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A POSTERIORI OPTIMIZATION OF COMPUTATIONAL GRIDS

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ABSTRACT

A method is described for a posteriori optimization of computational grids where grid non-orthogonality and grid overlap are minimized using an iterative optimization procedure. Desirable properties such as smoothness are at the same time maximized using the described technique. In this sense an optimal computational grid can be obtained, irrespective of the method used to generate the original grid. Thus, the user may generate a computational grid with whatever method he chooses. Then, if the grid is unacceptable for computations, it can be optimized in an a posteriori fashion. If the original grid has regions of overlap (non-positive Jacobian), the described method is capable of 'unravelling' the grid and making it useful for computations. Grid points on the boundary of the domain remain fixed, thereby allowing the correct resolution of regions of interest. The iterative optimization procedure is extremely fast due to the use of exact line searching and a conjugate direction method. The method can be applied to the optimization of two- or three-dimensional grids. Example grid optimization cases are shown for two-dimensional grids. The formulation of the method for three-dimensional grids is also given.

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Introduction

There has been a great deal of interest in the past few years in development of computational grid generation techniques[1] for use in discretizing complex regions for numerical solution of partial differential equations. The grid generation methods in common use have achieved a high degree of sophistication and ease of use. Nevertheless, the authors of this paper perceived a need for a method that would improve the quality of a given computational grid. In many cases a particular grid generation method works exceptionally well, but only for a small sub-class of problems. However, for more complex configurations, these methods do not always produce grids that are acceptable for computations. Grid quality deterioration is especially apparent in three-dimensional grid generation methods and when two-dimensional grids are combined to form a three-dimensional grid. In addition to grid quality problems, many methods suffer from computational inefficiency.

A possible alternative to optimize the cost-quality trade-off is to generate a non-perfect grid using an inexpensive and simple method and then to improve the grid in an a posteriori fashion. If the original grid is acceptable for computations then it can be directly used, but if the grid is not acceptable it should not be thrown away, and the particular grid generation program should not necessarily be abandoned. Rather, we can retain the grid as an initial guess for a grid improvement or optimization method. An efficient method for grid optimization is described in this paper.

ANALYSIS

The formulation of the grid optimization method will be illustrated as a two-dimensional grid optimization problem. The details of the method for the three-dimensional case are given in the Appendix.

Assume that we are given a computational grid which we wish to optimize. This initial grid is defined by its grid point coordinates, $(x_{i,j}, y_{i,j})$ where $1 \le i \le p$ and $1 \le j \le q$. The objective is to determine an iterative procedure that calculates corrections to $x_{i,j}$ and $y_{i,j}$ consistent with the goal of optimizing the grid.

An optimal grid can be defined as a grid posessing maximal local orthogonality and smoothness. An orthogonal conformal grid is everywhere orthogonal and entirely smooth with respect to the Laplace operator. Locally orthogonal grids can be generated efficiently using a variety of methods based on conformal mappings.[2 3 4] However, for conformal grids all grid points on all boundaries cannot be arbitrarily chosen by the user--some boundary points must be allowed to float. This can be a severe restriction in many cases. When it is desirable to specify and fix the points on the boundaries, many existing non-orthogonal grid generation methods can be used.[5 6 11] However, the specified distribution of boundary points is not always consistent with a smooth and maximally orthogonal grid. In addition, propagation of clustered regions into the rest of the domain can also be a problem.[7] Another problem with conformal grid generation techniques is the non-existence of general three-dimensional conformal mappings.

We will discuss the formulation of the grid optimizaton method by first looking at similarities with the Saltzman-Brackbill[8] variational grid generation method. In the variational method, two functionals are introduced that provide measures of grid smoothness

$$I_s = \iint (|\nabla_{xy}\xi|)^2 + (|\nabla_{xy}\eta|)^2 dxdy \qquad (1)$$

and grid orthogonality

$$I_o = \iint [(\nabla_{xy}\xi)\cdot(\nabla_{xy}\eta)]J^3 dxdy \qquad (2)$$

where

$\nabla_{xy} \equiv \frac{\partial}{\partial x}\vec{i} + \frac{\partial}{\partial y}\vec{j}$

