Requirements and Trends of Computational Fluid Dynamics as a Tool for Aircraft Design

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1 Introduction

Computational methods first began to have a significant impact on aerodynamics analysis and design in the period of 1965-75. This decade saw the introduction of panel methods which could solve the linear flow models for arbitrarily complex geometry in both subsonic and supersonic flow [54, 134, 165]. It also saw the appearance of the first satisfactory methods for treating the nonlinear equations of transonic flow [113, 112, 58, 59, 40, 50], and the development of the hodograph method for the design of shock free supercritical airfoils [15].

In a landmark paper of 1975 [31], Chapman, Mark and Pirtle anticipated that "computers should begin to supplant wind tunnels in the aerodynamic design and testing process". In effect, computers would ultimately provide a numerical wind tunnel. They listed three main objectives of computational aerodynamics:

1. To provide flow simulations that are either impractical or impossible to obtain in wind tunnels or other ground based experimental test facilities.

2. To lower the time and cost required to obtain aerodynamic flow simulations necessary for the design of new aerospace vehicles.

3. Eventually, to provide more accurate simulations of flight aerodynamics than wind tunnels can.

Chapman, Mark, and Pirtle also noted that the inherent limitations of computational and wind tunnel simulations are complementary. Wind tunnels are limited by the size of the models that can be placed in them, and by the density, temperature and velocity of the flow that they can sustain, with the consequence that flight-Reynolds numbers cannot be realized with complete models. Their accuracy is also limited by wall and support interference, and by aeroelastic distortion. Computers are not limited in any of these ways, but they are limited in speed and memory, which in turn limit the attainable complexity and resolution of the simulations.

Computational Fluid Dynamics (CFD) has now matured to the point at which it is widely accepted as a key tool for aerodynamic design. Algorithms have been the subject of intensive development for the past two decades. The principles underlying the design and implementation of robust schemes which can accurately resolve shock waves and contact discontinuities in compressible flows are now quite well established. It is also quite well understood how to design high order schemes for viscous flow, including compact schemes and spectral methods. Adaptive refinement of the mesh interval (h) and the order of approximations (p) has been successfully exploited both separately and in combination in the h-p method [116]. Despite these advances, CFD is still not being exploited as effectively as one would like in the design process. This is partially due to the long set-up times and high costs, both human and computational, of complex flow simulations. A

continuing obstacle to the treatment of configurations with complex geometry has been the problem of mesh generation. Several general techniques have been developed, including algebraic transformations and methods based on the solution of elliptic and hyperbolic equations. In the last few years methods using unstructured meshes have also begun to gain more general acceptance. The Dassault-INRIA group led the way in developing a finite element method for transonic potential flow. They obtained a solution for a complete Falcon 50 as early as 1982 [24]. Euler methods for unstructured meshes have been the subject of intensive development by several groups since 1985 [101, 75, 74, 152, 14], and Navier-Stokes methods on unstructured meshes have also been demonstrated [108, 109, 11].

The fidelity of mathematical modelling of high Reynolds number flows continues to be limited by computational costs , thus, accurate and cost-effective simulation of viscous flow at high Reynolds numbers associated with full scale flight remains a challenge. Improvements are still needed in a number of areas, including

1. mesh generation techniques to assure proper resolution of boundary layers
2. turbulence modeling for separated flows
3. algorithms to reduce computational costs.

Several routes are available toward the reduction of computational costs, including the reduction of mesh requirements by the use of higher order schemes, improved convergence to steady state by sophisticated acceleration methods, and the exploitation of massively parallel computers.

In addition to more accurate and cost-effective flow prediction methods, better optimization methods are also needed, so that not only can designs be rapidly evaluated, but directions of improvement can be identified which enable the rapid evaluation of a satisfactory design. Possession of techniques which result in a faster design cycle gives a crucial advantage in a competitive environment.

In the next section, this paper discusses steps needed for the implementation of computational simulation techniques which could meet industrial needs. A critical issue examined in Section 3 is the choice of mathematical models: what level of complexity is needed to provide sufficient accuracy for aerodynamic design, and what is the impact on cost and turn-around. Section 4 addresses issues in the formulation of numerical algorithms which provide the fundamental building blocks for a numerical wind tunnel. Section 5 presents the results of some numerical calculations which require moderate computer resources and could be completed with the fast turn around needed for effective industrial use. Section 6 discusses automatic design procedures which can be used to produce optimum aerodynamic designs. Finally, Section 7 discusses the outlook for achieving the goal of a numerical wind tunnel.

2 Steps Needed for the Implementation of Simulation Methods

The principal requirements of effective CFD methods for engineering design are

1. assured accuracy
2. acceptable computational cost
3. fast turn around.

Improvements are still needed in all three areas. Effective use of CFD for design is presently limited by the lack of good interfaces to CAD systems, which prevent full automation of the mesh generation process. This bottleneck needs to be eliminated and the CFD system should be fully integrated in a numerical design environment.

The core requirement for the successful exploitation of CFD is the development of the basic software for the computational simulation of complex fluid flows. A level of accuracy sufficient to assure confidence in the aerodynamic design must be achieved with acceptable computational costs and rapid turn around. Five principal steps can be identified in the development of software for aerodynamic simulation. These are:

1. Choice of a mathematical model appropriate to the requirements.

2. Mathematical analysis of the model to ensure that the problem is properly formulated (for example, definition of far field boundary conditions, conditions for uniqueness).

3. Formulation of a numerical approximation scheme.

4. Implementation as a computer program.

5. Validation.

All of these steps need to be carefully carried out to produce the reliable, robust, and accurate software that is needed.

Software which meets the basic requirements for the computational simulation of aerodynamic flows is the first step towards a numerical simulation system for design, but not by itself sufficient. The simulation software should also be embedded in a more comprehensive environment to provide user-friendly interfaces and efficient data management. The transfer of large volumes of data representing the geometries and computational results can become a major bottleneck. It is essential to develop procedures allowing the easy transfer of geometric data from computer aided design (CAD) systems. A numerical wind tunnel should also contain automatic measurement systems capable of determining the geometry of real objects. These interfaces should be general enough to allow the substitution of alternative CAD systems, and also of alternative aerodynamic simulation modules. Efficient methods for handling the output data are equally important. These must provide both for visualization of the results, and for their quantitative evaluation. Visualization is important because it can provide the designer with the insights needed to make an improvement, while quantitative evaluation is needed both for verification of the performance, and to allow optimization of the design.

3 Mathematical Models of Fluid Flow and Computational Costs

The choice of a model depends on the complexity of the flow, the level of accuracy required, and the computational cost. The Reynolds number of aerodynamic flows associated with the flight envelopes of full scale aircraft are very large (of the order of 10 million and up). Correspondingly the flows that need to be predicted are generally turbulent. The size of the smallest eddies in a turbulent flow may be estimated by dimensional analysis to be of the order of $Re^{\frac{3}{4}}$, where Re is the Reynolds number based on a representative global length scale. In a three-dimensional simulation, allowing for the need to resolve time scales which correspond to the smallest length scales, the computational complexity of a full simulation of a turbulent flow, down to the smallest scales in space and time, can therefore be estimated as proportional to the cube of the Reynolds number. Consequently a direct simulation of the full Navier-Stokes equations is not feasible, forcing the use of mathematical models with some level of simplification. Figure 1 indicates a hierarchy of models at different levels of simplification which have proved useful in practice. Efficient flight is generally achieved by the use of smooth and streamlined shapes which avoid flow separation and minimize viscous effects, with the consequence that useful predictions can be made using inviscid models. Inviscid calculations with boundary layer corrections can provide quite accurate predictions of lift and drag when the flow remains attached, but iteration between the inviscid outer solution and the inner boundary layer solution becomes increasingly difficult with the onset of separation. Procedures for solving the full viscous equations are likely to be needed for the simulation of arbitrary complex separated flows, which may occur at high angles of attack or with bluff bodies. In order to treat flows at high Reynolds numbers, one is generally forced to estimate turbulent effects by Reynolds averaging of the fluctuating components. This requires the introduction of a turbulence model. As the available computing power increases one may also aspire to large eddy simulation (LES) in which the larger scale eddies are directly calculated, while the influence of turbulence at scales smaller than the mesh interval is represented by a subgrid scale model.

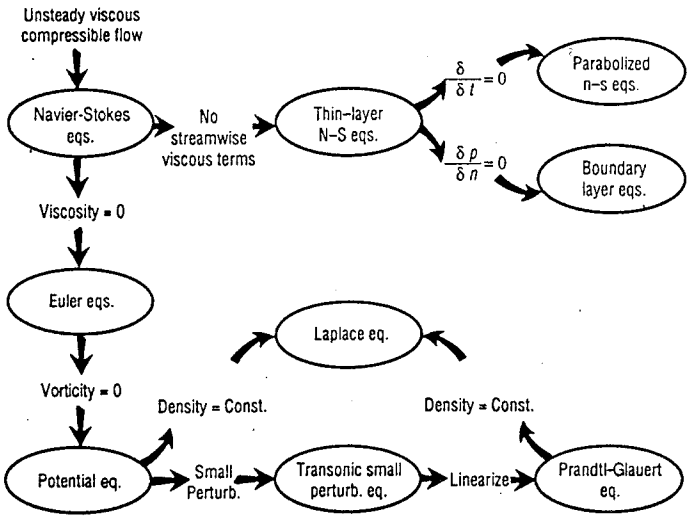


Figure 1: Equations of Fluid Dynamics for Mathematical Models of Varying Complexity (Supplied by Luis Miranda, Lockheed Corporation).

Computational costs vary drastically with the choice of mathematical model. Panel methods can be effectively implemented with higher-end personal computers (with an Intel 80486 microprocessor, for example). Studies of the dependency of the result on mesh refinement, performed by this author and others, have demonstrated that inviscid transonic potential flow or Euler solutions for an airfoil can be accurately calculated on a mesh with 160 cells around the section, and 32 cells normal to the section. Using multigrid techniques 10 to 25 cycles are enough to obtain a converged result. Consequently airfoil calculations can be performed in seconds on a Cray YMP, and can also be performed on 486-class personal computers. Correspondingly accurate three-dimensional inviscid calculations can be performed for a wing on a mesh, say with $192 \times 32 \times 48 = 294,912$ cells, in about 5 minutes on a single processor Cray YMP, or less than a minute with eight processors, or in 1 or 2 hours on a workstation such as a Hewlett Packard 735 or an IBM 560 model.

Viscous simulations at high Reynolds numbers require vastly greater resources. Careful two-dimensional studies of mesh requirements have been carried out at Princeton by Martinelli [105]. He found that on the order of 32 mesh intervals were needed to resolve a turbulent boundary layer, in addition to 32 intervals between the boundary layer and the far field, leading to a total of 64 intervals. In order to prevent degradations in accuracy and convergence due to excessively large aspect ratios (in excess of 1,000) in the surface mesh cells, the chordwise resolution must also be increased to 512 intervals. Reasonably accurate solutions can be obtained in a 512×64 mesh in 100 multigrid cycles. Figure 2 shows a comparison of experimental data with a calculated result for the RAE 2822 airfoil at a Mach number of 0.729, an angle of attack of 2.31° and a Reynolds number of 6 million. Translated to three dimensions, this would imply the need for meshes with 5–10 million cells (for example, $512 \times 64 \times 256 = 8,388,608$ cells). When simulations are performed on less fine meshes with, say, 500,000 to 1 million cells, it is very hard to avoid mesh dependency in the solutions as well as sensitivity to the turbulence model.

A typical algorithm requires of the order of 5,000 floating point operations per mesh point in one multigrid iteration. With 10 million mesh points, the operation count is of the order of 0.5×10^{11} per cycle. Given a computer capable of sustaining 10^{11} operations per second (100 gigaflops), 200 cycles could then be performed in 100 seconds. Simulations of unsteady viscous flows (flutter, buffet) would be likely to require 1,000–10,000 time steps. A further progression to large eddy simulation of complex configurations would require even greater resources. The following estimate is due to W.H. Jou [84]. Suppose that a conservative estimate of the size of

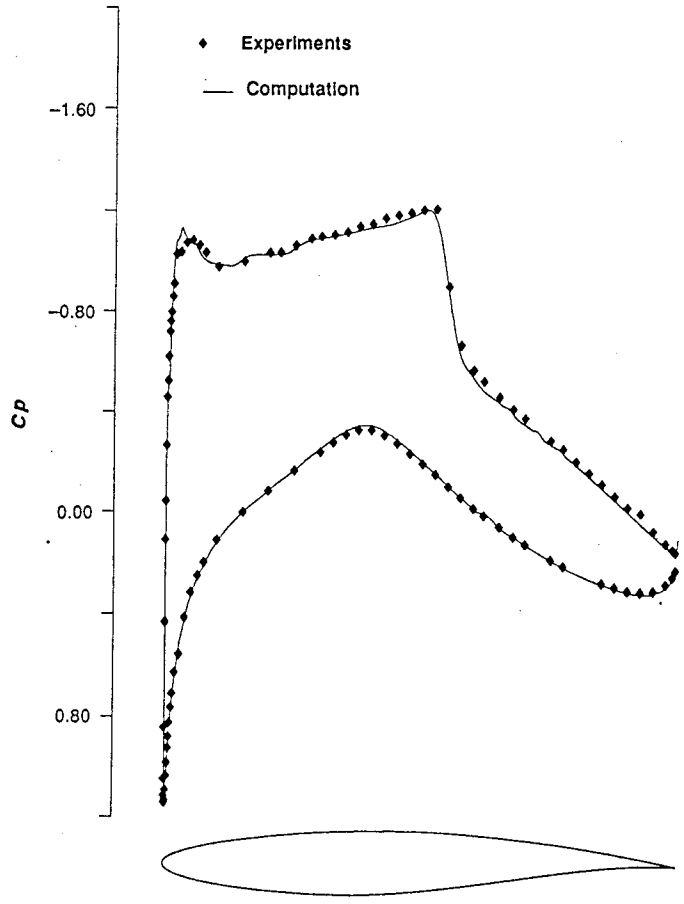


Figure 2: Comparison of the Calculated Result and Experimental Data for the RAE 2822 Airfoil at Mach 0.729 and 2.31° Angle of Attack (Supplied by Luigi Martinelli, Princeton University).

eddies in a boundary layer that ought to be resolved is 1/5 of the boundary layer thickness. Assuming that 10 points are needed to resolve a single eddy, the mesh interval should then be 1/50 of the boundary layer thickness. Moreover, since the eddies are three-dimensional, the same mesh interval should be used in all three directions. Now, if the boundary layer thickness is of the order of 0.01 of the chord length, 5,000 intervals will be needed in the chordwise direction, and for a wing with an aspect ratio of 10, 50,000 intervals will be needed in the spanwise direction. Thus, of the order of $50 \times 5,000 \times 50,000$ or 12.5 billion mesh points would be needed in the boundary layer. If the time dependent behavior of the eddies is to be fully resolved using time steps on the order of the time for a wave to pass through a mesh interval, and one allows for a total time equal to the time required for waves to travel three times the length of the chord, of the order of 15,000 time steps would be needed. Performance beyond the teraflop (10^{12} operations per second) will be needed to attempt calculations of this nature, which also have an information content far beyond what is needed for enginering analysis and design. The designer does not need to know the details of the eddies in the boundary layer. The primary purpose of such calculations is to improve the calculation of averaged quantities such as skin friction, and the prediction of global behavior such as the onset of separation. The current use of Navier-Stokes and large eddy simulations is to try to gain an improved insight into the physics of turbulent flow, which may in turn lead to the development of more comprehensive and reliable turbulence models.

It is doubtful whether a universally valid turbulence model, capable of describing all complex flows, could be devised [48]. Algebraic models [28, 9] have proved fairly satisfactory for the calculation of attached and slightly separated wing flows. These models rely on the boundary layer concept, usually incorporating separate formulas for the inner and outer layers, and they require an estimate of a length scale which depends on the thickness of the boundary layer. The estimation of this quantity by a search for a maximum of the

vorticity times a distance to the wall, as in the Baldwin-Lomax model, can lead to ambiguities in internal flows, and also in complex vortical flows over slender bodies and highly swept or delta wings [37, 106]. The Johnson-King model [82], which allows for non-equilibrium effects through the introduction of an ordinary differential equation for the maximum shear stress, has improved the prediction of flows with shock induced separation [135, 85].

Closure models depending on the solution of transport equations are widely accepted for industrial applications. These models eliminate the need to estimate a length scale by detecting the edge of the boundary layer. Eddy viscosity models typically use two equations for the turbulent kinetic energy k and the dissipation rate ϵ, or a pair of equivalent quantities [83, 164, 149, 1, 111, 33]. Models of this type generally tend to present difficulties in the region very close to the wall. They also tend to be badly conditioned for numerical solution. The $k - l$ model [143] is designed to alleviate this problem by taking advantage of the linear behaviour of the length scale l near the wall. In an alternative approach to the design of models which are more amenable to numerical solution, new models requiring the solution of one transport equation have recently been introduced [10, 148]. The performance of the algebraic models remains competitive for wing flows, but the one- and two-equation models show promise for broader classes of flows. In order to achieve greater universality, research is also being pursued on more complex Reynolds stress transport models, which require the solution of a larger number of transport equations.

