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THE IMPORTANCE OF BOUNDARY CONDITIONS
IN THE NUMERICAL TREATMENT OF HYPERBOLIC EQUATIONS

by

Gino Moretti

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NUMERICAL TREATMENT OF HYPERBOLIC EQUATIONS

Gino Moretti

Polytechnic Institute of Brooklyn
Farmingdale, New York

November 1968

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THE IMPORTANCE OF BOUNDARY CONDITIONS
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ABSTRACT

Many of the existing computations of initial-and-boundary value problems in fluid mechanics suffer from unrealistic treatment of boundary points. Three categories of boundaries are briefly discussed: rigid walls, arbitrary boundaries of a computational region in a subsonic flow, and shock waves. An attempt is made to show in what sense the numerical treatment of such boundaries may be physically wrong and what can be done instead. Examples from the blunt body problem, the transonic flow in a nozzle, the incompressible inviscid flow past a circle, and the quasi-one-dimensional flow in a Laval nozzle, are shown.

*

This paper was presented at the International Symposium on High-Speed Computing in Fluid Dynamics, Monterey, California, August 18-24, 1968.

1. INTRODUCTION

A great deal of work has been performed in the attempt to use numerical techniques to solve complicated problems in fluid mechanics, but too many results are far from being satisfactory. Failures are sometimes ascribed to such mysterious causes as "non-linear instability" (a term which is meaningless for lack of a definition and sounds very much like the "Hic sunt leones" label attached to unexplored lands in middle-age maps). I will try to show in this paper that in mixed initial-and-boundary-value problems major troubles arise if the boundary conditions are not properly handled.

Surprisingly, the difficulties of boundary-value problems so far seem to have been overestimated. Let us quote, for example, from page 128 of the authoritative book by Richtmyer and Morton¹: "For one thing the effect of boundary conditions has not so far been considered"; and from page 167: "To treat the more complex boundaries that can arise with more space dimensions is very much more difficult and little has so far been achieved in this area". Consequently, Richtmyer's book, which is a study in mathematical foundations, does not even attempt to attack the problem. Unfortunately, since nobody else does it in a book of the same level, oriented towards applications, the physicist and the engineer who face the task of solving a practical problem are led to believe that

what is not discussed by Richtmyer is a matter of no consequence. In other words, they tend to underestimate the importance of boundary conditions which are, instead, the governing elements of the entire computation.

The situation is worsened by the fact that the few examples of multi-dimensional problems given by Richtmyer in Chapter 13 (taken from the existing literature) show a number of troubles within the computational region whereas such troubles are generated at the boundaries.

There are, in fact, two classes of points to consider in a numerical computation: interior points and boundary points. As far as the interior points are concerned, many techniques are available. One can discuss their relative advantages or disadvantages in terms of, say, computational speed, accuracy, programming difficulty and so on. There are ways of determining such properties through a local analysis and some of the techniques, accurate to the second order, prove to be very good for all practical purposes. Nevertheless, many of the published computations show a progressive deterioration of results which is inconsistent with the good local qualities of the technique used for interior points and is then attributed to "non-linear instability". A "cure" for the latter is sought in damping devices ("artificial viscosity"); a procedure which is physically unjustified and which may provide smooth results at a very high

price, that is, the destruction of accuracy². In what follows, I would like to show a number of cases where there is no reason for introducing a concept of non-linear instability, conflicting with the local stability, if care is taken not to feed unrealistic perturbations from the boundaries. To emphasize the relevant arguments, the presentation will necessarily be sketchy and many details will be left unmentioned.

2. BOUNDARY CONDITIONS ON A RIGID WALL

Let us begin with few obvious statements.

(1) A fluid flow problem is described by a system of partial differential equations which are classically known as the indefinite equations of motion. Such equations are called indefinite because they apply to any problem in general but the equations per se do not define a specific problem.

(2) The problem is defined only when a proper set of initial and/or boundary conditions is given. The boundary conditions are such an important part of a definition of a problem that the patterns of two flow fields can be completely different from one another because of some differences in the flow boundaries, despite the fact that both flows obey the same system of indefinite partial differential equations.

(3) For each system of equations there are a number of necessary and sufficient boundary conditions. For example, for an inviscid flow the condition on a rigid, fixed wall is the

vanishing of the normal component of the velocity, V_n .

At the risk of appearing trivial, let me state that no other condition may be imposed on the rigid wall since the one above is sufficient to determine the flow field.

Now, let us see what happens when a problem of inviscid flow is treated by a numerical technique. A certain mesh is used. At the interior mesh-points the partial differential equations are substituted by finite-difference equations (and we will assume that the substitution satisfies all conditions for local stability and convergence). At each computational step, information is transmitted from each point to its neighboring points via the computation of finite differences. In this way, the boundary mesh-points influence their neighbors and transmit the effects of the boundary condition into the flow field.

For this to happen, the values of all physical quantities at boundary points must be known at each computational step. At a rigid, fixed boundary only the normal component of the velocity, V_n is clearly defined, but the tangential velocity, \vec{V}_t , the pressure, p , the density, ρ , are also required. At this point, we are required to find some way of computing them using information from interior points plus the boundary condition. In other words, we must solve finite difference approximations to the partial differential equations of motion in their limiting form as one approaches the boundary. If

we do not proceed properly, we face the risk of over-specifying the boundary conditions themselves and, in all probability, these overspecified boundary conditions will not be consistent with the nature of the boundary and the limiting forms of the equations of motion.

Unexpected procedures are found in the literature. In general, it seems that an "easy" way for solving the equations of motion at points on a rigid wall consists of adding an extra row of points behind the wall and computing the wall points with the same routine used for interior points. At each computational step, the problem is then shifted into that of defining values at the extra points which provide good derivatives at the wall points. To this effect, many authors use what they call a "reflection-principle" which is not a principle at all and should rather be called a reflection technique. I have been unable to find a precise definition of such a technique in the literature. In its crudest formulation, all physical parameters are specularly reflected on the rigid wall except V_n which is assumed as anti-symmetric. Bohachevsky et al.³, page 603 and 605; Bohachevsky et al.⁴, page 778; Burstein⁵, page 2114; Singleton⁶, page 2-2). Unfortunately, only the assumption regarding V_n is legitimate since it produces a vanishing V_n at the wall automatically and the normal derivatives of V_n so computed is the same as a one-sided derivative computed by finite differences, using

the interior point information (the accuracy so obtained is, however, very low). The other assumptions force the normal derivatives of the remaining quantities to vanish at the wall. These are redundant conditions and are physically wrong.

To show how far the real situation is from the assumed one, let us consider the case of a circular obstacle in a uniform flow, the flow being steady, two-dimensional, incompressible, and irrotational. With a proper scaling of the variables, the flow is described by the complex potential,

$$W = z + \frac{1}{z}$$

where $z = x + iy$ is the complex coordinate in the physical plane. Consequently, the complex velocity is

$$V = 1 - \frac{1}{z^2}$$

The velocity components in polar coordinates (u in the radial direction, v in the transverse direction) are

$$u = \left(1 - \frac{1}{r^2}\right) \cos \theta$$

$$v = \left(1 + \frac{1}{r^2}\right) \sin \theta$$

and the pressure coefficient is

$$C_p = -\frac{1}{r^4} + \frac{2 \cos 2\theta}{r^2}$$

The obstacle is defined by $r = 1$. The normal derivatives of pressure and velocity component at the obstacle wall are:

$$\left. \begin{aligned} \frac{\partial C_p}{\partial r} &= 8 \sin^2 \theta \\ \frac{\partial u}{\partial r} &= 2 \cos \theta \\ \frac{\partial v}{\partial r} &= -2 \sin \theta \end{aligned} \right\} \text{ at } r = 1$$

Obviously, such normal derivatives of pressure and v are far from vanishing, except at the stagnation points ($\theta = 0, \pi$). For example, Fig. 1 shows the distribution of C_p and v along the radius at $\theta = \pi/2$ (solid lines).