$J \equiv \xi_x\eta_y - \eta_x\xi_y$

(x,y) - physical coordinates

(ξ,η) - computational coordinates

The roles of dependent (ξ,η) and independent (x,y) coordinates are interchanged and the Euler-Lagrange equations are applied to the total functional

$$I = I(\xi,\eta) \equiv \lambda_s I_s + \lambda_o I_o \qquad (3)$$

where λ_s and λ_o are scalar weights for the smoothness and orthogonality measures respectively. The result of applying the Euler-Lagrange equations is a non-linear system of coupled differential equations of second order in the (x,y) physical coordinates that are solved by finite difference discretization. The transformed equations become

$$I_s = \iint [x_\xi^2+x_\eta^2+y_\xi^2+y_\eta^2]\ J\ d\xi d\eta \qquad (4)$$

$$I_o = \iint [x_\xi x_\eta+y_\xi y_\eta]^2\ d\xi d\eta \qquad (5)$$

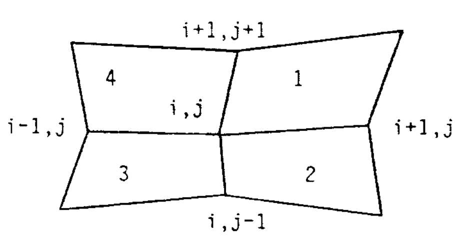
where $J = (x_\xi y_\eta - x_\eta y_\xi)^{-1}$

In theory, the same solutions of the Euler-Lagrange system can be achieved by direct discretization and minimization of the functional I. In this case, the derivatives can be replaced with finite differences and the integrals with simple summations over the grid points. However, after careful examination of eqs. 4 and 5 one can see that only first partial derivatives of x and y appear in the functional I. Therefore, a central finite difference discretizaton[9] of I of any order centered at the grid point $(x_{i,j}, y_{i,j})$ becomes independent of the values of $x_{i,j}$ and $y_{i,j}$. This leads to strong decoupling problems in the solution procedure which do not occur if the Euler-Lagrange system is solved since second order partial derivatives appear in the system.

The decoupling problem leads us to an alternative, more direct formulation of grid quality measures that are directly dependent on the central grid point $(x_{i,j}, y_{i,j})$. We define the smoothness measure qualitatively by stating that a smooth grid has minimal change in grid cell area from one grid cell to the next, in both the ξ and η directions. Similarly, a maximally orthogonal grid is one in which the grid lines of the families ξ=constant and η=constant intersect at right angles.

Grid Quality Measures

Consider the local problem of grid optimization for a master cell consisting of four elementary cells numbered 1,2,3 and 4



Assume that the grid points are connected with straight line segments defined by

$$\vec{r}_{i+1,j} = (x_{i+1,j}-x_{i,j})\vec{i} + (y_{i+1,j}-y_{i,j})\vec{j}$$
$$\vec{r}_{i,j+1} = (x_{i,j+1}-x_{i,j})\vec{i} + (y_{i,j+1}-y_{i,j})\vec{j}$$
$$\vec{r}_{i-1,j} = (x_{i-1,j}-x_{i,j})\vec{i} + (y_{i-1,j}-y_{i,j})\vec{j}$$
$$\vec{r}_{i,j-1} = (x_{i,j-1}-x_{i,j})\vec{i} + (y_{i,j-1}-y_{i,j})\vec{j} \quad (6)$$

The quantitative measure of local grid smoothness is given by

$$\sigma_{i,j} \equiv (V_1-V_2)^2+(V_2-V_3)^2+(V_3-V_4)^2+(V_4-V_1)^2 \quad (7)$$

where V_k is a measure of the area of the k'th elementary cell, e.g.

$$V_1 = |(\vec{r}_{i+1,j} \times \vec{r}_{i,j+1})| = [x_{i+1,j}y_{i,j+1} - y_{i+1,j}x_{i,j+1}] \quad (8)$$

