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GENERATION OF OPTIMUM THREE-DIMENSIONAL COMPUTATIONAL GRIDS

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Summary

A method for optimizing arbitrary three-dimensional boundary-conforming computational grids is presented. The smoothness and local orthogonality of the grid are maximized using a fast iterative procedure that allows for selective clustering of the grid. An optimal grid can be obtained, irrespective of the method used to generate the initial grid. Unacceptable and even overlapped grids can be made useful for computation using this method. Taking advantage of this unique property, a new concept for three- dimensional grid generation is proposed that consists in optimizing an imperfect first guess of the desired grid. The initial grid may thus be generated using a simple, inexpensive method. A new method for generating and optimizing multidimensional flow adaptive computational grids is also discussed that builds on the present grid optimization method.

Introduction

The quality of the computational grid is essential for the accurate and stable numerical simulation of gas dynamics problems using finite-difference methods. On one hand, the grid should be smooth, meaning that it should exhibit reasonable rates of change in spacing in each of the curvilinear coordinate directions. This will limit the diffusion-like truncation error introduced by nonuniform grids [1]. The grid cells should not be too skew, on the other hand, and orthogonality of the grid lines should be enforced at the boundaries for accurate implementation of the boundary conditions [2].

Grid generation methods explicitly based on these desirable grid qualities have been proposed [3,4,5,6]; our work represents an alternative, more heuristic formulation of the variational method of Brackbill and Saltzman [5,6] that has been successfully applied in two dimensions [7]. Its extension to three-dimensional problems and further development is discussed here. Satisfactory three-dimensional single grids about typical aircraft configurations are not easily obtained, since the slope discontinuities of the surface grid will result in highly skewed or even overlapped grid cells near the surface. In some simple cases it is possible to connect corresponding points on individual two-dimensional grids to obtain a "stacked" grid; for more complex configurations, the only practical alternative to a single grid consists in partitioning the domain and generating contiguous subgrids on the simpler three-dimensional regions, resulting in a "patched" grid. Apart from its complexity, this approach may bring grid quality problems at the boundaries between patches.

The method described here will optimize a given, arbitrary three-dimensional grid with respect to smoothness and local orthogonality while allowing local directional clustering of the resulting grid. Therefore, it may be applied as a post-processor for improving unacceptable grids to the point where they are useful for flow computations. However, its potential is best exploited when using it as a grid generator. In this case, a rough first guess of the desired grid is iteratively optimized, yielding a grid possessing the maximum possible smoothness and/or local orthogonality for the given configuration. The selective clustering capability built into the method has also led to the development of a new multidimensional flow adaptive grid generation method.

Analysis

The approach taken is one of nonlinear progamming. An objective function is defined as a composite weighted measure of departure from smoothness and local orthogonality over the grid, as follows. Let us consider a master cell centered at the grid point P(x(i,j,k), y(i,j,k), z(i,j,k)), the initial grid being given by the set of the coordinates of its points in the physical space. The master cell is shown in Fig.1. Quantitative measures for the departure from smoothness and orthogonality are respectively defined as:

$$SM_{ijk} = \kappa_1\|r_1\|^2 + \dots + \kappa_6\|r_6\|^2 \,, \tag{1}$$

$$ORT_{ijk} = (r_1 \cdot r_2)^2 + \dots + (r_6 \cdot r_4)^2 \,. \tag{2}$$

The positive scalars κ ($\kappa \geq 1$) in (1) allow the clustering of the resulting grid. Functional relationships of the general form $\kappa = \kappa(i, j, k)$ are chosen to cluster the grid towards selected boundaries of the grid. Grid adaptivity is obtained by defining a volume control functional VOC analogous to the smoothness measure, for which the κ's are given by the values of a positive weight function the grid is to adapt to, averaged between adjacent grid points. It is seen that both grid quality measures are minimal when the master cell is smooth (resp. orthogonal), and that minimizing (1) or the volume control functional is analogous to minimizing the energy of a system of connected tension springs (the grid vertices) of stiffness constants κ.

