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Transformation of Two and Three-Dimensional Regions by Elliptic Systems

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INTRODUCTION

Grid smoothing and orthogonalization procedures have been developed and implemented in the construction of two and three-dimensional grids. The procedures are based on the variational methods of grid generation. The results of this work are included in the attached paper which will be presented at the AIAA Aerospace Sciences Meeting in Reno. The two-dimensional examples were computed using the MSU IRIS Graphics Workstation. Color plots, which could not be included in the paper, will be presented at the meeting. The attached paper also contains some three-dimensional examples which are the product of some work done during the summer at the Air Force's Arnold Engineering Development Center. That work gave us the opportunity to test our methods on large three-dimensional grids without using any funds from the Grant.

There is one result of our work during this reporting period which is most significant. It has been demonstrated that the elliptic grid generation equations, with arbitrary forcing functions, can be solved, in their variational formulation, using a gradient method. Since gradient methods have a global convergence property, the divergence problems often encountered when using SOR iterative methods can be avoided. It is not to be concluded, however, that SOR methods should be abandoned, since gradient methods tend to converge very slowly. In fact, slow convergence was the major problem encountered in the three-dimensional grids.

Further progress has been made on the continuing effort to develop conservative interpolation formulas for overlapping grids. The basic algorithm was derived earlier and included in our previous semiannual report. Since then, our work has been directed toward solving some of the technical problems such as: how to efficiently find grid intersection points, how to store interpolation coefficients, and how to implement the extrapolation procedures at outflow points on the overlap boundary. Algorithms have been developed for solving these problems. Final verification of the algorithms has not been completed at this time. This work will continue into the next contract period and final results will be included in a future report.

EXPERIENCE IN GRID OPTIMIZATION*

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Abstract

Optimization methods are developed and analyzed for the solution of all the popular variational problems in grid generation. Comparisons are made between the different variational methods.

I. Introduction

Variational methods in grid generation have recently become a viable alternative to the more established elliptic methods. Their appeal is likely due to the geometric foundation of the variational methods. These methods were derived using grid properties such as distances between grid points, orthogonality of grid lines, and the volumes of grid cells. Because of the earlier successes of elliptic methods, the first solution algorithms consisted of converting the variational problem to a problem of solving the elliptic Euler equations. The Euler equations were then solved using available finite difference algorithms. This approach was used by Brackbill and Saltzman [1], and Roache and Steinberg [4]. One disadvantage in this procedure is that the Euler equations are considerably more complicated than the original variational integral. Due to the complexity of the Euler equations, they are difficult to solve and solution algorithms may not converge. These difficulties have led to the development of algorithms for the direct solution of the variational problem. This approach was followed by Kennon and Dulikravich [3] and Carcaillet et al. [2]. In these two reports, different discrete problems were formulated as unconstrained optimization problems and then solved using a conjugate gradient iterative method. There are several advantages in this alternative. The original geometric properties of the grid are stated precisely by the discrete problem. Thus there is no truncation error as there is in the numerical solution of the Euler equations. Also, the conjugate gradient and similar descent methods will always converge to a local extrema. However, the convergence rate may be very slow.

This report will present a survey of the types of integrals that may be included in a variational problem and the geometric properties that each integral imposes upon the grid. Optimization methods for the direct solution of the variational problems will also be covered. A Jacobi-Newton iterative method will be developed and compared with the Fletcher-Reeves conjugate gradient method. By combining the simpler Jacobi-Newton iteration with the direct solution of the variational problem, one has an algorithm which is easier to program than the Euler equations and requires less storage and less computer time per iteration than the conjugate gradient method.

II. Variational Integrals

Variational methods may be used to influence three geometric properties of a grid. These are the smoothness of the grid point distribution, the size of the grid cells, and the orthogonality of the grid lines. Each property, smoothness, cell volumes, and orthogonality, can be assigned a numerical value by evaluating an integral. Most of the results will deal with three-dimensional problems, and the physical and computational variables will be denoted by x, y, z and ξ, η, ζ, respectively.