The local measure of grid orthogonality is given by

$$\rho_{i,j} \equiv (\vec{r}_{i+1,j}\cdot\vec{r}_{i,j+1})^2 + (\vec{r}_{i,j-1}\cdot\vec{r}_{i+1,j})^2 + (\vec{r}_{i-1,j}\cdot\vec{r}_{i,j-1})^2 + (\vec{r}_{i,j+1}\cdot\vec{r}_{i-1,j})^2 \quad (9)$$

Clearly both the smoothness and orthogonality measures depend on the central grid point $(x_{i,j}, y_{i,j})$. We now define the total cost function F by

$$F \equiv \Sigma_{i=1}^{p} \Sigma_{j=1}^{q} [\alpha\rho_{i,j} + (1-\alpha)\sigma_{i,j}] \quad (10)$$
$$0 \le \alpha \le 1$$

Minimizing F will produce a grid that is optimally smooth (α=0) or orthogonal (α=1). Setting α to intermediate values between 0 and 1 gives different weights to the smoothness or orthogonality of the grid.

Iterative Optimization Procedure

To minimize F we use the following iterative optimization procedure. First, let us restate the problem in terms of the vector $z=(x,y)$ of length $2pq=2N$ that contains the x and y coordinates of the grid points in a natural ordering. Thus we must find the value $z=z^*$ such that $F(z^*)$ is a minimum. We use the Fletcher-Reeves conjugate direction procedure[10]

$$\delta z^{(0)} = -\nabla F(z^{(0)})$$

WHILE $|\nabla F| > \varepsilon$ DO

$$z^{(n+1)} = z^{(n)} + \omega^{(n)} \delta z^{(n)} \quad (11)$$
$$\delta z^{(n)} = -\nabla F(z^{(n)}) + \beta^{(n)} \delta z^{(n-1)}$$
$$\beta^{(n)} = |\nabla F^{(n)}|^2 \,/\, |\nabla F^{(n-1)}|^2$$

The factor ω in eq. 11 is the so-called line-search parameter and it is given by

$$\omega = \arg\,[\min_{\omega} \psi(\omega)] \quad (12)$$

where the scalar function $\psi(\omega)$ is given by

$$\psi(\omega) = F(z^{(n+1)}) = F(z^{(n)} + \omega \delta z^{(n)}) \quad (13)$$

Clearly, ω is found from a one-dimensional minimization of the scalar function $\psi(\omega)$. The determination of ω is usually the most costly portion of each step of an iterative optimization procedure since it involves many evaluations of the cost function $F(z)$. However, the parameter ω can be determined with minimal effort using concepts based on the Non-Linear Minimal Residual Method[11,12] for accelerating the iterative solution of differential systems.

Note that the orthogonality and smoothness measures are composed of simple polynomial expressions of the x and y grid point coordinates. Therefore, $\psi(\omega)$ is a fourth degree polynomial function in terms of ω. This follows by simple substitution of eq. 11 into eq. 13. To determine the value of ω that minimizes $\psi(\omega)$ we simply find and test the three roots of the cubic polynomial obtained from

$$\frac{\partial \psi}{\partial \omega} = 0 \quad (13)$$

The root that produces the minimum in ψ is used in eq. 11 to update the grid point coordinates. The iterative optimization procedure is halted when $|\nabla F|$ is less than a specified tolerance.

RESULTS

A computer program was developed to implement the grid optimization procedure for two-dimensional O-type grids. Note that all types of grids can be optimized in like manner.

The first test case was a non-staggered cascade of NACA 0012 airfoils at a gap-to-chord ratio of 1.0. The initial grid was generated using a complex-valued spline method[6,11] and is shown in fig. 1. The grid was then optimized using the weighting factor $\alpha=0.5$ with the result shown in fig. 2. One can see that the method is able to smooth this geometrically periodic grid and make it more orthogonal. This particular grid was specified to have 5 grid points at the upstream and downstream boundaries. We also applied the optimization procedure for a NACA 0012 cascade grid that had only 3 points at these boundaries (fig. 3). This grid has very large changes in cell areas near these boundaries. The grid was optimized and the result is shown in fig. 4. The optimized grid is smooth and useful for computations.

Another cascade example is shown in figs. 5 and 6, in this case a turbine cascade[13] at a gap-to-chord ratio of 1.0. The optimization method has greatly improved the grid, especially in regions where the original grid was highly non-orthogonal.

