Monte Carlo Simulation of Regular and Mach Reflection

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A numerical study was performed of the transition from regular to Mach reflection of oblique two-dimensional shock waves in the region of Mach number and deflection angle where both types of reflection are theoretically possible. The calculations have been carried out at the molecular level using the direct-simulation Monte Carlo method. The study confirms that this approach can provide a practical alternative to finite-difference and finite-element methods for the computation of continuum flows, especially when a dedicated minicomputer is used instead of a large machine in a general computing center. However, there are difficulties in the resolution of flow features that have characteristic dimensions that are small in comparison with those of the overall flowfield, and, in the present study, these precluded definitive conclusions about the type of reflection in the dual-solution region.

Introduction

CONSIDER the reflection at an ideal inviscid wall of the two-dimensional oblique shock wave produced by a deflection angle δ in a uniform supersonic stream of Mach number M_1, as shown in Fig. 1. In practice, a plane of symmetry acts as an ideal inviscid wall, and experiments show that regular reflection occurs for small deflection angles and Mach reflection occurs for large deflection angles. The conventional criterion for the onset of Mach reflection with increasing δ is that it occurs when δ becomes equal to the maximum deflection angle (or shock detachment angle) corresponding to the Mach number M_2 downstream of the incident shock.

The process is understood best if pressure p is plotted against flow angle θ in Fig. 2. Note that a downward flow deflection in Fig. 1 corresponds to a positive angle θ in Fig. 2. The upstream conditions are represented by point 1 at $p=p_1$, $\theta=0$, and any point downstream of an oblique shock wave of the positive family lies on the solid curve or "wave polar." The region downstream of the incident shock is represented by point 2, where $\theta_2=\delta$. Points behind a reflected shock wave in region 2 must lie on the appropriate dashed polar. For case A ($\theta_{2_A}=\delta_A$), regular reflection occurs, and the region (at $\theta=0$) downstream of the reflected shock is represented by the point 3_A. On the other hand, the reflected shock polar in case B does not reach the $\theta=0$ axis, and Mach reflection occurs. The flow properties are nonuniform in all of the regions downstream of the reflected wave complex, but points 3, 4, and 5 in the physical plane may be identified with the corresponding points in the p- θ plane. Note that corresponding points on opposite sides of a contact surface, such as 3 and 4, are coincident in the p- θ plane. The conventional criterion for the onset of Mach reflection is illustrated in Fig. 2 by the reflected wave polar C, corresponding to the deflection angle δ_C.

The overall configuration of wave polars in Fig. 2 is characteristic of high upstream Mach numbers. Mach reflection becomes possible for deflection angles equal to or greater than δ_D. This corresponds to the reflected shock polar D in Fig. 2, which intersects the $\theta=0$ axis at the normal shock point. This limiting case corresponds to a straight Mach stem and a contact surface parallel to the wall. For deflection angles between δ_D and δ_C, both regular and Mach reflection are possible, and the conventional criterion for the onset of Mach reflection implicitly assumes that regular reflection always occurs in this region. Recent wind-tunnel and shock-tube experiments have, however, led Henderson and Lozzi[1] to conclude that the conventional criterion is incorrect and that Mach reflection occurs as soon as it becomes possible, that is, at a deflection angle of δ_C. This effectively claims that Mach reflection always occurs in the range of deflection angle from δ_C to δ_D, where both types of reflection are theoretically possible.

Any supplement to the experimental data on the transition from regular to Mach reflection would appear to have to be numerical rather than analytical. The direct-simulation Monte Carlo method[2] already has been put forward[3] as an alternative to finite-difference methods for this type of continuum flow calculation. It is particularly suited to the reflected shock problem in that the boundary layers at the walls may be eliminated by the specification of specular reflection at the walls. At the same time, the model is viscous, and the structure of the shock waves is physically real. Outside the shock waves and contact surface, the flow is in local thermodynamic equilibrium, and, as long as there are sufficient collisions to keep it in equilibrium, the overall flow pattern is