The flow field described above can be considered as the asymptotic state of a time-dependent computation. If, in performing the latter, conditions are imposed at the boundary which are patently conflicting with the real nature of the solution, one is left to wonder why certain computations did not "explode". There are two reasons. One is that the departure from symmetry is not substantial in the vicinity of a stagnation point or along a wall which does not differ too much from an infinite straight line. The other, and more important, is that a very high artificial viscosity has been used -- an ill-advised procedure as I said before.

Results of the following example support the above arguments. Consider a blunt body with a circular nose in a supersonic stream ($M_\infty = 4$). The shock layer is computed first by a technique which I developed^{7,8,9}. No claim is made here for it as the only possible technique or the best one. However, a certain effort has been made to compute the boundary points with a physical insight:

(1) The pressure is determined by an equation where the relevant parameters are the pressure and the normal component of the velocity because the pressure waves sent to the wall in the normal directions bounce back from it due to the condition of impermeability ($V_n = 0$). The technique used is a modified method of characteristics in the plane defined by the normal to the wall and the time axis.

(2) The entropy is kept constant along the particle path on the wall; from pressure and entropy, the density follows.

(3) The tangential velocity is determined by a second-order accurate finite-different formulation of a momentum equation.

A 7×12 mesh is used to cover the computational region. The final results are reported at pages 48 and 49 of the report mentioned above⁹ and can be considered accurate at least to within one tenth of 1%. (Much better results are obtained with a 10×14 mesh -- See⁹ pages

50 and 51). Fig. 2 shows the pressure distributions between body and shock along five different radii ($\theta = 0$ is the symmetry line and θ increases from the symmetry line to the shoulder of the body). Here again the non-symmetrical behavior of p with respect to the rigid wall is evident (and is qualitatively similar to the incompressible case mentioned above). It may be expected that in repeating the computation after using symmetry rules at the body points (and, of course, leaving the rest unchanged) the results should not be too much affected near the symmetry line but should show a definite worsening with increasing θ . This is what actually happens. Fig. 3 shows the same lines as Fig. 2 as dashed lines, and the results of the second computation as solid lines. The slope of the p -curves at the wall is larger than the "exact" one, as a reaction of the numerical scheme to an attempt to enforce a vanishing slope. Wiggles are generated, which propagate through the shock layer, modify the shock shape and eventually get trapped between shock and body. Fig. 3 has been drawn at the 560th computational step, which is the last step computed⁹. After it, the results are practically frozen in both computations. In cases where the wall geometry is more complicated, the errors generated by the reflection technique may eventually make the results unstable.

Another technique for prescribing values on the extra row of points consists of extrapolating from inner points. Regardless of the order of curve-fitting used to extrapolate, it is easy to see that such a procedure is arbitrary, with no connection with the physical behavior of the flow. Consider three points, A, B, and C. The first is an interior point, the second is the point on the wall, and the third belongs to the auxiliary row, behind the wall. We know the values of a physical parameter, f at A and B and its value at C is obtained by extrapolation. In going from t to the next computational line, $t + \Delta t$, some derivatives are needed, for example $\partial f / \partial n$, $\partial^2 f / \partial n^2$ where n is a coordinate in the normal direction. The increment in f at B depends on those derivatives, which in turn depend on the geometrical nature of the fitting curve, not on physical properties.

For the sake of brevity, I do not present here any result obtained by using extrapolation techniques instead of the technique mentioned above⁹. They are particularly bad when strong curvature effects dominate the behavior of the flow in the vicinity of the wall. A more complete discussion of such effects will be published elsewhere.

Other attempts to deal with boundary points on a rigid wall, where the physical nature of the problem is not satisfied, can be found in the literature. Again in the blunt body problem, Lapidus¹⁰ introduces a diffusion along the boundary by averaging

certain values and arbitrarily corrects the momentum vector to make it parallel to the wall. The results, as the paper itself shows, are not very good.

3. PERMEABLE SUBSONIC BOUNDARIES

The second problem to be carefully considered refers to the handling of those boundaries which are not rigid walls but arbitrary, permeable limits of the computational region. For the sake of an argument, let us confine ourselves to the case of an inviscid, compressible flow.

The computational region must be finite. Since most of the practical problems deal with flows in an infinite domain, one is attempted to consider only a part of it by drawing arbitrary boundaries such as the ones shown in Fig. 4. The flow may enter the computational region or exit from it through such boundaries. In Fig. 4, CD, GH are "entry" boundaries, whereas AB, EF, and HL are "exit" boundaries.

If the flow is supersonic at all points of one of these lines, there are no difficulties. If the line is an entry boundary, all values can be prescribed along it. Making them consistent with the flow upstream of the boundary is a task independent of the numerical computation. Once such values are prescribed, there is no feedback into the region upstream from the computational region. If the line is an exit boundary, there is no feedback into the computational region from the

region downstream and there is no feedback either from the exit boundary onto the preceding row of points, so that the values at the exit boundary points can be determined, at each step, by a simple linear extrapolation from the inside of the computational region.

If the flow is subsonic on an entry line, any change in the computational region will send waves upstream through the line. These waves modify the upstream flow and the values on the entry line. At the next computational step, one should assume updated values on that line, but this implies bringing in the influence of the upstream flow. Thus, at least a part of the outer flow should be treated in the same way as the inner flow, which is inconsistent with the existence of a partition. Similar considerations can be made for a subsonic exit line.

Any permeable limit of a computational region with subsonic points and constant values assumed on it makes a time-dependent problem ill-posed. Disturbances are created which propagate inwards. Here again, there are cases where the results do not look so bad, because the arbitrary boundary is far from the region of interest and the computation is halted before the perturbation waves have a chance of piling up. But this is not a valid argument.

The only possible way out is to extend the computational region to where the physical values are well defined and unaffected by traveling waves, either going inwards or outwards.

This amounts to extending the region to infinity. In certain cases it is possible to do it. For example, in the case of a nozzle with a subsonic entrance, one may imagine the nozzle extended to an infinite reservoir, where the velocity vanishes and the other physical parameters take on their stagnation values. In the case of a flow about an obstacle, subsonic and uniform at infinity, the computation must be performed on the whole space. We can do this and yet keep the number of mesh points within reasonable limits by mapping the infinite physical domain into a finite region, a rectangle, say. Suppose that AB (Fig. 5) maps the infinity of the physical plane, where all physical parameters are given, constant values. The CD line maps some line lying in the physical plane at a large, but finite distance from the region of interest. The computation is performed on the rectangular mesh, obviously using the equations of motion after transformation in the auxiliary plane. To compute the values on the CD line we use information from the AB line and from the EF line. The information from the AB line brings in exact values. The geometrical stretching between CD and AB (and, consequently, the damping of outgoing waves and the absence of incoming waves) is included in the coefficients which affect the transformed equations. One may be skeptical about the amount of error introduced by a stretching where a local value of a coefficient should accurately represent the global

phenomenon actually taking place throughout an infinite region (such as the physical region mapped onto the strip, ABCD). However, the flow in the strip is nearly uniform. All derivatives are small and the local evaluation of the coefficients is sufficient to insure accuracy. The important point is that the calculation in the rectangle is physically well-posed.