To demonstrate the ability of the method to 'unravel' grids that contain overlap we optimized a grid for a space-shuttle cross-section[6] that was completely useless (fig. 7). The result of applying 25 iterations of the optimization method is shown in fig. 8. All regions of overlap have been 'unravelled' and the resulting grid is usable.

As a final example we show a uniform rectangular grid on which a uniform random error has been intentionally introduced (fig. 9a). The resulting iterative optimization sequence is shown in figs. 9b-9d. The overlapping grid was easily unravelled to produce the original uniform grid. These two-dimensional examples show that the method gives an efficient technique for improving non-optimal grids.

FUTURE RESEARCH

The most promising applications for the method are in the areas of three-dimensional grid optimization and flow adaptive grid generation. The three-dimensional problem can be solved with a direct extension of the two-dimensional analysis given in this paper. The three-dimensional grid optimization method is particularly suitable for grids that are based on stackings of two-dimensional grids.[2 3 4] In this case, the grid is probably fairly orthogonal within the stacking planes, but is usually quite non-orthogonal in the third direction. Nevertheless, the grid can be made as locally orthogonal as possible by applying the described grid optimization method.

Flow adaptive grid generation methods can also be formulated from the ideas presented in this paper. In this case, we would add an additional functional to $I(\xi,\eta)$, as done by Saltzman and Brackbill,[8] that is a weighted volume measure of a quantity that we wish the grid to adapt to (such as a pressure gradient). This functional would be minimized along with the grid quality measures. Thus, grid points would automatically cluster in regions of the flow domain requiring resolution while the grid would maintain a high degree of quality.

APPENDIX

This section presents the details of the method in three-dimensions.

Smoothness measure:

$$\sigma_{i,j,k} \equiv (V_1-V_2)^2+(V_2-V_3)^2+(V_3-V_4)^2+(V_4-V_1)^2+ (V_5-V_6)^2+(V_6-V_7)^2+(V_7-V_8)^2+(V_8-V_5)^2+ (V_1-V_5)^2+(V_2-V_6)^2+(V_3-V_7)^2+(V_4-V_8)^2 \quad \text{(A.1)}$$

where the V_k are appropriate volume measures for the eight elementary cells composing the master three-dimensional cell. For example,

$$V_1 = |\vec{r}_{i,j,k+1}\cdot(\vec{r}_{i+1,j,k} \times \vec{r}_{i,j+1,k})| \quad \text{(A.2)}$$

Orthogonality measure:

$$\rho_{i,j,k} \equiv (\vec{r}_{i+1,j,k}\cdot\vec{r}_{i,j+1,k})^2+(\vec{r}_{i,j-1,k}\cdot\vec{r}_{i+1,j,k})^2 + (\vec{r}_{i-1,j,k}\cdot\vec{r}_{i,j-1,k})^2+(\vec{r}_{i,j+1,k}\cdot\vec{r}_{i-1,j,k})^2 + (\vec{r}_{i+1,j,k}\cdot\vec{r}_{i,j,k-1})^2+(\vec{r}_{i,j-1,k}\cdot\vec{r}_{i,j,k-1})^2 + (\vec{r}_{i-1,j,k}\cdot\vec{r}_{i,j,k-1})^2+(\vec{r}_{i,j+1,k}\cdot\vec{r}_{i,j,k-1})^2 + (\vec{r}_{i+1,j,k}\cdot\vec{r}_{i,j,k+1})^2+(\vec{r}_{i,j-1,k}\cdot\vec{r}_{i,j,k+1})^2 + (\vec{r}_{i-1,j,k}\cdot\vec{r}_{i,j,k+1})^2+(\vec{r}_{i,j+1,k}\cdot\vec{r}_{i,j,k+1})^2 \quad \text{(A.3)}$$

Note that the smoothness measure $\sigma_{i,j,k}$ will produce a sixth order polynomial contribution to $\psi(\omega)$ (as opposed to fourth order in two-dimensions), while the orthogonality measure $\rho_{i,j,k}$ remains fourth order in ω. Thus, $\psi(\omega)$ will be sixth order and we will have to find the five roots of

$$\frac{\partial\psi}{\partial\omega} = 0 \qquad (A.4)$$

to perform the line searching part of the iterative optimization procedure.

