HAOT: A Python package for hypersonic aero-optics analysis

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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 for calculating optical properties are dispersed across various research papers, with no centralized repository consolidating these methods. Additionally, some of these calculations depend on spectroscopy constants, which are often inconsistently presented or unclear in the literature. To address this issue, this package includes a dedicated constants module that provides and documents numerous spectroscopy constants for diatomic molecules, ensuring consistency and accessibility.

HAOT was developed to facilitate the computation of aerodynamic quantities of interest from CFD results in a streamlined manner. The package has been employed in research, including the work by (Liza et al., 2023), where it was used to investigate nonequilibrium effects on aero-optics in hypersonic flows. By integrating relevant optical and aerodynamic calculations, HAOT severs as a valuable tool for researchers serves as a valuable tool for researchers studying the complex interactions between fluid dynamics and optical wave propagation in extreme flow conditions.

Algorithms

The HAOT package, contains five modules:

- Aerodynamics
- Optics
- Quantum Mechanics
- Constants
- Conversions

37 Each module can be imported independently, allowing for flexible usage depending on the
38 specific computational needs. The documentation provides detailed explanations of the
39 functions within each module, along with their proper usage. Additionally, docstrings are
40 included, making function prototypes and usage accessible within an interactive Python session
41 through built-in help functions.

42 To ensure accuracy and reliability, results obtained from these algorithms have been validated
43 against published literature. A comprehensive suite of unit tests has been developed to detect
44 potential issues and maintain code integrity.

Results

46 This section highlights some of the package's capabilities but does not encompass all of
47 them. For example HAOT can compute various compressible flow properties, including including
48 isentropic flow, normal shock relations, and oblique shock relations. For a complete list of
49 available functions and their descriptions, please refer to the documentation.

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

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

52 Where: K_1 and K_2 are empirically determined constants, $T(h)$ is the temperature as a function
53 of altitude, $p(h)$ is the atmospheric pressure, and $e(h)$ is the partial pressure of water vapor.
54 These constants are documented in the constants module.

55 The results obtained using Equation 1 are illustrated in Figure 1. This approximation provides
56 valuable insight into the altitudes where variations in the index of refraction most significantly
57 affect a seeker's performance. As expected, the critical region lies between 20 [km] and 30 [km]
58 above sea level, a range where atmospheric effects play a crucial role in optical tracking.
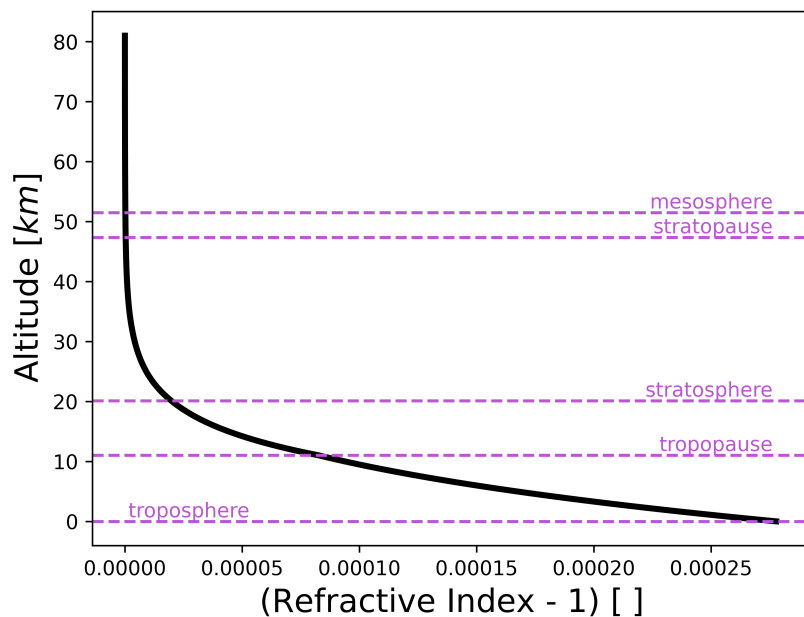

Figure 1: Atmospheric index of refraction for dry air.

The Gladstone-Dale constant is a key parameter used to calculate the index of refraction as given by Equation 2. This constant is directly related to the fluid's density and, in the case of hypersonic flows, must account for the contributions of multiple species due to the high-temperature chemical nonequilibrium effects present in such flows.