The global objective function is then defined by:

$$F = \Sigma_i \Sigma_j \Sigma_k [\alpha ORT_{ijk} + (1-\alpha) SM_{ijk} + \beta VOC_{ijk}] \ . \tag{3}$$

The unconstrained minimization of F using a first-order conjugate gradient method (Fletcher- Reeves method [8]) yields successive corrections to the physical coordinates of the grid points, so that the grid becomes smoother and/or more locally orthogonal, depending on the value of the weight parameter α $(0 \leq \alpha \leq 1)$. Adaptation of the grid to a specified weight function (such as $|\nabla p/p|$ for compressible flow problems with shocks) depends on the weight parameter β $(0 \leq \beta \leq 1)$.

The problem of minimizing F is recast in the following form: Minimize F(V), where V is the vector of length $N = 3\ Ni \times Nj \times Nk$ that contains the physical coordinates of all the grid points in a natural ordering; here, Ni, Nj, Nk are the number of grid points in each curvilinear coordinate direction. The iterative minimization method reduces the N-dimensional problem to a succession of one-dimensional searches. The so-called line-searching is here exact, since all components of F are polynomials in the grid point physical coordinates. The optimal grid is obtained when ∇F drops below a specified convergence tolerance. Further details on the algorithm, scaling procedures, treatment of boundary points are given in [9].

Results

The first test case presented concerns an initially uniform grid in the unit cube comprising 1000 cells. Random perturbations are added to the coordinates of each interior grid point, resulting in the severely overlapped grid shown in Fig.2. Some grid points even lie outside the cube. The optimization procedure for $\alpha = 0.5$ easily untangles the 271 overlapped master cells detected in the initial grid, in three iterations. The original cartesian grid is retrieved within fifty iterations (Figs.3-4). The influence of α on the untangling process is documented in Table 1 below.

Table 1: Randomized Cube Example: Influence of α

Iteration	Number of Overlapped Master Cells		
	$\alpha=0$	$\alpha=0.5$	$\alpha=1.0$
0	271	271	271
1	7	19	108
2	0	4	36
3	0	0	17
4	0	0	9
5	0	0	3
6	0	0	0

This example demonstrates the ability of the optimization method to treat an extremely poor initial grid effectively and shows it to converge rapidly towards the optimal grid (which, in this case, was known). It is also seen that the grid is most efficiently untangled when optimizing it in terms of smoothness only, as expected.

The second test case demonstrates the proposed concept for three-dimensional grid generation: Using an imperfect grid generated using a simple, inexpensive algebraic method as input, the optimization method is applied to obtain an acceptable grid. The configuration chosen resembles the Lockheed RPV "Aquila" (Fig.5). The initial grid is illustrated in Fig.6, evidencing unacceptable singularities. It is actually useless, possessing 67 overlapped master cells. Figures 7 and 8 illustrate the result of twenty iterations for α=0, the grid being untangled in four iterations. The improvement in smoothness is considerable. The visible differences between both figures result from implementing orthogonality at the vertical plane of symmetry and at the outflow boundary in the second case (Fig.8). Figure 9 shows the first body/wing conforming grid surface for the same optimized grid. Notice the high degree of smoothness achieved. Finally, the procedure is repeated for α=0.4 while enforcing clustering of the body/wing-conforming grid surfaces. Figure 10 shows the vertical plane of symmetry. The clustering effect is evident when comparing Fig.9 and Fig.11. The convergence history for this last example (Fig.12) shows the evolution of the global grid quality measures. The time required per iteration is 15s to process the 18.711 grid points, while the initial grid is generated in 12s. These values are for a Harris 800-II computer.

Finally, some preliminary results are shown for the adaptation of two-dimensional grids. Figures 13 through 15 present the grids obtained after twenty iterations for $\alpha=\beta=0.5$. It is seen that the volume control capability does not depend on the direction of the gradient of the sinusoidal weight function relative to the x and y coordinate directions. The comparison with identical test cases performed for the variational method [5] is favorable.

