Generation of Computational Grids Using Optimization

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A method for generation of computational grids using principles of nonlinear programming (optimization) is described. Grids are generated so that certain discrete measures of grid smoothness and orthogonality are maximized using a fast iterative optimization procedure. The method can also be used to improve an existing grid irrespective of the method used for its generation. If the original grid contains regions of overlap (nonpositive Jacobian), this method is capable of unraveling the grid and making it useful for computations. The iterative optimization procedure is efficient due to the use of a conjugate direction method with exact line searching. Examples are given of the application of this technique to two- and three-dimensional computational grids. The extension of the method to generate solution adaptive grids is discussed.

Introduction

IN the past few years, there has been a great deal of interest in the development of computational grid-generation techniques[1] for discretizing complex regions for the numerical solution of partial differential equations. The commonly used grid-generation methods have achieved a high degree of sophistication and ease of use. However, for complex configurations, the existing methods do not always produce acceptable grids 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.[2,3] In addition to grid-quality problems, many methods suffer from computational inefficiency. For these reasons, the authors have perceived a need for a grid-generation method that could be used to improve the quality of a given computational grid. In addition, the method should be capable of serving as a stand-alone grid-generation procedure, independent of other techniques.

The basic concept behind this grid-generation method is to assume from the outset that the grid to be generated or optimized consists of straight-line segments joining the nodal grid points. This is in contrast to methods that solve elliptic, parabolic, or hyperbolic partial differential equations or use conformal mapping. These methods are based on continuous, not discrete, coordinate transformations and, therefore, suffer from discretization errors for any grid consisting of a finite number of grid points. The grid-generation technique described herein formulates discrete measures of grid smoothness and orthogonality at each grid point and, therefore, does not suffer from truncation errors on coarse grids. These measures of grid quality are then minimized using a conjugate direction procedure with exact line searching. The resulting grids are optimal with respect to the particular smoothness and orthogonality measures chosen, and there are many possible choices for their exact forms.

The next section describes the formulation of the method followed by some typical results of using this method to improve existing grids or generate new grids. Finally, extensions of the method for generating solution adaptive grids are discussed, and other areas of possible future research are pointed out.

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Analysis

The formulation of the method will be illustrated for two-dimensional grids. The details of the method for the three-dimensional case are given in the Appendix.

We will discuss the grid-generation method by first noting similarities with the Saltzman-Brackbill[4] variational grid-generation method. In the variational method, two functionals are introduced that provide measures of grid smoothness

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

and grid orthogonality

$$I_o = \iint (\nabla_{xy}\xi) \cdot (\nabla_{xy}\eta) J^3 \, dx \, dy \qquad (2)$$

where

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

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

$$x,y = \text{physical coordinates}$$

$$\xi,\eta = \text{computational coordinates}$$

The roles of dependent (ξ,η) and independent (x,y) coordinates are interchanged, giving the transformed equations

$$I_s = \iint [x_\xi^2 + x_\eta^2 + y_\xi^2 + y_\eta^2] J \, d\xi \, d\eta \qquad (3)$$

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

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

Next the Euler-Lagrange equations are applied to the total functional

$$I = I(\xi,\eta) \equiv \lambda_s I_s + \lambda_o I_o \qquad (5)$$

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 nonlinear system of coupled differential equations of second order in the (x,y) physical coordinates that are solved by finite-difference discretization and iteration.

In theory, the same solutions of the Euler-Lagrange system can be achieved by direct discretization and minimization of the total functional $I(\xi,\eta)$. In this case, the derivatives can be replaced with finite differences, and the

integrals replaced with simple summations over the grid points. However, from Eqs. (3) and (4) one can see that only first partial derivatives of x and y appear in the functionals I_s and I_o. Therefore, a central difference discretization of I_s and I_o 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 otherwise do not occur if the Euler-Lagrange system is solved. This is because second-order partial derivatives appear in the Euler-Lagrange system and the central grid point $(x_{i,j}, y_{i,j})$ is strongly coupled to its neighboring grid points.