Another direction of research is the attempt to devise more rational models via renormalization group (RNG) theory [168, 144]. Both algebraic and two-equation $k - \epsilon$ models devised by this approach have shown promising results [107].

The selection of sufficiently accurate mathematical models and a judgment of their cost effectiveness ultimately rests with industry. Aircraft and spacecraft designs normally pass through the three phases of conceptual design, preliminary design, and detailed design. Correspondingly, the appropriate CFD models will vary in complexity. In the conceptual and preliminary design phases, the emphasis will be on relatively simple models which can give results with very rapid turn-around and low computer costs, in order to evaluate alternative configurations and perform quick parametric studies. The detailed design stage requires the most complete simulation that can be achieved with acceptable cost. In the past, the low level of confidence that could be placed on numerical predictions has forced the extensive use of wind tunnel testing at an early stage of the design. This practice was very expensive. The limited number of models that could be fabricated also limited the range of design variations that could be evaluated. It can be anticipated that in the future, the role of wind tunnel testing in the design process will be more one of verification. Experimental research to improve our understanding of the physics of complex flows will continue, however, to play a vital role.

4 Challenges for CFD Algorithms

The computational simulation of fluid flow presents a number of severe challenges for algorithm design. At the level of inviscid modeling, the inherent nonlinearity of the fluid flow equations leads to the formation of singularities such as shock waves and contact discontinuities. Moreover, the geometric configurations of interest are extremely complex, and generally contain sharp edges which lead to the shedding of vortex sheets. Extreme gradients near stagnation points or wing tips may also lead to numerical errors that can have global influence. Numerically generated entropy may be convected from the leading edge for example, causing the formation of a numerically induced boundary layer which can lead to separation. The need to treat exterior domains of infinite extent is also a source of difficulty. Boundary conditions imposed at artificial outer boundaries may cause reflected waves which significantly interfere with the flow. When viscous effects are also included in the simulation, the extreme difference of the scales in the viscous boundary layer and the outer flow, which is essentially inviscid, is another source of difficulty, forcing the use of meshes with extreme variations in mesh interval. For these reasons CFD, has been a driving force for the development of numerical algorithms.

4.1 Structured and Unstructured Meshes

The algorithm designer faces a number of critical decisions. The first choice that must be made is the nature of the mesh used to divide the flow field into discrete subdomains. The discretization procedure must allow for the treatment of complex configurations. The principal alternatives are Cartesian meshes, body-fitted curvilinear meshes, and unstructured tetrahedral meshes. Each of these approaches has advantages which have led to their use. The Cartesian mesh minimizes the complexity of the algorithm at interior points and facilitates the use of high order discretization procedures, at the expense of greater complexity, and possibly a loss of accuracy, in the treatment of boundary conditions at curved surfaces. This difficulty may be alleviated by using mesh refinement procedures near the surface. With their aid, schemes which use Cartesian meshes have recently been developed to treat very complex configurations [110, 136, 21, 88].

Body-fitted meshes have been widely used and are particularly well suited to the treatment of viscous flow because they readily allow the mesh to be compressed near the body surface. With this approach, the problem of mesh generation itself has proved to be a major pacing item. The most commonly used procedures are algebraic transformations [7, 41, 43, 145], methods based on the solution of elliptic equations, pioneered by Thompson [157, 158, 146, 147], and methods based on the solution of hyperbolic equations marching out from the body [150]. In order to treat very complex configurations it generally proves expedient to use a multiblock [163, 137] procedure, with separately generated meshes in each block, which may then be patched at block faces, or allowed to overlap, as in the Chimera scheme [18, 19]. While a number of interactive software systems for grid generation have been developed, such as EAGLE, GRIDGEN, GRAPE, and ICEM, the generation of a satisfactory grid for a very complex configuration may require months of effort.

The alternative is to use an unstructured mesh in which the domain is subdivided into tetrahedrons. This in turn requires the development of solution algorithms capable of yielding the required accuracy on unstructured meshes. This approach has been gaining acceptance, as it is becoming apparent that it can lead to a speed-up and reduction in the cost of mesh generation that more than offsets the increased complexity and cost of the flow simulations. Two competing procedures for generating triangulations which have both proved successful are Delaunay triangulation [38, 11], based on concepts introduced at the beginning of the century by Voronoi [161], and the moving front method [102].

4.2 Finite Difference, Finite Volume, and Finite Element Schemes

Associated with choice of mesh type is the formulation of the discretization procedure for the equations of fluid flow, which can be expressed as differential conservation laws. In the Cartesian tensor notation, let x_i be the coordinates, p, ρ, T, and E the pressure, density, temperature, and total energy, and u_i the velocity components. Each conservation equation has the form

$$\frac{\partial w}{\partial t} + \frac{\partial F_j}{\partial x_j} = 0. \tag{1}$$

For the mass equation

$$w = \rho, \quad F_j = \rho u_j.$$

For the i momentum equation

$$w_i = \rho u_i, \quad F_{ij} = \rho u_i u_j + p\delta_{ij} - \sigma_{ij},$$

where σ_{ij} is the viscous stress tensor. For the energy equation

$$w = \rho E, \quad F_j = (\rho E + p)u_j - \sigma_{jk}u_k - \kappa\frac{\partial T}{\partial x_j},$$

where κ is the coefficient of heat conduction. The pressure is related to the density and energy by the equation of state

$$p = (\gamma - 1)\rho\left(E - \frac{1}{2}u_i u_i\right)$$

in which γ is the ratio of specific heats. In the Navier-Stokes equations the viscous stresses are assumed to be linearly proportional to the rate of strain, or

$$\sigma_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \lambda\delta_{ij}\left(\frac{\partial u_k}{\partial x_k}\right), \tag{2}$$

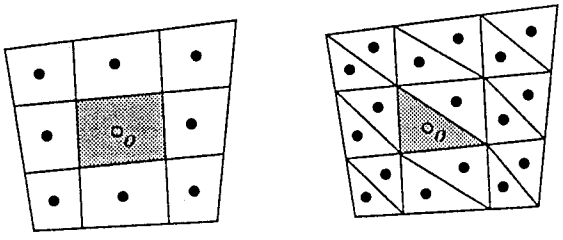
where μ and λ are the coefficients of viscosity and bulk viscosity, and usually $\lambda = -2\mu/3$.

The finite difference method, which requires the use of a Cartesian or a structured curvilinear mesh, directly approximates the differential operators appearing in these equations. In the finite volume method [103], the discretization is accomplished by dividing the domain of the flow into a large number of small subdomains, and applying the conservation laws in the integral form

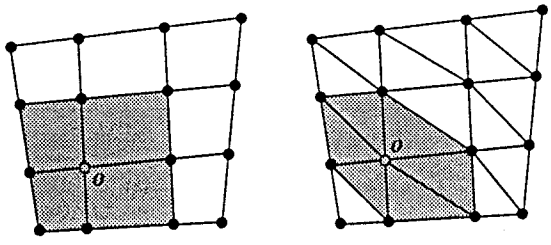
$$\frac{\partial}{\partial t}\int_\Omega w dV + \int_{\partial\Omega} \mathbf{F}\cdot d\mathbf{S} = 0.$$

Here $\mathbf{F}$ is the flux appearing in equation (1) and $d\mathbf{S}$ is the directed surface element of the boundary $\partial\Omega$ of the domain Ω. The use of the integral form has the advantage that no assumption of the differentiability of the solutions is implied, with the result that it remains a valid statement for a subdomain containing a shock wave. In general the subdomains could be arbitrary, but it is convenient to use either hexahedral cells in a body conforming curvilinear mesh or tetrahedrons in an unstructured mesh.

Alternative discretization schemes may be obtained by storing flow variables at either the cell centers or the vertices. These variations are illustrated in Figure 3 for the two-dimensional case. With a cell-centered scheme the discrete conservation law takes the form



3a: Cell Centered Scheme.



3b: Vertex Scheme.

Figure 3: Structured and Unstructured Discretizations.

$$\frac{d}{dt}wV + \sum_{\text{faces}} \mathbf{F}\cdot\mathbf{S} = 0, \tag{3}$$

where V is the cell volume, and $\mathbf{F}$ is now a numerical estimate of the flux vector through each face. $\mathbf{F}$ may be evaluated from values of the flow variables in the cells separated by each face, using upwind biasing to allow for the directions of wave propagation. With hexahedral cells, equation (3) is very similar to a finite difference scheme in curvilinear coordinates. Under a transformation to curvilinear coordinates X_j, equation (1) becomes

$$\frac{\partial}{\partial t}(Jw) + \frac{\partial}{\partial X_i}\left(J\frac{\partial X_i}{\partial x_j}F_j\right) = 0,$$

where J is the Jacobian determinant of the transformation matrix $\left[\frac{\partial x_i}{\partial X_j}\right]$. The transformed flux $J\frac{\partial X_i}{\partial x_j}F_j$ corresponds to the dot product of the flux $\mathbf{F}$ with a vector face area $J\frac{\partial X_i}{\partial x_j}$, while J represents the transformation of the cell volume. The finite volume form (3) has the advantages that it is valid for both structured and unstructured meshes, and that it assures that a uniform flow exactly satisfies the equations, because $\sum_{\text{faces}} \mathbf{S} = 0$ for a closed control volume. Finite difference schemes do not necessarily satisfy this constraint because of the discretization errors in evaluating $\frac{\partial X_i}{\partial x_j}$ and the inversion of the transformation matrix. A cell-vertex finite volume scheme can be derived by taking the union of the cells surrounding a given vertex as the control volume for that vertex [51, 66, 127]. In equation (3), V is now the sum of the volumes of the surrounding cells, while the flux balance is evaluated over the outer faces of the polyhedral control volume. In the absence of upwind biasing the flux vector is evaluated by averaging over the corners of each face. This has the advantage of remaining accurate on an irregular or unstructured mesh.

An alternative route to the discrete equations is provided by the finite element method. Whereas the finite difference and finite volume methods approximate the differential and integral operators, the finite element method proceeds by inserting an approximate solution into the exact equations. On multiplying by a test function ϕ and integrating by parts over space, one obtains the weak form

$$\frac{\partial}{\partial t}\iiint_\Omega \phi w d\Omega = \iiint_\Omega \mathbf{F}\cdot\nabla\phi d\Omega - \iint_{\partial\Omega} \phi\mathbf{F}\cdot d\mathbf{S} \tag{4}$$

which is also valid in the presence of discontinuities in the flow. In the Galerkin method the approximate solution is expanded in terms of the same family of functions as those from which the test functions are drawn. By choosing test functions with local support, separate equations are obtained for each node. For example, if a tetrahedral mesh is used, and ϕ is piecewise linear, with a nonzero value only at a single node, the equations at each node have a stencil which contains only the nearest neighbors. In this case the finite element approximation corresponds closely to a finite volume scheme. If a piecewise linear approximation to the flux $\mathbf{F}$ is used in the evaluation of the integrals on the right hand side of equation (4), these integrals reduce to formulas which are identical to the flux balance of the finite volume scheme.

Thus the finite difference and finite volume methods lead to essentially similar schemes on structured meshes, while the finite volume method is essentially equivalent to a finite element method with linear elements when a tetrahedral mesh is used. Provided that the flow equations are expressed in the conservation law form (1), all three methods lead to an exact cancellation of the fluxes through interior cell boundaries, so that the conservative property of the equations is preserved. The important role of this property in ensuring correct shock jump conditions was pointed out by Lax and Wendroff [91].

4.3 Non-oscillatory Shock Capturing Schemes

4.3.1 Local Extremum Diminishing (LED) Schemes

The discretization procedures which have been described in the last section lead to nondissipative approximations to the Euler equations. Dissipative terms may be needed for two reasons. The first is the possibility of undamped oscillatory modes. The second reason is the need for the clean capture of shock waves and contact discontinuities without undesirable oscillations. An extreme overshoot could result in a negative value of an inherently positive quantity such as the pressure or density. The development of non-oscillatory schemes has been a prime focus of algorithm research for compressible flow. Consider a general semi-discrete scheme of the form

$$\frac{d}{dt}v_j = \sum_{k\neq j} c_{jk}(v_k - v_j). \tag{5}$$

A maximum cannot increase and a minimum cannot decrease if the coefficients c_{jk} are non-negative, since at a maximum $v_k - v_j \leq 0$, and at a minimum $v_k - v_j \geq 0$. Thus the condition

$$c_{jk} \geq 0, \quad k \neq j \tag{6}$$

is sufficient to ensure stability in the maximum norm. Moreover, if the scheme has a compact stencil, so that $c_{jk} = 0$ when j and k are not nearest neighbors, a local maximum cannot increase and local minimum cannot decrease. This local extremum diminishing (LED) property prevents the birth and growth of oscillations. The one-dimensional conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0$$

provides a useful model for analysis. In this case waves are propagated with a speed $a(u) = \frac{\partial f}{\partial u}$, and the solution is constant along the characteristics $\frac{dx}{dt} = a(u)$. Thus the LED property is satisfied. In fact the total variation

$$TV(u) = \int_{-\infty}^{\infty} \left| \frac{\partial u}{\partial x} \right| dx$$

of a solution of this equation does not increase, provided that any discontinuity appearing in the solution satisfies an entropy condition [90]. Harten proposed that difference schemes ought to be designed so that the discrete total variation cannot increase [52]. If the end values are fixed, the total variation can be expressed as

$$TV(u) = 2 \left(\sum \text{ maxima } - \sum \text{ minima } \right).$$

Thus a LED scheme is also total variation diminishing (TVD). Positivity conditions of the type expressed in equations (5) and (6) lead to diagonally dominant schemes, and are the key to the elimination of improper oscillations. The positivity conditions may be realized by the introduction of diffusive terms or by the use of upwind biasing in the discrete scheme. Unfortunately, they may also lead to severe restrictions on accuracy unless the coefficients have a complex nonlinear dependence on the solution.

4.3.2 Artificial Diffusion and Upwinding

Following the pioneering work of Godunov [47], a variety of dissipative and upwind schemes designed to have good shock capturing properties have been developed during the past two decades [151, 22, 92, 93, 133, 120, 52, 119, 154, 5, 63, 169, 57, 166, 13, 12, 11]. If the one-dimensional scalar conservation law

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x} f(v) = 0 \tag{7}$$

is represented by a three point scheme

$$\frac{dv_j}{dt} = c^+_{j+\frac{1}{2}} (v_{j+1} - v_j) + c^-_{j-\frac{1}{2}} (v_{j-1} - v_j),$$

the scheme is LED if

$$c^+_{j+\frac{1}{2}} \geq 0, \quad c^-_{j-\frac{1}{2}} \geq 0. \tag{8}$$

A conservative semidiscrete approximation to the one-dimensional conservation law can be derived by subdividing the line into cells. Then the evolution of the value v_j in the jth cell is given by

$$\Delta x \frac{dv_j}{dt} + h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}} = 0, \tag{9}$$

where $h_{j+\frac{1}{2}}$ is an estimate of the flux between cells j and $j+1$. The simplest estimate is the arithmetic average $(f_{j+1} + f_j)/2$, but this leads to a scheme that does not satisfy the positivity conditions. To correct this, one may add a dissipative term and set

$$h_{j+\frac{1}{2}} = \frac{1}{2} (f_{j+1} + f_j) - \alpha_{j+\frac{1}{2}} (v_{j+1} - v_j). \tag{10}$$

In order to estimate the required value of the coefficient $\alpha_{j+\frac{1}{2}}$, let $a_{j+\frac{1}{2}}$ be a numerical estimate of the wave speed $\frac{\partial f}{\partial u}$,

$$a_{j+\frac{1}{2}} = \begin{cases} \frac{f_{j+1} - f_j}{v_{j+1} - v_j} & \text{if } v_{j+1} \neq v_j \\ \left. \frac{\partial f}{\partial v} \right|_{v=v_j} & \text{if } v_{j+1} = v_j \end{cases}. \tag{11}$$

Now

$$\begin{aligned} h_{j+\frac{1}{2}} &= f_j + \frac{1}{2}(f_{j+1} - f_j) - \alpha_{j+\frac{1}{2}}(v_{j+1} - v_j) \\ &= f_j - \left(\alpha_{j+\frac{1}{2}} - \frac{1}{2}a_{j+\frac{1}{2}}\right)(v_{j+1} - v_j), \end{aligned}$$

and similarly

$$h_{j-\frac{1}{2}} = f_j - \left(\alpha_{j-\frac{1}{2}} + \frac{1}{2}a_{j-\frac{1}{2}}\right)(v_j - v_{j-1}).$$

Then

$$\begin{aligned} h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}} &= +\left(\frac{1}{2}a_{j+\frac{1}{2}} - \alpha_{j+\frac{1}{2}}\right)\Delta v_{j+\frac{1}{2}} \\ &\quad + \left(\frac{1}{2}a_{j-\frac{1}{2}} + \alpha_{j-\frac{1}{2}}\right)\Delta v_{j-\frac{1}{2}}, \end{aligned}$$

where

$$\Delta v_{j+\frac{1}{2}} = v_{j+1} - v_j.$$

Thus the LED condition (8) is satisfied if

$$\alpha_{j+\frac{1}{2}} \geq \frac{1}{2}\left|a_{j+\frac{1}{2}}\right|. \tag{12}$$

If one takes

$$\alpha_{j+\frac{1}{2}} = \frac{1}{2}\left|a_{j+\frac{1}{2}}\right|,$$

the diffusive flux becomes

$$d_{j+\frac{1}{2}} = \frac{1}{2}\left|a_{j+\frac{1}{2}}\right|\Delta v_{j+\frac{1}{2}}$$

and one obtains the first order upwind scheme

$$h_{j+\frac{1}{2}} = \begin{cases} f_j & \text{if } a_{j+\frac{1}{2}} > 0 \\ f_{j+1} & \text{if } a_{j+\frac{1}{2}} < 0 \end{cases}.$$

This is the least diffusive first order scheme which satisfies the LED condition. In this sense upwinding is a natural approach to the construction of non-oscillatory schemes.

