Direct Simulation Monte Carlo Algorithms for Simulation of Non-equilibrium Gas Flows

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The emergence of Micro-Electro-Mechanical-Systems (MEMS) as a key enabling technology has led to the development of an increasing number of gas-phase microfluidic systems. Potential applications are numerous and include miniaturized heat exchangers, portable gas chromatography systems, miniaturized gas sensors and novel high-throughput gas flow cytometers. However, one of the most important issues influencing MEMS research is the growing realization that microflows are dominated by non-continuum or rarefaction effects. In this view, it becomes obvious that most of the classical fluid dynamics problems must be reconsidered when applied to flows through micro-channels or more complex micro-systems. Since the characteristic length of MEMS/NEMS is comparable with the mean free path of the gas molecules, the traditional computational fluid dynamics (CFD) methods, based on the Euler or Navier-Stokes equations, fail to predict the flows related with this devices. One of the most successful methods, developed for solving problems in rarefied gas dynamics and microfluidics, is the Direct Simulation Monte Carlo (DSMC) method, originally proposed by the Australian scientist G. Bird in 1963. Since then, DSMC has been applied to an impressive array of different problems ranging from hypersonic to subsonic flows.

The talk will report on some basic problems of the DSMC method concerning the accuracy estimation, the range of the numerical scheme parameters, within which correct results can be obtained, and some important parameter limits that restrict the method application. Several examples of application to rarefied dynamics and microfluidic problems taken from the author's practice will be given. The problems that will be considered belong to various application areas illustrating different flow regimes and requiring different degrees of rarefaction (Knudsen numbers), ranged from near-free molecular to near-continuum regimes. Some novel method modifications will be demonstrated.

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