

NASA Frontier Development Lab Technical Memorandum

Exploring the co-evolution of extraterrestrial atmospheres and alien biospheres

Authors: A. Bell^a, A. Chopra^b, W. Fawcett^c, R. Talebi^d

Mentors: D. Angerhausen^e, A. Berea^f, N.A. Cabrol^g, C. Kempes^h, M. Mascaroⁱ

^a *University of Tokyo, Tokyo, Japan*

^b *Australian National University, Canberra, Australia*

^c *Cavendish Laboratory, University of Cambridge, United Kingdom*

^d *Georgia Institute of Technology, Atlanta, USA*

^e *Center for Space and Habitability, Universität Bern, Bern, Switzerland*

^f *University of Central Florida, Florida, USA*

^g *The SETI Institute Carl Sagan Center, California, USA*

^h *Santa Fe Institute, New Mexico, USA*

ⁱ *Applied AI, Google, California, USA*



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NASA Frontier Development Lab

NASA Frontier Development Lab is a public / private research partnership between NASA, the SETI Institute and leaders in commercial AI and private space.

Hosted in Silicon Valley by the SETI Institute, the NASA FDL is an applied artificial intelligence research accelerator developed in partnership with NASA's Ames Research Center. Founded in 2016, the NASA FDL aims to apply AI technologies to challenges in space exploration by pairing machine learning expertise with space science and exploration researchers from academia and industry. These interdisciplinary teams address tightly defined problems and the format encourages rapid iteration and prototyping to create outputs with meaningful application to the space program and humanity.

SETI Institute

189 N. Bernardo Ave Suite 200
Mountain View, CA 94043

NASA Ames Space Portal

556 Edquiba Rd
Mountain View, CA 94043

Private Partner: Google Cloud

1 Introduction

The question “Is life on Earth alone in the universe?” motivates many current research themes in the astrobiology community (Domagal-Goldman et al., 2016; Stevenson and Large, 2017) and finding a second habitable Earth in order to become a multi-planet species will be important to ensure our survival in the long-term (Musk, 2017). Understanding the nature and distribution of habitable environments in the universe, and the life forms that may inhabit them, is increasingly part of the primary science goals of remote and *in situ* planetary exploration missions. Roadmaps such as Achenbach et al. (2015) and Des Marais et al. (2008) identify investigating the “co-evolution of life and the physical environment” and “identifying, exploring, and characterising environments for habitability and biosignatures” as two strategies to guide future astrobiology research at NASA. Here we present the results from the 2018 Frontier Development Lab (FDL) where we developed a scalable modelling framework to address three key science objectives:

1. Explore the parameter space of planetary atmospheres that are conducive to habitable conditions on the planetary surface.
2. Characterise the type and extent of chemical disequilibrium that planetary scale biological processes may impart on different planetary atmospheres.
3. Identify remotely detectable signatures in atmospheres of exoplanets that may be indicative of biological processes on the planetary surface.

The FDL scientific organising committee provided us with an initial prompt:

Can we anticipate exotic metabolic pathways using unsupervised (non human bias) machine learning approaches with a view to determining the chemistry of a biosphere – and ultimately ecological signatures that may suggest life, but ‘not as we know it’?

This memorandum describes how we refined the prompt to explore the extent to which surface biology can regulate the evolution of the host planet’s atmosphere, and if such biological influence could be detected by remote observations using future telescopes.

During the initial research phase, we explored a wide range of potential research questions where Machine Learning (ML) could be used to better understand “what is universally possible for life” (Cabrol et al., 2018). Using a method analogous to the Science Traceability Matrix (STM) (Weiss et al., 2005), we linked science objectives with expected outcomes and identified the measurement and functional requirements of each question.

It became clear in our early discussions that we lacked large empirical or simulated datasets usually necessary for application of machine learning techniques. Hence, our goal was to maximise science-return while developing a feasible framework for future scientifically compelling application of AI technologies in astrobiology.

The ideas we explored ranged from identifying differences between fractal patterns in biotic and abiotic imagery (Azúa-Bustos and Vega-Martínez, 2013), simulating the landscape of potential metabolic networks and microbial communities in extreme environments (Costello and Martin, 2018; Cuperlovic-Culf, 2018; Lesnik and Liu, 2017; Ravikrishnan et al., 2018), estimating the activation energies of the earliest biological reactions from quantum mechanical simulations (Amend and Shock, 2001; Black and Knowles, 2018), mapping the limits of life based on extremophile data (Cockell, 2011; Harrison et al., 2013), identifying a set of universally plausible monomers that could form polymers capable of catalytic functionality (such as RNA and peptides) and simulating the emergence of locomotion (Heess et al., 2017).

After considering accessible datasets, the domain expertise and skills that would be necessary and the scientific merit of the project, we identified one project that stood out as an exciting challenge within the time and compute resource constraints of FDL. Inspired by Cabrol (2017) and Lineweaver and Chopra (2012b), we decided to approach our challenge prompt, “Understanding what is universally possible for life”, by investigating the co-evolution of life and its habitable environments.

2 Background

The universe is filled with stars similar to our Sun (Robles et al., 2008). Exoplanet statistics suggest that rocky planets similar to our Earth are common (Bovaird et al., 2015; Burke et al., 2015; Petigura et al., 2013). Water, heat, chemical disequilibria, and energy sources would have been present on early wet rocky planets because of the universal nature of the processes that produced them (Chopra and Lineweaver, 2018; Lineweaver and Chopra, 2012a).

Since all life on Earth needs liquid water during some part of its life cycle, and the surface of the Earth is covered with it, the presence of liquid water on a planet’s surface is taken as a necessary (but not sufficient) condition for life (Lineweaver and Chopra, 2012b; McKay, 2014). Even if water is a constituent of the initial inventory of volatiles on rocky planets in the circumstellar habitable zones of their host stars, surface liquid water can exist only within the relatively narrow range of pressures and temperatures and thus may be only a transient feature of most habitable planets. The evolution of the luminosity of the host star and the redox chemistry of the planetary surface combined with the stochastic perturbations to the planetary atmosphere by impacts and changes to the type and magnitude of tectonic and volcanic activity together make the persistence of liquid water on the surface of planets over billions of years difficult. A fundamental aspect of life is its ability to stabilise its own environment in a homeorhetic mode as described by Margulis (1998). Thinking in this domain ranges from the original proposals by Lovelock and Margulis (1974) to the now widespread appreciation of the importance of niche construction in evolutionary processes (Laland et al., 2017).

