no added light elements. The output radii were then compared to known planetary values for validation.

Next, we explored how varying Fe/Mg influenced planetary structure. Using a fixed mass of 1.374 Earth masses (corresponding to Trappist-1b), we simulated planets with Fe/Mg values of 0.0, 0.2, 0.4, 0.6, 0.9, 1.2, and 1.5.

To assess the oxidation state of iron in the mantle, we varied `mol_frac_Fe_mantle` from 0.01 to 0.3, holding mass at 1.374 Earth masses and Fe/Mg at 0.9. This allowed us to examine how increasing mantle iron affects the core size and planetary radius.

We also tested the effect of incorporating light elements into the core. For each light element (Si, O, and S), we performed simulations with weight fractions of 0.01, 0.05, 0.10, 0.15, and 0.20. Other parameters were fixed at `mass = 1.374`, `FeMg = 0.9`, and `mol_frac_Fe_mantle = 0.0`, unless otherwise noted.

Finally, we examined how varying Si/Mg influences mantle mineralogy. With mass fixed at 1.374 Earth masses, we altered Si/Mg values (e.g., Si/Mg = 2.0) and observed changes in the proportions of silicates via the .tsv output files.

2.2 TRAPPIST-1b Modeling

To constrain the compositions of TRAPPIST-1b, we used the elemental abundances of its host star, TRAPPIST-1. Using the reported stellar metallicity ([Fe/H]) and empirical scaling relations from Griffith et al. (2021), we estimated [Mg/H] and [Si/H]. These logarithmic abundance values were converted to linear solar-scaled ratios using:

$$X_{rel} = 10^{[X/H]} \tag{1}$$

The resulting molar ratios were computed as:

$$Fe/Mg = (Fe/Mg)_{\odot} \times \left(\frac{Fe_{rel}}{Mg_{rel}} \right) \tag{2}$$

$$Si/Mg = (Si/Mg)_{\odot} \times \left(\frac{Si_{rel}}{Mg_{rel}} \right) \tag{3}$$

Assuming solar molar ratios of $(\mathrm{Fe/Mg})_{\odot} = 0.9$ and $(\mathrm{Si/Mg})_{\odot} = 0.9$, we found:

- Fe/Mg = 1.005
- Si/Mg = 0.902

We also placed Trappist-1b in context by comparing it with the terrestrial planets in our solar system. Using the equation:

$$S = \frac{L}{4\pi d^2} \tag{4}$$

we calculated surface irradiation, where L is stellar luminosity and d is the orbital distance. A provided Python script was used to generate comparative plots of planetary mass, radius, and insolation.

To simulate radius and density from refractory composition, we ran `ExoPlex` with:

- `mass = 1.374`
- `FeMg = 1.005`
- `SiMg = 0.902`

We accounted for the uncertainty in Trappist-1b's mass (± 0.069 $M_{\oplus}$) by simulating:

- `mass = 1.305` $M_{\oplus}$ (lower bound)
- `mass = 1.443` $M_{\oplus}$ (upper bound)

We then calculated planetary density using the formula:

$$\rho = \frac{m}{V} = \frac{m}{\frac{4}{3}\pi r^3} \tag{5}$$

2.3 Interior Structure Adjustment and Mineralogy

To reproduce both the observed mass (1.374 ± 0.069 $M_{\oplus}$) and radius (1.116 $R_{\oplus}$) of Trappist-1b, we iteratively adjusted:

- `FeMg` from 0.6 to 1.2
- `mol_frac_Fe_mantle` from 0.0 to 0.3
- `wt_frac_Si_core`, `wt_frac_O_core`, and `wt_frac_S_core` from 0.0 to 0.2

These simulations revealed parameter combinations that best matched the observed radius. We then analyzed the .tsv outputs to evaluate mantle mineralogy in these successful models, comparing the dominant silicate phases to Earth's mantle.

2.4 Summary of Parameters Used

Across different stages of the project, the following parameter ranges were used:

Parameter	Description	Values Used
`--mass`	Planetary mass ($M_\oplus$)	0.055–1.443
`--FeMg`	Iron-to-magnesium molar ratio	0.0–1.5
`--SiMg`	Silicon-to-magnesium molar ratio	0.9–2.0
`--mol_frac_Fe_mantle`	Molar fraction of Fe in mantle	0.0–0.3
`--wt_frac_Si_core`	Weight fraction of Si in core	0.0–0.2
`--wt_frac_O_core`	Weight fraction of O in core	0.0–0.2
`--wt_frac_S_core`	Weight fraction of S in core	0.0–0.2

Table 1: Summary of parameter ranges used in ExoPlex simulations.

