

## GRID ORTHOGONALIZATION FOR CURVILINEAR ALTERNATING-DIRECTION TECHNIQUES\*

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A method is developed for an a posteriori iterative improvement to an arbitrary computational grid. Local corrections to the coordinates of the grid points are used to form a global cost function which is minimized with respect to a single parameter. The local corrections and cost function can be constructed to maximize the local smoothness and/or the local orthogonality of the grid. The advantage of this method is that it allows the user to generate an initial grid using any inexpensive method, and then the grid can be improved with respect to both orthogonality and smoothness.

This technique was used to generate grids for a finite element alternating-direction method which uses curved elements. A sample transient diffusion problem was solved on a series of grids to investigate the sensitivity of the curvilinear alternating-direction method to grid orthogonalization. The initial grid was highly nonorthogonal and each grid produced by the automatic grid generation program was smoother and more orthogonal.

This work shows that the adaptive grid program can be easily used to generate nearly orthogonal grids and it shows that the curvilinear alternating-direction technique is not highly sensitive to nonorthogonality of the grid. It is shown that as long as a grid is somewhat reasonable, the alternating-direction method will perform quite well.

### 1. Introduction

Finite element methods are routinely used to model the solution of parabolic partial differential equations. Finite element techniques are extremely versatile and can be used easily on curved regions with very general boundary conditions. This is the primary reason that finite element methods have become extremely popular for modeling problems in solid mechanics, heat transfer, fluid mechanics, and structural dynamics. In 1971, Douglas and Dupont [1], motivated by previous finite difference work, formulated a finite element alternating-direction procedure to solve nonlinear parabolic problems posed on rectangular regions with uniform grid spacings. This method can solve large multidimensional problems as a series of one-dimensional problems. The storage and execution requirements are low since they are associated with one-dimensional problems. Dendy and Fairweather [2] extended these methods to unions of rectangles, and Hayes [3-7] generalized this method to nonrectangular regions composed of isoparametric finite elements. In this formulation, the Jacobian of the

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isoparametric map was obtained at the element nodes by a "patch approximation" and the alternating-direction parameter,  $\lambda$ , approximates the diffusion and the Jacobian.

The purpose of this paper is to investigate how sensitive the curvilinear alternating-direction method is to nonorthogonal grids. In this study, an automatic computational grid generation program was used to generate a series of optimized grids, each of which had increased smoothness and increased orthogonality. The final grid was a rectangular, uniform grid. A transient diffusion problem was solved on each of the grids using both the standard finite element method and the curvilinear alternating-direction technique. Errors on each of the grids are compared in order to analyze the sensitivity of the alternating-direction method to grid orthogonalization.

## 2. Optimized computational grid generation

Despite a wide variety of existing methods for automatic boundary fitted computational grid generation [8], it is often desirable to maintain maximum local grid orthogonality and smoothness in the variations of the grid cell sizes.

Recently, a new method has been developed for arbitrary two-dimensional [9] and three-dimensional [10] configurations that is capable of efficiently and reliably generating a grid, which is optimal in the sense of minimizing local nonsmoothness and nonorthogonality while keeping the boundary grid points fixed. Our optimal grid generation method has certain conceptual similarities with the existing variational grid generation method [11]. In the variational method, two functionals are introduced that provide measures of grid smoothness

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

and grid orthogonality

$$I_o = \iint [(\nabla_{xy} \xi) \cdot (\nabla_{xy} \eta)] J^3 dx dy . \quad (2)$$

Here,  $J = \xi_x \eta_y - \eta_x \xi_y$  is the Jacobian of the transformation from the  $(x, y)$  physical space to the uniformly discretized  $(\xi, \eta)$  computational space. The Euler-Lagrange equations of variational calculus are then applied to minimize the total cost functional

$$I(\xi, \eta) = \alpha I_o + (1 - \alpha) I_s , \quad (3)$$

where  $\alpha$  is a scalar weighting parameter ( $0 \leq \alpha \leq 1$ ).

Our optimal grid generation method differs from the variational method in that, instead of using straightforward finite difference representation of the partial derivatives in (1) and (2), the following approximations are used to evaluate local grid smoothness and orthogonality. Consider the local problem of grid optimization for a master cell consisting of four neighboring elementary cells numbered 1, 2, 3, and 4 as shown in Fig. 1. Define the position vectors

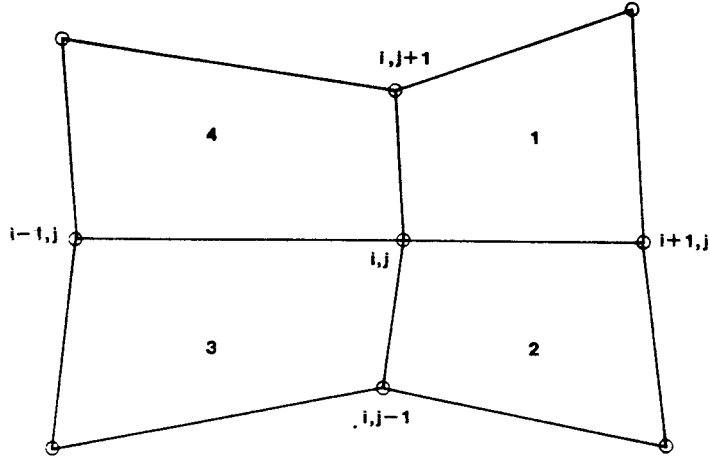


Fig. 1. Position vectors for a two-dimensional problem.