Although, wet rocky Earth-like planets are the focus of much current research (Barnes et al., 2018; Boutle et al., 2017; Cockell, 2016; Gaidos et al., 2005; Kaltenegger, 2017; Kasting and Catling, 2003; Kite and Ford, 2018; Kopparapu et al., 2013; Lammer et al., 2009; Nisbet et al., 2007; Seager, 2013; Zahnle et al., 2007), most work has focused on the astronomical and geophysical properties of the planet and host-star. The role of biology in enhancing or sustaining habitability has been explored by Harding and Margulis (2010) and Goldblatt (2016). It is possible that to be habitable, a planet needs to be inhabited (Goldblatt, 2017; Kasting, 2012). In contrast to traditional perspectives on habitability which suggest the presence of liquid water at the surface of a planet as an abiotic property, the presence of liquid water at the surface of a planet could be a biotic feature regulated by a biosphere.

The emergence of life's ability to regulate initially non-biological feedback mechanisms, called "Gaian regulation" after Lovelock and Margulis (1974), could be the most significant factor responsible for life's persistence on Earth over billions of years (Chopra and Lineweaver, 2016). Physical parameters such as insolation and escape velocity can be strongly modified by biotic regulation of albedo and greenhouse gas content of the atmosphere. It is plausible that soon after life emerged on Earth, its metabolisms may have had the potential to modulate the greenhouse gas composition of the atmosphere (Lyons et al., 2015). The biotic regulation of the carbon-silicate cycle is one example of feedback between life and its environment (Schwartzman and Volk, 1989; Walker, Hays et al., 1981). In contrast to abiotic regulation processes, biological regulation has the potential to have faster response rates to perturbations in the atmospheric compositions that may lead to runaway states.

3 Objectives

The exoplanetary science community has been studying factors that can influence habitability of exoplanets such as surface temperatures, densities, compositions, tectonic regimes, atmospheric chemistry, and albedos. While these studies help improve our understanding of planetary formation and evolution, our search for life on potentially habitable planets will depend on our ability to spectrally characterise and understand the abiotic and potentially biotic contributions to atmospheric chemical disequilibria (Kasting, Traub et al., 2009; Krissansen-Totton, Olson et al., 2018; Seager and Deming, 2010; Vázquez et al., 2010). If we are to find an unambiguous biosignature that can be remotely detected, and design instruments to detect them, we need to identify the range of atmospheres that should be priority targets for future observations (Catling et al., 2017; Kiang et al., 2018; Lovelock, 1965; Meadows, Reinhard et al., 2018; Schwieterman et al., 2017; Seager, 2017; Walker, Bains et al., 2018). We will also need develop understanding about what type and extent of biology could support, or at least be compatible with, the different atmospheres that could exist on exoplanets.

Planets within our solar system have strikingly different surface conditions, in large part because of the composition of the atmospheres they host. The next generation of telescopes will have the sensitivity required to determine the composition of exoplanetary atmospheres (Fujii et al., 2017; Venot et al., 2017; Wang et al., 2018). Remotely assessing the potential for life on the surface of a planet will require us to estimate the surface pressure and temperature to assess the likelihood of surface liquid water. The hyperspace of possible atmospheres on exoplanets is large and exploring it is computationally intensive.

Our plan was to develop a scalable framework to run models designed to study planetary atmospheres. We would then simulate a wide range of atmospheric compositions, particularly the abundances of biologically mediated gases, and stellar types that would yield stable (non-runaway) planetary atmospheres (Del Genio et al., 2018; Lenton and Bloh, 2001; Lucarini and Bódai, 2017). The derived flux estimates of the atmospheric gases would be coupled with a model for biological fluxes from communities of organisms in a range of environmental conditions. We would then characterise the potential role of biology in regulating planetary atmospheres (Harding and Margulis, 2010; Lenton, Daines et al., 2018).

Biological regulation of the atmosphere is considered to have been an important factor in stabilising the Earth's climate over billions of years. Such Gaian regulation could be a more important factor in extending the habitable lifetime of wet rocky planets in the circumstellar habitable zone than the luminosity of the host star, the composition of the atmosphere, or planetary geology. Estimating the magnitude of biological regulation on an exoplanet requires a better understanding of the biomass and metabolisms that could be viable in different extraterrestrial environments. Using simulations that couple planetary atmosphere models to biogeochemical models in the same manner as Kharecha et al. (2005) and Gebauer et al. (2017), would allow us investigate if biology can modulate the seasons of exoplanets (Olson et al., 2018) or delay the onset of runaway atmospheres.

Coupling biogeochemical models designed for terrestrial application to planetary atmosphere models is difficult and has limited utility for considering life forms and ecosystems that could be radically different to those we currently recognise on Earth. Hence, we also planned to build upon recent efforts that identified the dominant trends in organism physiology and which can be extended to constrain the range of potential biological rates (Kempes, Bodegom et al., 2017; Kempes, Dutkiewicz et al., 2012; Kempes, Wang et al., 2016). This work stemmed from the metabolic theory of ecology and generalised characteristics of life at distinct levels of biological complexity. An input to the biological portion of our model would be assumptions about the mix of life, combined with assumptions about a planetary environment in order to predict a specific range of feasible molecular fluxes over which we would perform broad parameter sweeps.

The generated distributions of exoplanetary atmospheres and the metabolisms and biomass necessary to explain the surface fluxes of gases in the atmospheres will enable us to estimate the likelihood of life being present within the ensemble of remotely characterised planets from future observations. Our approach will help transition from a zero-dimensional model of a circumstellar habitable zone to a more nuanced Gaussian distribution which can parametrise the extent of habitability (Lineweaver, Chopra and McIntyre, 2018).

