A Global Convergence Criterion for Steady State DSMC Simulations

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Abstract. A new global convergence criterion is presented to identify transient characteristics during the startup period of a steady state direct simulation Monte Carlo (DSMC) simulation. 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 have several limitations, and 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, and application to other types of flows is discussed.

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 involving translational nonequilibrium, and is commonly used to simulate a wide variety of rarefied flows. 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. Determining the number of time steps during the startup period 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. 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 convergence detection techniques for a rarefied nozzle/plume expansion flow, and application to other types of flow problems is discussed.

DETECTION OF CONVERGENCE TO STEADY STATE

As a starting point in procedures for global convergence detection, we intend to evaluate the maximum time variation in some local flow quantity throughout the simulation domain. A parameter based on this maximum variation should function similarly to the L-infinity norm commonly used in CFD calculations, but instead of approaching machine zero to indicate a converged solution, the parameter should approach a larger value associated with expected levels of statistical scatter. Global convergence is then assumed once the parameter reaches this predicted steady state value.

In the proposed convergence detection technique, two integer variables N_1 and N_2 are assigned to the data structure for each face (or, similarly, for each cell) along any external boundary of the computational grid. During particle movement operations performed for each simulation time step, the N_1 value at a given face will be incremented by one for every particle that exits the simulation domain (for inflow or outflow boundaries) or collides with a wall or symmetry boundary along this face. After a time period corresponding to a large number of simulation time steps, values of N_1 and N_2 are compared at each boundary face to calculate a global convergence parameter Q, after which N_2 is set to equal N_1 and N_1 is then reinitialized as zero. Thus, N_1 and N_2 represent the total number of particles with trajectories that intersect a boundary face over successive time periods. These periods should be long enough to capture any unsteady bulk motion in the flow; longer periods tend to better indicate transient behavior due to reduced statistical scatter associated with larger values of N_1 and N_2. Periods in the range of 1000 to 10,000 time steps should be appropriate for most DSMC applications.

In order to determine an appropriate convergence parameter Q, we assume that all trajectory-face intersections which contribute to N_1 are statistically independent and follow a Poisson distribution. The difference $N_1 - N_2$ therefore has a Skellam distribution [6] with a variance of approximately $N_1 + N_2$ and a mean value of zero at steady state. Thus, when steady state conditions have been attained along all boundary faces, the probability $P\left[|N_1 - N_2| / \sqrt{N_1 + N_2} < K\right]$ should be nearly equal at each face for any positive constant K. If M is the total number of boundary faces for which both N_1 and N_2 are nonzero, i is the boundary face index, and N_A and N_B are two integers independently sampled from the same Poisson distribution with mean and variance $\bar{N}$, it follows that the approximation

$$P\left[\max_{i\in[1,M]}\left\{\left(|N_1 - N_2| / \sqrt{N_1 + N_2}\right)_i\right\} < K\right] = \prod_{i=1}^{M} P\left[\left(|N_1 - N_2| / \sqrt{N_1 + N_2}\right)_i < K\right] \approx \left(P\left[|N_A - N_B| / \sqrt{2\bar{N}} < K\right]\right)^M \quad (1)$$

will be satisfied at steady state. Note in Eq. (1) that the variance of $N_1 - N_2$ is the sum of the expected mean values of N_1 and N_2 and is not exactly equal to $N_1 + N_2$. Next we define $K_{0.5}$ as a function of M such that

$$\left(P\left[|N_A - N_B| / \sqrt{2\bar{N}} < K_{0.5}(M)\right]\right)^M = 0.5 \quad (2)$$

By substituting $K_{0.5}$ for K in Eq. (1), we can show that $P[Q < 1] \approx 0.5$ if steady state conditions have been attained along all boundary faces, where

$$Q \equiv \max_{i \in [1,M]} \left\{ \left(\left| N_1 - N_2 \right| / \sqrt{N_1 + N_2} \right)_i \right\} \Big/ K_{0.5}(M) \tag{3}$$

Thus, at steady state, the quantity Q will have a median value of approximately one. Transient behavior along any boundary face will result in increased values of Q, and this parameter can therefore be used to evaluate the maximum departure from steady state conditions throughout the simulation domain. In general, steady state can be assumed once the condition $Q \leq 1$ (or, similarly, $Q \leq 1 + \varepsilon$ for some small tolerance $\varepsilon << 1$) has been satisfied.