$$\mathbf{r}_{i+1, j} = (x_{i+1, j} - x_{i, j})\mathbf{i} + (y_{i+1, j} - y_{i, j})\mathbf{j}, \quad (4)$$

$$\mathbf{r}_{i, j+1} = (x_{i, j+1} - x_{i, j})\mathbf{i} + (y_{i, j+1} - y_{i, j})\mathbf{j}, \quad (5)$$

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

$$\mathbf{r}_{i, j-1} = (x_{i, j-1} - x_{i, j})\mathbf{i} + (y_{i, j-1} - y_{i, j})\mathbf{j}, \quad (7)$$

where  $\mathbf{i}$  and  $\mathbf{j}$  are unit vectors in the  $x$ - and  $y$ -direction, respectively. The quantitative measure of local grid smoothness or change in cell area is given by

$$\sigma_{i, j} \equiv (A_1 - A_2)^2 + (A_2 - A_3)^2 + (A_3 - A_4)^2 + (A_4 - A_1)^2, \quad (8)$$

where  $A_k$  is an approximate measure of the area of the  $k$ th elementary cell, e.g.,

$$A_1 = |\mathbf{r}_{i+1, j} \times \mathbf{r}_{i, j+1}|. \quad (9)$$

The local measure of grid orthogonality is given by

$$\rho_{i, j} \equiv (\mathbf{r}_{i+1, j} \cdot \mathbf{r}_{i, j+1})^2 + (\mathbf{r}_{i, j-1} \cdot \mathbf{r}_{i+1, j})^2 \\ + (\mathbf{r}_{i-1, j} \cdot \mathbf{r}_{i, j-1})^2 + (\mathbf{r}_{i, j+1} \cdot \mathbf{r}_{i-1, j})^2. \quad (10)$$

Corner nodes are used to define area and orthogonality even for cells with curved sides.

Then we define the total cost function,  $F$ , as

$$F \equiv \sum_{i=1}^p \sum_{j=1}^q [\alpha \rho_{i, j} + (1 - \alpha) \sigma_{i, j}]. \quad (11)$$

The minimization problem can be restated in terms of the vector  $\mathbf{z} = (x, y)$  of length  $2pq = 2N$

that contains the  $x$ - and  $y$ -coordinates of the grid points in a natural ordering. Thus, one must find the value  $z = z^*$  such that  $F(z^*)$  is a minimum. Here, the Fletcher–Reeves conjugate direction procedure [12] was used to find  $F(z^*)$  from

$$z^{(n+1)} = z^{(n)} + \omega^{(n)} \delta z^{(n)}, \quad (12)$$

$$\delta z^{(n)} = -\nabla F(z^{(n)}) + \beta^{(n)} \delta z^{(n-1)}, \quad (13)$$

$$\beta^{(n)} = |\nabla F^{(n)}|^2 / |\nabla F^{(n-1)}|^2. \quad (14)$$

The parameter  $\omega$  in (12) is the so-called line-search parameter and it is given by

$$\omega = \arg [\min_{\omega} \psi(\omega)], \quad (15)$$

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

$$\psi(\omega) = F(z^{(n+1)}) = F(z^{(n)} + \omega \delta z^{(n)}). \quad (16)$$

The parameter  $\omega$  is determined with minimal effort using concepts based on the nonlinear minimal residual method [13] for accelerating the iterative solution of differential systems. By simple substitution of (12) into (16), it follows that  $\psi(\omega)$  is a fourth-degree polynomial function in terms of  $\omega$ . To determine the value of  $\omega$  that minimizes  $\psi(\omega)$ , one must find and test the three roots of the cubic polynomial obtained from

$$\partial \psi / \partial \omega = 0. \quad (17)$$

The root that produces the minimum in  $\psi$  is used to update the grid point coordinates.

Our method of grid generation using optimization has certain distinctive advantages over the method based on variational calculus. With our method, the initial grid can even be overlapped, that is, it can have regions of negative Jacobians. This situation very frequently

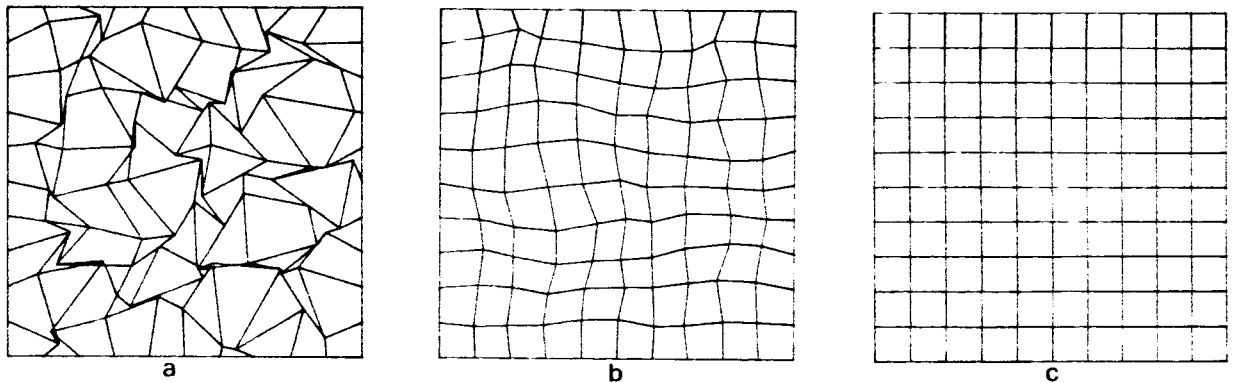


Fig. 2. (a) Initial two-dimensional grid with overlapped grid cells. (b) Grid after two iterations with an optimizer. (c) Grid after twenty iterations with an optimizer.