Conclusions

The discussion of the optimization method is as complete as space permits. More details and results for static grid optimization and flow adaptive grid generation are reported elsewhere [9]. Being independent of the technique used to generate the initial grid, both methods are widely applicable. They also are able to treat overlapped grids, which are a frequent problem when generating a grid about a complex three-dimensional configuration.

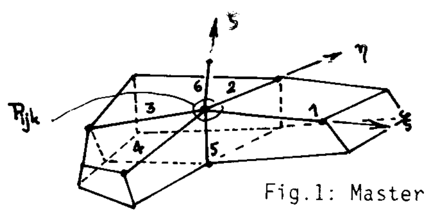

Fig.1: Master Cell.

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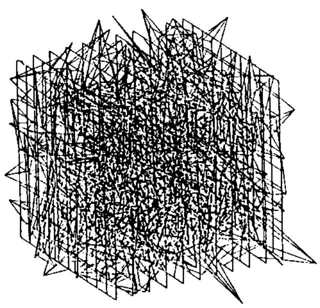


Fig.2: Randomized Initial Grid (271 Overlapped Cells).

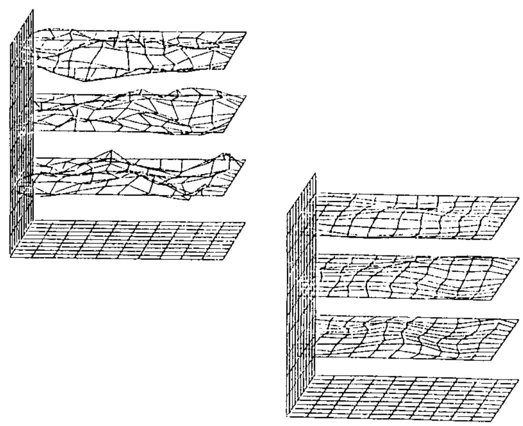


Fig.3: Grid after One Iteration (19 Overlapped Cells, Above) and after Three Iterations (No Overlapped Cells, Below).

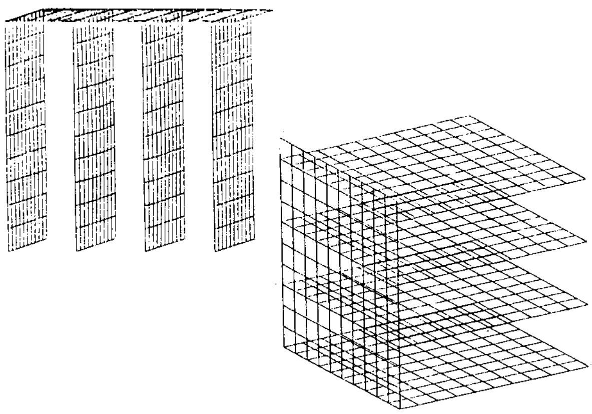


Fig.4: Grid after Twenty Iterations (nearly Uniform Grid, Above) and after Fifty Iterations (Cartesian Grid is recovered, Below).

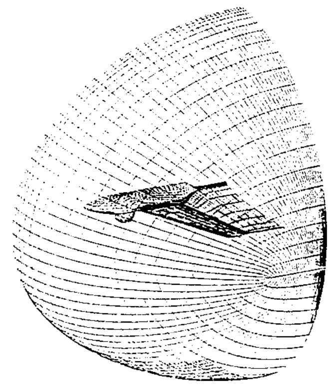
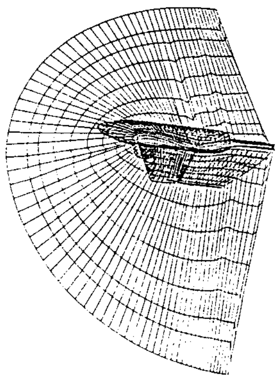


Fig.5: Inner and Outer Grid Surfaces for the "Aquila" Configuration.



