

Navier-Stokes and Monte Carlo Results for Hypersonic Flow

Lyle N. Long*

Pennsylvania State University, University Park, Pennsylvania 16802

As interest in hypersonic flight is once again growing, this is an opportune time to re-examine the applicability and limitations of our gasdynamic models. It is particularly important to address the flow regime between rarefied and continuum gasdynamics (the slip or transitional regime) because these flows may be common on future hypersonic vehicles and they are very poorly understood. This paper uses a full Navier-Stokes method and a molecular simulation method to analyze an indented nose cone at hypersonic Mach numbers. The Navier-Stokes code is based on a finite-volume, explicit Runge-Kutta time-marching scheme. The molecular simulation method is based on the direct simulation Monte Carlo method. Theoretical and numerical differences between the two methods are discussed. Heat-transfer predictions are compared to experimental data.

Nomenclature

CFL	= Courant-Friedrichs-Lewy number, $= c\Delta t/\Delta x$
c	= speed of sound
E	= total energy, $= (e + u^2/2)$
e	= internal energy
F	= vector of flow variables, $= [\rho, \rho u, \rho E]^T$
f	= velocity distribution function
f_0, f_1, f_2	= first, second, and third terms in Chapman-Enskog expansion of f , respectively
Kn_L	= Knudsen number based on L , $= \lambda/L$
$Kn_{\Delta x}$	= Knudsen number based on cell size, $= \lambda/\Delta x$
L	= characteristic length
M	= Mach number
n	= normal vector
p	= pressure
q	= heat transfer
q_n	= heat transfer normal to surface
Re_L	= Reynolds number based on characteristic length L , $= \rho UL/\mu$
$Re_{\Delta x}$	= Reynolds number based on cell size, Δx
S	= surface area
T	= temperature
t	= time
U	= characteristic velocity
u	= fluid velocity
u_n	= normal velocity, $= u \cdot n$
V	= volume
v	= molecular velocity
x	= position in space
y^+	= nondimensional distance from wall
ΔS	= incremental surface area (cell face area)
Δt	= time step size
ΔV	= incremental volume (cell volume)
Δx	= representative cell size
Δy	= representative cell size normal to wall
δ_{ij}	= Kronecker delta
λ	= mean free path
μ	= dynamic viscosity
μ_b	= bulk viscosity
ν	= kinematic viscosity
ν_w	= kinematic viscosity at wall
ρ	= density
ρ_w	= density at wall

τ	= shear stress tensor
τ_w	= shear stress at wall

Introduction

THE current interest in hypersonic vehicles makes it important to quantify some of the differences between predictions based on continuum (Navier-Stokes and Euler) equations and those based on kinetic theory [e.g., direct simulation Monte Carlo (DSMC)]. In addition, these predictions must be compared with experimental data in order to assess the merits of each method.

The purpose of the following paper is to discuss the merits and deficiencies of both Navier-Stokes and Monte Carlo codes from an engineering viewpoint. Neither continuum-based finite-difference methods nor the Monte Carlo code are ideally suited to the Reynolds number regime discussed here. Navier-Stokes codes often have difficulty at low Reynolds numbers, not only in simulating the physics but also in terms of numerical stability.

The Monte Carlo code, although able to model the physics well, requires a great deal of computer time (especially when the Reynolds numbers are not very small). Both types of codes were applied to the same geometry and compared to experimental data. This paper will discuss the pros and cons, limitations, and computer resources required for each method.

Another reason for performing this work was to evaluate the feasibility of using DSMC in the near-continuum regime. It is often stated that DSMC contains more of the physics than Navier-Stokes solutions. If this is the case, as computers get more and more powerful, DSMC might be used more and more in this regime. In order to assess its usefulness in the near-continuum regime, this paper presents results for the DSMC in a regime where it is not usually used.

Koppenwallner¹ has shown that Knudsen number or low density effects can have a significant impact on hypersonic vehicles. He shows that the nose-up pitching moment of the U.S. Space Shuttle was very poorly predicted due to Knudsen number effects. To correct for this, the body flap had to be deflected 15 deg, twice the expected amount. He claims that these effects on pitching moment cannot be neglected when $M/\sqrt{Re_L} > 0.01$. Our predictive capabilities in the transitional regime must be further developed and validated if we are to design vehicles that travel at the outer edges of the atmosphere.

This paper presents numerical predictions based on both continuum and kinetic theory for an axisymmetric indented nose cone. This particular configuration is called the Widhopf 1-10-10 configuration because it is made up of three radial arcs having radii of 1, 10, and 10, as shown in Fig. 1. Hypersonic vehicles experience extreme aerothermal heating over their

Presented as Paper 88-2730 at the AIAA Thermophysics, Plasmadynamics, and Lasers Conference, San Antonio, TX, June 27-29, 1988; received Jan. 9, 1989; revision received Oct. 23, 1989; second revision received Dec. 6, 1989; accepted for publication Dec. 26, 1989. Copyright © 1990 by the American Institute of Aeronautics and Astronautics, Inc. All rights reserved.

*Assistant Professor of Aerospace Engineering. Member AIAA.

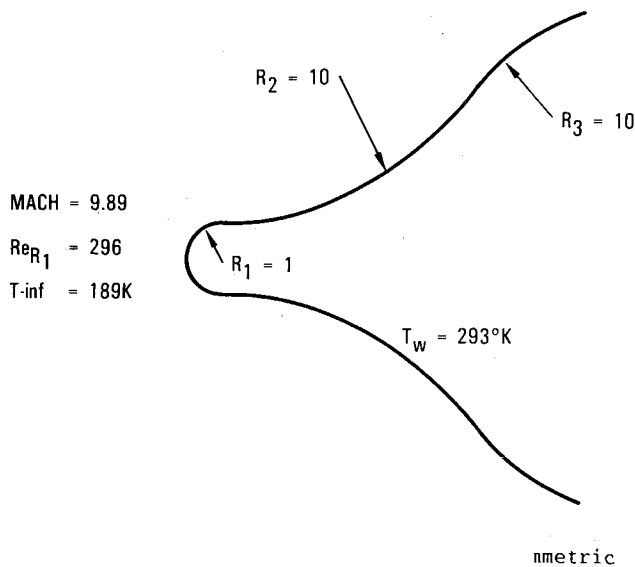


Fig. 1 Widhopf 1-10-10 axisymmetric indented nose cone.

