JOURNAL OF COMPUTATIONAL PHYSICS 80, 374–386 (1989)

On the Use of the Modified Nanbu Direct Simulation Scheme

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Received November 2, 1987; revised March 14, 1988

The application of direct simulation Monte Carlo methods to complex rarefied gas problems is well established. Several such methods now exist and these may be put into one of two categories, i.e., those which model the Boltzmann equation and those which model the Kac master equation. Previously, the latter methods have been in the ascendancy mainly due to their numerical efficiency. However, recent advances in using the Boltzmann equation as the kinetic model mean that the application of this solution technique warrants investigation. Our calculations show that the new DSMC method derived from the Boltzmann equation can achieve a processing time comparable with the more popular Monte Carlo schemes based on the Kac formulation.

1. INTRODUCTION

The direct simulation Monte Carlo method (DSMC) pioneered by Bird [1] is now a popular and successful solution technique in the field of near continuum and rarefied gas dynamics problems. In this method the large number of molecules in a real gas is represented by a much smaller statistical population of simulated particles. The essence of the method is that the collisions of these particles may be treated separately from their transverse motion over a small timestep Δt. This basic assumption is implemented many times in each of the cells describing physical space and a steady state solution is found by allowing the flow to relax until local equilibrium is reached in all parts of the flowfield.

Many complex and necessary aspects of molecular gas phenomena have been incorporated into the method including the ability to simulate:

(a) gas mixtures,
(b) internal energy modes,
(c) gas/surface interactions,
(d) chemical reactions.

The DSMC method of Bird is not unique: several schemes now exist and all of these have been categorised by Nanbu [2, 3]. The methods are classified according to whether they employ (A) the Kac master equation [4] as the mathematical model or (B) the Boltzmann equation. The essential differences in the schemes lie in the manner in which molecular collisions are performed.

0021-9991/89 $3.00

Bird's scheme falls into category (A) [2] although no conscious effort was made to solve the Kac equation. Instead, the driving force behind this method was the requirement to employ the minimum amount of computational effort while still obtaining engineering solutions to complex flow phenomena. In this respect the method has been highly successful.

The method of Nanbu [5] was the first DSMC method to fall into category (B). He derived his scheme in a mathematical manner directly from the Boltzmann equation. Nanbu's scheme has failed to achieve popularity due to the fact that it is very computationally intensive and also that energy and momentum are not conserved at the collision level. Later, however, Babovsky [6] proved in a strict mathematical sense that Nanbu's method achieves convergence, which has not been proven for the method of Bird.

The main differences in the implementation of the two methods may be deduced from the following brief descriptions of the respective schemes.

In Bird's method each collision is assigned a lifetime and a number of collisions calculated until the sum of these lifetimes is greater than Δt. In this way the expense of the method is found to be proportional to the number of molecules in the cell. In this scheme the first colliding molecule is chosen at random, after which the partner is defined in a probabilistic way and both molecules experience a change in state due to the collision. These points together imply that it is possible for each molecule to collide several times over Δt in Bird's method.

The method of Nanbu is quite different. The probability of collision for each molecule is found in turn by calculating $\overline{\sigma_T g}$, where σ_T is the total collision cross section and g is the relative velocity of two colliding bodies. As calculation of $\overline{\sigma_T g}$ requires the sum of N terms, the total expense of the method is found to be proportional to the square of the number of particles. The collision partner of the molecule presently under consideration may be defined in the same way as that in the Bird scheme, although only the first molecule undergoes change in the Nanbu method. Thus energy and momentum are not conserved molecule by molecule. However, on the grand scale, these quantities are seen to be conserved. Finally, in the Nanbu scheme, any changes in state due to intermolecular collisions are not implemented until all such calculations have been completed.

In a recent paper [7] the authors have made a thorough comparison of the two methods in an engineering context. In addition to finding excessive computational effort for the Nanbu scheme it was discovered that the implementation of this method may offer difficulties with respect to the initial choice of Δt. The problem was traced to the fact that in the Nanbu scheme each molecule may collide only once over the decoupling timestep. The choice of an appropriate value for Δt was only arrived at by a lengthy and expensive analysis of the particular flow problem, which would have to be repeated if the flow conditions were altered. It was concluded therefore that although in principle the method of Nanbu may be used to simulate engineering flows, in practise the difficulties in implementation and the poor computational performance make its application impracticable.

