JOURNAL OF COMPUTATIONAL PHYSICS **126,** 434–448 (1996)
ARTICLE NO. 0148

Statistical Error Analysis for the Direct Simulation Monte Carlo Technique

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Received April 21, 1995; revised February 5, 1996

The statistical error associated with the direct simulation Monte Carlo technique is studied when it is applied to nonequilibrium hypersonic and nozzle flows. A root mean square (rms) error is employed as an indicator of the level of the statistical fluctuations. The effects of number of particles per cell and sample size are analyzed and quantified. It is found that in order to adequately model the physics of interest, the number of particles in the simulation must be greater than a certain minimum. An equation is developed to model and analyze the rms errors. A range is provided of the appropriate number of particles to be employed in the simulation in order to achieve the smallest statistical error at a fixed computational cost. Values are also recommended for the maximum number of sampling time steps to be used for efficient computation on memory limited computers. The effects of collision model and of cloning particles on the statistical scatter are analyzed.

1. INTRODUCTION

The direct simulation Monte Carlo method (DSMC) is widely used as an effective method to simulate rarefied and nonequilibrium gas flows. In Bird's DSMC method [1], large numbers of particles are generated in the flow field to represent real physical molecules or atoms. The time step is sufficiently small so that the movement of the particles and interaction between them can be decoupled. In each time step a particle moves and is considered for collision when internal energy exchange occurs. After the steady state is established, time averaging is carried out in each cell to evaluate the macroscopic mean values of the flow properties. The physical model behind this method requires the cell size to be of the magnitude of the local mean-free path, which is usually a much smaller requirement than in other numerical methods. A sufficient number of particles must be maintained in the computational cells to simulate the collisions adequately and to keep the statistical noise low such that the mean macroscopic values obtained are reliable. To trace and calculate hundreds of thousands of particles makes the simulation expensive in terms of both machine memory and CPU time. So it is worthwhile to investigate efficient ways to perform DSMC computations while improving the quality of the solution.

This study is one of the stages in the development of a hybrid method in transitional flows involving both a particle method and a continuum approach. It is well known that the Monte Carlo method is physically accurate but relatively expensive to use, while traditional CFD methods become invalid for rarefied and strongly nonequilibrium flows. The hybrid numerical method may employ either the CFD or DSMC technique in various regions of the flow field based on local flow conditions. In the first step of this development, a continuum breakdown parameter was derived for predicting failure of the CFD approach [2]. This parameter indicates where in a flow field the switch should be made from the CFD to the DSMC technique. Another key issue in the hybrid scheme is the passing of information between these two methods. The DSMC technique is a statistical method and, hence, always has fluctuations associated with its solutions. If the level of these fluctuations is too high, it may cause divergence or other computational difficulties when information is communicated to the CFD part. From a practical standpoint, the numbers of particles and sampling steps that may be used in the DSMC component of a hybrid method are limited. Therefore, the goal of this study is to investigate ways to analyze and eventually minimize the statistical errors of the Monte Carlo method.

2. STATISTICAL ANALYSIS

Previous studies on error analysis of the DSMC technique include those of Garcia [3–5], Boyd and Stark [6], and Fallavollita *et al.* [7]. Discussions on the subject are also provided by Bird [8]. In the papers by Garcia, the correlation of hydrodynamic fluctuations was studied by employing the DSMC method, and the use of particle simulation in the study of hydrodynamic fluctuations for nonequilibrium systems was reviewed. In the study by Boyd and Stark, statistical errors for an expanding flow were compared for two different DSMC collision algorithms. In Ref. [7], statistical errors were generated for a hypersonic flow. It was concluded that the use of more particles is an efficient way to reduce the statistical errors

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and also to make the simulation less expensive. However, no attempt was made in Ref. [7] to model the statistical errors. Also, little attention was paid to the memory usage in the simulation. In the present study, the dependence of statistical scatter on both execution time and memory usage is considered and quantified. Statistical error analysis is performed on the basis of a simple model. Simulations are performed for three kinds of flows under rarefied conditions: low Mach number supersonic flow, hypersonic flow, and expansion nozzle flow. In addition, the use of particle cloning is investigated.

2.1. *Error Definition*

In the particle simulation, a macroscopic fluid quantity is determined from an average of data in a single cell as the simulation is advanced in time. The level of statistical fluctuations depends mainly on the number of particles and number of time steps. A physical property is determined by averaging over sample size $T * N_c$, where T and N_c are time steps and particles per cell, respectively. For convenience, this product is defined as sample size S. For a certain cell structure, sample size is proportional to the computational cost in the sampling stage, while N_c reflects the memory required for the calculation. The difficulty of the error analysis for this particle method is due to several reasons. First, random processes are used extensively in this method. All physical macroscopic properties of interest are related to these processes either directly or indirectly. It is too complicated to analyze these errors mathematically through the relations between them. The current computational facilities also pose a restriction on the size of simulations. The primary issue in this particle method is the nature of the sampling data dependence. Most statistical theories assume the original data for sampling are totally independent or dependent in a way that may be described by a certain function. However, this is not the case in DSMC simulations. A particle is often sampled several times with the same property in one cell before it collides with others and changes its properties. This degree of dependency is determined mainly by the collision rate. However, collision rate may vary greatly in a flow field, so it is difficult to develop a rigorous theory to analyze the statistical error.

To analyze the error, the first step is to find an appropriate quantity representing the statistical fluctuation, which is also relatively easy to evaluate. A dimensionless measure of relative rms error is introduced by writing

$$\varepsilon_q = \sqrt{\frac{1}{N_{\text{cell}}} \sum_{i=1}^{N_{\text{cell}}} \left(\frac{q_i - q_{\text{ref},i}}{q_{\max}} \right)^2}, \tag{1}$$

where q_i and $q_{\text{ref},i}$ refer to the computed and reference solutions in cell i. In this study, the reference solution will be provided by the highest accuracy DSMC result performed for a particular flow condition. The variable q can be any physical property such as density, temperature, or pressure. The error is estimated in each cell and averaged to give a root mean square error over all the cells. N_{cell} is the total number of the cells. $q_{\max}$ is the maximum value of q in the whole flow field, which is a constant for one specific flow.

The rms error can also be normalized by the local reference solution in each cell, i.e.,

$$\varepsilon_q^{\alpha} = \sqrt{\frac{1}{N_{\text{cell}}} \sum_{i=1}^{N_{\text{cell}}} \left(\frac{q_i - q_{\text{ref},i}}{q_{\text{ref},i}} \right)^2}. \tag{2}$$

It is clear that, in Eq. (1), ε_q is determined mainly by contributions from those cells with large errors, since these are heavily weighted in the calculation; thus, ε_q indicates the level of maximum error in the entire flow field. In evaluation of ε_q^{α}, errors from all cells are more evenly weighted. An alternative is to consider the dimensionless absolute error:

$$E_q = \frac{1}{N_{\text{cell}}} \sum_{i=1}^{N_{\text{cell}}} \frac{|q_i - q_{\text{ref},i}|}{q_{\max}}. \tag{3}$$

2.2. *Model Equation*

In the results to be presented later, statistical errors obtained from DSMC simulations under different flow conditions will be generated. To help extrapolate this limited set of data points it is useful to construct a model that provides an approximation to the behavior of the statistical fluctuations. From the theory of stochastic processes, it may be shown that for each cell i,

$$q_{\alpha,i} = q_{r,i} + \frac{a_i}{S^{1/2}} \theta + \frac{b_i}{N}, \tag{4}$$

where $q_{r,i}$ and $q_{\alpha,i}$ are the exact value and mean value averaged over N particles for specific run α, respectively; θ is a standardized variable (i.e., $\langle \theta \rangle = 0$ and $\langle \theta^2 \rangle = 1$). a_i and b_i are constants. This equation has been used successfully by Pope [9] to analyze statistical errors in turbulent flows. The particle method used in Ref. [9] provides an approximate numerical solution to the modeled evolution equation. The movement of particles is governed by the stochastic model equations. The macroscopic properties are obtained by averaging over particles properties. In terms of statistical behavior, it has some similarities to the current DSMC method.

In Eq. (4), the second term on the right-hand side is related to the standard deviation whereby error is reduced as the inverse of the sample size. The third term on the

right-hand side of Eq. (4) is the *bias*. This represents an additional component of the statistical error introduced by the use of a finite number of particles in the numerical algorithm. In the case of the DSMC technique, the *bias* is generated by particle collisions. In Appendix A, a derivation based on the procedures described by Pope [9] is provided for the form of the *bias* employed in Eq. (4). Using Eq. (4), it may be shown that

$$\frac{(q_{\alpha,i} - q_{\mathrm{ref},i})^2}{q_{\max}^2} \approx \frac{((a_i/S^{1/2})\,\theta + b_i/N)^2}{q_{\max}^2} \tag{5}$$

$$\left\langle \frac{(q_{\alpha,i} - q_{\mathrm{ref},i})^2}{q_{\max}^2} \right\rangle \approx \frac{1}{S}\left\langle \frac{a_i^2\,\theta^2}{q_{\max}^2} \right\rangle + \frac{1}{N^2}\left\langle \frac{b_i^2}{q_{\max}^2} \right\rangle, \tag{6}$$

where the bracket stands for the mean value. Therefore Eq. (1) can be modeled approximately by

$$\varepsilon_q^2 = \frac{A}{S} + \frac{B}{N_c^2}, \tag{7}$$

where N_c is the average number of particles per cell and A, B are constants. From the mathematical derivation, it is obvious that two conditions must be satisfied to make this approximation valid. First, $|q_{\mathrm{ref},i} - q_{r,i}|$ should be much smaller than $|q_{\alpha,i} - q_{r,i}|$, meaning the reference solution is qualitatively much better than the others. Second, the number of particles in different cells should not vary much. It is also worth noting that the contribution of size of time step to the statistical error is neglected in the present study.