I am indebted to Professor M. Van Dyke for pointing out to me after the oral presentation of this paper that a similar conclusion was reached by Wang and Longwell¹¹. There the authors compare the results of two calculations of incompressible viscous flow, one with an arbitrary truncation of the computational region and the other with a stretching of coordinates as described above. The results of the latter computation are undoubtedly closer to physical reality than those of the former one. Because of the nature of the problem, both sets of results are smooth. In the first case such smoothness provides a good example of how dangerous it may be to infer accuracy from smoothness.

For compressible inviscid flows wiggles build up as a consequence of the presence of subsonic boundaries. For example, Fig. 6 shows the pressure distribution along the wall of a two-dimensional Laval nozzle as assumed initially (dotted line) and after 300 computational steps. The technique used is the same as the one outlined⁹ for the blunt body problem. The wiggles in the results are a direct conse-

quence of an arbitrary limitation of the computed region. Waves traveling upstream are reflected at the boundary and trapped within the computational mesh. Results for an axisymmetric nozzle computed with the same technique but with a stretching of coordinates which let the nozzle emerge from an infinite reservoir are reported by Migdal et al.¹² and appear to be extremely good.

Another test of the infinite-stretching idea is currently in progress. The two-dimensional compressible inviscid flow about a circle in a stream, uniform at infinity, is being studied. For very low values of the free stream Mach number ($M = 0.1$, say), the flow is practically incompressible. The problem is analyzed as the time-dependent evolution of a flow, starting impulsively from rest. At the rigid boundary, the conditions are treated as outlined in the preceding section. A second-order accurate technique is used for the interior points. A number of stretching functions has been used in an attempt to optimize the clustering of mesh points near the body.¹³ The dots in Fig. 1 of this paper show the computed values of pressure and velocity at $\theta = \pi/2$, after 500 computational steps. The agreement with the theoretical values for an incompressible flow is extremely good, which proves that both boundary conditions, at the rigid wall and at infinity, are properly treated.

4. IMBEDDED SHOCKS

A third problem which should be mentioned when talking about the treatment of boundary conditions is the problem of discontinuity surfaces. I will confine myself to a brief analysis of shock waves. A shock can be considered as a boundary between two regions where the physical parameters are continuous and differentiable. In inviscid flows, shocks are discontinuities and should be handled as such since the jump conditions across a shock are not compatible with Euler's differential equations. One may anticipate, thus, that any attempt to compute a flow containing a shock by a numerical technique which closely approximates the inviscid differential equations is bound to fail (Richtmyer and Morton¹, pages 329, Fig. 12.4; Moretti²). It is well-known, however, that sharp transitions leading from the state ahead of a shock to the state behind it can be obtained as solutions of the Navier-Stokes equations and that the thickness of the transitional region is related to the Reynolds number of the flow. A similar result is obtainable by using difference equations obtained from the partial differential equations for inviscid flow, with the additions of an artificial viscosity (Richtmyer and Morton¹, page 327, Fig. 12.3). However, the Reynolds number is so high in most practical cases that, to obtain a good value of the shock thickness, one should use mesh

sizes many orders of magnitude smaller than the mesh sizes permitted by the capacity and speed of our present computers. A coarse mesh and a high viscosity (either natural or artificial) spreads the shock thickness unrealistically. In addition, the high viscosity affects the whole flow field and makes the solution depart substantially from the inviscid one (or the one corresponding to the actual, high Reynolds number). In this connection, a note of warning should be given to the reader of page 328 in Richtmyer's book. There the problem is that of a jump between two constant states, where all derivatives vanish. Obviously, the presence of viscosity does not affect a uniform flow and does not affect a numerical computation of a uniform flow either. However, the numerical solution of any other case treated as an inviscid flow with the addition of artificial viscosity is, in all practical calculation, extremely poor from the point of view of accuracy.

The Lax-Wendroff scheme (Richtmyer and Morton¹, page 330) is undoubtedly a closer approximation to the differential equations of inviscid flow than a first-order scheme with added artificial viscosity. In addition, it is consistent with the Rankine-Hugoniot conditions across a shock. Therefore, it is considered a powerful tool for the numerical analysis of shocked flows, and some interesting results have indeed been obtained. However, aside from the

unrealistic spreading of the shock thickness over several mesh points, it shows another disturbing feature, that is, at least on one side of the shock there are oscillations. Such a situation is clearly shown by Fig. 12.6 of Richtmyer's book¹, page 333. A reader, familiar with the theory of Fourier series, is reminded of a similar phenomenon which appears any time a Fourier expansion is attempted on a discontinuous function. See, for example, Fig. 7 where the Fourier expansions of a saw-tooth function, truncated at the tenth term and at the 50th term, are plotted in the vicinity of the discontinuity. The fact that such a Fourier expansion is not a suitable way of handling a discontinuity is proved by the Gibbs phenomenon¹⁴.

Now, when a Fourier expansion of a discontinuous function is needed, one proceeds first to eliminate the discontinuities by subtracting from the given function the proper number of saw-tooth functions with suitable values of the jumps, and then to expand the continuous function so obtained. The convergence is quick and the Gibbs phenomenon does not appear.

The same principle should inspire the numerical treatment of fluid flows containing shocks. The regions between shocks are smooth and can be handled with coarse meshes. The shocks (which, in a time-dependent case, must be left free to move) can be described with ease by

the Rankine-Hugoniot conditions plus one equation written from the inside of each region up to the shock. Such an equation must have the nature of the compatibility equation on a characteristic. In multi-dimensional problems, the method of characteristics has to be modified suitably. That this can be done is proved by the excellent results obtained⁹ if all the shock and body points are computed using such a technique.

Last year, I reported¹⁵ a preliminary approach to a more ambitious problem. A steady three-dimensional symmetric flow was studied, which is strongly compressed in a region and strongly expanded in another one. An imbedded shock builds up in a part of the flow and dies out somewhere.

In a simpler case, the possibility has been proved not only of fitting a moving shock so that the solution is extremely accurate despite the use of a coarse mesh, but also of predicting where and when the shock starts building up without resorting to coalescence of characteristics². In Fig. 8, some frames from a computer-made movie are shown, from which the formation of a shock appears together with its evolution and final freezing at the place where the steady shock should be, according to the geometry of the nozzle and the exit pressure.

5. CONCLUSIONS

Let us summarize now the basic points of the discussion.

(1) There are two classes of points in a numerical computation, interior points and boundary points.

(2) No conclusion can be drawn on the effectiveness of a technique for interior points unless one is sure that no disturbances are fed in from the boundaries.

(3) One can discuss the degree of accuracy of a particular technique for interior points; however, within the current state of the art, the question, as far as boundary points are concerned, is different, viz.: Is the technique used right or wrong?

(4) Cures for "non-linear instability" such as artificial viscosity decrease accuracy and conceal the nature of the trouble.

(5) Rigid wall points can be properly treated. Some examples are shown in this paper and warrant more intensive study.

(6) Preliminary examples show that, for certain flows with simple conditions at infinity, the use of a stretching technique provides satisfactory results.

(7) Imbedded shock waves should be treated as discontinuities, if one aims to achieve accuracy without having to resort to a prohibitively fine computational mesh.

(8) Beautiful results can be achieved on the present generation of computers, using a small number of mesh

points and consequently spending a short time to compute, if the boundary value problem is properly handled. In fact, I believe that finite-difference techniques for initial-and-boundary-value problems are a powerful, accurate, and inexpensive computation tool.