Another important requirement of discrete schemes is that they should exclude nonphysical solutions which do not satisfy appropriate entropy conditions [89], which require the convergence of characteristics towards admissible discontinuities. This places more stringent bounds on the minimum level of numerical viscosity [104, 156, 118, 121]. In the case that the numerical flux function is strictly convex, Aiso has recently proved [2] that it is sufficient that

$$\alpha_{j+\frac{1}{2}} > \max\left\{\frac{1}{2}\left|a_{j+\frac{1}{2}}\right|, \epsilon\,\mathrm{sign}(v_{j+1} - v_j)\right\}$$

for $\epsilon > 0$. Thus the numerical viscosity should be rounded out and not allowed to reach zero at a point where the wave speed $a(u) = \frac{\partial f}{\partial u}$ approaches zero. This justifies, for example, Harten's entropy fix [52].

It may be noted that the successful treatment of transonic potential flow also involved the use of upwind biasing. This was first introduced by Murman and Cole to treat the transonic small disturbance equation [113]. The author's rotated difference scheme [58], which extended their technique to treat the general transonic potential flow equation, proved to be very robust. TVD schemes can yield sharp discrete shock waves without oscillations, but in this simple form they are at best first order accurate.

Higher order schemes can be constructed by introducing higher order diffusive terms. Unfortunately these have larger stencils and coefficients of varying sign which are not compatible with the conditions (6) for a LED scheme, and it is known that schemes which satisfy these conditions are at best first order accurate in the neighborhood of an extremum. It proves useful in the following development to introduce the concept of essentially local extremum diminishing (ELED) schemes. These are defined to be schemes which satisfy the condition that in the limit as the mesh width $\Delta x \to 0$, local maxima are non-increasing, and local minima are non-decreasing.

4.3.3 High Resolution Switched Schemes: Jameson-Schmidt-Turkel (JST) Scheme

Higher order non-oscillatory schemes can be derived by introducing anti-diffusive terms in a controlled manner. An early attempt to produce a high resolution scheme by this approach is the Jameson-Schmidt-Turkel (JST) scheme [78]. Suppose that anti-diffusive terms are introduced by subtracting neighboring differences to produce a third order diffusive flux

$$d_{j+\frac{1}{2}} = \alpha_{j+\frac{1}{2}} \left\{ \Delta v_{j+\frac{1}{2}} - \frac{1}{2} \left(\Delta v_{j+\frac{3}{2}} + \Delta v_{j-\frac{1}{2}} \right) \right\}, \tag{13}$$

which is an approximation to $\frac{1}{2}\alpha\Delta x^3 \frac{\partial^3}{\partial x^3}$. The positivity condition (6) is violated by this scheme. It proves that it generates substantial oscillations in the vicinity of shock waves, which can be eliminated by switching locally to the first order scheme. The JST scheme therefore introduces blended diffusion of the form

$$\begin{aligned} d_{j+\frac{1}{2}} \quad = \quad & +\epsilon^{(2)}_{j+\frac{1}{2}} \Delta v_{j+\frac{1}{2}} \\ & -\epsilon^{(4)}_{j+\frac{1}{2}} \left(\Delta v_{j+\frac{3}{2}} - 2\Delta v_{j+\frac{1}{2}} + \Delta v_{j-\frac{1}{2}} \right), \end{aligned} \tag{14}$$

The idea is to use variable coefficients $\epsilon^{(2)}_{j+\frac{1}{2}}$ and $\epsilon^{(4)}_{j+\frac{1}{2}}$ which produce a low level of diffusion in regions where the solution is smooth, but prevent oscillations near discontinuities. If $\epsilon^{(2)}_{j+\frac{1}{2}}$ is constructed so that it is of order Δx^2 where the solution is smooth, while $\epsilon^{(4)}_{j+\frac{1}{2}}$ is of order unity, both terms in $d_{j+\frac{1}{2}}$ will be of order Δx^3.

The JST scheme has proved very effective in practice in numerous calculations of complex steady flows, and conditions under which it could be a total variation diminishing (TVD) scheme have been examined by Swanson and Turkel [153]. An alternative statement of sufficient conditions on the coefficients $\epsilon^{(2)}_{j+\frac{1}{2}}$ and $\epsilon^{(4)}_{j+\frac{1}{2}}$ for the JST scheme to be LED is as follows:

Theorem 1 (Positivity of the JST scheme)
Suppose that whenever either v_{j+1} or v_j is an extremum the coefficients of the JST scheme satisfy

$$\epsilon^{(2)}_{j+\frac{1}{2}} \geq \frac{1}{2} \left| \alpha_{j+\frac{1}{2}} \right|, \ \epsilon^{(4)}_{j+\frac{1}{2}} = 0. \tag{15}$$

Then the JST scheme is local extremum diminishing (LED).

Proof: *We need only consider the rate of change of v at extremal points. Suppose that v_j is an extremum. Then*

$$\epsilon^{(4)}_{j+\frac{1}{2}} = \epsilon^{(4)}_{j-\frac{1}{2}} = 0,$$

and the semi-discrete scheme (9) reduces to

$$\Delta x \frac{dv_j}{dt} = \left(\epsilon^{(2)}_{j+\frac{1}{2}} - \frac{1}{2} a_{j+\frac{1}{2}} \right) \Delta v_{j+\frac{1}{2}} - \left(\epsilon^{(2)}_{j-\frac{1}{2}} + \frac{1}{2} a_{j-\frac{1}{2}} \right) \Delta v_{j-\frac{1}{2}},$$

and each coefficient has the required sign. □

In order to construct $\epsilon^{(2)}_{j-\frac{1}{2}}$ and $\epsilon^{(4)}_{j-\frac{1}{2}}$ with the desired properties define

$$R(u,v) = \begin{cases} \left| \frac{u-v}{|u|+|v|} \right|^q & \text{if } u \neq 0 \text{ or } v \neq 0 \\ 0 & \text{if } u = v = 0, \end{cases} \tag{16}$$

where q is a positive integer. Then $R(u,v) = 1$ if u and v have opposite signs. Otherwise $R(u,v) < 1$. Now set

$$Q_j = R(\Delta v_{j+\frac{1}{2}}, \Delta v_{j-\frac{1}{2}}), \ Q_{j+\frac{1}{2}} = \max(Q_j, Q_{j+1}).$$

and

$$\epsilon^{(2)}_{j+\frac{1}{2}} = \alpha_{j+\frac{1}{2}} Q_{j+\frac{1}{2}}, \quad \epsilon^{(4)}_{j+\frac{1}{2}} = \beta_{j+\frac{1}{2}}(1 - Q_{j+\frac{1}{2}}), \tag{17}$$

where

$$\alpha_{j+\frac{1}{2}} \geq \frac{1}{2} \left| a_{j+\frac{1}{2}} \right|, \ \beta_{j+\frac{1}{2}} \text{is proportional to} \left| a_{j+\frac{1}{2}} \right|.$$

At a extremum $Q_j = 1$, since then $\Delta v_{j+\frac{1}{2}}$ and $\Delta v_{j-\frac{1}{2}}$ have opposite signs. Elsewhere $Q_j \leq 1$ and is of order Δx if the solution is smooth. Thus the conditions (15) for a LED scheme are satisfied, and if $q \geq 2$, $\epsilon^{(2)}_{j+\frac{1}{2}}$ is of order Δx^2 in smooth regions not containing an extremum.

4.3.4 Symmetric Limited Positive (SLIP) Scheme

An alternative route to high resolution without oscillation is to introduce flux limiters to guarantee the satisfaction of the positivity condition (6). The use of limiters dates back to the work of Boris and Book [22]. A particularly simple way to introduce limiters, proposed by the author in 1984 [63], is to use flux limited dissipation. In this scheme the third order diffusion defined by equation (13) is modified by the insertion of limiters which produce an equivalent three point scheme with positive coefficients. The original scheme [63] can be improved in the following manner so that less restrictive flux limiters are required. Let $L(u, v)$ be a limited average of u and v with the following properties:

P1. $L(u, v) = L(v, u)$

P2. $L(\alpha u, \alpha v) = \alpha L(u, v)$

P3. $L(u, u) = u$

P4. $L(u, v) = 0$ if u and v have opposite signs: otherwise $L(u, v)$ has the same sign as u and v.

Properties (P1–P3) are natural properties of an average. Property (P4) is needed for the construction of a LED or TVD scheme.

It is convenient to introduce the notation

$$\phi(r) = L(1, r) = L(r, 1),$$

where according to (P4) $\phi(r) \geq 0$. It follows from (P2) on setting $\alpha = \frac{1}{u}$ or $\frac{1}{v}$ that

$$L(u, v) = \phi\left(\frac{v}{u}\right) u = \phi\left(\frac{u}{v}\right) v.$$

Also it follows on setting $v = 1$ and $u = r$ that

$$\phi(r) = r\phi\left(\frac{1}{r}\right).$$

Thus, if there exists $r < 0$ for which $\phi(r) > 0$, then $\phi\left(\frac{1}{r}\right) < 0$. The only way to ensure that $\phi(r) \geq 0$ is to require $\phi(r) = 0$ for all $r < 0$, corresponding to property (P4).

Now one defines the diffusive flux for a scalar conservation law as

$$d_{j+\frac{1}{2}} = \alpha_{j+\frac{1}{2}} \left\{ \Delta v_{j+\frac{1}{2}} - L\left(\Delta v_{j+\frac{3}{2}}, \Delta v_{j-\frac{1}{2}}\right) \right\}. \tag{18}$$

Also define

$$r^+ = \frac{\Delta v_{j+\frac{3}{2}}}{\Delta v_{j-\frac{1}{2}}}, \quad r^- = \frac{\Delta v_{j-\frac{3}{2}}}{\Delta v_{j+\frac{1}{2}}}.$$

Then, the scalar scheme (9) reduces to

$$\begin{aligned}\Delta x\frac{dv_j}{dt} &= -\frac{1}{2}a_{j+\frac{1}{2}}\Delta v_{j+\frac{1}{2}} - \frac{1}{2}a_{j-\frac{1}{2}}\Delta v_{j-\frac{1}{2}} \\ &\quad +\alpha_{j+\frac{1}{2}}\left(\Delta v_{j+\frac{1}{2}} - \phi(r^+)\Delta v_{j-\frac{1}{2}}\right) \\ &\quad -\alpha_{j-\frac{1}{2}}\left(\Delta v_{j-\frac{1}{2}} - \phi(r^-)\Delta v_{j+\frac{1}{2}}\right) \\ &= +\left\{\alpha_{j+\frac{1}{2}} - \frac{1}{2}a_{j+\frac{1}{2}} + \alpha_{j-\frac{1}{2}}\phi(r^-)\right\}\Delta v_{j+\frac{1}{2}} \\ &\quad -\left\{\alpha_{j-\frac{1}{2}} + \frac{1}{2}a_{j-\frac{1}{2}} + \alpha_{j+\frac{1}{2}}\phi(r^+)\right\}\Delta v_{j-\frac{1}{2}}. \end{aligned} \tag{19}$$

Thus the scheme satisfies the LED condition if $\alpha_{j+\frac{1}{2}} \geq \frac{1}{2}\left|a_{j+\frac{1}{2}}\right|$ for all j, and $\phi(r) \geq 0$, which is assured by property (P4) on L. At the same time it follows from property (P3) that the first order diffusive flux is canceled when Δv is smoothly varying and of constant sign. Schemes constructed by this formulation will be referred to as symmetric limited positive (SLIP) schemes. This result may be summarized as

Theorem 2 (Positivity of the SLIP scheme)
Suppose that the discrete conservation law (9) contains a limited diffusive flux as defined by equation (18). Then the positivity condition (12), together with the properties (P1-P4) for limited averages, are sufficient to ensure satisfaction of the LED principle that a local maximum cannot increase and a local minimum cannot decrease. □

A variety of limiters may be defined which meet the requirements of properties (P1–P4). Define

$$S(u,v) = \frac{1}{2}\{\text{sign}(u) + \text{sign}(v)\}$$

so that

$$S(u,v) = \begin{cases} 1 & \text{if } u > 0 \text{ and } v > 0 \\ 0 & \text{if } u \text{ and } v \text{ have opposite sign} \\ -1 & \text{if } u < 0 \text{ and } v < 0. \end{cases}$$

Then two limiters which are appropriate are the following well-known schemes:

1. Minmod:
$$L(u,v) = S(u,v)\min(|u|,|v|)$$
2. Van Leer:
$$L(u,v) = S(u,v)\frac{2|u||v|}{|u|+|v|}.$$

In order to produce a family of limiters which contains these as special cases it is convenient to set

$$L(u,v) = \frac{1}{2}D(u,v)(u+v),$$

where $D(u,v)$ is a factor which should deflate the arithmetic average, and become zero if u and v have opposite signs. Take

$$D(u,v) = 1 - R(u,v) = 1 - \left|\frac{u-v}{|u|+|v|}\right|^q, \tag{20}$$

where $R(u,v)$ is the same function that was introduced in the JST scheme, and q is a positive integer. Then $D(u,v) = 0$ if u and v have opposite signs. Also if $q = 1$, $L(u,v)$ reduces to minmod, while if $q = 2$, $L(u,v)$ is equivalent to Van Leer's limiter. By increasing q one can generate a sequence of limited averages which approach a limit defined by the arithmetic mean truncated to zero when u and v have opposite signs.

When the terms are regrouped, it can be seen that with this limiter the SLIP scheme is exactly equivalent to the JST scheme, with the switch is defined as

$$\begin{aligned} Q_{j+\frac{1}{2}} &= R\left(\Delta v_{j+\frac{3}{2}}, \Delta v_{j+\frac{1}{2}}\right) \\ \epsilon^{(2)}_{j+\frac{1}{2}} &= \alpha_{j+\frac{1}{2}} Q_{j+\frac{1}{2}} \\ \epsilon^{(4)}_{j+\frac{1}{2}} &= \alpha_{j+\frac{1}{2}}\left(1 - Q_{j+\frac{1}{2}}\right). \end{aligned}$$

This formulation thus unifies the JST and SLIP schemes.

4.3.5 Essentially Local Extremum Diminishing (ELED) Scheme with Soft Limiter

The limiters defined by the formula (20) have the disadvantage that they are active at a smooth extrema, reducing the local accuracy of the scheme to first order. In order to prevent this, the SLIP scheme can be relaxed to give an essentially local extremum diminishing (ELED) scheme which is second order accurate at smooth extrema by the introduction of a threshold in the limited average. Therefore redefine $D(u,v)$ as

$$D(u,v) = 1 - \left|\frac{u-v}{\max(|u|+|v|, \epsilon\Delta x^r)}\right|^q, \tag{21}$$

where $r = \frac{3}{2}$, $q \geq 2$. This reduces to the previous definition if $|u| + |v| > \epsilon\Delta x^r$. Now

$$d_{j+\frac{1}{2}} = \alpha_{j+\frac{1}{2}}\left\{\Delta v_{j+\frac{1}{2}} - \frac{1}{2} D_{j+\frac{1}{2}}\left(\Delta v_{j+\frac{3}{2}} + \Delta v_{j-\frac{1}{2}}\right)\right\},$$

where

$$D_{j+\frac{1}{2}} = D\left(\Delta v_{j+\frac{3}{2}}, \Delta v_{j-\frac{1}{2}}\right).$$

In any region where the solution is smooth, $\Delta v_{j+\frac{3}{2}} - \Delta v_{j-\frac{1}{2}}$ is of order Δx^2. In fact if there is a smooth extremum in the neighborhood of v_j or v_{j+1}, a Taylor series expansion indicates that $\Delta v_{j+\frac{3}{2}}$, $\Delta v_{j+\frac{1}{2}}$ and $\Delta v_{j-\frac{1}{2}}$ are each individually of order Δx^2, since $\frac{dv}{dx} = 0$ at the extremum. Then $D_{j+\frac{1}{2}} = 1 - A$ where A is of order $\Delta x^{\frac{q}{2}}$, and

$$\begin{aligned} d_{j+\frac{1}{2}} &= \alpha_{j+\frac{1}{2}}\left(\Delta v_{j+\frac{1}{2}} - \frac{1}{2}\Delta v_{j+\frac{3}{2}} - \frac{1}{2}\Delta v_{j-\frac{1}{2}}\right) \\ &\quad + \alpha_{j+\frac{1}{2}} A\left(\Delta v_{j+\frac{3}{2}} + \Delta v_{j-\frac{1}{2}}\right), \end{aligned}$$

where the first term is of order Δx^3 and the second of order $\Delta x^{1+\frac{q}{2}}$. Therefore taking $q \geq 2$ is sufficient to ensure at least second order accuracy at a smooth extremum.