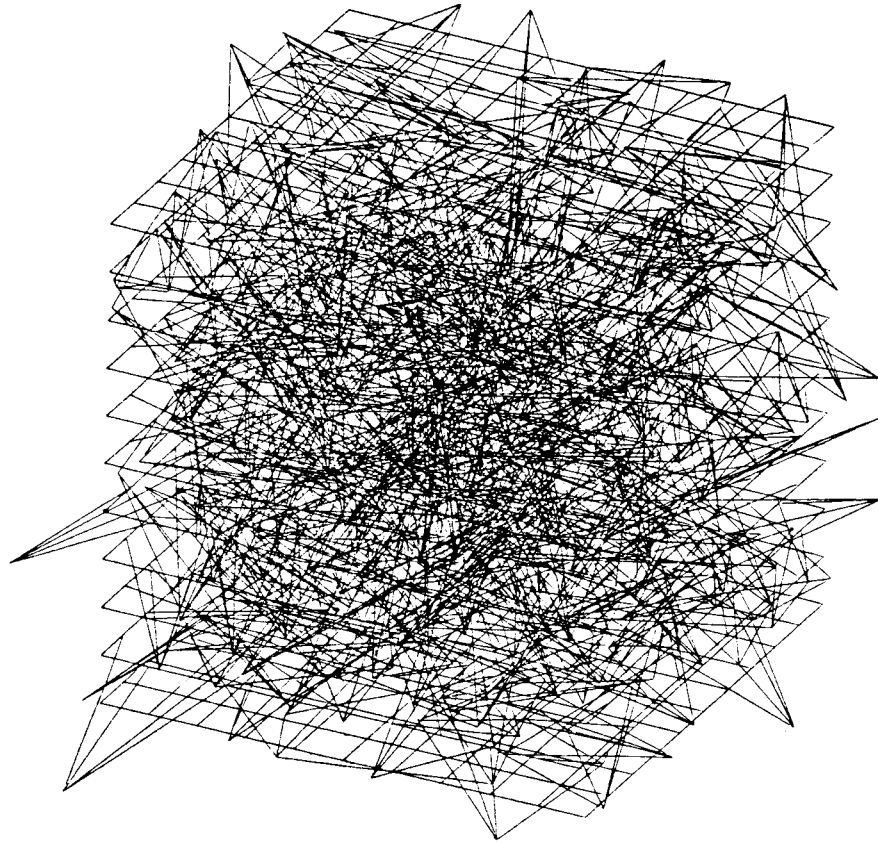


Fig. 3. Initial three-dimensional grid with overlapped grid cells.

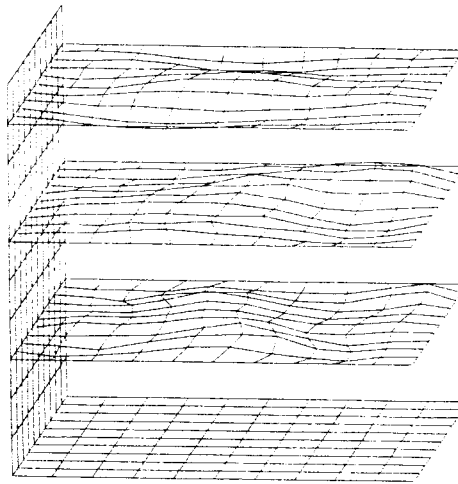


Fig. 4. Grid surfaces after two iterations with an optimizer.

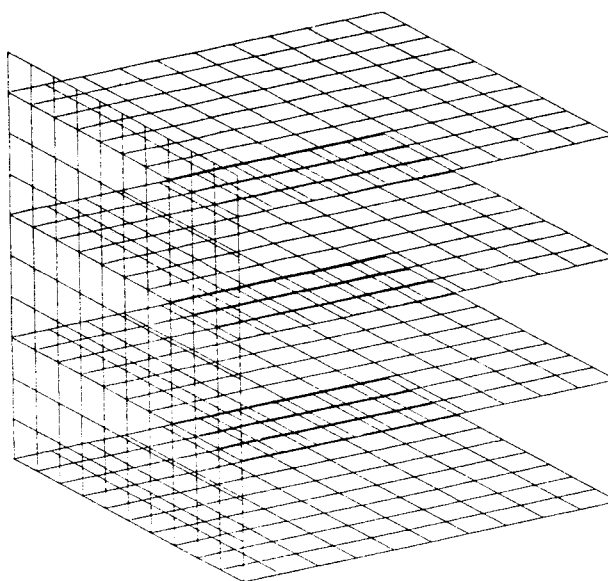


Fig. 5. Grid surfaces after twenty iterations with an optimizer.

occurs in three-dimensional problems involving highly irregular configurations. Figures 2 and 3–5 clearly demonstrate the capability of our optimal grid generation method to unravel two-dimensional and three-dimensional grids that were initially useless and to recover a grid that has maximum possible local smoothness and orthogonality.