ACKNOWLEDGMENT

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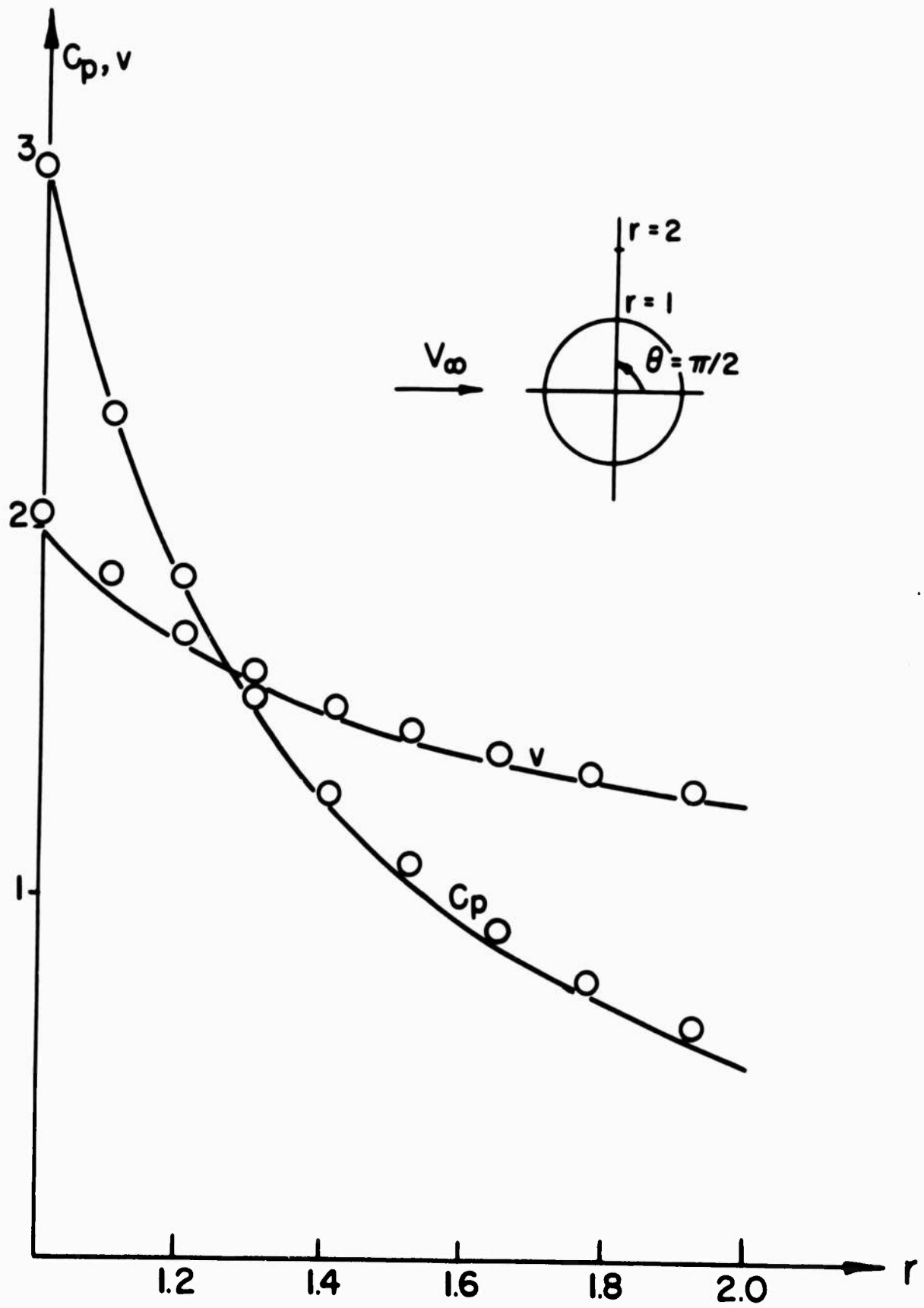


