ADVANCED NUMERICS FOR MULTI-DIMENSIONAL FLUID FLOW CALCULATIONS

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In recent years, there has been a growing interest in the development and use of mathematical models for the simulation of fluid flow, heat transfer and combustion processes in engineering equipment (ref. 1). The equations representing the multi-dimensional transport of mass, momenta and species are numerically solved by finite-difference or finite-element techniques. However despite the multitude of differencing schemes and solution algorithms, and the advancement of computing power, the calculation of multi-dimensional flows, especially three-dimensional flows, remains a mammoth task. The following discussion is concerned with the author's recent work on the construction of accurate discretization schemes for the partial derivatives, and the efficient solution of the set of nonlinear algebraic equations resulting after discretization. The present work has been jointly supported by the Ramjet Engine Division of the Wright Patterson Air Force Base, Ohio, and the NASA Lewis Research Center.

FINITE-DIFFERENCING

An efficient finite-difference scheme must represent the differential equations to a high accuracy and must be stable. In spite of the many formally higher order schemes that have been proposed, practical calculations have bee limited to the use of simple first order schemes. The reasons for this are that either the proposed schemes are unstable in general circumstances or they have limited range of formal accuracy. The complexities of the construction of accurate schemes stem from the following flow characteristics.

a) High grid Peclet number

b) Stream lines skewed with grid lines

c) Pressure gradients

d) Nonlinear source terms, also containing derivatives.

In designing any generally useful finite-difference calculation procedure, it is necessary to consider all of the above factors carefully.

The present work of the author is concerned with the integration of several individual ideas into a general purpose algorithm. Two promising schemes that are being considered are the influence scheme approach of Chen et al. (ref. 2) and of Raithby et al. (ref. 3) and the compact differencing approach of Kriess (ref. 4). In the influence scheme approach, the differential operator is analytically integrated over two (or three) dimensional subdomains after linearizing it with previous iterate values. A profile is assumed for variations along the boundaries. This results in an algebraic linear relation of the form

$$\phi_P = \sum_{i=1}^{8} C_I \phi_I + \sum_{i=1}^{9} D_I Q_I \tag{1}$$

where ϕ_I are neighbor values and Q_I represent the neighbor source terms. C_I and D_I represent coefficients. The advantages of the above approach are that it fully considers the multi-dimensional effects and is stable at high Peclet numbers.

In a compact differencing scheme the derivatives are represented to a fourth order accuracy but with a tridiagonal structure. The tridiagonal structure is advantageous for the solution of equations and for the treatment of boundary conditions. The compact differencing scheme however has been found in our preliminary work to be unstable (and inaccurate) at the high Peclet numbers of current interest. However the concept can still be used to represent the various other derivatives that occur in the source terms and the pressure gradients. The above two approaches are currently being pursued.

SOLUTION ALGORITHM

The solution of the nonlinear algebraic equations obtained after discretization is a mammoth task. The required computer times are large and convergence is not always assured. Current work in this direction has led to a fully-coupled solution of the nonlinear equations of momentum and continuity. The coupled set of nonlinear equations are solved with a Newton-Raphson method and efficient sparse matrix techniques. The turbulence equations are solved decoupled from the momentum and continuity equations. The equations are also arranged as blocks which are then preordered to reduce the computer storage and time. This algorithm has been extended to reacting flows and successful calculations have been made of isothermal turbulent flows and turbulent confined diffusion flames. The algorithm has been observed to be rapidly convergent and insensitive to variations in grid aspect ratio, flow Reynolds number and the number of finite-difference nodes.

Results of Some Calculations

Several calculations of laminar and turbulent recirculating flows have been made with different finite-difference grids. These have been documented in detail in Vanka (refs. 5, 6 and 7). In all the cases tested, rapid diminution of the residuals in the equations has been observed. Calculations have been made with finite-difference grids up to (80 x 95) size for turbulent flow in a sudden expansion. In the present report two tables are presented which demonstrate generally the observed rates of convergence. The first one is for a turbulent flow in a sudden expansion for the experiments of Craig et al. (ref. 8), with a (80 x 95) grid. The second one shows the rate of convergence for a confined diffusion flame for a configuration studied by Lockwood et al. (ref. 9). The latter calculations employed a (32 x 27) grid.

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Table 1. Convergence Rate for Craig's Sudden-expansion Flow, 80 x 95 Grid

Iter.	$\delta u/u_{in}$	$\delta v/u_{in}$	$\delta p/u_{in}^2$	δk	$\delta \varepsilon$
1	1.391E-1	2.904E-2	2.766E-1	5.846E-5	8.856E-5
5	2.879E-2	1.059E-2	1.155E-2	4.355E-5	3.344E-5
10	7.300E-2	5.500E-2	1.171E-1	4.584E-5	3.336E-4
15	2.717E-3	3.224E-4	8.086E-4	3.682E-5	5.972E-5
20	1.508E-5	1.360E-5	2.597E-5	4.246E-6	1.970E-6

Table 2. Convergence Rate for Confined Turbulent Diffusion Flame Calculations (Experiments of Lockwood et al.) with 32 x 27 grid

Iter.	$\delta u/u_c$	$\delta v/u_c$	$\delta p/\rho u_c^2$	δk	$\delta \varepsilon$	δf	δg
1	6.51E-1	3.25E-1	7.83E-1	1.75E-2	1.00E+0	2.00E-1	9.90E-2
5	6.75E-1	1.91E-1	5.85E-2	1.91E-4	1.31E-2	2.61E-1	3.32E-2
10	2.60E-2	6.55E-3	5.98E-3	2.67E-5	1.53E-3	1.31E-2	3.67E-3
15	2.48E-3	9.66E-4	3.56E-4	2.73E-6	1.13E-4	2.27E-3	4.66E-4
20	2.54E-4	1.79E-4	2.80E-5	1.39E-5	8.91E-5	2.62E-4	3.85E-5
25	4.34E-5	3.65E-5	1.54E-5	6.05E-7	4.58E-5	2.55E-5	4.95E-6