2.3. *Computational Efficiency*

In order to make recommendations for the numerical parameters to be used to minimize statistical fluctuations, some measure of the efficiency of the simulation must be provided. In the present study, this is provided by taking the derivative of Eq. (7),

$$2\varepsilon_q\,d\varepsilon_q = -\frac{A}{S^2}\,dS - \frac{2B}{N_c^3}\,dN_c. \tag{8}$$

One is mostly interested in the situation when S or N_c is constant. If $dN_c = 0$ then

$$2\varepsilon_q\,d\varepsilon_q = -\frac{A}{S^2}\,dS \tag{9}$$

$$f_N(S) = -\frac{d(\ln \varepsilon_q)}{d(\ln S)} = \frac{0.5}{1 + (B/AN_c^2)\,S} < 0.5, \tag{10}$$

where $f_N(S)$ is defined as computational efficiency for constant N_c. It is a function of sample size S. The larger the value of the computational efficiency, the more rapid will be the decrease in the rms error. It may be shown from Eq. (10) that sample size S must be at least four times the original value to reduce ε_q to $0.5\varepsilon_q$. Similarly, the efficiency for constant S is defined as

$$2\varepsilon_q\,d\varepsilon_q = -\frac{2B}{N_c^3}\,dN_c \tag{11}$$

$$f_S(N_c) = -\frac{d(\ln \varepsilon_q)}{d(\ln N_c)} = \frac{1}{1 + (A/BS)N_c^2} < 1; \tag{12}$$

$f_N(S)$ and $f_S(N_c)$ reveal the effectiveness of error reduction by two totally different approaches. One keeps constant the number of particles and samples over more time steps, while the other has a constant sample size and uses more particles, thus requiring fewer time steps. The statistical error is minimized by an increase of either execution time or memory usage. Equation (12) indicates that ε_q may be halved by using slightly more than double the number of particles if efficiency $f_S(N_c)$ is near 1. In terms of the upper bound of these two efficiencies, it is recommended to improve the accuracy of the solution by using more particles as long as f_S is greater than 0.5.

3. NUMERICAL SIMULATIONS

In the analyses that follow, a number of DSMC solutions are generated under the same flow conditions. The number of particles per cell and length of time-averaging are varied. The result of the highest quality, consisting of the largest number of particles and the longest time-averaging, is chosen as the reference DSMC solution. All other DSMC solutions are compared against it. It is indicated by Fallavollita *et al.* [7] that this approach is almost as effective in providing the error information as using the exact solution. The error ε_q was used in their evaluation to predict the statistical scatter for DSMC solutions.

3.1. *Hypersonic Flow*

Hypersonic flows over a sphere of radius 0.1 m are considered first for argon at Mach number 10. The flow employs a free stream temperature of 300 K and density of 2×10^{-5} kg/m^3 giving a Knudsen number of 0.02 based on sphere radius. The diffusive wall temperature is 300 K. The power of the temperature exponent for the viscosity coefficient of argon is modeled as $s = 0.72$ using the variable hard sphere (VHS) model [8]. The flow regime is specified to have 87 cells in the axial direction and 44 cells in the radial direction. The grid is structured and body-fitted with cells of variable size. The number of particles ranges from 5 to 80 per cell; thus the overall size of the simulation varies roughly from 19,000 to 300,000 particles. The time step employed is 6.0×10^{-8} s.

With regard to defining an rms error, it is expected that different macroscopic fluid quantities will exhibit different levels of statistical fluctuation, since they represent different moments of the velocity distribution function. Density is the zeroth moment of velocity, while temperature and pressure are second-order moments. In this investigation, rms errors are calculated based on the density and the translational temperature. The latter is calculated from the usual DSMC approach described in Ref. [1] in which:

$$\tfrac{3}{2}kT = \tfrac{1}{2}m(\langle u^2\rangle + \langle v^2\rangle + \langle w^2\rangle - \langle u\rangle^2 - \langle v\rangle^2 - \langle w\rangle^2), \quad (13)$$

where k is the Boltzmann constant, m is the molecular mass, and u, v, w are particle velocity components in three directions. The results presented here focus mainly on temperature, due to its higher sensitivity to statistical fluctuations. The peak temperature value of 9000 K inside the shock wave is used to normalize the errors. All the time steps are used in the sampling process once the steady state is established. The DSMC code is vectorized and computation is carried out on a Cray-C90.

Temperature contours of the Mach 10 shock wave flow are shown in Fig. 1. This simulation employs 80 particles per cell and 8192 time steps of sampling. It is taken as the reference solution for its highest degree of accuracy. The thick shock wave is due to the highly rarefied nature of the gas flow.

As described in the error definition equations, the contribution from each cell is accumulated and averaged to determine the values of ε_q, ε_q^α, and E_q to indicate the quality of the computation. However, there is a large variation in the density in different regions of the flow; thus the number of particles in each cell may also vary greatly. Different numbers of particles lead to different levels of statistical

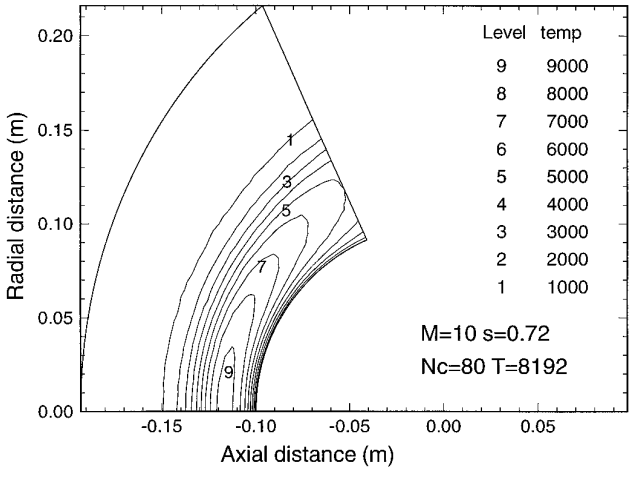

FIG. 1. Translational temperature contour for Mach 10 hypersonic flow over a sphere.

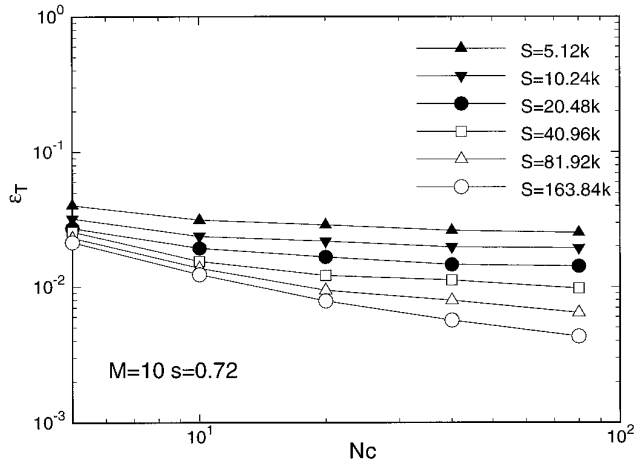

FIG. 2. Rms error ε_T based on translational temperature for Mach 10 hypersonic flow.

fluctuations. In order to make the rms and absolute errors reflect the statistical scatter in a more strict sense, the cell size is adapted to make each cell contain roughly the same number of particles. This is performed in the axial direction while the particle distribution in the radial direction is controlled by geometric weighting factors.

The rms error ε_T is provided in Fig. 2. The subscript T indicates that it is calculated based on the translational temperature. It is observed that for a fixed N_c, while the computation proceeds further in time, the rms error decreases monotonically, until an asymptotic value is reached. This means that with a limited number of particles to represent a large number of real physical molecules or atoms, even if the simulation is run forever, there still exists a deviation of the computed solution to the exact one. The deviation is what is usually called *bias* in stochastic processes. It is due mainly to an inadequate number of particles present in the simulation. The fewer the particles, the larger the deviation. In this case, the number of particles becomes a major factor affecting the accuracy of the solution, especially for small N_c. The existence of the *bias* is also attributed to simulation procedures that allow random walks in one or more of the variables. As sample size is proportional to the computational cost in the sampling stage, those data points joined by solid lines are obtained at the same cost. It is evident that more particles lead to higher accuracy. Hence, it is recommended to use the most particles permitted by machine memory for any simulation.