There are two basic smoothness integrals, one using the gradient of the physical variables and the other using the gradient of the computational variables. The integrals are denoted as S_1 and S_2 with D and R the computational and physical regions.

$$S_1 = \int_D P^2|r_\xi|^2 + Q^2|r_\eta|^2 + R^2|r_\zeta|^2 d\xi d\eta d\zeta \quad (1)$$

$$S_2 = \int_R P^2|\nabla\zeta|^2 + Q^2|\nabla\eta|^2 + R^2|\nabla\xi|^2 dxdydz$$

$$= \int_D (R^2|r_\eta x r_\zeta|^2 + Q^2|r_\zeta x r_\xi|^2 + P^2|r_\xi x r_\eta|^2)/J \, d\xi d\eta d\zeta \quad (2)$$

where J is the Jacobian $\frac{\partial(x,y,z)}{\partial(\xi,\eta,\zeta)}$ and $r = (x,y,z)$.

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The functions P, Q, and R, may be selected to control the grid point distribution. They directly affect the grid aspect ratio, and their influence can be readily seen by considering a one-dimensional transformation of any of the computational variables. The functions minimizing either of these integrals will define a smooth mapping between the physical and computational regions in the sense that the mapping functions are harmonic and therefore infinitely differentiable. However, the mapping defined by the minimization of S_1 may not be one-to-one. The mapping defined by the minimization of S_2 is one-to-one, but the construction of the mapping is more difficult. Current methods require the numerical solution of a system of nonlinear Euler equations.

For the two-dimensional case, there is a simple relation between the above integrals, (1) and (2), and the elliptic equations commonly used for grid generation. A two-dimensional version of S_2 in (2) may be written in the form

$$\int_R Q^2|\nabla\xi|^2 + P^2|\nabla\eta|^2 dxdy$$

$$= \int_D P^2|r_\xi|^2 + Q^2|r_\eta|^2)/J \, d\xi d\eta,$$

where J is the Jacobian $\frac{\partial(x,y)}{\partial(\xi,\eta)}$. The Euler equations for minimizing this integral may be written as

$$\nabla^2\xi = -(\ell nQ)_\xi|\nabla\xi|^2$$

$$\nabla^2\eta = -(\ell nP)_\eta|\nabla\eta|^2$$

or in computational space, with $r = (x,y)$, as

$$|r_\eta|^2(r_{\xi\xi} - (\ell nQ)_\xi r_\xi) + |r_\xi|^2(r_{\eta\eta} - (\ell nP)_\eta r_\eta)$$

$$- 2(r_\xi \cdot r_\eta)r_{\xi\eta} = 0.$$

This is the elliptic system with control functions

$$\phi = (\ell nQ)_\xi, \ \psi = (\ell nP)_\eta.$$

If ϕ and ψ are given, then the corresponding control functions for the variational integral are

$$P = \exp(\int\psi d\eta), Q = \exp(\int\phi d\xi).$$

A uniform distribution of grid cell volumes would not be appropriate in most practical applications. However, a near constant value of some weighted volume is often called for. The weight may depend on some desired distribution of volumes or a solution-dependent quantity used to define an adaptive grid. From a variational point of view, the optimal volume distribution could be defined by minimizing the integral

$$V_1 = \int_R G dxdydz$$
$$= \int_D GJ d\xi d\eta d\zeta \qquad (3)$$

where $G = Jw$, $w = w(\xi,\eta,\zeta)$.

While there is no guarantee that the variational problem will have a solution which gives a nonsingular mapping between physical and computational spaces, it can be noted that if such a solution exists, then the weighted Jacobian G will be constant. This follows from the Euler equations. The argument is simpler in the two-dimensional case. The Euler equations are then

$$G_\xi y_\eta - G_\eta y_\xi = 0$$

$$- G_\xi x_\eta + G_\eta x_\xi = 0,$$

and if it is assumed that the Jacobian $x_\xi y_\eta - x_\eta y_\xi \neq 0$, it follows that

$$G_\xi = G_\eta = 0$$

or G must be constant. The constant is determined by the physical region and the value of w since

$$\int_D G d\xi d\eta = \int_R w dxdy. \qquad (4)$$

There is one other volume integral that should be considered. If

$$V_2 = \int_D |\nabla G|^2 d\xi d\eta d\zeta, \qquad (5)$$

then the integrand is a second order differential expression in the physical variables x, y, and z. Consequently, the Euler equations are a system of fourth order equations. Now there must be two boundary conditions if a unique solution to the Euler equations is to be determined. One condition is imposed by fixing the boundary correspondence.