REFERENCES

1. Thompson, J. F., ed.. Numerical Grid Generation. Elsevier Science Publishing Co., Inc., 1982.

2. Ives, D. C., "Conformal Grid Generation." Numerical Grid Generation, J. F. Thompson ed., Elsevier Science Publishing Co., Inc., 1982.

3. Dulikravich, G. S., "GRID3O-Computer Program for Fast Generation of Multilevel, Three-Dimensional, O-Type, Boundary Conforming Computational Grids," NASA TP 1920, 1981.

4. Dulikravich, G. S., "Fast Generation of Three-Dimensional Computational Boundary-Conforming Periodic Grids of C-Type," in Numerical Grid Generation, J. F. Thompson ed., North-Holland, 1982, pp. 563-584.

5. Thompson, Joe F., "Elliptic Grid Generation," in Numerical Grid Generation, J. F. Thompson ed., North-Holland, 1982, pp. 79-105.

6. Kennon, S. R., "Direct Grid Generation Using Complex Spline Fitting," proceedings of the Fifth International Conference on Finite Elements and Flow Problems, University of Texas at Austin, Austin, Texas, January 23-26, 1984.

7. Ives, D. C., Lecture presented at University of Texas at Austin, October, 1984.

8. Saltzman, J. and J. Brackbill, "Applications and Generalizations of Variational Methods for Generating Adaptive Meshes," Numerical Grid Generation, J. F. Thompson ed., Elsevier Science Publishing Co., Inc., 1982.

9. Anderson, D. A. et. al. Computational Fluid Mechanics and Heat Transfer. McGraw-Hill, 1984

10. Zoutendijk, G. Mathematical Programming Methods. North-Holland, Amsterdam, 1976.

11. Kennon, S. R., "Novel Approaches to Grid Generation, Inverse Design, and Acceleration of Iterative Schemes," Master's thesis, Department of Aerospace Engineering and Engineering Mechanics, University of Texas at Austin, May, 1984.

12. Kennon, S. R. and G. S. Dulikravich, "Optimum Acceleration factors for Iterative Solution of Linear and Non-Linear Differential Systems," Computer Methods in Applied Mechanics and Engineering, (accepted for publication in 1984).

13. Hajjar, F. G., et. al., "Aerodynamics and Heat Transfer of Transonic Turbine Blades at Off-Design Angles of Incidence," M.I.T. Gas Turbine Laboratory report, 1978.