leading edges and nose cones. In some cases, the nose cone has ablated into a shape similar to that of the configuration considered here.²

The uneven ablation process is due to a complicated shock/shock and shock/boundary-layer interaction process that is not well understood. Once the ablation begins, it is further aggravated by the bow shock from the nose impinging on the indentation. This shape change can significantly alter the forces on the vehicle, and, consequently, its trajectory. Reference 3 presented experimental heat-transfer predictions for this configuration at $M = 9.89$ and $Re = 2.96 \times 10^3$ (based on nose radius). The Knudsen number based on the nose radius (0.05) indicates that the flowfield is within the near-continuum or slip regime. This is a rather small Knudsen number, and few Monte Carlo simulations have been attempted at these conditions because of the significant computer resources required. Of particular interest will be the differences between the continuum and kinetic theory approaches in the vicinity of the shock waves and how this affects the surface quantities.

References 4 and 5 analyzed this configuration using Navier-Stokes methods. Reference 6 compares DSMC and parabolized Navier-Stokes (PNS) predictions for similar configurations. The PNS approach requires that at least two different codes be used, one to start the solution in the nose region and one for the PNS marching solution. The present calculations were done by a single computer program based on the full Navier-Stokes equations.

Continuum vs Kinetic Theory Approaches

Gasdynamics can be modeled as a continuum or as a system of particles. The continuum approach is the most common, primarily because it is mathematically simpler and is valid for many fluid flows. However, the kinetic theory approach has a wider range of validity. The main limitations of kinetic theory are due to mathematical and numerical complexities that made it difficult to obtain numerical solutions with reasonable amounts of computer time.

The equation that governs the kinetic theory of binary collisions is the Boltzmann equation.⁷ The Boltzmann equation has only one unknown, the velocity distribution function f , but for a single-species monatomic gas, this is a function of seven variables $f(x, t, v)$. This distribution function represents the fraction of molecules in the volume between x and $x + \Delta x$ that have a velocity between v and $v + \Delta v$.

An important parameter in the kinetic theory of gases is the Knudsen number. The characteristic length must be based on

the flow gradients,⁸ e.g., $L = Q/(\nabla Q)$, where Q is a representative flow variable such as temperature or velocity. If the Reynolds number is based on the same characteristic length, then one can show that $Kn \approx 1.5M/Re$.

The continuum conservation equations (mass, momentum, and energy) are obtained by multiplying the Boltzmann equation by M , mv , and mv^2 , respectively, (where m is the molecule mass) and then integrating over all velocity space. However, they contain more unknowns than equations, and the real difficulty comes in deriving the constitutive relations for the shear stress tensor, τ and the heat transfer q . These are usually determined by expanding the distribution function as an asymptotic series in the Knudsen number.

Euler solutions are essentially the zeroth-order approximation to the Boltzmann equation and are only valid in the limit as $Kn \rightarrow 0$. The Navier-Stokes equations are the first-order approximation ($f_0 + Knf_1$), valid for $Kn \ll 1$. Since the Navier-Stokes equations are obtained by expanding f in an asymptotic expansion in Kn , they are only valid for small Knudsen numbers. Chapman and Enskog⁹ independently evaluated the second term f_1 to obtain expressions for the constitutive relations for the Navier-Stokes equations.

References 7-14 describe, in a variety of ways, the limitations of the continuum approach. The limitations are usually in the definition of the constitutive relations and not the mass, momentum, and energy conservation equations. That is, the equations that relate the shear stress and the heat transfer to the other variables break down.

Numerical Method Used to Solve the Navier-Stokes Equations

There are a wide range of approximations to the Navier-Stokes equations. These include inviscid (Euler), boundary-layer, parabolized Navier-Stokes, thin-layer Navier-Stokes, Reynolds-averaged Navier-Stokes (turbulent flow), and full Navier-Stokes equations. In addition to the various approximations, there are also many numerical approaches. The most common types can be classified as explicit, implicit, or spectral.

The present method is an explicit, finite-volume, Runge-Kutta time-marching scheme applied to the full Navier-Stokes equations. The flowfields are laminar and the perfect gas assumption is used. Because of the very small Reynolds number used here, the assumption of laminar flow is justified. This algorithm was originally developed for the Euler equations^{15,16} and has since been extended to the Navier-Stokes equations.

The code used here was developed by Lockheed and its capabilities were extended under contract to the Air Force Wright Aeronautical Laboratory.¹⁷ The code is called the Three-Dimensional Euler/Navier-Stokes Aerodynamic Method (TEAM) and is described completely in Ref. 17. However, the code used here was a very early version of the TEAM code; some of the performance estimates and capabilities described here have been significantly improved since this version was developed. The TEAM code solves the integral form of the Euler or Navier-Stokes equations¹⁸:

$$\frac{\partial}{\partial t} \iiint F dV = - \iint G dS$$

where

$$F = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}$$

$$G = \begin{pmatrix} \rho u_n \\ \rho u u_n + p n - n \cdot \tau \\ \rho H u_n - n \cdot \tau \cdot u + q_n \end{pmatrix}$$

where H is the total enthalpy. The shear stress tensor is given by

$$\tau_{ij} = \mu_i [(\partial u_i / \partial x_j) + (\partial u_j / \partial x_i)] + \mu_b - (2/3)\mu_i (\partial u_i / \partial x_i) \delta_{ij}$$

Typically, one assumes $\mu_b = 0$, but this is not necessarily valid for compressible (especially hypersonic) flows. The preceding equations simply state that the rate of change of the mass, momentum, and energy of the fluid within the volume V is equal to the flux of these quantities through the surface S bounding the region V .

The cell-face quantities are approximated by averaging the two cell-centered values on either side of each face. On a uniform mesh this is equivalent to a second-order-accurate central-difference scheme that has to be augmented by numerical dissipation to maintain stability. Jameson et al.¹⁵ developed an adaptive dissipation scheme that adjusts the dissipation depending on the strength of the pressure gradient.

