The Journal of Open Source Software

HAOT: A Python package for hypersonic aero-optics analysis

Martin E. Liza [1]

1 The University of Arizona

DOI: 10.xxxxxx/draft

Software

- Review
- Repository
- Archive

Editor: Open Journals

Reviewers:

- @openjournals

Submitted: 01 January 1970
Published: unpublished

Summary

Hypersonic flows present unique challenges due to the complex interplay of fluid dynamics, chemical reactions, and optical phenomena. As a signal from a Light Detection and Ranging (LiDAR) system travels through a hypersonic flow field, the beam is affected by the flow, potentially leading to errors in targeting and detection measurements.

`HAOT` is a Hypersonic Aerodynamics Optics Tools Python package developed to calculate different aerodynamic properties in a hypersonic medium. Its source code is available on GitHub, the documentation is available on Read the Docs and examples on the usage of the package are given on the documentation site under usage. These examples cover some easy examples such as the basic functionality of the tool and also cover examples using results from Computational Fluid Dynamics (CFD) simulations.

Statement of Need

Many techniques used to calculate optical properties are scattered across various papers, but there is no centralized repository containing all these calculations. Furthermore, some of these calculations require spectroscopy constants, which are often unclear or inconsistently presented in the literature. This package includes a constants module that provides and documents numerous spectroscopy constants for diatomic molecules.

`HAOT` was designed with the goal of being used to easily computed aerodynamic quantities of interest from CFD results. This package was used by (Liza et al., 2023). In this work, they investigate nonequilibrium effects on Aero-Optics in Hypersonic flows.

Algorithms

The `HAOT` package, contains five modules:

- Aerodynamics
- Optics
- Quantum Mechanics
- Constants
- Conversions

Each module can be imported independently. The documentation explains the functions in each module as well as their usage. Docstrings are include, so the function prototypes and usage can also be accessible in an interactive Python session. Results from these algorithms were compared with the literature, and a unit test was developed, which is located under the unit_test directory.

This section highlights some of the capabilities of the package but not all of them. For instance, the package can calculate various compressible flow properties, such as isentropic, normal shock, and oblique shock relations. Please refer to the documentation for a complete list of available functions.

Results

Equation 1 was introduced by (Smith & Weintraub, n.d.), and it provides an approximation for the index of refraction as a function of atmospheric altitude.

$$n(h) \approx 1 + \frac{K_1}{T(h)} \left(p(h) + K_2 \frac{e(h)}{T(h)} \right) \quad (1)$$

Where: K_1 and K_2 are constants, $T(h)$ is the temperature as a function of altitude, $p(h)$ is pressure as a function of altitude, and $e(h)$ is the partial pressure of water vapor.

Results for Equation 1 are provided in Figure 1. This approximation is a useful way of analyzing the region in which the index of refraction has the greatest impact on a seeker's performance. As expected, the critical region is between 20 $[\mathrm{km}]$ and 30 $[\mathrm{km}]$ above sea level, which is a region where a seeker's performance is particularly important.