As given in Eq. (3), evaluation of Q requires knowledge of the normalization value $K_{0.5}$ which satisfies Eq. (2). While it may be possible to find an exact expression for $K_{0.5}$ by inverting the Skellam cumulative distribution function, the approximate nature of the proposed convergence detection technique allows us to calculate $K_{0.5}$ with acceptable accuracy using a numerical correlation. One such correlation is found through the following procedure: Two integers N_A and N_B are independently sampled 10^7 times each from a Poisson distribution with a mean $\bar{N}$ of 100. Next, for each of 50 parameter values $(K_{0.5})_j$ = [0.1, 0.2, 0.3, ... 4.9, 5.0] a corresponding variable P_j is set to equal the fraction of (N_A, N_B) combinations for which $\left| N_A - N_B \right| < \sqrt{2\bar{N}} \left(K_{0.5} \right)_j$ is satisfied. We then compute $M_j = -\ln 2 / \ln P_j$ for all $j \in [1, 50]$.

For $M_j > 20$, the variation in $K_{0.5}$ with M is found to be closely approximated by a correlation of the form

$$K_{0.5}(M) = \sqrt{a + b \ln(M)} \tag{4}$$

where a and b are constants. From a least-squares curve fit, we find a = -1.23 and b = 1.85. In Fig. 1, the trend line given by Eq. (4) is plotted against a line between data points (M_j, $(K_{0.5})_j$) from the direct probabilistic solution to Eq. (2). In observing Fig. 1, we find a high level of agreement between the two curves over nearly five orders of magnitude variation in M. Discrepancies between the two curves for $M >> 1$ are primarily due to statistical scatter. However, relatively poor agreement is found for small values of M; the trend line underestimates $K_{0.5}$ by approximately 2%, 5% and 31% for M = 20, 10 and 3 respectively, and the above values for a and b give no real solution to Eq. (4) if M = 1. Such very small values of M correspond primarily to homogeneous flow problems, and are unlikely to be encountered in most DSMC applications.

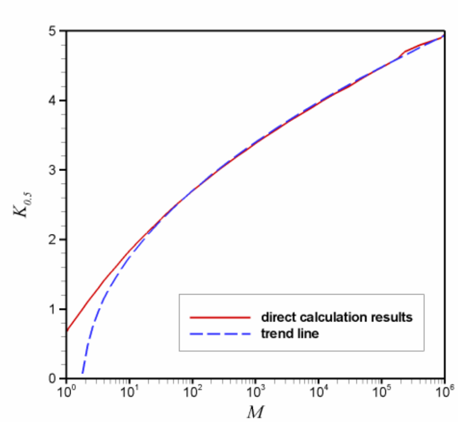

FIGURE 1. Variation in the normalization value $K_{0.5}$ with the number of boundary faces M.

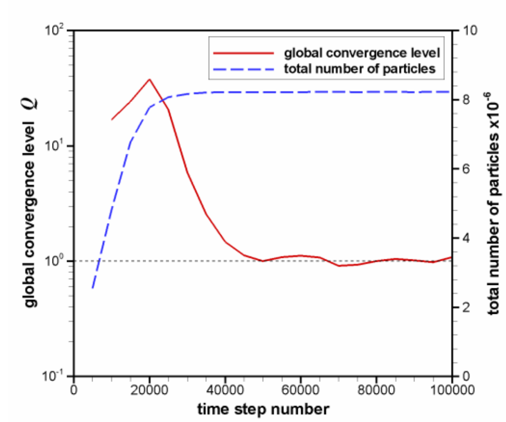

FIGURE 2. Time variation in the convergence parameter Q and the total number of particles.

Note that the effectiveness of the convergence parameter Q in assessing departure from steady state is subject to several assumptions: First, as described above, we assume that the sampling periods for N_1 and N_2 are not too short to capture unsteady characteristics at a given face due to either long transient time scales or excessive statistical scatter. Furthermore, we assume that unsteady characteristics at any point in the flow correspond to time variation in the unidirectional number flux along at least one boundary face. This implies that, as is generally the case, the region of slowest convergence is near some wall, symmetry, or inflow/outflow boundary. Finally, we assume that N_1 and N_2 follow a Poisson distribution, and that the mean value of $N_1 - N_2$ will asymptotically approach zero at all boundary faces during convergence to steady state.