The decoupling problem suggests the use of an alternative, more direct formulation of grid-quality measures that are directly dependent on the central grid point $(x_{i,j}, y_{i,j})$. The smoothness measure is defined 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 (i and j) directions. Similarly, a maximally orthogonal grid is one in which the grid lines of the families $\xi = $ const ($i = $ const) and $\eta = $ const ($j = $ const) 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 to 4 (Fig. 1). Assume that the grid points are connected with straight-line segments defined by the vectors:

$$r_{i+1,j} = (x_{i+1,j} - x_{i,j})i + (y_{i+1,j} - y_{i,j})j$$

$$r_{i,j+1} = (x_{i,j+1} - x_{i,j})i + (y_{i,j+1} - y_{i,j})j$$

$$r_{i-1,j} = (x_{i-1,j} - x_{i,j})i + (y_{i-1,j} - y_{i,j})j$$

$$r_{i,j-1} = (x_{i,j-1} - x_{i,j})i + (y_{i,j-1} - y_{i,j})j \qquad (6)$$

The quantitative measure of local grid smoothness, σ, is formed from the sum of the squares of differences in areas from one grid cell to the next. Thus σ is given by

$$\sigma_{i,j} \equiv (A_1 - A_2)^2 + (A_2 - A_3)^2 + (A_3 - A_4)^2 + (A_4 - A_1)^2 \qquad (7)$$

where A_k is a measure of the area of the kth elementary cell formed from cross products of the local position vectors, for example,

$$A_1 = |(r_{i+1,j} \times r_{i,j+1})| = |x_{i+1,j}y_{i,j+1} - y_{i+1,j}x_{i,j+1}| \qquad (8)$$

The quantitative measure of local grid orthogonality, ρ, is formed from dot products of the position vectors emanating from the central grid point and is given by

$$\rho_{i,j} \equiv (r_{i+1,j} \cdot r_{i,j+1})^2 + (r_{i,j-1} \cdot r_{i+1,j})^2$$

$$+ (r_{i-1,j} \cdot r_{i,j-1})^2 + (r_{i,j+1} \cdot r_{i-1,j})^2 \qquad (9)$$
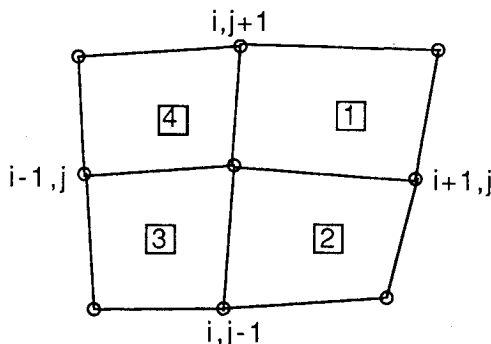

Fig. 1 Master cell.

Note that when the grid is smooth and orthogonal, σ and ρ will be minimized. Also note that the smoothness and orthogonality measures depend upon the central grid point $(x_{i,j}, y_{i,j})$ and, therefore, the decoupling problem discussed above is eliminated.

We now define the total cost function F as a linear combination of the smoothness and orthogonality measures

$$F \equiv \sum_i \sum_j \left\{ \frac{\alpha \rho_{i,j}}{\rho_{\max}} + (1 - \alpha) \frac{\sigma_{i,j}}{\sigma_{\max}} \right\} \qquad (10)$$

where

$$0 \le \alpha \le 1$$

$$\sigma_{\max} = \max_{i,j} [\sigma_{i,j}], \qquad \rho_{\max} = \max_{i,j} [\rho_{i,j}]$$

Minimizing F will produce a grid that is maximally smooth ($\alpha = 0$) or maximally orthogonal ($\alpha = 1$). Setting α to intermediate values between 0 and 1 gives different weights to the grid smoothness and orthogonality. The scaling of σ and ρ by their maximum values ensures that each measure will be of the same order of magnitude.