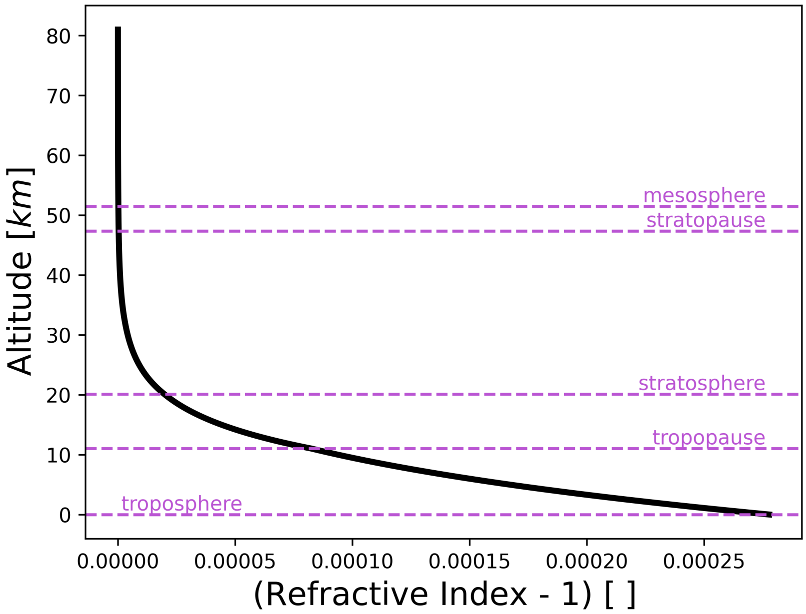


Figure 1: Atmospheric index of refraction for dry air.

The Gladstone-Dale constant is an important constant used to calculate the index of refraction (equation 2). For a dilute gas, the index of refraction can be approximated as:

$$n - 1 = \sum_{s=1}^{N} K_s \rho_s \quad (2)$$

Where: n is the index of refraction, K_s is the species' Gladstone-Dale constants, and ρ_s is the species density.

The Journal of Open Source Software

Figure 2 shows the Gladstone-Dale constants for a five-species gas. The species density was calculated using the CFD tool, SU2 (W. T. Maier et al., 2021), (W. Maier et al., 2023). These densities were then loaded into the `HAOT` tool to calculate Figure 2.

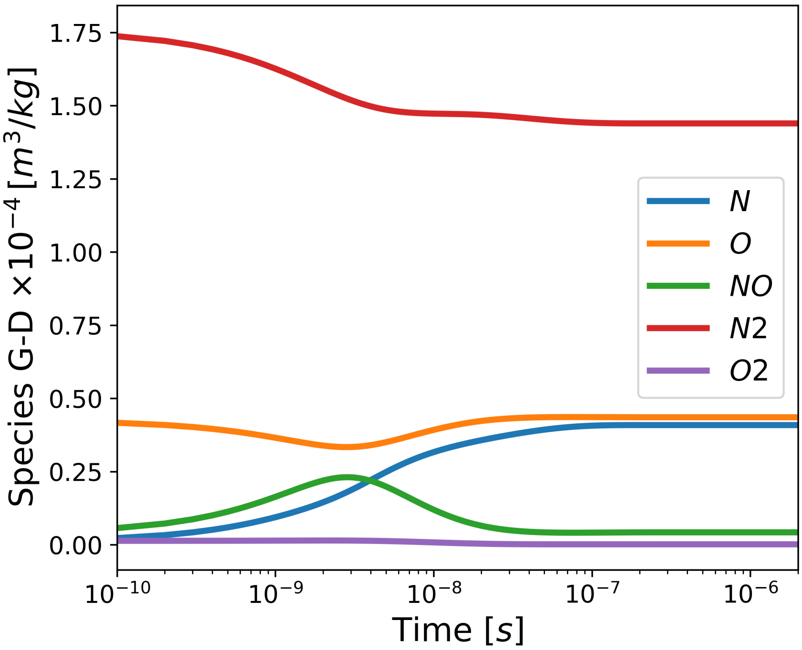


Figure 2: Species Gladstone-Dale constants for a five-species gas.

Another way of calculating the index of refraction is using the polarizability, as shown in equation 3.

$$n - 1 = \frac{1}{2\epsilon_0} \sum_{s=1} \alpha_s N_s \tag{3}$$

Where: ϵ_0 is the dielectric constant in vacuum, α_s is the species' polarizability constant, and N_s is the partial species mass fraction.

Figure 3 uses the extrapolation (equation 4) developed by (Kerl et al., 1992), based on the work of (Hohm & Kerl, 1986).

$$\alpha(\omega, T) = \frac{\alpha(0,0)}{1 - \left(\frac{\omega}{\omega_0}\right)^2} \left(1 + bT + cT^2\right) \tag{4}$$

Where: α is the polarizability as a function of the laser's frequency ω and temperature T. b and c are extrapolation constants, all of which are implemented in the `HAOT` package, and ω_0 is the oscillation frequency of the diatomic molecule.