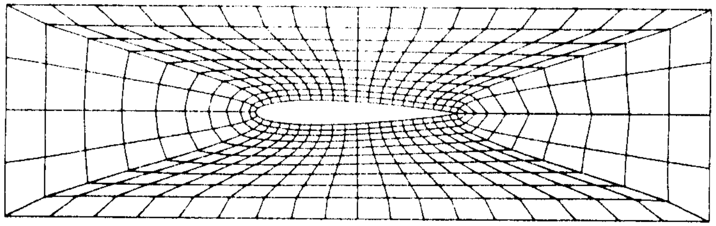


Fig. 1 NACA 0012 Cascade Grid - 5 points at infinities

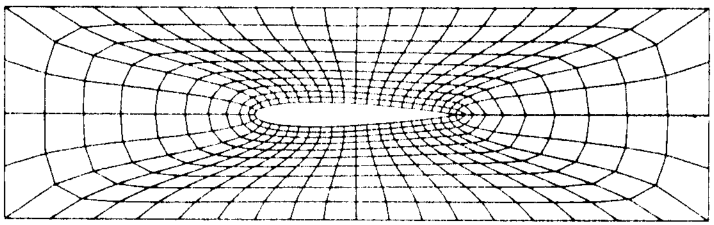


Fig. 2 Optimized NACA 0012 Cascade Grid

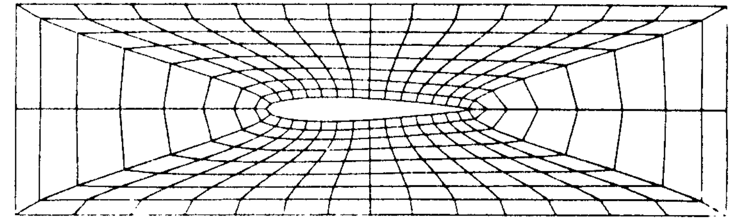


Fig. 3 NACA 0012 Cascade Grid - 3 points at infinities

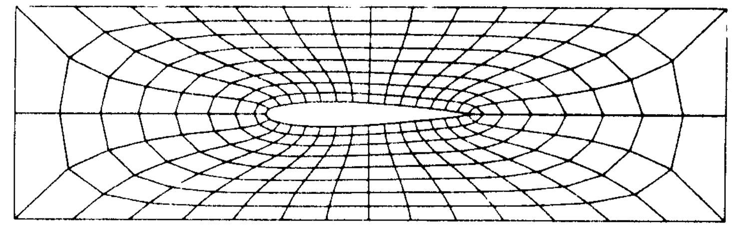


Fig. 4 Optimized NACA 0012 Grid - 3 points at infinities

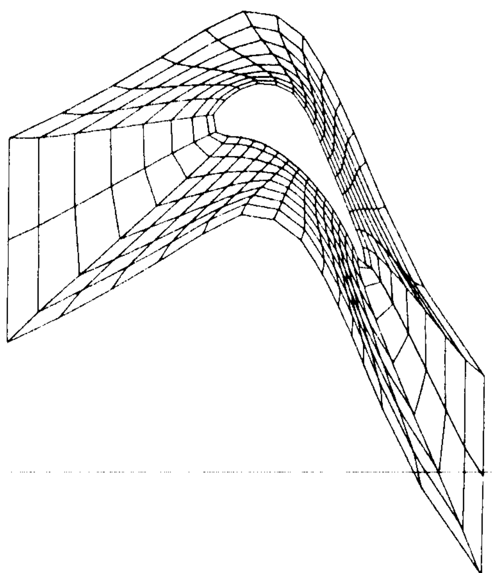


Fig. 5 Original Turbine Cascade Grid

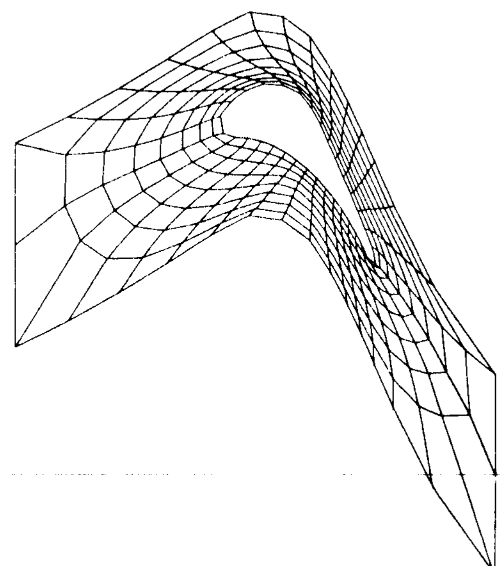