Iterative Optimization Procedure

To minimize F, the following iterative optimization procedure is used. First, let us restate the problem in terms of the vector $z = (x, y)$ of length $2i_{\max}j_{\max} = 2N$ that contains the x and y coordinates of the grid points in some convenient ordering. Thus we must find the value $z = z^*$ such that $F(z^*)$ is a minimum. We use the Fletcher-Reeves optimization procedure[5] since this is one of the only conjugate direction optimization procedures that does not require the storage of a $2N \times 2N$ matrix. The procedure can be summarized in algorithmic form as follows:

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

$$\text{WHILE} \quad |\nabla F(z^{(n)})| > \epsilon \quad \text{DO}$$

$$z^{(n+1)} = z^{(n)} + \omega_n \delta z^{(n)} \qquad (11)$$

where

$$\delta z^{(n)} = - \nabla F(z^{(n)}) + \beta^{(n)} \delta z^{(n-1)}$$

$$\beta^{(n)} = |\nabla F(z^{(n)})|^2 / |\nabla F(z^{(n-1)})|^2$$

The procedure is restarted if $n = 2N$, i.e., set $z^{(0)} = z^{(2N)}$ and continue the iteration procedure. The factor ω_n in Eq. (11) is the so-called line-search parameter given by

$$\omega_n = \arg\{ \min_\omega [\Psi(\omega)] \} \qquad (12)$$

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

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

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 Nonlinear Minimal Residual Method[6,7] for accelerating the convergence of iterative solutions of differential systems.

Note that the orthogonality and smoothness measures are composed of simple polynomial expressions in the x and y grid point coordinates. Therefore, $\Psi(\omega)$ is a fourth-degree polynomial in terms of ω. This follows by 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

$$\frac{\partial \Psi}{\partial \omega} = 0 \tag{14}$$

The real 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 $|\nabla F(z^{(n)})|$ is less than a specified tolerance.

Results

Computer programs were developed to implement the grid optimization procedure for two- and three-dimensional computational grids. The input to the programs consists of the the original grid point coordinates, the maximum number of optimization iterations to be performed, and the value of the weighting factor α. These programs keep the points fixed on the boundaries of the domains, although this is not a limitation of the technique.

The first test case is a periodic O-type grid for a nonstaggered 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[6,8] and is shown in Fig. 2. The grid was then optimized using the weighting factor $\alpha = 0.5$ with the result shown in Fig. 3. One can see that the method is able to smooth this grid and make it more orthogonal.

Another cascade example is shown in Figs. 4 and 5. This case presents a periodic O-type grid for a turbine cascade[9] 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 skewed.

To demonstrate the ability of the method to unravel grids that contain overlapping regions (nonpositive Jacobian), we optimized an O-type grid for a Space Shuttle cross section[7] that was originally useless (Fig. 6). The result of applying 50 iterations of the optimization method is shown in Fig. 7. All of the overlapped regions have been unraveled and the resulting grid is usable. Note that the grid points on the outer boundary and on the Space Shuttle surface were kept fixed.

As a final two-dimensional example, a uniform rectangular grid is shown, upon which a random error has been intentionally introduced (Fig. 8a). The resulting iterative optimization sequence is shown in Figs. 8b-8d. The overlapping grid was easily unraveled in 20 iterations to produce the original uniform grid.

The final example is for a three-dimensional grid inside a cube. The original grid was generated similarly to the one in Fig. 8, i.e., a uniform random error was added to each grid point of a uniform grid (Fig. 9). The modified smoothness measure (see Appendix) was used along with the three-dimensional orthogonality measure to optimize the grid. In
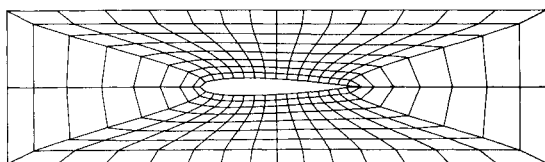

Fig. 2 Nonoptimal periodic O-type grid for NACA 0012 airfoil cascade, gap-to-chord ratio = 1.0, grid size 32 × 8.
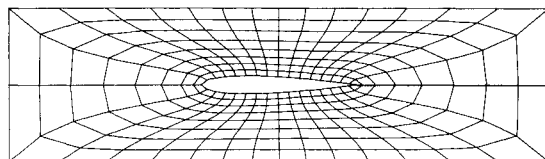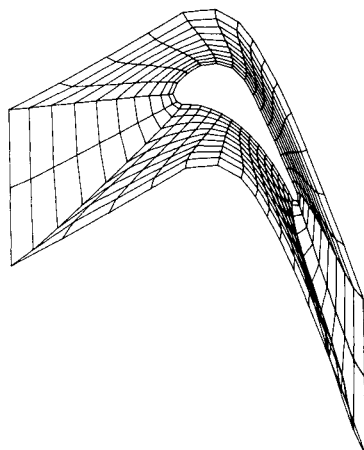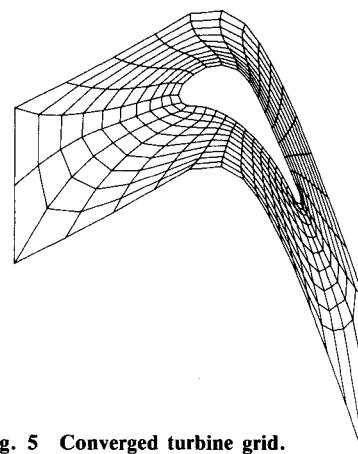

