Commun. Comput. Phys.
doi: 10.4208/cicp.080115.010515s

Vol. **18**, No. 4, pp. 1095-1121
October 2015

Modelling Rarefied Hypersonic Reactive Flows Using the Direct Simulation Monte Carlo Method

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Received 8 January 2015; Accepted (in revised version) 1 May 2015

Abstract. This paper presents the implementation, validation and application of TCE (total collision energy) model for simulating hypersonic reactive flows in a parallel direct simulation Monte Carlo code, named PDSC^{++}, using an unstructured grid. A series of benchmarking test cases, which include reproduction of theoretical rate constants in a single cell, 2D hypersonic flow past a cylinder and 2D-axisymmetric hypersonic flow past a sphere, were performed to validate the implementation. Finally, detailed aerothermodynamics of the flown reentry Apollo 6 Command Module at 105 km is simulated to demonstrate the powerful capability of the PDSC^{++} in treating realistic hypersonic reactive flow at high altitude.

AMS subject classifications: 76P05

Key words: DSMC, chemistry, non-equilibrium, TCE (total collision energy), hypersonic.

1 Introduction

Hypersonic aerothermodynamics (ATD) has become an increasingly important research topics because of increasing suborbital or orbital space activities worldwide (25 km and beyond). The detailed understanding of hypersonic ATD, such as catalytic reaction and oxidation of thermal protection layer, real-gas effects on shock-boundary layer interactions, blackout and real-gas effects, is especially important for those reentry space vehicles with high-enthalpy flow fields due to very high speed of the space vehicles. Even though there have been many ground wind tunnel experiments, e.g., HEG [1], F4 [2] and

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LENS [3] and relatively limited flight experiments, e.g., SHEFEX [4], it is well known that our understanding of hypersonic ATD, such as pitching moment anomaly and heat flux over dimensioning, is not enough for optimizing the design of reentry vehicles in an efficient way. Recently, some more thorough reentry flight experiments, e.g., EXPERT [5], are now under planning to obtain more detailed ATD data for reentry space vehicles using advanced in-situ measurement techniques. In addition to the aforementioned expensive ground tests and very expensive flight experiments, numerical modeling is considered to be the most attractive and affordable alternative in understanding these complex hypersonic ATD in detail, which would lead to a better design of the space vehicles. In this paper, we aim at implementing and validating chemical reaction module into a previously developed parallel direct simulation Monte Carlo (DSMC) code, named PDSC^{++} [6–8], that can used for general rarefied hypersonic flow simulation. At the end, we will demonstrate its capability in simulating a challenging 3D hypersonic Apollo Command Module reentry flow at an altitude of 105 km.

DSMC [9] is a particle-based simulation method, which employs fundamental collision kinetics and was shown to be equivalent to solving the Boltzmann equation when the number of simulation particles is large [10]. It has become a standard simulation method in either rarefied or thermal non-equilibrium gas dynamics. The computational cost of DSMC is generally high, especially when the flow is in the transitional and near-continuum regime. Fortunately, DSMC is a highly localized numerical scheme, which is especially suitable for parallel computing through domain decomposition, because binary collision occurs in a limited space (e.g., cell). In the community, there are several legacy DSMC codes which are parallelized using message passing interface (MPI). These may include DAC [11], MONACO [12], SMILE [13] and PDSC^{++}. For properly modeling hypersonic reactive flow under rarefied environment, efficient and accurate treatment of various kinds of chemical reactions in microscopic state is necessary and is described next.

For modeling chemical reactions in a rarefied hypersonic flow using DSMC, some special techniques are necessary. Among these, the total collision energy model (TCE) [9] is the most popular one, which converts the macroscopic Arrhenius rate equations to microscopic reaction cross sections at the microscopic level. It was used to calculate the reaction probabilities for dissociation and exchange reactions. In addition, a three-body collision model proposed by Boyd [14] was found to treat the recombination reaction reasonably well. The Larsen-Borgnakke model [15] was employed to handle the energy exchange between translational, rotational, and vibrational modes. In this paper, these models are used to model the chemical reaction within the framework of the PDSC^{++}, which is described in later section.

In the study, the implementation of chemical reaction module in PDSC^{++} is described in detail and validated by several benchmark problems. Finally, challenging hypersonic reactive flow past the Apollo Command Module was simulated to demonstrate the powerful capability of the PDSC^{++} in treating realistic hypersonic flows.