A large number of possible exoplanetary atmospheres were sampled, and the interplay of a simple biological model with the atmospheres was investigated during FDL.

4 Simulation of exoplanetary atmospheres with ATMOS

In order to scan the parameter space of atmospheres, we employed the `ATMOS` software package (Arney et al., 2016; Meadows, Arney et al., 2016), developed by the Virtual Planetary Laboratory (VPL). The `ATMOS` package, a coupled photochemistry-climate model, considers a 1-dimensional column of gas through the atmosphere. It is configurable with input parameters such as the concentration or surface fluxes of different species of gases, the star type of the planet's host star, the gravitational field strength of the planet, and the distance between the planet and the host star.

`ATMOS` uses a photochemical model to calculate the effect of UV radiation on the different gas species, and a climate model to calculate the temperature and pressure profile, as a function of altitude, of the different gases. The models of `ATMOS` can be described as a coupled set of differential equations and the software works to find a local 'steady state' solution for a given set of gas concentrations and fluxes as a function of altitude. A consequence of this is a strong dependence on the initial 'seeded' state of atmospheric concentrations. The software can only solve the set of differential equations provided that the next set of initial conditions is not *too* far from that of the previous set of initial conditions, and therefore one must make small steps in parameter space to get from one set of gas concentrations to another. Exactly how large this step size should be was determined empirically in past usage of this code by Arney et al. (2016) and therefore, in order to automate the process for a large parameter scan, studies were performed to determine step sizes and are documented in Appendix A.

In order to explore the parameter space of atmospheric concentrations, we had to search the space in a systematic manner such that a finished run would seed the initial states for the subsequent runs, which would solve the state for some small permutation in each gas relative to the previous state. The 'origin' state for the whole search process was defined by a `Modern Earth` template (a complete set of parameters corresponding to the present day atmosphere of the Earth) and subsequent runs computed the parameter space 'similar' to `Modern Earth`. The process would repeat until either the model failed or the full parameter space was scanned.

Gas	Scan range	Increment	Modern Earth value
O ₂	0.0–0.3	0.02	0.21
	0.3–1.0	0.05	
CO ₂	0.0–0.1	0.01	4.00 × 10 ⁻⁴
	0.1–1.0	0.05	
H ₂ O	0.0–0.9	0.05	1.23 × 10 ⁻²
CH ₄	0.0–0.1	0.005	1.63 × 10 ⁻⁶
H ₂	0.0–10 ⁻⁷	10 ⁻⁹	8.13 × 10 ⁻⁸
N ₂ +trace gases	—	—	0.78

Table 1: The (fractional) scan range and increments of gases varied in order to explore the parameter space of atmospheres. Note that N₂ was not varied systematically as with the other gases. It was instead used to fill the remainder of the atmosphere in cases where the other gas species did not sum to 1. The trace gases were not varied but always included with a fixed portion of the atmosphere.

Table 1 contains the list of scan ranges and increments which correspond to the step sizes, as well as the initial conditions corresponding to the Earth-values. The gas concentrations chosen to vary were O₂, H₂O, CH₄, CO₂, H₂ and N₂, which were known to have biogenic and greenhouse properties. In addition to these, a number of other trace gases which are important to the composition of Earth’s atmosphere were included, but not varied in the scan, and summed to a total of less than 1% of the Earth’s atmosphere.

The gases were scanned such that the total concentration of gasses summed to 100%, and all possible combinations of gases were considered. Note that in Table 1 N₂ is not varied stepwise as with the other gasses, but instead is used to ‘fill’ the remainder of the atmosphere if the combination of other gas concentrations did not sum to 100%.

5 Coupling biology with the atmosphere

In recent years, modelling of physical and biological coupled systems in oceanographic research has progressed significantly in terms of the spatial and temporal resolution and complexity. Such models now serve as useful tools to generate and test hypotheses about marine ecosystems (Werner et al., 2007). Similarly, regional and global climate models are also now beginning to incorporate biological sources and sinks to better characterise the influence of biota (Gnanadesikan et al., 2014).

Here, we attempted to couple `ATMOS` with a simple biological model as a proof-of-principle demonstration of how generalised biological models could be used to test hypotheses in astrobiology. This model estimated global biogenic CO₂ flux (uptake) for a given planetary surface temperature and energy density.

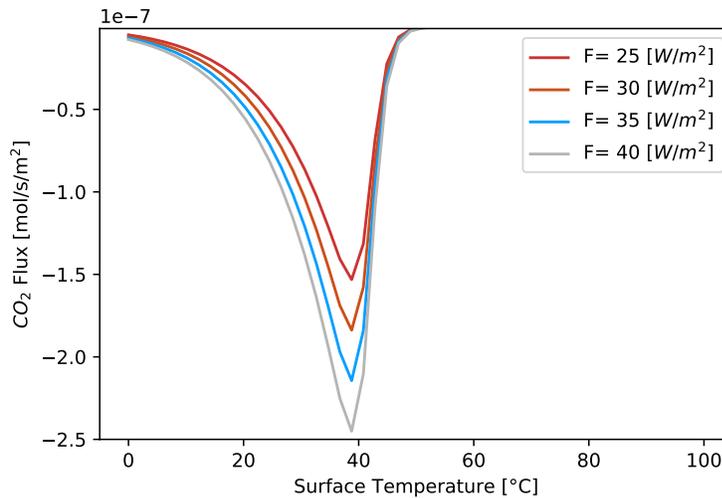


Figure 1: Biotic draw-down of CO₂ as a function of temperature and energy density. Curves describe preliminary models in which the flux of CO₂ is determined from the planetary surface temperature and energy density, F . The horizontal axis is the planetary surface temperature in Celsius, while the vertical axis is the CO₂ flux (uptake) due to biology. The various coloured curves indicate different levels of energy density on the surface.

Figure 1 shows the estimated values of CO₂ flux versus surface temperature, for several energy densities. We paired the `ATMOS` input and output with a general model for biogenic CO₂ flux, or CO₂ uptake as one might find on an Earth-like planet.

