# Bayesian Atmospheric Radiative Transfer (BART): An Open-Source Code for Atmospheric Characterization


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## Introduction

The Bayesian Atmospheric Radiative Transfer (BART) code infers atmospheric properties from spectroscopic and photometric observations. It uses a line-by-line method driven by an MCMC explorer, so it is useful for both high- and low-resolution data. BART provides robust uncertainty estimates, including correlations. If there are more parameters than data, BART will identify the allowed regions of phase space, indicating the relative likelihood of each region. Prior parameter knowledge can guide the MCMC. BART is optimized for fast calculation and reasonable memory use on multi-core machines, including high-end laptops for simpler problems, making it suitable for classroom use.

BART includes three independent packages and several auxiliary programs. The Thermochemical Equilibrium Abundances package (TEA, Blecic *et al.* 2016) calculates the likely initial state of the atmosphere. The Multi-Core Markov-Chain Monte Carlo (MC3) package is a parallel Differential-Evolution Monte Carlo phase-space explorer. Transit is a line-by-line radiative-transfer program optimized for parallel calculation of both emission (eclipse) and tangent-ray (transit) geometries.

This poster gives an overview of BART and briefly describes TEA and our Reproducible Research (RR) license. The PhD dissertations of P. Cubillos and J. Blecic (both at UCF in 2015) describe BART in more detail and apply it to HAT-P-11b and WASP-14b.

## Chemical Package: TEA

The Thermochemical Equilibrium Abundances calculates the mole mixing fractions of atomic and molecular gaseous species under thermochemical equilibrium. TEA implements the methods of White *et al.* (1958) and Eriksson (1971). Given the elemental abundances, temperature, and pressure values, TEA minimizes the Gibbs free energy of the system in an iterative, Lagrangian-optimization scheme. Blecic *et al.* (2016) used TEA to reproduce calculations with the Burrows & Sharp (1999) method, the Chemical Equilibrium with Applications (CEA) code (Fig. 4), and White *et al.* (1958). The TEA is available at http://github.com/dzesmin/TEA.

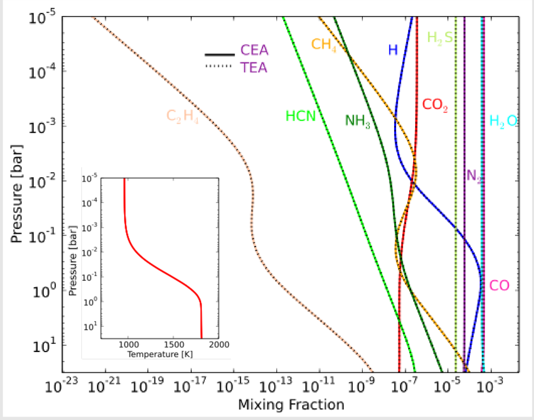


**Fig. 1:** Comparison of TEA (dotted curves) and CEA (solid curves) mixing fractions for a hot-Jupiter atmospheric profile (inset) with solar elemental composition. Both methods derive the equilibrium abundances by minimizing the Gibbs free energy. The colors indicate different chemical species.