Consider now the possible growth of the extrema. The limiter acts in the usual way if either $\left|\Delta v_{j+\frac{3}{2}}\right| > \epsilon\Delta x^r$ or $\left|\Delta v_{j-\frac{1}{2}}\right| > \epsilon\Delta x^r$. If v_j is a maximum, it may then be verified that

$$\Delta x \frac{dv_j}{dt} \leq \frac{1}{2}(\alpha_{j+\frac{1}{2}} + \alpha_{j-\frac{1}{2}})\epsilon\Delta x^r.$$

Therefore, if v_j is a maximum $\frac{dv_j}{dt} \leq B$, and similarly if v_j is a minimum $\frac{dv_j}{dt} \geq -B$, where $B \to 0$ as $\Delta x \to 0$ as long as $r > 1$. Thus the SLIP scheme with the limiter (21) is essentially local extremum diminishing (ELED).

The effect of the "soft limiter" is not only to improve the accuracy: the introduction of a threshold below which extrema of small amplitude are accepted also usually results in a faster rate of convergence to a steady state, and decreases the likelyhood of limit cycles in which the limiter interacts unfavorably with the corrections produced by the updating scheme. In a scheme recently proposed by Venkatakrishnan a threshold is introduced precisely for this purpose [160].

4.3.6 Upstream Limited Positive (USLIP) Schemes

By adding the anti-diffusive correction purely from the upstream side one may derive a family of upstream limited positive (USLIP) schemes. Corresponding to the original SLIP scheme defined by equation (18), a USLIP scheme is obtained by setting

$$d_{j+\frac{1}{2}} = \alpha_{j+\frac{1}{2}} \left\{ \Delta v_{j+\frac{1}{2}} - L\left(\Delta v_{j+\frac{1}{2}}, \Delta v_{j-\frac{1}{2}} \right) \right\}$$

if $a_{j+\frac{1}{2}} > 0$, or

$$d_{j+\frac{1}{2}} = \alpha_{j+\frac{1}{2}} \left\{ \Delta v_{j+\frac{1}{2}} - L\left(\Delta v_{j+\frac{1}{2}}, \Delta v_{j+\frac{3}{2}} \right) \right\}$$

if $a_{j+\frac{1}{2}} < 0$. If $\alpha_{j+\frac{1}{2}} = \frac{1}{2} \left| a_{j+\frac{1}{2}} \right|$ one recovers a standard high resolution upwind scheme in semi-discrete form. Consider the case that $a_{j+\frac{1}{2}} > 0$ and $a_{j-\frac{1}{2}} > 0$. If one sets

$$r^+ = \frac{\Delta v_{j+\frac{1}{2}}}{\Delta v_{j-\frac{1}{2}}}, \quad r^- = \frac{\Delta v_{j-\frac{3}{2}}}{\Delta v_{j-\frac{1}{2}}},$$

the scheme reduces to

$$\Delta x \frac{dv_j}{dt} = -\frac{1}{2} \left\{ \phi(r^+) a_{j+\frac{1}{2}} + \left(2 - \phi(r^-)\right) a_{j-\frac{1}{2}} \right\} \Delta v_{j-\frac{1}{2}}.$$

To assure the correct sign to satisfy the LED criterion the flux limiter must now satisfy the additional constraint that $\phi(r) \leq 2$.

The USLIP formulation is essentially equivalent to standard upwind schemes [120, 154]. Both the SLIP and USLIP constructions can be implemented on unstructured meshes [70, 72]. The anti-diffusive terms are then calculated by taking the scalar product of the vectors defining an edge with the gradient in the adjacent upstream and downstream cells.

4.3.7 Systems of Conservation Laws: Flux Splitting and Flux-Difference Splitting

Steger and Warming [151] first showed how to generalize the concept of upwinding to the system of conservation laws

$$\frac{\partial w}{\partial t} + \frac{\partial}{\partial x} f(w) = 0 \tag{22}$$

by the concept of flux splitting. Suppose that the flux is split as $f = f^+ + f^-$ where $\frac{\partial f^+}{\partial w}$ and $\frac{\partial f^-}{\partial w}$ have positive and negative eigenvalues. Then the first order upwind scheme is produced by taking the numerical flux to be

$$h_{j+\frac{1}{2}} = f_j^+ + f_{j+1}^-.$$

This can be expressed in viscosity form as

$$\begin{aligned} h_{j+\frac{1}{2}} &= +\frac{1}{2}\left(f_{j+1}^+ + f_j^+\right) - \frac{1}{2}\left(f_{j+1}^+ - f_j^+\right) \\ &\quad +\frac{1}{2}\left(f_{j+1}^- + f_j^-\right) + \frac{1}{2}\left(f_{j+1}^- - f_j^-\right) \\ &= \frac{1}{2}\left(f_{j+1} + f_j\right) - d_{j+\frac{1}{2}}, \end{aligned}$$

where the diffusive flux is

$$d_{j+\frac{1}{2}} = \frac{1}{2} \Delta (f^+ - f^-)_{j+\frac{1}{2}}. \tag{23}$$

Roe derived the alternative formulation of flux difference splitting [133] by distributing the corrections due to the flux difference in each interval upwind and downwind to obtain

$$\Delta x \frac{dw_j}{dt} + (f_{j+1} - f_j)^- + (f_j - f_{j-1})^+ = 0,$$

where now the flux difference $f_{j+1} - f_j$ is split. The corresponding diffusive flux is

$$d_{j+\frac{1}{2}} = \frac{1}{2}\left(\Delta f_{j+\frac{1}{2}}^+ - \Delta f_{j+\frac{1}{2}}^- \right).$$

Following Roe's derivation, let $A_{j+\frac{1}{2}}$ be a mean value Jacobian matrix exactly satisfying the condition

$$f_{j+1} - f_j = A_{j+\frac{1}{2}}(w_{j+1} - w_j). \tag{24}$$

$A_{j+\frac{1}{2}}$ may be calculated by substituting the weighted averages

$$u = \frac{\sqrt{\rho_{j+1}}u_{j+1} + \sqrt{\rho_j}u_j}{\sqrt{\rho_{j+1}} + \sqrt{\rho_j}}, H = \frac{\sqrt{\rho_{j+1}}H_{j+1} + \sqrt{\rho_j}H_j}{\sqrt{\rho_{j+1}} + \sqrt{\rho_j}} \tag{25}$$

into the standard formulas for the Jacobian matrix $A = \frac{\partial f}{\partial w}$. A splitting according to characteristic fields is now obtained by decomposing $A_{j+\frac{1}{2}}$ as

$$A_{j+\frac{1}{2}} = T\Lambda T^{-1}, \tag{26}$$

where the columns of T are the eigenvectors of $A_{j+\frac{1}{2}}$, and Λ is a diagonal matrix of the eigenvalues. Then

$$\Delta f^{\pm}_{j+\frac{1}{2}} = T\Lambda^{\pm}T^{-1}\Delta w_{j+\frac{1}{2}}.$$

Now the corresponding diffusive flux is

$$\frac{1}{2}\left|A_{j+\frac{1}{2}}\right|(w_{j+1} - w_j),$$

where

$$\left|A_{j+\frac{1}{2}}\right| = T\,|\Lambda|\,T^{-1}$$

and $|\Lambda|$ is the diagonal matrix containing the absolute values of the eigenvalues.

4.3.8 Alternative Splittings

Characteristic splitting has the advantages that it introduces the minimum amount of diffusion to exclude the growth of local extrema of the characteristic variables, and that with the Roe linearization it allows a discrete shock structure with s single interior point. To reduce the computational complexity one may replace $|A|$ by αI where if α is at least equal to the spectral radius $\max|\lambda(A)|$, then the positivity conditions will still be satisfied. Then the first order scheme simply has the scalar diffusive flux

$$d_{j+\frac{1}{2}} = \frac{1}{2}\alpha_{j+\frac{1}{2}}\Delta w_{j+\frac{1}{2}}. \tag{27}$$

The JST scheme with scalar diffusive flux captures shock waves with about 3 interior points, and it has been widely used for transonic flow calculations because it is both robust and computationally inexpensive.

An intermediate class of schemes can be formulated by defining the first order diffusive flux as a combination of differences of the state and flux vectors

$$d_{j+\frac{1}{2}} = \frac{1}{2}\alpha_{j+\frac{1}{2}}(w_{j+1} - w_j) + \frac{1}{2}\beta_{j+\frac{1}{2}}(f_{j+1} - f_j). \tag{28}$$

Schemes of this class are fully upwind in supersonic flow if one takes $\alpha_{j+\frac{1}{2}} = 0$ and $\beta_{j+\frac{1}{2}} = \text{sign}(M)$ when the absolute value of the Mach number M exceeds 1. The flux vector f can be decomposed as

$$f = uw + f_p, \tag{29}$$

where

$$f_p = \begin{pmatrix} 0 \\ p \\ up \end{pmatrix}. \tag{30}$$

Then

$$f_{j+1} - f_j = \bar{u}(w_{j+1} - w_j) + \bar{w}(u_{j+1} - u_j) + f_{p_{j+1}} - f_{p_j}, \tag{31}$$

where $\bar{u}$ and $\bar{w}$ are the arithmetic averages

$$\bar{u} = \frac{1}{2}(u_{j+1} + u_j), \quad \bar{w} = \frac{1}{2}(w_{j+1} + w_j).$$

Thus these schemes are closely related to schemes which introduce separate splittings of the convective and pressure terms, such as the wave-particle scheme [129, 8], the advection upwind splitting method (AUSM) [98, 162], and the convective upwind and split pressure (CUSP) schemes [71].

In order to examine the shock capturing properties of these various schemes, consider the general case of a first order diffusive flux of the form

$$d_{j+\frac{1}{2}} = \frac{1}{2}\alpha_{j+\frac{1}{2}} B_{j+\frac{1}{2}} (w_{j+1} - w_j), \tag{32}$$

where the matrix $B_{j+\frac{1}{2}}$ determines the properties of the scheme and the scaling factor $\alpha_{j+\frac{1}{2}}$ is included for convenience. All the previous schemes can be obtained by representing $B_{j+\frac{1}{2}}$ as a polynomial in the matrix $A_{j+\frac{1}{2}}$ defined by equation (24). According to the Cayley-Hamilton theorem, a matrix satisfies its own characteristic equation. Therefore the third and higher powers of A can be eliminated, and there is no loss of generality in limiting $B_{j+\frac{1}{2}}$ to a polynomial of degree 2,

$$B_{j+\frac{1}{2}} = \alpha_0 I + \alpha_1 A_{j+\frac{1}{2}} + \alpha_2 A^2_{j+\frac{1}{2}}. \tag{33}$$

The characteristic upwind scheme for which $B_{j+\frac{1}{2}} = \left|A_{j+\frac{1}{2}}\right|$ is obtained by substituting $A_{j+\frac{1}{2}} = T\Lambda T^{-1}$, $A^2_{j+\frac{1}{2}} = T\Lambda^2 T^{-1}$. Then α_0, α_1, and α_2 are determined from the three equations

$$\alpha_0 + \alpha_1 \lambda_k + \alpha_2 \lambda_k^2 = |\lambda_k|, \quad k = 1, 2, 3.$$

The same representation remains valid for three dimensional flow because $A_{j+\frac{1}{2}}$ still has only three distinct eigenvalues u, $u + c$, $u - c$.

4.3.9 Analysis of Stationary Discrete Shocks

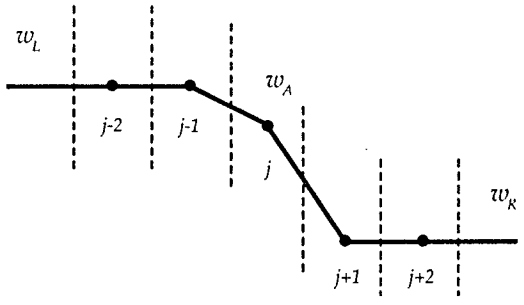


Figure 4: Shock structure for single interior point.

The ideal model of a discrete shock is illustrated in figure (4). Suppose that w_L and w_R are left and right states which satisfy the jump conditions for a stationary shock, and that the corresponding fluxes are $f_L = f(w_L)$ and $f_R = f(w_R)$. Since the shock is stationary $f_L = f_R$. The ideal discrete shock has constant states w_L to the left and w_R to the right, and a single point with an intermediate value w_A. The intermediate value is needed to allow the discrete solution to correspond to a true solution in which the shock wave does not coincide with an interface between two mesh cells. According to equation (22)

$$\int_0^L w(T)dx = \int_0^L w(0)dx - \int_0^T (f_{RB} - f_{LB})dt,$$

where f_{LB} and f_{RB} are the fluxes at the left and right boundaries. Assuming that the boundary conditions are compatible with a steady solution containing a stationary shock, the location x_s of the shock is fixed by

this equation, since

$$\int_0^L w(T)dx = x_s w_L + (L - x_s)w_R.$$

Similarly, in the semi-discrete system

$$\Delta x \sum_j w_j(T) = \Delta x \sum_j w_j(0) - \int_0^T (f_{RB} - f_{LB})dt. \tag{34}$$

Thus $\sum_j w_j(T)$ has a value which is determined by the initial and boundary conditions. In general it is not possible for this value to be attained by a discrete solution without an intermediate point, because then the sum would be quantized, increasing by $\Delta x(w_R - w_L)$ whenever the shock location is shifted one cell to the right.

Three diffusion models of varying complexity which belong to the class defined by equation (33) are examined in Reference [73] to determine their ability to support the ideal shock structure containing a single interior point. These correspond to one, two or three terms in equation (33). The analysis of these three cases shows that a discrete shock structure with a single interior point is supported by artificial diffusion that satisfies the two conditions that

1. it produces an upwind flux if the flow is determined to be supersonic through the interface

2. it satisfies a generalized eigenvalue problem for the exit from the shock of the form

$$(A_{AR} - \alpha_{AR} B_{AR})(w_R - w_A) = 0,$$

where A_{AR} is the linearized Jacobian matrix and B_{AR} is the matrix defining the diffusion for the interface AR. These two conditions are satisfied by both the characteristic schemes and also the CUSP scheme, provided that the coefficients of convective diffusion and pressure differences are correctly balanced. Scalar diffusion does not satisfy the first condition.

4.3.10 CUSP and Characteristic Schemes Admitting Constant Total Enthalpy in Steady Flow

In steady flow the stagnation enthalpy H is constant, corresponding to the fact that the energy and mass conservation equations are consistent when the constant factor H is removed from the energy equation. Discrete and semi-discrete schemes do not necessarily satisfy this property. In the case of a semi-discrete scheme expressed in viscosity form, equations (9) and (10), a solution with constant H is admitted if the viscosity for the energy equation reduces to the viscosity for the continuity equation with ρ replaced by ρH. When the standard characteristic decomposition (26) is used, the viscous fluxes for ρ and ρH which result from composition of the fluxes for the characteristic variables do not have this property, and H is not constant in the discrete solution. In practice there is an excursion of H in the discrete shock structure which represents a local heat source. In very high speed flows the corresponding error in the temperature may lead to a wrong prediction of associated effects such as chemical reactions.

The source of the error in the stagnation enthalpy is the discrepancy between the convective terms

$$u \begin{pmatrix} \rho \\ \rho u \\ \rho H \end{pmatrix},$$

in the flux vector, which contain ρH, and the state vector which contains ρE. This may be remedied by introducing a modified state vector

$$w_h = \begin{pmatrix} \rho \\ \rho u \\ \rho H \end{pmatrix}.$$

Then one introduces the linearization

$$f_R - f_L = A_h(w_{h_R} - w_{h_L}).$$

Here A_h may be calculated in the same way as the standard Roe linearization. Introduce the weighted averages defined by equation (25). Then

$$A_h = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{\gamma+1}{\gamma}\frac{u^2}{2} & \frac{\gamma+1}{\gamma}u & \frac{\gamma-1}{\gamma} \\ -uH & H & u \end{pmatrix}.$$

The eigenvalues of A_h are u, λ^+ and λ^- where

$$\lambda^{\pm} = \frac{\gamma+1}{2\gamma}u \pm \sqrt{(\frac{\gamma+1}{2\gamma}u)^2 + \frac{c^2-u^2}{\gamma}}. \tag{35}$$

Now both CUSP and characteristic schemes which preserve constant stagnation enthalpy in steady flow can be constructed from the modified Jacobian matrix A_h [73]. These schemes also produce a discrete shock structure with one interior point in steady flow. Then one arrives at four variations with this property, which can conveniently be distinguished as the E- and H-CUSP schemes, and the E- and H-characteristic schemes.