For every feedback cycle of the coupling:

- `ATMOS` generated a temperature-altitude profile from input gas concentrations (beginning with modern earth atmospheric composition)
- Surface temperature was extracted and the biogenic CO₂ flux was calculated at that temperature
- The atmospheric composition was updated according to the new CO₂ flux and a new surface temperature was determined with `ATMOS`

The results of this cycle are shown in Figure 2. This preliminary output of the feedback cycle demonstrates the concept for future experiments an atmosphere-biotic flux coupling which can be explored further to understand the potential habitability and likelihood of inhabitation of exoplanets.

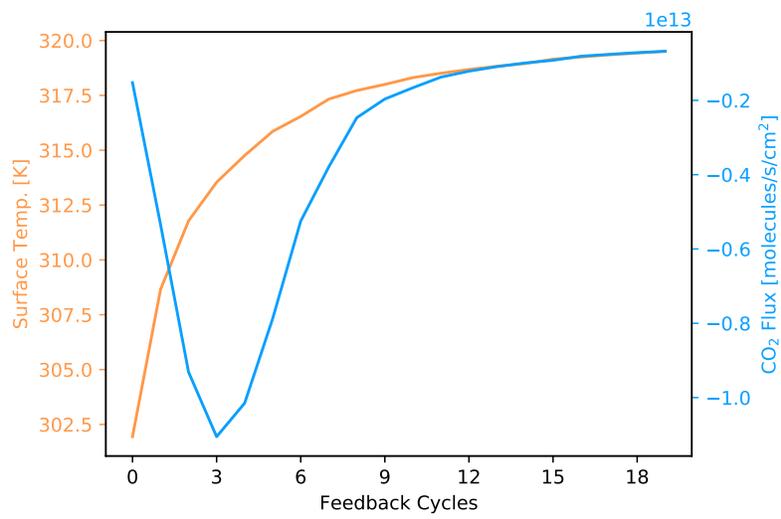


Figure 2: Testing of the efficacy of potential biotic feedback to perturbations via a CO₂ drawdown model in which the surface temperature in Kelvin (orange) output from *ATMOS* is coupled to a simple, generalised CO₂ biological uptake (blue) model. Curves are plotted over each iteration of the feedback loop.

6 Software and compute environment

The `ATMOS` software exhibits platform dependencies, in part attributable to its legacy piece-wise development. To streamline the `ATMOS` runs and maintain cross-platform consistency, we created a Docker image of `ATMOS` based on the Ubuntu Linux distribution. This image guaranteed consistent performance on all host platforms. To automate the process of configuring `ATMOS` for individual runs, we wrote a package called `PyAtmos` in Python 3 (chosen for its flexibility, extensive community-driven resources and potential for further development by end-users). `PyAtmos` allows one to easily configure `ATMOS`, run it, and extract the relevant results.

A Docker image loaded with `PyAtmos`, which inherited the original `ATMOS` image, was created to instantiate thousands of individual computers on the Google Cloud Platform (GCP), all of which worked in parallel to search the atmospheric parameter space. Additional Python scripts were written to supervise a work-queue and designed to manage the run-constraints of `ATMOS` outlined in Section 4. The work-queue is visualised in Figure 3. GCP instances spawned off thousands of identical virtual environments to compute the individual atmospheric concentrations with `PyAtmos`. Google Cloud Storage (GCS) hosted all the data output by each run and a GCP Structured Query Language (SQL) server stored a parsed log of all completed and queued runs. A Redis server tracked the completion of runs and allocated new work to each virtual machine.

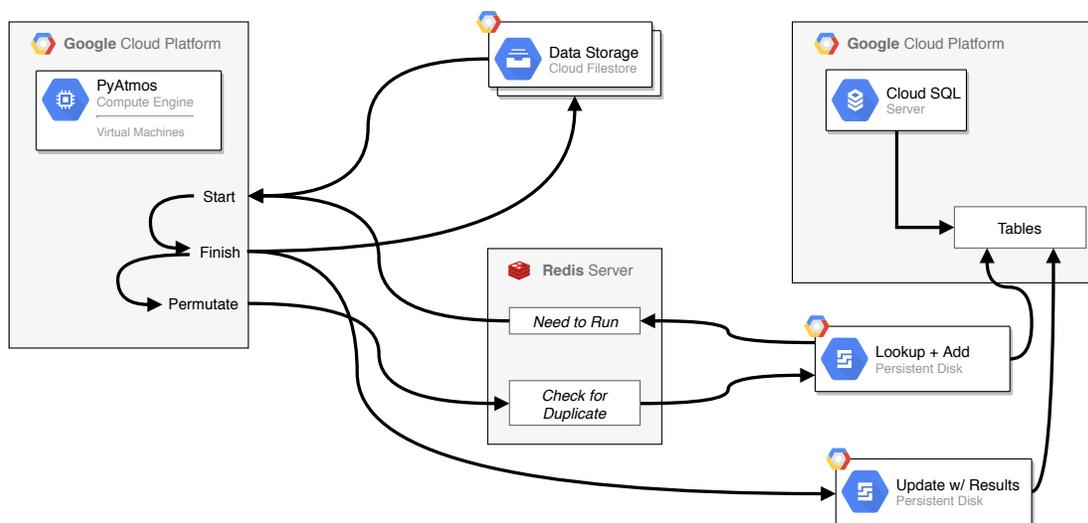


Figure 3: Computing setup for exploring a large parameter space of atmospheres.

7 Results of scanning the atmosphere parameter space

A total of 124,319 atmospheres were simulated according to the scan constraints described in Table 1. This represents a small fraction of the total space possible within the scan constraints and could be expanded for future studies. For each atmosphere, the temperatures and pressures at the planet surface were derived, and the distribution of these atmospheres is shown in Figure 4. Since the distribution is sensitive to the scan parameters employed in the search, only limited interpretations are possible with the initial results collected during FDL.

One inference was that amongst the simulated atmospheres, there were three “islands” of atmospheres on the plot, where the bottom left-most of these contained the atmosphere corresponding to present-day Earth (average surface temperature of 15 °C and pressure of 1.02 atm). As anticipated, we found that atmospheres with higher CO₂ concentrations were also those with higher temperatures and pressures. We found that surface temperatures and pressures were generally uncorrelated with increasing concentrations of the other gases varied. It is likely that this is due to the relatively small fraction of the atmospheres that were explored; and thus we may have been unable to truly identify the relative forcings of different atmospheric gases. Additional figures with information on the distribution of atmospheres simulated can be found in Appendix B.