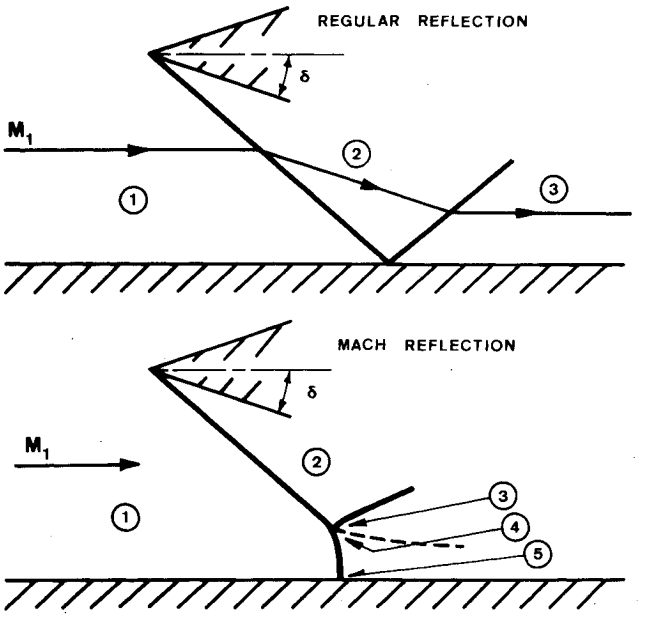

Fig. 1 Reflection of an oblique two-dimensional shock wave from a solid wall.

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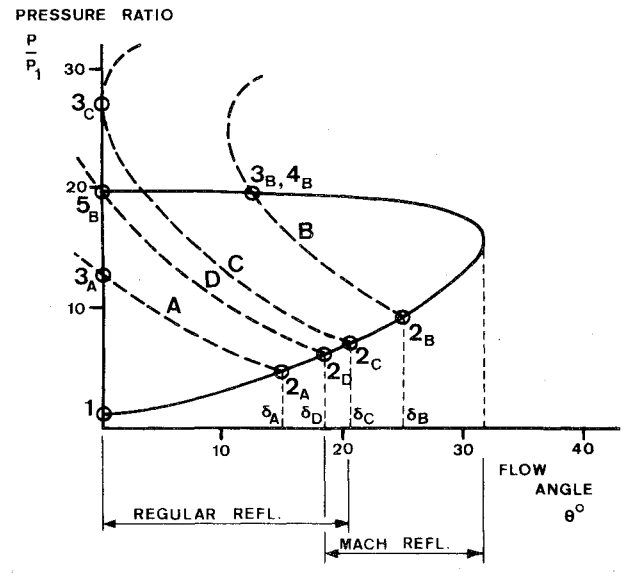

Fig. 2 Oblique shock-wave reflection in the pressure-flow-angle plane.

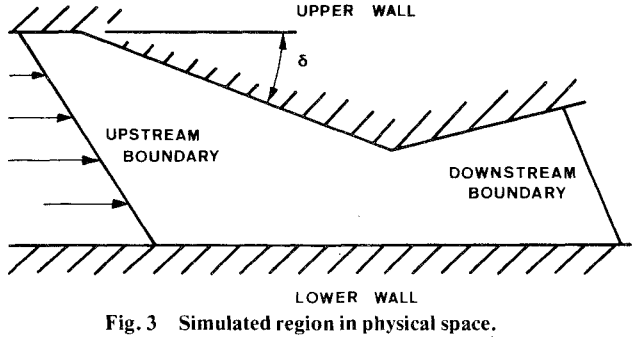

Fig. 3 Simulated region in physical space.

independent of Knudsen number. The shock waves in a conventional finite-difference solution are a direct consequence of second-order pseudoviscosity terms, and their structure is physically unreal. However, the major advantages of the molecular simulation are that an orthogonal grid or cell structure is not required and that stability problems are absent.

The disadvantage of molecular simulation is the large amount of computing time required to move around thousands of simulated molecules and to calculate millions of collisions amongst them. It was pointed out in the previous study[3] that this type of calculation would be performed in the most cost-effective manner by a dedicated minicomputer rather than by a large machine in a general computing center. A major objective of the present paper is to demonstrate the effectiveness of this approach.