FIG. 1

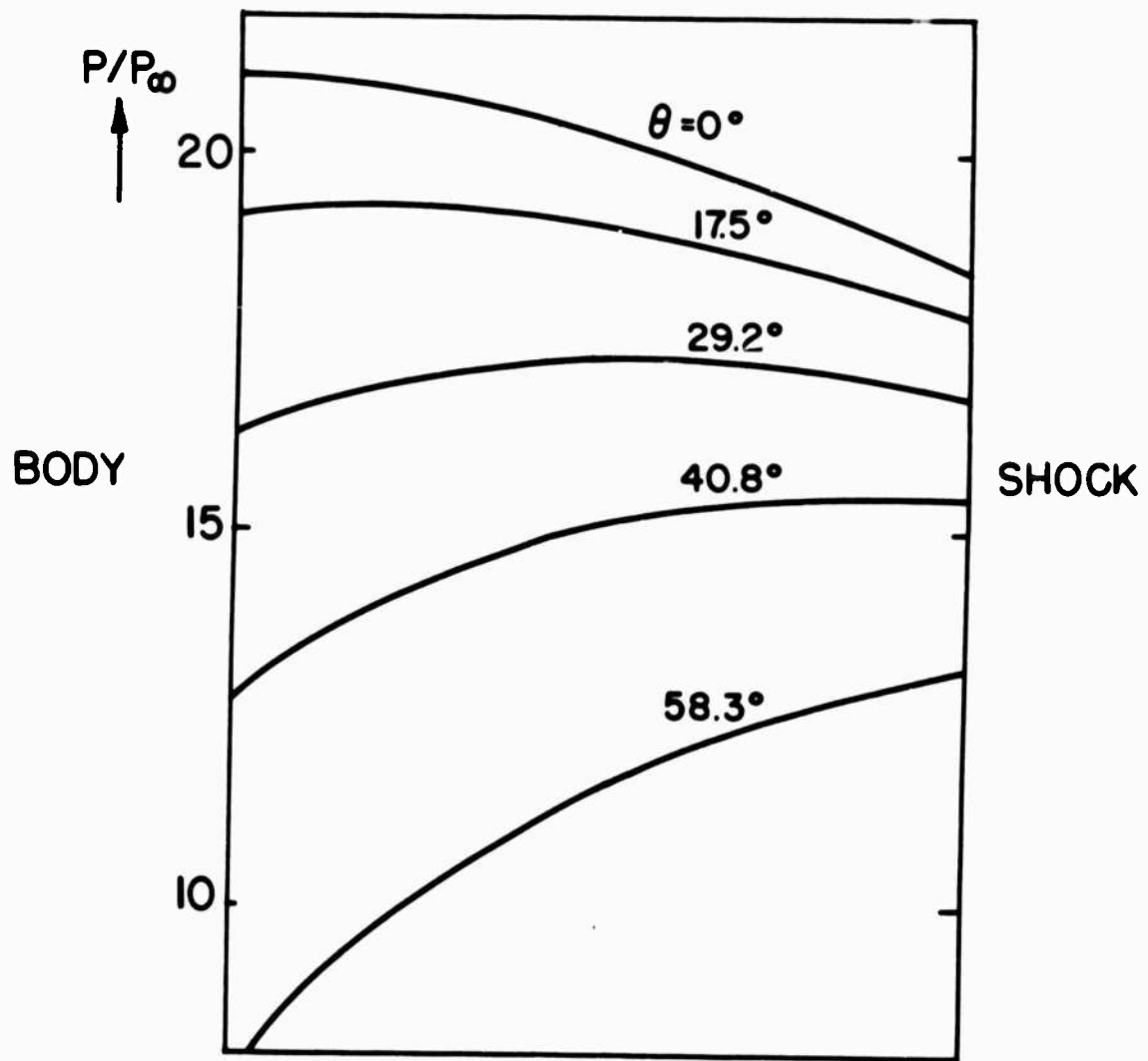


FIG. 2

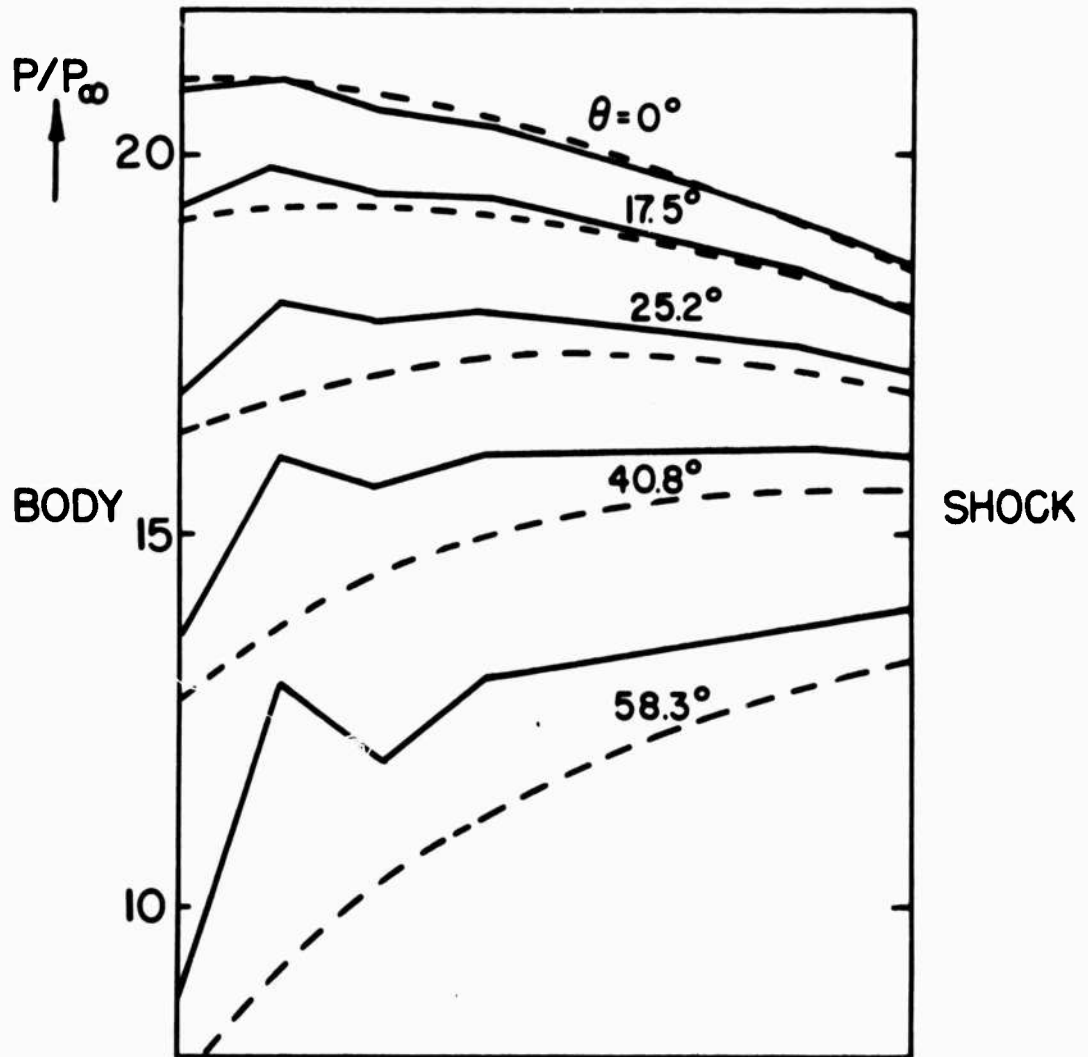


FIG. 3

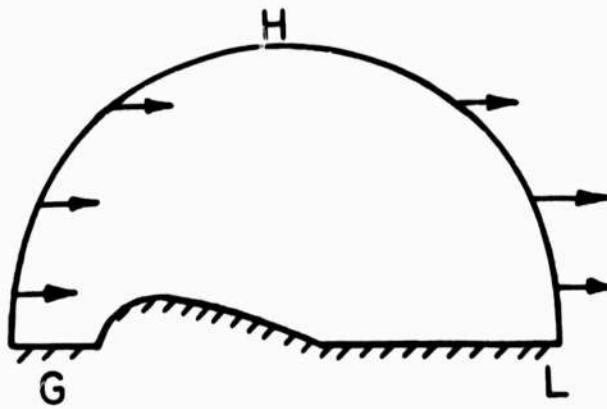
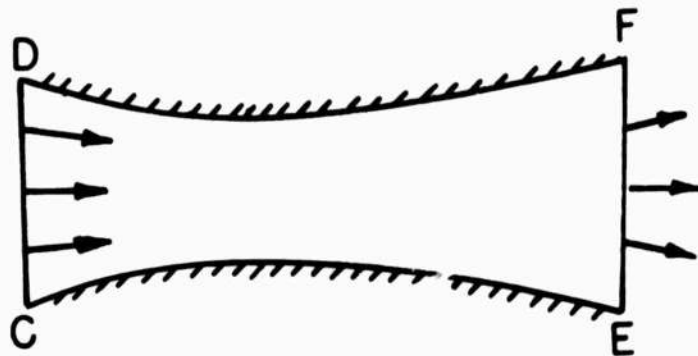
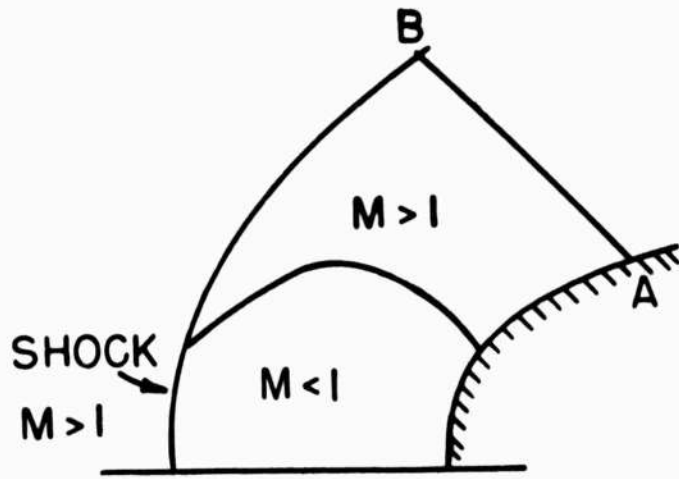