### 3. Curvilinear alternating-direction method

Complete details of the finite element alternating-direction method will not be given here, as they can be found in other references [4–7]; however, the key features of the method will be summarized. The alternating-direction method can be used to solve the transient differential equation

$$c(x, y)\partial u/\partial t - \nabla \cdot k(x, y)\nabla u + b(x, y)u = f(x, t) \quad \text{on } \Omega, \quad (18)$$

on a domain  $\Omega$  subject to either Dirichlet, Neumann, or mixed boundary conditions on the boundary of  $\Omega$ . The standard backward-difference finite element method used to approximate (18) is

$$(c(u^{n+1} - u^n)/\Delta t, v)_\Omega + (k\nabla u^{n+1}, \nabla v)_\Omega = (f^n, v)_\Omega \quad (19)$$

for all tensor product test functions  $v$  in the Sobolev space  $H^1(\Omega)$ . Note that the gradient,  $\nabla$ , in (19) is with respect to the physical  $(x, y)$  coordinates of  $\Omega$ . The alternating-direction method can be viewed as a perturbation of the left-hand side of the backward-difference equation (19) given by

$$\begin{aligned} & (c(u^{n+1} - u^n)/\Delta t, v)_\Omega + (\lambda \bar{\nabla}(u^{n+1} - u^n), \bar{\nabla}v) + \Delta t \lambda^2 (\partial^2(u^{n+1} - u^n)/\partial \xi \partial \eta, \partial^2 v/\partial \xi \partial \eta) \\ & = (f^{n+1}, v)_\Omega - (k \nabla u^n, \nabla v)_\Omega. \end{aligned} \quad (20)$$

The gradient,  $\bar{\nabla}$ , is taken with respect to the master coordinates  $(\xi, \eta)$  and  $\lambda = \lambda(\xi, \eta)$  is a Laplace-modified type parameter which approximates the diffusion term as well as the Jacobian of the isoparametric transformation. The higher-order, cross-derivative term has been added so that the coefficient matrix will factor into a convenient form [3-6].

The factored matrix problem has several attractive features [4, 7]. Problems which involve either two or three space dimensions are solved as a series of one-dimensional finite element problems. Therefore, both the storage requirement and the execution times increase linearly with the number of unknowns in the grid. Table 1 shows the storage requirements for tensor product, quadratic isoparametric elements in two and three space dimensions. The cases considered here correspond to isoparametric grids which are logically equivalent to rectangular grids with equal numbers of elements in each direction. In the alternating-direction method, the one-dimensional problems result in a pentadiagonal system for quadratic elements, so for each one-dimensional problem only five diagonals need to be stored. For the standard finite element technique, a band storage technique was used, and the storage increases with  $O(N^{3/2})$  for two-dimensional problems and  $O(N^{5/3})$  for three-dimensional problems. Table 1 shows that the savings in storage are substantial when using the alternating-direction method, even for relatively small problems.

Figure 6 shows the total time required on a Cray 1 to take 1,000 solution steps for the standard finite element backward-difference technique and 2,000 steps for the alternating-direction method using quadratic finite elements in two and three space dimensions.

In order to offset the error which was induced by adding the perturbation term to (19), the

Table 1  
Storage comparisons for quadratic tensor product elements

Number of elements	Number of nodes	Alternating-direction (words)	Finite element band storage (words)
2 Dimensions			
9	49	392	539
25	121	968	2904
64	289	2312	10404
81	361	2888	14440
121	529	4232	25392
225	961	7688	61504
324	1369	10952	104044
484	2025	16200	186300
900	3721	29768	461404
3 Dimensions			
8	125	1250	7750
27	343	3430	39102
64	729	7290	132678
125	1331	13310	354046