Since the completion of this work on the Nanbu method, the work of Babosky

[6] and Ploss [8] has been brought to our attention. Babovsky proves convergence of the Nanbu scheme by splitting the decoupling timestep Δt into an integer number of equal intervals. This immediately gave us the hope that the difficulties encountered with the initial choice of Δt could be eliminated. In addition, a further modification to Nanbu's scheme implemented by Ploss claimed to reduce the computational expense of the method. It is clear that these improvements to the Nanbu scheme may overcome the difficulties previously experienced [7] thus making its applicability more desirable. This scheme which has been designated the modified Nanbu method has therefore been investigated and its implementation is now described.

2. The Modified Nanbu Scheme

In the original scheme of Nanbu the collision probability for molecule i is given by

$$P_i = \sum_{j=1}^{N} P_{ij} = \sum_{j=1}^{N} \frac{n}{N} \Delta t \, \sigma_T(g_{ij}) \, g_{ij}, \tag{1}$$

where

n is the number density in the cell,

N is the number of simulated molecules in the cell,

and the total collision cross section is a function of the relative velocity g_{ij} of molecules i and j.

Over the decoupling timestep Δt, each particle is considered in turn as a candidate for collision so that each molecule may only collide once at most over each timestep. This aspect of the Nanbu scheme gave rise to the adverse effects reported in [7] and made choice of Δt difficult.

The first modification made to the method was to split the timestep Δt into L equal intervals, $\Delta\tau$. The collision algorithm is then called L times before molecular motion is again computed. This concept was introduced to prove convergence of Nanbu's method but it has the additional result of allowing each molecule to collide up to L times over the decoupling timestep Δt. This clearly allows the initial choice of Δt to be made in a less stringent manner although the appropriate choice of L still has to be dealt with.

The second modification leads to the expense of the method becoming proportional to the number of simulated molecules rather than the square. An explanation of the modifications may be found in [8]. It is sufficient here to confine ourselves to a description of the implementation.

In Nanbu's scheme the quantity P_i, which is the sum of all the P_{ij} terms, must be less than one for each molecule i, see Fig. 1a. On the line [0, 1] the subsection defined by $[P_i, 1]$ is the probability that the ith molecule does not collide. The

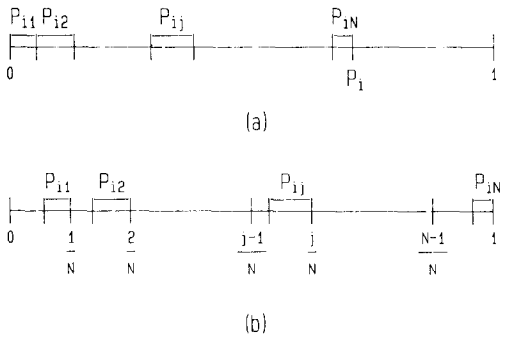

FIG. 1. Distributions of the probabilities P_{ij} over the unit interval for (a) the original Nanbu scheme and (b) the modified Nanbu scheme.

manner in which $[P_i, 1]$ is distributed is unimportant and so for convenience each of the P_{ij} are distributed at N identical intervals in $[0, 1]$ as shown in Fig. 1b. A random number $R \in [0, 1]$ is generated and used to define the possible collision partner in the following way: (i) if

$$R \in \left[\frac{j-1}{N}, \frac{j}{N}\right]$$

then j is the possible collision partner. P_{ij} is then computed using $\Delta\tau$ instead of Δt and, using the same random number, (ii) if

$$R > \frac{j}{N} - P_{ij}$$

a collision between molecules i and j is calculated.

The calculation of the collision then proceeds in the same manner as for the original method of Nanbu, i.e., only molecule i undergoes change, and the molecular properties are updated at the end of each call of the collision algorithm.

While in the original scheme Δt must be chosen with care so that P_i is always less than unity, in the modified method L must be chosen to satisfy

$$n \, \Delta t \, \sigma_T(g_{ij}) \, g_{ij} \leqslant L \tag{2}$$

for all i and j. This is clearly a more desirable criterion as the value of L will not affect the motion of the molecules while the choice of Δt has a direct effect.