FIG. 4

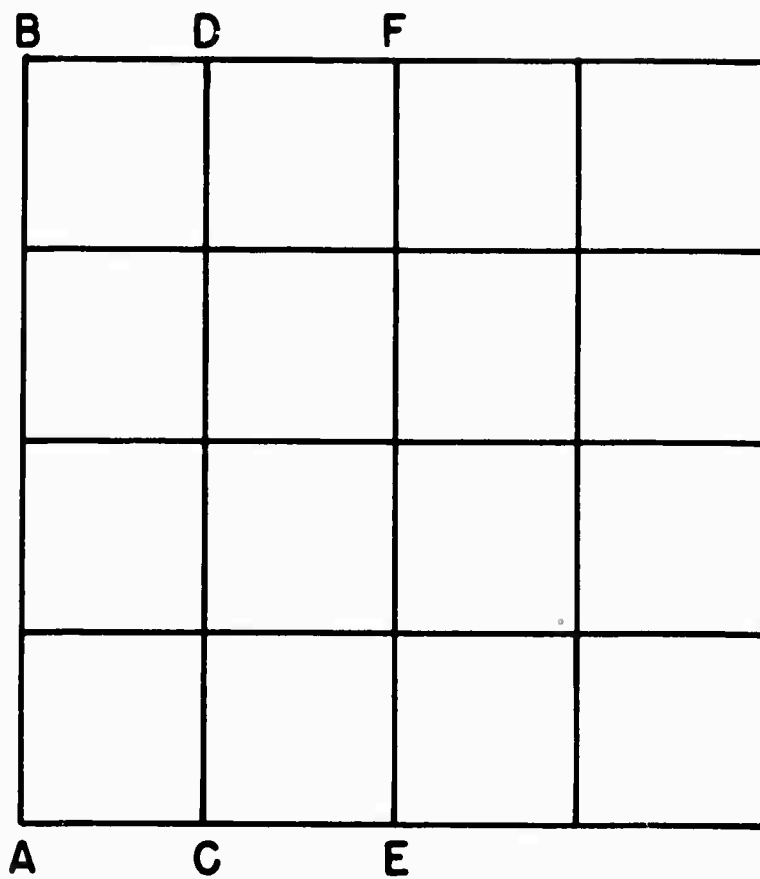


FIG. 5

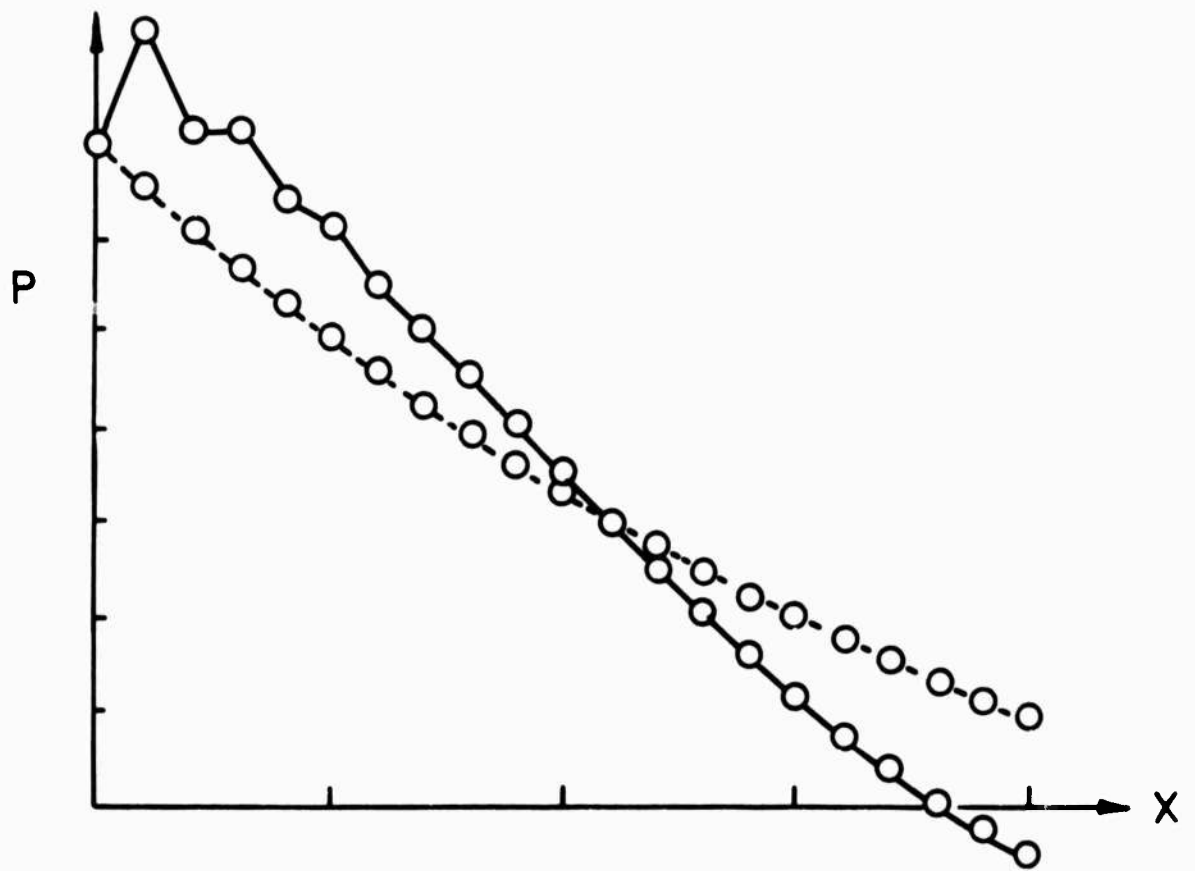


FIG. 6

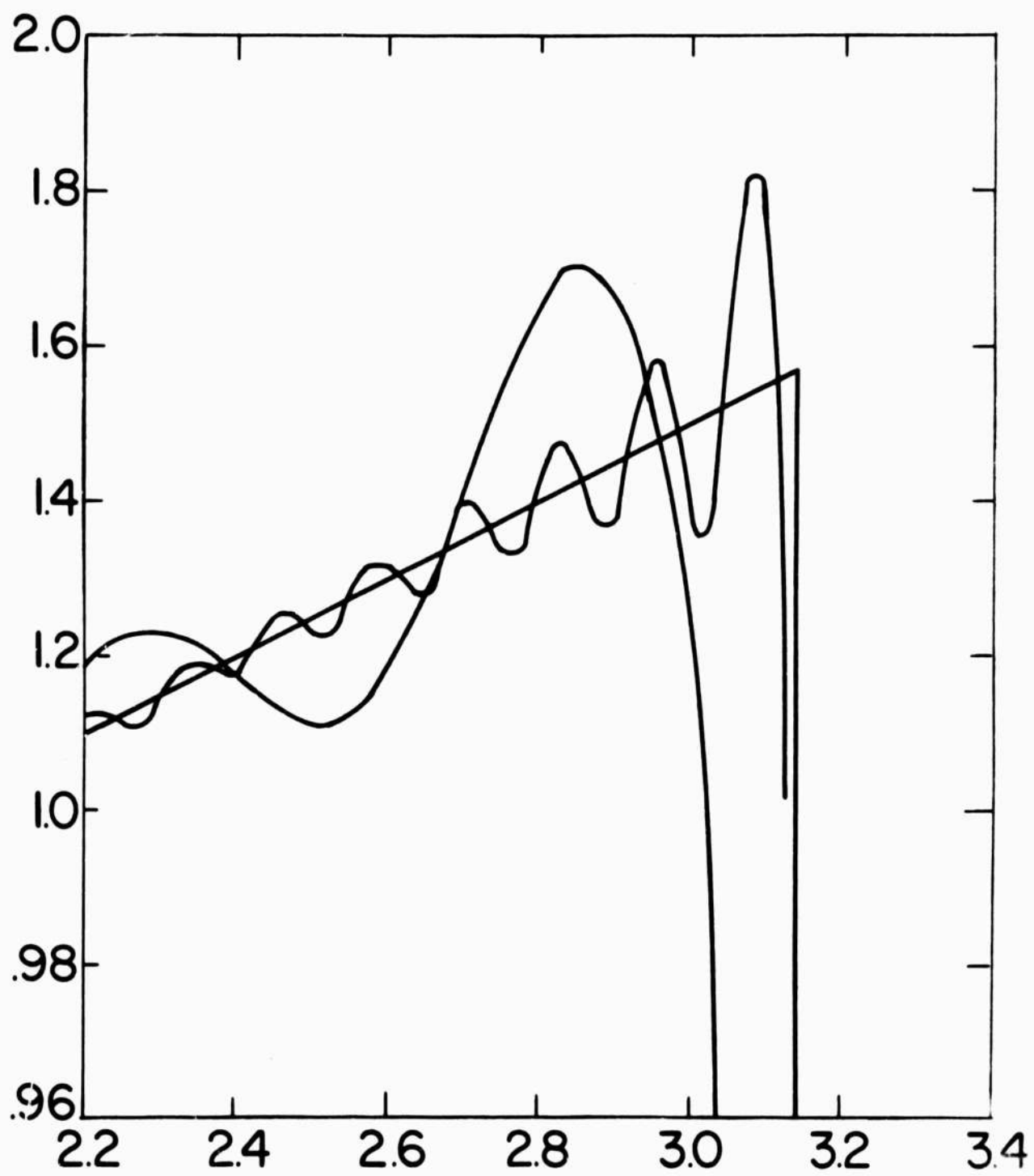


FIG. 7