We have also incorporated Roe's¹⁹ approximate Riemann solver, which is a characteristic-based upwind scheme into the TEAM code. This can be used in place of the adaptive dissipation scheme and is usually required at high Mach numbers. A subroutine was written to calculate dissipative fluxes using a form of the dissipation scheme described by Gnoffo.²⁰

The TEAM method can be used to analyze the flowfields around realistic complete aircraft configurations, including wings, canards, tails, fins, engine inlets, engine exhausts, fuselages, etc. This is possible because the computational domain can have a zonal structure, allowing it to be broken up into large regions (zones) as is necessary to generate suitable grids for realistic aircraft configurations.

Numerical Method Used to Solve Kinetic Theory

Several solution procedures for kinetic theory have been attempted with varying degrees of success. There are basically three types of numerical methods: numerical solutions to the Boltzmann equation,²¹ numerical solutions to model equations,²² and particle simulations.⁷ The attempts to numerically solve the Boltzmann equation have not been very successful for a number of reasons, as described in Refs. 7 and 21. However, a new and promising approach is described in Ref. 23. A new particle approach, cellular automata, is discussed in Ref. 24. The most common model equation approach is based on the BGK (Bhatnager, Gross, Krook) equation,²² which replaces the complicated collision integral with a much simpler algebraic function. This does reproduce the Boltzmann equation in the limit of very small or very large Knudsen numbers but is an approximation in the transition regime. It also yields a Prandtl number of 1.0.

The most widely used particle simulation method is the DSMC method of Bird.^{7,10,25} This method has had years of development and validation. The DSMC method does not actually solve the Boltzmann equation directly. However, this technique and the Boltzmann equation are derived in a similar manner. Nambu²⁶ shows that the DSMC method is equivalent to solving the Boltzmann equation. The DSMC, as implemented, is more general than the Boltzmann equation. It has been used to model chemical reactions, three-body collisions, catalytic reactions, radiation effects, and ionized flows. These effects would be very difficult to incorporate into a deterministic code.

In the DSMC method, the flowfield is broken into cells similar to those in finite-difference techniques. Simulated gas molecules are followed through a series of motions and collisions. The molecules move from one cell to another according to their own velocity. The cells are only used to decide which molecules will collide and for sampling.

In the past, the DSMC method was applied to either two-dimensional or axisymmetric problems. However, three-dimensional problems can now be solved using this approach.²⁷ The technique has been very successful despite its simplicity and the fact that it does not model the actual number of molecules.

The DSMC method has typically been applied to transitional or rarefied flows; however, with the ever-increasing power of computers, it may be used for fairly small Knudsen numbers as shown here. The primary disadvantage of this technique is the large amount of computer time required (several days of time on a minicomputer).

The DSMC uses array indexing schemes that do not vectorize, and consequently the Cray-XMP is only five times faster than a VAX 8600. Since the Cray costs much more than the VAX, it is not cost-effective for this code and was not used for the DSMC predictions. It is very important to pursue alternative methods both in terms of hardware (e.g., parallel processing) and software that may offer advantages in computational efficiency. Nearest neighbor-type problems such as explicit computational fluid dynamics methods or particle simulation methods are ideally suited to massively parallel processors such as the Connection Machine as shown in Refs. 28 and 29.

TEAM and DSMC Algorithmic Differences

There are numerous differences between the TEAM code and the DSMC code. A few of these will be elaborated here. They include accuracy considerations, user friendliness, grid requirements, and time-step constraints. The accuracies of the TEAM and DSMC codes are difficult to compare. TEAM, like all finite-difference schemes, is based on Taylor series expansions. It is second-order accurate, so the truncation error is $O(\Delta x^2)$. This description of the error analysis is only valid where the derivatives are smooth. Near shock waves or boundary layers the derivatives are very large and the solution cannot be approximated well by a Taylor series expansion. In these regimes, the numerical accuracy is difficult to estimate. These high-gradient regions are also where the continuum approximation will break down first. The numerical continuum approaches produce shock waves that are typically several Δx thick, when in fact they should only be a few mean free paths thick (depending on the Mach number).

The DSMC method also assumes the flow properties vary slowly across a cell because the molecular positions within the cells are ignored in the calculation of collisions. That is, a molecule within a cell can collide with any other molecule in that cell, even if the two are moving away from each other. However, a straightforward Taylor series expansion to determine the truncation terms may not be possible. The scheme should probably be classified as being between first-order and second-order accurate. The primary accuracy difference between DSMC and TEAM is that the DSMC method is a statistical approach, whereas TEAM is deterministic. Therefore, the accuracy of DSMC depends on the number of samples taken. In some cases this may have advantages in practical applications where an approximate solution may be useful, for instance in the early stages of design.

In finite-difference calculations, the intermediate solutions (prior to convergence) often have no meaning (since pseudo-time or iterative methods are used) and their accuracy cannot be quantified very easily. The deterministic approach may, in the end, be misleading since the actual flowfield is not deterministic anyway. The atmosphere is not completely predictable, and even at low altitudes there are turbulent components. At hypersonic speeds and high altitudes there are significant unknowns. The atmospheric density may vary up to 10%, and the chemical composition can also vary.

Since both codes assume that the flow properties vary slowly from cell to cell, the grids are very important. In fact, for high accuracy one must estimate where the gradients will be before the codes are run and then cluster the cells in that region. In some cases this is relatively easy (such as in a boundary layer), but in others (such as for complex reflected shock waves) it cannot be done ahead of time. The optimum approach would be some kind of adaptive grid scheme or adaptive grid refinement. This is being pursued for both Navier-Stokes and DSMC methods. As these methods are

applied to more and more complex geometries, grid adaptation will be essential.

Another major difference between TEAM and DSMC is the grids required. The TEAM method uses a structured zonal approach. Within each zone the cells are very ordered or structured. The DSMC method uses an unstructured zonal approach. Although the DSMC grids may be structured, this information is not used in the code. The different zones are primarily used to keep the number of simulated molecules per cell roughly constant from one region of the flowfield to another.

In the future we will be using unstructured tetrahedral grids in a three-dimensional DSMC code and a new Navier-Stokes code. The unstructured approach makes grid refinement fairly straightforward; cells can be simply subdivided. However, this approach makes it very difficult to develop programs that vectorize or parallelize. These tradeoffs must be addressed in the future for both finite-difference and Monte Carlo schemes.