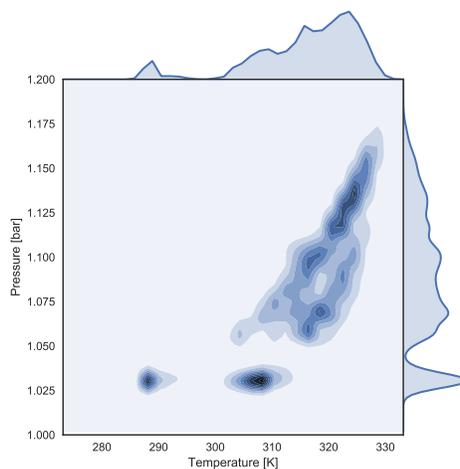


Figure 4: Distribution of atmospheres in the temperature versus pressure plane. The graphs above the upper and right axes are the 1-dimensional density profiles of temperature and pressure, respectively. Although the distribution is sensitive to the priors applied to the scan and the total number of atmospheres scanned, similar analyses with larger data sets could help infer the frequency of different classes of habitable exoplanetary atmospheres and enable interpretation of biosignatures.

Figure 5 shows 2D heatmaps and profile histograms for O_2 and CO_2 . The heatmaps show the number of atmospheres generated as a function of temperature and the gas mixing ratio, with darker regions indicating a greater proportion of atmospheres in a given histogram bin. The profile histograms (red bars) show the average temperature for all the atmospheres in that particular range of gas mixing ratio; for example, the first red point on Figure 5(a) corresponds to the average of all the atmospheres with O_2 mixing ratio between 0.00–0.05 (regardless of the concentrations of other gases). The red point shows the mean of the temperatures of the atmospheres and the error bars indicate the standard deviation.

Plots such as Figure 5 could give a simple way of determining the temperature of a planet to first order. For example, based on our current dataset, if we were to find that a planet had an O_2 mixing ratio between 0.35–0.40, then there would be a 68% chance that the temperature of that planet is in the range 30–50 °C – a potentially useful result given that liquid water on the surface of a planet may be an indicator for life (Lineweaver, Chopra and McIntyre, 2018). Further constraints on the temperatures could be provided by a concordance of results from other gases. However, to infer realistic surface temperatures, we would need to simulate a representative set of all possible exoplanetary atmospheres and expand our current dataset.

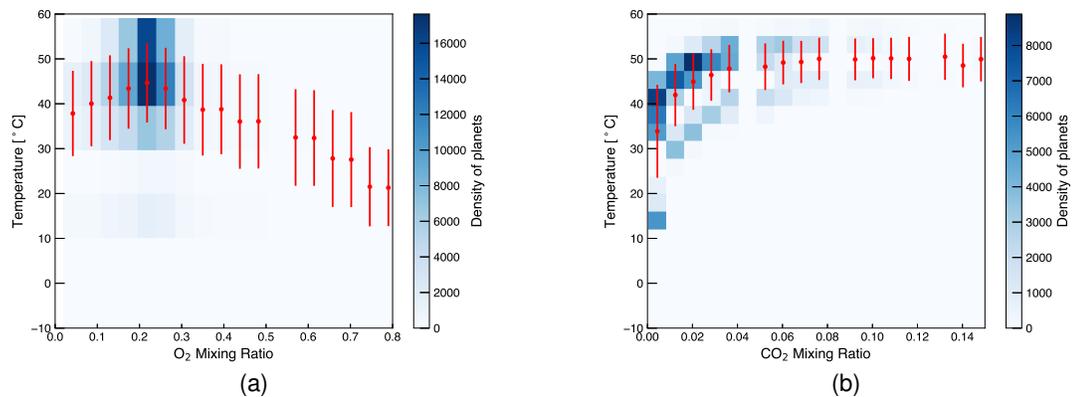


Figure 5: 2D histograms (heatmaps) of the density of scanned atmospheres in the surface temperature versus gas mixing ratio plane, overlain with the profile histogram of atmosphere temperatures as a function of the gas mixing ratio (O_2 -a, CO_2 -b). Each bin of gas mixing ratio contains many atmospheres, with all the combinations of other gasses that were simulated. Red points show the mean of the temperatures of the atmospheres in each bin, and the error bars show the standard deviation. As the heatmaps and the profile histograms depend significantly on the priors applied to the atmosphere scan and the number of scanned atmospheres, limited interpretation is possible with the current dataset and plots here only demonstrate the concept.

8 Future work using generalised biology models

During FDL, we explored biological feedback and metabolic cycle models such as Nicholson et al. (2018), which could be coupled with `ATMOS` or other global climate models. A schematic of one desired output from such exploration is shown in Figure 6. Our early results revealed that we could use such coupled analysis to predict atmospheric composition fluctuations for comparing inhabited and uninhabited planets. Further experiments could be designed to seek correlations between abiogenic CO_2 flux and biogenic CH_4 flux feedback cycles and determine if such correlations could remotely detectable through future observations.

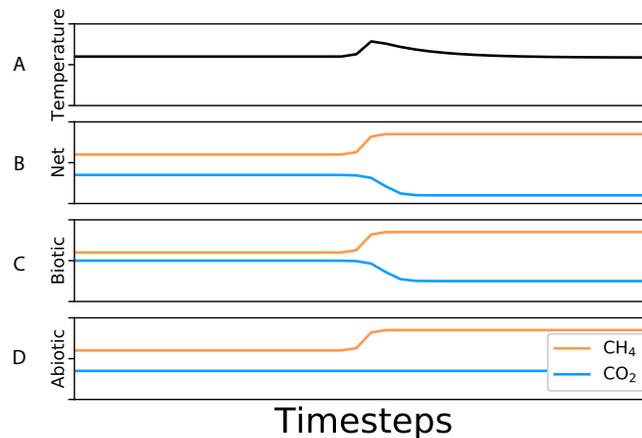


Figure 6: Schematic plot describing potential comparisons inhabited and uninhabited planets if the relative concentrations of CO_2 and CH_4 are known as a function of time. *A*: surface temperature as a function of time. *B*: the net CO_2 (blue) and CH_4 (orange) flux, from biotic and abiotic processes on the planet. *C*: CO_2 and CH_4 flux due to biological processes. *D*: fluxes due to abiological processes.