A second condition can be motivated by considering a lower order problem where G, the integrand of V_2, is a single dependent function of the variables ξ, η, and ζ. The Euler equation would then be Laplaces equation

$$\nabla^2 G = 0.$$

The equation has a unique solution if G is given on the boundary of the computational region. The function G would be uniquely determined up to a constant value if on the boundary,

$$G_\xi = 0 \text{ for } \xi = \text{constant}$$

$$G_\eta = 0 \text{ for } \eta = \text{constant}$$

$$G_\zeta = 0 \text{ for } \zeta = \text{constant}.$$

The constant value would again be determined by (4). Either of these types of boundary conditions could be advantageous in grid generation. Being able to specify the value of G along the boundary would aid in maintaining desired distributions of grid points near boundaries such as is needed in grids for the solution of problems with boundary layers. On the other hand, the derivative boundary conditions for G would be of value when several grids are patched together and it is desired that the cell sizes vary continuously from one subregion into another. The latter condition could also be used to generate a more uniform distribution of G over a single region.

If a grid is orthogonal, then

$$r_\xi \cdot r_\eta = r_\eta \cdot r_\zeta = r_\xi \cdot r_\zeta = 0,$$

where $r = (x,y,z)$. Therefore, one measure of skewness is the integral

$$A_1 = \int_D (r_\xi \cdot r_\eta)^2 + (r_\eta \cdot r_\zeta)^2 + (r_\xi \cdot r_\zeta)^2 d\xi d\eta d\zeta. \quad (6)$$

The integrand depends on the size of the grid cells since, for example,

$$r_\xi \cdot r_\eta = ||r_\xi||\ ||r_\eta|| \cos\theta$$

where θ is the angle of intersection between the ξ and η grid lines. As a result, minimizing the integral A_1 would have little effect in subregions with extremely small cells. For grids with widely varying cell volumes, the following integral would be more appropriate

$$A_2 = \int_D \left(\frac{r_\xi \cdot r_\eta}{||r_\xi||\ ||r_\eta||}\right)^2 + \left(\frac{r_\eta \cdot r_\zeta}{||r_\eta||\ ||r_\zeta||}\right)^2 + \left(\frac{r_\xi \cdot r_\zeta}{||r_\xi||\ ||r_\zeta||}\right)^2 d\xi d\eta d\zeta. \quad (7)$$

Irrespective of the solution algorithm selected, the minimization of A_2 is a more difficult problem since the integrand is a rational function of the physical derivatives rather than a multinomial as in A_1.

With the variational grid generation methods one selects a nonnegative linear combination of the form

$$I = \alpha S_i + \beta V_j + \gamma A_k, \quad (8)$$

where i, j, and k are either 1 or 2. Since the S_i, V_j, and A_k may be of differing magnitudes, the coefficients α, β, and γ may contain scaling factors. One method of scaling that can be used is to compute values $S_i^{(0)}$, $V_j^{(0)}$, and $A_k^{(0)}$ from an initial algebraic grid and then select non-negative numbers a, b, and c so that

$$a + b + c = 1.$$

Now if we choose

$$\alpha = a,\ \beta = b\,\frac{S_i^{(0)}}{V_j^{(0)}},\ \gamma = c\,\frac{S_i^{(0)}}{A_k^{(0)}},$$

then the initial value of I is the same for any combination of a, b, and c.