Figure 3 shows the change of polarizability as a function of temperature.

The Journal of Open Source Software

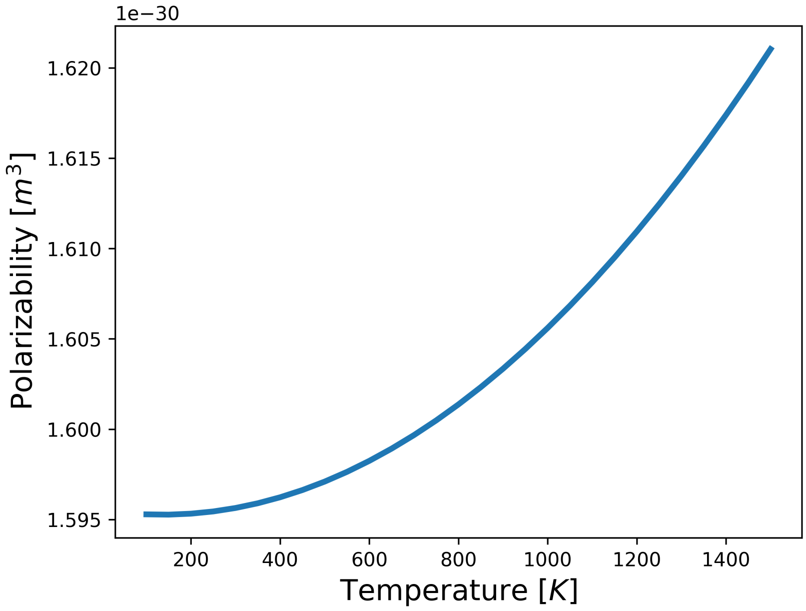


Figure 3: Polarizability of $O2$ using Kerl's method for a laser of $633[nm]$.

The results presented so far highlight some of the capabilities of the aerodynamics and optics modules. Figure 4 shows the results of the Boltzmann Distribution for N_2 (in the quantum mechanics module). Some aero-optics calculations (Buldakov et al., 2000), (Tropina et al., 2018) required a Boltzmann Distribution to calculate the polarizability and index of refraction for diatomic molecules.

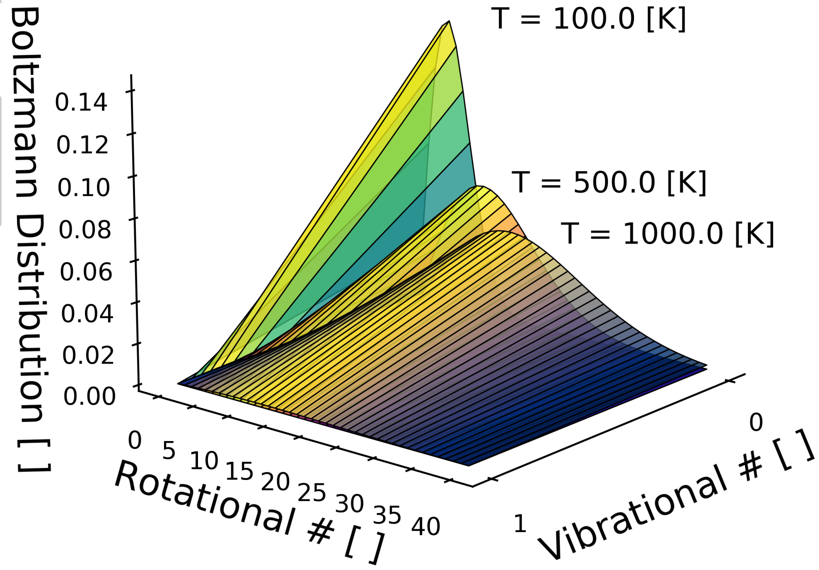
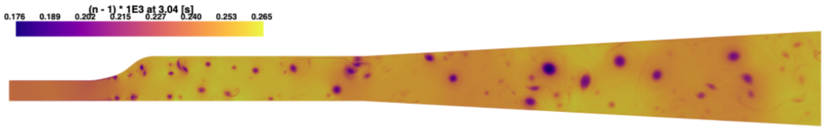