At some point in the foreseeable future, once we can reliably retrieve the atmospheric compositions of exoplanets from observed spectra, it may be possible to search for life in a statistical manner and constraint the likelihood of inhabitation of planets in the universe without necessarily detecting extraterrestrial life. In the equation formulated by Drake and Sobel (1992), this is the fraction of planets that could support life that actually develop life at some point (F_l). As a first step, one would target planets that are the most ‘similar’ to Earth: in mass, radius, composition, distance from host star and host star type. Then, if knowledge of how atmospheres form on such planets was sufficient, it would be possible to simulate distributions of properties of the expected atmospheres for these planets. In a manner similar to how exoplanets statistics from telescopes like Kepler have enabled comparative planetology of potentially habitable exoplanets (Bean et al., 2017), it may not be necessary to accurately predict the atmosphere of each planet so long as averaged properties can be accurately modelled.

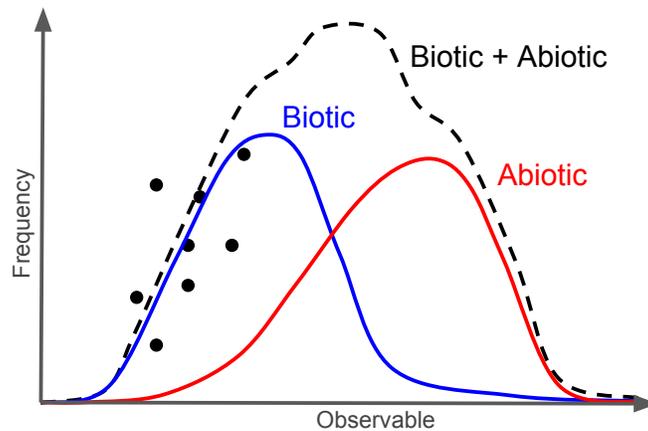


Figure 7: A schematic of how we could search for life using statistical methods. The red line represents the distribution of the given observable for the set of atmospheres (e.g. surface temperature) if no life would be present on all planets. The blue line is the same, except that it represents the distribution of the observable if life is present on all planets. The dashed line represents a combination of the biotic and abiotic hypotheses, which would vary according to the proportion of planets which have life. The black dots represent the hypothetical data of measured planets atmospheres.

Figure 7 gives a schematic of how such a distribution could be useful. In order to inform the actual distributions, parameters that constrain stellar, geological and atmospheric processes would be sufficient and no *a priori* knowledge of the type and extent life on a particular planets would be necessary. One could then test different hypothesis against the data (measured distribution of O₂ concentrations or other biogenic gases in exoplanetary atmospheres). If our confidence in the simulation of atmospheres was sufficient, the extent of agreement between the observed data and simulated distributions would yield a quantitative measure of the probability that life exists somewhere in the universe without being able to pinpoint on which planets actually life exists.

If it becomes possible to accurately couple biology to atmospheric models with sufficient confidence, then one could go a step further and model the atmospheres of potentially inhabited exoplanets to better understand the type and extent of metabolisms that are likely to be active on the surface. In this case, one could then test a number of 'Biotic + Abiotic' hypotheses with varying proportions and types of life (demonstrated by the blue line in Figure 7), and then test these against the observed data. One advantage of this approach is that a less sensitive telescope would be required to 'discover' alien life in this manner than one that would be required for detecting a strongly diagnostic biosignature on a single exoplanet.

9 Conclusion

Studies of habitability have traditionally focused on physical parameters; here we have demonstrated a proof-of-principle coupling of a model designed for planetary atmosphere studies with a biological energetics and flux model. It provides an avenue for connecting different metabolisms such as carbon fixation, methanogenesis and oxygenic respiration to global climate models, which may help to further elucidate the fundamental factors driving the evolution of planetary scale atmosphere dynamics and surface habitability. The scalability of our framework provides a mechanism to incorporate complex biogeochemical and global climate models to better understand the co-evolution of the atmosphere and biosphere.

In future work, we plan to include parameters such as star type, planet size and distance from the host star when evaluating the range of different atmospheres that may be habitable. We also plan to incorporate domain knowledge of biotic and abiotic fluxes and disequilibrium in the environment into models. Our work will be informed by realistic metabolisms to compare the abiotic and biotic fluxes that may be present on a planet which could stabilise and support co-evolution of the atmosphere and biosphere.

This project has also demonstrated how cloud computing capabilities can accelerate existing technologies and map out previously neglected parameter spaces. We succeeded in modelling tens-of-thousands of potential atmospheres over a few days, using software that was originally intended for use in single run applications. While we used relatively simple models such as `ATMOS` in this study, the framework developed is sufficiently flexible to enable more recently developed and more complex models such as `ROCKE-3D` (Way et al., 2017) to be incorporated into future models used in planetary habitability studies.

The full atmospheric composition dataset that could be generated will become a useful resource for the community to understand distributions of habitability parameters such as surface temperatures, photon and redox free energy availability for different classes of planetary systems. The dataset would enable better interpretations of future observations of exoplanet atmospheres and potential biosignatures.

The software product created during FDL has the potential to significantly improve the accessibility of `ATMOS` for a wide community of researchers, particularly for researchers with limited experience in handling `FORTRAN` source code. The parameter search approach, enabled by GCP, could be adopted by the community to simulate more atmospheres and/or modified to rapidly iterate on other problems that utilise `ATMOS`. More generally, we anticipate that the approach of containerising legacy or hard-to-use software, executing it over massively parallel processing, and setting up a procedural execution algorithms could become a template for similar parameter search problems in and beyond astrobiology.