Only one P_{ij} calculation is made for each molecule, so that it may be seen that the expense of the modified Nanbu method is proportional to N, thus making it considerably more efficient than the original scheme. However, the increased parallel nature of the modified algorithm results in a further powerful reduction in computational expense through the application of vector computers. A full description of the vectorization procedure for part of the algorithm is included in [8].

This new DSMC scheme has been implemented and tested on a CRAY 1-S and utilises the vectorization facilities available. When analysing a new computational method the choice of the test case is important. The two flow problems investigated here allow many aspects of the Monte Carlo method to be inspected with respect to the modified algorithm. Specifically, the one-dimensional Rayleigh problem and the sonic expansion of nitrogen through a small nozzle have been tested. With the experience gained from these simulations a simple method for estimating the number of subdivisions of the timestep was developed and is described.

3. The Rayleigh Problem

The Rayleigh problem is a well-known, theoretical, one-dimensional, unsteady flow problem. A semi-infinite volume of homogeneous gas of density ρ_∞ and temperature T_∞ is at rest above the diffusely reflective plane $y=0$. This plane instantaneously acquires a temperature T_w and a velocity in the positive x direction U_w at time $t=0$. In the present case T_w and U_w are chosen to coincide with the finite-difference solution of Chu [9] who solved the non-linear Krook equation for the problem. Specifically, U_w is taken as twice the most probable thermal speed of the stationary gas and T_w is taken as 1.6 times the gas temperature.

Results are presented at $tv_0=5$ and $tv_0=10$ where v_0 is the collision rate in the undistrubed gas. The simulation region extends to $20\lambda_0$, where λ_0 is the mean free path before displacement occurs, and the number of cells employed is 80. As the flow is unsteady, each set of results is averaged by running the simulation from the initial conditions through to $tv_0=10$ over a large number of repetitions (typically 200). In this study, hard-sphere molecules have been employed and the initial configuration follows that of Bird [1, Appendix G].

In this problem the surface properties at the diffusely reflecting plate are also of

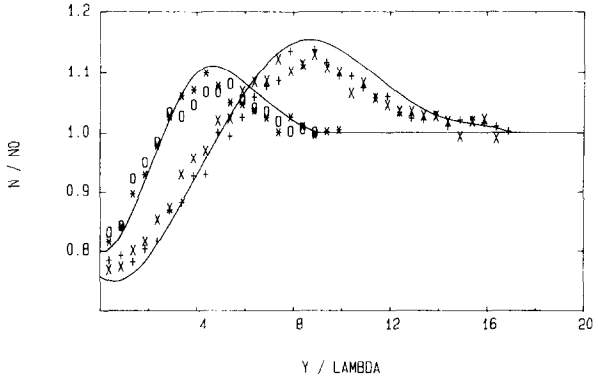

FIG. 2. Number density plots for the Rayleigh problem. *, modified Nanbu, $tv_0=5$; 0, Bird, $tv_0=5$; +, modified Nanbu, $tv_0=10$; X, Bird, $tv_0=10$; ———, Chu [9].

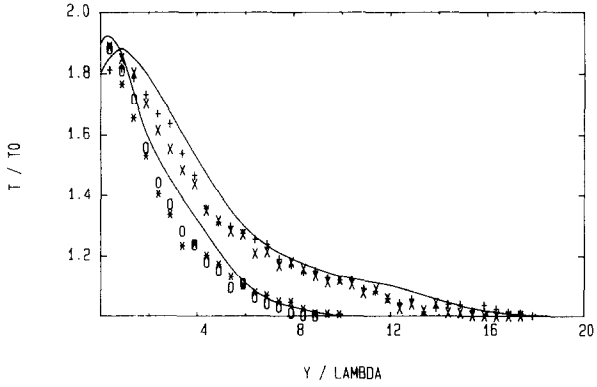

FIG. 3. Temperature plots for the Rayleigh problem. *, modified Nanbu, $tv_0 = 5$; 0, Bird, $tv_0 = 5$; +, modified Nanbu, $tv_0 = 10$; X, Bird, $tv_0 = 10$; ———, Chu [9].

