FROSTIE: An open source modelling and retrieval package for spectroscopic data of planetary surfaces

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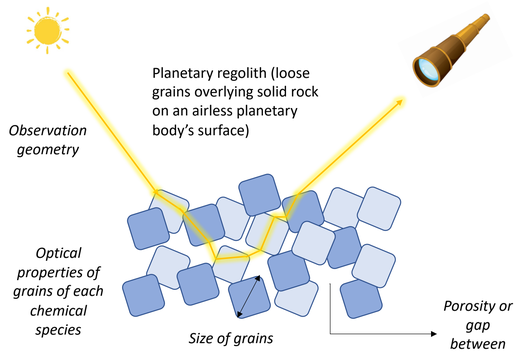
Scientific Motivation

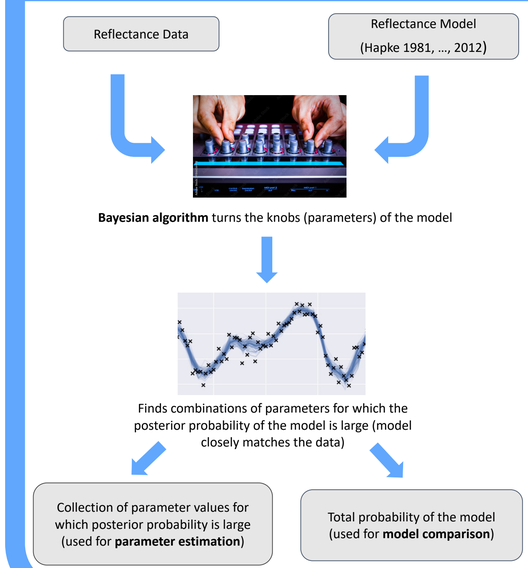
- Spectroscopic modelling enables us to derive key inferences from data such as abundances of various surface species of a planetary body.
- However, abundances are degenerate with other physical parameters such as grain-size and porosity of the planetary regolith[1], increasing the number of free parameters.
- Bayesian inference helps explore a complicated parameter space in an efficient way and sheds light on parameter degeneracy.
- However, an easy-to-use, open-source software for this kind of analysis is missing from public domain.

The Hapke Bi-Directional Reflectance Model

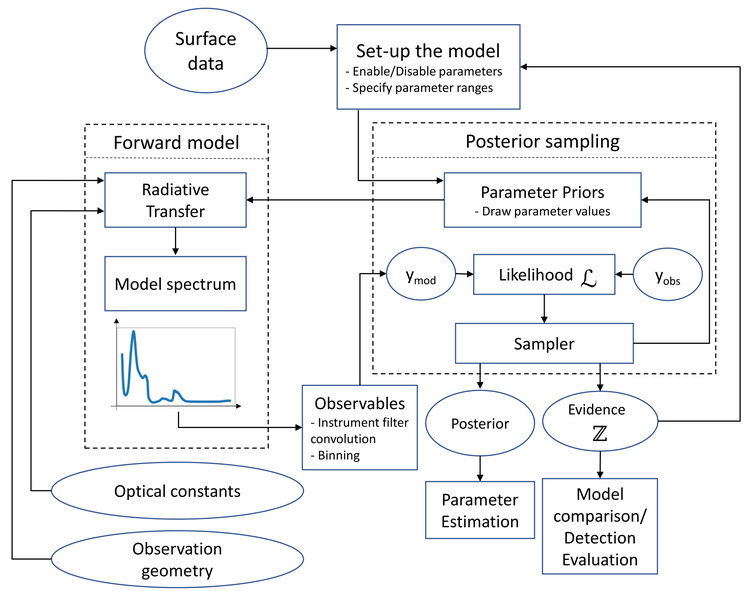
Reflectance of an airless surface as a function of various parameters



Bayesian Inference



FROSTIE, written in python, is an easy-to-use software that enables spectroscopic modelling and retrieval with the Hapke reflectance model[1], and comes with good documentation and various tutorial notebooks.



Architecture of *FROSTIE*

Scan to see an application[2] of *FROSTIE*:

FROSTIE

Planned *FROSTIE* v1.0.0 Features

- Hapke reflectance modelling with multiple endmember species
- Generating simulated data from model spectra using instrument convolution functions
- Full Bayesian model comparison analysis using the nested sampling package *dynesty*[3]
- Various plotting functions to produce publication-quality figures of parameter distributions, best-fit model, etc.
- Core functionality walkthrough with detailed Jupyter notebooks that can be run on cloud (e.g., Google Collab)
- An interactive tool for controlling model parameters and visualizing their effects on the model

Software Development Status

	Core functions	Docstrings	Testing	Tutorials
Forward-model module	✓	✓		✓
Retrieval module	✓			
Plotting module	✓			
Interactive model plotting module				

Journal of Open Source Software (JOSS) submission requirements:

Requirements	**How *FROSTIE* will satisfy it**
Repository	Hosted on GitHub (currently private)
License file	BSD 3-Clause License
Statement of Need	*FROSTIE* has been used in published and cited works
Installation Instructions	Via GitHub repo. download; PyPI to be added
Core Functionality Documentation	Python docstrings; Sphinx for documentation website
Automated Tests	Pytest; Continuous Integration options like Travis-CI
Tutorials/Example Usage	Jupyter Notebooks; Collab/Docker for online usage

Future Work

- Additional parameters/functionality for the Hapke model such as opposition effect, macroscopic roughness, internal scatterers, coated particles, multi-layer regolith, etc.
- Module to invert refractive indices from reflectance spectrum.
- Test with a retrieval algorithm with GPU support.
- Any suggestions?

Acknowledgements

I would like to acknowledge the support of of the the NASA FINESST grant 80NSSC20K1381 that supported my graduate work when most of the core code of *FROSTIE* was written. I am also thankful to the Europa Clipper Project at JPL for supporting the continued development of *FROSTIE* and sponsoring this trip. Finally, I am grateful to the Code/Astro workshop (https://semaphorep.github.io/codeastro/), participating in which motivated me to start converting my chaotic *FROSTIE* code into a high-quality open source software.

References

[1] Hapke, B. JGR: Solid Earth 86, 3039–3054 (1981)
[2] Mishra,I. et al. PSJ, 2, 183 (2021)
[3] Speagle, J.S., MNRAS, 493, 3132–3158 (2020)

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