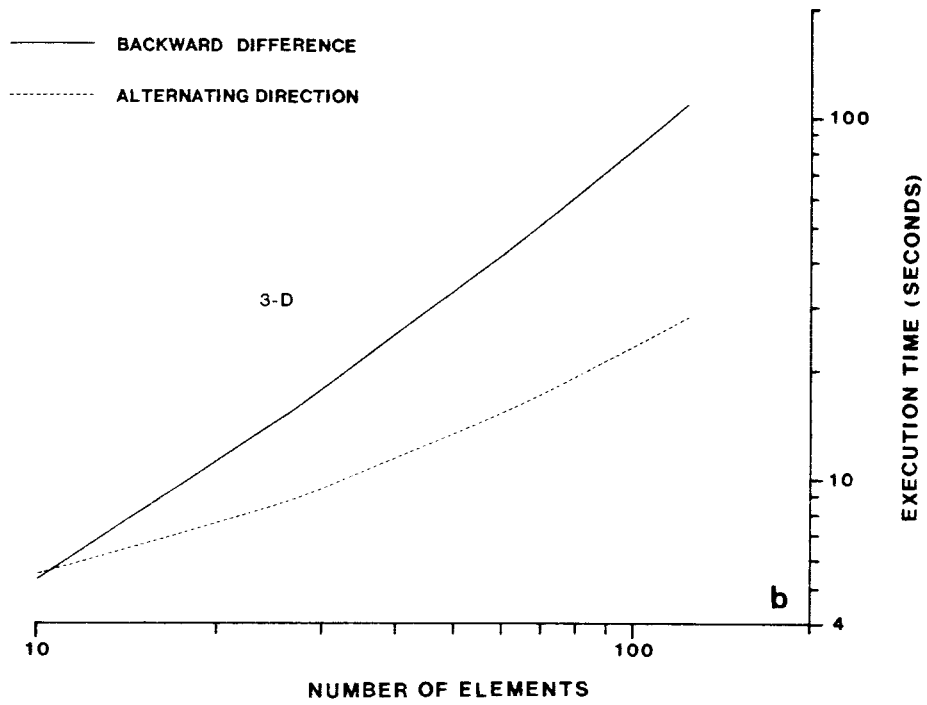
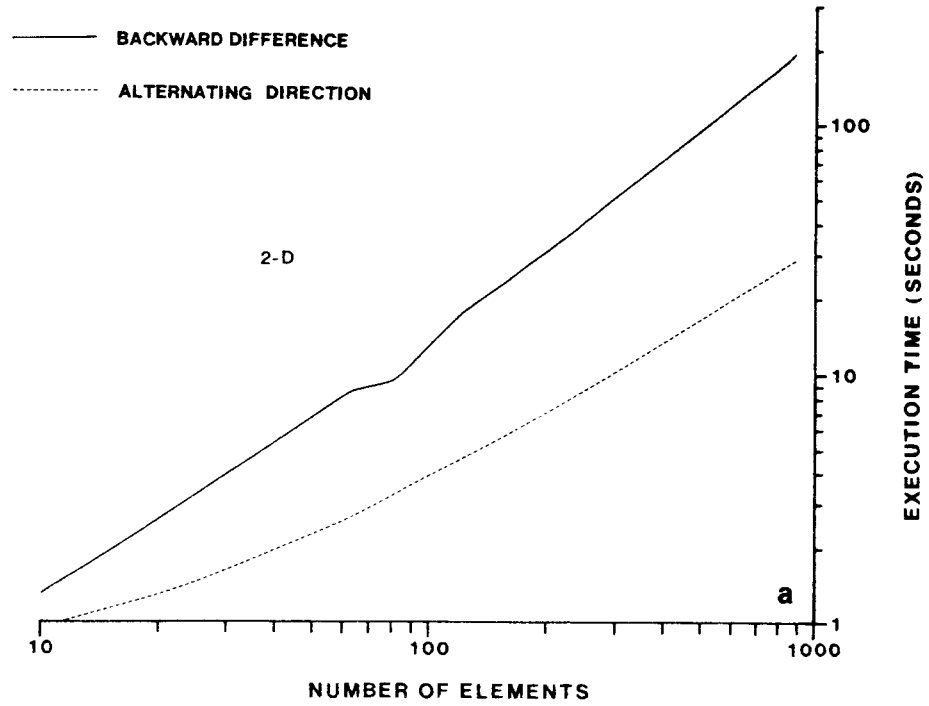


Fig. 6. Solution time for a linear problem. (a) Two dimensions. (b) Three dimensions.



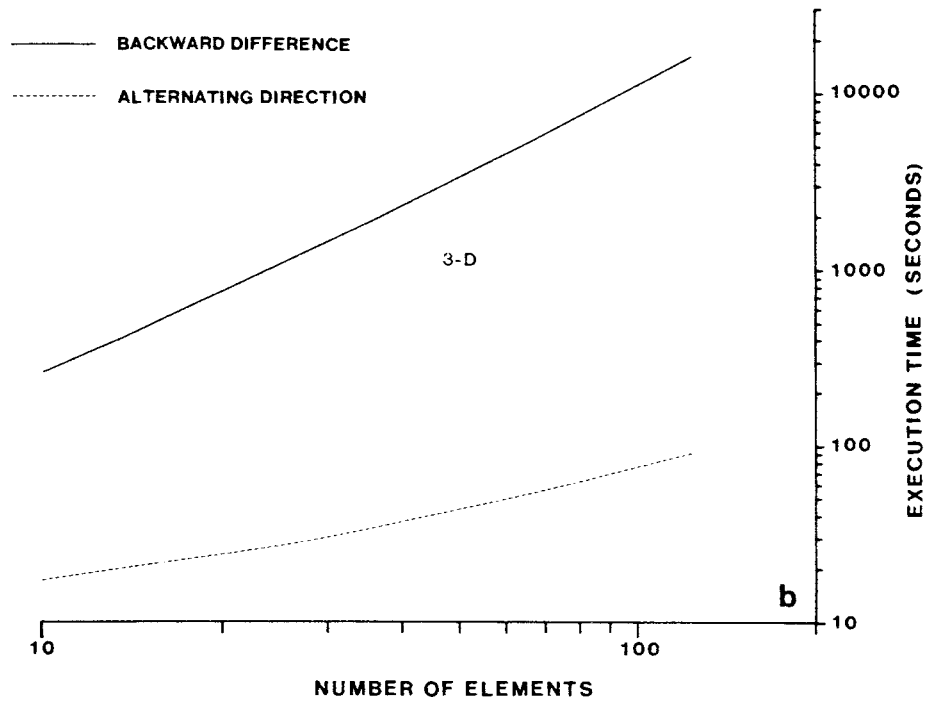
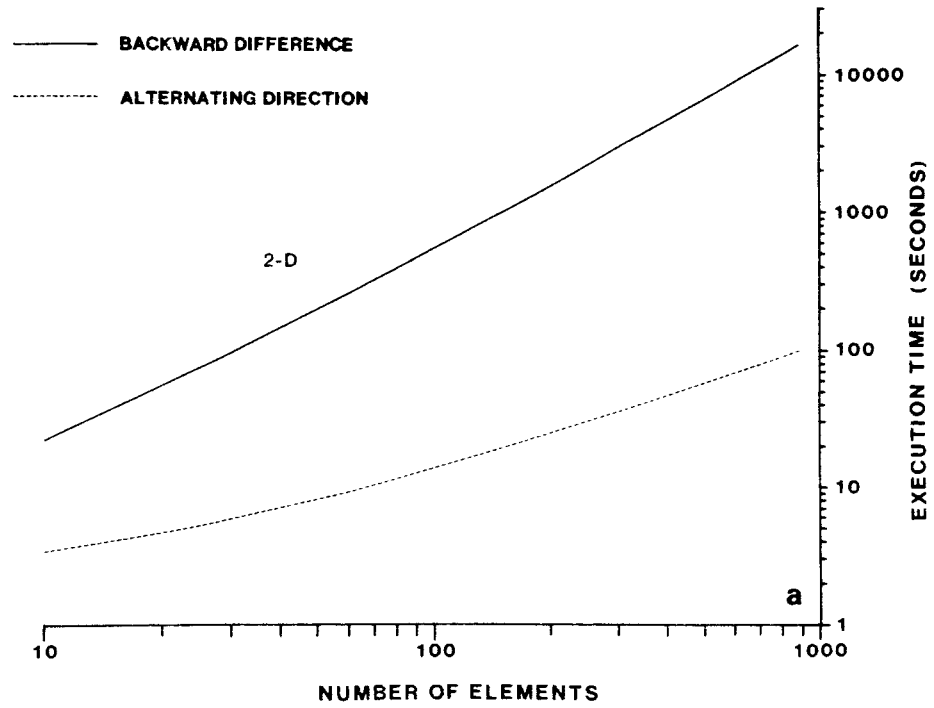