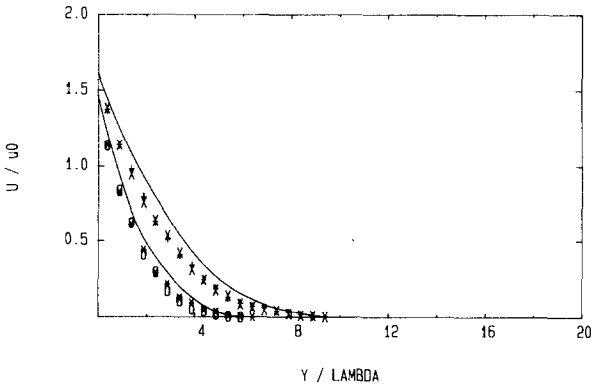

FIG. 4. Shear velocity plots for the Rayleigh problem. *, modified Nanbu, $tv_0 = 5$; 0, Bird, $tv_0 = 5$; +, modified Nanbu, $tv_0 = 10$; X, Bird, $tv_0 = 10$; ———, Chu [9]. u_0 is the most probable thermal velocity in the undisturbed gas.

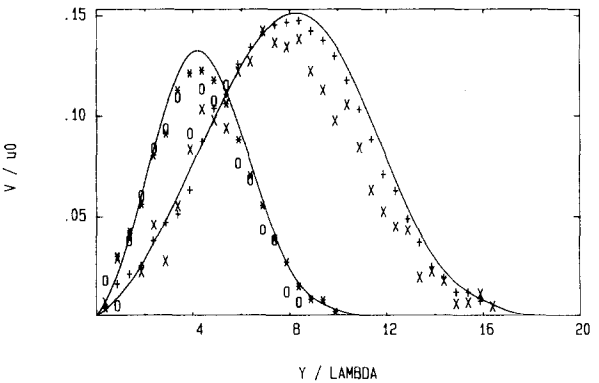

FIG. 5. Normal velocity plots for the Rayleigh problem. *, modified Nanbu, $tv_0 = 5$; 0, Bird, $tv_0 = 5$; +, modified Nanbu, $tv_0 = 10$; X, Bird, $tv_0 = 10$; ———, Chu [9].

interest. Bird [1, p. 152] calculated a number of time-independent collisionless properties and claimed that his DSMC results could be extrapolated to these values. Specifically, number flux, pressure, shear stress, and heat flux were investigated. However, these extrapolations are by no means conclusive. To investigate this phenomenon in more detail a larger number of flow cells has been employed in our simulations.

Calculations were made with both the Bird and modified Nanbu simulation schemes. The most efficient value for L in the modified method was found to be three. Employing larger values gave self-consistent results with increasingly longer execution times. Smaller values gave unsatisfactory results. The modified Nanbu calculations required about 20% more processing time than that for the Bird method.

Flowfield results for number density, temperature, and the velocities in the shear and normal directions are shown for the two methods together with Chu's calculations in Figs. 2–5. Excellent agreement exists for the two DSMC techniques. The main deviation of the Monte Carlo results from Chu's calculations occur for the normal velocity. It is interesting to note in this respect that the results obtained with the modified method show a much improved correspondence with the finite difference solution than do those of Bird. In addition these results show much less scatter.

Although it is by no means certain, this improved scatter phenomena may be due to the increased deterministic nature of the modified scheme. It is certainly true that the modified Nanbu method produces results which are consistent with Bird's calculations, thus showing that the violation of conservation of energy and momentum at the molecular level does not seem to have an adverse effect on the results.

4. Sonic Expansion

Having established confidence in the modified method through the one-dimensional experiments it was decided to re-investigate the two-dimensional flow discussed in [7]. It would then be possible to assess the modified method against those of both Bird and Nanbu. In addition, these calculations include the transfer of energy between internal modes using the Larsen–Borgnakke [10] phenomenological model. It is of great importance that such aspects of the DSMC method are proved to function correctly within the structure of the new scheme. This model is implemented in the usual manner in that the total collision energy of the colliding molecules is used to sample post-collision values from local equilibrium distribution functions. In keeping with the general concept of the Nanbu algorithm, only one molecule undergoes change as a result of each inelastic collision calculated. In the present study, the collision number is assumed to be constant and has a value of 5.