The last assumption may be problematic in flows – such as those involving long oblique shocks or shock-boundary layer interactions – which potentially allow scatter-induced fluctuations in the location of shocks or other high gradient regions. Such fluctuations may increase steady state $|N_1 - N_2|$ values for a small number of boundary faces well beyond physically expected levels. To simulate these types of flows, the parameter Q can be modified, if necessary, to depend on only wall boundary faces or to exclude boundary faces near the shock.

Given the above assumptions and limitations, it should be emphasized that the parameter Q is not proposed as a universal solution to the convergence detection problem for all DSMC simulations, but instead as a reasonable balance between simplicity, efficiency, ease of implementation and fidelity for a range of simulation types.

EVALUATION FOR A RAREFIED EXPANSION FLOW

For initial evaluation of the proposed convergence criterion $Q \leq 1$, we consider the rarefied expansion of molecular nitrogen through a divergent nozzle into a vacuum. An axisymmetric simulation is performed using the DSMC code MONACO [7]. At simulation startup, the entire flowfield is initialized as a vacuum, and the variable hard sphere (VHS) model is used along with adaptive subcell procedures for collision partner selection [1]. Vibrational excitation is neglected, and a model of Boyd is used for rotational-translational energy exchange [8]. Inflow properties include a Mach number of 1.3 and a temperature of 500 K, and the nozzle surface is modeled as a diffusely reflecting isothermal wall at 500 K. The nozzle has a uniform divergence half angle of 20°, an exit to throat area ratio of 80 and an exit diameter of 0.0036 m. (The flowfield geometry is shown below in Fig. 4.) The inflow density is 0.014 kg/m^3, which corresponds to an inflow Knudsen number based on local nozzle diameter of 0.0014 and a centerline Knudsen number of approximately 0.005 at the nozzle exit. The computational grid consists of 55,409 quadrilateral cells and 917 external grid boundary faces, with cell sizes roughly adapted to the local mean free path. The global convergence parameter Q is evaluated once every 5000 time steps over the course of the simulation, with a negligible impact on both computational expense and memory requirements.

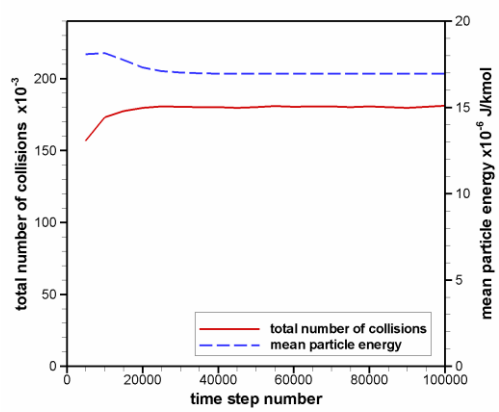

FIGURE 3. Time variation in the total number of collisions and the mean particle energy.

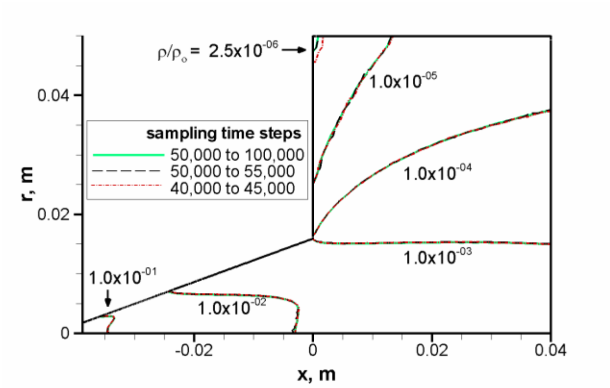

FIGURE 4. Normalized density contours based on three different sampling periods.