Fig. 3 Converged NACA 0012 grid.

Fig. 4 Nonoptimal periodic O-type grid for MIT turbine airfoil cascade, gap-to-chord ratio = 1.0, grid size 32 × 10.
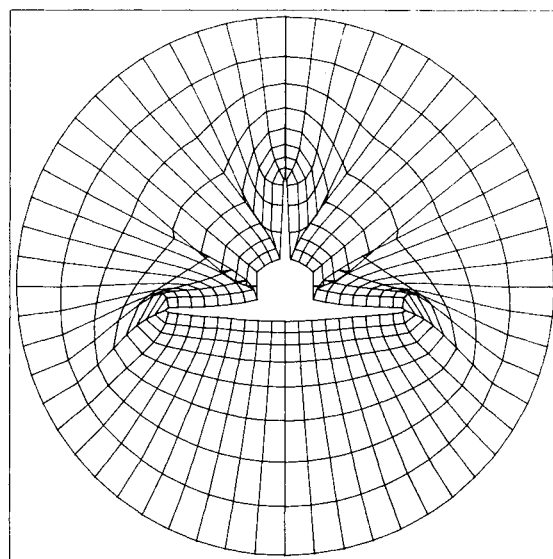

Fig. 5 Converged turbine grid.

Fig. 6 Nonoptimal O-type grid for Space Shuttle cross section, grid size 56 × 8.

20 iterations, the original uniform grid was retrieved as shown in Fig. 10.

Finally, a typical plot of the optimization procedure convergence history is shown in (Fig. 11). The convergence of the smoothness, orthogonality, and total cost function is shown for the Space Shuttle case (Fig. 6) with a weighting factor of $\alpha = 0.5$. It can be seen that the quantitative measures of the grid quality were reduced by acceptable amounts before the convergence rate slowed. The CPU time for this case was 44.65 s (≈ 0.002 s per iteration per grid point) on a Harris 800 computer (roughly equivalent in speed to a VAX 11/780 computer).

Future Research

The most promising applications for the method are in the areas of three-dimensional grid generation and flow adaptive optimized grid generation. The three-dimensional grid-generation method would be particularly suitable for grids that are based on stackings of two-dimensional grids.[2] In
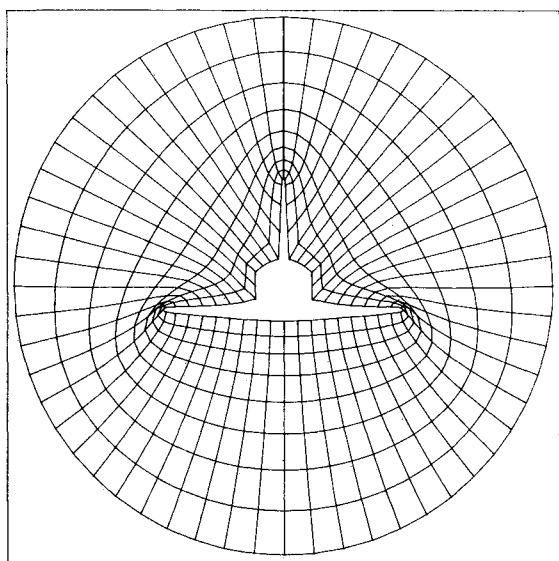

Fig. 9   Three-dimensional randomized grid in the unit cube.

Fig. 7   Converged Space Shuttle grid.