The errors E_T and ε_T^α are shown in Figs. 3 and 4 for the same simulations. These values are different but show the same trend and essentially predict the same behavior of the statistical scatter. This is consistent with the results of Fallavollita *et al.* [7]. As mentioned previously, rms errors were also evaluated based on the density solution. These generally gave similar trends to the results based on tem-

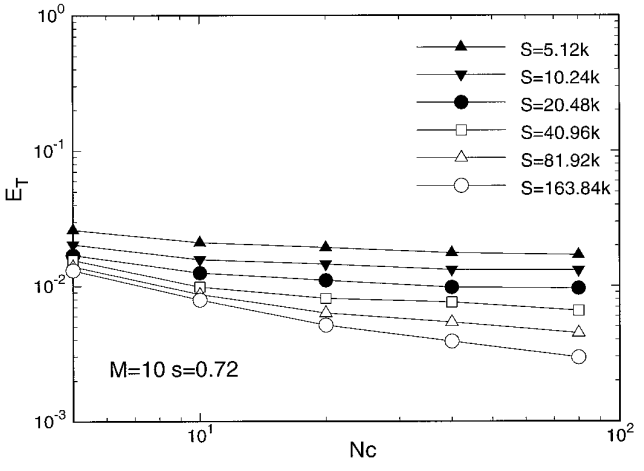

FIG. 3. Absolute error E_T based on translational temperature for Mach 10 hypersonic flow.

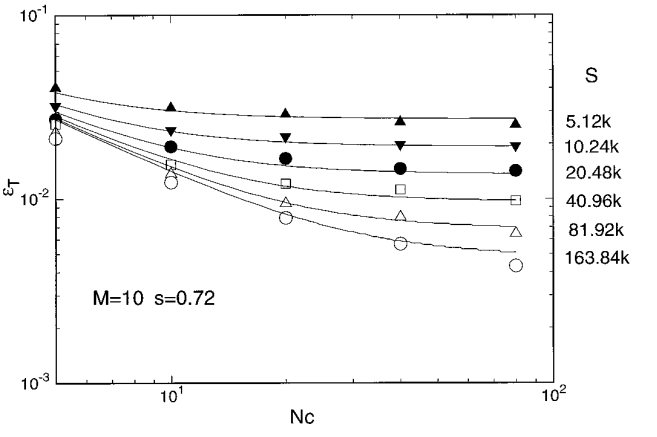

FIG. 5. Comparison of original rms error ε_T and fitted curves for Mach 10 hypersonic flow.

perature. As expected, however, the magnitude of the statistical error was smaller for density.

Any one of these three parameters can be adopted to estimate the statistical fluctuations, since the focus in this work is on how the rms level of the statistical fluctuation is affected by different values of N_c and S, rather than the exact values of those errors. The rms error ε_q is used in this analysis.

As discussed previously, the model equation is valid when the number of particles does not vary much from cell to cell and when the reference solution closely resembles the true solution. To meet the requirements, the reference solution is achieved through sampling of more time steps. In addition, the mesh is adapted after a test run to balance the number of particles in each cell. As a result, less CPU time is consumed in the computation through this improvement. It is clear from Eq. (7), when S tends to infinity, the limiting value of the rms error is $\sqrt{B}/N_c$. This indicates that the *bias* in Fig. 2 is inversely proportional to the number of particles used.

The least squares method is used to fit the rms errors by Eq. (7). The coefficients are $A = 3.789$ and $B = 0.0179$. Comparisons between the original data points and the fitting curves are shown in Fig. 5. They show very good agreement, which indicates the validity of the curve fitting approach. Here, the data for $N_c = 5$ are not used for the curve fitting. It is believed that this small number of particles introduces further statistical fluctuations into the DSMC algorithm that are not apparent at higher values. Their use in the curve fits would then cause inaccuracy in the values derived for A and B.

In order to study the errors associated with changes in physical models, the simulation is repeated for Maxwellian gas ($s = 1.0$) and hard sphere modules ($s = 0.5$). These two special cases represent limits for ''soft'' and ''hard'' molecules, respectively.

For the Maxwellian gas, the collision probability for a particular particle is independent of velocity. This gives rise to a thicker shock wave and further extension of the shock wave in the upstream direction. In order to keep the cell sizes less than a local mean free path, approximately 160×44 cells are required. After the grid is properly adapted, however, only 87×44 cells are needed. Up to 50% of the CPU time is saved through this improvement. The time step used here is 5.9×10^{-8} s. Compared with the $s = 0.72$ gas, Maxwellian molecules have a lower collision rate, so in each time step, fewer particles have collisions. This solution is therefore expected to exhibit more statistical fluctuations due to the higher degree of data dependency. On the other hand, hard-sphere molecules interact more strongly and thus the solution should have less statistical scatter. In this case, the shock thickness

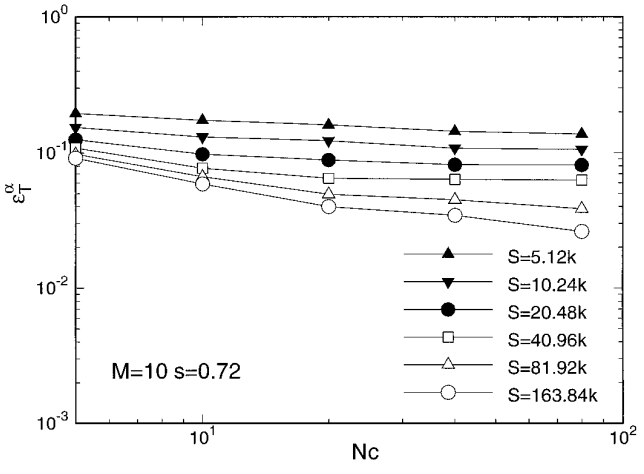

FIG. 4. Rms error ε_T^α based on translational temperature for Mach 10 hypersonic flow.

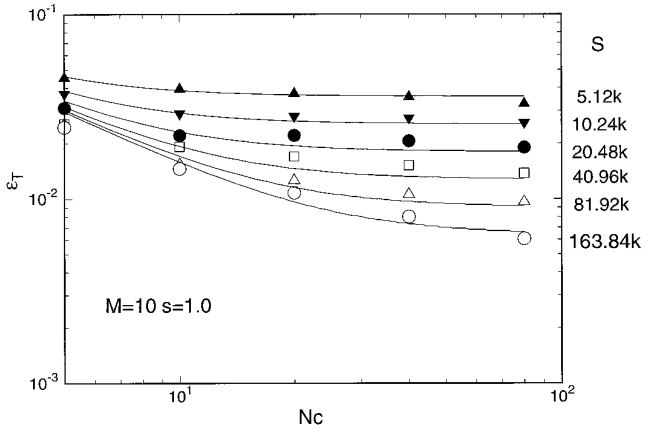

FIG. 6. Comparison of original rms error ε_T and fitted curves for Mach 10 hypersonic flow using Maxwell molecules.

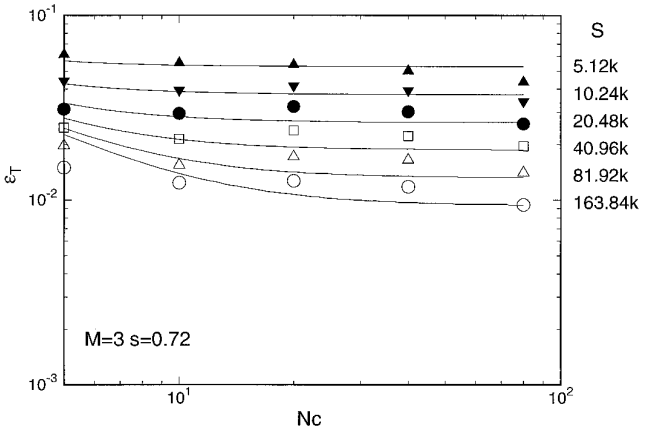

FIG. 8. Comparison of original rms error ε_T and fitted curves for Mach 3 hypersonic flow.

decreases because the collision probability has a strong dependence on the relative velocity. Actually, fewer computational cells are needed for this computation. For the purpose of comparison, the same number of cells 87×44 is still kept in the computation. The time step for hard-sphere molecules is 6.3×10^{-8} s. The rms errors for these two special cases are shown in Figs. 6 and 7. The relative trends of the results are exactly as expected. For corresponding simulations with the same S and N_c, the Maxwellian gas has the larger rms error, while the hard-sphere gas exhibits a smaller degree of statistical fluctuations. Since the time steps for hard-sphere and Maxwellian molecules differ only slightly, the effect of time step is considered negligible here. The modeling equation is successful in fitting the original data sets. The consistency between the theoretical prediction and numerical evaluation proves the validity of this approach to study the statistical error in particle methods.

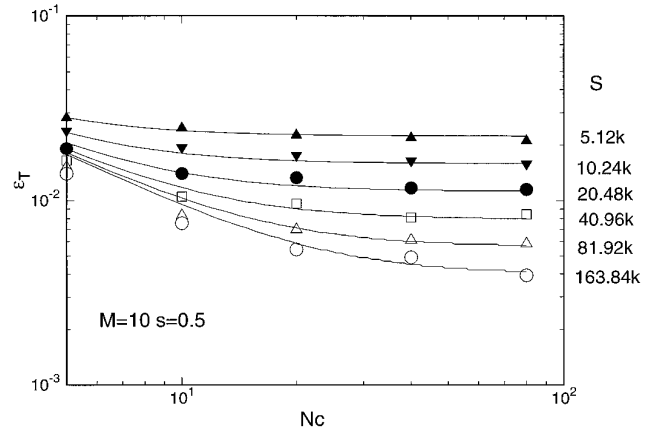

FIG. 7. Comparison of original rms error ε_T and fitted curves for Mach 10 hypersonic flow using hard-sphere molecules.