Figure 2 shows the variation in the global convergence parameter Q as a function of time step number. The total number of simulated particles is plotted for comparison. As shown in the figure, the number of particles rapidly increases during the first several thousand time steps after simulation startup, and reaches a plateau around 8.22×10^6 at steady state. At step 25,000, the number of particles is within 2.2% of the time-averaged steady state value, and total particle populations are within 1% and 0.1% of this value at steps 30,000 and 40,000 respectively. In contrast, the value of Q is shown in Fig. 2 to vary between 17 and 37 during the first 25,000 steps, with a value of approximately 1.50 at step number 40,000. The convergence criterion $Q \leq 1$ is not satisfied until step 50,000, after which the median value of Q is very close to one (indicated by the dotted line in Fig. 2) as expected at steady state. For additional comparison, the total number of collisions per time step and the mean energy per particle are plotted as functions of the time step number in Fig. 3. Both quantities are found to be less sensitive to transient behavior than the total number of particles; the number of collisions is within 1% of the corresponding steady state value at step 20,000, and the mean energy is within 1% of the steady state value at step 25,000.

A comparison of the four curves in Figs. 2 and 3 indicates that the convergence parameter Q exhibits far greater sensitivity to transient characteristics than other quantities commonly used to detect global convergence to steady state. As an additional advantage relative to the other quantities plotted in Figs. 2 and 3, the approximate median value of Q at steady state is known a priori. In contrast, steady state values of nearly any other relevant global value can usually be determined only from time-averaged simulation results. One further advantage of the parameter Q is that, by retaining the center coordinates of the face j for which

$$\left(\left|N_1 - N_2\right| / \sqrt{N_1 + N_2}\right)_j = \max_{i \in [1,M]} \left\{ \left(\left|N_1 - N_2\right| / \sqrt{N_1 + N_2}\right)_i \right\} \tag{5}$$

during each evaluation of Eq. (3), we can find the approximate location of maximum temporal variation during each summation period. Applying this procedure to the expansion flow problem, we identify the location of slowest convergence – where Eq. (5) is satisfied between steps 35,000 and 45,000 – as the area furthest from the symmetry axis along the nozzle exit plane. Standard DSMC convergence detection techniques are expected to be particularly insensitive to transient characteristics in this area due to the low density, while convergence should be especially slow here as a result of the large relative distance from the nozzle inflow boundary.

The lack of a converged solution over a sampling period between time steps 40,000 and 45,000 is observed in Fig. 4, where density iso-contour lines are shown for this sampling period along with lines based on additional periods from step 50,000 to 55,000 and from step 50,000 to 100,000. Note that all density values in Fig. 4 are normalized by the stagnation density of 0.029 kg/m^3. As shown in the figure, excellent agreement is found in the region of slowest convergence between results from the latter two sampling periods, whereas the earlier sampling period gives noticeably lower densities in this region. At the point (x = 0 m, r = 0.05 m) the sampling period between steps 40,000 and 45,000 is found to underestimate the density by 6.6% relative to the steady state value (as taken from the 50,000 to 100,000 step sampling period) while a much smaller underestimate of 0.5% is found for the sampling period between steps 50,000 and 55,000. It follows that global steady state conditions can be safely assumed after 50,000 steps, as predicted by the convergence criterion $Q \leq 1$, but significant transient characteristics are observed at step number 40,000.

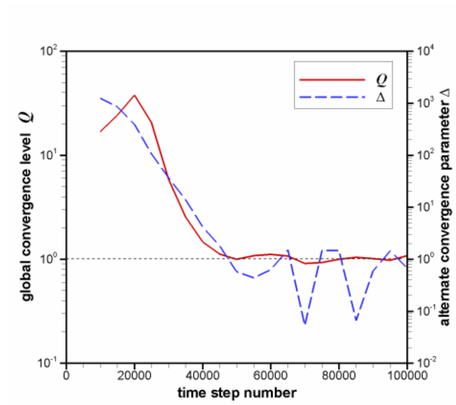

FIGURE 5. Variation Time variation in convergence parameters Q and Δ.