Fig. 6 Optimized Turbine Cascade Grid

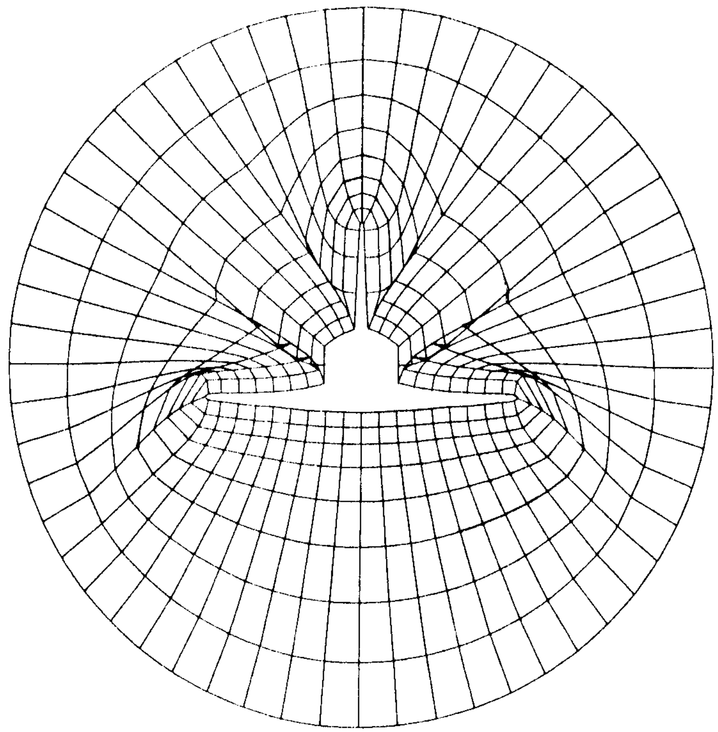


Fig. 7 Original Space Shuttle Cross-Section Grid

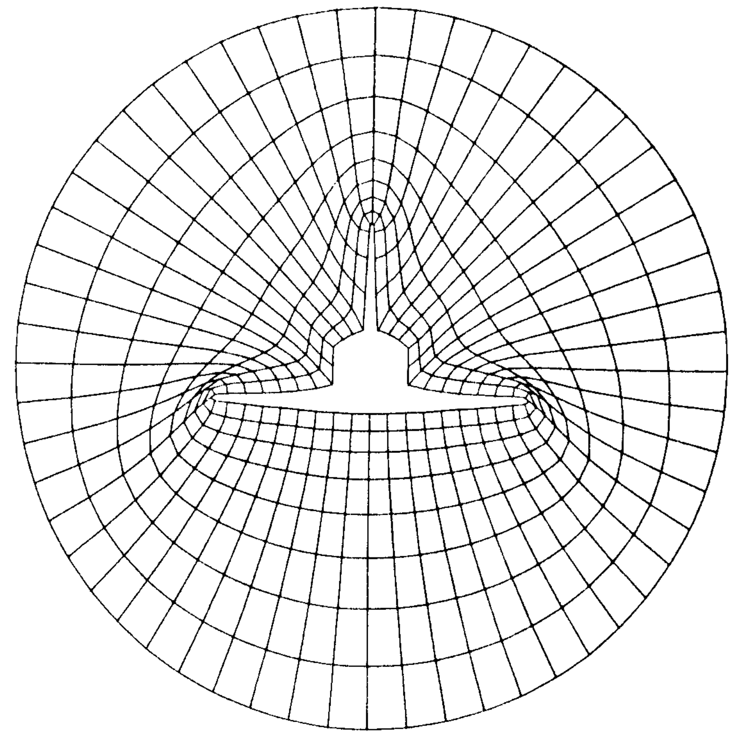


Fig. 8 Optimized Space Shuttle Cross-Section Grid

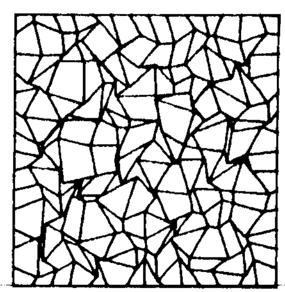


Fig. 9a Original grid

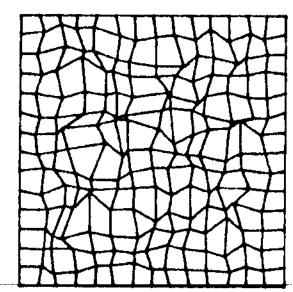


Fig. 9b One iteration

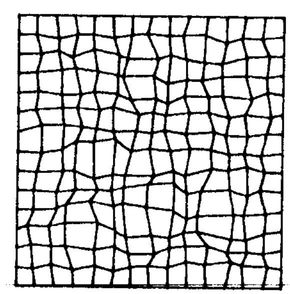


Fig 9c Two iterations

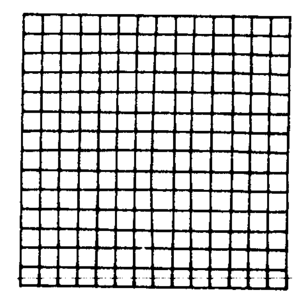


Fig. 9d Optimized Grid after 50 iterations