In order to compare the cell-size requirements (which are related to computer memory and speed requirements) for the two approaches, it is instructive to perform some order-of-magnitude estimates. In Navier-Stokes methods, one can describe cell size in terms of a cell Reynolds (or Peclet) number,²⁰ which is a key parameter in determining the stability and accuracy of the method [in addition to the Courant-Friedrichs-Lewy (CFL) or Courant number]. The cell Reynolds number is defined as

$$Re_{\Delta x} = \rho U \Delta x / \mu$$

Since

$$Re_{\Delta x} \approx 1.5M\Delta x/\lambda$$

we can write

$$\Delta x/\lambda = 2Re_{\Delta x}/3M$$

where M should be interpreted as a local Mach number. This now puts the Navier-Stokes cell Reynolds number in a form comparable to that discussed in the DSMC literature: cell size and mean free path. Ideally, in the DSMC method, one would like to have $\Delta x < \lambda$, but more work should be done in determining the effects of exceeding this limit.

One constraint on the Navier-Stokes cell size is the minimum required to accurately predict surface heat transfer and skin friction. One rule³¹ is that the first cell should correspond to a $y^+ < 1$, where

$$y^+ = \frac{y}{\nu_w} \sqrt{\frac{\tau_w}{\rho_w}}$$

The quantity y is the distance normal to the wall. One empirical formula to meet this criteria is to set the first cell size using $\Delta y \leq 0.05L/\sqrt{Re_L}$, but this will be problem dependent.

Since $L \approx \lambda Re_L/1.5M$, the preceding equation can be rewritten as

$$\Delta y/\lambda \leq 0.03\sqrt{Re_L}/M$$

For example, if $M = 0.05$ (e.g., in a boundary layer) and $Re_L = 100$, then $\Delta y \approx 6\lambda$. Considering that the DSMC method has been used for $\Delta y > \lambda$, the preceding equation shows that the Navier-Stokes methods can require cells that are of the same size as DSMC in some cases, especially at low Reynolds numbers.

The other key parameter is the time step required by the two methods. In Navier-Stokes methods, one normally speaks in terms of a CFL number and a cell Reynolds number. For a four-stage Runge-Kutta-scheme, the viscous time step limit (based on a one-dimensional model equation) is given by

$$CFL/Re_{\Delta x} = \nu \Delta t / \Delta x^2 < 0.7$$

or

$$\Delta t < 0.7\Delta x^2/\nu$$

To compare the preceding to the DSMC conditions, we can approximate the kinematic viscosity by $\nu \approx (2/3)\lambda c$, which gives

$$\Delta t \leq 2.1\Delta x^2/\lambda c$$

Now, the mean collision time is approximately given by $t_c \approx 0.75\lambda/c$, which means the preceding becomes

$$\Delta t \leq 1.4t_c/Kn_{\Delta x}^2$$

or

$$\Delta t/t_c \leq 1.4(M/Re_{\Delta x})^2$$

where M and $Re_{\Delta x}$ are local flow quantities. This puts the Navier-Stokes code time-step limit in a form similar to the DSMC code. Ideally, one should use a time step on the order of the mean molecular collision time in DSMC. This can be exceeded without a major loss in accuracy in some cases. There are no stability problems with the DSMC method, but most Navier-Stokes methods are very sensitive to their stability limits. For highly nonlinear problems, such as those with strong shocks, or complex three-dimensional flowfield, these stability limits cannot be predicted very well. But when the local cell Reynolds number and Mach number are of the same order, the time step will have to be on the order of the mean collision time even in the Navier-Stokes code. During the initial stages of a DSMC calculation, one can use quite large time steps, and they can be reduced once the problem approaches convergence. This cannot be done with Navier-Stokes methods due to the stability constraints. Also, one must compare the number of computations per time step; the Navier-Stokes method has thousands of floating point operations to perform per time step.

It should be pointed out that the Reynolds number depends on a continuum concept and one should be careful in developing criteria for rarefied flow using such ideas. This is clearly an approximation but often is the best one can do.

In another area, ease of use, neither of these codes can be considered a "black box" that could be turned over to someone with little or no background in gasdynamics. One difficult aspect of the DSMC method is specifying the ratio between the number of physical and simulated molecules. One would like this number as low as possible, but computer memory limitations usually force this to be quite high (e.g., 10^{15}). In order to set this number, one must almost estimate the amount of mass in the final flowfield solution and then divide by the flowfield volume. For complex geometries this is simply not possible and one must resort to trial and error. If the number is set too low then the number of simulated molecules will increase to the number that the Fortran array was dimensioned to. Above this point, the solution will be in error. It would be useful if this process could be automated.

One must also specify the time step to use in the DSMC method. Ideally, this should be computed automatically within the code based on accuracy constraints. The ratio of the mean collision time and the time step can be easily printed out. But one must manually adjust the time step if it becomes too large. In codes such as TEAM, the time step is automatically calculated according to the CFL number that was input and this time step can be different for each cell (for a steady-state problem).

The complexities of the TEAM and DSMC computer programs are also quite different. The TEAM code contains roughly 10 times more lines of Fortran than DSMC (20,000 vs 2000). The TEAM solver has impressive geometric capabilities and is well documented, but complex three-dimensional grids

are very difficult to develop for it. Some grids can take several months to develop. The DSMC code now is fairly well documented, but, since it is essentially an unstructured grid solver, it will be much easier to generate complex three-dimensional grids for it. The DSMC method includes more physics as well, such as thermal and chemical nonequilibrium (finite-rate chemistry). In general, Monte Carlo methods result in much simpler codes than finite-difference methods. This can be an important point since code maintenance and modifications can be quite costly. The length of the code can also be a measure of how accessible it is to the user(s).