3 Results

This section presents the findings from our ExoPlex simulations and analytical work for Project 4: *Build-a-Planet*, focusing on the rocky exoplanet TRAPPIST-1b.

3.1 Stellar Composition and Molar Ratios

We began by estimating the refractory composition of TRAPPIST-1b based on the measured stellar abundances of its host star. Using a reported Fe/H value of 0.04 and the stellar scaling relationships from Griffith et al. (2021), we calculated [Mg/H] = –0.008 and [Si/H] = –0.007. These correspond to linear abundances relative to solar values of Fe = 1.096, Mg = 0.982, and Si = 0.984. From these values, we derived the molar ratios necessary for ExoPlex inputs: **Fe/Mg = 1.005** and **Si/Mg = 0.902**.

3.2 Comparison to Solar System Rocky Planets

We contextualized TRAPPIST-1b by comparing its physical characteristics to those of rocky planets in our solar system. Using values of 1.116 Earth radii ($\sim$ 7110 km) and 1.374 Earth masses ($\sim 8.206 \times 10^{24}$ kg), we found that TRAPPIST-1b is larger than Earth in both size and mass. Its calculated surface irradiation is approximately 4.25 times that of Earth, consistent with its close orbital proximity to its host star. A comparative plot titled *"Comparison of Rocky Planet Properties"* illustrates this context through subplots of radius, mass, and surface irradiation.

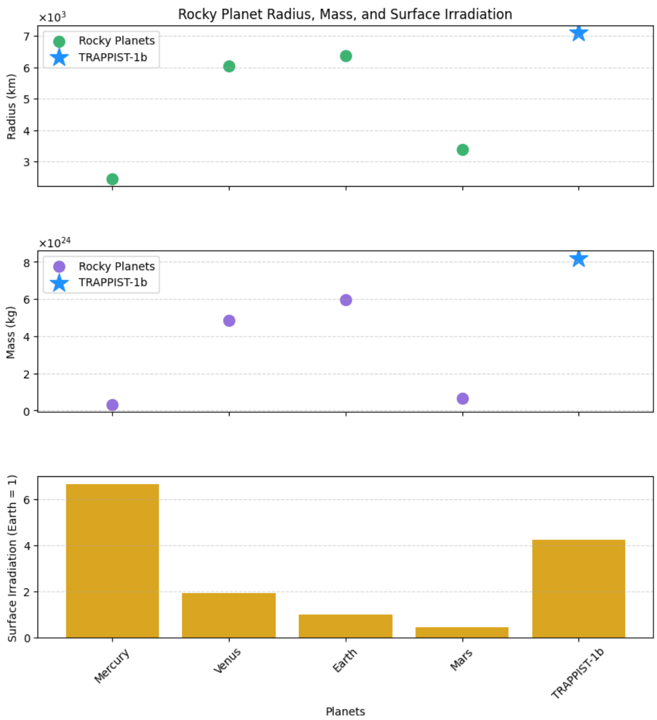

Figure 1: Comparison of Rocky Planet Properties

3.3 Expected Radius and Density Based on Stellar Composition

Next, we used ExoPlex to simulate TRAPPIST-1b's radius and density under the assumption that it shares the same refractory ratios as its host star. We ran simulations using three mass values that span the reported uncertainty range (1.305, 1.374, and 1.443 $M_\oplus$). The results are summarized in Table 2.

Mass ($M_\oplus$)	**Radius ($R_\oplus$)**	**Density (kg/m^3)**	**Core Mass Fraction (%)**	**CMB Pressure (GPa)**
1.305	1.071	5856.67	35.40	176.98
1.374	1.086	5914.33	35.27	181.93
1.443	1.101	5960.91	35.13	186.82

Table 2: ExoPlex results assuming stellar composition

All of these simulations underpredict the observed radius of 1.116 $R_\oplus$, suggesting that TRAPPIST-1b may deviate from a planet formed with solar-like refractory composition.

3.4 Tuning Planetary Composition to Match Observations

To better match TRAPPIST-1b's observed mass and radius, we adjusted several compositional parameters in ExoPlex. First, by decreasing the Fe/Mg ratio to **0.60**, we obtained a radius of **1.116** $R_\oplus$ for a mass of 1.374 $M_\oplus$. This simulation resulted in a reduced core mass fraction of 24.69% and a core-mantle boundary pressure of 202.47 GPa.

