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Convergence Detection in Direct Simulation Monte Carlo Calculations for Steady State Flows

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Abstract. A new criterion is presented to detect global convergence to steady state, and to identify local transient characteristics, during rarefied gas flow simulations performed using the direct simulation Monte Carlo (DSMC) method. Unlike deterministic computational fluid dynamics (CFD) schemes, DSMC is generally subject to large statistical scatter in instantaneous flow property evaluations, which prevents the use of residual tracking procedures as are often employed in CFD simulations. However, reliable prediction of the time to reach steady state is necessary for initialization of DSMC sampling operations. Techniques currently used in DSMC to identify steady state convergence are usually insensitive to weak transient behavior in small regions of relatively low density or recirculating flow. The proposed convergence criterion is developed with the goal of properly identifying such weak transient behavior, while adding negligible computational expense and allowing simple implementation in any existing DSMC code. Benefits of the proposed technique over existing convergence detection methods are demonstrated for representative nozzle/plume expansion flow, hypersonic blunt body flow and driven cavity flow problems.

AMS subject classifications: 65C05, 76M28

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1 Introduction

The direct simulation Monte Carlo (DSMC) method [1] has been developed over the past several decades as a general simulation scheme for dilute gas flows with signifi-

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cant translational nonequilibrium, and is commonly used to simulate a wide variety of rarefied flows. In contrast to typical computational fluid dynamics (CFD) schemes based on discrete approximations for a system of partial differential equations, DSMC employs Lagrangian particle tracking along with probabilistic collision procedures to replicate underlying physical processes in the governing Boltzmann equation. In DSMC simulations of steady state flows, output quantities of interest are typically sampled over a large number of time steps in order to reduce statistical scatter. For accurate results, sampling should be initiated only after steady state conditions have been realized across the entire simulated flowfield, following some transient startup period during which bulk flow quantities may evolve over time. The determination of convergence to steady state is usually at the discretion of the DSMC code user, and statistical scatter generally prevents residual tracking of the type often used to measure solution convergence in deterministic CFD simulations. This tends to result in a tradeoff between simulation efficiency and accuracy, as a more conservative estimate of the transient time interval reduces the probability of initiating sampling while the flow is still evolving, but may lead to unnecessarily high simulation expense.

Common techniques for estimating convergence to steady state in DSMC include tracking the time variation in the total number of simulated particles [2] or the total number of simulated collisions per time step. The transient period may also be estimated by calculating the approximate time for acoustic waves to pass through the simulation domain, then applying a safety factor which depends strongly on the type of flow being simulated [3]. An alternate technique, implemented in recent DSMC codes of Bird [4], involves comparison of normalized differences in the total number of particles over large time intervals to some fixed tolerance value. Yet another technique, for use when aerodynamic coefficients are the main output parameters of interest, compares net momentum and energy fluxes along external grid boundaries to the total force and total heat transfer acting on an immersed solid body [5]. While such techniques may often give a reasonably good estimate of the time required to reach steady state, resulting information must be judged with the above accuracy/efficiency tradeoff in mind, and determination of solution convergence can be regarded as one of the more difficult concepts for inexperienced DSMC users. Consideration of the total number of simulated particles or collisions may be particularly problematic when applied to flows involving large local variation in gas density, recirculating regions, or an isolated volume (such as a driven cavity or one dimensional channel flow) through which particles cannot enter or escape.

In this paper, a new global convergence parameter is proposed to quantify the maximum departure from steady state conditions over the full simulation domain. Compared to existing techniques for DSMC convergence detection, the new parameter should be more sensitive to temporal changes within small flowfield regions or within regions of relatively low density, and should function very similarly to CFD residuals in tracking solution convergence for a wide variety of flows. In the following sections, a new procedure for convergence detection is outlined, and underlying approximations and assumptions are described. The new procedure is then evaluated through comparison with existing