PRISM Seminar Series – Spring 2012

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AAE Special Seminar

"Modeling of High-Temperature Chemical Reactions in Air "

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Armstrong Hall of Engineering
ARMS 1021

Abstract: The direct simulation Monte Carlo (DSMC) method is traditionally used to study rarefied flows with a significant degree of thermal and chemical nonequilibrium. Presently, one of the most challenging problems in terms of the DSMC method development and improvement is related to the need to effectively and reliably simulate nonequilibrium chemical reactions especially in high-temperature conditions of atmospheric reentry with velocities above 10 km/s. Many DSMC models of chemical reactions were suggested in the literature. The models differ in the area of applicability, derivation, and accuracy. A model for DSMC computations taking into account high-temperature nonequilibrium chemical reactions in an air mixture was developed and implemented in the SMILE++ software system. The vibrationally specific cross sections of chemical reactions (required for DSMC modeling) are obtained as functions of the sum of translational and rotational energies on the basis of the known two-temperature reaction rate constant in the form of N.M. Kuznetsov. The reaction cross sections are found numerically as an approximate, but stable solution of the integral equation containing this reaction rate constant in its right part.

An important feature of the proposed model is the possibility of using it in hybrid continuum/DSMC codes. In this case, chemical reactions in the continuum module are modeled using the two-temperature rate constant, which is a procedure typical for continuum approaches, whereas the model suggested here is used in DSMC computations. Such a methodology allows taking into account the processes of high-temperature dissociation in hybrid codes.

***Bio**: Professor Mikhail Ivanov* is the Head of Computational Aerodynamics Laboratory at the Institute of Theoretical and Applied Mechanics (ITAM) of the Siberian Branch of Russian Academy of Sciences in Novosibirsk. He got a MS degree in Computational Mechanics from Moscow State University in 1968 and a PhD degree from Institute of Theoretical and Applied Mechanics in 1979 and a Doctor of Science degree in 1994. He has led development of widely used DSMC solver SMILE utilized by Russian Space Corporation Energiya, European Space Agency and other licensees. He has co-authored over 200 journal and conference papers in the areas of high-altitude aerothermo-dynamics, shock physics and other applications of rarefied gas dynamics. In 2007 Mikhail Ivanov has been a recipient of Krylov Prize, the award for seminal work in Computational Mechanics given by Russian Academy of Sciences. He is a Fellow of American Institute of Aeronautics and Astronautics.

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