Hypersonic flows at Mach 10 involve strong nonequilibrium and large gradients of the macroscopic properties. For comparison, a gas flow with less nonequilibrium is also investigated. Specifically, a Mach 3 flow over the same sphere and at the same density as before is investigated. The rms errors for this flow are provided in Fig. 8. The time step used for this case is 1.8×10^{-7} s. For a constant N_c, the rate of reduction of errors is smaller as the sample size grows larger in comparison to the Mach 10 flow. On the other hand, the rms errors along the constant sample size line are quite different from the high Mach number case. They are almost independent of the number of particles N_c. The free stream velocity here is about one-third of the Mach 10 flow. The same amount of velocity perturbation will therefore make up a larger portion of the mean velocity. Thus the accuracy of translational temperature, a second-order moment of the velocity distribution, also has a higher degree of uncertainty. This may be one reason that the necessary information for the error analysis is difficult to obtain. The application of Eq. (7) is also less appropriate because of the inferior quality of the reference solution. In this flow, the quality of the solution is only improved very slowly as more time steps of sampling are used. It is prohibitive to run this simulation further with limited computation resources.

As shown in the previous figures, the rms error can be reduced by either using more particles or by running the simulation further, i.e., increasing the sample size. The problem raised is how much is gained from these two processes. If the simulation is run with twice the number of time steps or twice the number of particles, to what extent is the rms error decreased? DSMC simulations usually face two difficulties posed by computational resources: limited machine memory, and restriction of CPU time. When the simulation is performed on a local workstation or other machines with limited memory, the total number

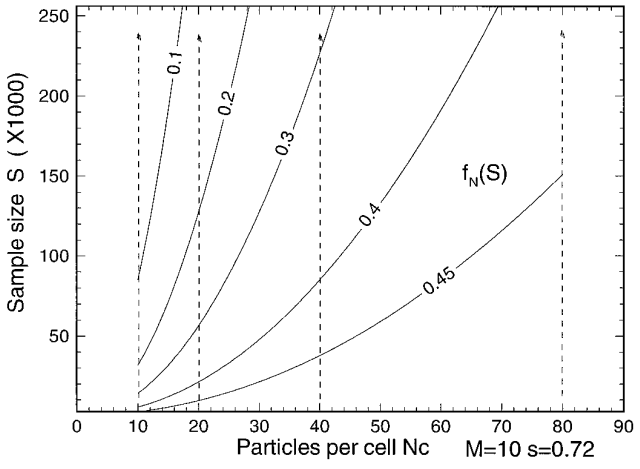

FIG. 9. Computational efficiency with constant number of particles per cell N_c for Mach 10 hypersonic flow.

of particles employed is restricted. However, by using the work station as a dedicated computer, a large number of averaging time steps may be executed. The strategy for computation on such machines is to first choose an appropriate number of particles governed by available memory and then to sample for a long time to reduce the error. It would be helpful to have in advance an indication of how much computational effort is needed to reach the desired level of accuracy. The computational efficiency changes while the simulation proceeds. When the computational efficiency becomes small, little is gained by consuming additional amounts of CPU time. At this point, the computation should be terminated. Figure 9 shows how the computational efficiency for constant N_c varies with the sample size, which is an indication of the total cost. A value of $f_N(S) = 0.2$ is used to define the boundary between efficient computation and inefficient computation. The value of 0.2 means each time that the effort is doubled, only a 13% reduction of statistical error is achieved, which can be derived from Eq. (10). In other words, to reduce the rms error by 50%, 32 times the effort is needed. It is advised not to run the simulation beyond the point where the efficiency is less than 0.2. Any real computation will proceed in the direction shown by the arrows in Fig. 9. For example, the second arrow from the left displays the process when $N_c = 20$. At the beginning of sampling, the efficiency is near 0.50. As time progresses, $f_N(S)$ declines very rapidly, until it reaches a value of 0.2 at $S \approx 120{,}000$. Therefore this computation should be stopped somewhere around 6000 time steps. Further calculation beyond this point will be inefficient. To quantify this argument, simply let $f_N(S_{\max}) = 0.2$. From Eq. (10), it is easily found that $S_{\max} = 1.5AN_c^2/B$, i.e., $T_{\max} = 1.5AN_c/B$. If $S_{\max}$ is substituted into Eq. (7), the rms error is $\varepsilon_q = \sqrt{5/3}\,(\sqrt{B}/N_c)$, which is 29% larger than the asymptotic value of $\sqrt{B}/N_c$ when S tends to infinity. For $N_c = 20$, the rms error obtained is about 0.009, which is close to the asymptotic value of 0.007.

The other situation encountered is when a large memory system is accessible but the CPU time is limited to a certain level, especially when external supercomputer facilities are used. In this case the simulation sample size is restricted. Again the question is how many particles should be used to run the simulation in an efficient way. The procedure is to find an appropriate number of particles first and then run the simulation with this value of N_c particles per cell and a sample size S. Intuitively, simulation with a small number of particles should be avoided, since it does not take advantage of the large memory system, and the final solution will be heavily biased. On the other hand, when more particles are used, a sufficiently high computational efficiency should be maintained to ensure the memory is used efficiently. The variation of $f_S(N_c)$ is provided in Fig. 10. Comparison of separate simulations with different values of N_c is highlighted along the direction of the arrows. When considering the use of more particles, the efficiency is calculated as an indication of the associated cost of memory. Consider $S = 81.92k$ as an example. The efficiency $f_S(N_c)$ is about 0.8 for $N_c = 10$. A simulation with an average of 10 particles per cell can have its rms error reduced through the increase of sample size by an efficiency $f_N(S) < 0.5$. Thus it is advised to use more particles because the current $f_S(N_c)$ is greater than 0.5. As a general recommendation, all simulations should use more particles if they have $f_S(N_c) > 0.5$. In this example, at least 20 particles per cell should be used. The maximum value of N_c suggested by the figure is 40, where $f_S(N_c)$ drops to 0.2. Use of more particles will only decrease the efficiency to an unacceptable level and should be avoided. Here $N_{c\max}$ and $N_{c\min}$ can be calculated from $f_S(N_{c\max}) = 0.2$ and $f_S(N_{c\min}) = 0.5$

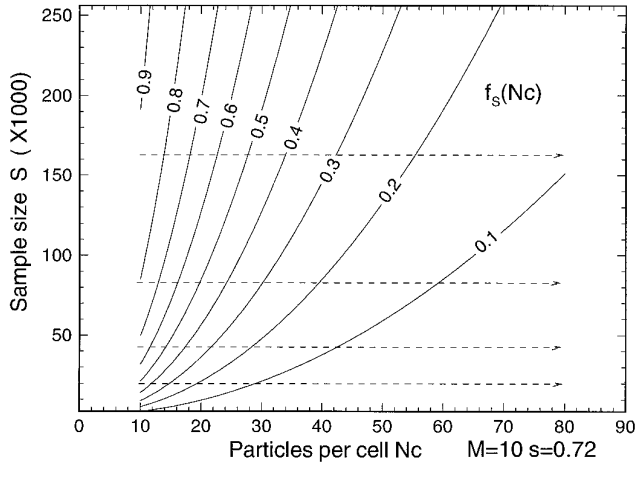

FIG. 10. Computational efficiency with constant sample size S for Mach 10 hypersonic flow.

in Eq. (12). Their values are found to be $N_{c\min} = \sqrt{BS/A}$ and $N_{c\max} = 2N_{c\min} = 2\sqrt{BS/A}$. In practical computation, it is advised to use a number of particles between $N_{c\min}$ and $N_{c\max}$. The lower and upper bounds of N_c correspond to rms errors of $\sqrt{2}\sqrt{A/S}$ and $\sqrt{5/4}\sqrt{A/S}$, respectively. The asymptotic value when N_c tends to infinity is $\sqrt{A/S}$. If memory permits, $N_{c\max}$ should be used, so that the highest accuracy is achieved, which is 12% away from the asymptotic value. The number of time steps T is estimated to be $0.5\sqrt{AS/B} < T < \sqrt{AS/B}$. For $S = 81.92k$, the smallest rms error is approximately 0.008, which is very close to the asymptotic value of 0.007.

The preceding studies considered the statistical error of the DSMC method when applied to strong compression flows. The quantity ε_T was adopted to indicate the level of statistical fluctuations. A sample equation was derived through stochastical theories and observed to be effective in numerical analysis.

3.2. *Nozzle Flow*

In order to assess the generality of the results presented in the previous section for hypersonic compressed flows, an expansion flow is now investigated. A resistojet is a low thrust rocket in which an inert propellant is heated and expanded through a nozzle to produce thrust. This is a basic form of electrothermal propulsion used on satellites. A resistojet consists of propellant storage and handling system, power supply, a heater and a nozzle. Continuous supply of heat and propellant are the source of the thrust. Here the numerical investigation is performed for H_2 in the nozzle and near field of the plume expansion.