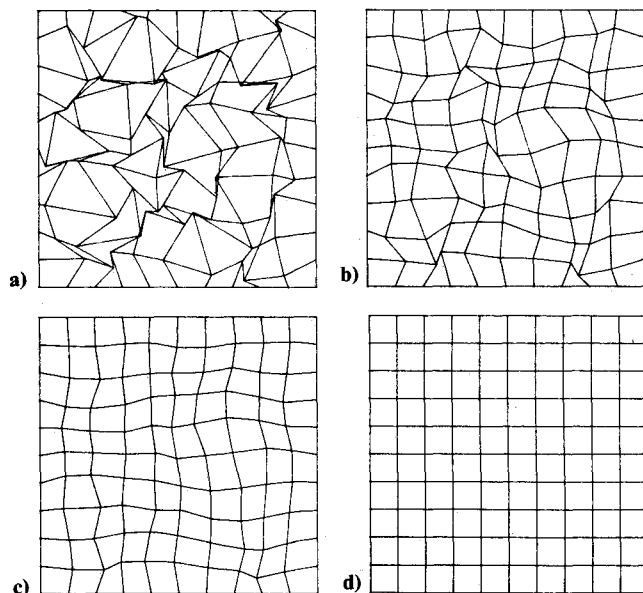Fig. 10   Optimized three-dimensional grid (20 iterations).

Fig. 8   a) Original uniform grid with a uniform random error; b) Grid after one iteration; c) Grid after two iterations; and d) Converged grid (20 iterations).
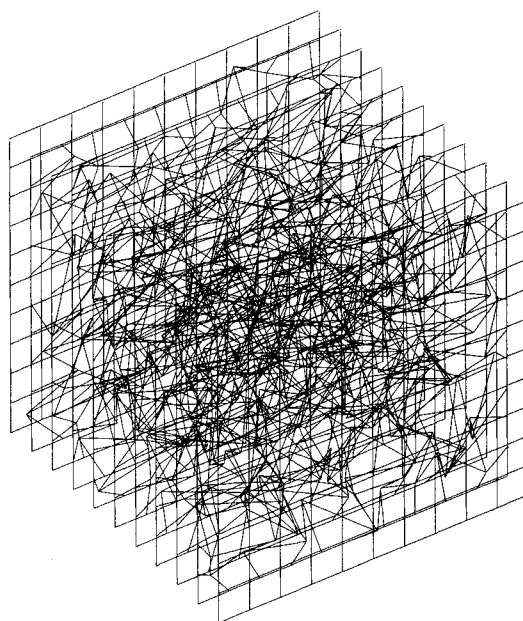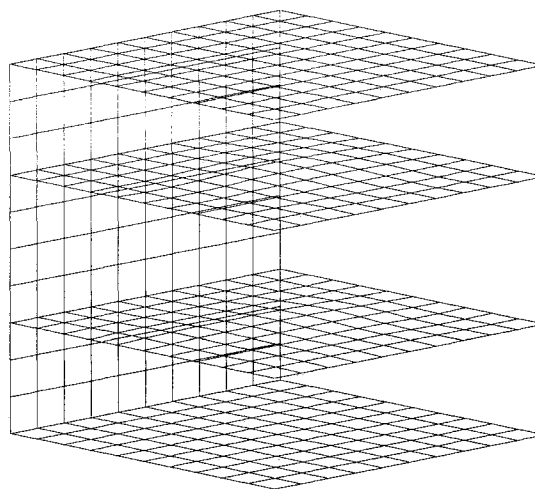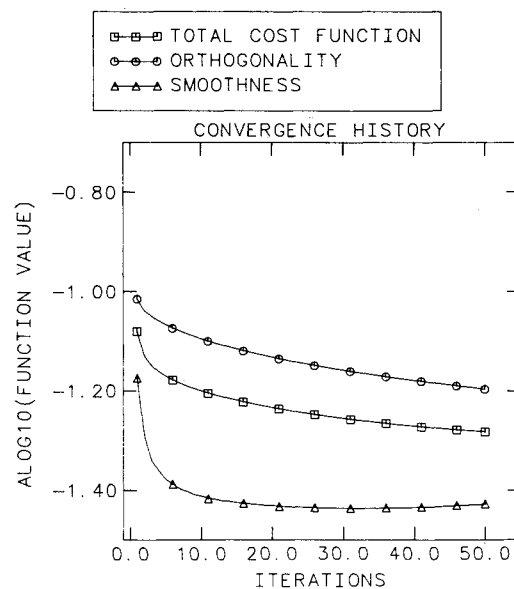