4.3.11 Multidimensional Upwinding, High Order Godunov Schemes, and Kinetic Flux Splitting

A substantial body of current research is directed toward the implementation of truly multi-dimensional upwind schemes [55, 123, 94]. Some of the most impressive simulations of time dependent flows with strong shock waves have been achieved with higher order Godunov schemes [166]. In these schemes the average value in each cell is updated by applying the integral conservation law using interface fluxes predicted from the exact or approximate solution of a Riemann problem between adjacent cells. A higher order estimate of the solution is then reconstructed from the cell averages, and slope limiters are applied to the reconstruction. An example is the class of essentially non-oscillatory (ENO) schemes, which can attain a very high order of accuracy at the cost of a substantial increase in computational complexity [30, 140, 138, 139]. Methods based on reconstruction can also be implemented on unstructured meshes [13, 12]. Recently there has been an increasing interest in kinetic flux splitting schemes, which use solutions of the Boltzmann equation to predict the interface fluxes [39, 34, 42, 124, 167].

4.4 Discretization of the Viscous Terms

The discretization of the viscous terms of the Navier Stokes equations requires an approximation to the velocity derivatives $\frac{\partial u_i}{\partial x_j}$ in order to calculate the tensor σ_{ij}, equation (2). Then the viscous terms may be included in the flux balance (3). In order to evaluate the derivatives one may apply the Gauss formula to a control volume V with the boundary S.

$$\int_V \frac{\partial u_i}{\partial x_j} dv = \int_S u_i n_j ds$$

where n_j is the outward normal. For a tetrahedral or hexahedral cell this gives

$$\overline{\frac{\partial u_i}{\partial x_j}} = \frac{1}{\text{vol}} \sum_{\text{faces}} \overline{u}_i \, n_j \, s \tag{36}$$

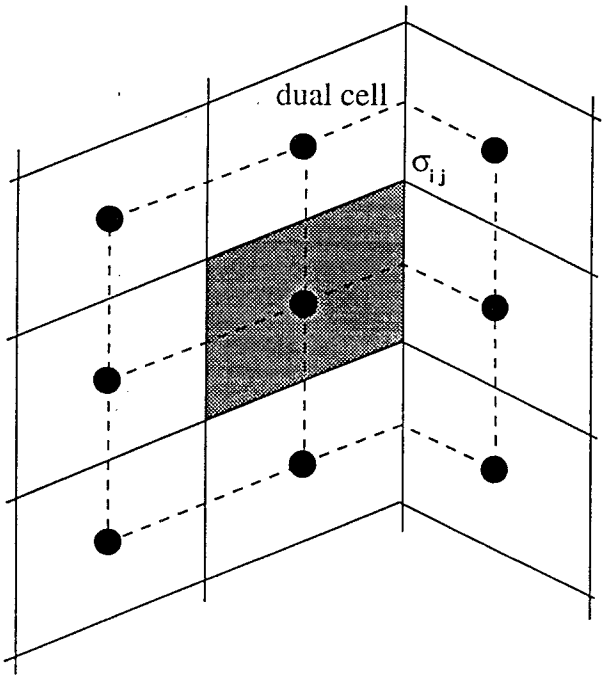
where $\overline{u}_i$ is an estimate of the average of u_i over the face. If u varies linearly over a tetrahedral cell this is exact. Alternatively, assuming a local transformation to computational coordinates X_j, one may apply the chain rule

$$\frac{\partial u}{\partial x} = \left[\frac{\partial u}{\partial X}\right]\left[\frac{\partial X}{\partial x}\right] = \frac{\partial u}{\partial X}\left[\frac{\partial x}{\partial X}\right]^{-1} \tag{37}$$

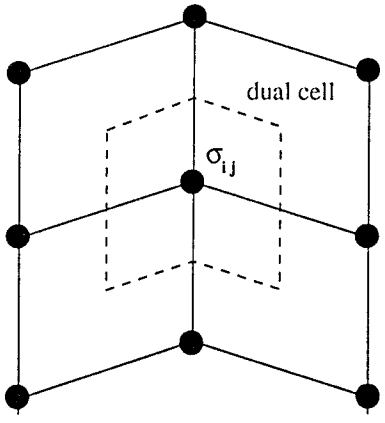
Here the transformation derivatives $\frac{\partial x_i}{\partial X_j}$ can be evaluated by the same finite difference formulas as the velocity derivatives $\frac{\partial u_i}{\partial X_j}$ In this case $\frac{\partial u}{\partial X}$ is exact if u is a linearly varying function.

For a cell-centered discretization (figure 5a) $\frac{\partial u}{\partial X}$ is needed at each face. The simplest procedure is to evaluate $\frac{\partial u}{\partial X}$ in each cell, and to average $\frac{\partial u}{\partial X}$ between the two cells on either side of a face [81]. The resulting discretization does not have a compact stencil, and supports undamped oscillatory modes. In a one dimensional calculation, for example, $\frac{\partial^2 u}{\partial x^2}$ would be discretized as $\frac{u_{i+2}-2u_i+u_{i-2}}{4\Delta x^2}$. In order to produce a compact stencil $\frac{\partial u}{\partial x}$ may be estimated from a control volume centered on each face, using formulas (36) or (37) [131]. This is computationally expensive because the number of faces is much larger than the number of cells. In a hexahedral mesh with a large number of vertices the number of faces approaches three times the number of cells.

This motivates the introduction of dual meshes for the evaluation of the velocity derivatives and the flux balance as sketched in figure 5. The figure shows both cell-centered and cell-vertex schemes. The dual mesh



5a: Cell-centered scheme. σ_{ij} evaluated at vertices of the primary mesh



5b: Cell-vertex scheme. σ_{ij} evaluated at cell centers of the primary mesh

Figure 5: Viscous discretizations for cell-centered and cell-vertex algorithms.

connects cell centers of the primary mesh. If there is a kink in the primary mesh, the dual cells should be formed by assembling contiguous fractions of the neighboring primary cells. On smooth meshes comparable results are obtained by either of these formulations [105, 106, 80]. If the mesh has a kink the cell-vertex scheme has the advantage that the derivatives $\frac{\partial u_i}{\partial x_j}$ are calculated in the interior of a regular cell, with no loss of accuracy.

A desirable property is that a linearly varying velocity distribution, as in a Couette flow, should produce a constant stress and hence an exact stress balance. This property is not necessarily satisfied in general by finite difference or finite volume schemes on curvilinear meshes. The characterization k-exact has been proposed for schemes that are exact for polynomials of degree k. The cell-vertex finite volume scheme is linearly exact if the derivatives are evaluated by equation (37), since then $\frac{\partial u_i}{\partial x_j}$ is exactly evaluated as a constant, leading to constant viscous stresses σ_{ij}, and an exact viscous stress balance. This remains true when there is a kink in the mesh, because the summation of constant stresses over the faces of the kinked control volume sketched in

figure 5 still yields a perfect balance. The use of equation (37) to evaluate $\frac{\partial u_i}{\partial x_j}$, however, requires the additional calculation or storage of the nine metric quantities $\frac{\partial u_i}{\partial x_j}$ in each cell, whereas equation (36) can be evaluated from the same face areas that are used for the flux balance.

In the case of an unstructured mesh, the weak form (4) leads to a natural discretization with linear elements, in which the piecewise linear approximation yields a constant stress in each cell. This method yields a representation which is globally correct when averaged over the cells, as is proved by energy estimates for elliptic problems [15]. It should be noted, however, that it yields formulas that are not necessarily locally consistent with the differential equations, if Taylor series expansions are substituted for the solution at the vertices appearing in the local stencil. Figure 6 illustrates the discretization of the Laplacian $u_{xx} + u_{yy}$ which is obtained with linear elements. It shows a particular triangulation such that the approximation is locally consistent with $u_{xx} + 3u_{yy}$. Thus the use of an irregular triangulation in the boundary layer may significantly degrade the accuracy.

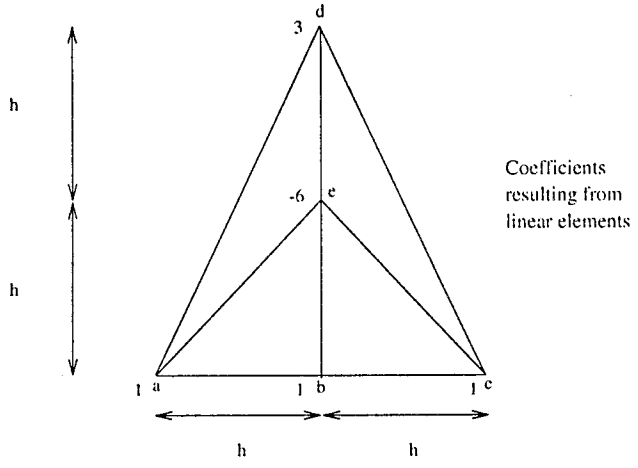


Figure 6: Example of discretization $u_{xx} + u_{yy}$ on a triangular mesh. The discretization is locally equivalent to the approximation $u_{xx} = \frac{u_a - 2u_b + u_c}{h^2}, 3u_{yy} = \frac{3u_d - 6u_e + 3u_b}{h^2}$.

4.5 Time Stepping Schemes

If the space discretization procedure is implemented separately, it leads to a set of coupled ordinary differential equations, which can be written in the form

$$\frac{d\mathbf{w}}{dt} + \mathbf{R}(\mathbf{w}) = 0, \tag{38}$$

where $\mathbf{w}$ is the vector of the flow variables at the mesh points, and $\mathbf{R}(\mathbf{w})$ is the vector of the residuals, consisting of the flux balances defined by the space discretization scheme, together with the added dissipative terms. If the objective is simply to reach the steady state and details of the transient solution are immaterial, the time-stepping scheme may be designed solely to maximize the rate of convergence. The first decision that must be made is whether to use an explicit scheme, in which the space derivatives are calculated from known values of the flow variables at the beginning of the time step, or an implicit scheme, in which the formulas for the space derivatives include as yet unknown values of the flow variables at the end of the time step, leading to the need to solve coupled equations for the new values. The permissible time step for an explicit scheme is limited by the Courant-Friedrichs-Lewy (CFL) condition, which states that a difference scheme cannot be a convergent and stable approximation unless its domain of dependence contains the domain of dependence of the corresponding differential equation. One can anticipate that implicit schemes will yield convergence

in a smaller number of time steps, because the time step is no longer constrained by the CFL condition. Implicit schemes will be efficient, however, only if the decrease in the number of time steps outweighs the increase in the computational effort per time step consequent upon the need to solve coupled equations. The prototype implicit scheme can be formulated by estimating $\frac{\partial \mathbf{w}}{\partial t}$ at $t + \mu\Delta t$ as a linear combination of $\mathbf{R}(\mathbf{w^n})$ and $\mathbf{R}(\mathbf{w^{n+1}})$. The resulting equation

$$\mathbf{w}^{n+1} = \mathbf{w}^n - \Delta t \left\{ (1-\mu)\,\mathbf{R}\left(\mathbf{w^n}\right) + \mu \mathbf{R}\left(\mathbf{w}^{n+1}\right) \right\}$$

can be linearized as

$$\left(\mathbf{I} + \mu\Delta t \frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right) \delta\mathbf{w} + \Delta t \mathbf{R}\left(\mathbf{w}^n\right) = 0.$$

If one sets $\mu = 1$ and lets $\Delta t \to \infty$ this reduces to the Newton iteration , which has been successfully used in two-dimensional calculations [159, 46]. In the three-dimensional case with, say, an $N \times N \times N$ mesh, the bandwidth of the matrix that must be inverted is of order N^2. Direct inversion requires a number of operations proportional to the number of unknowns multiplied by the square of the bandwidth of the order of N^7. This is prohibitive, and forces recourse to either an approximate factorization method or an iterative solution method.

Alternating direction methods, which introduce factors corresponding to each coordinate, are widely used for structured meshes [17, 125]. They cannot be implemented on unstructured tetrahedral meshes that do not contain identifiable mesh directions, although other decompositions are possible [99]. If one chooses to adopt the iterative solution technique, the principal alternatives are variants of the Gauss-Seidel and Jacobi methods. A symmetric Gauss-Seidel method with one iteration per time step is essentially equivalent to an approximate lower-upper (LU) factorization of the implicit scheme [79, 115, 29, 170]. On the other hand, the Jacobi method with a fixed number of iterations per time step reduces to a multistage explicit scheme, belonging to the general class of Runge-Kutta schemes [32]. Schemes of this type have proved very effective for wide variety of problems, and they have the advantage that they can be applied equally easily on both structured and unstructured meshes [77, 62, 64, 132].

If one reduces the linear model problem corresponding to (38) to an ordinary differential equation by substituting a Fourier mode $\hat{w} = e^{ipx_j}$, the resulting Fourier symbol has an imaginary part proportional to the wave speed, and a negative real part proportional to the diffusion. Thus the time stepping scheme should have a stability region which contains a substantial interval of the negative real axis, as well as an interval along the imaginary axis. To achieve this it pays to treat the convective and dissipative terms in a distinct fashion. Thus the residual is split as

$$R(w) = Q(w) + D(w),$$

where $Q(w)$ is the convective part and $D(w)$ the dissipative part. Denote the time level $n\Delta t$ by a superscript n. Then the multistage time stepping scheme is formulated as

$$\begin{aligned}
w^{(n+1,0)} &= w^n \\
&\cdots \\
w^{(n+1,k)} &= w^n - \alpha_k \Delta t \left(Q^{(k-1)} + D^{(k-1)} \right) \\
&\cdots \\
w^{n+1} &= w^{(n+1,m)},
\end{aligned}$$

where the superscript k denotes the k-th stage, $\alpha_m = 1$, and

$$\begin{aligned}
Q^{(0)} &= Q\left(w^n\right), \; D^{(0)} = D\left(w^n\right) \\
&\cdots \\
Q^{(k)} &= Q\left(w^{(n+1,k)}\right) \\
D^{(k)} &= \beta_k D\left(w^{(n+1,k)}\right) + (1-\beta_k) D^{(k-1)}.
\end{aligned}$$

The coefficients α_k are chosen to maximize the stability interval along the imaginary axis, and the coefficients β_k are chosen to increase the stability interval along the negative real axis.

These schemes do not fall within the standard framework of Runge-Kutta schemes, and they have much larger stability regions [64]. Two schemes which have been found to be particularly effective are tabulated below. The first is a four-stage scheme with two evaluations of dissipation. Its coefficients are

$$\begin{array}{ll} \alpha_1 = \frac{1}{3} & \beta_1 = 1 \\ \alpha_2 = \frac{4}{15} & \beta_2 = \frac{1}{2} \\ \alpha_3 = \frac{5}{9} & \beta_3 = 0 \\ \alpha_4 = 1 & \beta_4 = 0 \end{array} . \tag{39}$$

The second is a five-stage scheme with three evaluations of dissipation. Its coefficients are

$$\begin{array}{ll} \alpha_1 = \frac{1}{4} & \beta_1 = 1 \\ \alpha_2 = \frac{1}{6} & \beta_2 = 0 \\ \alpha_3 = \frac{3}{8} & \beta_3 = 0.56 \\ \alpha_4 = \frac{1}{2} & \beta_4 = 0 \\ \alpha_5 = 1 & \beta_5 = 0.44 \end{array} . \tag{40}$$

4.6 Multigrid Methods

4.6.1 Acceleration of Steady Flow Calculations

Radical improvements in the rate of convergence to a steady state can be realized by the multigrid time-stepping technique. The concept of acceleration by the introduction of multiple grids was first proposed by Fedorenko [44]. There is by now a fairly well-developed theory of multigrid methods for elliptic equations based on the concept that the updating scheme acting as a smoothing operator on each grid [23, 49]. This theory does not hold for hyperbolic systems. Nevertheless, it seems that it ought to be possible to accelerate the evolution of a hyperbolic system to a steady state by using large time steps on coarse grids so that disturbances will be more rapidly expelled through the outer boundary. Various multigrid time-stepping schemes designed to take advantage of this effect have been proposed [114, 60, 51, 66, 27, 6, 53, 76, 87].

One can devise a multigrid scheme using a sequence of independently generated coarser meshes by eliminating alternate points in each coordinate direction. In order to give a precise description of the multigrid scheme, subscripts may be used to indicate the grid. Several transfer operations need to be defined. First the solution vector on grid k must be initialized as

$$w_k^{(0)} = T_{k,k-1} w_{k-1},$$

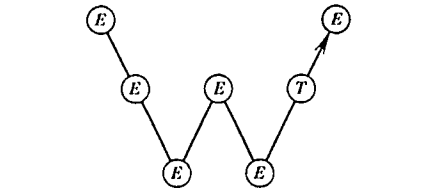
where w_{k-1} is the current value on grid $k-1$, and $T_{k,k-1}$ is a transfer operator. Next it is necessary to transfer a residual forcing function such that the solution grid k is driven by the residuals calculated on grid $k-1$. This can be accomplished by setting

$$P_k = Q_{k,k-1} R_{k-1}\left(w_{k-1}\right) - R_k\left[w_k^{(0)}\right],$$

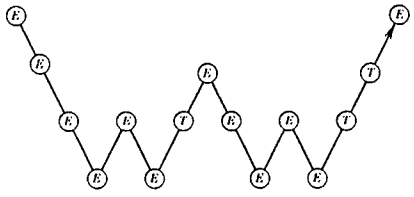
where $Q_{k,k-1}$ is another transfer operator. Then $R_k(w_k)$ is replaced by $R_k(w_k) + P_k$ in the time- stepping scheme. Thus, the multistage scheme is reformulated as

$$\begin{aligned} w_k^{(1)} &= w_k^{(0)} - \alpha_1 \Delta t_k \left[R_k^{(0)} + P_k\right] \\ \cdots & \quad \cdots \\ w_k^{(q+1)} &= w_k^{(0)} - \alpha_{q+1} \Delta t_k \left[R_k^{(q)} + P_k\right]. \end{aligned}$$

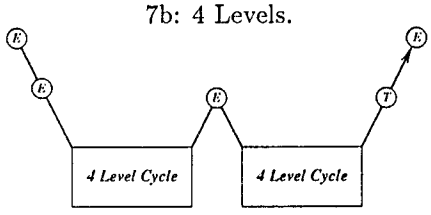
The result $w_k^{(m)}$ then provides the initial data for grid $k+1$. Finally, the accumulated correction on grid k has to be transferred back to grid $k-1$ with the aid of an interpolation operator $I_{k-1,k}$. With properly



7a: 3 Levels.