III. OPTIMIZATION

In the direct solution of the variational problem each integral is approximated on a square grid in computational space. Thus the continuous problem of minimizing I is reduced to the discrete problem of finding a minimum value of an objective function

$$F = \sum F_{i,j,k} \quad (9)$$

where i, j, k ranges over the indices of the grid points. The grid points on the boundary would be included although it is assumed that these points are fixed. Each term $F_{i,j,k}$ is to contain all difference approximations centered at the grid point $r_{i,j,k}$ which are used in the formation of the objective function F. The optimal grid is found by obtaining the unconstrained minimizer of the objection function F. There are many algorithms for solving optimization problems. An algorithm which has been successfully implemented in grid generation is the Fletcher-Reeves conjugate gradient method. The method can be used with any of the variational integrals of the previous section. Since the approximations of (2) and (7) involve quotients, it is possible that somewhere in the iteration scheme a division by a number close to zero may occur. This problem can be easily avoided by placing a lower bound on the denominators. Only a two-dimensional grid problem using (2) has been attempted because the three-dimensional integral becomes very complicated when transformed to computational space.

The conjugate gradient and related descent methods have the attractive feature of always converging to a grid which represents a local minimum value for the objective function. Their use in the solution of large three-dimensional grid generation problems may not be very efficient. At each iteration a one-dimensional minimization problem must be solved to determine the optimal step-size in the descent direction. The step-size problem can not be easily solved and frequently requires several evaluations of the objective function. This is especially true when the integrals in (2) and (7) are included. Therefore, alternate solution algorithms have been investigated. The application of Newton or quasi-Newton methods for nonlinear minimization problems in grid generation does not appear to be practical because of the number of matrix operations. Motivated by algorithms which are used to solve the discretized Euler equations, a Jacobi-Newton method has been selected as an alternate algorithm for solving the optimization problem. The following development covers the basic steps of the algorithm.

A local minimum value of F occurs at points where

$$\nabla F = 0,$$

or writing this system in component form

$$\left.\frac{\partial F}{\partial x}\right|_{i,j,k} = 0$$

$$\left.\frac{\partial F}{\partial y}\right|_{i,j,k} = 0 \qquad (10)$$

$$\left.\frac{\partial F}{\partial z}\right|_{i,j,k} = 0.$$

The system of nonlinear equations is solved using a Jacobi-Newton iterative method. At each point, Newton's method is used to approximately solve the three equations given in (10). In all of our examples, only one Newton iteration was performed. In fact, for certain variational integrals, the system is linear and the exact solution is obtained in one iteration.

The Jacobi-Newton iterative method described above has been used to solve a wide range of two and three-dimensional grid generation problems. So far, it has not been used with the variational integrals S_2 and A_2 because the quotients would cause the Newton iteration equations to be very lengthy. Convergence problems have not been encountered except in some cases where the grid folded. It is often necessary to use under-relaxation for larger problems.

IV. RESULTS

The following examples are presented to demonstrate the effect of the grid optimization procedure when applied to a large-scale three-dimensional grid. As can be seen, the success of the optimization process depends primarily on the proper choice of the variational integrals included in (8). When a decision had to be made between efficiency and robustness, it was the policy to develop a robust algorithm. A numerical step-size determination was used in the conjugate gradient iteration even though it was sometimes possible to calculate the exact optimal step-size.

All of the variational integrals have been used in the optimization of small two-dimensional grids. In all cases the objective was to improve an algebraic grid while keeping the basic grid point distribution. Thus the functions P and Q of integrals S_1 and S_2 are defined simply as

$$P^2 = \frac{|r_\eta^{(0)}|}{|r_\xi^{(0)}|}, \quad Q^2 = \frac{1}{P^2}$$

and the weight function w in V_1 and V_2 is

$$w(\xi,\eta) = (|r_\xi^{(0)}|\ |r_\eta^{(0)}|)^{-1}$$

where the superscript (0) is used to indicate that these functions are computed from the coordinates of the initial algebraic grid. One-sided differences have been used in the approximation of all variational integrals. Consequently, at each grid point there are four possible approximations for each integrand. In order to retain any grid symmetry, the average of these four values is used as the approximation of the integrand.