Results

This section will present results from both the TEAM (Navier-Stokes) code and the DSMC method. Additional results and color pictures of the flowfield are presented in Ref. 32. The configuration to be analyzed is shown in Fig. 1. The freestream static and wall temperatures were 189 and 293 deg, respectively. The flow conditions were $M = 9.89$, $Kn = 0.05$, and $Re = 2.96 \times 10^3$, based on nose radius. The Navier-Stokes predictions assumed a perfect gas, and no finite-rate chemistry was used in the DSMC predictions. No-slip boundary conditions were used for the Navier-Stokes, and fully diffuse reflections were used in DSMC.

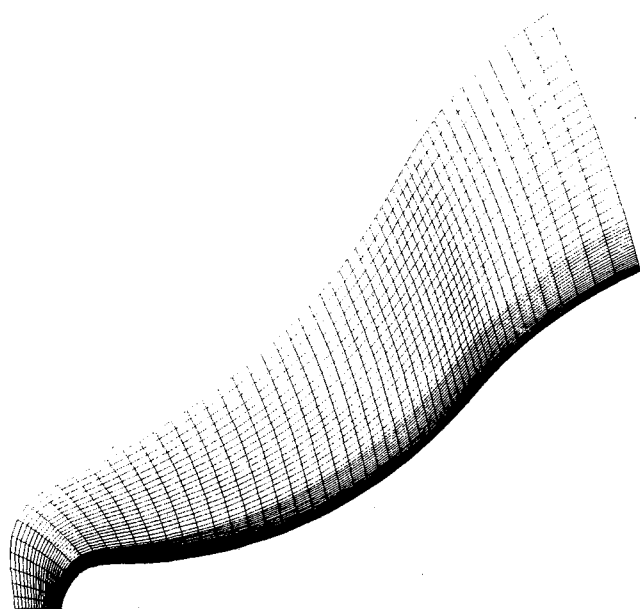


Fig. 2 Grid used in Navier-Stokes code ($72 \times 127 \times 11$).

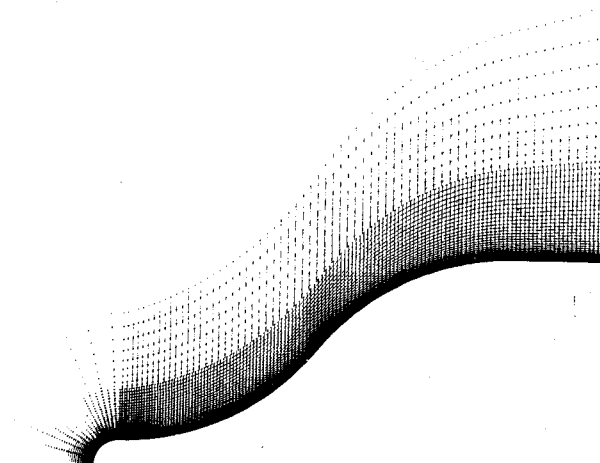


Fig. 3 Two-zone grid used in DSMC Code (39×150 and 9×75).

The grids used in this study were different for the Navier-Stokes and DSMC method. However, since the two are very different, the grid requirements for each are different. Therefore, although it would have been interesting to have used the same grid for the two, it did not seem essential. For the Navier-Stokes predictions, a three-dimensional grid with $72 \times 127 \times 11$ nodes in the normal, streamwise, and radial directions were used, as shown in Fig. 2. Since TEAM does not include an axisymmetric option, it had to be modeled as a

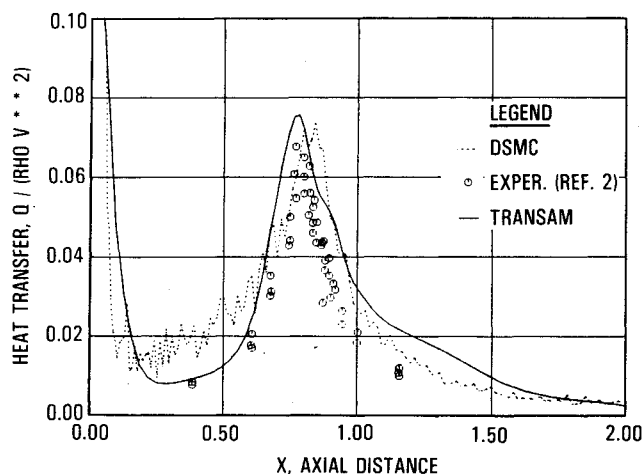


Fig. 4 DSMC and TEAM heat-transfer predictions compared to experimental data.³

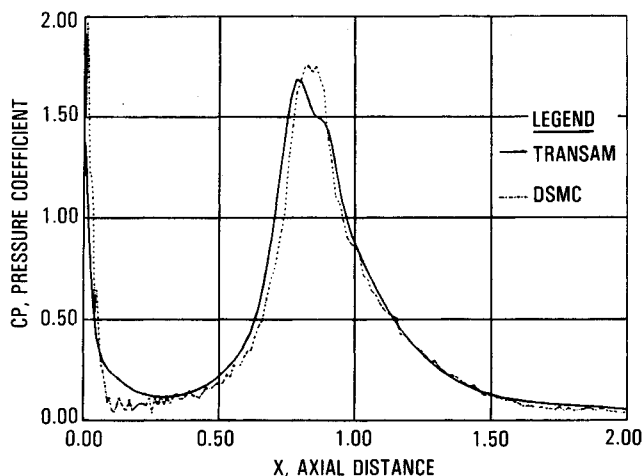


Fig. 5 Surface pressure predictions for DSMC and TEAM codes.

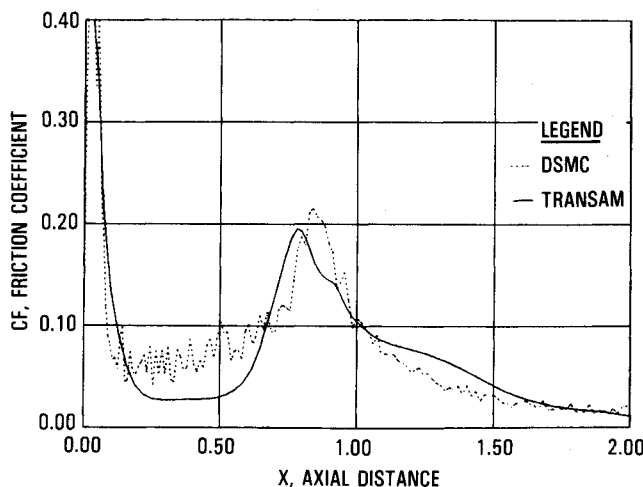


Fig. 6 Skin-friction predictions from DSMC and TEAM codes.

three-dimensional shape. This will allow us to investigate this configuration at angle of attack in the future.