Fig. 7. Solution time for a nonlinear problem. (a) Two dimensions. (b) Three dimensions.

time step,  $\Delta t$ , for the alternating-direction method was half as large as the one used for the backward-difference method. In the alternating-direction method, the pentadiagonal matrices are stacked and solved in a vector mode, and the standard finite element equations are solved using a LINPACK band solver. The computation rates for the alternating-direction method are  $O(N)$ , and the savings in computation times will increase as the problem size increases. Figure 7 shows corresponding timing data for a nonlinear problem where an average of three iterations is taken per time step. An IMSL routine was used for the solution of the standard finite element equations because it is superior to the LINPACK routines for the decomposition of a matrix which must be done on each iteration. Again, the differences in computation speeds will increase with the problem size. This data was obtained using a vector computer; however, similar ratios of computation time would be obtained on sequential machines.

#### 4. Numerical results

It is evident that the alternating-direction method offers certain computational advantages over standard finite element techniques. However, when using curvilinear grids, one might be concerned with the sensitivity of the alternating-direction method to the degree of grid nonorthogonality and nonsmoothness. In order to address this question, the following problem was solved numerically:

$$\partial u / \partial t - \Delta u = x(x-1)y(y-1) - 2t[y(y-1) + x(x-1)], \quad (21)$$

on a unit square where  $u$  is prescribed to be zero on the boundary. The analytic solution for this problem is given as

$$u = tx(x-1)y(y-1). \quad (22)$$

This test problem has the advantage that on a rectangular grid the standard finite element backward-difference method can match the analytic solution exactly. Therefore, it is possible to investigate the inherent error due to the perturbing equation (21) so that it will factor into alternating-direction form. One can then look at errors on the other computational grids to investigate the additional error that is introduced due to curvilinear, nonorthogonal, and nonsmooth grids.

Figure 8(a) shows the original finite element grid which was input to the optimal grid generation program. It is a strongly nonorthogonal grid with a high degree of curvature in each of the elements. Figure 8(b) shows the grid which was produced from the optimal grid generation program in one iteration. Although this grid still has elements which are quite nonorthogonal, it is a great improvement over the initial grid. Figures 8(c) and 8(d) show the grids produced after three and five optimization iterations, respectively. Figure 8(e) shows the grid produced by the optimal grid generation program after fifty iterations. It is a uniform rectangular grid. The optimization procedure is demonstrated in Figs. 9 and 10, which show the decrease in the objective functions during the iterative process for the two grid sequences shown in Figs. 2 and 8, respectively. There is a significant decrease in the objective functions during the first few iterations. Table 2 shows the errors for both the standard finite element

