A. Munafo'*, J. R. Haack†, I. M. Gamba^, T. E. Magin+

* Department of Aerospace Engineering
University of Illinois at Urbana-Champaign, Talbot Lab, 104 S. Wright St., Urbana, IL 61801, USA
munafo@illinois.edu

† Computational Physics Group (CCS-2) and Center for Non Linear Studies (T-CNLS)
Los Alamos National Laboratories, Los Alamos, NM 87544, USA
haack@lanl.gov

^ Department of Mathematics and The Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin, 201 E. 24th Street, Austin, TX 78712, USA
gamba@math.utexas.edu

+ Aeronautics and Aerospace department
von Karman Institute for fluid Dynamics, Chaussée de Waterloo 72, 1640 Rhode-Saint-Genèse, Belgium
magin@vki.ac.be

A CONSERVATIVE SPECTRAL-LAGRANGIAN BOLTZMANN SOLVER FOR MULTI-COMPONENT AND MULTI-ENERGY LEVEL GASES

Rarefied gas-dynamics has a broad domain of applications ranging from the study of the early phase of spacecraft entry into planetary atmospheres to the investigation of evaporation and condensation phenomena [1].

The degree of rarefaction in a flow depends on the local value of the Knudsen number Kn [1]. When the Knudsen number exceeds values of the order of 0.01, rarefied gas effects begin to become important and attempts to compute rarefied flows by means of a hydrodynamic description based on the Navier–Stokes equations can give inaccurate results. This is precisely due to the failure of Newton's and Fourier's law for the stress tensor and the heat flux vector, respectively, in the rarefied regime. When the gas is dilute, the Boltzmann equation provides an adequate kinetic description [1]. The Boltzmann equation is an integro-differential equation that describes the evolution in the phase-space of the velocity distribution function. Once the velocity distribution function is known, it is possible to compute macroscopic observables such as density, hydrodynamic velocity and heat flux by means of suitable moments.

The solution of the Boltzmann equation represents a computational challenge. This is due to the integro-differential nature of the equation. Another source of difficulty is the high-dimensionality of the problem, since numerical solutions must be sought in the phase-space.

In this work a spectral-Lagrangian method is presented for the full, non-linear Boltzmann equation for multi-component gases with discrete internal energy levels (treated as separate species) [2]. Both elastic and and inelastic collisions (leading to transitions among the internal states) are accounted for. The advantage of the spectral-Lagrangian method lies in the generality of the algorithm in use for the evaluation of the collision operator, as well as the conservation of mass, momentum and energy during collisions. The latter is realized through the solution of constrained optimization problems. The computational procedure is based on the Fourier transform of the partial elastic and inelastic collision operators and exploits the fact that these can be written as weighted convolutions in Fourier space with no restriction on the cross-section model. The proposed numerical method is applied to solve both space homogeneous and in-homogeneous problems. Computational results are compared with those obtained by means of the DSMC method in order to assess the accuracy of the proposed spectral-Lagrangian method.

REFERENCES

[1] C. Cercignani, Rarefied Gasdynamics, Cambridge University Press, 2000.
[2] A. Munafo', J. R. Haack, I. M. Gamba. T. E. Magin, . "A spectral-Lagrangian Boltzmann solver for a multi-energy level gas", *J. Comput. Phys.*, **264**, 152-176 (2014).