The value of y^+ in the Navier-Stokes code was <1 in the cells near the wall. For the cases run herein, the TEAM code used approximately 62 words of memory per cell and in full-Navier-Stokes mode required approximately 0.0001 CPU s/cell/cycle using the adaptive dissipation scheme (on a single processor Cray-XMP). However, the newer version of the TEAM code runs significantly faster (for thin shear-layer calculations it only uses 0.000025 CPU s/cell/cycle). The results presented here used 33,000 cycles and 98,406 cells. The CFL number had to be quite small (0.1). The second-order-accurate upwind scheme requires roughly 50% more CPU time per cycle but is more robust than the adaptive dissipation scheme at hypersonic Mach numbers.

For the DSMC predictions, a two-dimensional two-zone grid of 39×150 and 9×75 nodes was used (Fig. 3). There were a total of 6477 cells in the flowfield. The ratio of simulated to real molecules was different in the two zones, in order to minimize the number in the far field. The DSMC grid was finer in the freestream direction. The solution was assumed converged when the number of simulated molecules leveled off at some level. The DSMC code used here required approximately 290 words of memory per cell. In the calculations made here, approximately 115,000 simulated molecules were

used. A VAX 8600 was used for the calculations. It was able to calculate approximately 3000 simulated collisions (and move approximately 7000 molecules) per CPU s. Several weeks of VAX time was used for the present calculations.

Heat-transfer predictions of Holden³ are compared to predictions in Fig. 4. These data were taken in a Calspan shock tunnel. Both TEAM and DSMC predicted the peak heating rate quite well, but there are minor differences away from the point of peak heating. Figure 5 shows excellent agreement between the surface pressure predictions from the DSMC code and the Navier-Stokes code (TEAM). Figure 6 shows the predicted skin friction; this quantity is the least correlated (between the two prediction methods) of the flow quantities. The large amount of scatter in the DSMC predictions is because in the expansion region after the nose there are very few molecules. One should probably have a separately defined zone of cells there with a higher ratio of simulated to real molecules. Also, the code could have been run for a longer time, which was not possible here.

The robustness of the DSMC method is illustrated by these results. That is, the DSMC code (in this author's experience) can be run for a short time or with few molecules, and the results will be approximately correct but exhibit statistical scatter. On the other hand, Navier-Stokes codes can fail less gracefully but will display nice smooth curves and 64-bit num-

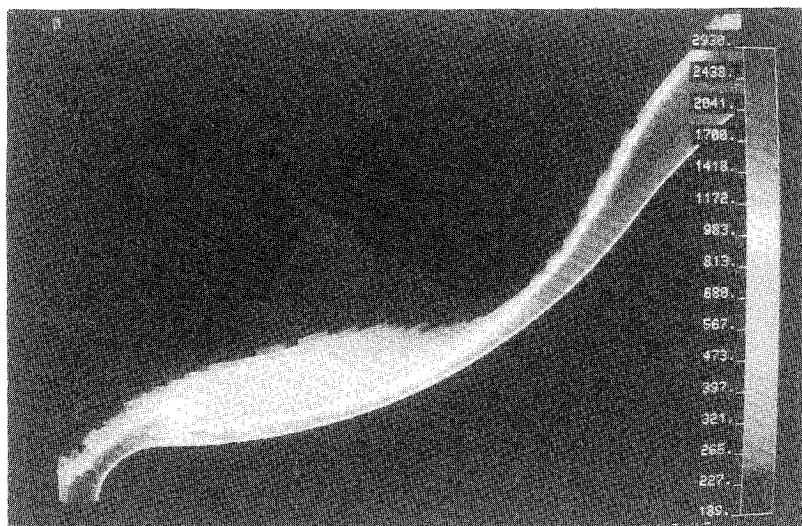


Fig. 7 DSMC predicted temperature contours (K).

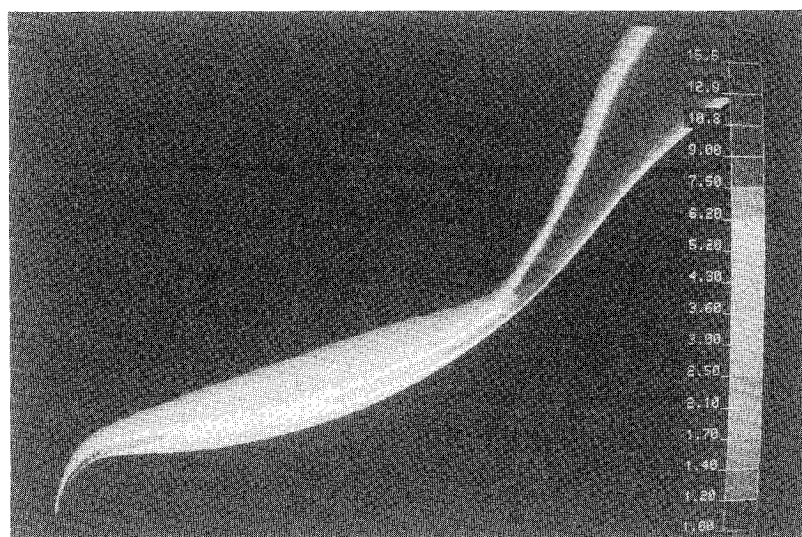


Fig. 8 TEAM predicted temperature contours, T/T_∞ .