The flow consists of the sonic expansion of hot nitrogen gas through a small nozzle which provides parallel flow at the exit plane. The exit radius is taken as 15

mean free paths; the flow is two-dimensional having a specularly reflecting centreline. The initial temperature and pressure of the nitrogen is taken as 2000 K and 5000 Nm^{-2}, respectively. The steady state solution to this problem is achieved by averaging the flow properties over a suitable sample size. In the current calculations, each cell in the flowfield typically contains 20–30 simulated molecules and a minimum sample size of 4000 is employed in the averaging process.

As in [7] the effect of different collision models was investigated using the variable hard sphere (VHS) formation of Bird [11]. In this model the total collision cross section is given as a function of the relative collision velocity

$$\sigma_T = \sigma_R[\tfrac{1}{2}m_r g^2/\{(2-\omega)kT_R\}]^{-\omega} \tag{3}$$

where

σ_R is a reference cross section calculated at temperature T_R

m_r is the reduced mass of the collision

k is Boltzmann's constant

ω defines the particular collision interaction.

In the present work we were particularly interested in discovering the relationship between the value of L and that of ω. In particular, for direct comparison with results presented in [7], the values of ω investigated were $\omega = 0$, 0.24, and 0.5. An efficient value of L was discovered through a series of numerical experiments. For each value of ω chosen, an initial value of L was guessed. The modified algorithm was run and results averaged over the same number of loops as for the simulation which employed the Bird method. The calculations for the two methods were then compared. In particular, number density and translational and rotational temperature contours together with the collision rates in the various regions of the flowfield were analysed. If good agreement in the results was found then the value

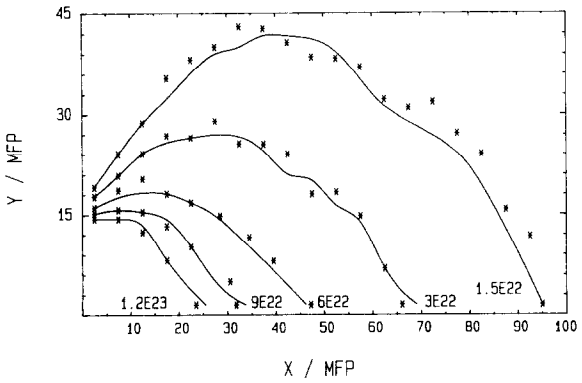

FIG. 6. Density plots for the sonic expansion of hot nitrogen: ———, Bird method [7]; *, modified Nanbu method.

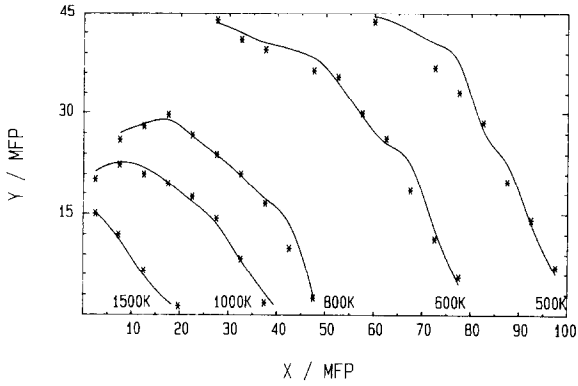

FIG. 7. Temperature plots for the sonic expansion of hot nitrogen: ———, Bird method; *, modified Nanbu method.

of L was reduced until the calculations for the two methods began to diverge. Alternatively, if the results for our initial value for L did not agree then L was increased until satisfactory results were obtained. In this manner a correspondence between L and ω was obtained.

Results for density and temperature contours are shown in Figs. 6 and 7 for typical calculations. It can be seen that good agreement exists for the two methods. The rotational temperature contours showed similar agreement. In addition, it was found that the computational cost of the new method was up to eight times faster than the original Nanbu scheme, and just 25% more expensive than the method of Bird. The relative CPU times required for these calculations using the Bird, Nanbu, and modified Nanbu schemes, for the three values of ω investigated are shown in Table I. This confirms the claims of Nanbu [3] that the modified method should be considered seriously as an altenative simulation method to that of Bird.

