



The DSMC Method

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Direct Simulation Monte Carlo is a well-established method for the computer simulation of a gas flow at the molecular level. While there is a limit to the size of the flow-field with respect to the molecular mean free path, personal computers now allow solutions well into the continuum flow regime. The method can be applied to basic problems in gas dynamics and practical applications range from microelectromechanics systems (MEMS) to astrophysical flows. DSMC calculations have assisted in the design of vacuum systems, including those for semiconductor manufacture, and of many space vehicles and missions. The method was introduced by the author fifty years ago and it has been the subject of two monographs that have been published by Oxford University Press. It is now twenty years since the second of these was written and, since that time, most DSMC procedures have been superseded or significantly modified. In addition, visual interactive DSMC application programs have been developed that have proved to be readily applicable by non-specialists to a wide variety of practical problems. The computational variables are set automatically within the code and the programs report whether or not the criteria for a good calculation have been met. This book is concerned with the theory behind the current DSMC molecular models and procedures, with their integration into general purpose programs, and with the validation and demonstration of these programs. The DSMC and associated programs, including all source codes, can be freely downloaded through links that are provided in the book. The main accompanying program is simply called the "DSMC program" and, in future versions of the book, it will be applicable to homogeneous (or zero-dimensional) flows through to three-dimensional flow. All DSMC simulations are time-accurate unsteady calculations, but the flow may become steady at large times. The current version of the DSMC code is applicable only to zero and one-dimensional flows and the older DS2V code is employed for the two-dimensional validation and demonstration cases. It is because of this temporary use of the older and well-proven program that the DS2V source code is made freely available for the first time. Most of the homogeneous flow cases are validation studies, but include internal mode relaxation studies and spontaneous and forced ignition leading to combustion in an oxygen-hydrogen mixture. The one-dimensional cases include the structure of a re-entry shock wave that takes into account electronic excitation as well as dissociation, recombination and exchange reactions. They also include a spherically imploding shock wave and a spherical blast wave. The two-dimensional and axially-symmetric demonstration cases range from a typical MEMS flow to aspects of the flow around rotating planets. Intermediate cases include the formation and structure of a combustion wave, a vacuum pump driven by thermal creep, a typical vacuum processing chamber, and the flow around a typical re-entry vehicle

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