7b: 4 Levels.



7c: 5 Levels.

Figure 7: Multigrid W-cycle for managing the grid calculation. E, evaluate the change in the flow for one step; T, transfer the data without updating the solution.

optimized coefficients multistage time-stepping schemes can be very efficient drivers of the multigrid process. A W-cycle of the type illustrated in Figure 7 proves to be a particularly effective strategy for managing the work split between the meshes. In a three-dimensional case the number of cells is reduced by a factor of eight on each coarser grid. On examination of the figure, it can therefore be seen that the work measured in units corresponding to a step on the fine grid is of the order of

$$1 + 2/8 + 4/64 + \ldots < 4/3,$$

and consequently the very large effective time step of the complete cycle costs only slightly more than a single time step in the fine grid.

4.6.2 Multigrid Implicit Schemes for Unsteady Flow

Time dependent calculations are needed for a number of important applications, such as flutter analysis, or the analysis of the flow past a helicopter rotor, in which the stability limit of an explicit scheme forces the use of much smaller time steps than would be needed for an accurate simulation. In this situation a multigrid explicit scheme can be used in an inner iteration to solve the equations of a fully implicit time stepping scheme [69].

Suppose that (38) is approximated as

$$D_t w^{n+1} + R(w^{n+1}) = 0.$$

Here D_t is a k^{th} order accurate backward difference operator of the form

$$D_t = \frac{1}{\Delta t} \sum_{q=1}^{k} \frac{1}{q} (\Delta^-)^q,$$

where

$$\Delta^- w^{n+1} = w^{n+1} - w^n.$$

Applied to the linear differential equation

$$\frac{dw}{dt} = \alpha w$$

the schemes with $k = 1, 2$ are stable for all $\alpha\Delta t$ in the left half plane (A-stable). Dahlquist has shown that A-stable linear multi-step schemes are at best second order accurate [35]. Gear however, has shown that the schemes with $k \leq 6$ are stiffly stable [45], and one of the higher order schemes may offer a better compromise between accuracy and stability, depending on the application.

Equation (38) is now treated as a modified steady state problem to be solved by a multigrid scheme using variable local time steps in a fictitious time t^*. For example, in the case $k = 2$ one solves

$$\frac{\partial w}{\partial t^*} = R^*(w),$$

where

$$R^*(w) = \frac{3}{2\Delta t} w + R(w) + \frac{2}{\Delta t} w^n - \frac{1}{2\Delta t} w^{n-1},$$

and the last two terms are treated as fixed source terms. The first term shifts the Fourier symbol of the equivalent model problem to the left in the complex plane. While this promotes stability, it may also require a limit to be imposed on the magnitude of the local time step Δt^* relative to that of the implicit time step Δt. In the case of problems with moving boundaries the equations must be modified to allow for movement and deformation of the mesh.

This method has proved effective for the calculation of unsteady flows that might be associated with wing flutter [3, 4]. It has the advantage that it can be added as an option to a computer program which uses an explicit multigrid scheme, allowing it to be used for the efficient calculation of both steady and unsteady flows.

4.7 High Order Schemes and Mesh Refinement

The need both to improve the accuracy of computational simulations, and to assure known levels of accuracy is the focus of ongoing research. The main routes to improving the accuracy are to increase the order of the discrete scheme, and reduce the mesh interval. High order difference methods are most easily implemented on Cartesian, or at least extremely smooth grids. The expansion of the stencil as the order is increased leads to the need for complex boundary conditions. Compact schemes keep the stencil as small as possible [128, 96, 26]. On simple domains, spectral methods are particularly effective, especially in the case of periodic boundary conditions, and can be used to produce exponentially fast convergence of the error as the mesh interval is decreased [117, 25]. A compromise is to divide the field into subdomains and introduce high order elements. This approach is used in the spectral element method [86].

High order difference schemes and spectral methods have proven particularly useful in direct Navier-Stokes simulations of transient and turbulent flows. High order methods are also beneficial in computational aero-acoustics, where it is desired to track waves over long distances with minimum error. If the flow contains shock waves or contact discontinuities, the ENO method may be used to construct high order non-oscillatory schemes.

In multi-dimensional flow simulations, global reduction of the mesh interval can be prohibitively expensive, motivating the use of adaptive mesh refinement procedures which reduce the local mesh width h if there is an indication that the error is too large [20, 36, 100, 56, 126, 95]. In such h-refinement methods, simple error indicators such as local solution gradients may be used. Alternatively, the discretization error may be estimated by comparing quantities calculated with two mesh widths, say on the current mesh and a coarser mesh with double the mesh interval. Procedures of this kind may also be used to provide *a posteriori* estimates of the error once the calculation is completed.

This kind of local adaptive control can also be applied to the local order of a finite element method to produce a p-refinement method, where p represents the order of the polynomial basis functions. Finally, both h- and p- refinement can be combined to produce an h-p method in which h and p are locally optimized to

yield a solution with minimum error [116]. Such methods can achieve exponentially fast convergence, and are well established in computational solid mechanics.

5 Current Status of Numerical Simulation

This section presents some representative numerical results which confirm the properties of the algorithms which have been reviewed in the last section. These have been drawn from the work of the author and his associates. They also illustrate the kind of calculation which can be performed in an industrial environment, where rapid turn around is important to allow quick assessment of design changes, and computational costs must be limited.

5.1 One dimensional shock

In order to verify the discrete structure of stationary shocks, calculations were performed for a one dimensional problem with initial data containing left and right states compatible with the Rankine Hugoniot conditions. An intermediate state consisting of the arithmetic average of the left and right states was introduced at a single cell in the center of the domain. With this intermediate state the system is not in equilibrium, and the time dependent equations were solved to find an equilibrium solution with a stationary shock wave separating the left and right states. Table 1 shows the result for a shock wave at Mach 20. This calculation used the H-CUSP scheme, which allows a solution with constant stagnation enthalpy. The SLIP construction was used with the limiter defined by equation (21), and $q = 3$. The table shows the values of ρ, u, H, p, M and the entropy $S = \log \frac{p}{\rho^\gamma} - \log\left(\frac{p_L}{\rho_L^\gamma}\right)$. A perfect one point shock structure is displayed. The entropy is zero to 4 decimal places upstream of the shock, exhibits a slight excursion at the interior point, and is constant to 4 decimal places downstream of the shock. It may be noted that the mass, momentum and energy of the initial data are not compatible with the final equilibrium state. According to equation (34) the total mass, momentum and energy must remain constant if the outflow flux f_R remains equal to the inflow flux f_L. Therefore f_R must be allowed to vary according to an appropriate outflow boundary condition to allow the total mass, momentum and energy to be adjusted to values compatible with equilibrium.

5.2 Airfoil calculations

The results of transonic flow calculations for two well known airfoils, the RAE 2822 and the NACA 0012, are presented in figures (10-13). The H-CUSP scheme was again used with the SLIP construction. The limiter defined by equation (21) was used with $q = 3$. The 5 stage time stepping scheme (40) was augmented by the multigrid scheme described in section 4.2 to accelerate convergence to a steady state. The equations were discretized on meshes with O-topology extending out to a radius of about 100 chords. In each case the calculations were performed on a sequence of successively finer meshes from 40x8 to 320x64 cells, while the multigrid cycles on each of these meshes descended to a coarsest mesh of 10x2 cells. Figure 10 shows the inner parts of the 160x32 meshes for the two airfoils. Figures 11-13 show the final results on 320x64 meshes for the RAE 2822 airfoil at Mach .75 and 3° angle of attack, and for the NACA 0012 airfoil at Mach .8 and 1.25° angle of attack, and also at Mach .85 and 1° angle of attack. In the pressure distributions the pressure coefficient $C_p = \frac{p-p_\infty}{\frac{1}{2}\rho_\infty q_\infty^2}$ is plotted with the negative (suction) pressures upward, so that the upper curve represents the flow over the upper side of a lifting airfoil. The convergence histories show the mean rate of change of the density, and also the total number of supersonic points in the flow field, which provides a useful measure of the global convergence of transonic flow calculations such as these. In each case the convergence history is shown for 100 cycles, while the pressure distribution is displayed after a sufficient number of cycles for its convergence. The pressure distribution of the RAE 2822 airfoil converged in only 25 cycles. Convergence was slower for the NACA 0012 airfoil. In the case of flow at Mach .8 and 1.25° angle of attack, additional cycles were needed to damp out a wave downstream of the weak shock wave on the lower surface.

I	ρ	u	H	p	M	s
12	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
13	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
14	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
15	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
16	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
17	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
18	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
19	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
20	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
21	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
22	4.1924	7.3248	283.4960	307.4467	0.7229	40.3353
23	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
24	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
25	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
26	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
27	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
28	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
29	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
30	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
31	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
32	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355

Table 1: Shock Wave at Mach 20

As a further check on accuracy the drag coefficient should be zero in subsonic flow, or in shock free transonic flow. Table 2 shows the computed drag coefficient on a sequence of three meshes for three examples. The first two are subsonic flows over the RAE 2822 and NACA 0012 airfoils at Mach .5 and 3° angle of attack. The third is the flow over the shock free Korn airfoil at its design point of Mach .75 and 0° angle of attack. In all three cases the drag coefficient is calculated to be zero to four digits on a 160x32 mesh.

Mesh	RAE 2822 Mach .50 α 3°	NACA 0012 Mach .50 α 3°	Korn Airfoil Mach .75 α 0°
40x8	.0062	.0047	.0098
80x16	.0013	.0008	.0017
160x32	.0000	.0000	.0000

Table 2: Drag Coefficient on a sequence of meshes

5.3 Three dimensional calculations for a swept wing

As a further test of the performance of the H-CUSP scheme, the flow past the ONERA M6 wing was calculated on a mesh with C-H topology and 192x32x48 = 294912 cells. Figure 14 shows the result at Mach .84 and 3.06° angle of attack. This again verifies the non-oscillatory character of the solution, and the sharp resolution of shock waves. In this case 50 cycles were sufficient for convergence of the pressure distributions.

6 Aerodynamic Design

6.1 The Design Problem as a Control Problem

Aerodynamic design has traditionally been carried out on a cut and try basis, with the aerodynamic expertise of the designer guiding the selection of each shape modification. Although considerable gains in aerodynamic performance have been achieved by this approach, continued improvement will most probably be much more difficult to attain. The subtlety and complexity of fluid flow is such that it is unlikely that repeated trials in an interactive analysis and design procedure can lead to a truly optimum design. Automatic design techniques are therefore needed in order to fully realize the potential improvements in aerodynamic efficiency.

Numerical optimization methods have been applied successfully to some simplified cases, such as two-dimensional airfoils in viscous flows [130] and wings in inviscid flows. However, this approach requires the computation of a large number of flow solutions before an optimum point can be located in the design space.

An alternative approach is to cast the design problem as a search for the shape that will generate the desired pressure distribution. This inverse approach recognizes that the designer usually has an idea of the the kind of pressure distribution that will lead to the desired performance. Thus, it is useful to consider the inverse problem of calculating the shape that will lead to a given pressure distribution. The method is advantageous, since only one flow solution is required to obtain the desired design. Unfortunately, a physically realizable shape may not necessarily exist, unless the pressure distribution satisfies certain constraints. Thus the problem must be very carefully formulated.

A particularly attractive way to circumvent the difficulty that the objective may be unattainable is to regard the design problem as a control problem in which the control is the shape of the boundary. A variety of alternative formulations of the design problem can then be treated systematically within the framework of the mathematical theory for control of systems governed by partial differential equations [97]. This approach to optimal aerodynamic design was introduced by Jameson [67, 68], who examined the design problem for compressible flow with shock waves, and devised adjoint equations to determine the gradient for both potential flow and also flows governed by the Euler equations. More recently Ta'asan, Kuruvila, and Salas, implemented a one shot approach in which the constraint represented by the flow equations is only required to be satisfied by the final converged solution [155]. Pironneau has studied the use of control theory for optimum shape design of systems governed by elliptic equations [122], while adjoint methods have also been used by Baysal and Eleshaky [16].

Suppose that the control is defined by a function $\mathcal{F}(\xi)$ of some independent variable ξ or in the discrete case a vector with components $\mathcal{F}_i$. Also suppose that the desired objective is measured by a cost function I. This may, for example, measure the deviation from a desired surface pressure distribution, but it can also represent other measures of performance such as lift and drag. Thus the design problem is recast into a numerical optimization procedure. This has the advantage that if the objective, say, of a target pressure distribution, is unattainable, it is still possible to find a minimum of the cost function. Now a variation $\delta\mathcal{F}$ in the control produces a variation δI in the cost. Following control theory, δI can be expressed to first order as an inner product

$$\delta I = (\mathcal{G}, \delta\mathcal{F}),$$

where the gradient $\mathcal{G}$ is independent of the particular variation $\delta\mathcal{F}$, and can be determined by solving an adjoint equation. For a discrete system of equations

$$(\mathcal{G}, \delta\mathcal{F}) \equiv \sum \mathcal{G}_i \delta\mathcal{F}_i$$

and for an infinitely dimensional system

$$(\mathcal{G}, \delta\mathcal{F}) \equiv \int \mathcal{G}(\xi)\, \delta\mathcal{F}\, d\xi.$$

In either case, if one makes a shape change

$$\delta\mathcal{F} = -\lambda\mathcal{G}, \tag{41}$$

where λ is sufficiently small and positive, then

$$\delta I = -\lambda (\mathcal{G}, \mathcal{G}) < 0$$

assuring a reduction in I.

For flow about an airfoil or wing, the aerodynamic properties which define the cost function are functions of the flow-field variables (w) and the physical location of the boundary, which may be represented by the function $\mathcal{F}$, say. Then

$$I = I(w, \mathcal{F}),$$

and a change in $\mathcal{F}$ results in a change

$$\delta I = \frac{\partial I^T}{\partial w} \delta w + \frac{\partial I^T}{\partial \mathcal{F}} \delta \mathcal{F}, \tag{42}$$

in the cost function. Brute force methods evaluate the gradient by making a small change in each design variable separately, and then recalculating both the grid and flow-field variables. This requires a number of additional flow calculations equal to the number of design variables. Using control theory, the governing equations of the flowfield are introduced as a constraint in such a way that the final expression for the gradient does not require reevaluation of the flow field. In order to achieve this, δw must be eliminated from (42). The governing equation R expresses the dependence of w and $\mathcal{F}$ within the flowfield domain D,

$$R(w, \mathcal{F}) = 0,$$

Thus δw is determined from the equation

$$\delta R = \left[\frac{\partial R}{\partial w}\right] \delta w + \left[\frac{\partial R}{\partial \mathcal{F}}\right] \delta \mathcal{F} = 0. \tag{43}$$

Next, introducing a Lagrange Multiplier ψ, we have

$$\begin{aligned} \delta I &= \frac{\partial I^T}{\partial w} \delta w + \frac{\partial I^T}{\partial \mathcal{F}} \delta \mathcal{F} - \psi^T \left(\left[\frac{\partial R}{\partial w}\right] \delta w + \left[\frac{\partial R}{\partial \mathcal{F}}\right] \delta \mathcal{F} \right) \\ &= \left\{ \frac{\partial I^T}{\partial w} - \psi^T \left[\frac{\partial R}{\partial w}\right] \right\} \delta w + \left\{ \frac{\partial I^T}{\partial \mathcal{F}} - \psi^T \left[\frac{\partial R}{\partial \mathcal{F}}\right] \right\} \delta \mathcal{F} \end{aligned}$$

Choosing ψ to satisfy the adjoint equation

$$\left[\frac{\partial R}{\partial w}\right]^T \psi = \frac{\partial I}{\partial w} \tag{44}$$

the first term is eliminated, and we find that

$$\delta I = \mathcal{G} \delta \mathcal{F} \tag{45}$$

where

$$G = \frac{\partial I^T}{\partial \mathcal{F}} - \psi^T \left[\frac{\partial R}{\partial \mathcal{F}}\right].$$

The advantage is that (45) is independent of δw, with the result that the gradient of I with respect to an arbitrary number of design variables can be determined without the need for additional flow-field evaluations. The main cost is in solving the adjoint equation (44). In general, the adjoint problem is about as complex as a flow solution. If the number of design variables is large, the cost differential between one adjoint solution and the large number of flowfield evaluations required to determine the gradient by brute force becomes compelling. Instead of introducing a Lagrange multiplier, ψ, one can solve (43) for δw as

$$\delta w = -\left[\frac{\partial R}{\partial w}\right]^{-1} \left[\frac{\partial R}{\partial \mathcal{F}}\right] \delta \mathcal{F},$$

and insert the result in (42). This is the implicit gradient approach, which is essentially equivalent to the control theory approach, as has been pointed out by Shubin and Frank [141, 142]. In any event there is an advantage in determining the gradient $\mathcal{G}$ by the solution of the adjoint equation.