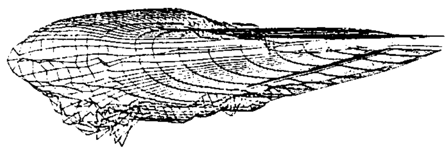
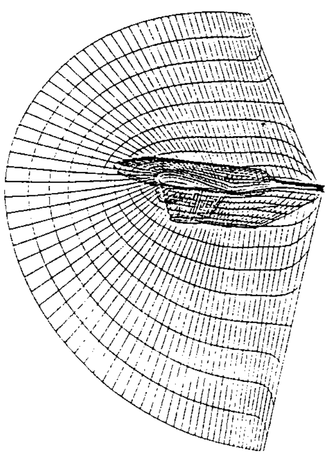


Fig.6: Initial Three-Dimensional Grid Showing Unacceptables Irregularities. One of the Quasi-Meridional Grid Surfaces (j=cst) and the Second Body-Conforming Grid Surface (k=cst) are shown.



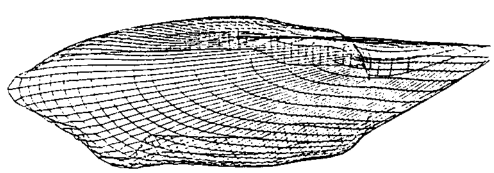


Fig.7: Same Grid Surfaces for the Optimized Grid Obtained after Twenty Iterations for $\alpha=0$. Points on the Outflow Boundary and on the Vertical Plane of Symmetry are Kept Fixed.

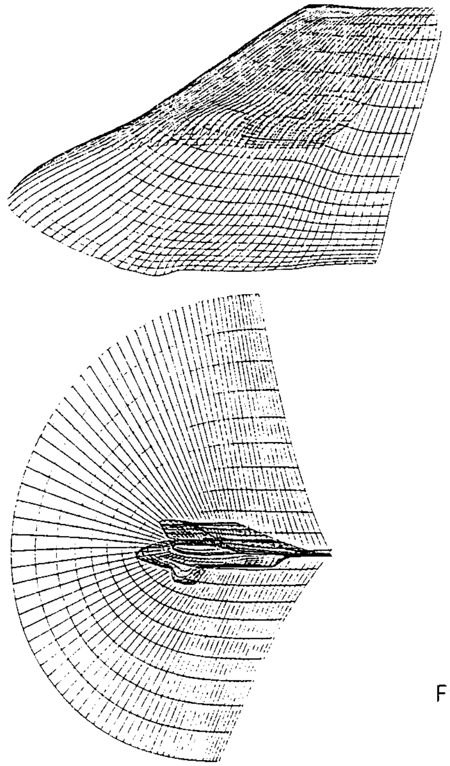


Fig.8: Same Grid Surfaces for the Optimized Grid Obtained after Twenty Iterations for $\alpha=0$ with Orthogonality Enforced at the Outflow Boundary and at the Vertical Plane of Symmetry.

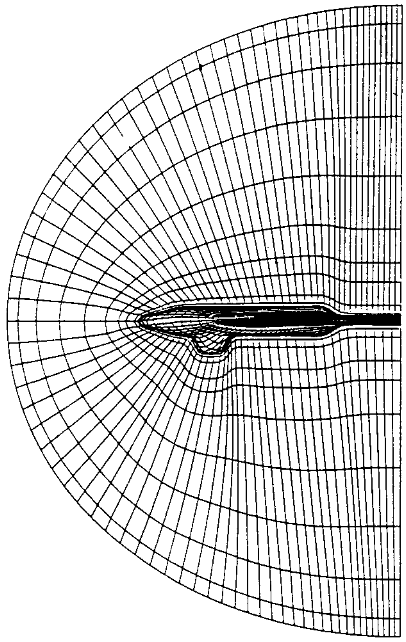


Fig.10: Optimized Grid Obtained after 20 Iterations for $\alpha=0.4$ With Clustering of the Body-Conforming Grid Surfaces Towards the Body.

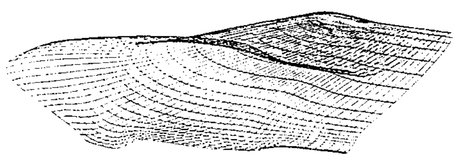


Fig.9: For the Same Optimized Grid: First Body/Wing Conforming Grid Surface, Showing High Degree of Smoothness.