We also explored the role of mantle iron content via the `mol_frac_Fe_mantle` parameter. Increasing this to 0.355 (while maintaining Fe/Mg = 1.005 and Si/Mg = 0.902) decreased the core mass fraction to 21.96%. Although this adjustment affects the oxidation state and density of the mantle, we did not achieve the exact observed radius using this single parameter change alone.

Further, we explored the effect of adding light elements to the iron core. Adding silicon (`wt_frac_Si_core = 0.105`) led to a modest reduction in core mass fraction. Adding oxygen (`wt_frac_O_core = 0.1`) significantly expanded the core and increased the overall radius, while sulfur (`wt_frac_S_core = 0.22`) had a more moderate effect. These simulations indicate that light elements in the core can help increase the planetary radius without drastically changing the overall mass.

Ultimately, the simulation best matching TRAPPIST-1b's observed properties used the following inputs:

- `--mass = 1.374`
- `--FeMg = 0.60`
- `--SiMg = 0.902`
- `--wt_frac_O_core = 0.1`
- `--wt_frac_S_core = 0.22`

This run demonstrates that a reduced Fe/Mg ratio and an oxygen and sulfur rich core offer a viable compositional model for the planet.

3.5 Mantle Mineralogy and Comparison to Earth

In our initial simulations using solar-like compositions, the predicted mantle mineralogy consisted of ~52.6% SiO_2, ~39.1% MgO, ~4.4% Al_2O_3, ~3.8% CaO, and negligible FeO. When we lowered the Fe/Mg ratio or increased `mol_frac_Fe_mantle`, the FeO content in the mantle rose significantly. For example, a simulation with Fe/Mg = 0.9 and `mol_frac_Fe_mantle = 0.3` produced a mantle with 15.86% FeO.

These results suggest that TRAPPIST-1b may possess a mantle with more FeO than Earth's, especially if it has undergone different oxidation or differentiation processes. A more detailed phase and mineral analysis using the ExoPlex `.tsv` files would be needed to fully interpret these mineralogies across planetary depth.

4 Conclusion

Through our simulations with `ExoPlex`, we gained a deeper understanding of how a rocky exoplanet's internal composition influences its bulk structure, particularly its mass and radius. By systematically adjusting parameters such as Fe/Mg, Si/Mg, and the distribution of iron between the core and mantle, we observed clear, physically consistent trends that shaped our understanding of TRAPPIST-1b.

Lowering the Fe/Mg ratio resulted in a smaller core and an increased planetary radius, while higher Fe/Mg values produced denser planets with more massive cores. Likewise, increasing the fraction of iron incorporated into the mantle (`mol_frac_Fe_mantle`) led to a denser silicate layer which corresponded to a smaller core. This demonstrated how mantle oxidation states influence core size and planetary density.

Incorporating light elements into the core, such as silicon, oxygen, and sulfur, provided further insights. Silicon decreased the core mass fraction and slightly increased the radius due to its lower density. Oxygen significantly expanded the core and raised the overall radius, suggesting a strong impact on core structure. Sulfur, while increasing the core mass, had a more subtle effect on the radius. These simulations highlight the potential variability in planetary structure arising from differences in core composition and elements.

We also found that variations in the Si/Mg ratio altered the mantle mineralogy, influencing the proportions of major silicate minerals. These mineralogical changes, while secondary to bulk density effects, have implications for the planet's thermal structure and geodynamics.

We encountered several limitations with `ExoPlex`. The software showed sensitivity to nonstandard inputs, occasionally leading to crashes when compositional parameters exceeded the grid of supported mineral solutions. This reflects a broader constraint of the accuracy and reliability of simulation outcomes. In many cases, significantly different input compositions produced similar output radii, which may mask subtle internal differences between otherwise similar planets.

Future development of planetary interior models would benefit from expanding the range of supported compositions, improving the flexibility of input parameters, and incorporating uncertainty propagation to model distributions rather than single-point outcomes. Enhancements to mineralogical modeling and phase equilibrium calculations would also help improve resolution at key boundaries like the core-mantle interface.

Overall, our work with `ExoPlex` demonstrates the importance of internal composition in shaping observable planetary properties. By connecting stellar abundances to planetary structures, we move closer to interpreting the growing catalog of exoplanets in physically meaningful ways and to understand the diversity of worlds beyond our solar system.