KAPPA: an object-oriented C++ library for kinetic theory computations

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Abstract

Kappa is an object-oriented C++ library for calculation of physico-chemical relaxation rates and transport coefficients in various approximations of kinetic theory, including multi-temperature and state-to-state approximations suited for flows with strong non-equilibrium. The design of the library allows it to be easily included in existing CFD codes, and is aimed at ease of use and code readability. The object-oriented scheme used in the library, along with the implemented models of state-resolved physico-chemical relaxation rates are presented. Sample code for the calculation of a non-equilibrium flow shock wave and transport coefficients in the flow is given.

1. Introduction

Computational fluid dynamics solvers typically utilize simplified engineering models for transport coefficients and thermochemical relaxation rates, such as Wilke's rule for shear viscosity of mixture, Fick's law for diffusion velocities, Eucken's factor, the Landau–Teller expression for vibrational relaxation, and the Arrhenius law for chemical reactions. However, an increase in computational performance has recently led to the implementation of more accurate kinetic theory models in existing solvers,[21,23] including a realization of a state-specific approach in the ANSYS Fluent solver.[10] However, implementation of accurate kinetic theory models in solvers is hindered by the complexity of the algorithms involved (for example, the calculation of transport coefficients requires computation of specific heat capacities, collision integrals and solution of systems of linear algebraic equations) and the need for rigorous verification of the models being implemented, as well as handling of edge cases (vanishing components). This problem can be solved by using external libraries for computation of the transport coefficients and relaxation rates, and calling them from the solver.

Currently, several such libraries exist, such as SoVA,[9] EGLIB,[6] Cantera,[8] Mutation.[22] However, none of the mentioned software libraries provide methods for computation of state-specific process rates and transport coefficients, and thus, are not well-suited for strongly non-equilibrium flows; moreso, most of these products used simplified or outdated models interaction models. Thus, a software library which would implement well-tested interaction models and accurate kinetic theory algorithms, and allow not only for multi-temperature and one-temperature flow modeling, but also for state-specific flow computations, and which also could account for excited electronic states, would significantly ease the study of strongly non-equilibrium flows with the help of existing CFD solvers.

2. Library functionality

KAPPA (Kinetic Approach to modeling of re-entry Processes in Planetary Atmospheres) is a library written in C++ for computation of transport coefficients, thermodynamic properties, and physico-chemical process rates in arbitrary mixtures, which can include charged particles. The library can compute these quantities in state-to-state as well as multi-temperature and one-temperature approximations; it can account for chemical, vibrational non-equilibrium and electronic excitation. An overview of the library and its functionality is given below

KAPPA: A LIBRARY FOR KINETIC THEORY COMPUTATIONS

2.1 OOP Scheme

The library provides the following classes:

- Atom and Molecule classes which hold particle-specific data, such as particle masses, diameters, electronic, rotational and vibrational energy levels, etc.

- An Interaction class which contains parameters for an interaction of two particles (collision-reduced mass, collision diameter, Arrhenius law constants, etc.)

- Approximation, ApproximationMultiT, ApproximationOneT classes, which provide functions to compute various properties for a single species or a specific interaction (partition functions, relaxation times, rate coefficients, specific heats)

- Mixture, MixtureMultiT, MixtureOneT classes built on top of corresponding Approximation classes which provide functions to compute transport coefficients (thermal conductivity, shear and bulk viscosities, diffusion coefficients), relaxation rates, specific heats in arbitrary mixtures

2.2 Particle and interaction databases

The KAPPA project includes not only a library, but also two databases: a particles database, which includes data such as masses, diameters, oscillator reduced masses, electronic, rotational and vibrational states (energies and degeneracies), dissociation and ionization energies for C, N, O, N^+, O^+, N_2, O_2, N_2^+, O_2^+, C_2, NO, CO, e^-; and an interaction database, which contains parameters of various interaction models for elastic and inelastic collisions (such as Variable Soft Sphere parameters, Arrhenius law constants, etc.) Both databases are in human-readable YAML format (easy to view and edit).

2.3 Interaction models

The following elastic and inelastic collision models are currently available in the code:

- For computation of elastic collision integrals, the Rigid Sphere, Variable Soft Sphere, Lennard–Jones potential, Born–Mayer potential, ESA phenomenological potential[5] are implemented

- For computation of VT and VV-exchanges probabilities, cross-sections and rate coefficients, the SSH and FHO models are implemented, as well as approximations based on QCT data[1,4,7]

- For computation of exchange reaction rate coefficients, the Arrhenius law, as well as the Rusanov-Fridman,[20] Polak,[18] Warnatz[19] models, along with Aliat's[2] model for gases with electronic excitation are implemented

- For calculation of dissociation reaction probabilities, cross-sections and rate coefficients, the Rigid Sphere, Variable Soft Sphere, Arrhenius law, Treanor–Marrone model[13] (along with its modification based on QCT data[1,7] and its modification for gases with electronic excitation[2]), as well as approximations based on QCT data[1,4,7]

- For calculation of ionization reaction rate coefficients, the Arrhenius law is implemented

- For computation of relaxation times, Parker's model[17] for rotational relaxation, the Millikan–White model[14] for vibrational relaxation and Park's correction[16] are implemented

The following models are planned to be implemented in the code in the near future:

- A more realistic model valid for vibrational relaxation times, suitable for high-temperature flows, based on kinetic theory definitions[11]

- Various models for electronic excitation and vibrational-electron energy exchanges

- Modifications of the Treanor–Marrone model for dissociation based on newly available QCT data[3]

- Modifications of the Aliat model for exchange reactions, accounting for the vibrational excitation of the molecular reaction product, based on QCT data

All physico–chemical process rates can be computed either in the state-to-state approximation, or in multi- and one-temperature approximations (averaged over vibrational and electronic level distributions).