For a dilute gas, the index of refraction can be approximated as:

$$n - 1 = \sum_{s=1}^{N} K_s \rho_s \tag{2}$$

Where: n is the index of refraction, K_s represents the Gladstone-Dale constant for species s, and ρ_s is the corresponding species density.

Figure 2 presents the Gladstone-Dale constants for a five-species gas. The species densities were computed using the CFD tool, SU2 (W. T. Maier et al., 2021), (W. Maier et al., 2023). These computed densities were then imported into the HAOT tool to generate Figure 2.
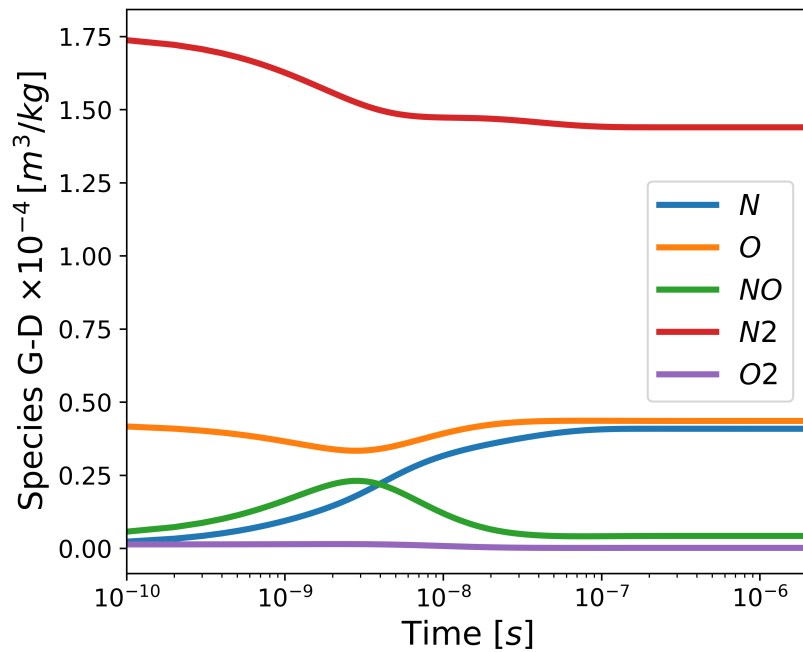

Figure 2: Species Gladstone-Dale constants for a five-species gas.

An alternative method for calculating the index of refraction involves using polarizability, as expressed 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 polarizability constant for species s, and N_s represents the number density of species s.

Figure 3 presents results obtained using an extrapolation method (Equation 4) developed by (Kerl et al., 1992), based on the work of (Hohm & Kerl, 1986). This method provides a temperature-dependent correction to the static polarizability, improving accuracy for high-temperature conditions relevant to hypersonic flows and aero-optical calculations.

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

77 Where: $\alpha(\omega, T)$ represents the polarizability as a function of laser's frequency ω and temperature
78 T. The parameters b and c are empirical extrapolation constants, and ω_0 is the characteristic
79 oscillation frequency of the diatomic molecule. These values are implemented in the `HAOT`
80 package, allowing for easy computation of temperature-dependent polarizability.

81 Figure 3 illustrates the variation of polarizability with temperature for oxygen (O_2) at a laser
82 wavelength of $633\,nm$, demonstrating the effectiveness of Kerl's method in modeling optical
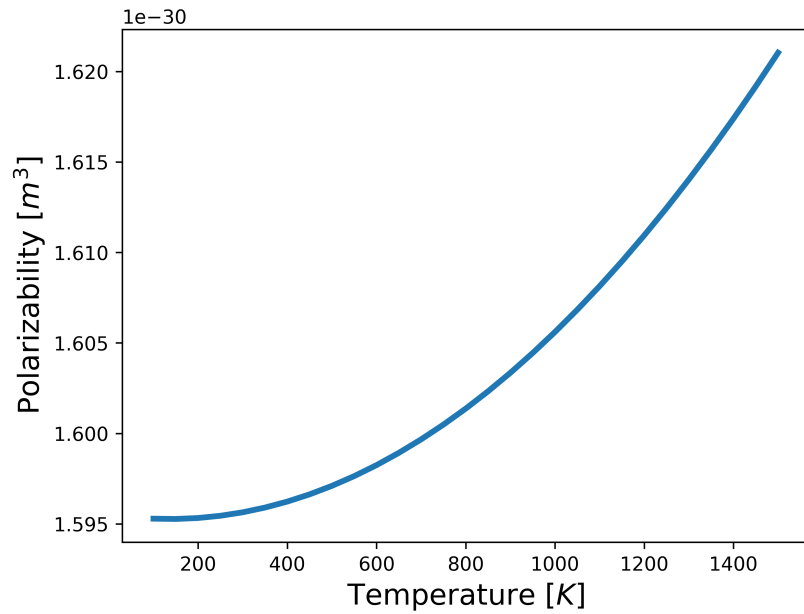83 properties under varying thermodynamic conditions.