Method and Problem Description

The direct-simulation Monte Carlo method[2] is a technique for the computer modeling of a real-gas flow by some thousands of simulated molecules. The velocity components and position coordinates of the simulated molecules are stored in the computer and are modified with time as the molecules are followed concurrently through representative collisions and boundary interactions in simulated physical space. The flow under consideration is two-dimensional in the x y plane, and only the x and y position coordinates need be stored for each molecule. All three velocity components must be stored, since the collisions are treated as three-dimensional. The hard-sphere molecular model was used for the calculations so that the results apply to a monatomic gas with a specific heat ratio of 5/3. The energy sink model[2] with two internal degrees of freedom was used in the previous study[3] to enable direct comparisons to be made with experiments employing a diatomic gas, but, since the molecular model has no qualitative effect on the transition from regular to Mach reflection, the simpler model has been preferred.

The simulated region in physical space is illustrated in Fig. 3. It is bounded by upstream and downstream flow boundaries and by upper and lower specularly reflecting walls. Molecules enter the upstream boundary with typical velocity components and position coordinates appropriate to a uniform supersonic flow in the x direction. The lower wall is everywhere parallel to the x axis, and the incident shock wave is generated at a sharp deflection of the upper wall through the angle δ. This convergence of the duct is reversed by a sharp divergent angular change at a location downstream of the point at which the incident shock strikes the lower wall. This insures that the downstream flow boundary is sufficiently supersonic for there to be virtually no upstream moving molecules. The flowfield is initially a vacuum, and the molecules commence entering the upstream boundary at zero time. This leads to a physically real unsteady flow, and it was found that, as long as the upper wall divergence is sufficiently far forward (leading to a reasonably large area minimum of the channel), a steady flow pattern is set up as the large-time solution. If the minimum area was set too small, it was found that a blocked flow was set up such that a strong incident shock moved right back to the upstream boundary, and the desired wave reflection pattern was not established.

The flowfield generally was divided into 20 rows, each containing 50 cells, although several runs were made with 25 rows of 100 cells. The total number of simulated molecules within the flowfield at any instant ranged from 6,000 to 10,000. Unit length was defined by the initial height of the channel, and the mean free path in the undisturbed gas was of the order of 0.01. This meant that the cell width was larger than the undisturbed mean free path, thus leading to some "smearing" of the shock-wave profiles.

The calculations were carried out on a disk based PDP 11/40 system. The memory size is 32K of 16-bit words or 16K of 32-bit floating point variables. The number of molecules and cells in these calculations would require 120K to run within the core. It therefore was necessary to divide the flow into blocks and to have only one of these in core at any instant. Appropriate buffer storage was set up for molecules transferring from one block to another. The machine time for these calculations was divided almost equally between central processor operations and the data transfer to and from the disks. The number of collisions calculated per hour in a collision-dominated (low Knudsen number) flow provides a useful measure fo computer speed. When used in the disk-core transfer mode to cope with the large-scale computations, the PDP 11/40 system calculates between 100,000 and 200,000 collisions/hr. This may be compared with the rate of approximately 5×10^6 collisions/hr on the CDC6600 that was used for the previous study.[3] It has proved to be entirely practical to run the system without any operator 24 hr a day, seven days a week. A typical run for the present study involves some 15×10^6 collisions, or approximately 100 hr of computation. This represents less than 2% of the annual utilization of a system, with a purchase price of the order of $40,000. If the machine is written off over 7 yr and a 10% maintenance cost is assumed, the cost of each run is less than $200. The same run would require some 3 hr on a CDC 6600 or 40 min on a CDC 7600.

Results

Attention was concentrated on wave reflections in a monatomic gas at a Mach number of 4. Figure 2 has, in fact, been drawn to scale for this case, and the numerical values apply directly to it. The simulation results are presented most effectively through plots of the pressure contours in the x y plane.