The nozzle geometry is specified as a conical divergent section with a throat diameter of 0.654 mm, a length of 8.53 mm, and a divergent half angle of 20°. Hydrogen is supplied at a constant mass flow rate of 3.5×10^{-6} kg/s, giving a number density of 2.4×10^{24} m^{-3} and a temperature of 230.9 K at the throat. The stagnation temperature and pressure are 295 K and 134 torr, respectively. The VHS model is employed with viscosity temperature exponent of 0.67. Knudsen number scaled by the throat diameter is 1.6×10^{-3}. The computational regime is extended to 14 mm downstream of the nozzle exit to include a portion of the plume.

As mentioned previously, the size of computational cells is scaled by the mean free path in the DSMC technique. Since local mean free path is inversely proportional to flow density, high density flows demand more computational cells. This means that more particles are simulated and more collisions are computed. The simulation of the nozzle flow is quite expensive due to the relatively high density flow near the throat, which is in the continuum regime. As the gas expands through the nozzle, flow density drops drastically. The ratio of the densities in the throat and exit plane is of the order of 10^3. Therefore, the cells in the downstream region are about three orders of magnitude larger than those near the throat. Due to the supersonic nature of the flow, the gas accelerates all along the nozzle. However, this acceleration is small compared with the rate of increase of the cell size. As a result, a particle takes much more time to cross a cell in the downstream region than upstream near the throat. It appears as if the particles are frozen in the large cells. They require several hundred steps to cross a cell, while undergoing very few collisions. One difficulty caused by this situation is that it takes the computation a long time before the whole system reaches steady state. This aspect makes nozzle flows one of the most difficult categories of computations undertaken by the DSMC method.

In order to overcome this difficulty, a variable time step scheme is employed in the code. The computational domain employs a structured grid with 387 cells in the axial direction, including 370 cells inside the nozzle, and 51 cells in the radial direction. Every 10 cells along the axial direction, the time step is increased so that downstream particles are allowed to move further in one iteration. Specifically, from the nozzle throat to the nozzle exit plane, the time step varies from 6.8×10^{-11} s to 7.3×10^{-9} s. With this approach, a steady state is established with significantly less computational cost compared to use of a constant time step. In addition, these increases in time step scale approximately with the local increase in the mean time between collisions caused by the decrease in flow density.

A number of simulations are carried out for the same grid structure and for a range of N_c from 5 to 80. The total number of particles employed varies from 100,000 to 1.6 million. Only the statistical errors inside the nozzle are studied, thus N_c refers to the average number of particles per cell inside the nozzle. The simulation requires 20,000 time steps before the entire flow reaches the steady state. Again, all errors are calculated through comparison of translational temperature in each cell. The stagnation temperature of 295 K is used to nondimensionalize the errors.

Here cell size is scaled by the local mean-free path, instead of being adapted by the number of particles. In the simulation, many particles congregate near the nozzle throat. Near the symmetry line, the number of particles in each cell is kept reasonably large by use of weighting factors. By comparison, particles are distributed sparsely in those cells near the wall. Hence, there is a large variation in the number of particles per cell in the flow field. This computation is performed in a more natural and practical sense than the hypersonic compressed flows, without any intention to fit the requirement of error analysis.

Temperature contours inside the nozzle are shown in Fig. 11. This solution has the highest degree of accuracy employing an average of 80 particles per cell in the nozzle and 4096 steps of sampling. The total number of particles

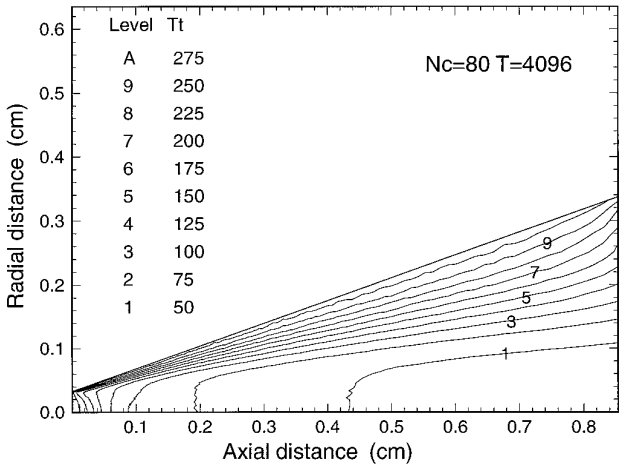

FIG. 11. Translational temperature contours inside a resistojet nozzle.

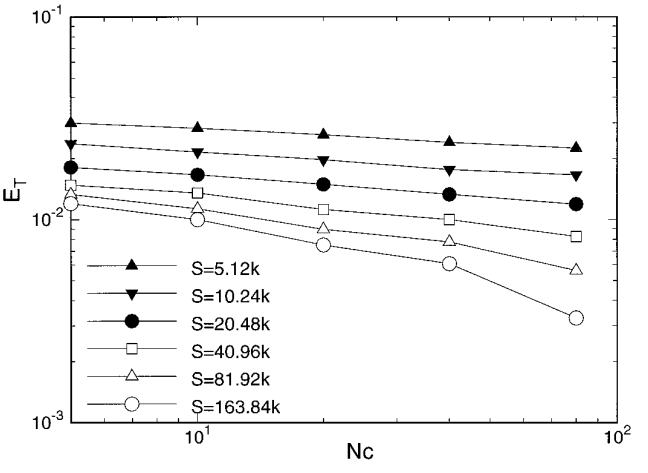

FIG. 13. Absolute error E_T based on translational temperature for nozzle flow.

present in the flow is about 1.6 million. The results of this computation are considered as an approximation to the exact solution against which all other DSMC solutions are compared.

The three errors ε_T, E_T, and ε_T^α are evaluated in the same manner as before and results are provided in Figs. 12–14. In Fig. 12, for a constant N_c, while the computation progresses, sample size increases linearly with the number of time steps. It is observed that ε_T approaches an asymptotic value which is determined by the number of particles itself. The computed rms errors are biased, especially when N_c is small. If attention is focused on those errors along a line of constant sample size, it is clear that use of more particles results in a smaller rms error at the same computational cost. Thus, use of more particles is favored in the simulation as long as machine memory permits. Review of Figs. 12–14 indicates that these three statistical errors are consistent in the sense that they have the same trend and provide the same information on the statistical behavior of the simulation. Based on this observation, ε_T is chosen for further study.

The rms errors in Fig. 12 may be fitted by the equation $\varepsilon_q^2 = A/S + B/N_c^2$, where $A = 6.9248$ and $B = 0.02384$. Comparison between the original data and fitted curves is presented in Fig. 15 which indicates general agreement. The consistency is not very satisfactory for those simulations which have $N_c = 80$ and relatively large sample size. This is explained as the result of the inadequate accuracy of the reference solution. Equation (7) is developed under the assumption that the reference solution is qualitatively much better than those solutions under study. However, it is not true for those solutions obtained with the same number of particles and slightly fewer time steps of sam-

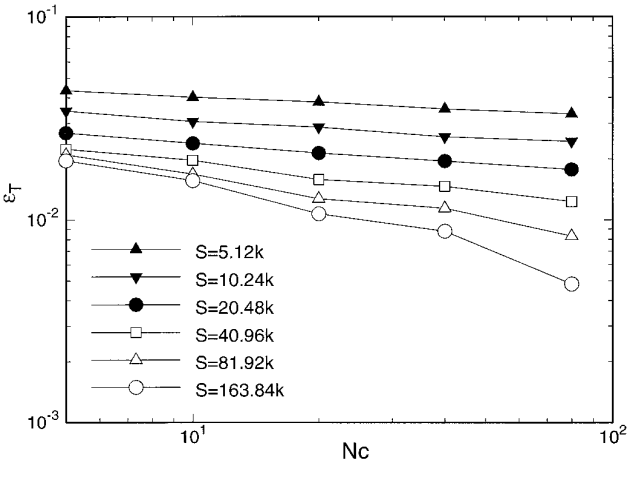

FIG. 12. Rms error ε_T based on translational temperature for nozzle flow.

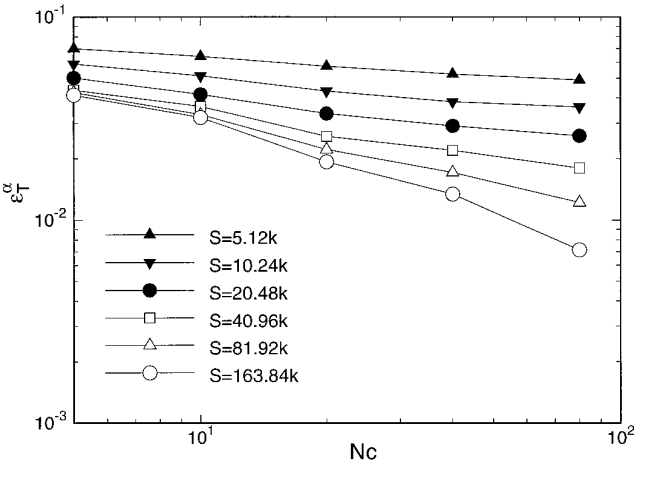

FIG. 14. Rms error ε_T^α based on translational temperature for nozzle flow.