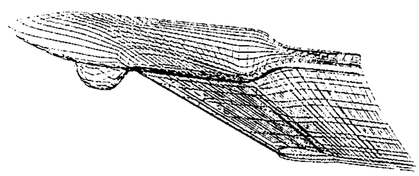


Fig.11: For the Same Optimized Grid: First Body-Conforming Grid Surface, Showing High Degree of Smoothness (Compare to Fig.9).

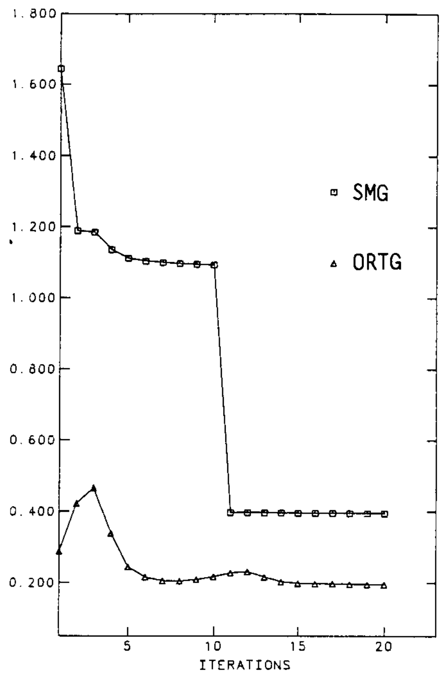


Fig.12: Convergence History for the Optimization Procedure of Fig.10-11 (SMG=Global Weighted Smoothness Measure, ORTG=Global Orthogonality Measure).

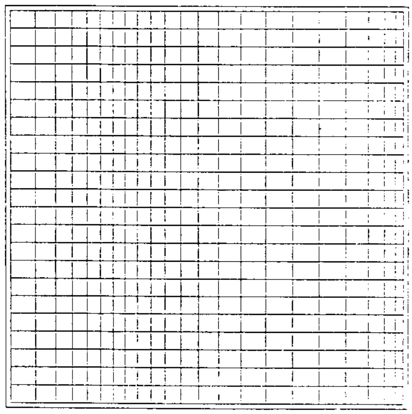


Fig.13: Adapted Grid,
$W = \sin(2\pi x) + 1/\sigma_o$,
$\alpha = 0.5$, $\beta = 0.5$, $\sigma_o = 100$.

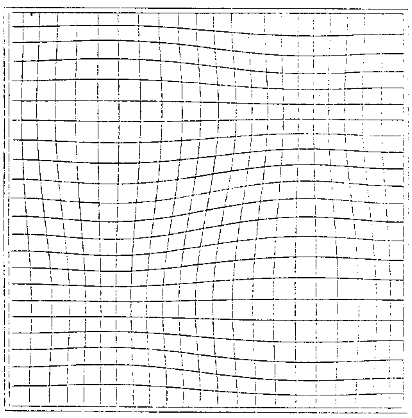


Fig.14: Adapted Grid,
$W = \sin(2\pi x)\times\sin(2\pi y) + 1/\sigma_o$
$\alpha = 0.5$, $\beta = 0.5$, $\sigma_o = 100$.

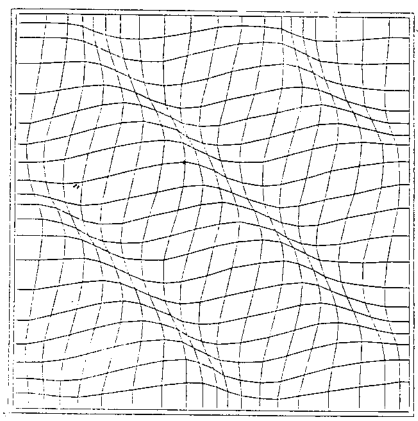


Fig.15: Adapted Grid,
$W = \sin[4\pi(x+y)] + 1/\sigma_o$,
$\alpha = 0.5$, $\beta = 0.5$, $\sigma_o = 100$.