PPFM: An Object-Oriented C++ Library for Thermodynamic and Transport Properties Calculation

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Abstract: PPFM (Plasma Properties for Many) is an object-oriented C++ tool for composition, thermodynamic and transport properties calculation of LTE and NLTE plasmas, with minimal user input. Its modular design ensures flexibility, extensibility, efficiency and accuracy for on-the-fly properties calculation or database generation.

1. Introduction

Modelling of plasma processes requires the solution of several physics equations which describe the transport of physical quantities, with constitutive relations describing the material behavior, function of some physical quantities (e.g., temperature, concentration) by means of different models (e.g., Fourier law, Fick's law), providing a continuum approximation of the phenomena occurring at molecular scale. In plasma field, thermodynamic and transport properties required for constitutive relations closure are customary calculated by analytical methods based on the first order perturbation of the Boltzmann equation, starting from interaction potential data, while thermodynamic properties are obtained from atomic and molecular data. However, the calculation required to compute quantities such as partition functions, collision integrals, inelastic collisions, are quite cumbersome, requiring significant efforts.

Plasma modelers are often limited by the availability (or the lack) of a property database for specific species mixtures. Moreover, addition of new species, or an interaction potential update, require ad hoc recalculation of the properties, an activity that is nowadays a prerogative of few relevant research groups. While, for LTE plasmas, several relevant mixtures property databases are available, thermal or chemical non-equilibrium greatly increases the computational challenge and limits database availability. Several approaches to handle thermal NLTE rely on a 2 temperature (2T) description of the plasma, one for electrons and one for the heavy species, each group with its own set of properties, function of the species and the non-equilibrium parameter; the chemical non-equilibrium contributes to increase the degrees of freedom of the databases.. In non-equilibrium cases, the modeler can opt for: a) on-the-fly calculations of the properties based on the local compositionand the non-equilibrium parameter, or b) large multidimensional databases function of species concentrations. For these reasons the development of software tools for the in-situ calculation of transport properties may be beneficial for the over-all plasma community, removing barriers that may prevent the uptake of modelling in more complex, non-equilibrium, scenarios.

2. Methods

PPFM is a library for building transport properties calculation workflows, i.e. gathering or compute chemical species partition functions and interaction collision integrals for equilibrium composition and transport properties calculation, addressing abovementioned needs based on the algorithms validated in [1,2]. It implements property calculations for both LTE and NLTE, with a modular design and advanced C++ programming techniques. Users can stream the workflow bottom-to-top from interaction potential to transport properties. PPFM provides two Chapman-Enskog based approaches: the classical Devoto [3] and the more advanced Zhang and Murphy [4] approaches. The modular structure of the library makes it very intuitive for both users and developers. Verbose class hierarchies with clearly separated interfaces ensures the extensibility and scalability of the program so that new methods can be easily added by deriving interface classes. Container classes and template meta-programming techniques allow automation of the data handling. In addition, they offer a clear platform for the user to operate on problem definitions.

3. Results and Discussion

PPFM validation process consisted in confronting our code computed values of composition (particle densities), thermodynamic (mass density, constant pressure specific heat, SoS) and transport coefficients (thermal conductivities, viscosity, electrical conductivity and diffusion coefficients) with values from published studies available in the literature. The pure gases confronted are Hydrogen, Nitrogen and Argon, considering the chemical species H,H^+,H_2 and e-; N,N^+,N^{+2},N^{+3},N_2 and e- and Ar, Ar^+,Ar^{+2} and e- respectively. Mixtures of ArH_2 and N_2H_2 with the chemical species listed above have also been validated with H_2 concentrations equal to 0.01%, 25%, 50%, 75% and 99.99% in volume for the first and fixed to 5% for the second. PPFM values perfectly matched those from the literature in both LTE and NLTE conditions with the non-equilibrium parameter $\theta=T_e/T_h$ being equal to 1,2 and 3 in any case except for the Argon gas for which θ=1,2,3,5,7 and 10 have been adopted. Development is still ongoing to extend species and models capabilities.

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References

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