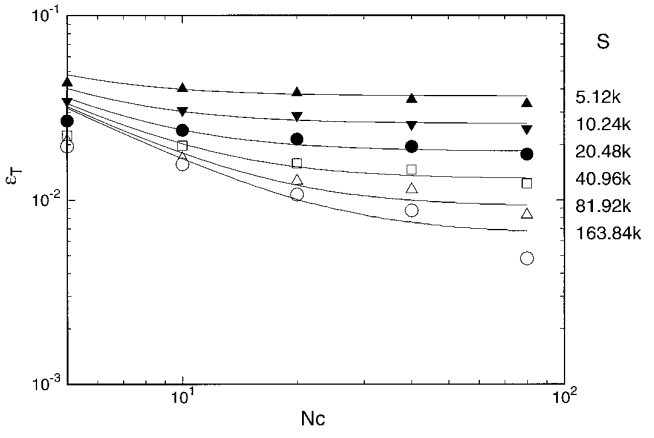

FIG. 15. Comparison of original rms error ε_T and fitted curves for nozzle flow.

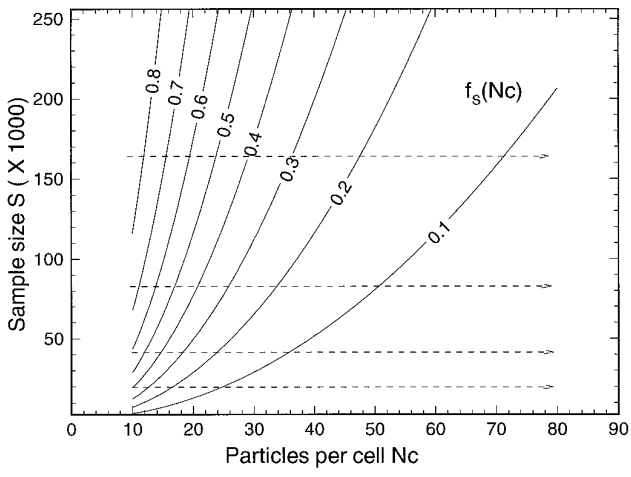

FIG. 17. Computational efficiency with constant sample size S for nozzle flow.

pling in this nozzle flow. Better agreement can be achieved by simply running the reference simulation further or by employing more particles. It is worth noting that the particle distribution also varies greatly under this flow condition. Hence, the two requirements for using the model equation are both violated to a small degree. Despite this, the fitting curves still provide a reasonably good approximation to the computed rms errors. Based on this curve-fitting function, analysis of the computational efficiency is carried out in the same way as before.

The computational efficiencies $f_N(S)$ and $f_S(N_c)$ are presented in Figs. 16–17. They exhibit similar behavior as the hypersonic simulations. For this specific flow, the suggested number of particles employed in the simulation is between $0.06\sqrt{S}$ and $0.12\sqrt{S}$ for restricted sample size S. The minimum error is then $2.942/\sqrt{S}$. If the number of particles is held constant, the recommended maximum sample size is 435.7 N_c^2, corresponding to a total of 435.7 N_c time steps and an rms error of $0.199/N_c$.

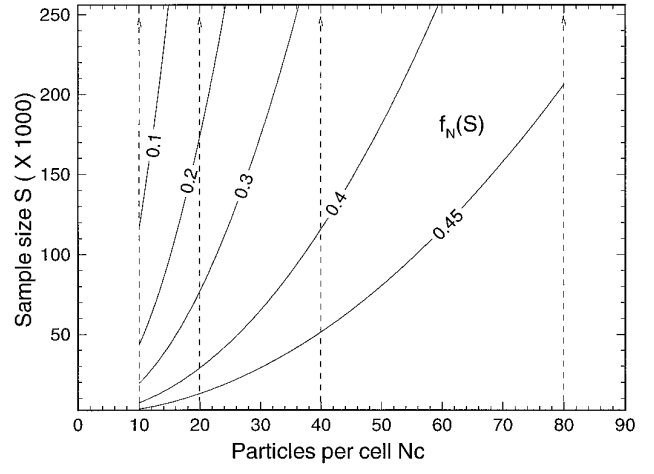

FIG. 16. Computational efficiency with constant number of particles per cell N_c for nozzle flow.

In order to evaluate the quality of the model equation (7), the relative deviation δ of error for each pair of sample size S and particle number N_c is calculated as $\delta = (\varepsilon_{T,f} - \varepsilon_T)/\varepsilon_T$, where $\varepsilon_{T,f}$ is the corresponding error computed from the curve-fitting function. The average values of $|\delta|$ for four different flows studied here are given in Table I. All of the average values of $|\delta|$ are less than 8%, which indicates that the model equation provides a good approximation to the original data.

The studies on the expansion nozzle flow reveal consistency with the previous results for hypersonic bow shock waves. Thus, the validity and generality of this error analysis approach are proved.

Three very different flow conditions are considered here: a strong expansion nozzle flow, one bow shock wave with strong nonequilibrium ($M = 10$), and one with weak nonequilibrium ($M = 3$). Recommendations are made for the appropriate sample size and number of particles to be used for efficient computation in each case. When an intermediate number of particles ($N_c = 20$) is used in the simulations, the statistical analysis for these three flow conditions recommends maximum sample sizes of $S_{\max} = 174k$, $127k$,

TABLE I

Statistical Analysis of Curve Fits

Flow	VHS parameter s	Average of $\|\delta\|$
Mach 10 bow shock	0.5	6.1%
Mach 10 bow shock	0.72	5.4%
Mach 10 bow shock	1.0	6.9%
Nozzle flow	0.67	7.3%

and 800k, respectively. The corresponding numbers of time steps are 8.7k, 6.4k, and 40k. This implies that for hypersonic flows and nozzle flows, the optimal number of time steps for sampling is of the order of several thousand iterations. It is also clear that the Mach 3 shock wave demands far more time steps than the other two. For an intermediate sample size (S = 163.84k), the estimated optimal values for N_c are 24 ~ 48, 28 ~ 56, and 10 ~ 20, respectively. This indicates that under most conditions the strong nonequilibrium flows require roughly 30 ~ 50 particles per cell to achieve best computational efficiency. This value is about 2 times larger than the usually accepted value of $N_c = 20$. The recommended value of N_c for the Mach 3 shock wave is less than 20 at this sample size. Thus it is less effective to reduce the error by using more particles in this flow when the total computational cost is limited. In addition, the values for this low Mach number case may be less accurate for the reasons mentioned before. However, they still provide qualitative information for efficient computation.

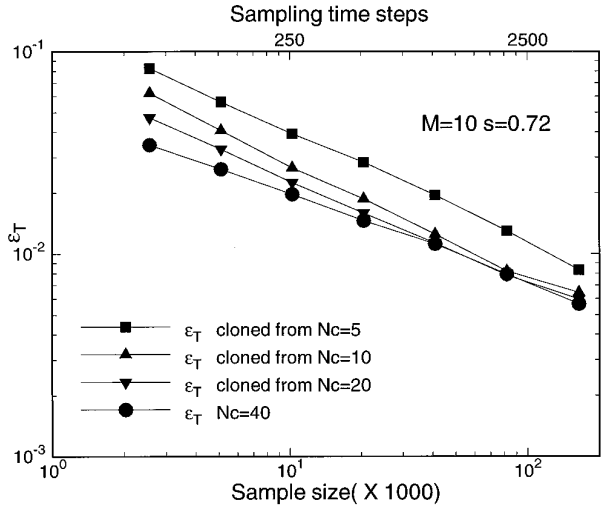

FIG. 18. Comparison of ε_T with respect to sample size S and sampling time steps T for cloned simulations of Mach 10 hypersonic flow.

3.3. *Particle Cloning*

The statistical errors were analyzed and ways to reduce the computational cost in the sampling stage were considered in the previous sections. From the practical viewpoint, the computational cost in the transient period is also of much importance, since many simulations require significant CPU time during this stage. An effective technique in DSMC to minimize the computational expense in this stage is to clone the particles. In other words, immediately after the steady state is established, particles are cloned so that more particles participate in the time averaging process. This technique is capable of saving CPU time in the transient stage by factors of 2 or more.

One problem associated with a cloned simulation is that it may involve a high degree of data dependency. This occurs because the cloned particles have the same properties as the original ones. The only way for the new particles to change their properties is through interaction with other particles. As a result, the level of statistical fluctuations in the cloned simulations remains constant (i.e., does not decrease) within the first several hundred time steps of sampling. As the simulation progresses, the distinction between cloned and uncloned computations will finally vanish after a large number of iterations. To be beneficial, the simulations with fewer particles in the transient period must reproduce the statistical fluctuations in the large scale simulation as early as possible after the sampling process is started. It is interesting to see when the distinction between these two simulations starts to vanish. Here rms errors are again employed as an indication of the level of statistical fluctuation of the solution. If the rms errors have the same values for two simulations, then the mean macroscopic properties obtained from them are treated as being equally accurate. The Mach 10 bow-shock flow is taken as the example, and the same reference solution is used as before.

Four separate simulations are started with average numbers of particles of 5, 10, 20, and 40. When the steady state is established, the particles in the first three simulations are cloned to the average level of $N_c = 40$. The error ε_T is calculated and the results are presented in Fig. 18. It is clear that those errors connected by the $N_c = 40$ line have the least rms error. Simulations involving fewer particles in the transient stage contain larger statistical fluctuations at the beginning of the sampling. The results show that the cloned simulations originally employing $N_c = 10$ and 20 particles do not differ significantly from the $N_c = 40$ case after about 1000 and 500 time steps, respectively. Hence, these two cloned simulations can replace the original large scale simulation without any loss of accuracy. By comparison, if particles are cloned three times, the statistical fluctuation is still much higher than the desired level after 4000 time steps of sampling. In this case, many more time steps of iteration are required to reach the required accuracy.

