Monte Carlo Simulations of Biophysical Factors for Viability of Life in Exoplanetary Atmospheres

Maximillian S. Westphal[1] and Anil K. Pradhan[2]

[1]*Biophysics Graduate Program, The Ohio State University, Columbus, OH 43210, USA;* `westphal.21@osu.edu`

[2]*Dept. of Astronomy, The Ohio State University, Columbus, OH 43210, USA;* `pradhan.1@osu.edu`

Abstract. In astrobiology, we propose to adapt the GEANT4 Monte Carlo package, developed by CERN, to simulate the effects of the stellar radiation fields on exoplanet atmospheres, and explore the possibility of DNA-based biosignatures and lifeforms. Stellar spectral profiles from cool dwarfs will be subject to quasi-monochromatic intensity modulations by the chemical constituents of exoplanetary atmospheres, represented as phantoms using Earth-like compositions as well as those observed and theorized for exoplanets. We will consider radiation penetration in the atmosphere using available molecular opacities of prime atmospheric constituents such as H_2O and CO_2, and study biophysical effects on DNA survival and strand breaking at varying elevations.

1. Introduction

As more stars are discovered and more Earth-like exoplanets orbiting those stars are detected, the aspiration to determine their viability for supporting life has grown (Cassan et al. 2012; Seager 2014). But the question that remains is what biosignatures might look like should we observe them from Earth. Because the Earth is currently the only known planet to support life, this problem can be approached by focusing on Earth in addition to exoplanets. What would the Earth look like if we observed it from a faraway exoplanet? GEANT4 is an open-source toolkit developed by CERN that uses the Monte Carlo method to simulate particle passage, including photons, through matter, and could lead to the answer of these questions (Agostinelli et al. 2003; Allison et al. 2006, 2016).

In astrobiology GEANT4 would be used to simulate transmission spectroscopy of exoplanetary atmospheres. Until recently GEANT4 has been most commonly used in high-energy applications such as X-ray and hadron radiation therapy, X-ray astronomy, and particle collisions. However, the energy range of transmission spectroscopy for astrobiology (optical and near infrared) is generally in the low-energy regime of GEANT4, less than 1000 eV. GEANT4 is generally less accurate in this low-energy regime unless specific data and physics packages are employed, e.g., GEANT4-DNA (Incerti et al. 2010). This add-on has shown significant improvements in accuracy in low-energy interactions between particles and liquid water (Incerti et al. 2010). Other groups have adapted GEANT4-DNA for use in materials and environments where accuracy at low-energies is important, e.g., silicon for microelectronics (Valentin et al.

2010; Raine et al. 2012; Valentin et al. 2012). In order to use GEANT4 for transmission spectroscopy related to astrobiology, it would require a new low-energy package for many of the most common molecular species indicative of life such as O_2, H_2O, N_2O, CH_4, CH_2SH, CH_2Cl, N_2, and CO_2 (Seager 2014). The most important data set this package would need to contain would be monochromatic opacities for each molecule in the ultraviolet, visible, and infrared.

Furthermore, the GEANT4-DNA package allows for simulations of radiation-induced damage to DNA, which could be also extended to DNA-macromolecule viability when exposed to the blackbody radiation of different stellar types and atmosphere compositions (Incerti et al. 2010). These sections of the package will prove useful for determining viability of macromolecules that are the precursors to DNA, which may have been recently observed in protostars (Codella et al. 2017).

We propose to use the Monte Carlo code GEANT4 to simulate what the spectroscopic signature of Earth's and other life-supporting exoplanets' atmospheres might look like should they be observed.

2. Methods

We will begin by modeling Earth and our own Sun with GEANT4. As can be seen in Fig. 1, the solar spectrum does not match a perfect blackbody (Pradhan & Nahar 2011), and this is most noticeable in the ultraviolet wavelengths. We will use the spectrum shown in Fig. 1 split into many energy bands to facilitate launching multiple photon energies simultaneously. This will also allow us to modify the scale height of different parts of the spectrum if necessary.

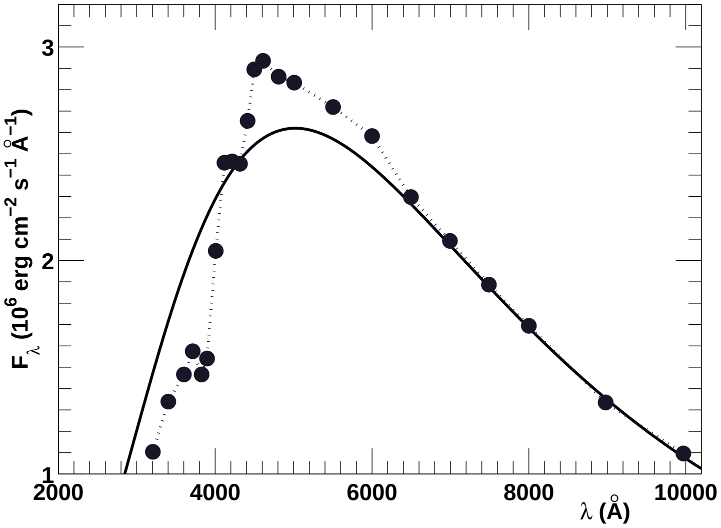

Figure 1. Blackbody radiation at 5770 K (solid line) compared to the emitted solar flux (dashed-dot line). Reproduced from Fig. 10.1 of Pradhan & Nahar (2011) with permission from Cambridge University Press.