## The BART Chart

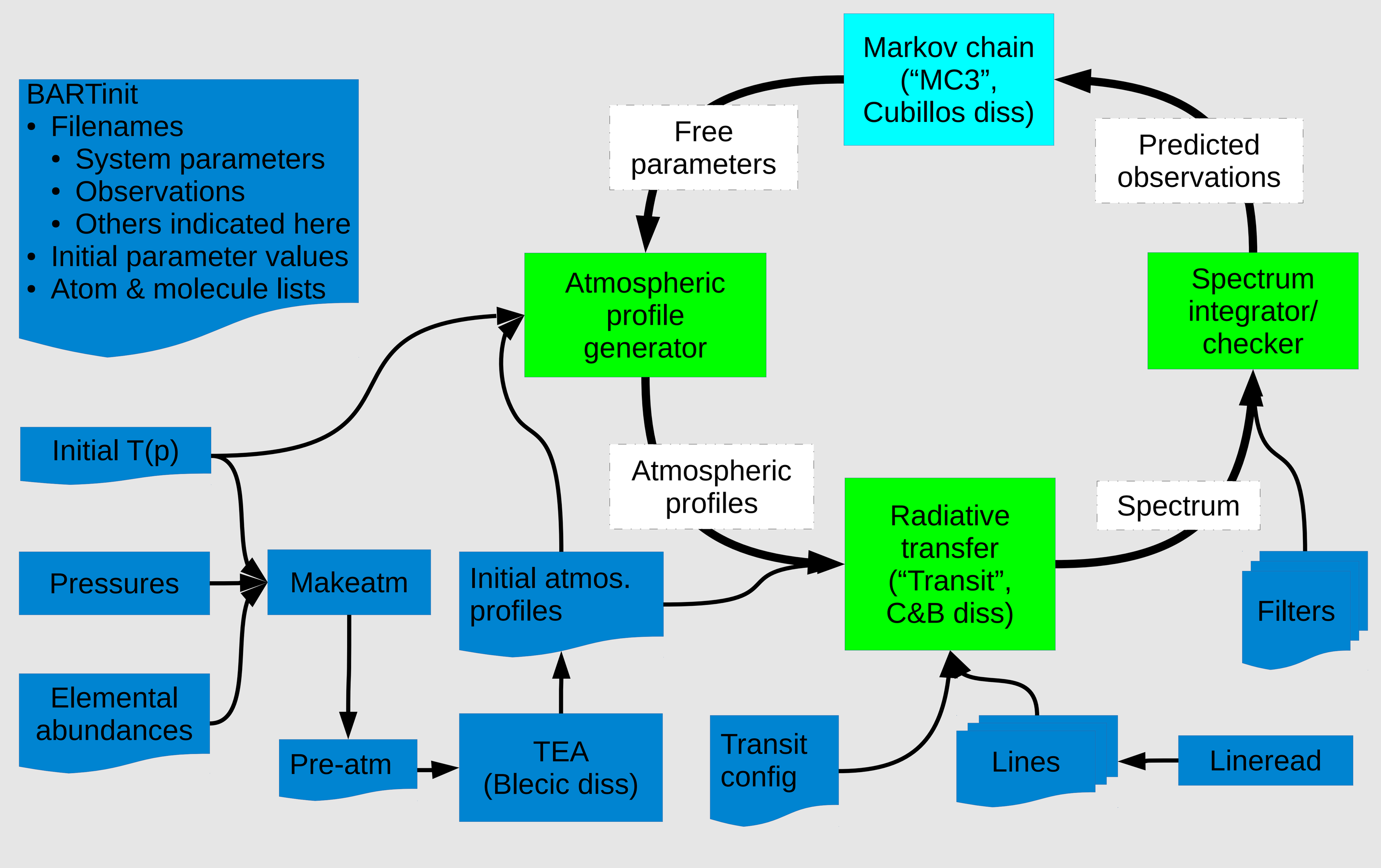


**Fig. 2:** The BART Chart. Programs are boxes. Files have wavy bottoms. Transmitted information is white.

The initialization routines read planetary and stellar parameters and the user's configuration file to generate the initial atmosphere and to configure the component codes. The initial atmosphere may be in thermochemical equilibrium at all levels, may be set to constant mixing ratios based on equilibrium, or may be set to constant or variable abundances of the user's choosing. Currently, BART scales these initial profiles with one parameter per chemical, but parameterized abundance profiles could be used, as several options for parameterized thermal profiles already are.

Pylineread converts molecular line lists into Transit's internal format. One can easily add new line-list formats, mix and match them, and test how different lists for the same chemical affect the results.

MC3 drives BART's main loop, generating free atmospheric parameters. These include abundance scale factors and T(p) (temperature-pressure) profile parameters. The atmospheric profile generator makes profiles of chemical abundances and temperatures vs. pressure and radius. Transit accepts these and calculates the emission or absorption spectrum. BART integrates the spectrum over observational bandpasses, which values return to MC3 for comparison to data, and the cycle repeats. MC3 calculates the Gelmann-Rubin convergence criterion. On completion, MC3 produces plots for the best-fit spectrum and thermal profile, contribution functions, the MCMC traces, and the 1D and 2D posterior marginalizations.

## Open Source, Open Development

BART is an open-source, open-development, reproducible-research package written in Python and C. Designed from inception for community use and development, BART and its component codes are well structured and well documented for both users and developers. The flexible design allows a variety of creative uses without changes to the code, and many more-involved changes can be made without modifying the portions written in C.

"Open source" means you can contribute and get credit for your improvements to the code through Github's pull-request mechanism. There are email lists for users and developers, which can be digested so you receive at most one per day (traffic is now much lower than that). Contributions must meet the project's documentation standard and must integrate cleanly into the existing design.

"Open development" means we have developed BART from day 1 in public on Github, taking input and testing from the community, and will continue to do so.

## Reproducible Research

With the advent of complex computer codes, irreproducible research has become an increasing problem (see, e.g., Hansen, Schwartz, and Cowan 2014). Even if a paper could describe a calculation fully, verification is impossible and bugs are likely. In practice, two codes described similarly often compute differently. Code sharing would solve this problem, but what protects investigators' interests?

Originating in computer science, the Reproducible Research (RR) movement states that science builds on the progress of each investigation, and gives credit with citations. Code often represents the majority of a study's creative input and time, and should be no different. If everyone did it, the playing field would be level.

Our RR license states that if you publish a result from BART, you must also publish an electronic compendium of the inputs, code, and outputs you used, including all code modifications. This ensures that nobody can make a private, improved version and not share it. More importantly, it allows community verification and review of new methods. It will be released and will take effect when we publish. Until then, the community may download, run, and modify BART, but may not share or publish results from it.

We feel that all journals should require such compendia for all published calculations. Our RR license is a step in that direction.


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