After making such a modification, the gradient can be recalculated and the process repeated to follow a path of steepest descent (41) until a minimum is reached. In order to avoid violating constraints, such as a minimum acceptable wing thickness, the gradient may be projected into the allowable subspace within which the constraints are satisfied. In this way one can devise procedures which must necessarily converge at least to a local minimum, and which can be accelerated by the use of more sophisticated descent methods such as conjugate gradient or quasi-Newton algorithms. There is the possibility of more than one local minimum, but in any case the method will lead to an improvement over the original design. Furthermore, unlike the traditional inverse algorithms, any measure of performance can be used as the cost function.

6.2 Implementation for Swept Wings

In order to illustrate the application of control theory to aerodynamic design problems we present a three-dimensional wing design using the inviscid Euler equations as the mathematical model for compressible flow. Since three dimensional calculations require substantial computational resources, it is extremely important for the practical implementation of the method to use fast solution algorithms for the flow and the adjoint equations. In this case the author's FLO87 computer program has been used as the basis of the design method. FLO87 solves the three dimensional Euler equations with a cell-centered finite volume scheme, and uses residual averaging and multigrid acceleration to obtain very rapid steady state solutions, usually in 25 to 50 multigrid cycles [61, 65]. Upwind biasing is used to produce non-oscillatory solutions, and assure the clean capture of shock waves. This is introduced through the addition of carefully controlled numerical diffusion terms, with a magnitude of order Δx^3 in smooth parts of the flow. The adjoint equations are treated in the same way as the flow equations. The fluxes are first estimated by central differences, and then modified by downwind biasing through numerical diffusive terms which are supplied by the same subroutines that were used for the flow equations.

The method has been tested for the optimization of a swept wing. The wing planform was fixed while the sections were free to be changed arbitrarily by the design method, with a restriction on the minimum thickness. The wing has a unit semi-span, with 38 degrees leading edge sweep. It has a modified trapezoidal planform, with straight taper from a root chord of 0.38, and a curved trailing edge in the inboard region blending into straight taper outboard of the 30 percent span station to a tip chord of 0.10, with an aspect ration of 9.0. The initial wing sections were based on a section specifically designed by the author's two dimensional design method [67] to give shock free flow at Mach 0.78 with a lift coefficient of 0.6. The pressure distribution is displayed in figure 15. This section, which has a thickness to chord ration of 9.5 percent, was used at the tip. Similar sections with an increased thickness were used inboard. The variation of thickness was non-linear with a more rapid increase near the root, where the thickness to chord ratio of the basic section was multiplied by a factor of 1.47. The inboard sections were rotated upwards to give the initial wing 3.0 degrees twist from root to tip.

The two dimensional pressure distribution of the basic wing section at its design point was introduced as a target pressure distribution uniformly across the span. This target is presumably not realizable, but serves to favor the establishment of relatively benign pressure distribution. The total inviscid drag coefficient, due to the combination of vortex and shock wave drag, was also included in the cost function. Calculations were performed with the lift coefficient forced to approach a fixed value by adjusting the angle of attack every fifth iteration of the flow solution. It was found that the computational costs can be reduced by using only 15 multigrid cycles in each flow solution, and in each adjoint solution. Although this is not enough for full convergence, it proves sufficient to provide a shape modification which leads to an improvement. Figures 16 and 17 show the result of a calculation at Mach number of 0.85, with the lift coefficient forced to approach a value of 0.5. This calculation was performed on a mesh with 192 intervals in the ξ direction wrapping around the wing, 32 intervals in the normal η direction and 48 intervals in the spanwise ζ direction, giving a total of 294912 cells. The wing was specified by 33 sections, each with 128 points, giving a total of 4224 design variables. The plots show the initial wing geometry and pressure distribution, and the modified geometry and

pressure distribution after 10 design cycles. The total inviscid drag was reduced from 0.0209 to 0.0119. The initial design exhibits a very strong shock wave in the inboard region. It can be seen that this is completely eliminated, leaving a very weak shock wave in the outboard region. The drag reduction is mainly accomplished in the first four design cycles but the pressure distribution continues to be adjusted to become more like the target pressure distribution. To verify the solution, the final geometry, after 10 design cycles, was analyzed with another method using the computer program FLO67. This program uses a cell-vertex formulation, and has recently been modified to incorporate a local extremum diminishing algorithm with a very low level of numerical diffusion [71]. When run to full convergence it was found that the redesigned wing has a drag coefficient of 0.0096 at Mach 0.85 at a lift coefficient of 0.5, with a corresponding lift to drag ratio of 52. The result for $\alpha = 0.0°$ and $C_L = 0.505$ is illustrated in Figure 18: this seems to be the nearest to a shock free condition. A calculation at Mach 0.500 shows a drag coefficient of 0.0089 for a lift coefficient of 0.5. Since in this case the flow is entirely subsonic, this provides an estimate of the vortex drag for this planform and lift distribution, which is just what one obtains from the standard formula for induced drag, $C_D = {C_L}^2/\epsilon\pi AR$, with an aspect ratio $AR = 9$, and an efficiency factor $\epsilon = 0.97$. Thus the design method has reduced the shock wave drag coefficient to about 0.0007 at a lift coefficient of 0.5. For a representative transport aircraft the parasite drag coefficient of the wing due to skin friction is about 0.0045. Also the fuselage drag coefficient is about 0.0050, the nacelle drag coefficient is about 0.0015, the empennage drag coefficient is about 0.0020, and excrescence drag coefficient is about 0.0010. This would give a total drag coefficient $C_D = 0.0236$ for a lift coefficient of 0.5, corresponding to a lift to drag ratio $L/D = 21$. This would be a substantial improvement over the values obtained by currently flying transport aircraft. These results suggest that the method can be a very useful tool for the design of new airplanes. Even in the case of three dimensional flows, the computational requirements are so moderate that the calculations can be performed with workstations such as the IBM RISC 6000 series. A design cycle on a 192x32x48 mesh takes about $1\frac{1}{2}$ hours on an IBM model 530 workstation, allowing overnight completion of a design calculation for a swept wing.

7 Outlook and Conclusions

Better algorithms and better computer hardware have contributed about equally to the progress of computational science in the last two decades. In 1970 the Control Data 6600 represented the state of the art in computer hardware with a speed of about 10^6 operations per second (one megaflop), while in 1990 the 8 processor Cray YMP offered a performance of about 10^9 operations per second (one gigaflop). Correspondingly, steady-state Euler calculations which required 5,000–10,000 steps prior to 1980 could be performed in 10–50 steps in 1990 using multigrid acceleration. With the advent of massively parallel computers it appears that the progress of computer hardware may even accelerate. Teraflop machines offering further improvement by a factor of 1,000 are likely to be available within a few years. Parallel architectures will force a reappraisal of existing algorithms, and their effective utilization will require the extensive development of new parallel software.

In parallel with the transition to more sophisticated algorithms, the present challenge is to extend the effective use of CFD to more complex applications. A key problem is the treatment of multiple space and time scales. These arise not only in turbulent flows, but also in many other situations such as chemically reacting flows, combustion, flame fronts and plasma dynamics. Another challenge, is presented by problems with moving boundaries. Examples include helicopter rotors, and rotor-stator interaction in turbomachinery. Algorithms for these problems can be significantly improved by innovative concepts, such as the idea of time inclining. It can be anticipated that interdisciplinary applications in which CFD is coupled with the computational analysis of other properties of the design will play an increasingly important role. These applications may include structural, thermal and electromagnetic analysis. Aeroelastic problems and integrated control system and aerodynamic design are likely target areas.

The development of improved algorithms continues to be important in providing the basic building blocks for

numerical simulation. In particular, better error estimation procedures must be developed and incorporated in the simulation software to provide error control. The basic simulation software is only one of the needed ingredients, however. The flow solver must be embedded in a user-friendly system for geometry modeling, output analysis, and data management that will provide a complete numerical design environment. These are the ingredients which are needed for the full realization of the concept of a numerical wind tunnel. Figures 8 and 9 illustrate the way in which a numerical wind tunnel might evolve from current techniques, which involve massive data handling tasks, to a fully integrated design environment.

In the long run, computational simulation should become the principal tool of the aerodynamic design process because of the flexibility it provides for the rapid and comparatively inexpensive evaluation of alternative designs, and because it can be integrated with a multi-disciplinary optimization (MDO) procedure. Experimental facilities are likely to be used principally for fundamental investigations of the basic physics of fluid flow, and for final verification of the design prior to flight testing. This is already the accepted procedure in the structural design process.

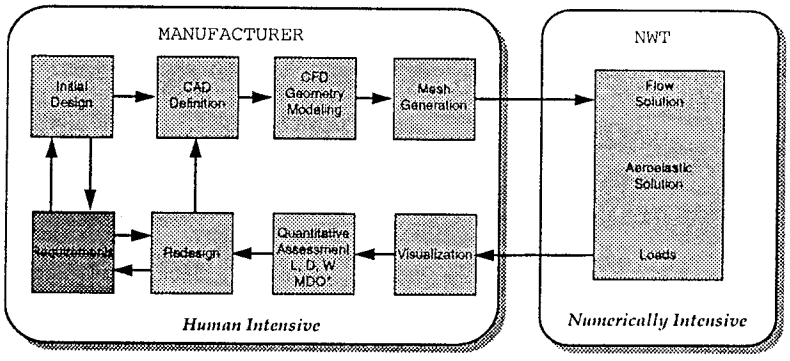


Figure 8: Concept for a numerical wind tunnel.

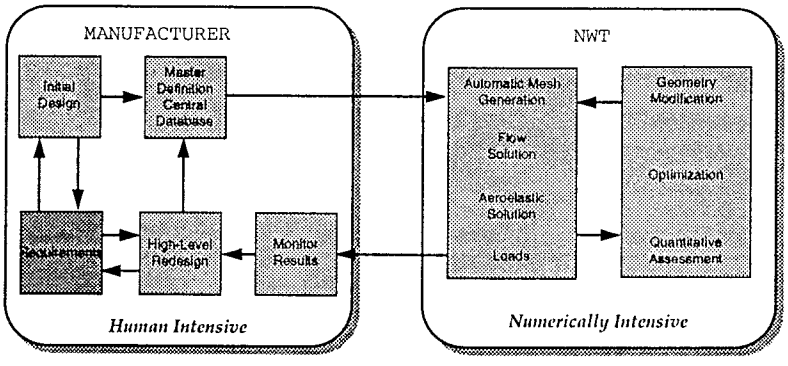


Figure 9: Advanced numerical wind tunnel.

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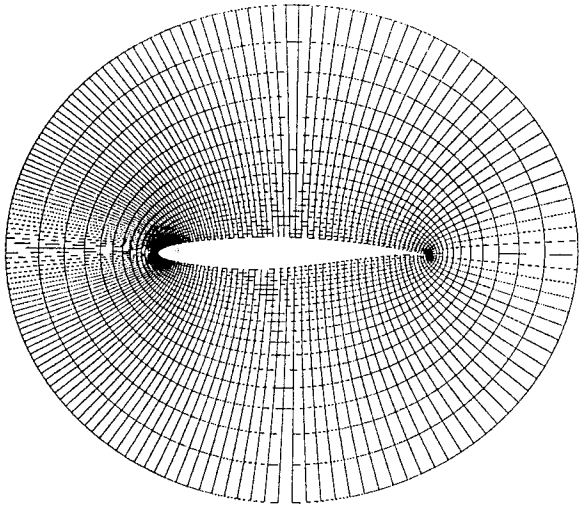
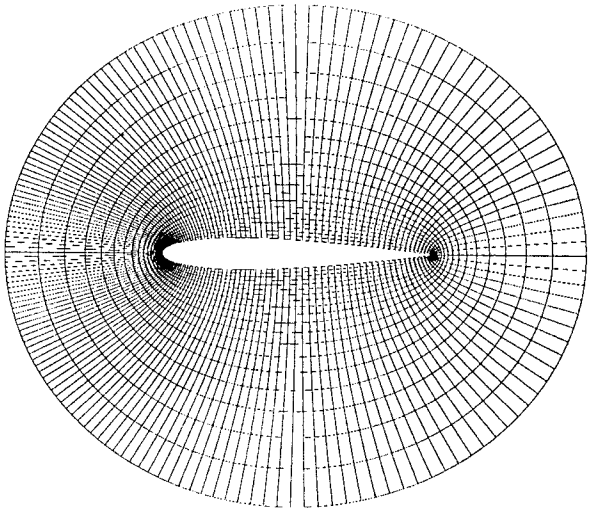
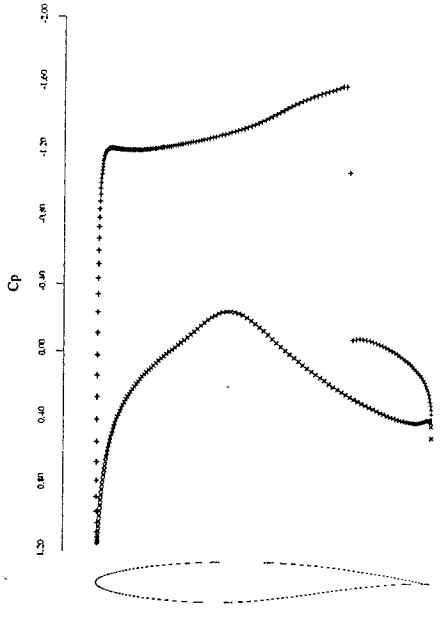


10a: RAE-2822 Airfoil

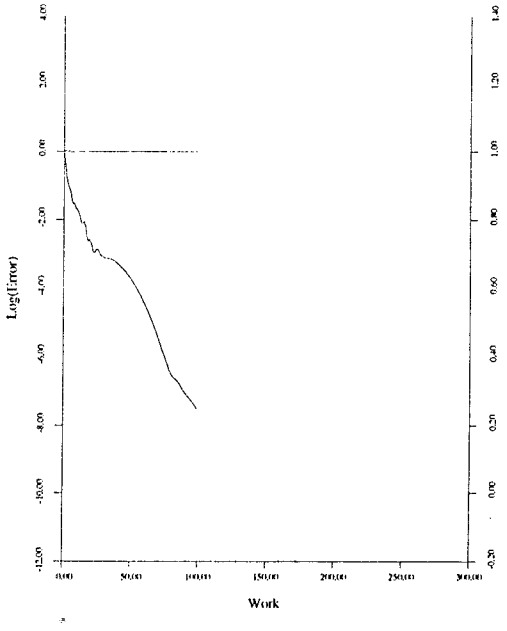


10b: NACA-0012 Airfoil

Figure 10: O-Topology Meshes, 160x32

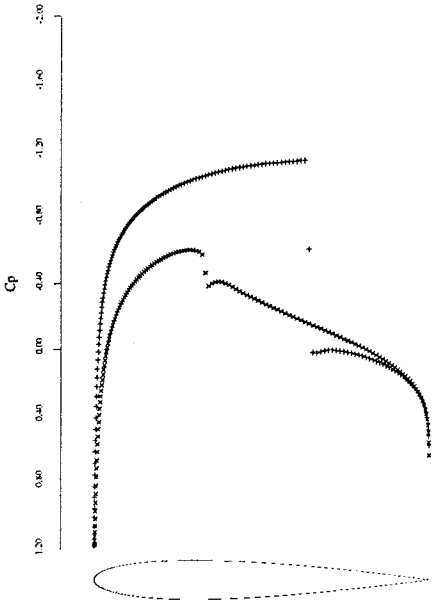


11a: C_p after 25 Cycles.
$C_l = 1.1312$, $C_d = 0.0469$.

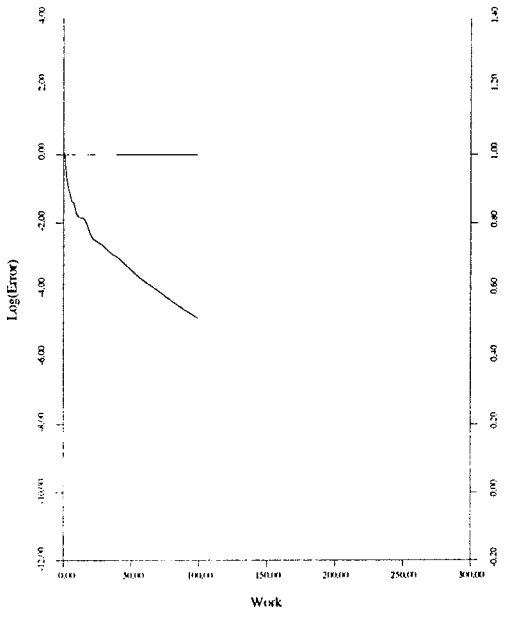


11b: Convergence.

Figure 11: RAE-2822 Airfoil at Mach 0.750 and $\alpha = 3.0°$
H-CUSP Scheme.