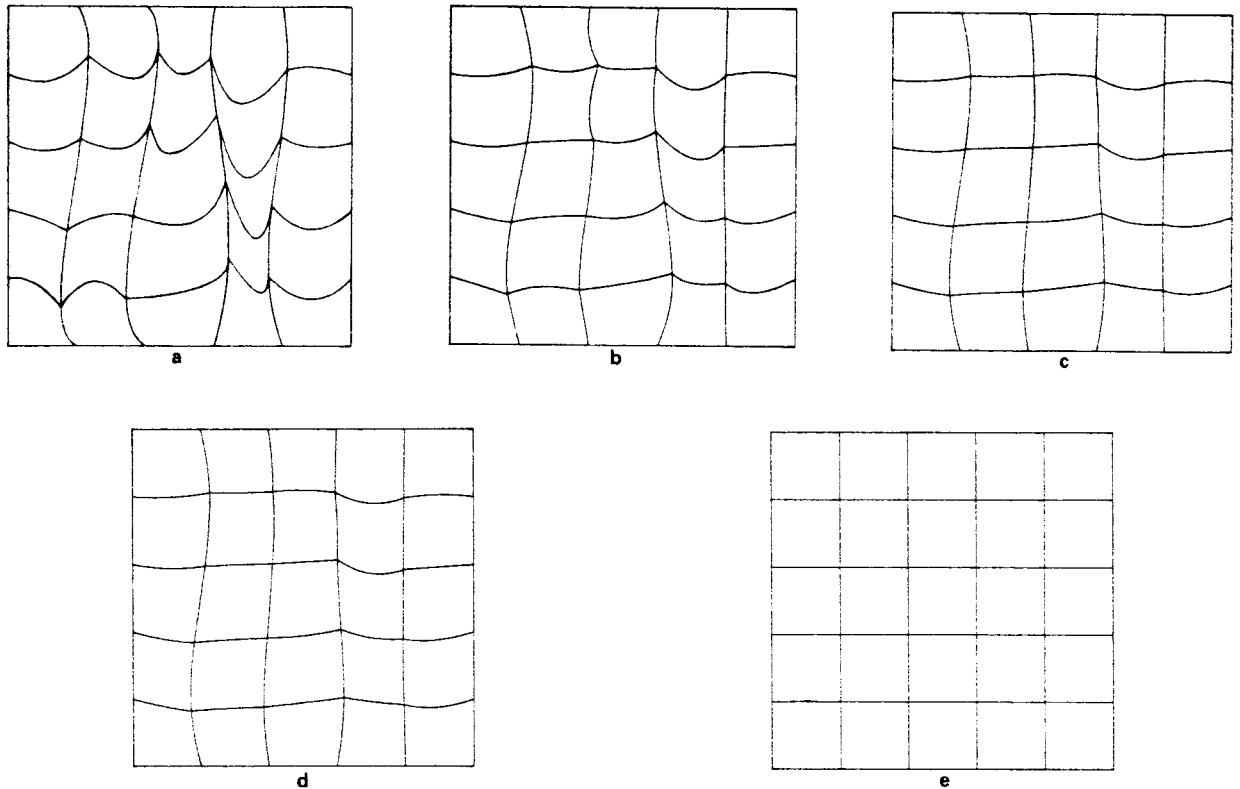


Fig. 8. (a) Original grid. (b) The grid after 1 iteration of smoothing and orthogonalization. (c) The grid after 3 iterations of smoothing and orthogonalization. (d) The grid after 5 iterations of smoothing and orthogonalization. (e) The grid after 50 iterations.

method (FEM) and the alternating-direction method (ALT-DIR). The analytic solution is linear in time and the finite element backward-difference method can match the transient behavior exactly. Therefore, all of the errors displayed in Table 2 for FEM are independent of the time step,  $\Delta t$ . In ALT-DIR, the perturbation term which was added to (21) corresponds to adding

$$\Delta t^2 \lambda^2 \partial^5 u / \partial t \partial x^2 \partial y^2 \quad (23)$$

in the differential operator. For the problem considered here, (21), the ALT-DIR perturbation term corresponds to  $4\Delta t^2 \lambda^2$  which is nonzero. Table 2 contains the  $H^0$  Sobolev norm,  $\|e\|_0$ , which measures the error in a solution, the  $H^1$  Sobolev norm,  $\|e\|_1$ , which measures the error both in the solution and in the gradient, and the infinity norm error,  $\|e\|_\infty$ , which measures the maximum error in the solution at the nodal points. Ten time steps were taken with  $\Delta t = 0.1$  and 100 time steps were taken with  $\Delta t = 0.01$ . On the uniform rectangular grid (50 iterations), the FEM calculates the analytic solution to machine accuracy on the Cyber 175 as expected. The values given for the ALT-DIR on the uniform grid indicate the inherent error which was introduced by the perturbation term which was added to (21). The errors for

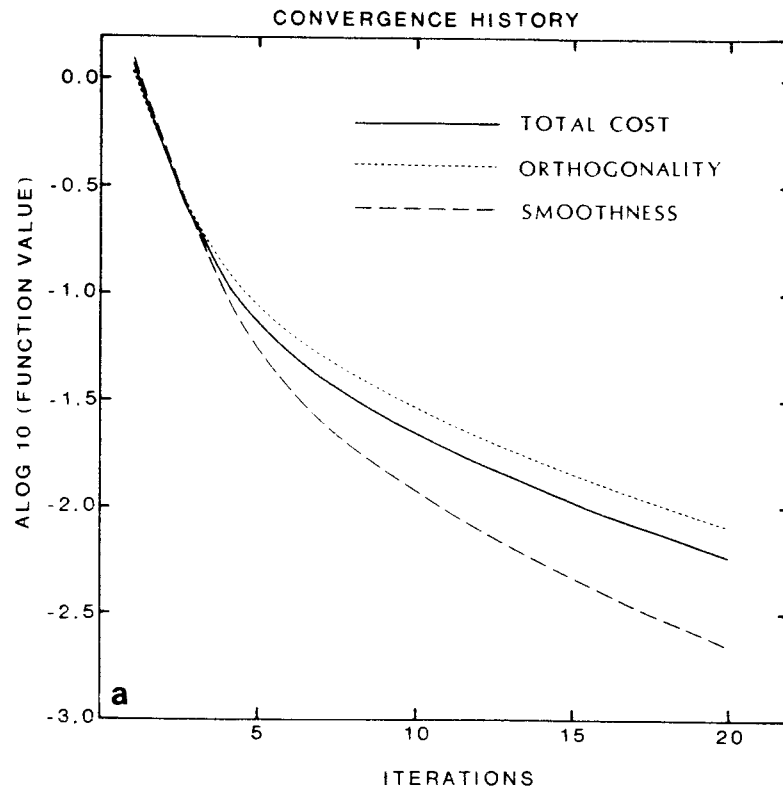


Fig. 9. Measures of grid quality for the grid shown in Fig. 2.