Acknowledgements

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Acronyms

FDL Frontier Development Lab. 3, 4, 7, 12, 14, 16, 17, 21

GCP Google Cloud Platform. 11, 16

GCS Google Cloud Storage. 11

KEGG Kyoto Encyclopedia of Genes and Genomes. 21

ML Machine Learning. 3, 21

SQL Structured Query Language. 11

STM Science Traceability Matrix. 3

VPL Virtual Planetary Laboratory. 7

A Step-size variation tests

We implemented a test to explore the dependence of `ATMOS` output on the size of gas concentration increments. Figure 8 shows how the steady-state surface temperature evolved when CH_4 concentration was increased with different increments. We tested four increment sizes: 0.1% (light blue), 0.25 (orange), 0.5 (pink), and 1.0% (black), in the range of 0 to 5% CH_4 atmospheric concentration. For each of the four step-size runs, CH_4 was sequentially increased and each time CH_4 was incremented, the output atmosphere state of the previous run was taken as the initial state.

The purpose of this test was to justify our procedural parameter search to demonstrate why we were unable to perform a simple brute-force, broadcasted parameter search. If the `ATMOS` simulations were deterministic, producing a unique output for a given atmospheric composition, regardless of starting conditions, we would have been able to run all simulations without the need for feedback between runs. The results of the test, shown in Figure 8, indicate that at least to the extent tested here, (in the range from 0 to 5% CH_4 composition) the `ATMOS` output is not deterministic. If it were, we would expect all of the points to fall on the same curve. Smaller increment sizes also appear to lead to a more consistent surface-temperature output.

Future work could explore the extent to which output depends on which gases are varied, and in which direction. The exploration of the search parameter space could also be optimised by application of machine learning methods.

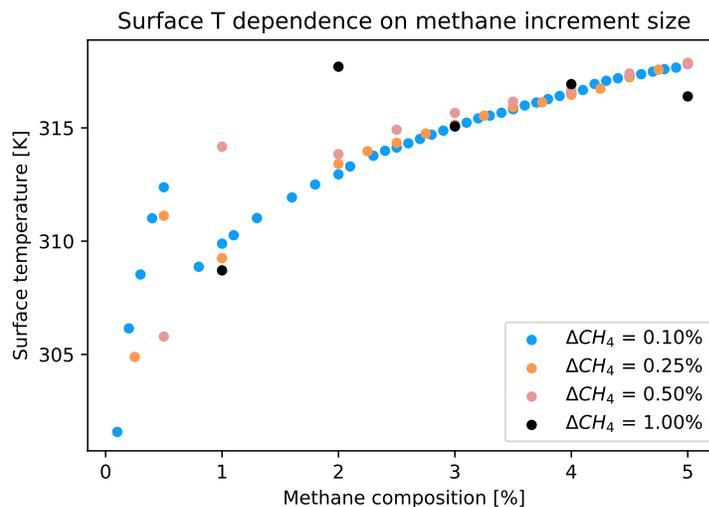


Figure 8: Temperatures resulting from successive `ATMOS` runs at four different CH_4 concentration increment sizes, each starting at 0% CH_4 . Smaller increments yield more consistent and quicker results.

B Distributions of sampled atmospheres

This section displays some of the properties of the 124,319 sampled atmospheres. Figure 9 shows 2-dimensional histograms of the gas mixing ratios. Figure 10 shows histograms of the number of atmospheres generated versus the mixing ratio of the input gas. A black arrow is added to each histogram to show the corresponding Earth-value for each gas concentration. For simplicity, three planes were chosen: CH₄-O₂, H₂-H₂O and O₂-CO₂.

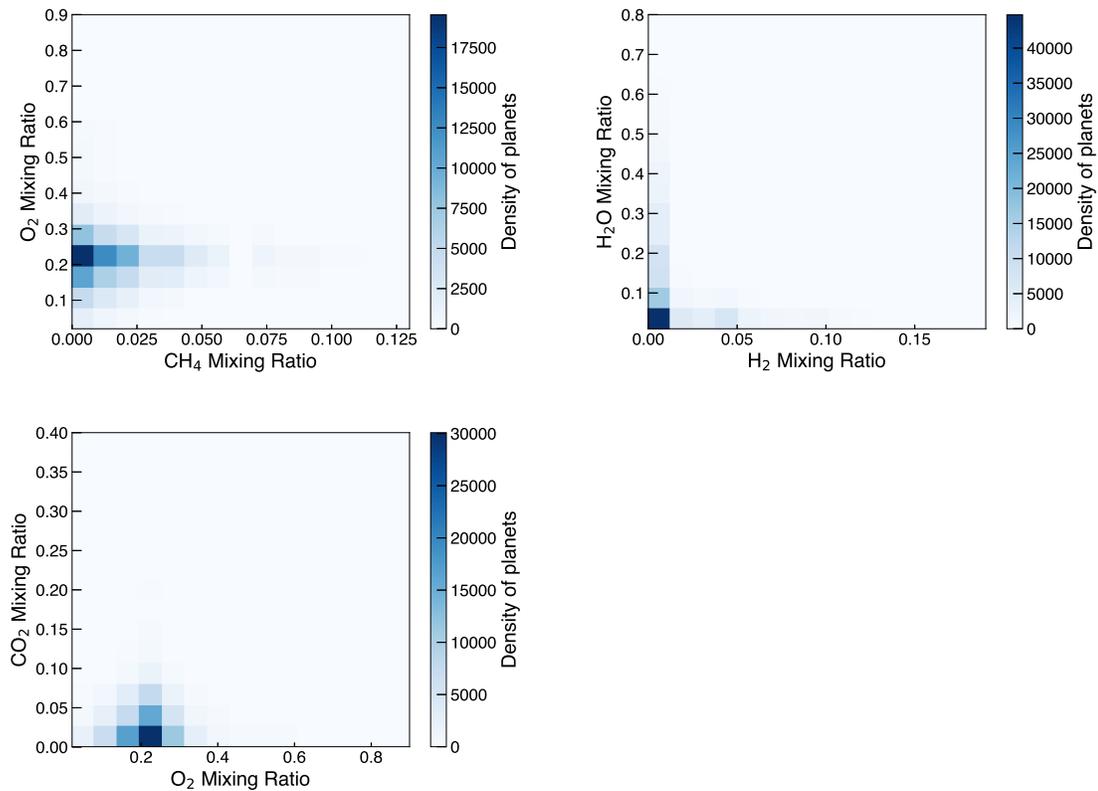


Figure 9: Two-dimensional histograms showing the density of simulated atmospheres in the CH₄-O₂, H₂-H₂O and O₂-CO₂ planes.