Results for the rms error based on flow density are shown as ε_D in Fig. 19. As expected, the magnitude of these fluctuations is smaller than those based on translational temperature. Statistical fluctuations of density for the four simulations studied previously are evaluated. Maximum density used to normalized the error is 1.2×10^{-3} kg/m^3. It is observed that within 2000 time steps of sampling, the rms errors for all cloned simulations decrease to the same level as the $N_c = 40$ case.

To assess the total computational cost, it is also worthwhile to relate the computed rms errors with the real CPU

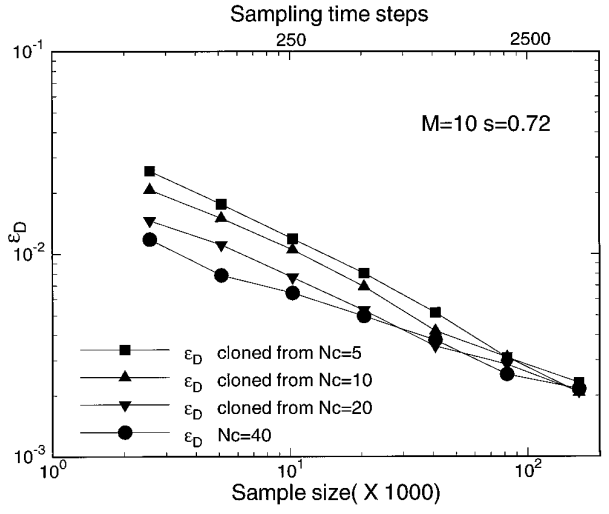

FIG. 19. Comparison of ε_D with respect to sample size S and sampling time steps T for cloned simulations of Mach 10 hypersonic flow.

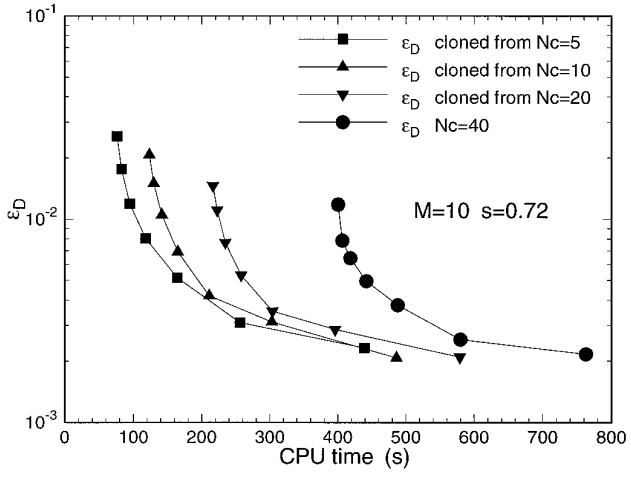

FIG. 21. Comparison of ε_D with respect to CPU time for cloned simulations of Mach 10 hypersonic flow.

time. Variation of ε_T and ε_D against the CPU time are presented in Figs. 20–21. The CPU time consumed in the transient stage for these four simulations are roughly of ratio 1 : 2 : 4 : 8. The same amount of CPU time is spent on the sampling period in each simulation. Using these results, the CPU time for each simulation to reach a fixed level of rms error may be compared. It is found that for $\varepsilon_T > 0.02$, the $N_c = 5$ case is the least expensive. It takes less than half of the time required by the $N_c = 40$ simulation. However, if a smaller ε_T is required, which is usually the case, then the $N_c = 10$ simulation has the best performance. However, for the density variation, Fig. 21 reveals that in the current region of study, the $N_c = 5$ case is most efficient, achieving the same rms error at the least cost. It may be concluded

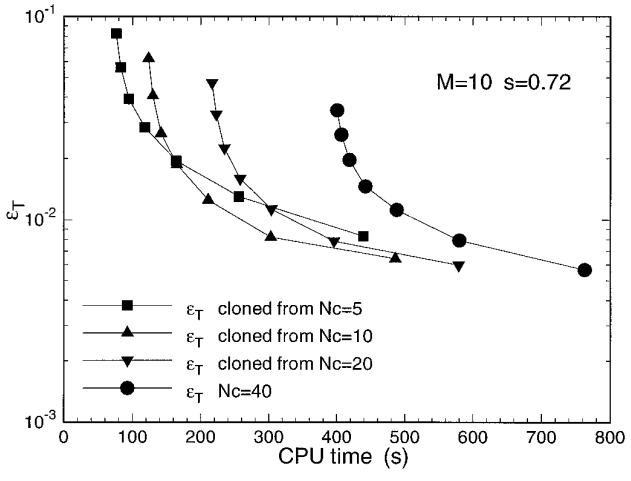

FIG. 20. Comparison of ε_T with respect to CPU time for cloned simulations of Mach 10 hypersonic flow.

that the statistical fluctuations in density and temperature are affected by cloning to a different extent. This effect is more pronounced for higher order moments of the velocity distribution function. Generally, if the particles are cloned no more than 2 times, the statistical fluctuation will decrease to the desired level within a reasonable number of time steps. If the particles are cloned more than 3 times, a large number of time steps of sampling may be required to reduce the original statistical uncertainty, especially for higher moments of the velocity distribution.

For the Mach 10 hypersonic flow, the ratio of sampling time to transient time is about 1 : 1. For those simulations demanding more time during the transient period, such as the expansion flow in the nozzle, the use of fewer particles in the transient stage plays a more important role in minimizing the computational expense. Figures 22–23 give the rms errors for the cloned simulations of expansion flow inside nozzle. The density of 8.0×10^{-3} kg/m^3 at the throat is used to nondimensionalize the rms error. It is observed that both temperature and density may be calculated from the cloned simulations after 4000 time steps. In this case, the behavior of the temperature errors is similar to those for density. Under this flow condition, the computational time in the transient stage is about 2.5 times larger than that in the sampling stage. Figures 24–25 indicate that the simulation that started with only five particles per cell is the most efficient one. To reach a value of $\varepsilon_T = 0.02$, the CPU time is only 40% of that needed by the $N_c = 40$ simulation. This large difference occurs because the transient stage consumes a significant portion of the total computational effort in this flow. Any saving achieved during the transient period will have a significant effect on the total computational cost. Thus, cloning is highly recommended for this kind of simulation.

In practical simulation, when both computational cost

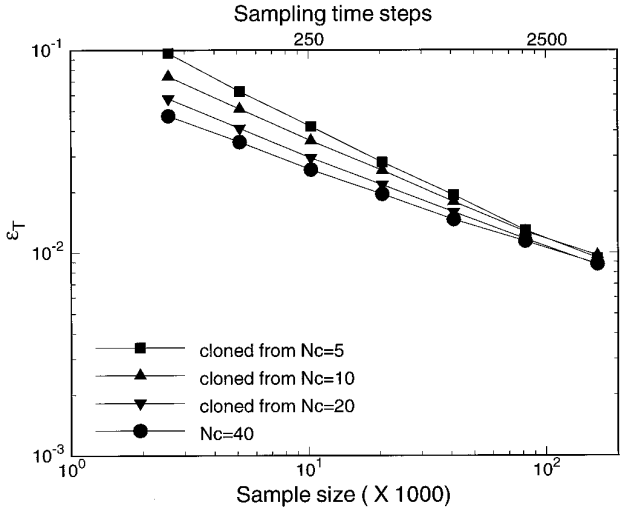

FIG. 22. Comparison of ε_T with respect to sample size S and sampling time steps T for nozzle flow.

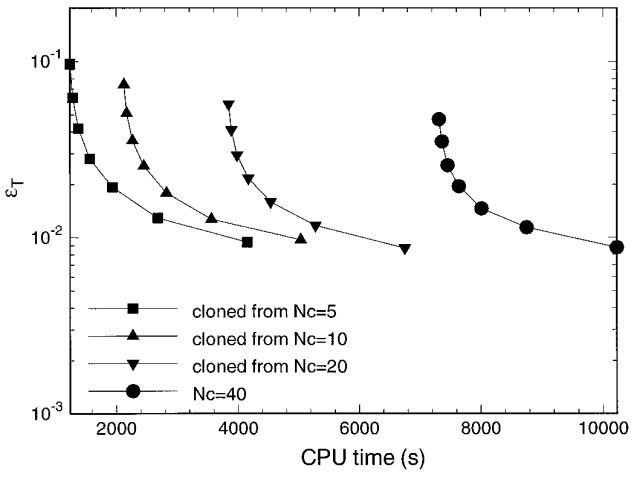

FIG. 24. Comparison of ε_T with respect to CPU time for nozzle flow.

and memory are restricted, the simulations for the strong nonequilibrium bow shock wave ($M = 10$) and expansion nozzle flows are recommended to be performed in the following way: first, use few particles in the transient stage; then, once steady state is reached, clone the particles once or twice to an average level of $N_c = 30 \sim 50$; finally, run the simulation for another $4k \sim 12k$ time steps for sampling. For those flows involving weak nonequilibrium ($M = 3$ shock wave), cloning particles is again recommended. However, there is no point in using more than 20 particles per cell after cloning. More than $10k$ time steps of sampling is required to reduce the statistical error to an acceptable level. Due to the wide variety of geometrics and flow conditions for which DSMC is applied, it is difficult to develop universal recommendations. The results presented here are intended to provide guidelines to achieve efficient DSMC computations for similar flow conditions.

