Multi-Scale Models of Nonequilibrium Gas Flows

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Abstract

Simulation of the environment around a spacecraft or hypersonic vehicle during flight in the upper atmosphere is a challenging problem due to abundance of physical and chemical effects in the shock-heated air. The flow is often found in a state of chemical and thermal nonequilibrium when a physical process does not reach an equilibrium state due to short characteristic time of a system. Current models of aerothermochemistry adopt a large number of empirical parameters and assumptions. This often leads to a poor agreement of computational data and experimental measurements. Moreover, the experimental data gathered from the ground test facilities often does not cover the input parameters of interest.

In order to increase the repeatability and robustness of the future hypersonic flight experience, a significant progress in the accuracy of gasdynamic models is required. Ideally, such models should be derived from the first principles, i.e. via a direct modeling of collisions between atoms and molecules, as shown in the figure above. Recently, this research direction came to life due to ever-increasing computational power and advances in theoretical chemistry. This seminar presents the recent progress in aerothermochemistry spans length scales from the ab initio principles in molecular dynamics to multi-dimensional high speed gas flows.

Daniil Andrienko, Ph.D.
Postdoctoral Research Fellow
Nonequilibrium Gas & Plasma Dynamics Laboratory
Department of Aerospace Engineering
University of Michigan

Dr. Daniil Andrienko received his Ph.D. from Wright State University (Dayton, OH) in Mechanical and Materials Engineering in 2014 and Cand.Sci (Ph.D. equivalent) from Moscow Institute of Physics and Technology in Applied Physics of Gas and Plasma in 2013. Currently he is a postdoctoral research fellow in the Nonequilibrium Gas & Plasma Dynamics Laboratory, Department of Aerospace Engineering, University of Michigan.