The integral S_2 generates the only optimal grid which is smooth and unfolded in the neighborhood of concave corners. Such a grid is plotted in Figure 1. The volume integrals V_1 and V_2 would not generate smooth grids and the integral S_1 would generate a grid which folds over the corner. However, S_1 does generate acceptable grids near convex corners. For most regions, the orthogonality integrals, A_1 and A_2, cannot be used alone to solve grid generation problems. An improved grid can often be generated by choosing the objective function as a convex combination of an orthogonality integral and either a smoothness or volume integral. The second integral is used to prevent grid folding. Figures 2 and 3 demonstrate the characteristics of the two orthogonality integrals. The grid in Figure 2 is generated using A_1 and S_1. Note the effect of including A_1. While there is some decrease in skewness where the grid is coarse, there are other regions where the grid lines are even more skewed than in the original interpolated grid. That is not the case when A_2 and S_1 are used to form the objective function. That grid is plotted in Figure 3. In order to emphasize the effect of the orthogonality integrals in the last two examples, only enough smoothness was included to prevent grid lines from crossing. The volume integral V_1 has been very helpful in the generation of grids near singularities. An example of a grid generated by minimizing V_1 is presented in Figure 4. Figures 5 and 6 give two more examples where the grid optimization process can reduce skewness in a grid without destroying the grid point distribution. The integral V_2 was generally less effective in these examples. Convergence was also slower, as might be expected with a method involving higher order derivatives.

Most of the grid optimization options have been incorporated in a state-of-the-art grid generation code developed at AEDC. The following examples illustrate the optimization of large three-dimensional grids for practical geometric configurations. Figure 7 represents the grid for an internal flow problem. Figure 8 gives a view of a part of a grid surface after optimization. Figure 9 is the grid for an external flow problem. The effect of the grid optimization process is illustrated in Figure 10.

It should be mentioned that the term "volume" used in this report is actually a misnomer. The Jacobian in equations (3) and (4) should always be computed from the definition and the appropriate difference approximations. If the cell areas (or volumes) are substituted for the Jacobians, then the optimal grid may contain triangular or even non-convex cells.

V. CONCLUSIONS

The successful application of variational methods in grid optimization depends on tailoring the integral to be minimized to the shape of the physical region and the desired distribution of grid points. If an algebraically generated grid is to be optimized, control functions can be defined using the arc length distribution of points along each family of grid lines. The solution of the variational problem can be computed using the traditional optimization methods or by iterative methods similar to those currently being used to solve elliptic partial differential equations. The convergence rate for either iterative method is generally slow when applied to large three-dimensional grids.

REFERENCES

1. J. U. Brackbill and J. S. Saltzman, "Adaptive Zoning for Singular Problems in Two Dimensions," Journal of Computational Physics 46 (1982), 342-368.

2. R. Carcaillet, "Optimization of Three-Dimensional Computational Grids and Generation of Flow Adaptive Computational Grids," AIAA Paper 86-0156, AIAA 24th Aerospace Sciences Meeting, Reno, Nevada, 1986.

3. S. R. Kennon and G. S. Dulikravich," A Posteriori Optimization of Computational Grids," AIAA Paper 85-0483, AIAA 23rd Aerospace Sciences Meeting, Reno, Nevada, 1985.

4. P. J. Roache and S. Steinberg, "A New Approach to Grid Generation Using a Variational Formulation," AIAA Paper 85-1527, AIAA 7th Computational Fluid Dynamics Conference, Cincinnati, Ohio, 1985.