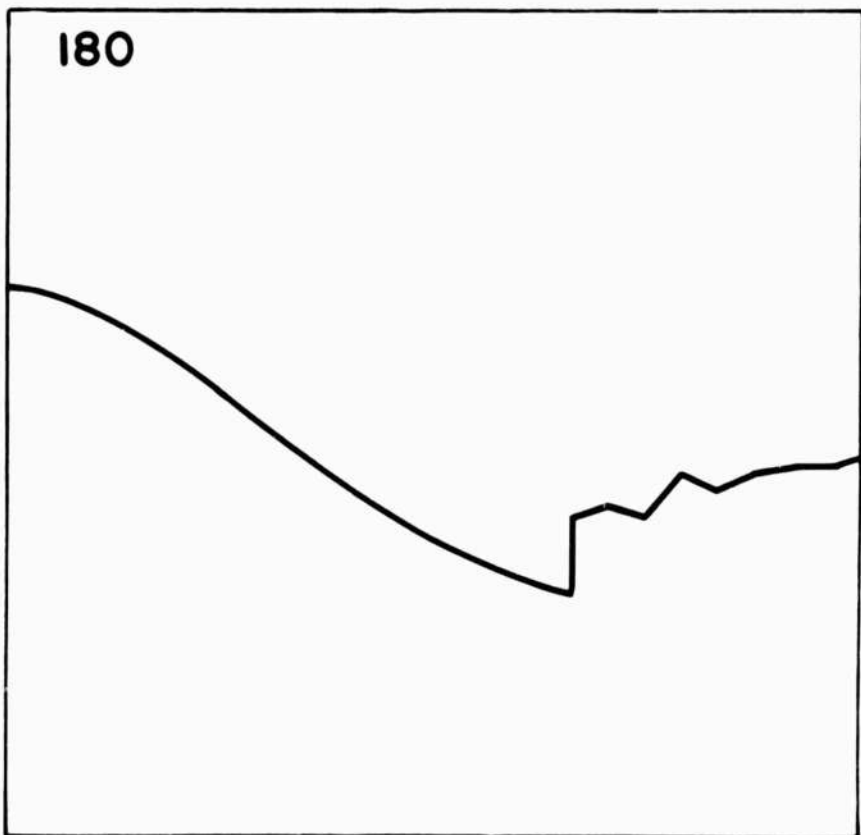
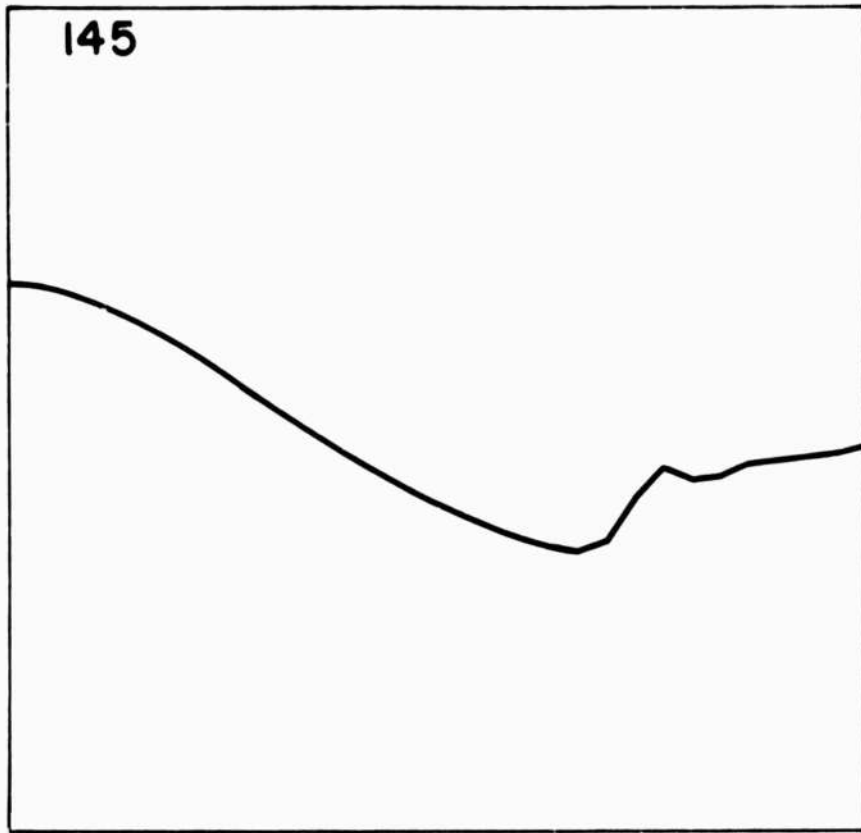


FIG. 8

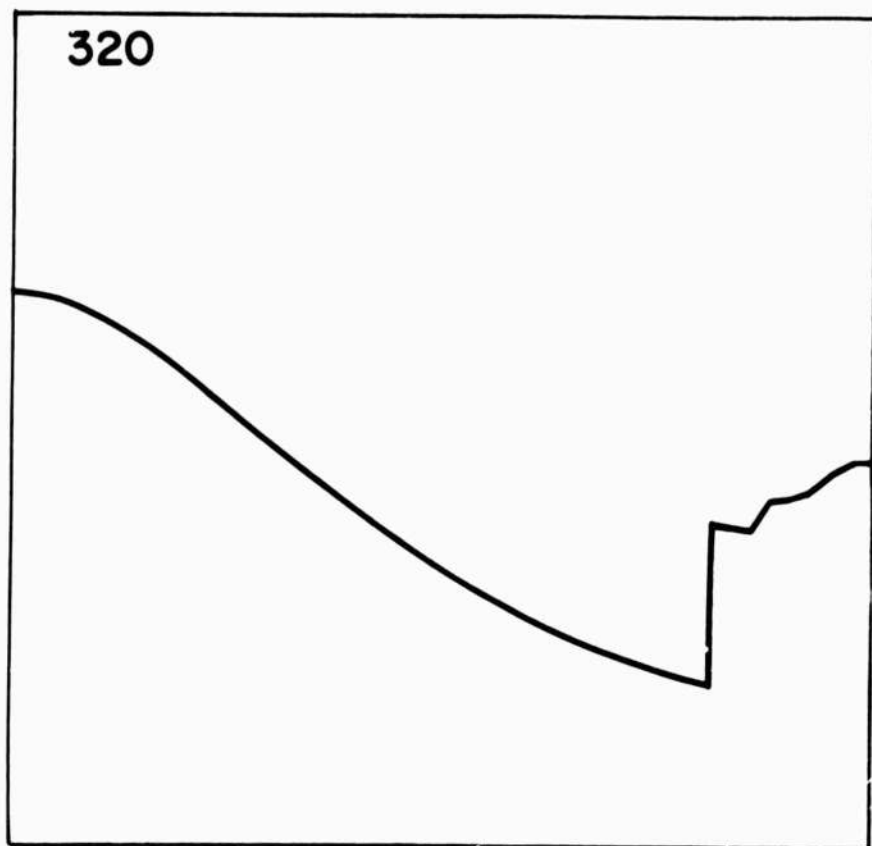
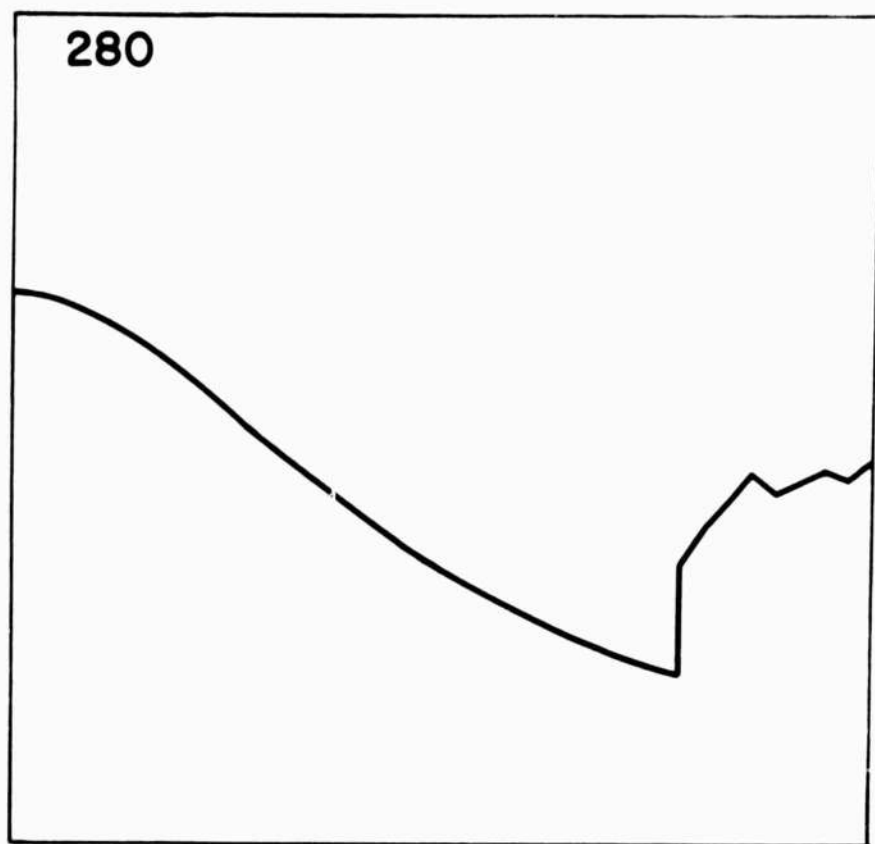