It is clear that the ability to choose L rather than having to alter Δt is much preferable. It is concluded that the modified Nanbu direct simulation method may be used to solve engineering problems providing a suitable value of L is determined. To avoid unnecessary computational cost it is clear that a method of determining L from the initial flow conditions is desirable. Such a method is now described.

TABLE I

Problem	Coll. model (ω)	CPU relative to Bird		
		Bird	Nanbu	Modified Nanbu
$1-d$	0.00	1.000	—	1.193
$2-d$	0.00	1.000	4.341	1.235
$2-d$	0.24	1.000	7.565	1.260
$2-d$	0.50	1.000	9.822	1.245

5. Approximate Method for Calculating L

The determination of an effective value for L in the modified Nanbu scheme through numerical experimentation is a very expensive procedure. It is clearly desirable that a value for L should be predicted from the initial flow properties prior to simulation. A simple method for prescribing L is now described.

Consider the form of Eq. (2) for the VHS collision model

$$L \geqslant n\,\Delta t\,\sigma_R (g_{ij})^{1-2\omega} [\tfrac{1}{2} m_r / \{(2-\omega)\,kT_R\}]^{-\omega}. \tag{4}$$

The number density may be replaced by N/V, where V is the volume of the current cell. For a particular flow problem, an estimate of the maximum value of the expression in (4) is required. In particular, the maximum value of

$$n(g_{ij})^{1-2\omega} \equiv \frac{N}{V}(g_{ij})^{1-2\omega} \tag{5}$$

must be found. In the range of operation of ω, i.e., $\omega \in [0, 0.5]$ the expression $1-2\omega > 0$ so that the maximum value of g_{ij} coincides with that of $(g_{ij})^{1-2\omega}$. When $1-2\omega = 0$, the expression in (4) is constant, so that the following analysis is unnecessary.

The thermal velocities u' of colliding molecules are assumed to have a Maxwellian distribution given by the temperature T in each cell, i.e.,

$$f(u') = \frac{\beta}{\pi^{1/2}} \exp(-\beta^2 u'^2), \tag{6}$$

where

$$\beta^{-1} = \left(\frac{2kT}{m}\right)^{1/2}$$

is the most probable thermal velocity and m is the molecular mass. Hence the maximum value for the total velocity in any one direction may be approximated by

$$u_{\max} = U + 3\beta^{-1}$$

and the minimum velocity by

$$u_{\min} = U - 3\beta^{-1},$$

where U is the component of the stream velocity.

It should be noted that in the Maxwellian distribution (6), a maximum argument equal to $3\beta^{-1}$ accounts for 99.99% of probable velocities and is the usual cut-off value used when sampling from such a distribution.

The maximum value for the relative velocity between two colliding molecules in any one direction is then given by

$$(u_{\text{rel}})_{\max} = (U + 3\beta^{-1}) - (U - 3\beta^{-1}) = 6\beta^{-1}.$$

An approximate value for the maximum relative velocity calculated over all three components is now

$$(g_{ij})_{\max} = [(6\beta^{-1})^2 + (6\beta^{-1})^2 + (6\beta^{-1})^2]^{1/2} = (108)^{1/2}\beta^{-1}. \tag{7}$$

Substituting into expression (5) reveals that the maximum collision probability occurs at the maximum value of

$$\frac{N}{V}[(108)^{1/2}\beta^{-1}]^{1-2\omega} \equiv \frac{N}{V}\left(216\frac{kT}{m}\right)^{1/2-\omega}. \tag{8}$$

It is therefore essential that the maximum values of N and T be estimated before commencing the Monte Carlo simulation. In the case of the Rayleigh problem these parameters may be obtained from Chu's solutions. The other necessary values may be obtained from initial conditions and substitution into (8) and (4) results in $L > 2.1$ which is in good agreement with our value of $L = 3$ obtained by experiment.