3.4. *Effect of Time Step*

An additional parameter that affects the statistical fluctuations in DSMC computations is the time step, Δt. Generally there are two constraints on the size of Δt. First, it should be smaller than the mean time between collisions. This is required to permit decoupling of particle motion and particle collisions. Second, the time step should be small enough so that particles never cross a cell in one iteration of the algorithm. Typically, particles should spend three to five iterations in each cell. In low speed flows, the

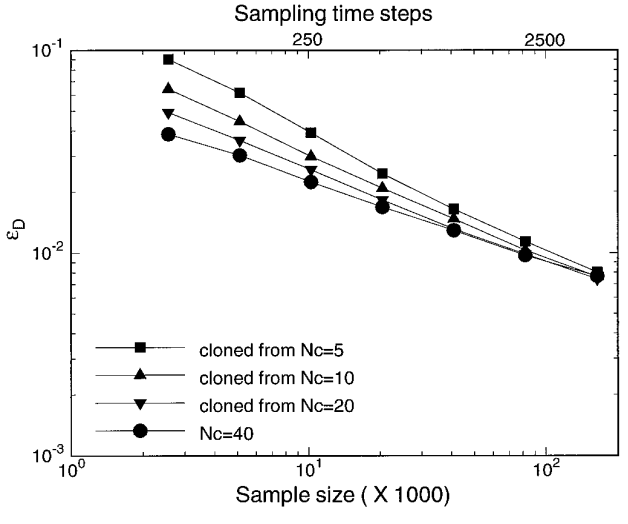

FIG. 23. Comparison of ε_D with respect to sample size S and sampling time steps T for nozzle flow.

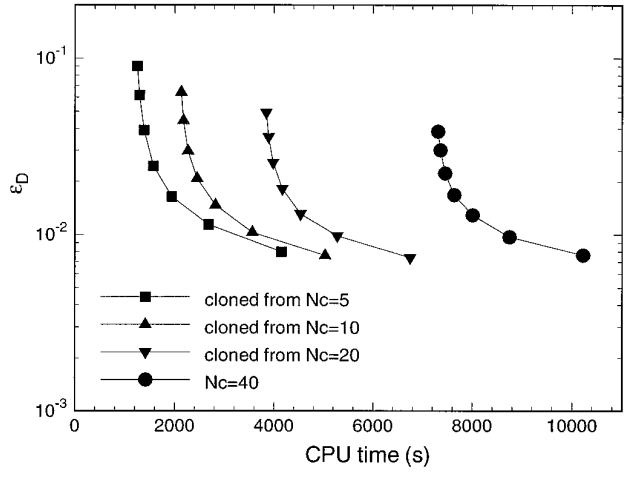

FIG. 25. Comparison of ε_D with respect to CPU time for nozzle flow.

first criterion is dominant, whereas in high speed flows it is the second criterion that limits the size of Δt.

Within these constraints, the size of the time step employed also affects the computational cost and the statistical fluctuations. A larger time step will require simulation of more collisions per iteration of the algorithm. If the total execution time is measured over a fixed sample size (rather than a fixed amount of physical time) then use of a larger Δt will require a longer execution time.

The degree of statistical independence of the DSMC results is affected by the size of the time step. As indicated above, the value of Δt is normally chosen so that particles take several iterations to traverse a cell. Thus, if particle properties are sampled every iteration, there is a strong degree of correlation in the data. At an early point in this study, a test was performed where sampling was performed every second iteration. It was found that the statistical errors associated with the macroscopic flow quantities of density and temperature were not significantly different compared to the results presented here. Obviously, there is a significant increase in numerical cost associated with this procedure and so this issue was not pursued further.

The effect of the value of the time step on the statistical fluctuations is an important aspect of DSMC computations and should be investigated in more detail. The primary goal of the present study is to provide model equations with which to analyze the fluctuations of DSMC computations of large scale flows.

4. CONCLUDING REMARKS

Statistical errors were studied in the DSMC method when it is applied to both bow-shock and expansion flows under rarefied conditions. It was found that an rms error based on translational temperature is a suitable quantity for indicating the level of statistical fluctuations in this particle method. Dependence of the statistical behavior on number of particles per cell and total sample size was investigated. It was observed that the computed solution may be biased when a limited number of particles is employed in the simulation. This deviation is inversely proportional to the number of particles per cell. A simple equation was introduced to analyze the behavior of the statistical errors associated with variation of the number of particles per cell and total sample size. The reliability of this approach is subject to the accuracy of the reference solution. Computational efficiencies f_N and f_S were defined to measure the quality of simulation with respect to both computational cost and rate of reduction of statistical scatter. The results demonstrated that a larger number of particles are necessary to perform the simulation in a more efficient way. Appropriate numbers of particles and sampling time steps for efficient computation were also proposed, under the conditions of limited machine memory or restricted computational time.

Statistical fluctuations arising in simulations where particle cloning is employed were also investigated. Based on these studies, it was recommended that few particles be used in the transient period of the simulation. These should be cloned when the steady state is established. Most macroscopic properties could be obtained through cloning without loss of accuracy after several thousand time steps of sampling. A large amount of CPU time was saved through this procedure. For those flows demanding longer time in the transient stage, the reduction in CPU time was more significant. It was found that different moments of the velocity distribution fuction exhibited different sensitivities to the statistical scatter in the original small scale simulation before cloning.

Finally, the statistical errors associated with different intermolecular models were analyzed. It was found that the errors were smallest for hard-sphere interaction. This occurred because this model produces the highest collision rate. This suggests that statistical scatter may be minimized by selecting numerical parameters that allow the largest number of collisions to be simulated while preserving the physical validity of the computation.

APPENDIX A

The following derivation is based on the work reported by Pope [9]. In the DSMC technique, the statistical fluctuations that are manifested as *bias* arise through intermolecular collisions. In a purely collisionless flow, particles are entirely statistically independent and hence the only statistical error is due to the sample size employed for ensemble averaging. In application of the DSMC technique to a collisional flow, any ensemble-average statistic $\langle Q \rangle_{N_c}$ has a *bias* B_Q caused by the use of a finite number of particles, N_c, in a cell to simulate the collisions. From kinetic theory, it may be shown that the number of collisions that must be simulated over time step Δt, for a cell with N_c particles, and a physical number density n is given by

$$N_{\text{coll}} = \tfrac{1}{2} N_c \Delta t \langle n \sigma g \rangle, \tag{14}$$

where σ is the collision cross section and g is the relative collision velocity. There are several popular schemes employed to simulate this number of collisions in the DSMC technique. All of these schemes are statistical rather than deterministic such that the variation of N_{coll} over each iteration of the DSMC algorithm is a random variable that depends on N_c. Hence, the number of collisions may be written

$$N_{\text{coll}} = N^o_{\text{coll}} + \varepsilon \psi N_c^{-1/2}, \tag{15}$$

where ψ is a standardized random variable (i.e., $\langle \psi \rangle = 0$, $\langle \psi^2 \rangle = 1$), ε is the standard error, and it is assumed to first

order that N^o_{coll} and ε are independent of N_c. It is further assumed that the dependence of the property $\langle Q\rangle_{N_c}$ on the number of collisions may be expressed by the conditional expectation:

$$q(\hat{N}_c) \equiv \langle \langle Q\rangle_{N_c} | N_{\text{coll}} = \hat{N}_{\text{coll}}\rangle. \tag{16}$$

This allows the expectation $\langle\langle Q\rangle_{N_c}\rangle$ to be written

$$\langle\langle Q\rangle_{N_c}\rangle = \langle q(N_{\text{coll}})\rangle = \langle q(N^o_{\text{coll}} + \varepsilon\psi N_c^{-1/2}\rangle. \tag{17}$$

Now, expanding about N^o_{coll},

$$\langle\langle Q\rangle_{N_c}\rangle = \langle q(N^o_{\text{coll}})\rangle + \langle q'(N^o_{\text{coll}})\varepsilon\psi N_c^{-1/2}\rangle + \tfrac{1}{2}\langle q''(N^o_{\text{coll}})\varepsilon^2\psi^2 N_c^{-1}\rangle + O(N^{-3/2}) \tag{18}$$

$$\langle\langle Q\rangle_{N_c}\rangle = \langle q(N^o_{\text{coll}})\rangle + \tfrac{1}{2}q''(N^o_{\text{coll}})\varepsilon^2 N_c^{-1} + O(N_c^{-3/2}). \tag{19}$$

Thus it is found that the *bias* scales as N_c^{-1} to leading order as assumed in Eq. (4).

ACKNOWLEDGMENTS

This study was motivated through discussions with Stephen B. Pope and his contributions are gratefully acknowledged. Financial support was provided by NASA Ames Research Center under University Consortium Agreement NCA2-820 to Cornell University. Computer time on the Cray-C90 was provided by the Minnesota Supercomputing Center.

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