

A Probabilistic Automatic Steady State Detection Method for the Direct Simulation Monte Carlo

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Received 8 August 2015; Accepted 24 March 2016

Abstract. The statistical error associated with sampling in the DSMC method can be categorized as type I and II, which are caused by the incorrect rejection and acceptance of the null hypothesis, respectively. In this study, robust global and local automatic steady state detection methods were developed based on an ingenious method based purely on the statistics and kinetics of particles. The key concept is built upon probabilistic automatic reset sampling (PARS) to minimize the type II error caused by incorrect acceptance of the samples that do not belong to the steady state. The global steady state method is based on a relative standard variation of collisional invariants, while the local steady state method is based on local variations in the distribution function of particles at each cell. In order to verify the capability of the new methods, two benchmark cases — the one-dimensional shear-driven Couette flow and the two-dimensional high speed flow past a vertical wall — were extensively investigated. Owing to the combined effects of the automatic detection and local reset sampling, the local steady state detection method yielded a substantial gain of 30-36% in computational cost for the problem studied. Moreover, the local reset feature outperformed the automatic detection feature in overall computational savings.

AMS subject classifications: 82B80, 76P05

Key words: Direct simulation Monte Carlo, statistical error, type II error, steady state detection, reset sampling.

1 Introduction

The direct simulation Monte Carlo (DSMC) method is considered as one of the most successful computational methods to solve the Boltzmann equation based on direct statistical simulation of the molecular processes described by the gas kinetic theory [1,2]. It has

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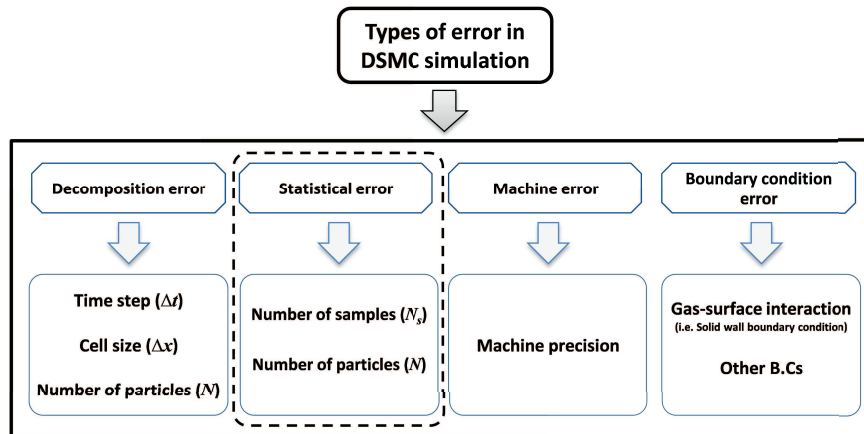


Figure 1: Computational errors, including the statistical error, in the DSMC simulation.

also been mathematically and empirically proved that the DSMC solution will converge to the true solution of the Boltzmann equation for a gas undergoing binary collisions between gas particles, if critical computational parameters — time-step, cell-size, and the number of particles — are chosen properly and when no wall surface boundary condition is involved in the simulation [3, 4]. Owing to robustness and ease of incorporating various collision mechanisms into the algorithm, DSMC has expanded its way into diverse applications, including hypersonic gas flows, micro-scale gases, chemical reactions, and material processing [5–8].

Four types of computational error are in general present in the DSMC simulation [4]: decomposition (or discretization), statistical [9,10], machine (or round-off), and boundary condition errors, as summarized in Fig. 1. In particular, the statistical error — the focus of the present work — is caused by the random fluctuation and statistical uncertainty inherent in the DSMC method. In a recent study of the verification method for DSMC [4], based on the exact physical laws of conservation, it was shown that the statistical error is dominant in the first phase of error convergence and the rate of its decrease is inversely proportional to the square root of the sample steps. In the second phase, the combination of boundary condition and decomposition errors becomes prominent in comparison with the statistical error. To reduce the statistical uncertainty and noise arising in evaluating the mean value of the random variables during the DSMC simulation, an appropriate probability sampling process is required [1, 4, 11].

The statistical error associated with the sampling procedure can be further categorized as type I and type II. In order to statistically analyze these errors, a null hypothesis [12] is defined as the DSMC samples belonging to the steady state. An *incorrect rejection* of the null hypothesis — not considering the samples that belong to the steady state — leads to *type I error*, which can be minimized by including more independent steady state samples. On the other hand, an *incorrect acceptance* of the null hypothesis — con-