As an additional means of assessing convergence to steady state, we consider a modification to Eq. (3) based on the total number of particles in the grid. A new parameter Δ is defined such that

$$\Delta \equiv \frac{1}{K_{0.5}(1)} \left|\eta_1 - \eta_2\right| / \sqrt{\eta_1 + \eta_2} \tag{6}$$

where η_1 is the total number of particles during the current time step and η_2 is the corresponding value at some previous time step. Assuming the time interval between these two steps is large compared to the mean particle residence time within the simulation domain, η_1 and η_2 may be treated as statistically independent Poisson distributed quantities. The variance of $\eta_1 - \eta_2$ can therefore be approximated as $\eta_1 + \eta_2$. Similar reasoning to that used above for Q can be employed to argue that, at steady state, Δ should have a median value near one. As found in Fig. 1, the normalization coefficient $K_{0.5}(1)$ in Eq. (6) is approximately 0.676. Note that a very similar normalized difference $\left|\eta_1 - \eta_2\right| / \sqrt{\eta_1 + \eta_2}$ has been used for automatic initiation of steady state sampling procedures in a DSMC code developed by Bird [4].

In Fig. 5, the two convergence parameters Q and Δ are plotted as functions of the time step number. The dotted line denotes expected median values at steady state for both Q and Δ. While Q exhibits far less scatter at steady state than Δ, the latter parameter varies over a larger range during the startup period. As with the condition $Q \leq 1$, the condition $\Delta \leq 1$ is not satisfied until step number 50,000, which seems to indicate comparable sensitivity to local transient characteristics within a small, low density region. However, the median steady state value of Δ is known with considerably less certainty than that of Q, because any individual particles that contribute to both η_1 and η_2 tend to reduce the variance of $\eta_1 - \eta_2$. As a result, smaller time intervals used in the evaluation of Eq. (6) can lead to smaller values of Δ at steady state. Although the relative effectiveness of the two parameters Δ and Q may be problem dependent, both increased scatter and reduced expectation accuracy at steady state should, in general, make Δ a less reliable indicator of steady state conditions than Q.

CONCLUSIONS

A new technique for assessing global convergence to steady state in DSMC simulations has been presented. Relative to other DSMC convergence indicators, the proposed convergence parameter Q should generally provide increased sensitivity to weak transient characteristics in small or low density regions of the simulated flowfield. Other advantages of the new technique include simple implementation, negligible impact on simulation expense or memory requirements, a priori knowledge of the expected median parameter value at steady state, and the ability to determine the location of slowest convergence. These characteristics of the new technique have been demonstrated for an expansion flow through a divergent nozzle into a vacuum.

Extension to other types of flows should generally be straightforward, although modifications may be required for improved sensitivity. In particular, inflow/outflow boundary faces near farfield shocks may need to be excluded from the calculation of Q for hypersonic external flow simulations, due to stochastic fluctuations in farfield shock position which are larger than expected for steady state fluctuations in Poisson distributed quantities. In the current implementation, all faces along inflow/outflow boundaries are automatically excluded from the calculation of Q during simulations for this type of flow. While the potential need to exclude inflow/outflow boundary faces from convergence parameter evaluations for such flows may be seen as a weakness in the proposed technique, this highlights another valuable indication provided by the parameter Q: If Q fails to approach one after steady state conditions have presumably been reached, then unsteady effects (e.g. vortex shedding) or strong macroscopic fluctuations (e.g. a drifting bow shock) are likely present but not visible in time-averaged simulation results. The proposed technique may therefore be used to detect any smearing effects associated with the use of time averaging.

A different problem arises in subsonic flows or other flows involving characteristic transient times much longer than the residence time for acoustic waves. In this case, very long time sampling periods may be required for evaluation of N_1 and N_1 values used in Eq. (3), to avoid satisfying the convergence criterion $Q \approx 1$ long before steady state conditions have been reached throughout the simulated flowfield.

As discussed above, the parameter Q is not proposed as a universal indicator for global convergence in all DSMC simulations of steady state flows. Instead, Q is intended as an easily computed and more sensitive alternative to global quantities, such as the number of particles or the number of collisions per time step, which are often used for convergence detection in DSMC. Despite significant limitations, the proposed convergence detection technique should hold promise as a simple means of reliably predicting steady state convergence for a range of DSMC simulations. Improved reliability in convergence detection can in turn reduce user input requirements through increased automation of DSMC numerical procedures. In addition, a reliable indicator of the time to reach steady state may allow improvements in either efficiency or accuracy, as uncertainty in this time typically leads to either unnecessarily long startup periods or accuracy loss due to a lack of convergence at initiation of time-averaged sampling routines.

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