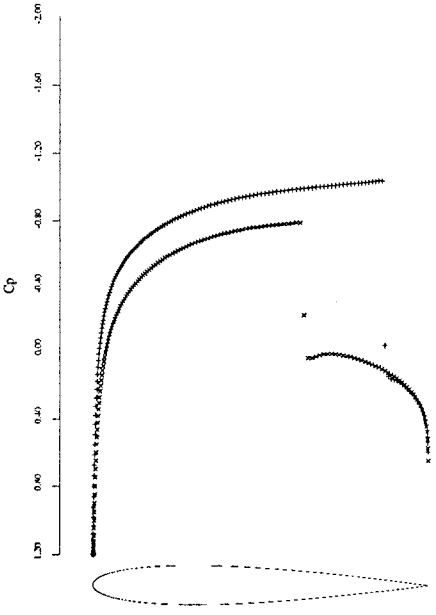


12a: C_p after 35 Cycles.
$C_l = 0.3654$, $C_d = 0.0232$.

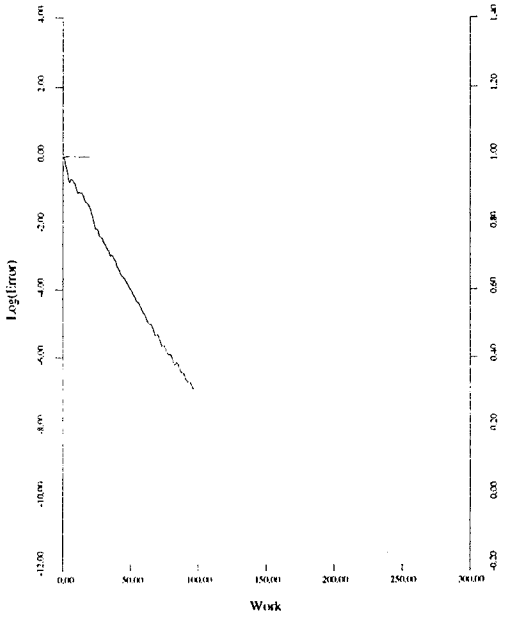


12b: Convergence.

Figure 12: NACA-0012 Airfoil at Mach 0.800 and $\alpha = 1.25°$
H-CUSP Scheme.

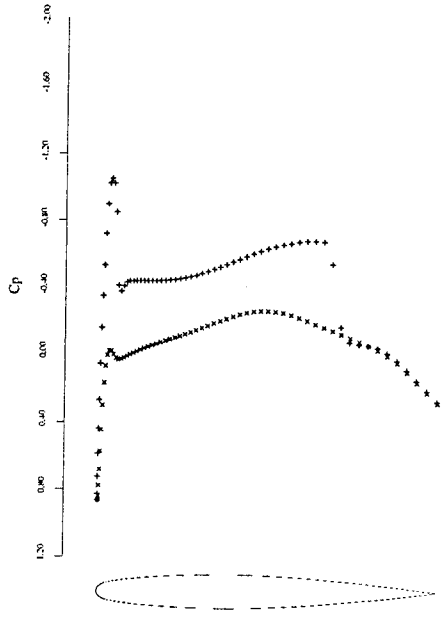


13a: C_p after 35 Cycles.
$C_l = 0.3861$, $C_d = 0.0582$.

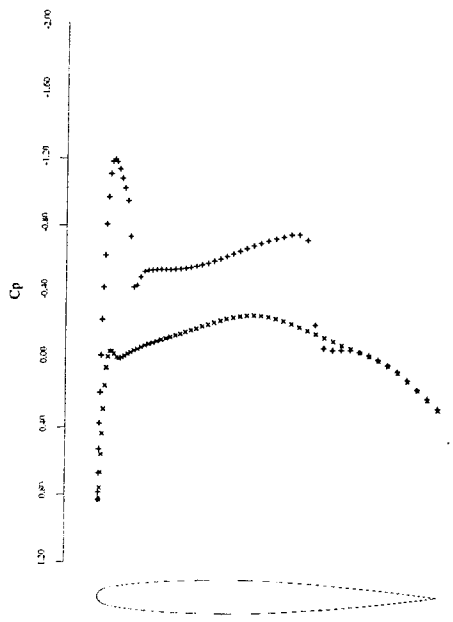


13b: Convergence.

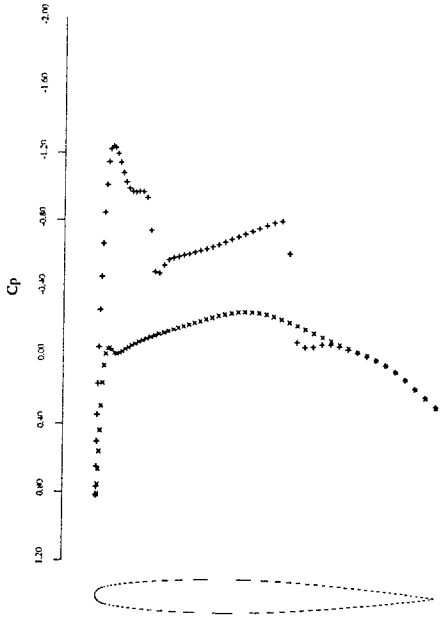
Figure 13: NACA-0012 Airfoil at Mach 0.850 and $\alpha = 1.0°$
H-CUSP Scheme.



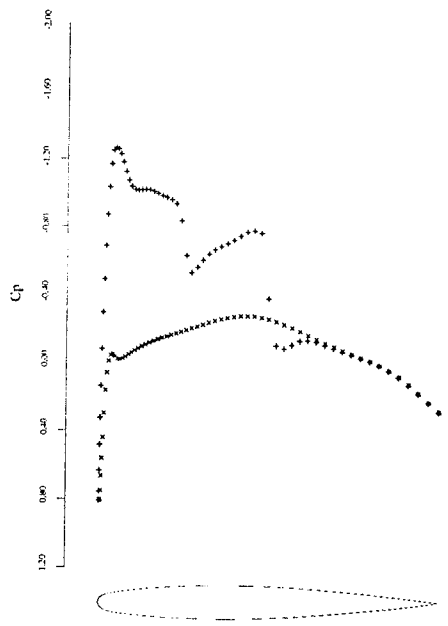
14a: 12.50% Span.
$C_l = 0.2933$, $C_d = 0.0274$.



14b: 31.25% Span.
$C_l = 0.3139$, $C_d = 0.0159$.



14c: 50.00% Span.
$C_l = 0.3262$, $C_d = 0.0089$.



14d: 68.75% Span.
$C_l = 0.3195$, $C_d = 0.0026$.

Figure 14: Onera M6 Wing.
Mach 0.840, Angle of Attack 3.06°, 192×32×48 Mesh.
$C_L = 0.3041$, $C_D = 0.0131$.
H-CUSP scheme.

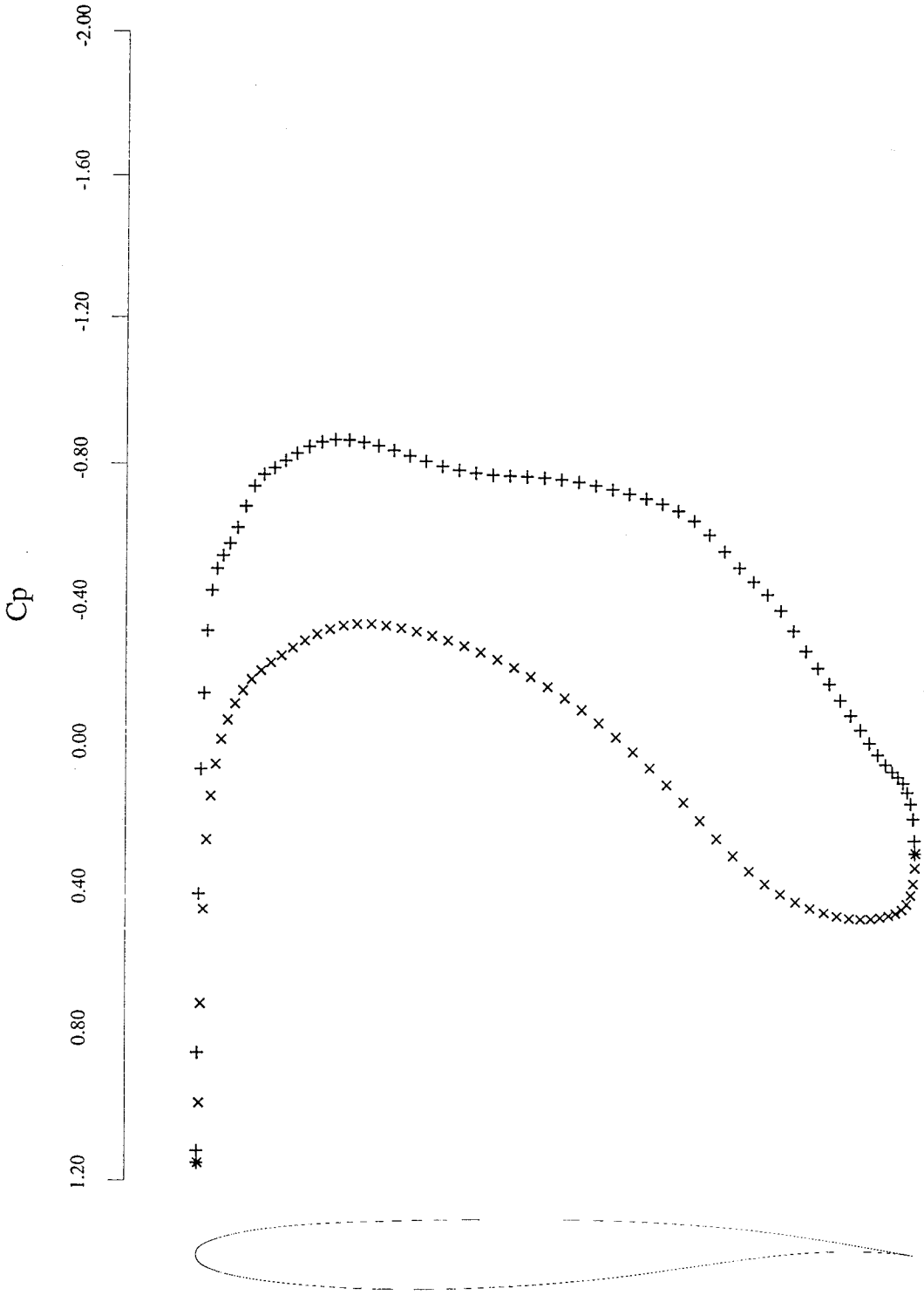
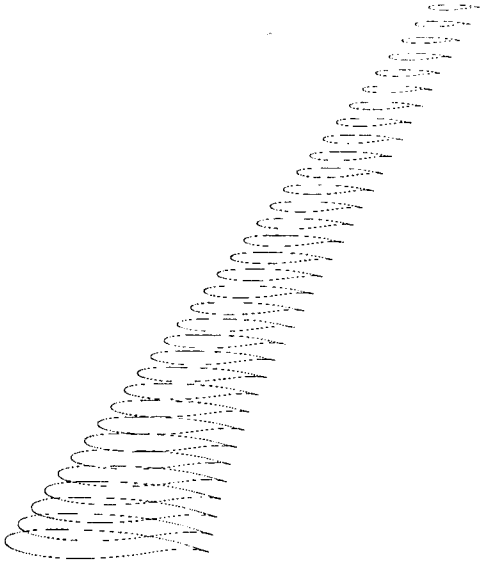
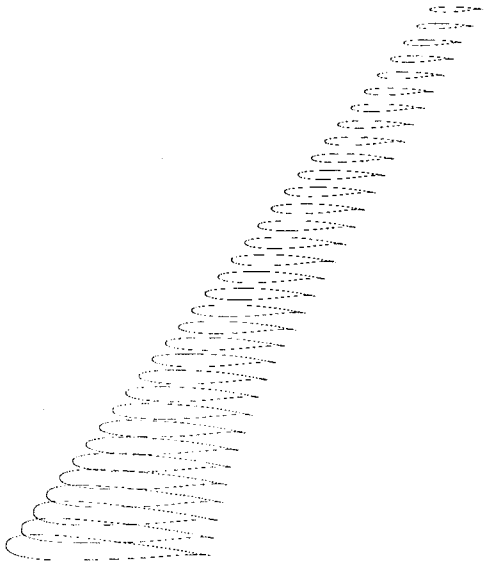


Figure 15: Initial Wing Section and Target Pressure Distribution





16a: Initial Wing
$C_l = 0.5000$, $C_d = 0.0209$, $\alpha = -1.349°$

16b: 10 Design Iterations
$C_l = 0.5000$, $C_d = 0.0119$, $\alpha = 0.033°$

Figure 16: Lifting Design Case, $M = 0.85$, Fixed Lift Mode.
Drag Reduction

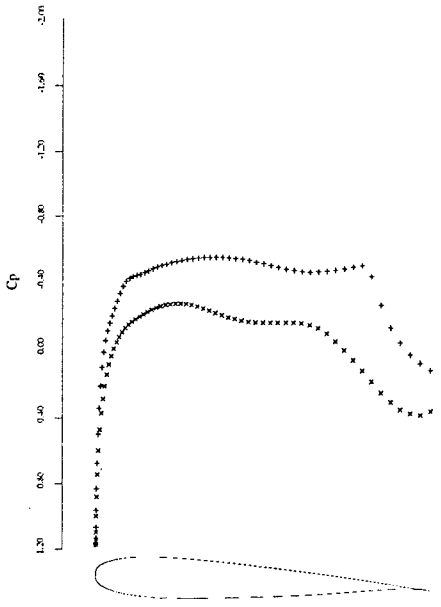
UPPER SURFACE PRESSURE

17a: Initial Wing
Lifting Design Case, $M = 0.85$, Fixed Lift Mode.
$C_L = 0.5000$, $C_D = 0.0209$, $\alpha = -1.349°$
Drag Reduction

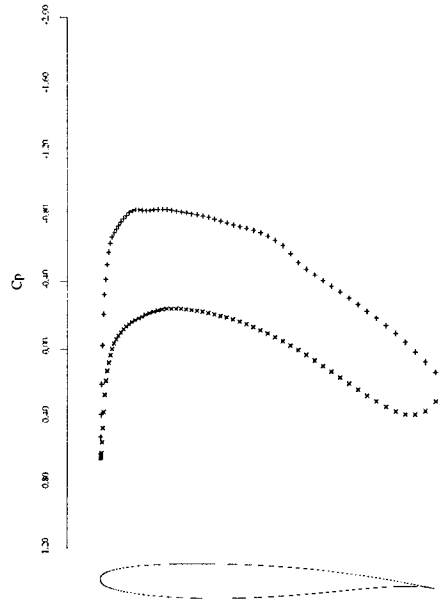
UPPER SURFACE PRESSURE

17b: 10 Design Iterations
Lifting Design Case, $M = 0.85$, Fixed Lift Mode.
$C_L = 0.5000$, $C_D = 0.0119$, $\alpha = 0.033°$
Drag Reduction

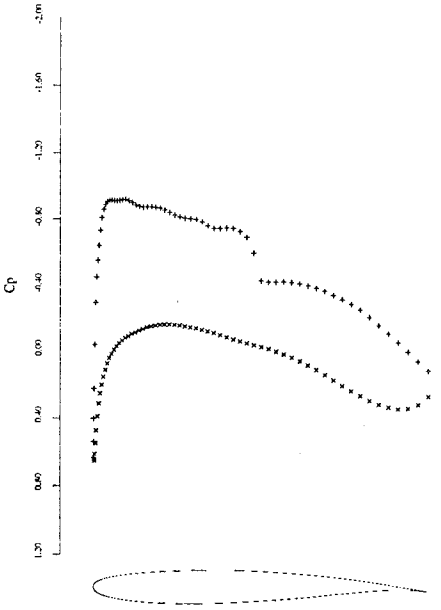
Figure 17: Lifting Design Case, $M = 0.85$, Fixed Lift Mode.
Drag Reduction



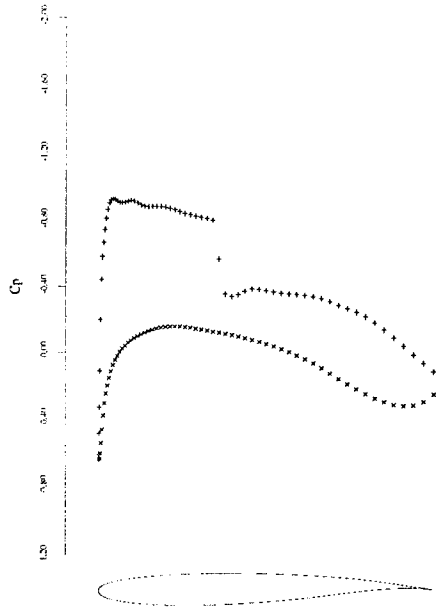
18a: span station $z = 0.00$



18b: span station $z = 0.312$



18c: span station $z = 0.625$



18d: span station $z = 0.937$

Figure 18: FLO67 check on redesigned wing.
$M = 0.85$, $C_L = 0.5051$, $C_D = 0.0099$, $\alpha = 0.0°$.