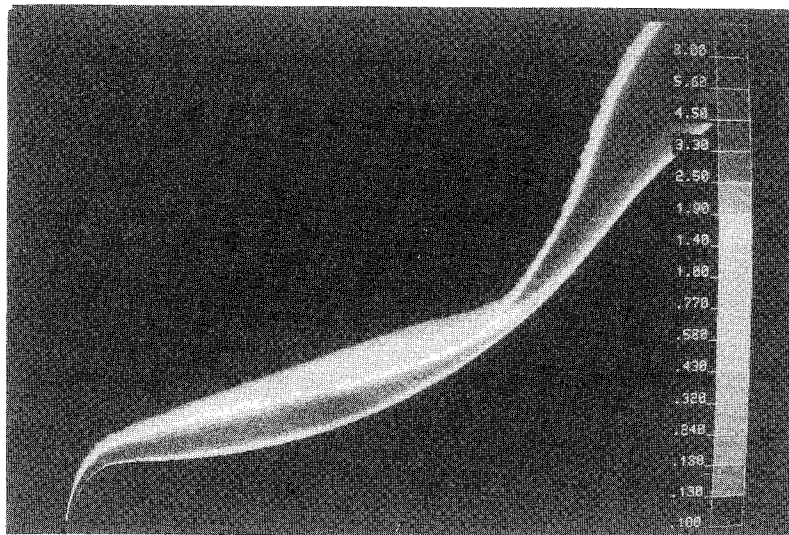


Fig. 9 TEAM predicted entropy contours, $\Delta s/s_\infty$.

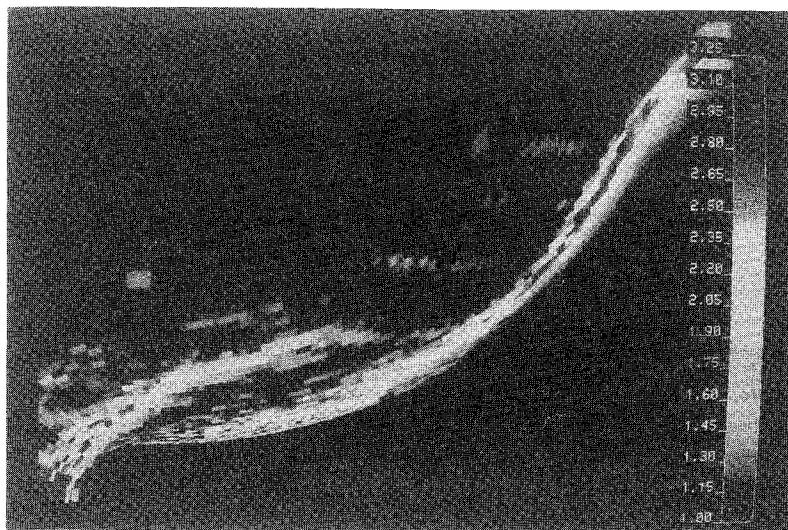


Fig. 10 Ratio of translational temperature to internal temperature from DSMC code.

bers that are significantly in error. The DSMC-predicted flowfield around the nose cone, shaded according to temperature, is shown in Fig. 7. The Navier-Stokes flowfield predictions (T/T_∞) are displayed in Fig. 8, where $T_\infty = 189$ K. In the region of the shock/shock interaction, the temperatures exceeded 2900 K. Both codes predict qualitatively similar flowfields, but the shock layer downstream of the impingement point is thicker in the Navier-Stokes solution.

The flowfields in the nose regions are quite different in the TEAM and DSMC predictions. DSMC predicts a fairly thick shock, whereas TEAM predicts a very sharp shock. The DSMC predictions are expected to be more realistic here since the nose radius is only 20 (freestream) mean free paths, and the actual characteristic length will be even smaller than the nose radius. As shown in Ref. 25, the continuum approach starts becoming a poor approximation at these Knudsen numbers due to the large local Knudsen numbers that occur in the shock wave. The freestream Knudsen number is a poor indicator of when the continuum approximation will break down.

Figure 9 shows the TEAM predictions for entropy change (measured from the freestream entropy). The values are very high in the shock waves and near the body. The layers directly adjacent to the body show an entropy decrease due to the cooled (constant temperature) wall. The well-known entropy-layer effect typical of hypersonic blunt-body flows is visible in this figure. Of particular interest is Fig. 10, which shows the

ratio of the translational temperature and the internal temperature from the DSMC code. This shows significant statistical scatter. The air was modeled as O_2 and N_2 diatomic molecules with vibrational and rotational degrees of freedom. At equilibrium, the energy will be equally distributed between the various degrees of freedom and there will only be one temperature. The ratio shown in this figure is a measure of the thermal nonequilibrium in the flowfield, which cannot be predicted by the TEAM code at this time. As expected, it is highest near the body and in the shock waves.

It should be stressed that no grid or algorithmic parameters were adjusted to make the predictions agree better with experiment. Although most codes will give the correct solution with enough coaxing, it is very important to have prediction methods (as opposed to "postdiction"). Also, in engineering environments where these codes will be used, it is very important that they be used with confidence when the solution is not known. The solutions presented here could, of course, be improved by iterating on the grid or clustering points near the gradients.

Conclusions

This paper has described some of the differences and similarities between a Navier-Stokes code (TEAM) and the direct simulation Monte Carlo code. Both programs appear to be quite effective for hypersonic flowfields. However, both re-

quire substantial computer time. In the flow regimes where both are applicable, one must evaluate which one is better suited to meeting the user's requirements. In some cases, it will depend on the cost of engineering man-hours compared to computer hours. The DSMC method has been used and validated extensively in the aerospace community and should be part of every organization's toolbox of codes. For the same level of physics modeling, the DSMC code will be easier to write, maintain, and use.

However, as the Reynolds number gets larger, the DSMC will require much more computer time than the Navier-Stokes methods. These results do show that the DSMC method can be used in the near-continuum regime. As computer power increases, the DSMC method will be used at higher and higher Reynolds numbers because it is earlier to include all the complicated physics and chemistry of high-speed flows. Much more work should be done toward adapting the DSMC method to vector and parallel computers.

Acknowledgments

This work was sponsored by Lockheed Independent Research and Development Project 88006730. I would like to thank C. Olling and G.A. Bird for very useful and informative discussions.