2.1. Representative Atmospheric Phantom

The Earth and its atmosphere will be modeled as a layered spherical phantom similar to those used in modeling X-ray radiation therapy and imaging (Westphal et al. 2017). The atmosphere will follow the structure of the Earth's atmosphere, and we will launch photons from the modulated blackbody spectrum into it to observe the absorption spectrum as if the Earth were an exoplanet itself. The solar flux interacting with the atmosphere will be modeled as in Fig. 2.

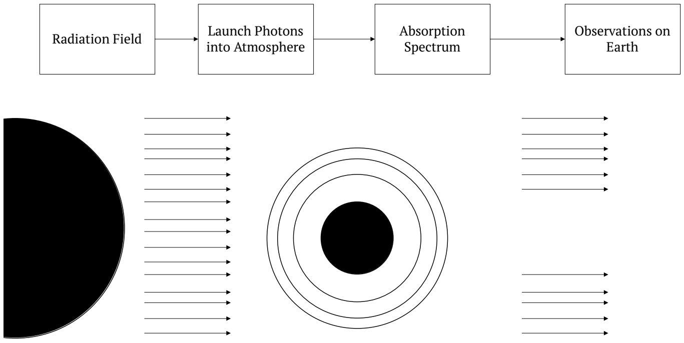

Figure 2. The radiation field is launched from a large sun-like source across GEANT4's vacuum material, where it will interact with molecular gases around a planet's atmosphere. The radiation passing through the material can then be studied immediately on the other side of the atmosphere, as well as after passing through very large distances of the vacuum material before arriving at Earth.

The radiation field will be launched from a spherical star-shaped source similar to the modulated blackbody spectrum in Fig. 1. The photons from this source will pass through a "galactic" material, which is made of hydrogen at density 10^{-25} g/cm^3, temperature 2.73 K, and pressure 3×10^{-18} Pa. The planet will first be modeled after the Earth with air in the atmosphere changing in density, temperature, and composition at higher elevations. The default air material in GEANT4 is a simple mixture of N, O, and Ar, but will be altered to better reflect the gases in the Earth's atmosphere.

Following these initial Earth-based simulations, we will add expected biosignatures, chemicals likely to indicate the presence of life to the atmosphere, and modify the atmosphere to see how combinations of gases alter the absorption spectrum. Some of the best candidates for biosignatures include O_2, H_2O, N_2O, CH_4, CH_2SH, CH_2Cl, N_2, and CO_2 (Seager 2014).

2.2. Modifying GEANT4

GEANT4-DNA is designed for low-energy liquid water simulations, which means that transmission spectroscopy simulations need to be accurate in the energy range of absorbed ultraviolet, visible, and infrared light. To modify GEANT4-DNA, we will use molecular spectroscopy databases, e.g., ExoMol, and calculate the biosignature monochromatic opacities to be imported into GEANT4 (Tennyson et al. 2016). This will result in a new dataset for use in GEANT4 in a similar fashion to how the GEANT4-MicroElec dataset was created.

It has been shown that stars of different temperatures and sizes have greatly varying habitable “Goldilocks zones” (Gillon et al. 2017). The UV opacity is uncertain in many of these cooler stars. Furthermore, different sized planets, e.g., Hot Jupiters, can also contain biosignatures such as water, so an additional toolkit for confirming observational data would be beneficial to astronomers in general (Tinetti et al. 2007). This additional GEANT4 dataset will allow us to bypass expensive experiments and help verify currently existing datasets.

2.3. Strand Breaks and DNA Survival

Following modifications of GEANT4 and GEANT4-DNA, we will be able to simulate more accurately radiation-induced DNA damage in atmospheres. It has been shown that very low-energy electrons (3–20 eV) cause resonant formations of DNA strand breaks (Boudaiffa et al. 2000). These energies will serve to calibrate the incident host-star radiation field and the UV intensity and wavelength input. The low-energy additional data will allow for tests on the viability of this DNA strand-breaking and of other macromolecules in a variety of atmospheric environments. In addition, the cell survival modules of GEANT4-DNA will allow us to determine whether individual cells are capable of living within an atmosphere exposed to a star’s radiation field.

3. Conclusion

To the best of our knowledge, GEANT4 has not yet been used for exoplanetary biosignature simulations. By expanding its datasets to include low-energy monochromatic molecular opacities similarly to GEANT4-DNA, we should be able to simulate exoplanetary atmospheres and their interactions with low-energy stellar radiation.

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