Table 2  
Errors using finite element and alternating-direction methods

Grid	Method	$\Delta t$	$\ e\ _0$	$\ e\ _1$	$\ e\ _2$
Original	FEM	0.1	0.57E-3	0.14E-1	0.17E-2
	ALT-DIR	0.1	—	—	—
		0.01	—	—	—
After 1 iteration	FEM	0.1	0.23E-3	0.81E-3	0.40E-3
	ALT-DIR	0.1	0.93E-2	0.49E-1	0.17E-1
		0.01	0.60E-3	0.85E-2	0.13E-2
After 3 iterations	FEM	0.1	0.81E-4	0.32E-2	0.55E-4
	ALT-DIR	0.1	0.91E-2	0.42E-1	0.17E-1
		0.01	0.44E-3	0.37E-2	0.82E-3
After 5 iterations	FEM	0.1	0.88E-4	0.34E-2	0.63E-4
	ALT-DIR	0.1	0.92E-2	0.43E-1	0.16E-1
		0.01	0.44E-3	0.39E-2	0.83E-3
After 50 iterations (uniform grid)	FEM	0.1	0.52E-12	0.10E-10	0.10E-9
	ALT-DIR	0.1	0.91E-2	0.42E-1	0.16E-1
		0.01	0.39E-3	0.18E-2	0.74E-3

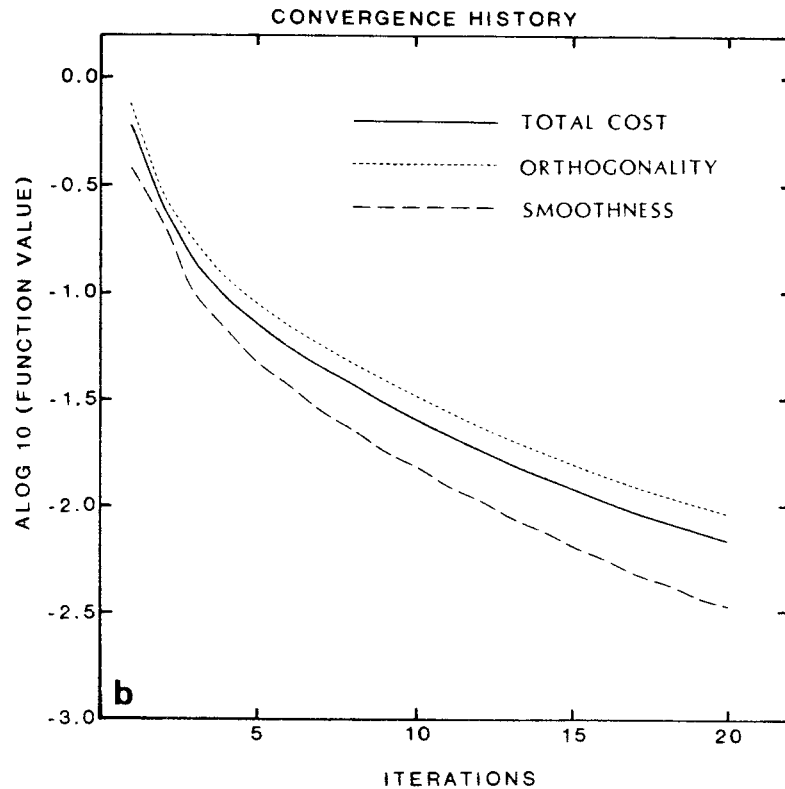


Fig. 10. Measures of grid quality for the grid shown in Fig. 8.

$\Delta t = 0.01$  indicate that this error can be reduced by taking a smaller time step. The errors could also be reduced by redefining the spatial grid.

The FEM errors produced on the original grid indicate the error which is inherent in the finite element method for that grid. The errors for  $\Delta t = 0.01$  indicate that this error can be reduced by taking a smaller time step. The alternating-direction method could not be used on the original grid with any time step as it produced highly oscillatory, divergent results. A striking result is evident when one compares the error using ALT-DIR on the grids produced after 1, 3, and 5 grid optimization iterations. The errors are essentially the same on all three optimized grids and they differ very little from the errors produced on the uniform rectangular grid. On each of these grids, the difference between the FEM and the ALT-DIR errors is the extra error induced by the alternating-direction perturbation. One can deduce from these results that the alternating-direction method is not highly sensitive to grid orthogonalization as long as a somewhat reasonable grid is used. Therefore, one does not need to devote an excessive amount of time to generating smooth, orthogonal curvilinear grids to be used by the alternating-direction method.

## 5. Conclusions

An automatic optimal grid generation program is used which can accept any initial grid and iteratively improve it using a cost function which can be weighted in terms of grid smoothness and grid orthogonality. This program is very easy to use and is very effective in removing nonsmoothness and nonorthogonality from a computational grid.

This program was used on an original grid which was highly nonorthogonal to produce a series of optimized computational grids. The alternating-direction and finite element methods were applied to an example problem on these grids in order to compare the resulting numerical errors. This comparison study shows that the curvilinear alternating-direction method is not highly sensitive to grid smoothness and grid orthogonality. One simply needs to input a grid which is somewhat reasonable, and the alternating-direction method will produce solutions that are essentially as good as if the method had been implemented on a uniform rectangular grid.

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