References

- ¹Koppenwallner, G., "Low Reynolds Number Influence on Aerodynamic Performance of Hypersonic Lifting Vehicles," AGARD-CP-428; *Aerodynamics of Hypersonic Lifting Vehicles*, Bristol, UK, 1987, pp. 11-1-11-14.
- ²Holden, M. S., "A Review of Aerothermal Heating Problems Associated with Hypersonic Flight," AIAA Paper 86-0267, Jan. 1987.
- ³Holden, M. S., "Studies of the Heat Transfer and Flow Characteristics of Rough and Smooth Indented Noses—Part I. Steady Flows," AIAA Paper 86-0384, Jan. 1986.
- ⁴Widhopf, G. F., and Victoria, K. J., "Numerical Solution of the Unsteady Navier-Stokes Equations for the Oscillatory Flow over a Concave Body," *Proceedings of the Fourth International Conference on Numerical Methods in Fluid Dynamics*, June 1974, pp. 431-444.
- ⁵Conti, R. J., and Kirch, H. R., "Navier-Stokes Simulation of Hypersonic Flow About Indented Nosesets," AIAA Paper 87-0489, Jan. 1987.
- ⁶Bartel, T. J., Homicz, G. F., and Walker, M. A., "Comparisons of Monte-Carlo and PNS Calculations for Rarefied Flow Over Reentry Vehicle Configurations," AIAA Paper 88-0465, Jan. 1988.
- ⁷Bird, G. A., *Molecular Gas Dynamics*, Clarendon, Oxford, 1976.
- ⁸Smolderen, J. J., "The Evolution of the Equations of Gas Flow at Low Density," *Progress in Aeronautical Sciences*, Vol. 6, edited by D. Kuchemann and L. H. G. Sterne, Pergamon, Oxford, 1965, Chap. 1.
- ⁹Chapman, S., and Cowling, T. G., *The Mathematical Theory of Non-Uniform Gases*, Cambridge University Press, Cambridge, UK, 1952.
- ¹⁰Bird, G. A., "Monte Carlo Simulation of Gas Flows," *Annual Review of Fluid Mechanics*, Vol. 10, 1978, pp. 11-31.
- ¹¹Vincenti, W. G., and Kruger, C. H., *Introduction to Physical Gas Dynamics*, Wiley, New York, 1965.
- ¹²Dorrance, W. H., *Viscous Hypersonic Flow*, McGraw-Hill, New York, 1962.
- ¹³Kogan, M. N., "Molecular Gas Dynamics," *Annual Review of Fluid Mechanics*, Vol. 5, 1973, pp. 383-404.
- ¹⁴Sherman, F. S., "The Transition from Continuum to Free-Molecular Flow," *Annual Review of Fluid Mechanics*, Vol. 1, 1969, pp. 317-340.
- ¹⁵Jameson, A., Schmidt, W., and Turkel, E., "Numerical Solutions of the Euler Equations by Finite Volume Methods Using Runge-Kutta Time-Stepping Schemes," AIAA Paper 81-1259, June 1981.
- ¹⁶Agarwal, R. K., and Deese, J. E., "Transonic Wing-Body Calculations Using Euler Equations," AIAA Paper 83-0501, Jan. 1983.
- ¹⁷Raj, P., Brennan, J. E., Keen, J. M., Long, L. N., Mani, K., Olling, C. R., Sikora, J. S., and Singer, S. W., "Three-Dimensional Aerodynamic Method (TEAM)," Vols. I, II, and III, AFWAL-TR-87-3074, June 1989.
- ¹⁸Thompson, P. A., *Compressible-Fluid Dynamics*, McGraw-Hill, New York, 1972.
- ¹⁹Roe, P. L., "Approximate Riemann Solvers, Parameter Vector, and Difference Schemes," *Journal of Computational Physics*, Vol. 43, 1981, pp. 357-372.
- ²⁰Gnoffo, P. A., "Application of Program LAURA to Three-Dimensional AOTV Flowfields," AIAA Paper 86-0565, Jan. 1986.
- ²¹Yen, S. M., "Numerical Solution of the Nonlinear Boltzmann Equation for Nonequilibrium Gas Flows," *Annual Review of Fluid Mechanics*, Vol. 16, 1984, pp. 67-97.
- ²²Liepmann, H., Narasimha, R., and Chanine, M. T., "Structure of a Plane Shock Layer," *Physics of Fluids*, Vol. 5, No. 11, 1962, p. 1313.
- ²³Tan, Z., Chen Y. K., Varghese, P. L., and Howell, J. R., "A New Numerical Strategy to Evaluate the Collision Integral of the Boltzmann Equation," Sixteenth International Symposium on Rarefied Gas Dynamics, Pasadena, CA, 1988.
- ²⁴Long, L. N., Coopersmith, R. M., and McLachlan, B. G., "Cellular Automata Applied to Gas Dynamic Problems," AIAA Paper 87-1384, June 1987.
- ²⁵Moss, J. N., Cuda, V., and Simmonds, A. L., "Nonequilibrium Effects for Hypersonic Transitional Flows," AIAA Paper 87-0404, Jan. 1987.
- ²⁶Nambu, K. S., "Theoretical Basis of the Direct Simulation Monte Carlo Method," *Journal of the Physical Society of Japan*, Vol. 52, 1983, p. 3382.
- ²⁷Celenligil, M. C., Bird, G. A., Moss, J. A., "Direct Simulation of Three-Dimensional Hypersonic Flow About Intersecting Blunt Wedges," AIAA Paper 88-0463, Jan. 1988.
- ²⁸Long, L. N., "A Three-Dimensional Navier-Stokes Code for the Connection Machine," *Proceedings of the Conference on Scientific Applications of the Connection Machine*, World Scientific, Singapore, June 1989.
- ²⁹Long, L. N., Khan, M. M. S., and Sharp, H. T., "A Massively Parallel Euler/Navier-Stokes Method," *Proceedings of the AIAA Computational Fluid Dynamics Conference*, AIAA, Washington, DC, June 1989.
- ³⁰Thompson, H. D., Webb, B. W., and Hoffman, J. D., "The Cell Reynolds Number Myth," *International Journal for Numerical Methods in Fluids*, Vol. 5, 1985, pp. 305-310.
- ³¹Anderson, D. A., Tannehill, J. C., and Pletcher, R. H., *Computational Fluid Dynamics and Heat Transfer*, McGraw-Hill, Washington, DC, 1984.
- ³²Long, L. N., "A Comparison of Navier-Stokes and Monte Carlo Methods for Hypersonic Flows," AIAA Paper 88-2730, June 1988.