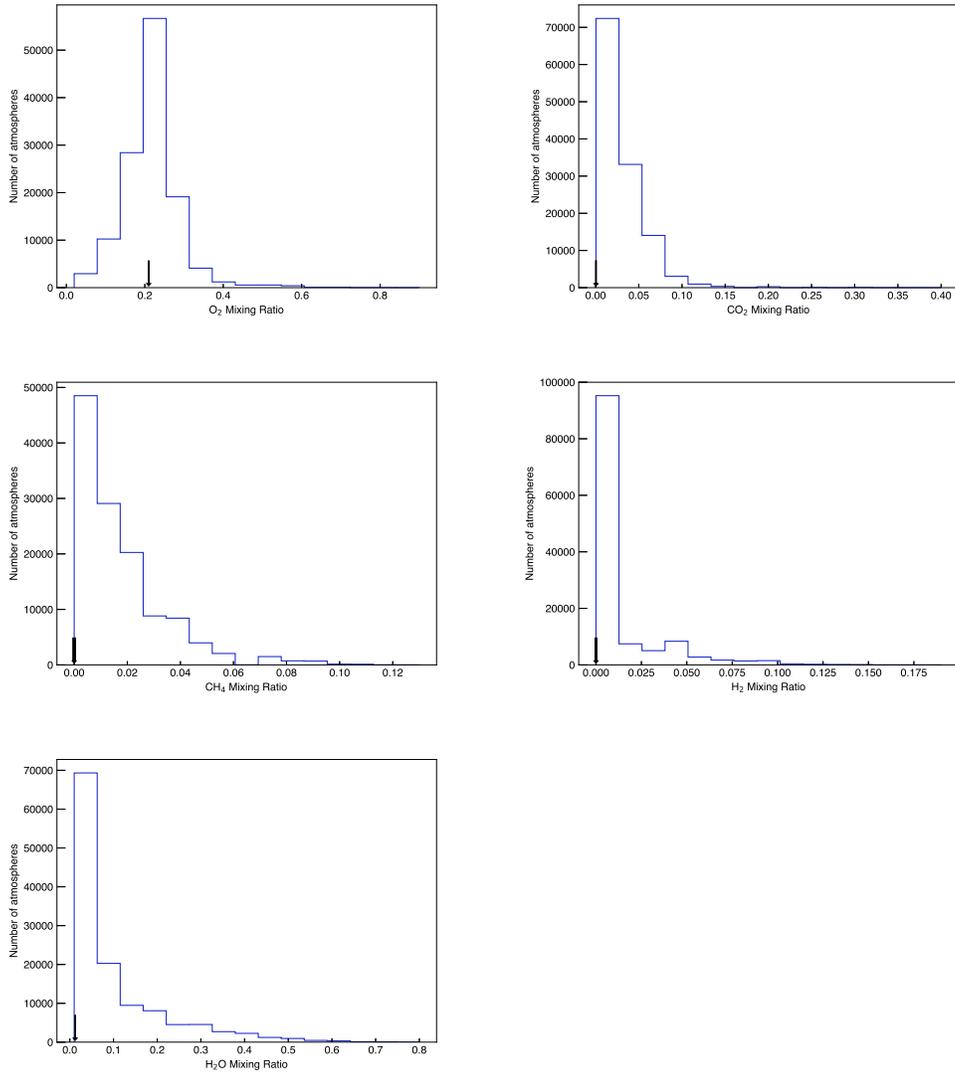


Figure 10: Distributions of the number of atmospheres generated as a function of the input gas mixing ratio. The arrow indicates the concentration of the gas on Earth.

C Additional research concepts

During the problem definition phase of FDL, we explored a range of potential research concepts. Table 2 provides an outline of five of these concepts, should these be useful as a starting point for future iterations of FDL and the wider astrobiology community.

<i>Project</i>	<i>Description</i>	<i>References</i>
Fractal-based generalised image recognition of life	Training a neural network to classify biological and non-biological images at various scales by extracting and comparing fractal properties. Interpreting the trained model to find generalised properties of life on Earth.	Obsert et al. (1990); Våge and Thingstad (2015)
Mapping the space of possible biopolymers	Considering polymers as a likely universal requirement for life, and using machine learning to accelerate searches for viable polymers, e.g those which may be able to form backbones for alpha-helix-like structures.	Saladino et al. (2007); Tavenor et al. (2016); Wu et al. (2018)
Entropic recognition of life	Detecting life via entropy may be useful to remote measurement experiments. Modelling biological entropy patterns may be a fundamental foundation for establishing theoretical probabilities of life based on other observables.	Aoki (2006); Goldenfeld and Woese (2011); Krissansen-Totton, Bergsman et al. (2016); Krissansen-Totton, Olson et al. (2018); Loudon et al. (2016)
Accelerated activation energy searches for proteins	Establish general patterns for protein activation energies using ML learning based predictions. Investigate changes in activation energies over evolutionary timescales.	Andzelm et al. (1995); Caspi et al. (2012); Cohen et al. (2008); Faber et al. (2017); Gilmer et al. (2017); Ramakrishnan et al. (2014); Schuch and Verstraete (2009); Sinitskiy and Pande (2018)
Generalised properties of metabolic networks	Extract fundamental patterns in metabolic network data (e.g. Kyoto Encyclopedia of Genes and Genomes (KEGG)) to help develop a generalised theory of biology. Analysis of complex networks may be accelerated with auto-encoding neural networks.	Caspi et al. (2012); Kempe, Bodegom et al. (2017); Ogata et al. (1999)

Table 2: Brief descriptions of the alternate astrobiology project ideas conceptualised during FDL 2018. Relevant references to aid future work studies.

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