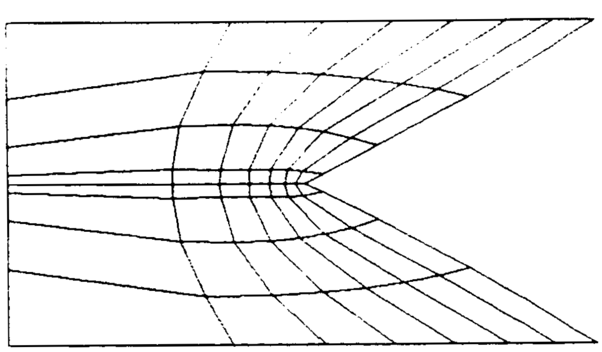

Figure 1. Optimized grid using S_2

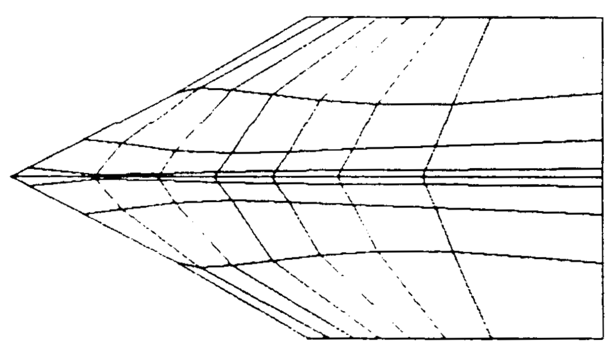

Figure 2. Optimized grid using S_1 and A_1

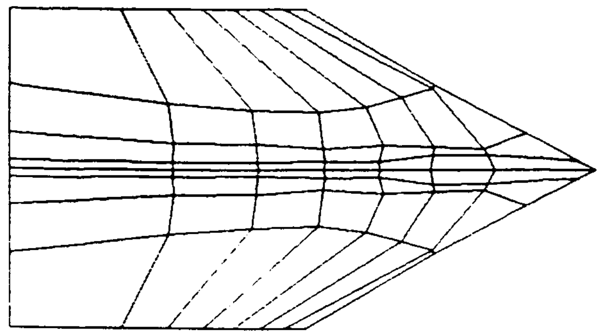

Figure 3. Optimized grid using S_1 and A_2

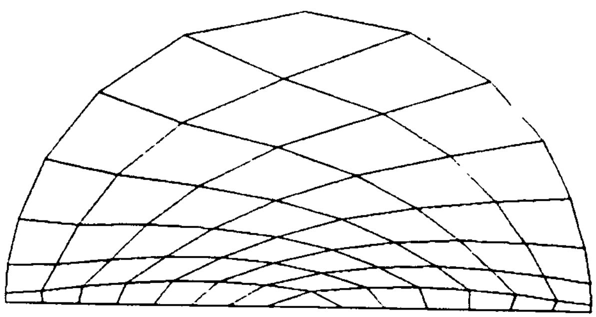

Figure 4. Optimized grid using V_1

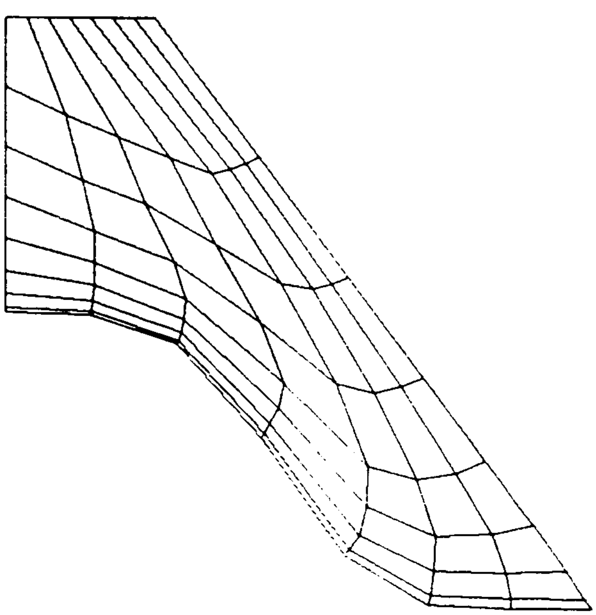

Figure 5. Optimized grid using S_2 and A_2