FIG. 8

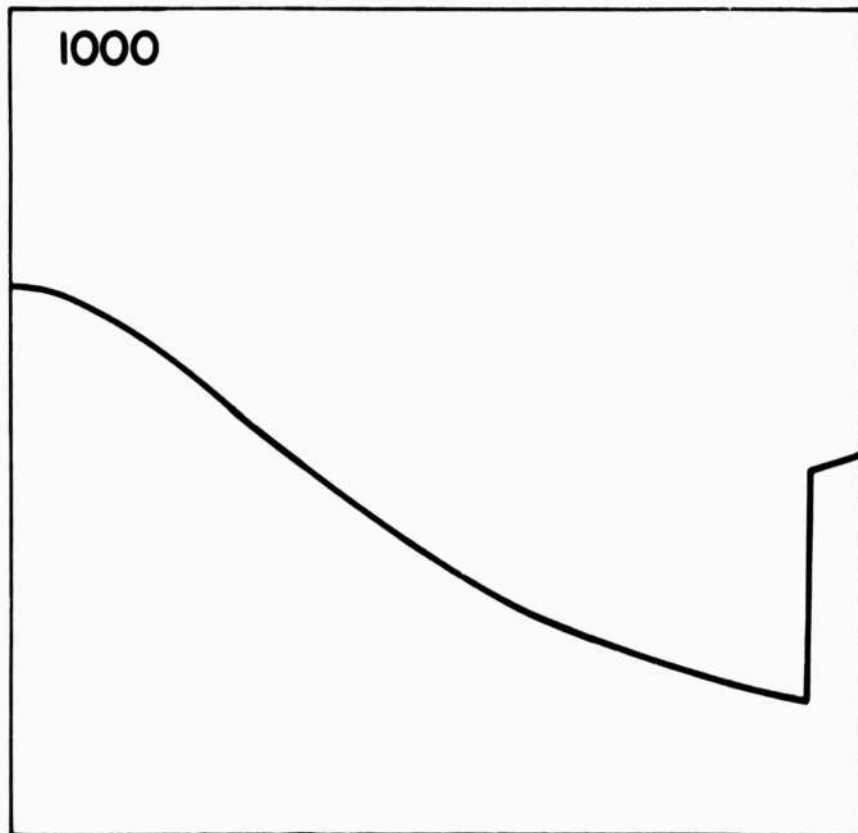
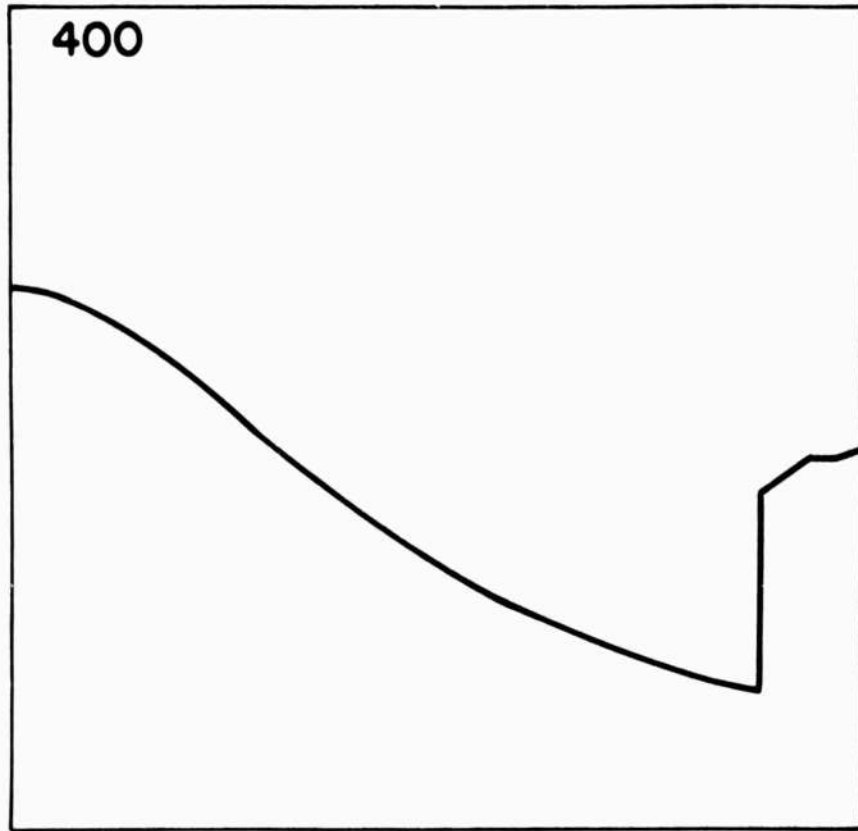


FIG. 8

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13. ABSTRACT
Many of the existing computations of initial-and-boundary value problems in fluid mechanics suffer from unrealistic treatment of boundary points. Three categories of boundaries are briefly discussed: rigid walls, arbitrary boundaries of a computational region in a subsonic flow, and shock waves. An attempt is made to show in what sense the numerical treatment of such boundaries may be physically wrong and what can be done instead. Examples from the blunt body problem, the transonic flow in a nozzle, the incompressible inviscid flow past a circle, and the quasi-one-dimensional flow in a Laval nozzle, are shown.

14. KEY WORDS	LINK A		LINK B		LINK C	
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