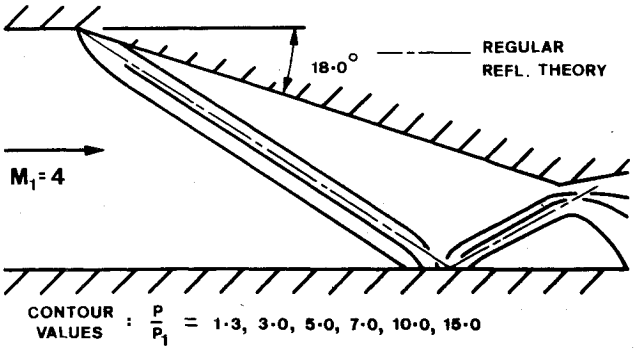

Fig. 4 Pressure contours from the simulation of the $\delta = 18°$ case.

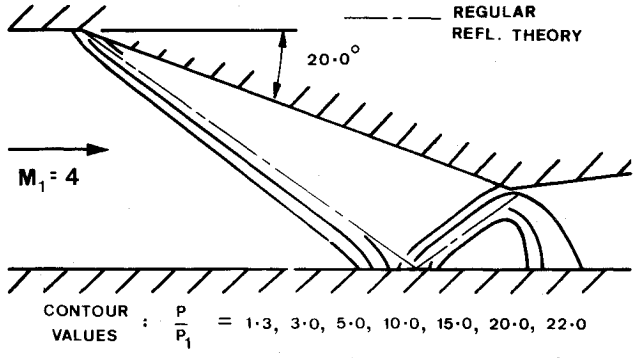

Fig. 5 Pressure contours from the simulation of the $\delta = 20°$ case.

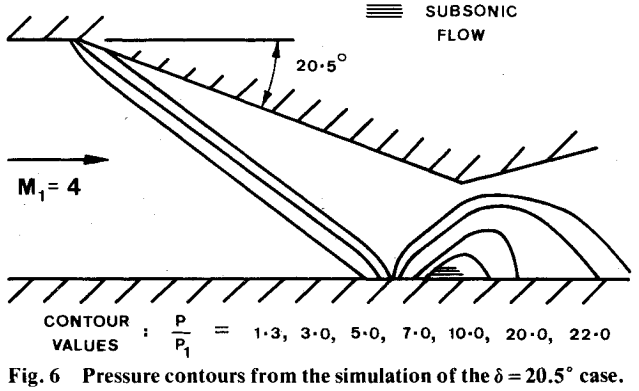

Fig. 6 Pressure contours from the simulation of the $\delta = 20.5°$ case.

Figure 4 shows the pressure contours for a deflection angle δ of 18°, for which only regular reflection is possible. The general form of these contours is similar to those previously obtained[4] for the corresponding one-dimensional unsteady problem of the reflection of a normal shock wave from a wall. The corresponding pressure contours for the $\delta = 20°$ case are shown in Fig. 5. This deflection angle is in the range for which both regular and Mach reflection are possible, but the contours are qualitatively similar to those for the $\delta = 18°$ case. Note that the pressure in a large region of this flow is substantially higher than the $19.75p_1$ corresponding to the compression of a Mach 4 monatomic gas flow by a normal shock wave.

The two sets of contours in Figs. 6 and 7 are for deflection angles of 20.5° and 21.5°, respectively. These angles are both above the value of 20.4° at which Mach reflection must occur. For $\delta = 20.5$, the contours are hardly different from those for regular reflection, and the region of subsonic flow is very small. For $\delta = 21.5$, the central contours of the reflecting shock remain near normal for a larger distance above the wall, and the region of subsonic flow is more extensive. Note that the pressure behind the shock continues to exceed the normal shock value. This can be attributed to the subsonic

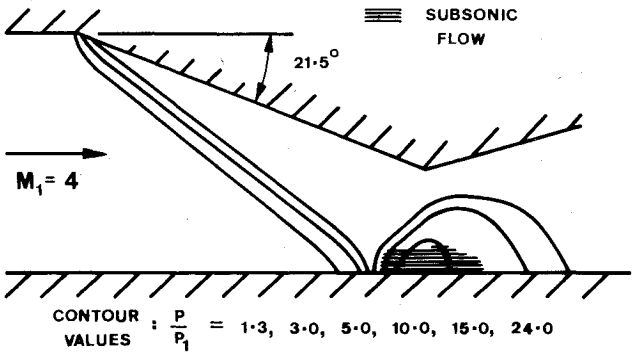

Fig. 7 Pressure contours from the simulation of the $\delta = 21.5°$ case.