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

84 The results presented thus far highlight some of the key capabilities of the aerodynamics and
85 optics modules within 'HAOT". Additionally, Figure 4 presents the Boltzmann distribution for
86 nitrogen (N_2), implemented in the quantum mechanics module. Several aero-optics studies
87 (Buldakov et al., 2000), (Tropina et al., 2018) have incorporated Boltzmann distribution
88 calculations to determine the polarizability and index of refraction for diatomic molecules,
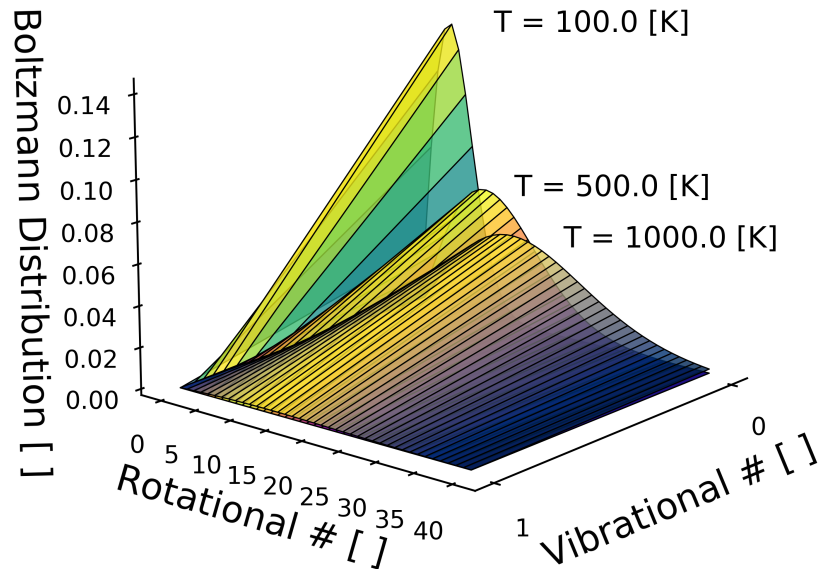89 demonstrating its significance in hypersonic flow modeling.

Figure 4: Boltzmann Distribution for $N2$.

These tools can be readily applied to the results obtained from a CFD simulation. Below, we present calculations for the index of refraction, Gladstone-Dale constant, and dielectric properties using the HAOT package. A low-speed, compressible Large Eddy Simulation (LES) was performed using OpenFOAM to generate the results shown below. The primary objective here is not to provide a detailed description of the CFD setup, but rather to demonstrate the capabilities of the HAOT tool in processing and analyzing flow-field optical properties.
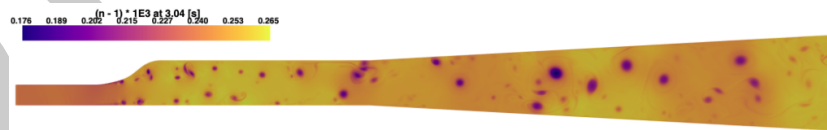
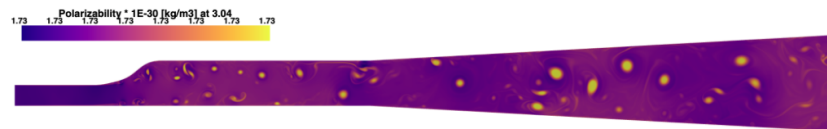

Figure 5: Index of Refraction.
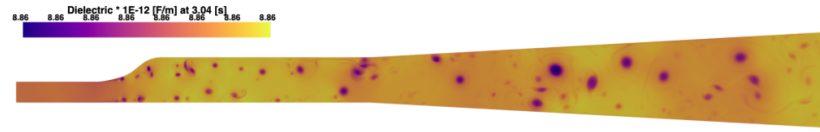

Figure 6: Index of Refraction.

Figure 7: Dielectric medium.

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