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

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Summary

The Radiative Transfer Equation (RTE) models the processes of absorption, scattering and emission as electromagnetic radiation propagates through a medium. Consider a plane-parallel, horizontally homogeneous atmosphere with vertical coordinate τ (optical depth) increasing from top to bottom, directional coordinates ϕ for the azimuthal angle (positive is counterclockwise), and $\mu = \cos\theta$ for the polar direction (θ 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, namely blackbody emission from the atmosphere $s(\tau)$, scattering from a collimated beam of starlight with intensity I_0 as well as incident azimuthal and cosine polar angles ϕ_0 and μ_0, respectively, and 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 direction (μ, ϕ) is described by the 1D RTE (Chandrasekhar, 1960; K. Stamnes et al., 1988)

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

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

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

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

where γ is the scattering angle, g_ℓ is the ℓth Legendre coefficient of the phase function p, and P_ℓ is the Legendre polynomial of order ℓ. These address the ϕ' integral in (1) and decompose the problem into solving the equation

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

for each Fourier mode of u. The D^m terms are derived from p and are thus also independent of τ. The Q^m terms are derived from the direct beam source. The second key step is to discretize the μ' integral using a 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 are made to reduce the errors incurred by the truncation of the phase function Legendre series (Nakajima & Tanaka, 1988; Wiscombe, 1977).

My package `PythonicDISORT` is a Python 3 reimplementation of `DISORT` that replicates most of its functionality while being easier to install, use and modify, though at the cost of computational speed. It has `DISORT`'s main features: multi-layer solver, delta-M scaling, Nakajima-Tanaka corrections, only flux option, direct beam source, isotropic internal source (blackbody emission), Dirichlet boundary conditions (diffuse flux boundary sources), Bi-Directional Reflectance Function for surface reflection, as well as additional features like actinic flux computation and integration of the solution functions with respect to optical depth. `PythonicDISORT` has been tested against `DISORT` on `DISORT`'s own test problems. While packages that wrap `DISORT` in Python already exist (Connour & Wolff, 2020; Hu, 2017), `PythonicDISORT` is the first reimplementation of `DISORT` from scratch in Python.

Statement of need

`PythonicDISORT` is not meant to replace `DISORT`. Due to fundamental differences between Python and FORTRAN, `PythonicDISORT`, though quite optimized, remains 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-spherical correction.

`PythonicDISORT` is instead designed with three goals in mind. First, it is meant to be a 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 who are experienced in the field may find it useful to experiment with `PythonicDISORT` before upscaling with `DISORT`. Installation of `PythonicDISORT` through `pip` should be system agnostic as `PythonicDISORT`'s core dependencies are only `NumPy` (Harris 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 and manual memory allocation, has a lengthy and system-dependent installation, and each call requires a 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 accessible to more people than `DISORT`'s FORTRAN code. Moreover, `PythonicDISORT` comes with a Jupyter Notebook (Kluyver et al., 2016) – its *Comprehensive Documentation* – that breaks down both the mathematics and code behind the solver. Users can in theory follow the Notebook to 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 `DISORT`. This should expedite research and development for `DISORT` and similar algorithms.

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

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