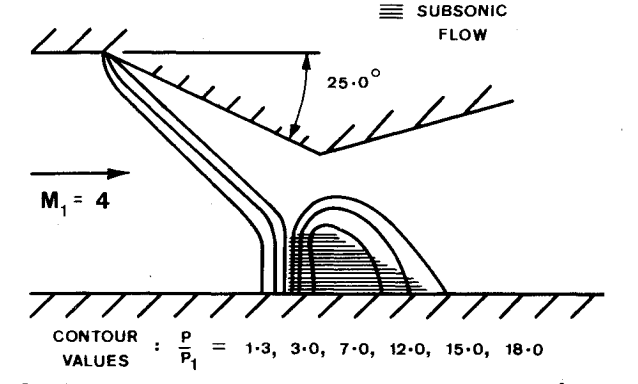

Fig. 8 Pressure contours from the simulation of the $\delta = 25°$ case.

compression that generally occurs behind the Mach stem, and, in this case, the Knudsen number is such that this region is merged with the shock wave.

Finally, Fig. 8 shows the pressure contours for the well-established Mach reflection corresponding to $\delta = 25°$. The triple point now has moved a significant distance from the wall, and the Mach stem is quite distinct. However, the expansion at the upper wall has had to be placed so far upstream that the reflected shock is affected quickly, and the area of further compression behind the Mach stem is small.

Discussion and Conclusions

The transition from regular to Mach reflection of an oblique shock wave has been computed at the molecular level. This gives the internal structure of the waves, but, since the main emphasis is on the macroscopic rather than the microscopic aspects of the flow, a cell size has been chosen such that the shock-wave thickness is approximately 50% too large. Even so, the resolution of the waves is similar to that in finite-difference calculations of the related unsteady flow[5] in which the shock thickness is a consequence of pseudoviscosity effects. The ease of application and the absence of stability problems make Monte Carlo simulation an attractive alternative to finite-difference and finite-element methods for some continuum-flow problems. It is particularly suited to this type of problem involving complex shock-wave configurations with inviscid boundaries. The cost of the enormous number of calculations required by the application of the direct-simulation Monte Carlo method to low-Knudsen-number flows brought down to a reasonable figure if they are carried out on a dedicated minicomputer system rather than on a large computer in a general computing center.

Figures 5-8 suggest that regular reflection can occur in the range of deflection angles for which both types of reflection are possible. It is possible that the early transition to Mach reflection which is observed in experiments[1] results from disturbances that are absent in an idealized numerical model. However, it is also possible that the apparent regular reflection in Fig. 5 is a consequence of the comparatively high

Knudsen number (0.01 based on the channel height), and a Mach reflection pattern would emerge at lower Knudsen numbers. This possibility arises as a result of the shortness of the Mach stem in the reflections in the dual-solution region, which would translate to the order of the upstream mean free path in the present calculations. In presenting the results, emphasis has been placed on the pressure because of the large difference between the regular and Mach reflection values for the downstream pressure. Figure 2 shows that the pressure just behind the Mach reflection is $19.75p$, that for case C is $26p_1$. The extent of the pressure contour for $p/p_1 = 22$ in Fig. 5 might appear to rule out Mach reflection, but it should be remembered that there is a recompression behind the Mach stem. Therefore, although the Monte Carlo simulation is adequate for regular reflection or for Mach reflection when the length of the Mach stem is a significant fraction of the channel height, as in Fig. 8, it is unable to resolve flow details with a characteristic dimension that is very small in comparison with this height. These difficulties with respect to resolution are associated with the cell or mesh size and apply to finite-difference as well as to Monte Carlo calculations.

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