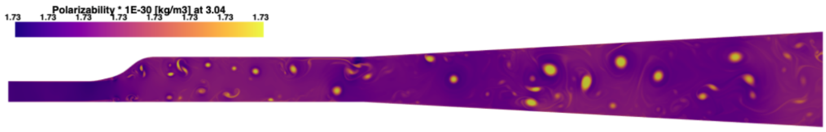
Figure 4: Boltzmann Distribution for $N2$.

These tools can be applied to the results from a CFD code fairly easy results of calculating the index of refraction, Gladstone Dale Constant and dielectric medium are below. A low speed compressible Large Eddys Simulation was used with OpenFOAM to perform results below, the goal of this is not to go into very especific details of the CFD ssetup but to showcase the ablity of the HAOT tool.



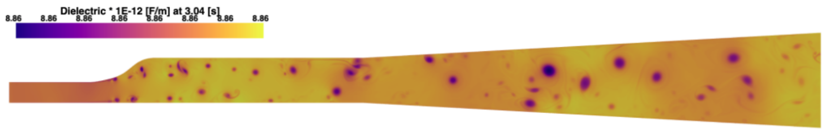
\begin{figure}[h!]

\caption{Index of Refraction. \end{figure}



\begin{figure}[h!]

\caption{Index of Refraction. \end{figure}



\begin{figure}[h!]

\caption{Dielectric medium. \end{figure}

References

Buldakov, M. A., Matrosov, I. I., & Cherepanov, V. N. (2000). Temperature dependence of polarizability of diatomic homonuclear molecules. *Optics and Spectroscopy*, *89*, 37–41. https://doi.org/10.1134/BF03355985

Hohm, U., & Kerl, K. (1986). Temperature dependence of mean molecular polarizability of gas molecules. *Molecular Physics*, *58*, 541–550. https://doi.org/10.1080/00268978600101351

Kerl, K., Hohm, U., & Varchmin, H. (1992). Polarizability α (ω, T , ρ) of small molecules in the gas phase. *Berichte Der Bunsengesellschaft Für Physikalische Chemie*, *96*, 728–733. https://doi.org/10.1002/bbpc.19920960517

Liza, M., Tumuklu, O., & Hanquist, K. M. (2023, June). Nonequilibrium effects on aero-optics in hypersonic flows. *AIAA AVIATION 2023 Forum*. https://doi.org/10.2514/6.2023-3736

Maier, W. T., Needels, J. T., Garbacz, C., Morgado, F., Alonso, J. J., & Fossati, M. (2021). SU2-NEMO: An open-source framework for high-mach nonequilibrium multi-species flows. *Aerospace*, *8*, 193. https://doi.org/10.3390/aerospace8070193

Maier, W., Needels, J. T., Alonso, J. J., Morgado, F., Garbacz, C., Fossati, M., Tumuklu, O., & Hanquist, K. M. (2023). Development of physical and numerical nonequilibrium modeling capabilities within the SU2-NEMO code. *AIAA AVIATION 2023 Forum*. https://doi.org/10.2514/6.2023-3488

Smith, E., & Weintraub, S. (n.d.). https://doi.org/10.1109/JRPROC.1953.274297

Tropina, A., Wu, Y., Limbach, C., & Miles, R. B. (2018). Aero-optical effects in non-equilibrium air. *2018 Plasmadynamics and Lasers Conference*. https://doi.org/10.2514/6.2018-3904