2.4 Approximations

Algorithms for transport coefficient and physico-chemical relaxation rate computation are implemented in the library for the state-to-state, multi-temperature and one-temperature approximations. The state-to-state and one-temperature approximations can also take into account electronic excitation.

3. State-to-state modeling of thermal conductivity

In state-to-state computations, molecules are assumed to be rigid rotators (rotational degrees of freedom are independent of vibrational). This allows for significant simplification of thermal conductivity computation in the state-to-state approximation,[12, 15] however, KAPPA allows to compute the thermal conductivity without such simplifications. In a binary flow, the simplified computational scheme requires solving a system of 5 linear equations, while using the full state-to-state approach requires solving a system of 146 linear equations for a N_2/N flow or 110 linear equations for O_2/O flow (if an anharmonic oscillator model is used for the vibrational spectrum). While solving systems of such size is unfeasible in real-life CFD computations (since that would require solving these linear systems in each grid cell at each calculation step), it is of interest to compare thermal conductivity computed via the simplified linear system with the thermal conductivity computed via the full state-to-state system. Such an analysis has not been performed before, and would help to assess whether the coupling of rotational and vibrational degrees of freedom has a significant influence on the thermal conductivity.
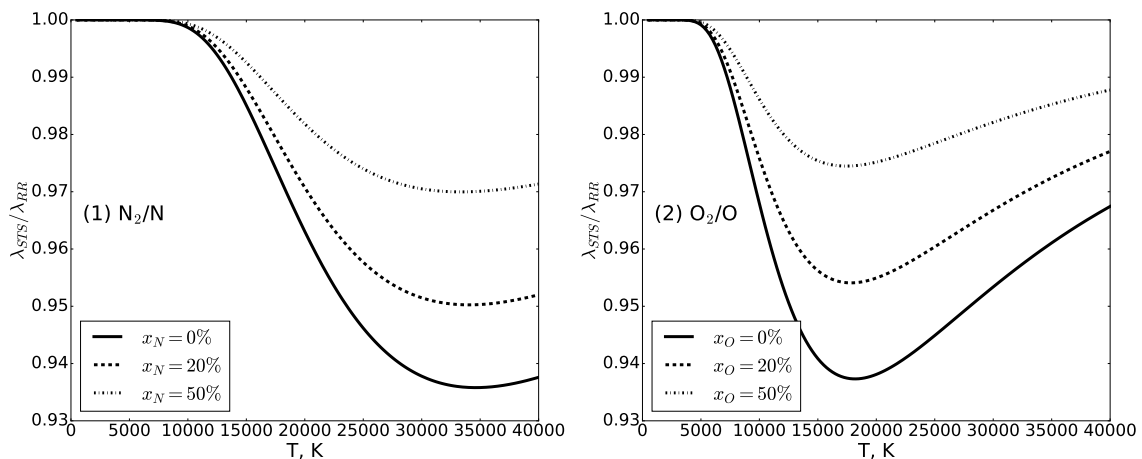

Figure 1: Ratio of thermal conductivity computed using the state-to-state model to the thermal conductivity computed using a rigid rotator approximation in binary mixtures of nitrogen (1) and oxygen (2) for different values of the molar concentration of atomic species as a function of temperature T (assuming a Boltzmann distribution over the vibrational states).

From Figures 3, 3 it can be seen that accounting for the dependence of rotational spectrum on the vibrational does not significantly affect the thermal conductivity, the difference being less than 7%. Thus, it can be concluded that even in conditions of extremely high temperatures, the simplified model for the thermal conductivity coefficient is valid. While the presented calculations have been performed for a Boltzmann distribution over the vibrational levels, in real-life flows the discrepancy between the full state-to-state model and the simplified model would be even lower: in flows behind strong shockwaves, where $T_v < T$, the higher vibrational states are even less densely populated than in the considered case, and thus, the effects of the dependence of the rotational degrees of freedom on the vibrational degrees of freedom (which are pronounced only for the upper vibrational levels) would have little influence on the thermal conductivity. For nozzle flows, while the upper vibrational levels are more densely populated, the temperatures are quite low, and thus, the effects of the rovibrational coupling will also be insignificant.

4. Conclusions

A library for kinetic theory computations in strongly non-equilibrium flows is presented, its capabilities, structure, and the implemented models are discussed. Results of the computation of thermal conductivity utilizing a complete state-to-state approach and a simplified rigid rotator model are given. It is shown that the dependence of rotational degrees
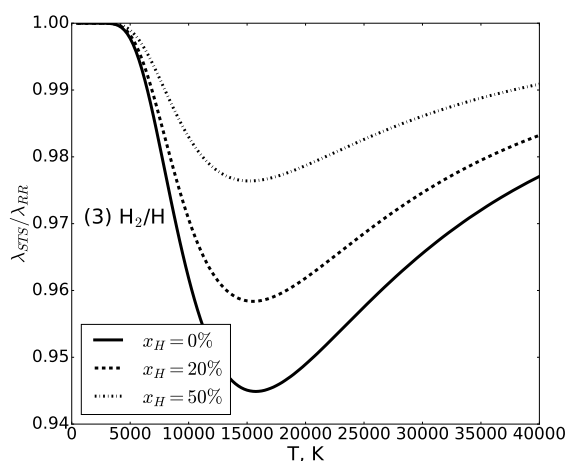
Figure 2: Ratio of thermal conductivity computed using the state-to-state model to the thermal conductivity computed using a rigid rotator approximation in a binary mixtures of hydrogen for different values of the molar concentration of atomic species as a function of temperature T (assuming a Boltzmann distribution over the vibrational states).

of freedom on the vibrational degrees of freedom has a negligible effect on the thermal conductivity.

5. Acknowledgments

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