

PythonicDISORT: A Python reimplementation of the Discrete Ordinate Radiative Transfer package DISORT

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Summary

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The Radiative Transfer Equation (RTE) models the processes of absorption, scattering and emission as electromagnetic radiation propagates through a medium. Consider a planeparallel, horizontally homogeneous atmosphere with vertical coordinate τ (optical depth) increasing from top to bottom and directional coordinates ϕ for the azimuthal angle (positive is counterclockwise) and $\mu=\cos heta$ for the polar direction (heta is the polar angle measured from the surface normal), with $\mu > 0$ pointing up following the convention of (K. Stamnes et al., 1988). Given three possible sources: blackbody emission from the atmosphere $s(\tau)$; scattering from a collimated beam of starlight with intensity I_0 and incident azimuthal and cosine polar angles ϕ_0, μ_0 ; radiation from other atmospheric layers or the Earth's surface which is modeled by Dirichlet boundary conditions, the diffuse intensity $u(\tau, \mu, \phi)$ propagating in 15 direction (μ, ϕ) is described by the 1D RTE (Chandrasekhar, 1960; K. Stamnes et al., 1988):

$$\mu \frac{\partial u(\tau, \mu, \phi)}{\partial \tau} = u(\tau, \mu, \phi) - \frac{\omega}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} p(\mu, \phi; \mu', \phi') u(\tau, \mu', \phi') d\phi' d\mu' - \frac{\omega I_0}{4\pi} p(\mu, \phi; -\mu_0, \phi_0) \exp(-\mu_0^{-1}\tau) - s(\tau)$$
(1)

Here ω is the single-scattering albedo and p the scattering phase function. These are assumed 17 to be independent of τ , i.e. homogeneous in the atmospheric layer. An atmosphere with 18 au-dependent ω and p can be modeled by a multi-layer atmosphere with different ω and p for 19 each layer. 20

The RTE is important in many fields of science and engineering, for example, in the retrieval 21 of optical properties of the medium from measurements (McGuire et al., 2008; Teng et al., 22 2020; Torricella et al., 1999). The gold standard for numerically solving the 1D RTE is the 23 Discrete Ordinate Radiative Transfer package DISORT which was coded in FORTRAN 77 and 24 first released in 1988 (K. Stamnes et al., 1988; S. Stamnes, 1999). It has been widely used, 25 for example by MODTRAN (Berk et al., 2014), Streamer (Key & Schweiger, 1998), and SBDART 26 (Ricchiazzi et al., 1998), all of which are comprehensive radiative transfer models that are 27 themselves widely used in atmospheric science, and by the three retrieval papers Torricella 28 et al. (1999); McGuire et al. (2008); Teng et al. (2020). DISORT implements the Discrete 29 Ordinates Method which has two key steps. First, the diffuse intensity function u and phase 30 function p are expanded as the Fourier cosine series and Legendre series respectively: 31

$$\begin{split} u\left(\tau,\mu,\phi\right) &\approx \sum_{m=0} u^m\left(\tau,\mu\right)\cos\left(m\left(\phi_0-\phi\right)\right)\\ p\left(\mu,\phi;\mu',\phi'\right) &= p\left(\cos\gamma\right) \approx \sum_{\ell=0}^{m=0} (2\ell+1)g_\ell P_\ell\left(\cos\gamma\right) \end{split}$$

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Software

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where γ is the scattering angle. These address the ϕ' integral in (1) and decompose the problem into solving

$$\mu \frac{\partial u^m(\tau,\mu)}{\partial \tau} = u^m(\tau,\mu) - \int_{-1}^1 D^m\left(\mu,\mu'\right) u^m\left(\tau,\mu'\right) \mathrm{d}\mu' - Q^m(\tau,\mu) - \delta_{0m} s(\tau)$$

- for each Fourier mode of u. The terms D^m are derived from p and are thus also independent of τ . The second key step is to discretize the μ' integral using some quadrature scheme. DISORT uses the double-Gauss quadrature scheme from Sykes (1951). This results in a system of ordinary differential equations that can be solved using standard methods, and post-hoc corrections (Nakajima & Tanaka, 1988; Wiscombe, 1977) are made to reduce the errors incurred by the truncation of the phase function Legendre series.
- My package PythonicDISORT is a Python 3 reimplementation of DISORT that replicates most 40 of its functionality while being easier to install, use and modify, though at the cost of 41 computational speed. It has DISORT's main features: multi-layer solver, delta-M scaling, 42 Nakajima-Tanaka (NT) corrections, only flux option, direct beam source, isotropic internal 43 source (blackbody emission), Dirichlet boundary conditions (diffuse flux boundary sources), 44 Bi-Directional Reflectance Function (BDRF) for surface reflection, as well as additional features 45 like actinic flux computation and integration of the solution functions with respect to optical 46 depth. PythonicDISORT has been tested against DISORT on DISORT's own test problems. While 47 packages that wrap DISORT in Python already exist (Connour & Wolff, 2020; Hu, 2017), 48 PythonicDISORT is the first time DISORT has been reimplemented from scratch in Python. 49

50 Statement of need

⁵¹ PythonicDISORT is not meant to replace DISORT. Due to fundamental differences between

⁵² Python and FORTRAN, PythonicDISORT, though quite optimized, remains a few times slower

than DISORT. Thus, projects that prioritize computational speed should still use DISORT. In addition, PythonicDISORT currently lacks DISORT's latest features, most notably its pseudo-

55 spherical correction.

PythonicDISORT is instead designed with three goals in mind. First, it is meant to be a 56 pedagogical and exploratory tool. PythonicDISORT's ease of installation and use makes it a low-barrier introduction to Radiative Transfer and Discrete Ordinates Solvers. Even researchers 58 who are experienced in the field may find it useful to experiment with PythonicDISORT before 59 deciding whether and how to upscale with DISORT. Installation of PythonicDISORT through 60 pip should be system agnostic as PythonicDISORT's core dependencies are only NumPy (Harris 61 et al., 2020) and SciPy (Virtanen et al., 2020). In addition, using PythonicDISORT is as simple as calling the Python function pydisort. In contrast, DISORT requires FORTRAN compilers 63 and manual memory allocation, has a lengthy and system dependent installation, and each call 64 requires shell script for compilation and execution.

Second, PythonicDISORT is designed to be modified by users to suit their needs. Given that
 Python is a widely-used high-level language, PythonicDISORT's code should be understandable,
 at least more so than DISORT's FORTRAN code. Moreover, PythonicDISORT comes with a
 Jupyter Notebook (Kluyver et al., 2016) – its *Comprehensive Documentation* – that breaks down

⁷⁰ both the mathematics and code behind the solver. Users can in theory follow the Notebook to

⁷¹ recode PythonicDISORT from scratch; it should at least help them make modifications.

- Third, PythonicDISORT is intended to be a testbed. For the same reasons given above, it should be easier to implement and test experimental features in PythonicDISORT than in
- 74 DISORT. This should expedite research and development for DISORT and similar algorithms.
- PythonicDISORT was first released on PyPl and GitHub on May 30, 2023. It was used in Ho
 & Pincus (2024) and is being used in at least three ongoing projects: on the Two-Stream



- 77 Approximations, on atmospheric photolysis, and on the topographic mapping of Mars through
- 78 photoclinometry. I will continue to maintain and upgrade PythonicDISORT. The latest version:
- ⁷⁹ PythonicDISORT v0.9.3 was released on October 13, 2024.

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