Fig. 11   Convergence history for Space Shuttle grid.

this case, the grid is probably fairly orthogonal within the stacking surfaces, but it could be quite nonorthogonal 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, an additional functional should be added to F as done by Saltzman and Brackbill.[4] The new functional should represent a weighted volume measure of a quantity, such as the pressure gradient, that we wish the grid to adapt to. This functional would be minimized along with the grid-quality measures, thus forcing the grid points to automatically cluster in regions of the flow domain requiring resolution, while maintaining a high degree of grid smoothness and orthogonality. Note also that automatic grid clustering in specified regions could be implemented in the same fashion.

Since there are many ways to formulate the smoothness and orthogonality measures (e.g., the orthogonality measure could be formulated in terms of cross products of the position vector r), other formulations could be tested to find those that are best in terms of computational efficiency and grid quality. Furthermore, other grid-quality measures such as grid-cell aspect ratios could be added to F to further improve grid quality.

Appendix

This section presents the details of the grid-generation/optimization method in the three-dimensional case.
Smoothness measure:

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

$$+ (V_5 - V_6)^2 + (V_6 - V_7)^2 + (V_7 - V_8)^2 + (V_8 - V_5)^2$$

$$+ (V_1 - V_5)^2 + (V_2 - V_6)^2 + (V_3 - V_7)^2 + (V_4 - V_8)^2 \quad \text{(A1)}$$

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

$$V_1 \equiv |r_{i,j,k+1} \cdot (r_{i+1,j,k} \times r_{i,j+1,k})| \quad \text{(A2)}$$

Orthogonality measure:

$$\rho_{i,j,k} \equiv (r_{i+1,j,k} \cdot r_{i,j+1,k})^2 + (r_{i,j-1,k} \cdot r_{i+1,j,k})^2 + (r_{i-1,jk} \cdot r_{i,j-1,k})^2$$

$$+ (r_{i,j+1,k} \cdot r_{i-1,j,k})^2 + (r_{i+1,j,k} \cdot r_{i,j,k-1})^2 + (r_{i,j-1,k} \cdot r_{i,j,k-1})^2$$

$$+ (r_{i-1,j,k} \cdot r_{i,j,k-1})^2 + (r_{i,j+1,k} \cdot r_{i,j,k-1})^2 + (r_{i+1,j,k} \cdot r_{i,j,k+1})^2$$

$$+ (r_{i,j-1,k} \cdot r_{i,j,k+1})^2 + (r_{i-1,j,k} \cdot r_{i,j,k+1})^2 + (r_{i,j+1,k} \cdot r_{i,j,k+1})^2$$

$$\text{(A3)}$$

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. Since $\Psi(\omega)$ is of

sixth order we have to find the five roots of

$$\frac{\partial \Psi}{\partial \omega} = 0 \quad \text{(A4)}$$

to perform the line-searching part of the iterative optimization procedure.
Alternative smoothness measure:

An alternative smoothness measure can be formulated, which is both easier to implement and requires much less computational effort than the standard smoothness measure. This alternative smoothness measure was used for the three-dimensional grid-optimization example shown in the Results section. The alternative smoothness measure is a measure of the relative distance between a grid point and its surrounding neighbors, and is given by

$$\sigma^*_{i,j,k} = (r_{i+1,j,k} \cdot r_{i+1,j,k}) + (r_{i,j-1,k} \cdot r_{i,j-1,k}) + (r_{i-1,j,k} \cdot r_{i-1,j,k})$$

$$+ (r_{i,j+1,k} \cdot r_{i,j+1,k}) + (r_{i,j,k+1} \cdot r_{i,j,k+1}) + (r_{i,j,k-1} \cdot r_{i,j,k-1}) \quad \text{(A5)}$$

Note that σ^* is much simpler and, therefore, less expensive to compute than the standard smoothness measure σ. Also note that σ^* contributes only second-order terms to $\Psi(\omega)$.

Acknowledgments

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