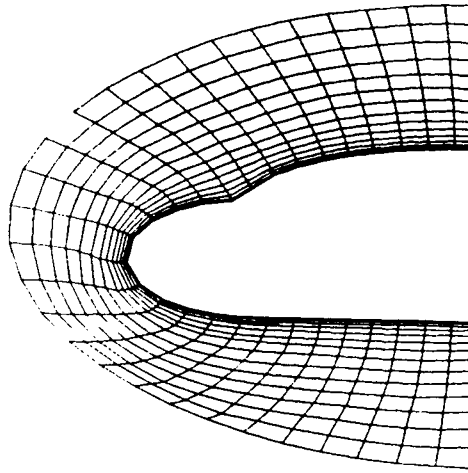

Figure 6. Optimized grid using S_2 and A_2

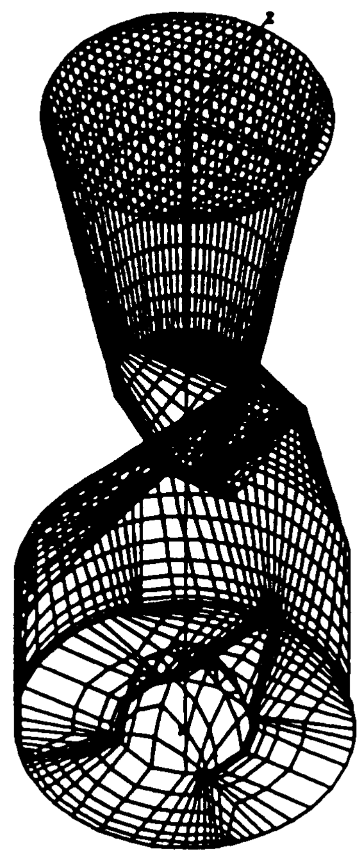

Figure 7. Grid for a three-dimensional duct

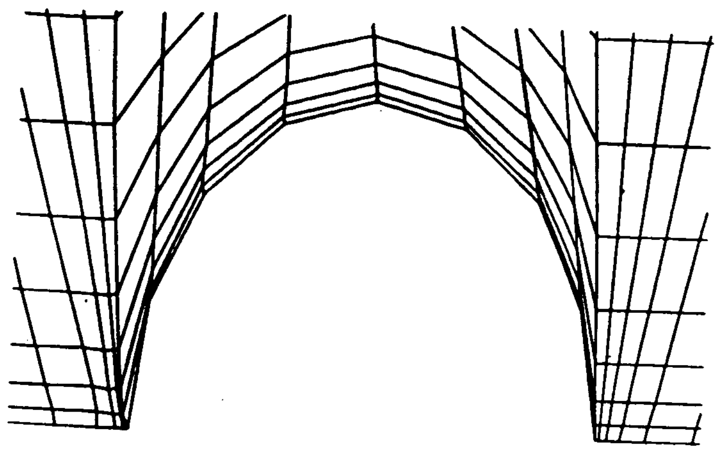

Figure 8. Optimization using S_1, A_2, and V_2

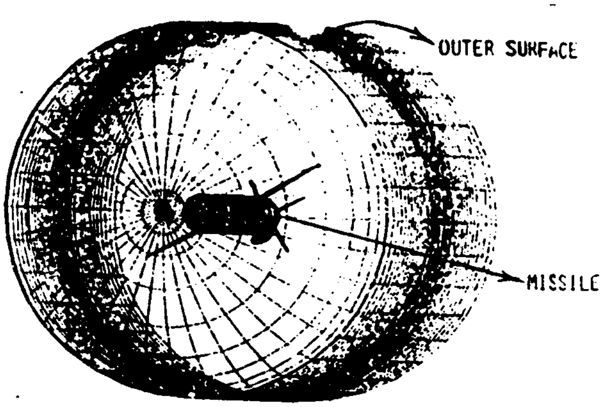

Figure 9. Grid about a missile

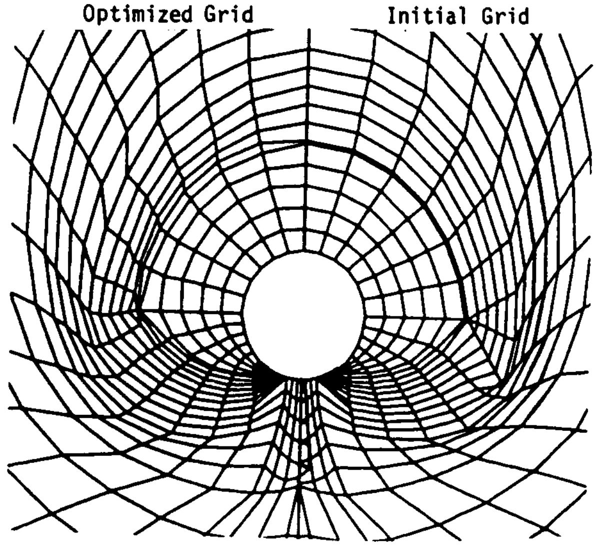

Figure 10. Optimization using V_2