In the calculations for the sonic expansion the conditions at the nozzle exit are used to determine L as both N and T have their maximum values at this part of the flowfield. The full expression for the determination of L is

$$L \geqslant \Delta t \frac{N}{V}\left(\frac{216kT}{m}\right)^{1/2-\omega} \sigma_R[\tfrac{1}{2}m_r/\{(2-\omega)\,kT_R\}]^{-\omega}. \tag{9}$$

Thus it can be seen that the choice of ω will directly affect the value of L required to ensure that the modified algorithm functions correctly.

The calculations made at the nozzle exit using this equation together with the values of L found by numerical experiment are shown in Table II. The expression is plotted as a function of ω in Fig. 8.

TABLE II

Problem	Coll. model (ω)	L calculated	L experiment
$1-d$	0.00	2.10	3
$2-d$	0.00	55.60	50
$2-d$	0.05	42.64	41
$2-d$	0.15	24.87	24
$2-d$	0.24	15.16	15
$2-d$	0.35	8.17	9
$2-d$	0.50	3.55	5

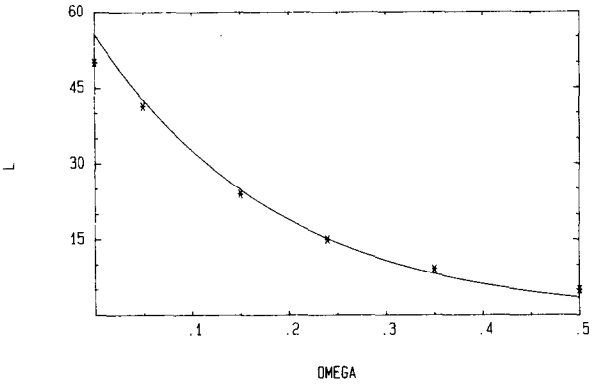

FIG. 8. Number of subdivisions of the timestep Δt in the modified Nanbu scheme as a function of the VHS collision model parameter ω: ———, Eq. (9); *, result found from numerical experiment.

It is clear that excellent agreement exists between the values, so that it is felt that an effective value for L may be obtained using this simple method for any given conditions. For large engineering problems in which there are large differences in local mean free path at different points in the flowfield it is necessary to employ different decoupling timesteps. In such problems it will also be necessary to calculate different values of L for each of these flow regions.

An identical time increment Δt has been employed for each value of ω investigated in the calculations. The large variation in the required value of L observed in the numerical experiments and predicted by Eq. (9) indicates that for ideal simulation the decoupling timestep should be recalculated whenever ω is altered. This introduces another useful aspect of Eq. (9) which may be used to identify an appropriate Δt for a chosen value of L.

It should be noted that the large values of L required for when $\omega < 0.25$ suggests that in many cases the particles should collide several times over Δt. This emphasises the improvement made to the Nanbu method by the subdivision of the decoupling timestep.

6. CONCLUDING REMARKS

In the present work the usefulness of the modified Nanbu direct simulation Monte Carlo method has been illustrated. This method offers great improvements on the original scheme of Nanbu both in terms of performance and implementation by allowing the decoupling timestep to be split into a number of L equal subdivisions.

The method has successfully predicted results for one- and two-dimensional flows with additional computational costs of less than 25% compared with those incurred with the method of Bird. It should be noted, however, that the parallel

nature of the modified algorithm may lead to further reductions in computational effort. Results for diffuse reflection from a hot surface and for internal energy transfer are found to be consistent with those of Bird.

The statistical fluctuations inherent in the two methods should also be considered. In Bird's scheme, the first of the two collision partners is chosen in a completely random fashion. It is therefore possible for molecules to be overlooked which have high collision probabilities. On the other hand, in the Nanbu schemes, the collision probability of each molecule is considered, so that a better determination of the molecules which collide is achieved. Thus the modified scheme is a more deterministic method than that of Bird and it would be expected that its results would show less scatter. In the DSMC method this would mean that reasonable averages could be obtained over a smaller statistical sample. This aspect of the Monte Carlo method has not been properly investigated and a requirement for the future is that such an analysis should be performed with respect to problems for which theoretical or experimental results are well established.

ACKNOWLEDGMENT

One of the authors (I. D. Boyd) gratefully acknowledges the financial support of an SERC/IBM CASE Award.

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